Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 04:03 pm BST

PDB ID	:	8BAA / pdb_00008baa
EMDB ID	:	EMD-15944
Title	:	CryoEM structure of GroEL-GroES-ADP.AlF3-Rubisco, class II.
Authors	:	Gardner, S.; Saibil, H.R.
Deposited on	:	2022-10-11
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

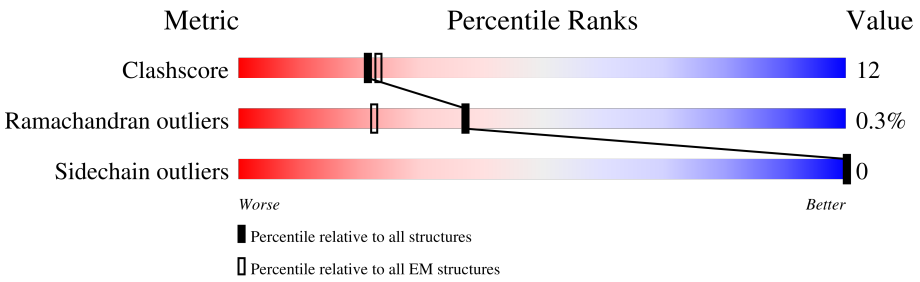
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

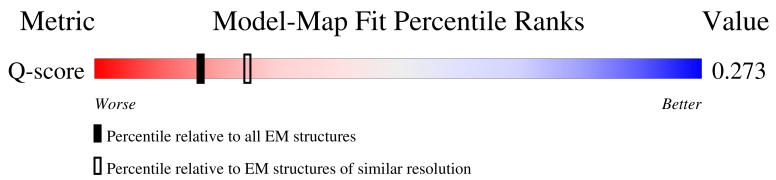
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	547	77% 19%
1	B	547	79% 17%
1	C	547	78% 18%
1	D	547	76% 20%

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Mol	Chain	Length	Quality of chain
1	E	547	7% 76% 20%
1	F	547	7% 76% 20%
1	G	547	76% 20%
1	H	547	12% 77% 18%
1	I	547	12% 72% 23%
1	J	547	12% 73% 22%
1	K	547	12% 75% 20%
1	L	547	11% 73% 22%
1	M	547	11% 72% 24%
1	N	547	11% 76% 19%
2	O	97	27% 49% 48%
2	P	97	18% 62% 36%
2	Q	97	24% 64% 34%
2	R	97	14% 56% 43%
2	S	97	15% 74% 24%
2	T	97	13% 61% 36%
2	U	97	22% 66% 33%
3	Z	466	37% 65% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AF3	A	601	-	-	X	-
4	AF3	C	602	-	-	X	-
4	AF3	D	602	-	-	X	-
4	AF3	G	601	-	-	X	-
6	ADP	I	2002	X	-	-	-
6	ADP	M	2003	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 127465 atoms, of which 64540 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chaperonin GroEL.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	524	7834	2397	3979	665	773	20	0	0
1	B	524	7834	2397	3979	665	773	20	0	0
1	C	524	7834	2397	3979	665	773	20	0	0
1	D	524	7834	2397	3979	665	773	20	0	0
1	E	524	7834	2397	3979	665	773	20	0	0
1	F	524	7834	2397	3979	665	773	20	0	0
1	G	524	7834	2397	3979	665	773	20	0	0
1	H	523	7817	2391	3972	664	770	20	0	0
1	I	523	7817	2391	3972	664	770	20	0	0
1	J	523	7817	2391	3972	664	770	20	0	0
1	K	523	7817	2391	3972	664	770	20	0	0
1	L	523	7817	2391	3972	664	770	20	0	0
1	M	523	7817	2391	3972	664	770	20	0	0
1	N	523	7817	2391	3972	664	770	20	0	0

- Molecule 2 is a protein called Co-chaperonin GroES.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	O	97	1490	454	762	127	145	2	0	0

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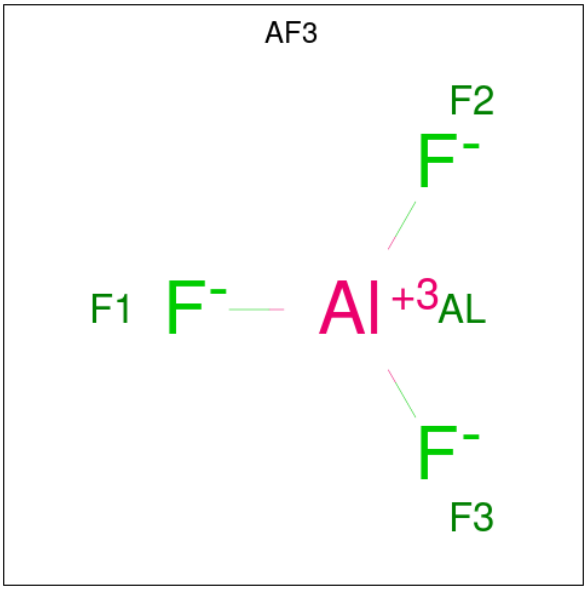
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	P	97	1490	454	762	127	145	2	0	0
2	Q	97	1490	454	762	127	145	2	0	0
2	R	97	1490	454	762	127	145	2	0	0
2	S	97	1490	454	762	127	145	2	0	0
2	T	97	1490	454	762	127	145	2	0	0
2	U	97	1490	454	762	127	145	2	0	0

- Molecule 3 is a protein called Ribulose bisphosphate carboxylase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	Z	459	6883	2213	3381	613	658	18	0	0

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
4	A	1	4	1	3	0
4	B	1	4	1	3	0

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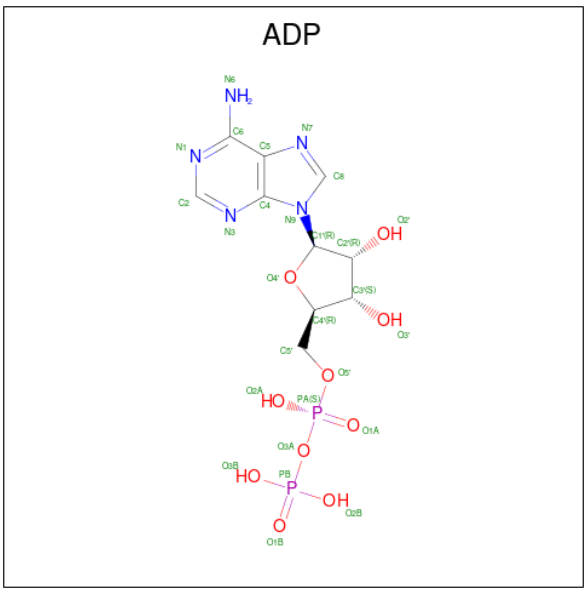
Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
4	C	1	4	1	3	0
4	D	1	4	1	3	0
4	E	1	4	1	3	0
4	F	1	4	1	3	0
4	G	1	4	1	3	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0
5	B	1	1	1	0
5	C	1	1	1	0
5	D	1	1	1	0
5	E	1	1	1	0
5	F	1	1	1	0
5	G	1	1	1	0
5	H	1	1	1	0
5	I	1	1	1	0
5	J	1	1	1	0
5	K	1	1	1	0
5	L	1	1	1	0
5	M	1	1	1	0
5	N	1	1	1	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
6	A	1	39	10	12	5	10	2	0
6	B	1	39	10	12	5	10	2	0
6	C	1	39	10	12	5	10	2	0
6	D	1	39	10	12	5	10	2	0
6	E	1	39	10	12	5	10	2	0
6	F	1	39	10	12	5	10	2	0
6	G	1	39	10	12	5	10	2	0
6	H	1	39	10	12	5	10	2	0
6	I	1	39	10	12	5	10	2	0
6	J	1	39	10	12	5	10	2	0
6	K	1	39	10	12	5	10	2	0
6	L	1	39	10	12	5	10	2	0
6	M	1	39	10	12	5	10	2	0

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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
6	N	1	39	10	12	5	10	2	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

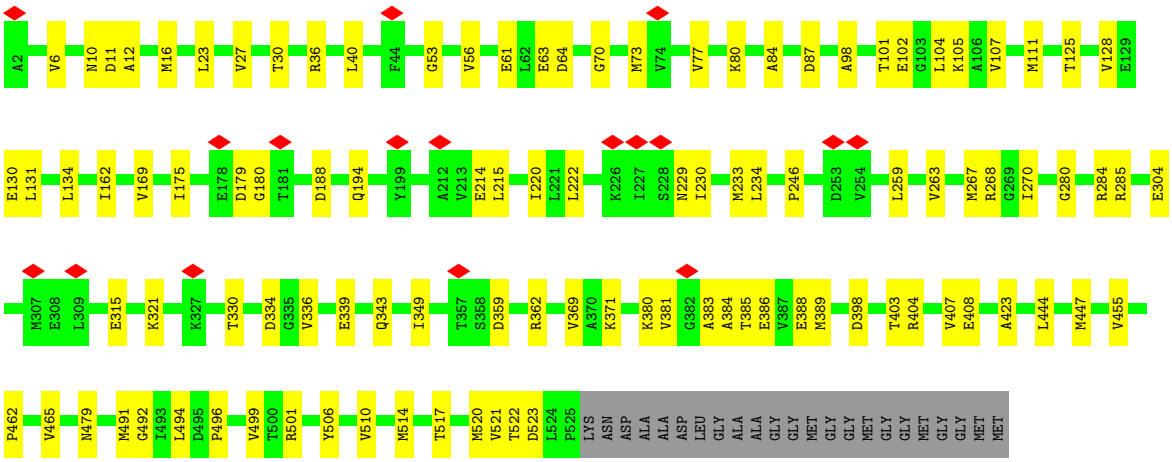
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
7	H	1	1	1	0
7	I	1	1	1	0
7	J	1	1	1	0
7	K	1	1	1	0
7	L	1	1	1	0
7	M	1	1	1	0
7	N	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

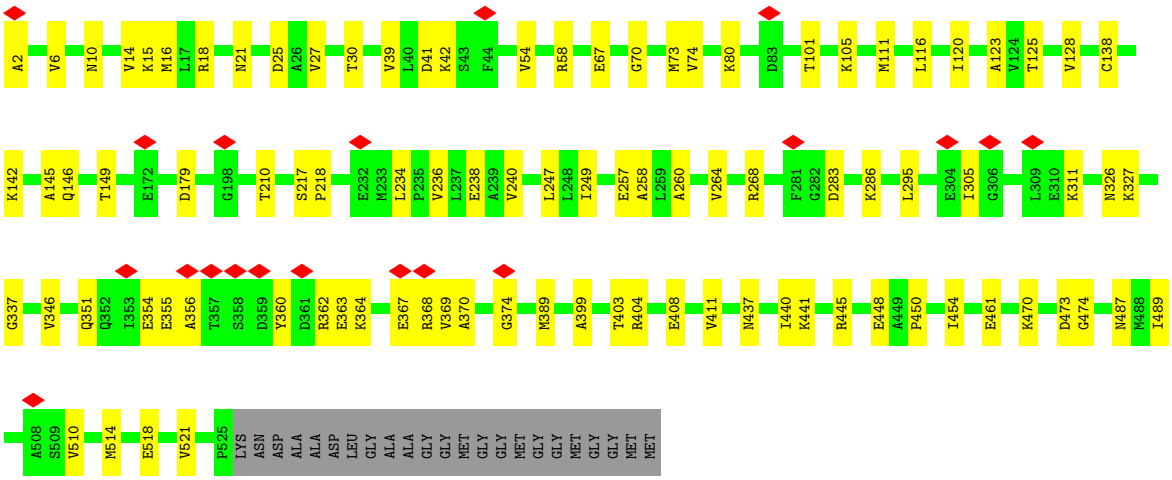
• Molecule 1: Chaperonin GroEL

Chain A: 77% 19%



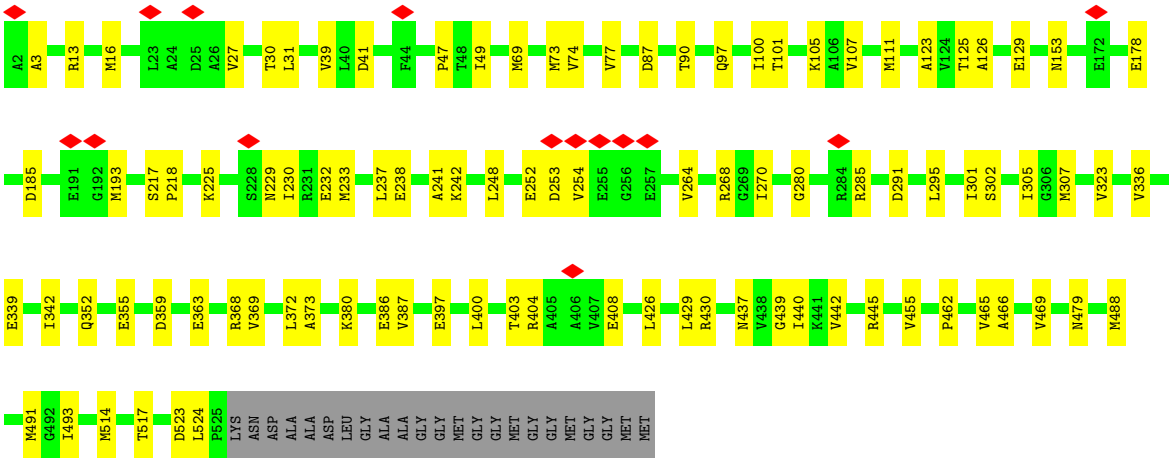
• Molecule 1: Chaperonin GroEL

Chain B: 79% 17%



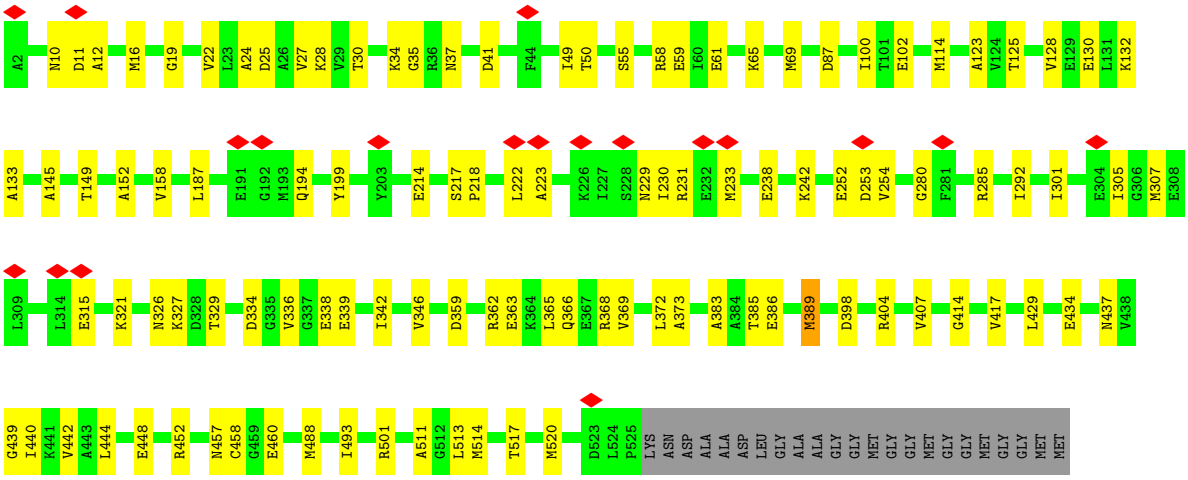
• Molecule 1: Chaperonin GroEL

Chain C:



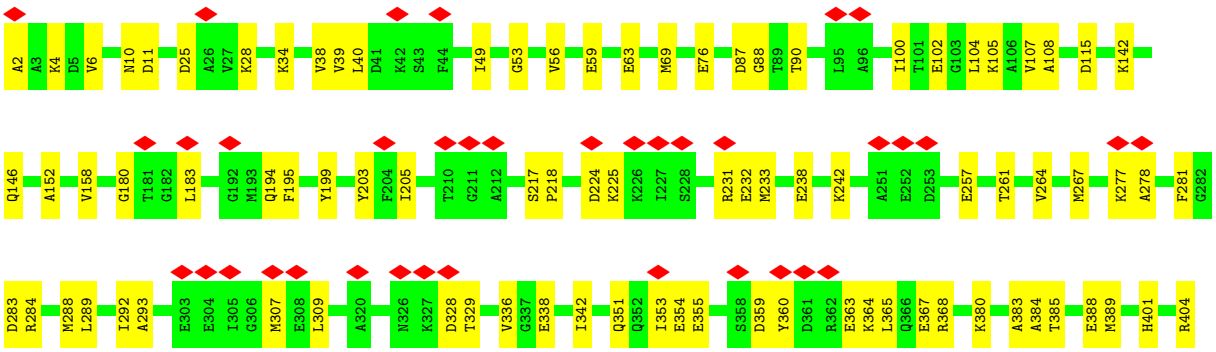
- Molecule 1: Chaperonin GroEL

Chain D:



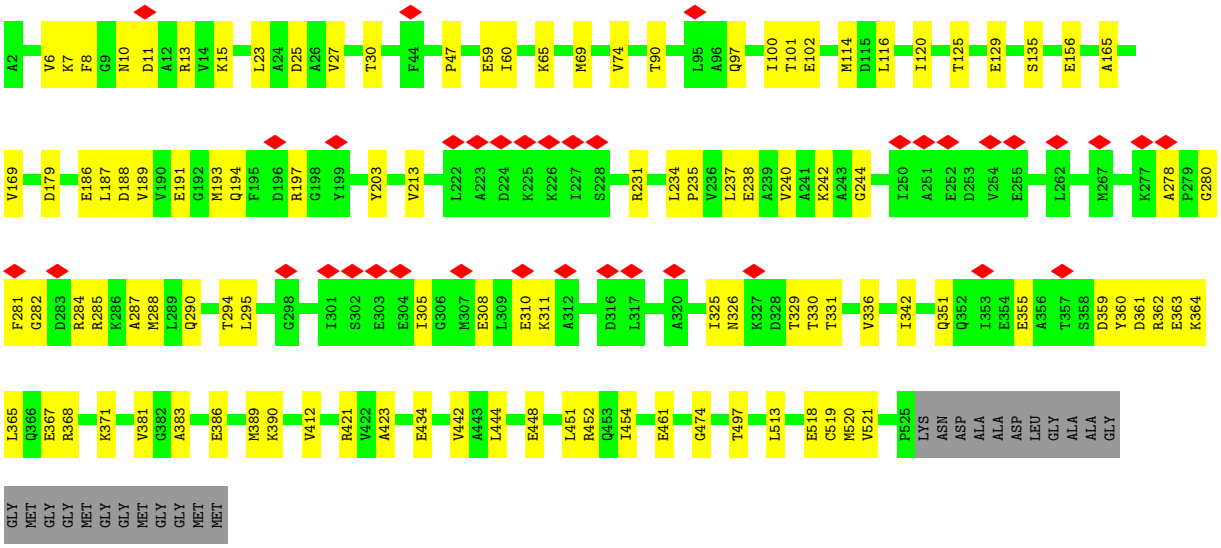
- Molecule 1: Chaperonin GroEL

Chain E:



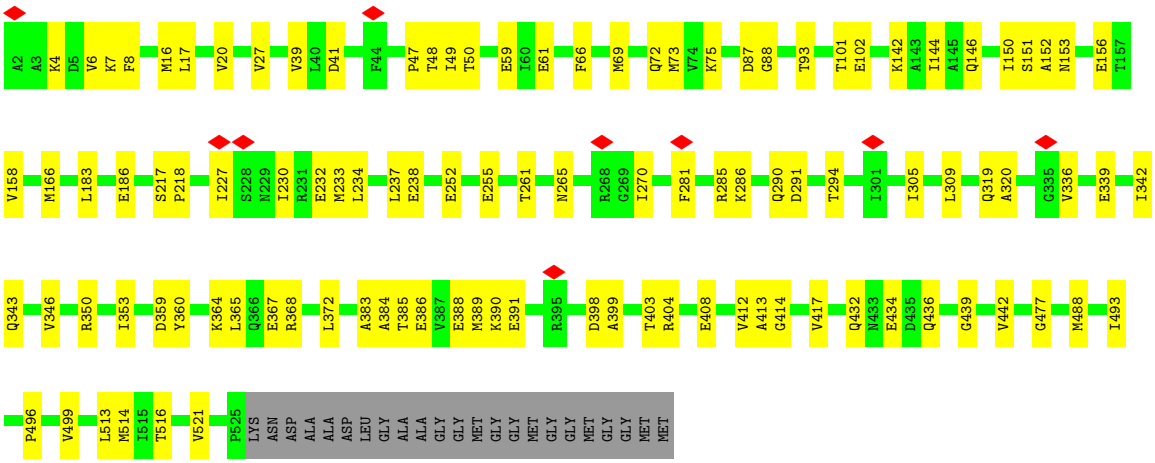
• Molecule 1: Chaperonin GroEL

Chain F:



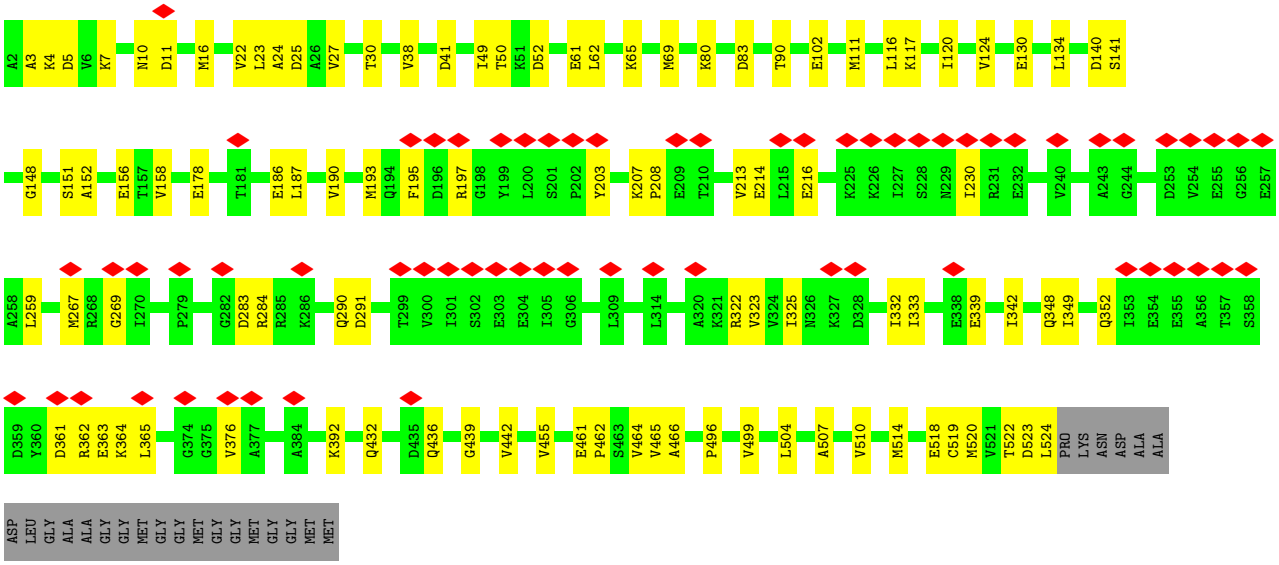
• Molecule 1: Chaperonin GroEL

Chain G:



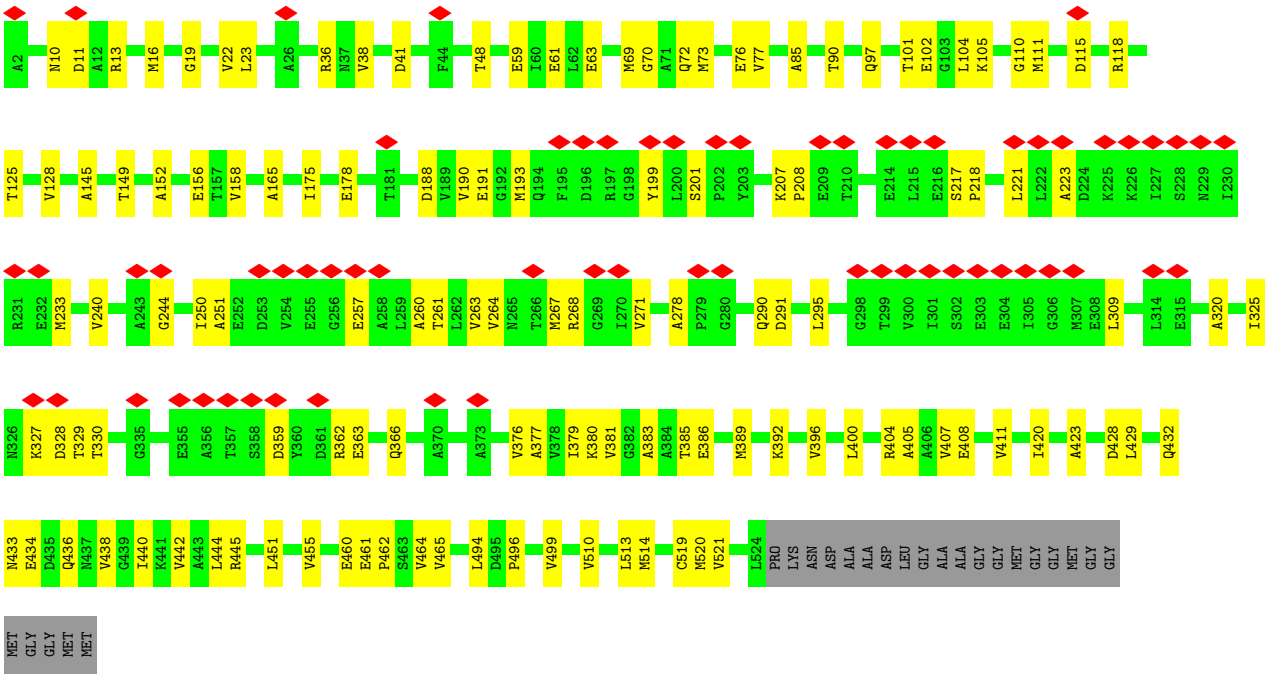
• Molecule 1: Chaperonin GroEL

Chain H:



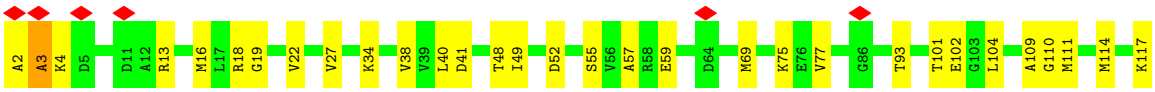
• Molecule 1: Chaperonin GroEL

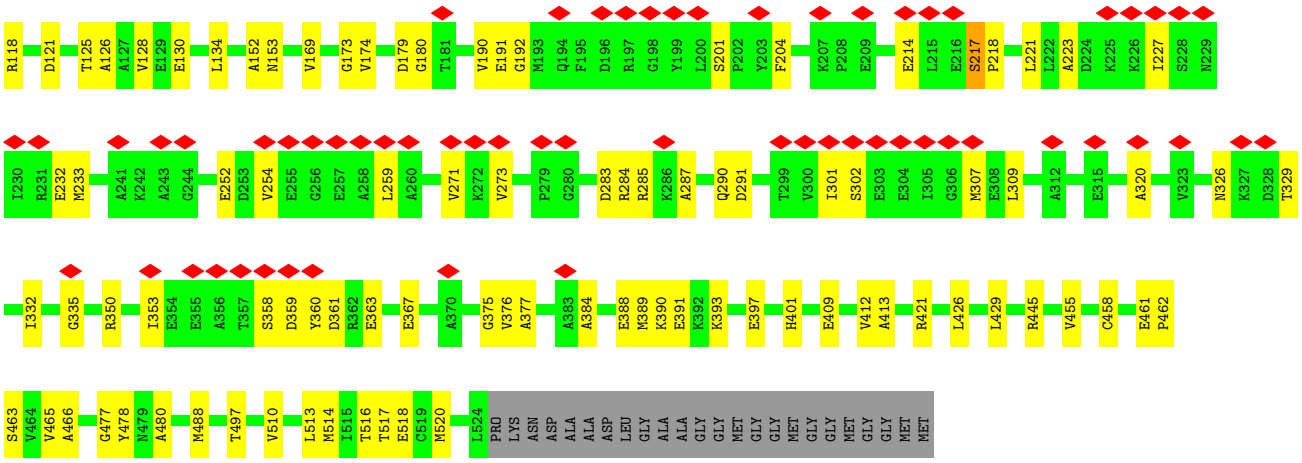
Chain I:



• Molecule 1: Chaperonin GroEL

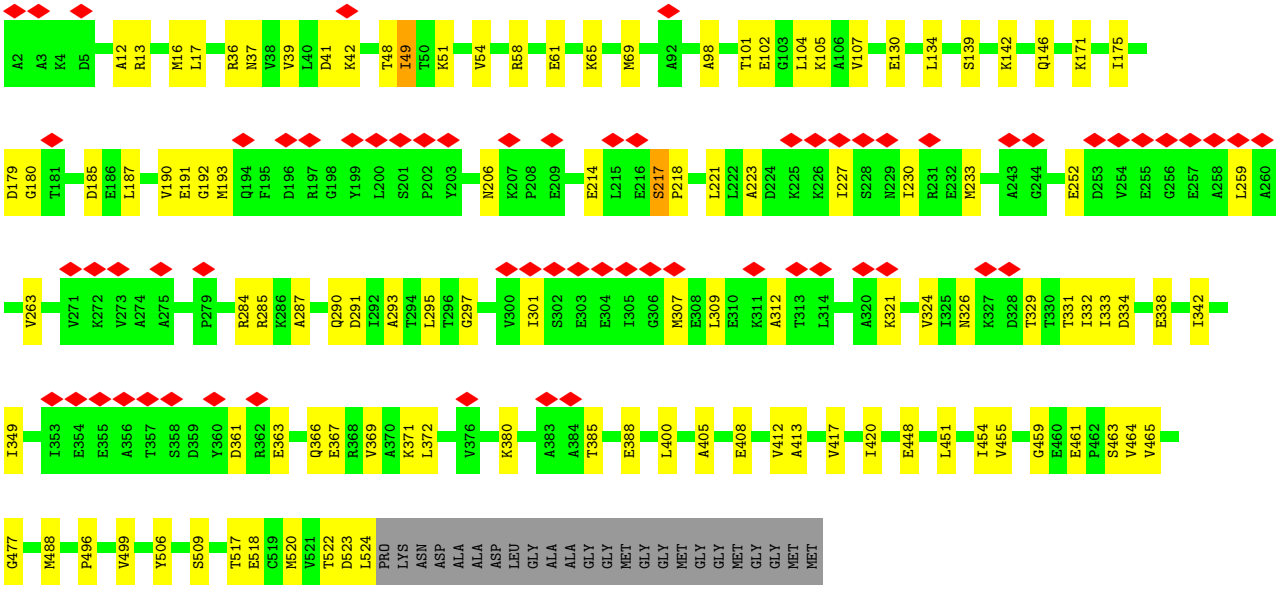
Chain J:





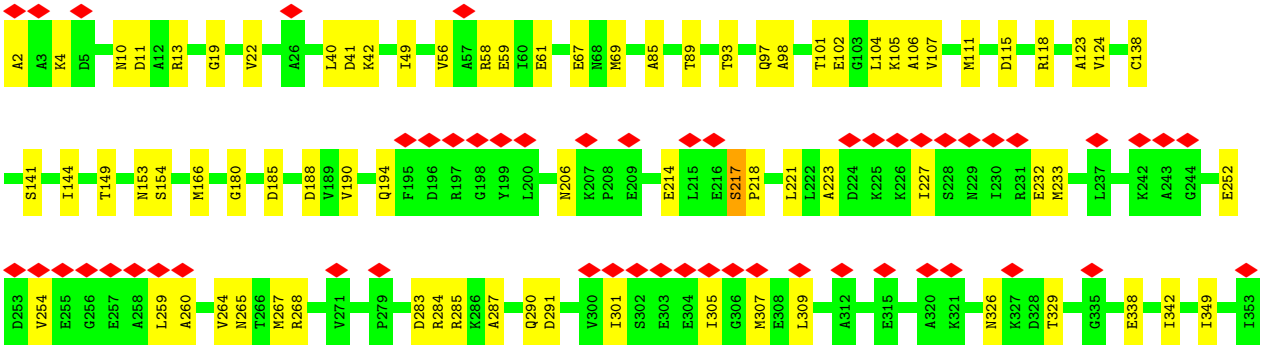
• Molecule 1: Chaperonin GroEL

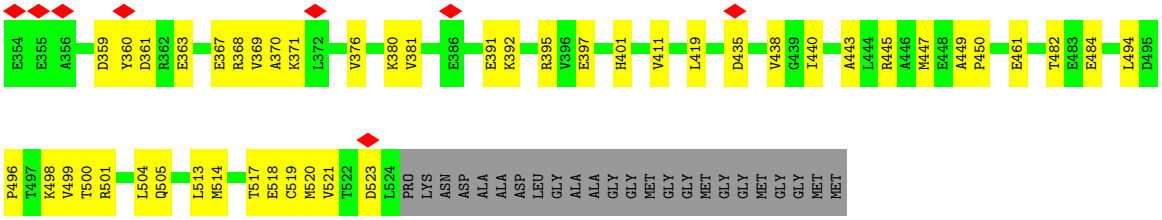
Chain K:



• Molecule 1: Chaperonin GroEL

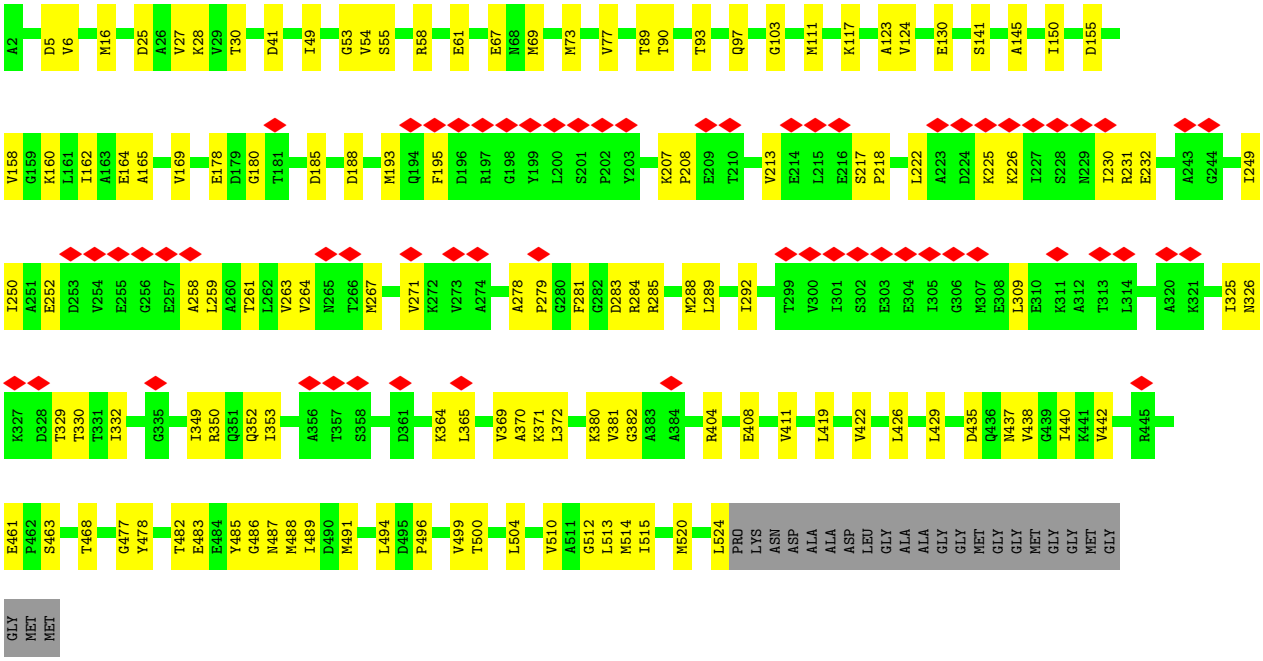
Chain L:





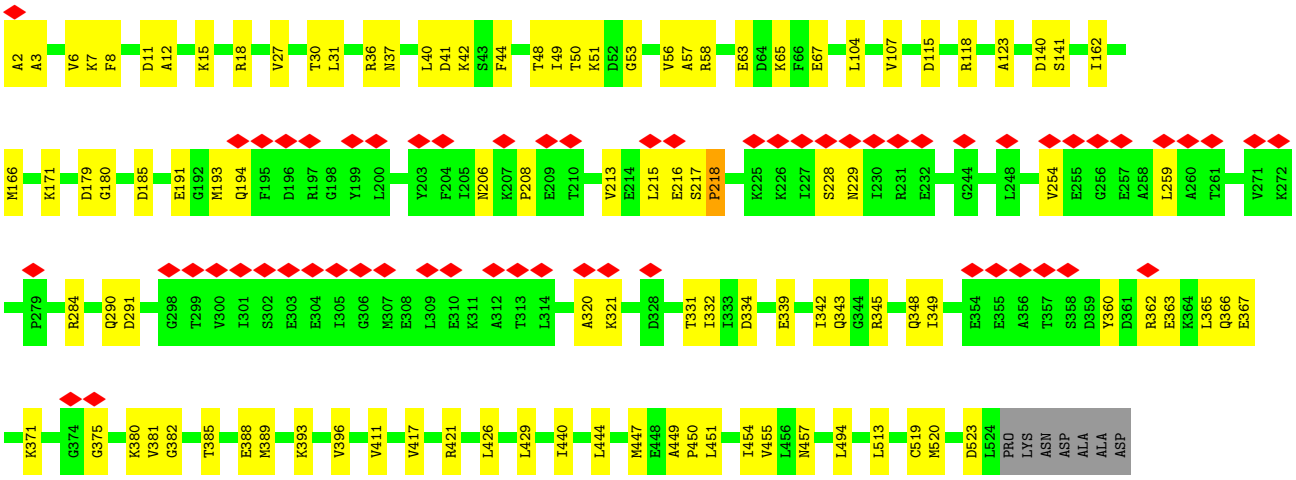
• Molecule 1: Chaperonin GroEL

Chain M:



• Molecule 1: Chaperonin GroEL

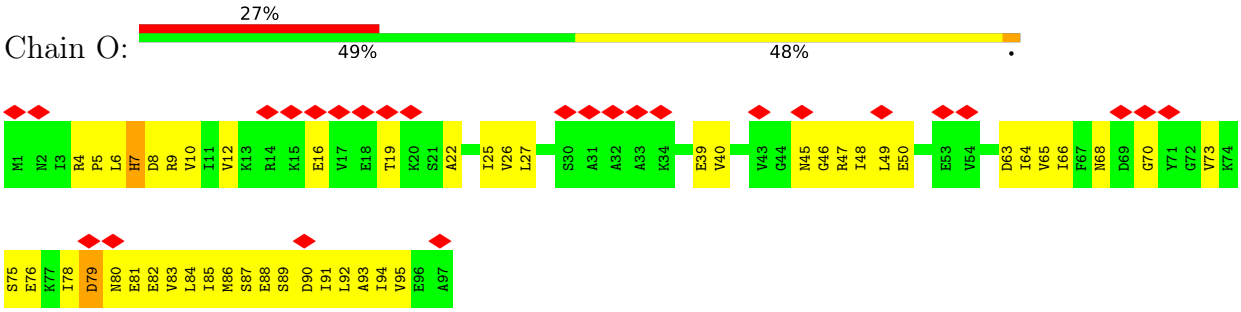
Chain N:



LEU GLY ALA ALA GLY GLY MET GLY GLY MET GLY GLY MET GLY GLY MET MET

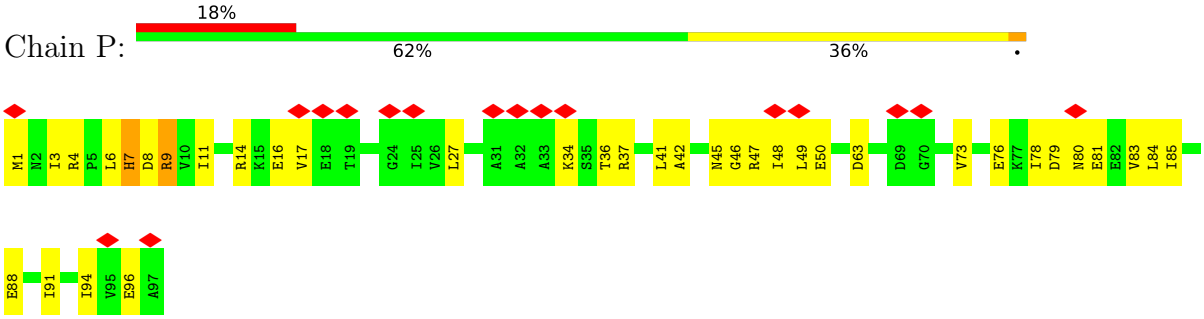
- Molecule 2: Co-chaperonin GroES

Chain O:



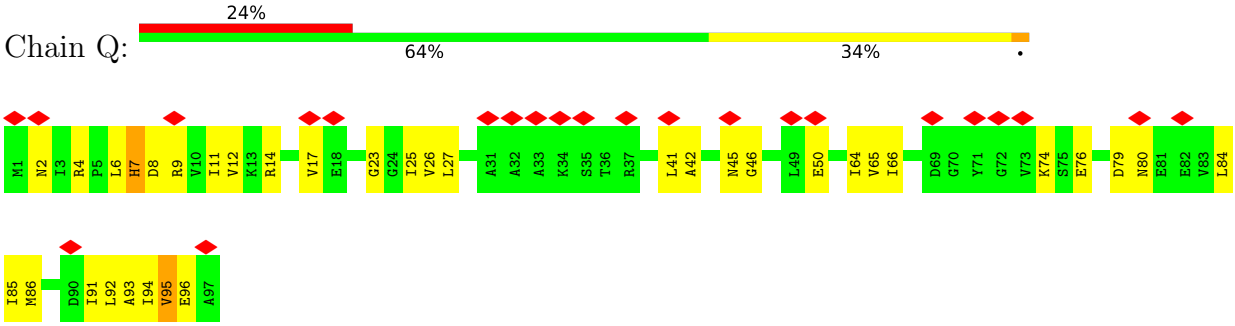
- Molecule 2: Co-chaperonin GroES

Chain P:



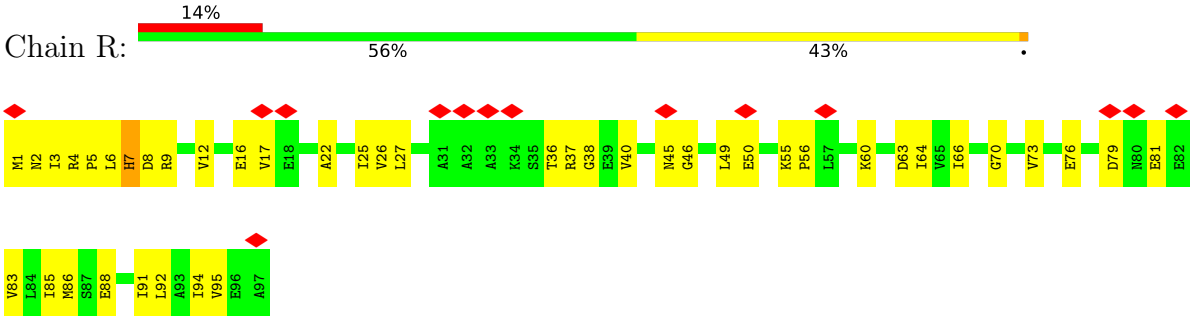
- Molecule 2: Co-chaperonin GroES

Chain Q:



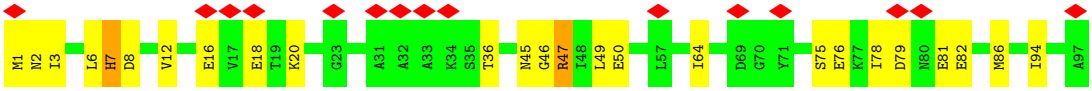
- Molecule 2: Co-chaperonin GroES

Chain R:



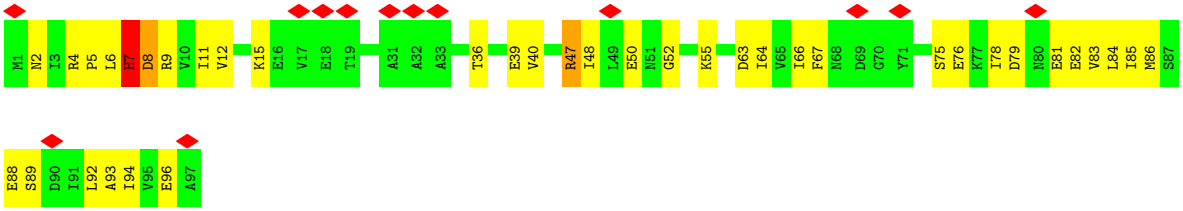
- Molecule 2: Co-chaperonin GroES

Chain S:



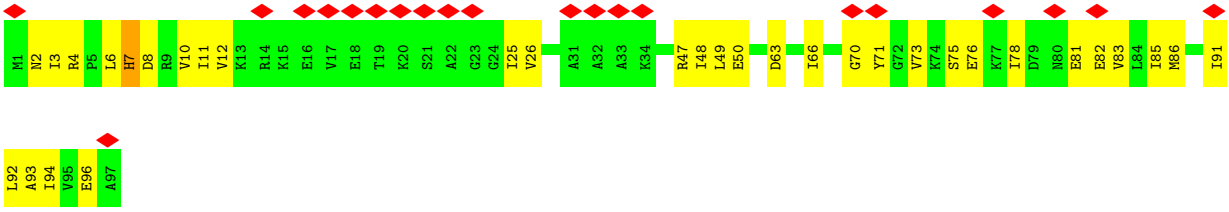
• Molecule 2: Co-chaperonin GroES

Chain T:



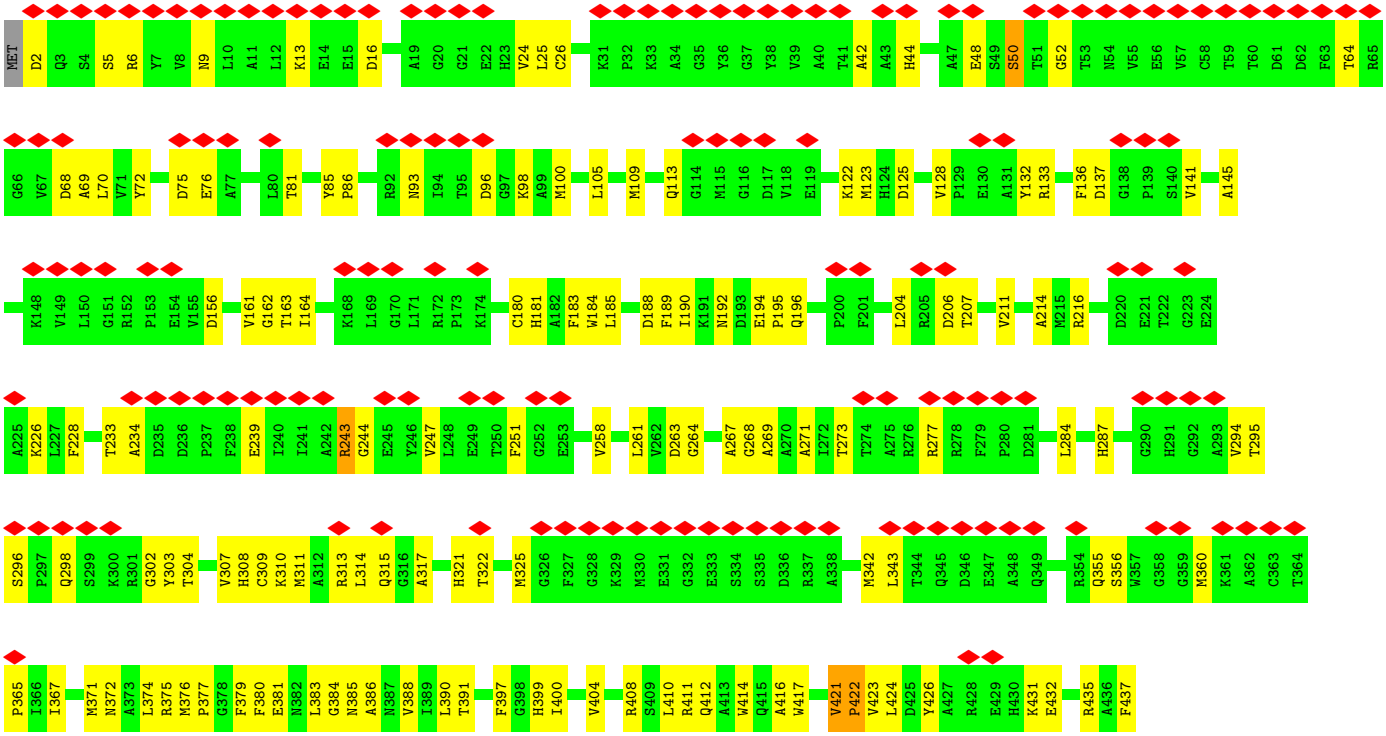
• Molecule 2: Co-chaperonin GroES

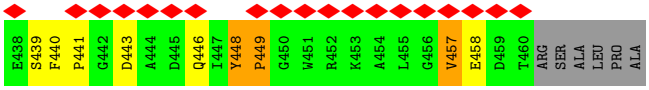
Chain U:



• Molecule 3: Ribulose bisphosphate carboxylase

Chain Z:




E438
S439
F440
P441
G442
D443
A444
D445
Q446
I447
Y448
P449
G450
W451
R452
K453
A454
L455
G456
V457
E458
D459
T460
ARG
SER
ALA
LEU
PRO
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.2	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.369	Depositor
Minimum map value	-0.738	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	380.52225, 380.52225, 380.52225	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84938, 0.84938, 0.84938	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, K, AF3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.14	0/3883	0.41	0/5243
1	B	0.14	0/3883	0.42	0/5243
1	C	0.15	0/3883	0.41	0/5243
1	D	0.17	0/3883	0.44	1/5243 (0.0%)
1	E	0.15	0/3883	0.42	0/5243
1	F	0.14	0/3883	0.41	0/5243
1	G	0.14	0/3883	0.40	0/5243
1	H	0.13	0/3872	0.41	0/5227
1	I	0.16	0/3872	0.42	0/5227
1	J	0.15	0/3872	0.43	0/5227
1	K	0.15	0/3872	0.44	0/5227
1	L	0.15	0/3872	0.43	0/5227
1	M	0.16	0/3872	0.45	0/5227
1	N	0.15	0/3872	0.41	1/5227 (0.0%)
2	O	0.22	0/732	0.72	2/983 (0.2%)
2	P	0.25	0/732	0.84	2/983 (0.2%)
2	Q	0.22	0/732	0.71	1/983 (0.1%)
2	R	0.21	0/732	0.56	0/983
2	S	0.16	0/732	0.51	0/983
2	T	0.17	0/732	0.56	2/983 (0.2%)
2	U	0.21	0/732	0.60	0/983
3	Z	0.16	0/3586	0.52	2/4859 (0.0%)
All	All	0.16	0/62995	0.45	11/85030 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	O	0	1
2	S	0	1
2	T	0	1
3	Z	0	1
All	All	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	448	TYR	C-N-CD	-9.36	86.62	125.00
3	Z	421	VAL	C-N-CD	-7.09	95.92	125.00
2	P	80	ASN	N-CA-C	6.65	123.83	113.72
1	N	218	PRO	CA-N-CD	-6.26	103.24	112.00
1	D	389	MET	CA-CB-CG	6.00	126.11	114.10
2	O	79	ASP	CA-C-N	5.58	132.20	121.54
2	O	79	ASP	C-N-CA	5.58	132.20	121.54
2	P	9	ARG	CA-CB-CG	-5.57	102.97	114.10
2	Q	95	VAL	N-CA-C	5.39	116.14	107.73
2	T	7	HIS	CA-C-N	5.27	131.61	121.54
2	T	7	HIS	C-N-CA	5.27	131.61	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	231	ARG	Sidechain
2	O	47	ARG	Sidechain
2	S	47	ARG	Sidechain
2	T	47	ARG	Sidechain
3	Z	243	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	3979	3976	83	0
1	B	3855	3979	3976	67	0
1	C	3855	3979	3976	77	0
1	D	3855	3979	3976	97	0
1	E	3855	3979	3976	85	0
1	F	3855	3979	3976	89	0
1	G	3855	3979	3976	87	0
1	H	3845	3972	3967	86	0
1	I	3845	3972	3967	101	0
1	J	3845	3972	3967	102	0
1	K	3845	3972	3967	93	0
1	L	3845	3972	3967	85	0
1	M	3845	3972	3967	103	0
1	N	3845	3972	3967	78	0
2	O	728	762	762	56	0
2	P	728	762	762	37	0
2	Q	728	762	762	35	0
2	R	728	762	762	52	0
2	S	728	762	762	22	0
2	T	728	762	762	35	0
2	U	728	762	762	39	0
3	Z	3502	3381	3380	129	0
4	A	4	0	0	3	0
4	B	4	0	0	1	0
4	C	4	0	0	2	0
4	D	4	0	0	2	0
4	E	4	0	0	1	0
4	F	4	0	0	1	0
4	G	4	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	27	12	12	1	0
6	B	27	12	12	1	0
6	C	27	12	12	1	0
6	D	27	12	12	0	0
6	E	27	12	12	1	0
6	F	27	12	12	2	0
6	G	27	12	12	0	0
6	H	27	12	12	1	0
6	I	27	12	12	2	0
6	J	27	12	12	0	0
6	K	27	12	12	0	0
6	L	27	12	12	0	0
6	M	27	12	12	1	0
6	N	27	12	12	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
All	All	62925	64540	64483	1507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:MET:HE2	1:G:309:LEU:HD21	1.40	1.02
1:F:59:GLU:O	1:G:4:LYS:NZ	1.98	0.95
1:H:522:THR:OG1	1:I:41:ASP:OD2	1.85	0.94
2:S:75:SER:OG	2:S:82:GLU:OE2	1.84	0.94
1:I:61:GLU:OE1	1:I:72:GLN:NE2	2.01	0.94
1:L:284:ARG:NH2	1:L:361:ASP:OD1	2.03	0.92
1:N:63:GLU:O	1:N:65:LYS:NZ	2.04	0.91
1:N:385:THR:OG1	1:N:388:GLU:OE1	1.88	0.90
2:U:75:SER:OG	2:U:82:GLU:OE2	1.93	0.87
1:G:151:SER:OG	1:G:398:ASP:OD2	1.94	0.86
2:O:16:GLU:OE2	2:O:19:THR:OG1	1.93	0.86
1:J:518:GLU:OE2	1:K:36:ARG:NE	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:ASP:OD2	1:H:284:ARG:NH1	2.12	0.83
1:J:130:GLU:N	1:J:130:GLU:OE1	2.12	0.82
1:D:363:GLU:OE1	1:D:366:GLN:NE2	2.13	0.82
1:F:90:THR:OG1	6:F:603:ADP:O3B	1.97	0.81
1:G:186:GLU:N	1:G:186:GLU:OE1	2.14	0.80
1:H:214:GLU:OE1	1:H:322:ARG:NH1	2.14	0.80
1:N:180:GLY:O	1:N:389:MET:HE1	1.83	0.79
1:G:432:GLN:NE2	1:G:436:GLN:OE1	2.17	0.78
1:H:290:GLN:NE2	1:H:291:ASP:OD1	2.16	0.78
1:B:116:LEU:O	1:B:120:ILE:HD12	1.83	0.78
1:F:461:GLU:N	1:F:461:GLU:OE1	2.17	0.78
1:F:129:GLU:N	1:F:129:GLU:OE2	2.16	0.77
1:C:123:ALA:HB2	1:C:440:ILE:HD12	1.66	0.77
1:G:384:ALA:N	1:G:388:GLU:OE2	2.17	0.76
1:H:432:GLN:NE2	1:H:436:GLN:OE1	2.19	0.76
1:E:115:ASP:OD1	1:E:436:GLN:NE2	2.18	0.76
1:B:27:VAL:O	1:B:30:THR:HG22	1.85	0.76
2:O:12:VAL:HG12	2:O:86:MET:HE1	1.67	0.76
1:K:385:THR:OG1	1:K:388:GLU:OE1	2.04	0.75
3:Z:233:THR:HG23	3:Z:267:ALA:HB2	1.69	0.75
1:B:326:ASN:OD1	1:B:327:LYS:N	2.19	0.75
2:R:27:LEU:HD12	2:R:27:LEU:O	1.86	0.75
1:E:49:ILE:HG21	1:F:513:LEU:HD21	1.67	0.75
1:A:339:GLU:O	1:A:343:GLN:NE2	2.20	0.75
1:G:434:GLU:OE1	1:G:434:GLU:N	2.20	0.74
1:M:188:ASP:OD1	1:M:380:LYS:NZ	2.19	0.74
1:L:326:ASN:OD1	1:L:329:THR:N	2.21	0.73
4:B:602:AF3:F1	6:B:603:ADP:O2B	1.96	0.73
1:C:232:GLU:OE1	1:C:232:GLU:N	2.21	0.73
1:D:434:GLU:OE1	1:D:434:GLU:N	2.20	0.73
1:E:384:ALA:N	1:E:388:GLU:OE2	2.21	0.73
2:P:79:ASP:OD1	2:P:81:GLU:OE1	2.07	0.73
1:M:90:THR:OG1	6:M:2003:ADP:O1B	2.05	0.73
1:D:383:ALA:HB3	1:D:389:MET:HE2	1.69	0.73
1:E:108:ALA:O	1:L:105:LYS:NZ	2.22	0.73
1:I:188:ASP:OD2	1:I:380:LYS:NZ	2.22	0.73
1:L:13:ARG:NH2	1:L:518:GLU:OE1	2.22	0.72
1:M:429:LEU:HD23	1:M:440:ILE:HD11	1.70	0.72
1:C:49:ILE:HD12	1:D:513:LEU:HD13	1.71	0.72
1:L:188:ASP:OD1	1:L:380:LYS:NZ	2.22	0.72
1:F:434:GLU:OE2	1:F:434:GLU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:VAL:HG11	1:J:510:VAL:HG11	1.72	0.72
1:K:326:ASN:OD1	1:K:329:THR:N	2.22	0.72
3:Z:371:MET:O	3:Z:376:MET:HE3	1.90	0.72
1:M:461:GLU:OE2	1:M:463:SER:OG	2.06	0.71
1:H:156:GLU:N	1:H:156:GLU:OE1	2.22	0.71
1:L:194:GLN:O	1:L:371:LYS:NZ	2.23	0.71
1:B:473:ASP:OD1	1:B:474:GLY:N	2.24	0.71
2:R:36:THR:O	2:R:37:ARG:NH2	2.24	0.71
3:Z:309:CYS:HB3	3:Z:343:LEU:HD11	1.72	0.71
1:K:290:GLN:NE2	1:K:291:ASP:OD1	2.23	0.71
4:A:601:AF3:F2	6:A:603:ADP:O2B	1.98	0.71
1:J:290:GLN:NE2	1:J:291:ASP:OD1	2.24	0.71
2:T:7:HIS:O	2:T:8:ASP:OD1	2.08	0.70
1:K:179:ASP:OD1	1:K:180:GLY:N	2.25	0.70
1:C:408:GLU:OE1	1:C:408:GLU:N	2.24	0.70
1:C:386:GLU:N	1:C:386:GLU:OE1	2.24	0.70
1:L:290:GLN:NE2	1:L:291:ASP:OD1	2.23	0.70
1:F:295:LEU:HA	1:F:342:ILE:HD11	1.73	0.70
1:M:513:LEU:HD11	1:N:49:ILE:CD1	2.21	0.70
2:T:15:LYS:HZ3	2:T:64:ILE:HG23	1.57	0.70
1:C:73:MET:HB3	1:C:514:MET:HE1	1.72	0.70
1:M:16:MET:SD	1:M:514:MET:SD	2.90	0.70
1:N:284:ARG:NH1	1:N:360:TYR:O	2.25	0.70
1:G:513:LEU:O	1:G:516:THR:HG22	1.91	0.70
1:B:123:ALA:HB2	1:B:440:ILE:HD12	1.73	0.69
1:J:326:ASN:OD1	1:J:329:THR:N	2.25	0.69
1:I:327:LYS:NZ	1:J:384:ALA:O	2.23	0.69
2:T:12:VAL:HG22	2:T:86:MET:HE1	1.74	0.69
1:B:41:ASP:OD2	1:C:69:MET:HE1	1.93	0.69
1:I:77:VAL:HG11	1:I:510:VAL:HG21	1.74	0.69
2:R:12:VAL:HG22	2:R:86:MET:HE1	1.75	0.68
1:F:191:GLU:N	1:F:191:GLU:OE1	2.26	0.68
1:M:89:THR:O	1:M:93:THR:HG23	1.93	0.68
1:D:87:ASP:OD1	4:D:602:AF3:F3	2.00	0.68
1:K:363:GLU:OE1	1:K:366:GLN:NE2	2.25	0.68
3:Z:26:CYS:HB3	3:Z:123:MET:HE2	1.75	0.68
1:G:238:GLU:HG2	2:R:25:ILE:HD11	1.74	0.68
2:S:16:GLU:OE2	2:S:20:LYS:NZ	2.27	0.68
1:G:496:PRO:O	1:G:499:VAL:HG12	1.93	0.68
1:J:397:GLU:O	1:J:401:HIS:ND1	2.27	0.68
1:M:158:VAL:O	1:M:162:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:6:LEU:HD12	2:O:6:LEU:O	1.93	0.68
2:R:36:THR:OG1	2:R:37:ARG:NH2	2.27	0.67
1:G:233:MET:HE2	1:G:309:LEU:CD2	2.20	0.67
1:L:397:GLU:O	1:L:401:HIS:ND1	2.27	0.67
1:N:345:ARG:NH2	1:N:348:GLN:OE1	2.28	0.67
2:O:79:ASP:O	2:O:80:ASN:OD1	2.12	0.67
2:U:12:VAL:HG22	2:U:86:MET:HE1	1.75	0.67
1:H:90:THR:OG1	6:H:2002:ADP:O1B	2.12	0.67
1:J:284:ARG:NH2	1:J:361:ASP:OD1	2.27	0.67
1:L:4:LYS:NZ	1:L:523:ASP:OD1	2.27	0.67
2:Q:64:ILE:O	2:Q:95:VAL:HG22	1.95	0.67
1:L:59:GLU:O	1:L:61:GLU:OE1	2.14	0.66
1:D:214:GLU:N	1:D:214:GLU:OE1	2.29	0.66
1:D:55:SER:O	1:D:59:GLU:OE1	2.14	0.66
1:H:111:MET:HB3	1:H:116:LEU:HD11	1.76	0.66
3:Z:457:VAL:HG12	3:Z:458:GLU:H	1.59	0.66
1:D:386:GLU:OE1	1:D:386:GLU:N	2.28	0.66
2:T:6:LEU:HD12	2:T:6:LEU:O	1.95	0.66
2:O:76:GLU:N	2:O:76:GLU:OE1	2.28	0.66
3:Z:303:TYR:CZ	3:Z:311:MET:SD	2.89	0.66
1:B:448:GLU:OE2	1:B:470:LYS:NZ	2.29	0.66
1:J:214:GLU:N	1:J:214:GLU:OE1	2.29	0.65
2:S:78:ILE:O	2:S:79:ASP:OD1	2.13	0.65
1:L:185:ASP:OD1	1:L:392:LYS:NZ	2.30	0.65
1:I:10:ASN:OD1	1:I:11:ASP:N	2.30	0.65
1:M:25:ASP:HA	1:M:28:LYS:HZ2	1.62	0.65
4:E:601:AF3:F2	6:E:603:ADP:O2B	2.04	0.65
1:K:192:GLY:O	1:K:193:MET:HE2	1.97	0.65
1:K:193:MET:HE1	1:K:371:LYS:O	1.97	0.65
2:R:6:LEU:HD12	2:R:6:LEU:O	1.96	0.65
1:I:190:VAL:O	1:I:376:VAL:N	2.29	0.65
2:P:4:ARG:O	2:P:4:ARG:NH1	2.30	0.65
1:F:156:GLU:OE1	1:F:156:GLU:N	2.29	0.65
2:R:36:THR:HG23	2:R:37:ARG:CZ	2.27	0.65
1:H:362:ARG:NH2	1:H:363:GLU:OE2	2.29	0.64
2:O:78:ILE:O	2:O:79:ASP:OD2	2.15	0.64
1:F:351:GLN:O	1:F:355:GLU:OE1	2.16	0.64
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.79	0.64
1:N:41:ASP:OD1	1:N:42:LYS:N	2.31	0.64
1:N:290:GLN:NE2	1:N:291:ASP:OD1	2.30	0.64
1:N:179:ASP:O	1:N:380:LYS:NZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:36:THR:HG23	2:R:37:ARG:NH1	2.12	0.64
1:N:166:MET:HE2	1:N:171:LYS:HA	1.80	0.64
1:E:152:ALA:CB	1:E:158:VAL:HG21	2.28	0.64
1:F:179:ASP:OD1	1:F:389:MET:HE3	1.98	0.64
1:N:18:ARG:NH2	1:N:67:GLU:OE2	2.30	0.64
1:H:49:ILE:HG21	1:N:513:LEU:HD12	1.80	0.64
2:P:37:ARG:NH2	2:Q:76:GLU:OE2	2.31	0.64
1:C:429:LEU:HD23	1:C:430:ARG:N	2.13	0.63
1:M:404:ARG:O	1:M:408:GLU:OE1	2.15	0.63
3:Z:5:SER:O	3:Z:6:ARG:HG2	1.97	0.63
1:E:39:VAL:HG11	1:F:520:MET:HE3	1.80	0.63
1:C:87:ASP:OD1	4:C:602:AF3:F3	2.06	0.63
2:U:47:ARG:HE	2:U:49:LEU:HD13	1.63	0.63
1:C:225:LYS:N	1:C:252:GLU:OE1	2.31	0.63
2:O:27:LEU:O	2:O:27:LEU:HD12	1.99	0.63
1:H:152:ALA:CB	1:H:158:VAL:HG21	2.29	0.62
1:K:214:GLU:N	1:K:214:GLU:OE1	2.32	0.62
3:Z:192:ASN:ND2	3:Z:196:GLN:OE1	2.31	0.62
2:T:50:GLU:OE2	2:T:55:LYS:NZ	2.32	0.62
1:K:193:MET:SD	1:K:371:LYS:O	2.57	0.62
1:N:426:LEU:HD23	1:N:444:LEU:HD21	1.80	0.62
1:D:429:LEU:HD23	1:D:440:ILE:HD11	1.82	0.62
1:E:487:ASN:OD1	1:E:489:ILE:HG22	1.99	0.62
1:D:342:ILE:HG23	1:D:372:LEU:HD21	1.82	0.62
3:Z:161:VAL:HG13	3:Z:410:LEU:HD11	1.81	0.62
1:I:263:VAL:HG22	1:I:267:MET:SD	2.40	0.62
1:N:115:ASP:OD1	1:N:118:ARG:NH2	2.32	0.62
3:Z:381:GLU:OE1	3:Z:417:TRP:NE1	2.32	0.62
1:C:16:MET:HE3	1:C:514:MET:SD	2.40	0.61
4:C:602:AF3:F3	6:C:603:ADP:O3B	2.08	0.61
1:G:87:ASP:OD1	4:G:601:AF3:F2	2.07	0.61
2:T:47:ARG:HH12	2:U:48:ILE:HD12	1.65	0.61
1:E:53:GLY:O	1:E:56:VAL:HG12	1.99	0.61
2:R:38:GLY:O	2:R:64:ILE:HD12	1.99	0.61
1:M:232:GLU:OE2	1:M:309:LEU:N	2.30	0.61
1:N:11:ASP:OD1	1:N:15:LYS:NZ	2.30	0.61
1:H:364:LYS:HG3	1:H:365:LEU:HD22	1.83	0.61
1:J:191:GLU:OE2	1:J:335:GLY:N	2.34	0.61
1:E:360:TYR:O	1:E:363:GLU:HG3	2.01	0.61
1:D:19:GLY:O	1:D:22:VAL:HG12	2.00	0.61
1:H:518:GLU:N	1:H:518:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:ILE:HG23	1:J:49:ILE:O	2.00	0.61
1:L:461:GLU:OE1	1:L:461:GLU:N	2.34	0.61
1:I:175:ILE:HG23	1:I:400:LEU:HD11	1.82	0.61
1:D:222:LEU:HD21	1:D:292:ILE:HG23	1.82	0.60
1:D:315:GLU:OE1	1:D:315:GLU:N	2.34	0.60
2:T:94:ILE:O	2:U:3:ILE:HD12	2.00	0.60
1:I:455:VAL:HG21	1:I:465:VAL:HG11	1.83	0.60
3:Z:416:ALA:HB2	3:Z:426:TYR:CD1	2.37	0.60
1:C:105:LYS:NZ	1:J:109:ALA:O	2.27	0.60
1:E:283:ASP:OD1	1:E:284:ARG:N	2.34	0.60
1:B:360:TYR:O	1:B:363:GLU:HG3	2.01	0.60
1:H:10:ASN:OD1	1:H:11:ASP:N	2.35	0.60
1:B:437:ASN:O	1:B:440:ILE:HG22	2.01	0.60
1:I:290:GLN:NE2	1:I:291:ASP:OD1	2.34	0.60
1:C:49:ILE:HD11	1:C:387:VAL:O	2.02	0.60
1:E:383:ALA:HB3	1:E:389:MET:SD	2.41	0.60
3:Z:284:LEU:HD22	3:Z:317:ALA:HA	1.84	0.60
1:L:482:THR:OG1	1:L:484:GLU:OE1	2.18	0.60
2:Q:6:LEU:HD12	2:Q:6:LEU:O	2.01	0.60
2:T:47:ARG:NH1	2:U:48:ILE:HD12	2.15	0.60
1:I:77:VAL:HG11	1:I:510:VAL:CG2	2.32	0.60
2:S:45:ASN:OD1	2:S:46:GLY:N	2.35	0.60
1:F:15:LYS:HE2	1:F:15:LYS:HA	1.84	0.60
2:P:96:GLU:OE2	2:Q:4:ARG:NE	2.35	0.60
3:Z:93:ASN:ND2	3:Z:98:LYS:O	2.34	0.60
1:D:398:ASP:OD2	4:D:602:AF3:F1	2.09	0.59
1:J:513:LEU:HD21	1:K:49:ILE:HD13	1.83	0.59
1:N:381:VAL:O	1:N:389:MET:HE3	2.02	0.59
3:Z:386:ALA:HB2	3:Z:414:TRP:CD1	2.37	0.59
1:H:190:VAL:O	1:H:376:VAL:N	2.34	0.59
1:L:58:ARG:NE	1:L:59:GLU:OE2	2.34	0.59
1:C:73:MET:CB	1:C:514:MET:HE1	2.32	0.59
1:L:484:GLU:OE1	1:L:484:GLU:N	2.34	0.59
1:G:156:GLU:N	1:G:156:GLU:OE1	2.33	0.59
1:G:350:ARG:O	1:G:353:ILE:HG22	2.02	0.59
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.85	0.59
1:G:87:ASP:OD1	1:G:88:GLY:N	2.36	0.59
1:G:232:GLU:HB3	1:G:309:LEU:HD23	1.84	0.59
1:K:193:MET:HE3	1:K:295:LEU:HD13	1.84	0.59
1:K:193:MET:O	1:K:332:ILE:N	2.36	0.59
1:D:61:GLU:N	1:D:61:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:MET:SD	1:H:269:GLY:N	2.75	0.59
1:M:195:PHE:CZ	1:M:250:ILE:HD12	2.37	0.59
1:A:383:ALA:HB3	1:A:389:MET:SD	2.43	0.58
1:B:210:THR:O	1:B:210:THR:HG22	2.02	0.58
1:F:27:VAL:O	1:F:30:THR:HG22	2.02	0.58
1:G:142:LYS:O	1:G:146:GLN:OE1	2.21	0.58
1:K:284:ARG:NH2	1:K:361:ASP:OD1	2.36	0.58
1:A:80:LYS:NZ	1:G:384:ALA:O	2.35	0.58
1:H:348:GLN:NE2	1:H:352:GLN:OE1	2.36	0.58
3:Z:188:ASP:OD1	3:Z:411:ARG:NH2	2.35	0.58
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.85	0.58
1:D:440:ILE:O	1:D:444:LEU:HD12	2.04	0.58
2:R:37:ARG:NH2	2:R:66:ILE:HG23	2.19	0.58
1:A:77:VAL:CG2	1:A:510:VAL:HG11	2.32	0.58
1:F:290:GLN:NE2	1:F:294:THR:OG1	2.36	0.58
1:H:148:GLY:O	1:H:151:SER:OG	2.19	0.58
1:M:16:MET:HE3	1:M:520:MET:HE1	1.86	0.58
1:I:221:LEU:CD2	1:I:223:ALA:HB2	2.34	0.58
1:G:336:VAL:HG12	1:G:336:VAL:O	2.03	0.58
2:O:91:ILE:O	2:P:6:LEU:HD21	2.03	0.58
2:T:75:SER:OG	2:T:82:GLU:OE2	2.16	0.58
3:Z:311:MET:HE2	3:Z:315:GLN:HE21	1.69	0.58
1:H:507:ALA:O	1:H:510:VAL:HG12	2.04	0.58
1:J:152:ALA:O	1:J:153:ASN:OD1	2.21	0.58
3:Z:109:MET:HG3	3:Z:303:TYR:CZ	2.39	0.58
1:H:5:ASP:OD2	1:H:7:LYS:NZ	2.36	0.57
1:L:447:MET:HE3	1:L:504:LEU:HD11	1.84	0.57
1:C:49:ILE:HD12	1:D:513:LEU:CD1	2.34	0.57
3:Z:13:LYS:O	3:Z:16:ASP:OD1	2.22	0.57
1:A:514:MET:O	1:A:517:THR:HG23	2.04	0.57
1:D:100:ILE:HD11	1:D:511:ALA:HA	1.85	0.57
1:G:383:ALA:HB1	1:G:388:GLU:HG3	1.84	0.57
2:R:70:GLY:O	2:R:73:VAL:HG12	2.04	0.57
2:U:25:ILE:HG13	2:U:26:VAL:N	2.20	0.57
1:E:104:LEU:HA	1:E:107:VAL:HG12	1.86	0.57
1:I:438:VAL:O	1:I:442:VAL:HG23	2.04	0.57
1:J:271:VAL:HG12	1:J:273:VAL:HG23	1.85	0.57
1:L:363:GLU:O	1:L:367:GLU:OE1	2.22	0.57
1:E:496:PRO:O	1:E:499:VAL:HG12	2.05	0.57
1:F:13:ARG:NH1	1:F:518:GLU:OE1	2.37	0.57
1:C:129:GLU:OE1	1:C:129:GLU:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:96:GLU:HG3	2:R:4:ARG:CZ	2.35	0.57
2:Q:45:ASN:OD1	2:Q:46:GLY:N	2.38	0.56
1:F:360:TYR:O	1:F:363:GLU:HG2	2.06	0.56
1:D:493:ILE:O	1:D:493:ILE:HG13	2.06	0.56
1:E:4:LYS:HA	1:E:4:LYS:HE3	1.87	0.56
1:I:420:ILE:HD11	1:I:451:LEU:HB3	1.88	0.56
1:K:461:GLU:OE2	1:K:463:SER:HB3	2.05	0.56
2:P:6:LEU:O	2:P:6:LEU:HG	2.05	0.56
2:Q:66:ILE:O	2:Q:92:LEU:N	2.31	0.56
3:Z:325:MET:HE3	3:Z:379:PHE:CD2	2.41	0.56
2:O:12:VAL:CG1	2:O:86:MET:HE1	2.34	0.56
3:Z:372:ASN:ND2	3:Z:443:ASP:OD2	2.37	0.56
1:K:496:PRO:O	1:K:499:VAL:HG12	2.05	0.56
1:C:369:VAL:O	1:C:373:ALA:N	2.39	0.56
3:Z:313:ARG:HG2	3:Z:360:MET:HE3	1.86	0.56
1:C:359:ASP:O	1:C:363:GLU:OE1	2.23	0.56
1:D:458:CYS:HB2	1:D:460:GLU:OE1	2.06	0.56
1:J:477:GLY:HA3	1:J:488:MET:HE2	1.87	0.56
1:K:252:GLU:OE2	1:K:285:ARG:NH2	2.37	0.56
1:M:69:MET:HE1	1:N:41:ASP:HA	1.86	0.56
2:O:64:ILE:O	2:O:94:ILE:HD12	2.05	0.56
2:P:11:ILE:HG23	2:P:41:LEU:HB2	1.88	0.56
1:D:369:VAL:O	1:D:373:ALA:N	2.37	0.56
1:K:16:MET:HE1	1:K:517:THR:HG21	1.87	0.56
1:K:193:MET:HE3	1:K:295:LEU:CD1	2.36	0.56
1:A:104:LEU:HA	1:A:107:VAL:HG12	1.86	0.56
1:D:41:ASP:OD1	1:E:69:MET:SD	2.64	0.56
1:I:250:ILE:HG23	1:I:250:ILE:O	2.06	0.56
1:J:69:MET:HE1	1:K:41:ASP:HA	1.88	0.56
1:L:252:GLU:OE2	1:L:285:ARG:NH2	2.35	0.55
1:F:234:LEU:O	1:F:238:GLU:OE1	2.24	0.55
1:I:178:GLU:N	1:I:379:ILE:O	2.35	0.55
1:M:486:GLY:HA3	1:M:491:MET:HE1	1.87	0.55
1:F:284:ARG:O	1:F:288:MET:SD	2.64	0.55
2:S:12:VAL:HG22	2:S:86:MET:HE1	1.88	0.55
3:Z:162:GLY:HA2	3:Z:189:PHE:O	2.06	0.55
2:O:25:ILE:HG13	2:O:26:VAL:HG23	1.87	0.55
2:Q:96:GLU:HG3	2:R:4:ARG:NH1	2.21	0.55
2:R:94:ILE:O	2:S:3:ILE:HD12	2.06	0.55
3:Z:424:LEU:HD12	3:Z:424:LEU:H	1.72	0.55
1:E:203:TYR:CE2	1:F:305:ILE:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:45:ASN:OD1	2:R:46:GLY:N	2.39	0.55
1:D:123:ALA:HB2	1:D:440:ILE:HD12	1.88	0.55
1:G:365:LEU:O	1:G:368:ARG:HG2	2.05	0.55
1:I:115:ASP:OD1	1:I:118:ARG:NH2	2.38	0.55
1:M:160:LYS:O	1:M:164:GLU:OE1	2.24	0.55
1:N:444:LEU:HA	1:N:447:MET:HE3	1.88	0.55
1:A:386:GLU:HA	1:A:389:MET:HG2	1.87	0.55
1:B:286:LYS:H	1:B:286:LYS:HD2	1.71	0.55
2:P:11:ILE:HG22	2:P:42:ALA:HB3	1.89	0.55
2:R:4:ARG:HD3	2:R:4:ARG:N	2.21	0.55
1:B:21:ASN:O	1:B:25:ASP:OD1	2.25	0.55
1:F:421:ARG:NH2	1:F:474:GLY:O	2.39	0.55
1:H:80:LYS:O	1:H:83:ASP:OD1	2.25	0.55
1:J:252:GLU:OE2	1:J:285:ARG:NH2	2.36	0.55
1:M:49:ILE:HG13	1:M:49:ILE:O	2.07	0.55
1:G:72:GLN:OE1	1:G:75:LYS:NZ	2.23	0.55
1:L:419:LEU:HD12	1:L:447:MET:HE2	1.89	0.55
1:M:510:VAL:O	1:M:514:MET:N	2.33	0.55
2:O:73:VAL:HG23	2:O:86:MET:HE3	1.88	0.55
2:S:18:GLU:O	2:S:18:GLU:HG2	2.07	0.55
1:B:311:LYS:HE3	1:B:311:LYS:HA	1.88	0.55
1:F:23:LEU:CD2	1:F:74:VAL:HG23	2.38	0.55
1:H:111:MET:CB	1:H:116:LEU:HD11	2.37	0.55
1:A:304:GLU:OE1	1:A:304:GLU:N	2.35	0.54
1:A:315:GLU:N	1:A:315:GLU:OE1	2.39	0.54
1:J:52:ASP:O	1:J:55:SER:OG	2.20	0.54
1:K:363:GLU:O	1:K:367:GLU:OE1	2.24	0.54
2:T:39:GLU:OE2	2:T:40:VAL:N	2.40	0.54
1:C:253:ASP:OD1	1:C:254:VAL:N	2.39	0.54
1:I:405:ALA:HA	1:I:408:GLU:OE1	2.07	0.54
1:J:390:LYS:O	1:J:393:LYS:HG2	2.07	0.54
1:D:437:ASN:O	1:D:440:ILE:HG22	2.07	0.54
2:O:5:PRO:HB2	2:O:9:ARG:HB2	1.89	0.54
1:K:193:MET:O	1:K:331:THR:HA	2.08	0.54
2:U:70:GLY:O	2:U:73:VAL:HG12	2.07	0.54
1:E:233:MET:HE1	1:E:309:LEU:HD13	1.90	0.54
1:J:518:GLU:CD	1:K:36:ARG:HE	2.16	0.54
1:C:27:VAL:O	1:C:30:THR:HG22	2.07	0.54
1:I:90:THR:OG1	6:I:2002:ADP:O1B	2.16	0.54
1:K:455:VAL:HG21	1:K:465:VAL:HG21	1.89	0.54
1:C:238:GLU:O	1:C:242:LYS:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ILE:O	1:D:305:ILE:HG22	2.08	0.54
1:J:307:MET:HA	1:J:307:MET:HE2	1.90	0.54
3:Z:457:VAL:HG12	3:Z:458:GLU:N	2.23	0.54
1:D:128:VAL:HG23	1:D:501:ARG:HG2	1.90	0.54
1:J:126:ALA:O	1:J:130:GLU:OE1	2.25	0.54
1:L:391:GLU:OE2	1:L:395:ARG:HD2	2.08	0.54
1:N:215:LEU:HB2	1:N:218:PRO:HG3	1.88	0.54
2:O:45:ASN:OD1	2:O:46:GLY:N	2.41	0.54
1:B:6:VAL:HG12	1:B:521:VAL:HG12	1.90	0.53
1:C:493:ILE:O	1:C:493:ILE:HG23	2.08	0.53
1:F:8:PHE:O	1:F:11:ASP:OD1	2.27	0.53
1:F:194:GLN:HE21	1:F:329:THR:HG23	1.73	0.53
1:I:152:ALA:CB	1:I:158:VAL:HG21	2.38	0.53
1:I:199:TYR:OH	1:I:327:LYS:HD2	2.09	0.53
1:I:267:MET:SD	1:I:267:MET:O	2.66	0.53
1:K:13:ARG:NH2	1:K:518:GLU:OE2	2.42	0.53
2:R:76:GLU:OE2	2:R:85:ILE:HG13	2.08	0.53
1:A:73:MET:CE	1:G:47:PRO:HD2	2.37	0.53
1:A:522:THR:HG23	1:G:41:ASP:OD2	2.09	0.53
1:C:229:ASN:O	1:C:232:GLU:OE1	2.27	0.53
1:E:100:ILE:HD13	1:E:515:ILE:HG23	1.91	0.53
2:O:87:SER:OG	2:O:89:SER:OG	2.21	0.53
2:P:6:LEU:O	2:P:7:HIS:CG	2.62	0.53
3:Z:133:ARG:NH1	3:Z:356:SER:O	2.42	0.53
1:H:4:LYS:HA	1:H:523:ASP:HA	1.90	0.53
1:J:114:MET:SD	1:K:459:GLY:HA3	2.49	0.53
1:K:477:GLY:C	1:K:488:MET:HE3	2.33	0.53
1:K:506:TYR:O	1:K:509:SER:OG	2.17	0.53
1:L:98:ALA:O	1:L:102:GLU:OE1	2.25	0.53
1:L:284:ARG:N	1:L:284:ARG:HD2	2.23	0.53
1:B:351:GLN:O	1:B:355:GLU:OE1	2.27	0.53
1:E:10:ASN:OD1	1:E:11:ASP:N	2.42	0.53
2:S:86:MET:SD	2:S:86:MET:N	2.82	0.53
3:Z:325:MET:HG3	3:Z:371:MET:SD	2.48	0.53
1:A:270:ILE:HG12	2:Q:27:LEU:HD13	1.90	0.53
1:D:69:MET:HE3	1:D:69:MET:HA	1.90	0.53
1:M:28:LYS:NZ	1:M:97:GLN:OE1	2.36	0.53
2:Q:94:ILE:O	2:R:3:ILE:HD12	2.07	0.53
1:D:242:LYS:HE2	1:D:242:LYS:HA	1.91	0.53
1:K:98:ALA:O	1:K:102:GLU:OE1	2.27	0.53
3:Z:185:LEU:O	3:Z:408:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLN:HA	1:C:100:ILE:HG22	1.90	0.53
1:D:383:ALA:HB3	1:D:389:MET:CE	2.36	0.53
1:E:284:ARG:O	1:E:288:MET:SD	2.67	0.53
1:L:359:ASP:O	1:L:363:GLU:OE1	2.26	0.53
2:O:92:LEU:HD23	2:P:9:ARG:HH11	1.72	0.53
3:Z:400:ILE:HD11	3:Z:435:ARG:HD3	1.91	0.53
1:D:114:MET:HE3	1:D:114:MET:HA	1.89	0.53
1:E:439:GLY:O	1:E:442:VAL:HG12	2.09	0.53
1:H:69:MET:SD	1:H:520:MET:HE3	2.48	0.53
1:I:48:THR:HG23	1:I:48:THR:O	2.09	0.53
1:N:104:LEU:HA	1:N:107:VAL:HG12	1.89	0.53
1:C:153:ASN:OD1	1:C:153:ASN:O	2.26	0.53
1:M:103:GLY:HA3	1:M:515:ILE:HD11	1.91	0.53
2:R:22:ALA:N	2:R:26:VAL:O	2.39	0.53
2:S:1:MET:SD	2:S:2:ASN:O	2.67	0.53
3:Z:377:PRO:HB2	3:Z:448:TYR:CE2	2.44	0.53
1:J:223:ALA:HB1	1:J:227:ILE:HD11	1.91	0.52
1:A:404:ARG:O	1:A:408:GLU:OE1	2.27	0.52
1:B:73:MET:SD	1:B:73:MET:C	2.92	0.52
1:C:105:LYS:NZ	1:J:110:GLY:HA3	2.25	0.52
1:F:10:ASN:OD1	1:F:11:ASP:N	2.42	0.52
1:G:217:SER:OG	1:G:319:GLN:NE2	2.42	0.52
1:H:130:GLU:O	1:H:134:LEU:HD23	2.09	0.52
1:M:289:LEU:HA	1:M:292:ILE:HG22	1.91	0.52
2:U:76:GLU:OE1	2:U:76:GLU:N	2.42	0.52
1:D:102:GLU:HB3	1:D:442:VAL:HG23	1.91	0.52
1:F:6:VAL:HG12	1:F:521:VAL:HG12	1.91	0.52
4:F:601:AF3:F3	6:F:603:ADP:O3A	2.16	0.52
1:J:125:THR:O	1:J:128:VAL:HG12	2.09	0.52
2:R:66:ILE:HD13	2:S:3:ILE:HD11	1.91	0.52
3:Z:109:MET:HG3	3:Z:303:TYR:CE1	2.44	0.52
3:Z:156:ASP:O	3:Z:414:TRP:CH2	2.62	0.52
1:F:135:SER:OG	1:F:497:THR:HG21	2.09	0.52
1:M:252:GLU:OE1	1:M:285:ARG:NE	2.42	0.52
2:O:88:GLU:HA	2:O:91:ILE:HD13	1.91	0.52
1:D:336:VAL:HG12	1:D:336:VAL:O	2.09	0.52
1:F:364:LYS:O	1:F:368:ARG:HG3	2.09	0.52
1:J:130:GLU:O	1:J:134:LEU:HD23	2.09	0.52
1:K:69:MET:HE1	1:K:522:THR:HG22	1.91	0.52
1:N:185:ASP:OD1	1:N:382:GLY:N	2.36	0.52
3:Z:109:MET:CE	3:Z:123:MET:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:GLY:O	1:F:285:ARG:NH2	2.39	0.52
1:I:125:THR:O	1:I:128:VAL:HG12	2.08	0.52
1:J:510:VAL:O	1:J:514:MET:N	2.36	0.52
2:O:4:ARG:NH2	2:U:96:GLU:OE2	2.35	0.52
3:Z:376:MET:HE1	3:Z:390:LEU:HD22	1.92	0.52
1:C:100:ILE:HD12	1:C:514:MET:HG2	1.91	0.52
3:Z:233:THR:HG1	3:Z:263:ASP:H	1.55	0.52
3:Z:371:MET:HE2	3:Z:375:ARG:HB3	1.91	0.52
1:J:232:GLU:HG3	1:J:309:LEU:HB2	1.91	0.52
1:N:30:THR:OG1	1:N:51:LYS:O	2.28	0.52
1:N:53:GLY:HA2	1:N:56:VAL:HG12	1.91	0.52
2:Q:6:LEU:O	2:Q:7:HIS:CG	2.63	0.52
1:B:145:ALA:O	1:B:149:THR:HG23	2.09	0.52
1:L:267:MET:O	1:L:268:ARG:NH2	2.43	0.52
2:T:6:LEU:O	2:T:7:HIS:CG	2.63	0.52
1:D:194:GLN:HE21	1:D:329:THR:HG23	1.75	0.52
1:J:191:GLU:O	1:J:191:GLU:CD	2.53	0.52
1:C:233:MET:HE2	1:C:237:LEU:HD21	1.92	0.51
1:D:253:ASP:OD1	1:D:254:VAL:N	2.42	0.51
1:E:142:LYS:O	1:E:146:GLN:NE2	2.42	0.51
1:E:364:LYS:O	1:E:367:GLU:HG2	2.10	0.51
1:F:308:GLU:HG3	1:F:310:GLU:OE1	2.09	0.51
3:Z:184:TRP:HB3	3:Z:226:LYS:HD3	1.92	0.51
3:Z:234:ALA:HB2	3:Z:239:GLU:OE1	2.10	0.51
1:L:482:THR:CB	1:L:484:GLU:OE1	2.59	0.51
1:M:411:VAL:HG21	1:M:494:LEU:HD12	1.92	0.51
2:P:3:ILE:HD11	2:P:78:ILE:HG12	1.91	0.51
2:Q:23:GLY:O	2:Q:25:ILE:HD12	2.09	0.51
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.93	0.51
1:D:301:ILE:HD11	1:D:307:MET:HB3	1.92	0.51
1:E:38:VAL:HG22	1:F:519:CYS:SG	2.51	0.51
1:E:217:SER:N	1:E:218:PRO:HD3	2.26	0.51
1:J:461:GLU:OE2	1:J:463:SER:OG	2.27	0.51
1:L:10:ASN:OD1	1:L:11:ASP:N	2.44	0.51
3:Z:311:MET:O	3:Z:315:GLN:N	2.41	0.51
1:B:105:LYS:HD2	1:I:111:MET:CE	2.40	0.51
1:D:439:GLY:O	1:D:442:VAL:HG12	2.10	0.51
1:E:433:ASN:OD1	1:E:436:GLN:OE1	2.27	0.51
1:F:114:MET:HE3	1:F:114:MET:HA	1.92	0.51
1:H:504:LEU:C	1:H:504:LEU:HD23	2.35	0.51
1:I:175:ILE:HD12	1:I:377:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:MET:HE1	1:J:520:MET:SD	2.50	0.51
1:M:130:GLU:HG2	1:M:422:VAL:HG23	1.93	0.51
1:J:169:VAL:HG12	1:J:173:GLY:HA3	1.93	0.51
1:J:174:VAL:HG13	1:J:376:VAL:HG23	1.92	0.51
1:J:426:LEU:HD12	1:J:429:LEU:HD22	1.93	0.51
1:K:12:ALA:HB1	1:K:520:MET:HE3	1.93	0.51
1:L:232:GLU:HG3	1:L:309:LEU:HB2	1.93	0.51
1:N:451:LEU:O	1:N:454:ILE:HG22	2.10	0.51
2:O:10:VAL:HG21	2:O:91:ILE:HD11	1.93	0.51
2:T:96:GLU:OE2	2:U:4:ARG:NH1	2.35	0.51
1:E:25:ASP:OD2	1:F:8:PHE:CE2	2.63	0.51
1:F:287:ALA:HB1	1:F:368:ARG:HH22	1.74	0.51
1:I:102:GLU:OE1	1:I:442:VAL:HG21	2.11	0.51
1:L:513:LEU:HD11	1:M:49:ILE:HD13	1.91	0.51
1:M:16:MET:HE3	1:M:520:MET:CE	2.40	0.51
1:M:263:VAL:HG13	1:M:264:VAL:N	2.26	0.51
2:O:25:ILE:HG13	2:O:26:VAL:N	2.26	0.51
1:M:27:VAL:O	1:M:30:THR:HG22	2.10	0.51
1:M:123:ALA:HB2	1:M:440:ILE:HD12	1.93	0.51
2:S:6:LEU:O	2:S:7:HIS:CG	2.64	0.51
1:H:50:THR:HG22	1:H:52:ASP:H	1.76	0.51
1:J:233:MET:HB2	1:J:309:LEU:HD13	1.92	0.51
1:K:230:ILE:HG21	1:K:259:LEU:HD13	1.93	0.51
1:L:411:VAL:HG21	1:L:494:LEU:HD23	1.93	0.51
1:A:111:MET:HA	1:A:111:MET:HE2	1.92	0.51
1:C:125:THR:O	1:C:129:GLU:OE1	2.28	0.51
1:N:36:ARG:NH2	1:N:457:ASN:O	2.44	0.51
1:A:384:ALA:N	1:A:388:GLU:OE2	2.43	0.51
1:K:130:GLU:O	1:K:134:LEU:HD23	2.11	0.51
1:K:175:ILE:HG23	1:K:400:LEU:HD11	1.92	0.51
2:Q:12:VAL:HG22	2:Q:86:MET:HE1	1.92	0.51
1:F:97:GLN:O	1:F:101:THR:HG23	2.12	0.50
1:M:478:TYR:O	1:M:488:MET:HE1	2.11	0.50
3:Z:204:LEU:HD13	3:Z:243:ARG:HD3	1.93	0.50
1:A:77:VAL:HG21	1:A:510:VAL:HG11	1.93	0.50
1:D:59:GLU:O	1:D:61:GLU:OE1	2.29	0.50
1:G:233:MET:CE	1:G:309:LEU:HD21	2.28	0.50
1:H:323:VAL:HG22	1:H:332:ILE:HD12	1.92	0.50
1:I:267:MET:HE1	1:I:271:VAL:O	2.11	0.50
1:L:153:ASN:O	1:L:154:SER:OG	2.22	0.50
2:O:22:ALA:N	2:O:26:VAL:O	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ILE:HD11	1:C:372:LEU:HD22	1.93	0.50
1:G:16:MET:SD	1:G:514:MET:HE1	2.51	0.50
1:H:392:LYS:HA	1:H:392:LYS:HE2	1.93	0.50
2:T:36:THR:OG1	2:T:67:PHE:O	2.27	0.50
3:Z:69:ALA:HA	3:Z:86:PRO:HD3	1.93	0.50
1:B:111:MET:HE2	1:B:111:MET:N	2.27	0.50
1:D:102:GLU:HA	1:D:102:GLU:OE1	2.11	0.50
1:H:349:ILE:HG23	1:H:365:LEU:CD1	2.42	0.50
1:A:423:ALA:HB2	1:A:447:MET:HE3	1.93	0.50
1:D:359:ASP:OD1	1:D:362:ARG:NH1	2.40	0.50
1:G:398:ASP:OD1	4:G:601:AF3:F1	2.19	0.50
1:I:102:GLU:OE1	1:I:442:VAL:CG2	2.59	0.50
1:I:149:THR:HG22	1:I:156:GLU:HA	1.93	0.50
1:J:101:THR:HG23	1:J:102:GLU:N	2.26	0.50
1:L:115:ASP:OD1	1:L:118:ARG:NH1	2.44	0.50
2:T:79:ASP:HB2	2:T:81:GLU:OE1	2.11	0.50
1:G:364:LYS:O	1:G:367:GLU:HG3	2.12	0.50
1:H:349:ILE:O	1:H:365:LEU:HD12	2.11	0.50
1:J:217:SER:N	1:J:218:PRO:HD3	2.26	0.50
1:K:193:MET:CE	1:K:371:LYS:O	2.59	0.50
1:L:360:TYR:HA	1:L:363:GLU:OE1	2.11	0.50
1:A:359:ASP:OD1	1:A:362:ARG:NH2	2.44	0.50
1:I:16:MET:CG	1:I:520:MET:HE1	2.42	0.50
1:J:152:ALA:C	1:J:153:ASN:OD1	2.55	0.50
1:N:27:VAL:O	1:N:30:THR:HG22	2.11	0.50
1:E:351:GLN:O	1:E:354:GLU:HG3	2.12	0.50
1:H:27:VAL:O	1:H:30:THR:HG22	2.12	0.50
1:L:367:GLU:O	1:L:371:LYS:N	2.45	0.50
1:A:61:GLU:OE1	1:B:2:ALA:O	2.29	0.50
1:D:230:ILE:HA	1:D:233:MET:HE2	1.94	0.50
1:F:451:LEU:O	1:F:454:ILE:HG22	2.12	0.50
1:H:349:ILE:HG23	1:H:365:LEU:HD13	1.94	0.50
1:I:423:ALA:O	1:I:444:LEU:HD12	2.12	0.50
1:K:324:VAL:HG23	1:K:333:ILE:HD11	1.93	0.50
1:L:141:SER:OG	1:L:166:MET:HE1	2.11	0.50
3:Z:216:ARG:HH11	3:Z:216:ARG:HA	1.77	0.50
1:G:50:THR:HA	1:G:391:GLU:OE2	2.11	0.49
2:U:12:VAL:O	2:U:83:VAL:HG13	2.12	0.49
3:Z:109:MET:HE2	3:Z:123:MET:HE3	1.93	0.49
1:I:16:MET:HE3	1:I:514:MET:SD	2.53	0.49
1:L:223:ALA:HB1	1:L:227:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:180:GLY:HA2	1:N:380:LYS:HG2	1.94	0.49
1:N:216:GLU:O	1:N:218:PRO:HD3	2.12	0.49
2:T:75:SER:HB2	2:T:84:LEU:HD23	1.94	0.49
3:Z:343:LEU:HD12	3:Z:365:PRO:HG3	1.94	0.49
3:Z:416:ALA:HB1	3:Z:422:PRO:O	2.12	0.49
1:A:80:LYS:NZ	1:G:385:THR:HA	2.28	0.49
1:A:220:ILE:HG22	1:A:222:LEU:CD2	2.43	0.49
1:B:367:GLU:OE2	1:B:368:ARG:HG3	2.13	0.49
1:B:408:GLU:OE1	1:B:408:GLU:N	2.39	0.49
1:C:437:ASN:O	1:C:440:ILE:HG22	2.12	0.49
1:D:338:GLU:OE2	1:D:339:GLU:N	2.44	0.49
1:E:38:VAL:HG13	1:F:519:CYS:SG	2.53	0.49
1:F:231:ARG:H	1:F:231:ARG:HD3	1.78	0.49
1:H:333:ILE:HA	1:H:376:VAL:HG21	1.94	0.49
1:K:349:ILE:HG22	1:K:369:VAL:HG13	1.94	0.49
2:R:88:GLU:HA	2:R:91:ILE:HD13	1.94	0.49
1:E:40:LEU:HD22	1:E:59:GLU:HG3	1.95	0.49
1:E:105:LYS:HE2	1:L:111:MET:HG2	1.94	0.49
1:E:414:GLY:O	1:E:417:VAL:HG12	2.13	0.49
1:E:428:ASP:O	1:E:428:ASP:OD1	2.30	0.49
1:G:227:ILE:O	1:G:255:GLU:OE1	2.30	0.49
1:I:309:LEU:HD12	1:I:309:LEU:H	1.77	0.49
1:E:261:THR:O	1:E:264:VAL:HG12	2.11	0.49
1:K:321:LYS:NZ	1:K:334:ASP:OD2	2.44	0.49
1:M:250:ILE:HD11	1:M:279:PRO:HD3	1.94	0.49
2:T:94:ILE:CG2	2:U:4:ARG:HG2	2.42	0.49
3:Z:261:LEU:HD11	3:Z:287:HIS:HB2	1.95	0.49
1:A:27:VAL:O	1:A:30:THR:HG22	2.12	0.49
1:E:34:LYS:HE2	1:E:458:CYS:SG	2.52	0.49
1:I:233:MET:O	1:I:233:MET:SD	2.71	0.49
1:J:201:SER:HB3	1:J:204:PHE:CE2	2.48	0.49
1:N:193:MET:O	1:N:332:ILE:N	2.46	0.49
1:N:349:ILE:HA	1:N:365:LEU:HD12	1.94	0.49
1:D:37:ASN:HD21	1:D:49:ILE:HB	1.77	0.49
1:D:488:MET:CE	1:D:493:ILE:HD11	2.43	0.49
1:F:23:LEU:HD23	1:F:74:VAL:HG23	1.95	0.49
1:F:311:LYS:O	1:F:311:LYS:HD3	2.12	0.49
1:A:284:ARG:NH2	3:Z:75:ASP:OD1	2.45	0.49
1:A:284:ARG:NH1	3:Z:76:GLU:OE1	2.43	0.49
1:F:197:ARG:O	1:F:330:THR:HG23	2.13	0.49
1:F:242:LYS:O	1:F:242:LYS:NZ	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:448:GLU:OE1	1:F:452:ARG:NE	2.46	0.49
1:N:216:GLU:C	1:N:218:PRO:CD	2.86	0.49
1:I:513:LEU:HD21	1:J:49:ILE:HD13	1.94	0.49
1:K:12:ALA:HB1	1:K:520:MET:CE	2.43	0.49
1:K:193:MET:CE	1:K:295:LEU:CD1	2.91	0.49
1:K:206:ASN:ND2	1:K:214:GLU:OE1	2.46	0.49
1:M:437:ASN:O	1:M:440:ILE:HG22	2.12	0.49
1:B:283:ASP:HA	1:B:286:LYS:HD3	1.94	0.48
1:F:361:ASP:O	1:F:365:LEU:HD23	2.12	0.48
1:H:38:VAL:HG13	1:N:519:CYS:SG	2.53	0.48
1:J:55:SER:O	1:J:59:GLU:OE1	2.31	0.48
1:L:40:LEU:HD21	1:L:56:VAL:HG22	1.95	0.48
1:L:41:ASP:OD1	1:L:42:LYS:N	2.46	0.48
1:L:221:LEU:HD12	1:L:301:ILE:HD13	1.95	0.48
1:M:213:VAL:O	1:M:213:VAL:HG13	2.12	0.48
2:O:85:ILE:CD1	2:U:92:LEU:HD13	2.43	0.48
1:A:194:GLN:OE1	1:A:330:THR:O	2.31	0.48
1:A:479:ASN:HD22	1:A:491:MET:HE2	1.78	0.48
1:B:142:LYS:O	1:B:146:GLN:NE2	2.46	0.48
1:G:384:ALA:HB3	1:G:388:GLU:OE2	2.13	0.48
1:K:193:MET:N	1:K:332:ILE:O	2.38	0.48
1:L:260:ALA:O	1:L:264:VAL:HG23	2.12	0.48
2:P:91:ILE:HG22	2:Q:6:LEU:HD21	1.94	0.48
1:H:61:GLU:OE2	1:N:2:ALA:O	2.30	0.48
1:H:69:MET:HE2	1:I:41:ASP:OD1	2.14	0.48
1:K:61:GLU:O	1:K:61:GLU:OE1	2.31	0.48
3:Z:294:VAL:HG23	3:Z:295:THR:H	1.78	0.48
1:A:280:GLY:O	1:A:285:ARG:NH2	2.45	0.48
1:D:448:GLU:CD	1:D:452:ARG:HE	2.21	0.48
1:E:233:MET:HE1	1:E:309:LEU:CD1	2.43	0.48
1:G:144:ILE:HD13	1:G:166:MET:HG2	1.95	0.48
1:G:342:ILE:HB	1:G:372:LEU:HD21	1.94	0.48
2:S:36:THR:OG1	2:T:76:GLU:OE2	2.26	0.48
3:Z:379:PHE:CZ	3:Z:383:LEU:HD22	2.48	0.48
1:B:73:MET:HE3	1:B:514:MET:HE3	1.95	0.48
1:J:520:MET:SD	1:K:39:VAL:HB	2.53	0.48
1:K:13:ARG:HB3	1:K:104:LEU:HD12	1.96	0.48
1:M:61:GLU:O	1:M:61:GLU:CD	2.56	0.48
1:M:482:THR:C	1:M:483:GLU:OE1	2.57	0.48
3:Z:386:ALA:O	3:Z:388:VAL:N	2.40	0.48
1:A:385:THR:O	1:A:388:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ALA:O	1:D:389:MET:HE1	2.13	0.48
1:G:383:ALA:H	1:G:389:MET:HE1	1.79	0.48
1:H:519:CYS:SG	1:I:38:VAL:HG22	2.54	0.48
1:I:102:GLU:O	1:I:105:LYS:HG2	2.14	0.48
1:J:191:GLU:OE2	1:J:335:GLY:O	2.32	0.48
1:J:221:LEU:HD12	1:J:301:ILE:HD13	1.96	0.48
1:K:61:GLU:O	1:K:61:GLU:CD	2.56	0.48
1:K:101:THR:HG23	1:K:102:GLU:N	2.28	0.48
1:K:193:MET:HE1	1:K:372:LEU:HA	1.94	0.48
1:L:104:LEU:O	1:L:107:VAL:HG12	2.13	0.48
1:L:233:MET:HB2	1:L:309:LEU:HD13	1.95	0.48
1:M:150:ILE:HD11	1:M:494:LEU:O	2.12	0.48
1:A:87:ASP:OD1	4:A:601:AF3:F1	2.21	0.48
1:A:102:GLU:O	1:A:105:LYS:HB3	2.13	0.48
1:C:217:SER:N	1:C:218:PRO:HD3	2.29	0.48
1:E:100:ILE:HD13	1:E:515:ILE:CG2	2.43	0.48
1:J:4:LYS:NZ	1:K:61:GLU:OE2	2.36	0.48
1:J:412:VAL:HG22	1:J:413:ALA:N	2.29	0.48
1:M:283:ASP:OD1	1:M:283:ASP:C	2.57	0.48
2:P:14:ARG:CZ	2:P:34:LYS:HE2	2.44	0.48
2:P:76:GLU:N	2:P:83:VAL:O	2.47	0.48
1:D:35:GLY:HA2	1:D:457:ASN:HD21	1.78	0.48
1:H:352:GLN:HB2	1:H:365:LEU:HD11	1.95	0.48
1:I:381:VAL:O	1:I:389:MET:HE2	2.14	0.48
2:P:96:GLU:OE2	2:Q:4:ARG:CZ	2.61	0.48
2:U:66:ILE:HG23	2:U:92:LEU:HB2	1.95	0.48
1:E:365:LEU:HD22	1:E:368:ARG:NH2	2.29	0.48
1:G:339:GLU:HA	1:G:342:ILE:HG12	1.96	0.48
1:G:359:ASP:OD1	1:G:360:TYR:N	2.46	0.48
1:M:426:LEU:HD12	1:M:429:LEU:HD22	1.96	0.48
2:O:6:LEU:O	2:O:7:HIS:CG	2.66	0.48
2:U:11:ILE:HD11	2:U:83:VAL:HG11	1.96	0.48
2:U:63:ASP:HB3	2:U:94:ILE:CD1	2.43	0.48
1:A:6:VAL:HG12	1:A:521:VAL:HG12	1.95	0.48
1:D:187:LEU:HD23	1:D:187:LEU:H	1.79	0.48
1:M:5:ASP:OD1	1:M:6:VAL:N	2.47	0.48
2:T:64:ILE:O	2:T:94:ILE:HD12	2.14	0.48
1:A:73:MET:CB	1:A:514:MET:HE1	2.43	0.47
1:A:80:LYS:HE3	1:A:506:TYR:CD1	2.49	0.47
1:A:455:VAL:HG11	1:A:465:VAL:HG11	1.96	0.47
1:D:35:GLY:HA2	1:D:457:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:GLU:O	1:E:261:THR:HG23	2.14	0.47
1:E:460:GLU:OE1	1:E:460:GLU:N	2.46	0.47
1:H:178:GLU:N	1:H:178:GLU:OE1	2.47	0.47
1:J:118:ARG:O	1:J:121:ASP:OD1	2.32	0.47
2:R:49:LEU:C	2:R:50:GLU:HG2	2.39	0.47
2:T:66:ILE:O	2:T:92:LEU:N	2.45	0.47
2:U:6:LEU:HG	2:U:6:LEU:O	2.14	0.47
3:Z:412:GLN:NE2	3:Z:432:GLU:OE2	2.41	0.47
1:E:277:LYS:HD3	1:E:278:ALA:O	2.13	0.47
1:E:477:GLY:C	1:E:488:MET:HE3	2.40	0.47
1:J:254:VAL:HA	1:J:259:LEU:HD23	1.97	0.47
1:K:102:GLU:HA	1:K:105:LYS:HZ2	1.79	0.47
1:L:214:GLU:OE1	1:L:214:GLU:N	2.47	0.47
1:M:496:PRO:O	1:M:499:VAL:HG12	2.14	0.47
2:P:49:LEU:C	2:P:50:GLU:HG3	2.39	0.47
2:Q:4:ARG:O	2:Q:4:ARG:HG3	2.14	0.47
1:B:404:ARG:O	1:B:408:GLU:OE1	2.32	0.47
1:G:391:GLU:OE2	1:G:391:GLU:HA	2.13	0.47
1:L:519:CYS:SG	1:L:520:MET:N	2.86	0.47
2:R:25:ILE:HG13	2:R:26:VAL:N	2.28	0.47
3:Z:6:ARG:NH1	3:Z:64:THR:O	2.47	0.47
3:Z:9:ASN:HB2	3:Z:70:LEU:HD12	1.97	0.47
3:Z:239:GLU:CD	3:Z:243:ARG:HE	2.22	0.47
1:D:10:ASN:OD1	1:D:11:ASP:N	2.47	0.47
1:D:58:ARG:HB3	1:D:58:ARG:HH11	1.79	0.47
2:R:6:LEU:O	2:R:7:HIS:CG	2.67	0.47
2:R:66:ILE:CD1	2:S:3:ILE:HD11	2.44	0.47
2:U:6:LEU:O	2:U:7:HIS:CG	2.67	0.47
3:Z:416:ALA:O	3:Z:421:VAL:HG22	2.14	0.47
1:A:53:GLY:O	1:A:56:VAL:HG12	2.15	0.47
1:B:364:LYS:O	1:B:367:GLU:HG3	2.15	0.47
1:D:346:VAL:CG2	1:D:372:LEU:HD22	2.44	0.47
1:G:342:ILE:HG13	1:G:343:GLN:N	2.29	0.47
1:G:439:GLY:O	1:G:442:VAL:HG12	2.14	0.47
1:H:4:LYS:N	1:I:63:GLU:OE2	2.29	0.47
1:K:49:ILE:O	1:K:49:ILE:HG23	2.14	0.47
1:K:54:VAL:HG12	1:K:58:ARG:HH12	1.80	0.47
1:M:222:LEU:HD23	1:M:250:ILE:CG2	2.44	0.47
2:O:12:VAL:HG23	2:O:39:GLU:C	2.40	0.47
2:R:12:VAL:CG2	2:R:86:MET:HE1	2.43	0.47
1:B:18:ARG:NE	1:B:67:GLU:OE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HG13	1:B:58:ARG:NH2	2.30	0.47
1:G:69:MET:O	1:G:73:MET:HG2	2.15	0.47
1:H:117:LYS:O	1:H:120:ILE:HG22	2.15	0.47
1:I:521:VAL:CG2	1:J:40:LEU:HD13	2.45	0.47
1:J:360:TYR:O	1:J:363:GLU:HG3	2.15	0.47
1:L:307:MET:HA	1:L:307:MET:HE2	1.97	0.47
1:M:207:LYS:HG3	1:M:208:PRO:HD3	1.97	0.47
2:O:95:VAL:CG2	2:P:1:MET:HG2	2.44	0.47
2:T:15:LYS:NZ	2:T:64:ILE:HG23	2.28	0.47
1:A:349:ILE:HG21	1:A:369:VAL:HG13	1.96	0.47
1:C:47:PRO:HG3	1:D:69:MET:HE1	1.96	0.47
1:C:339:GLU:HA	1:C:342:ILE:HG22	1.97	0.47
1:E:87:ASP:OD1	1:E:88:GLY:N	2.48	0.47
1:E:354:GLU:OE2	1:E:355:GLU:HG3	2.15	0.47
1:H:61:GLU:OE2	1:N:3:ALA:HA	2.14	0.47
1:H:213:VAL:HG13	1:H:213:VAL:O	2.14	0.47
1:I:240:VAL:O	1:I:244:GLY:N	2.47	0.47
1:I:251:ALA:O	1:I:278:ALA:N	2.42	0.47
1:J:409:GLU:O	1:J:497:THR:OG1	2.25	0.47
1:K:223:ALA:HB1	1:K:227:ILE:HD11	1.95	0.47
1:L:254:VAL:HA	1:L:259:LEU:HD23	1.96	0.47
2:U:25:ILE:HG13	2:U:26:VAL:H	1.80	0.47
1:A:386:GLU:H	1:B:80:LYS:HZ1	1.62	0.47
1:C:439:GLY:O	1:C:442:VAL:HG12	2.15	0.47
1:F:280:GLY:O	1:F:285:ARG:NE	2.42	0.47
1:G:217:SER:N	1:G:218:PRO:HD3	2.30	0.47
1:A:16:MET:HE2	1:A:16:MET:HA	1.97	0.47
1:C:280:GLY:O	1:C:285:ARG:NH2	2.44	0.47
1:E:39:VAL:O	1:E:39:VAL:HG13	2.15	0.47
1:K:461:GLU:OE1	1:K:464:VAL:HG23	2.15	0.47
1:K:523:ASP:OD1	1:K:524:LEU:N	2.48	0.47
1:L:89:THR:O	1:L:93:THR:HG23	2.15	0.47
1:M:77:VAL:HG11	1:M:510:VAL:HG21	1.96	0.47
1:M:130:GLU:CG	1:M:422:VAL:HG23	2.45	0.47
1:M:513:LEU:HD11	1:N:49:ILE:HD12	1.97	0.47
2:P:91:ILE:HD12	2:P:91:ILE:H	1.81	0.47
1:E:383:ALA:HB1	1:E:388:GLU:HG3	1.97	0.46
1:G:265:ASN:OD1	1:G:270:ILE:HB	2.15	0.46
1:I:69:MET:HE1	1:J:41:ASP:OD1	2.15	0.46
1:M:77:VAL:HG11	1:M:510:VAL:CG2	2.45	0.46
1:A:398:ASP:OD2	4:A:601:AF3:F1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:SER:O	1:C:305:ILE:HG22	2.15	0.46
1:F:364:LYS:O	1:F:367:GLU:HG2	2.15	0.46
1:I:19:GLY:O	1:I:22:VAL:HG12	2.16	0.46
1:N:206:ASN:C	1:N:208:PRO:HD2	2.39	0.46
3:Z:163:THR:HB	3:Z:183:PHE:CE1	2.51	0.46
3:Z:267:ALA:HB1	3:Z:271:ALA:CB	2.45	0.46
3:Z:416:ALA:HB3	3:Z:423:VAL:HA	1.98	0.46
1:A:180:GLY:HA2	1:A:380:LYS:HE3	1.97	0.46
1:C:400:LEU:O	1:C:403:THR:HG22	2.16	0.46
1:I:199:TYR:CE1	1:I:327:LYS:HA	2.49	0.46
1:K:193:MET:CE	1:K:295:LEU:HD13	2.46	0.46
1:M:193:MET:N	1:M:332:ILE:O	2.39	0.46
1:M:230:ILE:HD13	1:M:249:ILE:HG12	1.97	0.46
1:M:350:ARG:O	1:M:353:ILE:HG22	2.15	0.46
1:N:30:THR:HG21	1:N:53:GLY:CA	2.46	0.46
1:N:216:GLU:C	1:N:218:PRO:HD2	2.41	0.46
2:P:36:THR:HG23	2:P:37:ARG:HE	1.80	0.46
2:R:25:ILE:HG13	2:R:26:VAL:HG23	1.97	0.46
1:B:445:ARG:HB2	1:B:445:ARG:NH1	2.31	0.46
1:E:63:GLU:OE1	1:E:63:GLU:N	2.33	0.46
1:F:102:GLU:HB3	1:F:442:VAL:HG23	1.97	0.46
1:G:59:GLU:O	1:G:61:GLU:OE1	2.33	0.46
1:I:101:THR:HG23	1:I:102:GLU:N	2.30	0.46
1:M:213:VAL:HG13	1:M:325:ILE:HB	1.97	0.46
1:N:7:LYS:HD2	1:N:11:ASP:OD2	2.16	0.46
1:B:370:ALA:O	1:B:374:GLY:N	2.40	0.46
1:C:466:ALA:O	1:C:469:VAL:HG12	2.16	0.46
1:F:7:LYS:O	1:F:8:PHE:CD1	2.69	0.46
1:G:27:VAL:HG11	1:G:93:THR:HG21	1.96	0.46
1:H:3:ALA:CB	1:I:63:GLU:HG3	2.46	0.46
1:H:102:GLU:OE1	1:H:442:VAL:HG23	2.15	0.46
1:K:58:ARG:HH11	1:K:58:ARG:HB2	1.80	0.46
1:N:179:ASP:OD1	1:N:389:MET:HE2	2.15	0.46
1:N:254:VAL:HG13	1:N:259:LEU:HD23	1.96	0.46
2:S:78:ILE:O	2:S:81:GLU:N	2.46	0.46
2:T:12:VAL:HA	2:T:39:GLU:O	2.15	0.46
2:U:49:LEU:O	2:U:50:GLU:HG3	2.16	0.46
3:Z:380:PHE:CD2	3:Z:414:TRP:HD1	2.33	0.46
1:A:267:MET:HE2	1:B:305:ILE:HD13	1.98	0.46
1:C:268:ARG:HD2	2:O:27:LEU:HD21	1.97	0.46
1:D:229:ASN:OD1	1:D:231:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:445:ARG:O	1:E:448:GLU:OE1	2.34	0.46
1:K:259:LEU:HD12	1:K:263:VAL:HG23	1.98	0.46
1:M:513:LEU:HD11	1:N:49:ILE:HD13	1.96	0.46
3:Z:414:TRP:NE1	3:Z:417:TRP:CE3	2.84	0.46
1:D:128:VAL:HG22	1:D:132:LYS:NZ	2.31	0.46
1:H:16:MET:HE2	1:H:514:MET:SD	2.55	0.46
1:H:496:PRO:O	1:H:499:VAL:HG12	2.15	0.46
1:I:455:VAL:HG22	1:I:460:GLU:HB2	1.98	0.46
1:J:283:ASP:OD1	1:J:284:ARG:HD2	2.16	0.46
1:L:265:ASN:HA	1:L:268:ARG:HH22	1.80	0.46
2:Q:96:GLU:HB2	2:R:1:MET:HE2	1.96	0.46
2:R:5:PRO:HB2	2:R:9:ARG:HB2	1.98	0.46
3:Z:303:TYR:CD1	3:Z:307:VAL:HG12	2.51	0.46
1:B:399:ALA:O	1:B:403:THR:HG22	2.16	0.46
1:C:185:ASP:OD1	1:C:185:ASP:N	2.49	0.46
1:H:352:GLN:HB2	1:H:365:LEU:CD1	2.46	0.46
1:I:404:ARG:O	1:I:407:VAL:HG12	2.16	0.46
1:M:369:VAL:HG23	1:M:370:ALA:N	2.30	0.46
2:U:49:LEU:C	2:U:50:GLU:HG3	2.41	0.46
3:Z:44:HIS:O	3:Z:48:GLU:OE1	2.34	0.46
3:Z:184:TRP:CZ2	3:Z:190:ILE:HD12	2.50	0.46
1:A:23:LEU:HD23	1:A:23:LEU:C	2.41	0.46
1:C:111:MET:N	1:C:111:MET:HE2	2.31	0.46
1:D:27:VAL:O	1:D:30:THR:HG22	2.16	0.46
1:G:101:THR:HG23	1:G:102:GLU:N	2.31	0.46
1:I:73:MET:O	1:I:76:GLU:HG3	2.15	0.46
1:J:57:ALA:C	1:J:75:LYS:HZ3	2.24	0.46
1:K:104:LEU:HA	1:K:107:VAL:HG12	1.98	0.46
1:M:283:ASP:OD1	1:M:284:ARG:N	2.49	0.46
2:Q:79:ASP:O	2:Q:80:ASN:CG	2.59	0.46
2:Q:93:ALA:HB1	2:R:3:ILE:HG13	1.98	0.46
3:Z:181:HIS:HB2	3:Z:214:ALA:HB1	1.96	0.46
1:D:372:LEU:HD23	1:D:372:LEU:C	2.40	0.46
1:F:294:THR:HG22	1:F:342:ILE:HD13	1.98	0.46
1:G:399:ALA:O	1:G:403:THR:HG22	2.16	0.46
1:H:455:VAL:HG11	1:H:465:VAL:HG11	1.98	0.46
1:J:445:ARG:HA	1:J:445:ARG:NE	2.31	0.46
1:M:326:ASN:OD1	1:M:329:THR:N	2.46	0.46
2:U:63:ASP:HB3	2:U:94:ILE:HD11	1.98	0.46
1:A:455:VAL:HG21	1:A:465:VAL:HG11	1.98	0.45
1:D:326:ASN:CG	1:D:327:LYS:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB1	1:G:158:VAL:HG21	1.99	0.45
1:I:190:VAL:N	1:I:376:VAL:O	2.36	0.45
1:K:420:ILE:HD12	1:K:448:GLU:OE2	2.16	0.45
1:L:19:GLY:HA2	1:L:67:GLU:HG3	1.97	0.45
1:L:190:VAL:O	1:L:376:VAL:N	2.47	0.45
1:M:165:ALA:O	1:M:169:VAL:HG12	2.17	0.45
1:M:438:VAL:O	1:M:442:VAL:HG23	2.16	0.45
1:A:105:LYS:HE3	1:H:111:MET:CE	2.45	0.45
1:A:259:LEU:O	1:A:263:VAL:HG23	2.17	0.45
1:E:433:ASN:N	1:E:436:GLN:OE1	2.49	0.45
1:G:346:VAL:CG2	1:G:372:LEU:HD22	2.47	0.45
1:H:284:ARG:HH22	1:H:361:ASP:HA	1.80	0.45
1:I:16:MET:SD	1:I:70:GLY:HA2	2.57	0.45
1:I:59:GLU:OE2	1:I:59:GLU:O	2.33	0.45
1:J:455:VAL:HG11	1:J:465:VAL:HG11	1.97	0.45
1:L:19:GLY:O	1:L:22:VAL:HG22	2.16	0.45
2:T:93:ALA:HB1	2:U:3:ILE:HD11	1.98	0.45
3:Z:24:VAL:HG21	3:Z:136:PHE:HZ	1.80	0.45
1:C:264:VAL:HG12	2:O:27:LEU:HD11	1.98	0.45
1:D:238:GLU:HA	2:U:25:ILE:HD11	1.98	0.45
1:F:383:ALA:HB3	1:F:389:MET:SD	2.57	0.45
1:L:206:ASN:ND2	1:L:214:GLU:OE1	2.49	0.45
1:L:496:PRO:O	1:L:499:VAL:HG12	2.16	0.45
2:R:66:ILE:HG22	2:R:92:LEU:HB2	1.98	0.45
2:S:49:LEU:C	2:S:50:GLU:HG3	2.41	0.45
3:Z:161:VAL:O	3:Z:189:PHE:N	2.49	0.45
3:Z:206:ASP:OD1	3:Z:207:THR:N	2.47	0.45
3:Z:374:LEU:HD11	3:Z:437:PHE:CZ	2.51	0.45
1:A:102:GLU:OE1	1:A:102:GLU:HA	2.17	0.45
1:E:307:MET:SD	1:E:307:MET:N	2.90	0.45
1:E:359:ASP:OD1	1:E:360:TYR:N	2.49	0.45
1:G:384:ALA:CA	1:G:388:GLU:OE2	2.64	0.45
1:H:152:ALA:HB3	1:H:158:VAL:HG21	1.98	0.45
2:O:95:VAL:O	2:O:95:VAL:HG13	2.15	0.45
3:Z:2:ASP:N	3:Z:52:GLY:O	2.48	0.45
1:B:125:THR:O	1:B:128:VAL:HG12	2.16	0.45
1:C:270:ILE:CD1	2:O:27:LEU:HD23	2.47	0.45
1:D:488:MET:HE3	1:D:493:ILE:HD11	1.99	0.45
1:F:281:PHE:O	1:F:284:ARG:HG2	2.16	0.45
1:I:191:GLU:HB3	1:I:295:LEU:HD11	1.97	0.45
1:I:199:TYR:CD2	1:I:201:SER:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:19:GLY:O	1:J:22:VAL:HG12	2.16	0.45
1:L:2:ALA:O	1:L:4:LYS:N	2.50	0.45
2:O:75:SER:HB3	2:O:82:GLU:OE2	2.16	0.45
2:O:76:GLU:OE2	2:O:85:ILE:HG23	2.16	0.45
2:R:7:HIS:C	2:R:9:ARG:H	2.25	0.45
1:B:356:ALA:O	1:B:362:ARG:NE	2.49	0.45
1:G:404:ARG:O	1:G:408:GLU:OE1	2.34	0.45
1:I:519:CYS:SG	1:J:38:VAL:HG13	2.57	0.45
1:N:191:GLU:HA	1:N:375:GLY:HA2	1.98	0.45
2:T:8:ASP:OD1	2:T:9:ARG:HD2	2.15	0.45
1:A:214:GLU:C	1:A:215:LEU:HD22	2.41	0.45
1:A:230:ILE:HA	1:A:233:MET:HE2	1.98	0.45
1:A:268:ARG:O	1:A:268:ARG:HG3	2.17	0.45
1:E:384:ALA:HB3	1:E:388:GLU:OE2	2.16	0.45
1:I:145:ALA:O	1:I:149:THR:HG23	2.16	0.45
1:I:386:GLU:HA	1:I:389:MET:HG3	1.99	0.45
1:K:412:VAL:HG22	1:K:413:ALA:N	2.32	0.45
1:M:524:LEU:C	1:M:524:LEU:HD23	2.41	0.45
2:Q:74:LYS:O	2:Q:84:LEU:HA	2.17	0.45
3:Z:371:MET:CE	3:Z:375:ARG:HB3	2.46	0.45
1:A:522:THR:HG22	1:A:523:ASP:N	2.31	0.45
1:C:237:LEU:O	1:C:241:ALA:N	2.35	0.45
1:D:513:LEU:C	1:D:513:LEU:HD23	2.42	0.45
1:E:328:ASP:OD1	1:E:329:THR:HG23	2.16	0.45
1:K:69:MET:CE	1:L:41:ASP:OD2	2.64	0.45
1:M:487:ASN:O	1:M:491:MET:HE3	2.17	0.45
1:N:367:GLU:HB3	1:N:371:LYS:NZ	2.32	0.45
2:U:66:ILE:O	2:U:92:LEU:N	2.40	0.45
1:C:352:GLN:HA	1:C:355:GLU:HG3	1.98	0.45
1:E:445:ARG:O	1:E:445:ARG:HD3	2.17	0.45
1:H:25:ASP:OD2	1:H:25:ASP:O	2.34	0.45
1:L:501:ARG:NH1	1:L:505:GLN:OE1	2.48	0.45
1:M:54:VAL:CG2	1:M:89:THR:HG21	2.44	0.45
2:P:7:HIS:HB3	2:P:45:ASN:OD1	2.17	0.45
2:R:76:GLU:N	2:R:76:GLU:OE1	2.49	0.45
3:Z:440:PHE:N	3:Z:441:PRO:HD3	2.32	0.45
1:E:180:GLY:HA2	1:E:380:LYS:HE3	1.99	0.45
1:G:17:LEU:O	1:G:20:VAL:HG12	2.16	0.45
1:J:388:GLU:HA	1:J:391:GLU:HG3	1.99	0.45
2:R:2:ASN:OD1	2:R:2:ASN:C	2.59	0.45
2:R:76:GLU:OE2	2:R:83:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:301:ILE:O	1:J:302:SER:HB3	2.17	0.44
1:L:367:GLU:O	1:L:370:ALA:N	2.50	0.44
1:L:513:LEU:CD1	1:M:49:ILE:HD13	2.47	0.44
2:P:48:ILE:O	2:P:48:ILE:HG22	2.17	0.44
3:Z:244:GLY:O	3:Z:247:VAL:HG12	2.17	0.44
1:C:100:ILE:HG23	1:C:101:THR:N	2.31	0.44
1:H:61:GLU:O	1:H:61:GLU:CD	2.61	0.44
1:H:69:MET:CE	1:I:41:ASP:OD1	2.65	0.44
1:J:478:TYR:O	1:J:488:MET:HE1	2.17	0.44
1:K:37:ASN:OD1	1:K:51:LYS:NZ	2.28	0.44
1:M:231:ARG:O	1:M:231:ARG:NH1	2.42	0.44
2:P:81:GLU:OE1	2:P:81:GLU:N	2.50	0.44
2:P:94:ILE:CG2	2:Q:4:ARG:HG2	2.46	0.44
1:A:73:MET:HE2	1:A:73:MET:HA	1.99	0.44
1:C:301:ILE:HD11	1:C:307:MET:HB3	1.99	0.44
1:F:235:PRO:HA	1:F:238:GLU:OE2	2.18	0.44
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.99	0.44
1:H:193:MET:SD	1:H:195:PHE:HD1	2.40	0.44
1:I:23:LEU:C	1:I:23:LEU:HD23	2.41	0.44
1:I:445:ARG:HA	1:I:445:ARG:NE	2.32	0.44
1:J:13:ARG:HB3	1:J:104:LEU:HD12	2.00	0.44
1:M:55:SER:HA	1:M:58:ARG:NH2	2.33	0.44
1:N:217:SER:HA	1:N:320:ALA:O	2.18	0.44
1:N:339:GLU:HA	1:N:342:ILE:HG12	2.00	0.44
3:Z:156:ASP:O	3:Z:414:TRP:HH2	1.99	0.44
3:Z:267:ALA:HB1	3:Z:271:ALA:HB3	1.99	0.44
1:C:429:LEU:HD23	1:C:429:LEU:C	2.42	0.44
1:D:238:GLU:HG2	2:U:25:ILE:HD11	1.98	0.44
1:E:487:ASN:OD1	1:E:489:ILE:CG2	2.65	0.44
1:F:65:LYS:O	1:F:69:MET:HE2	2.17	0.44
1:G:291:ASP:OD2	1:G:368:ARG:NH2	2.50	0.44
1:H:439:GLY:O	1:H:442:VAL:HG12	2.18	0.44
1:I:268:ARG:HD2	1:I:268:ARG:O	2.18	0.44
1:I:411:VAL:HG21	1:I:494:LEU:HD12	1.99	0.44
1:J:180:GLY:HA3	1:J:389:MET:HE2	2.00	0.44
1:J:223:ALA:HB1	1:J:227:ILE:CD1	2.48	0.44
1:J:516:THR:O	1:J:518:GLU:OE1	2.36	0.44
1:K:221:LEU:HD12	1:K:301:ILE:HD13	2.00	0.44
1:K:461:GLU:OE1	1:K:461:GLU:O	2.36	0.44
1:N:228:SER:OG	1:N:229:ASN:N	2.50	0.44
2:R:64:ILE:HG23	2:R:95:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:6:LEU:O	2:S:6:LEU:HG	2.18	0.44
2:T:63:ASP:HB3	2:T:94:ILE:CD1	2.47	0.44
2:U:66:ILE:CG2	2:U:93:ALA:HB3	2.47	0.44
1:E:238:GLU:O	1:E:242:LYS:N	2.43	0.44
1:E:401:HIS:CD2	1:E:404:ARG:HH12	2.35	0.44
1:L:349:ILE:HG22	1:L:369:VAL:HG13	1.99	0.44
1:M:325:ILE:HG13	1:M:330:THR:HG23	1.99	0.44
2:O:25:ILE:CG1	2:O:26:VAL:N	2.79	0.44
2:P:88:GLU:HA	2:P:91:ILE:HD13	1.99	0.44
3:Z:188:ASP:HA	3:Z:226:LYS:HG2	1.99	0.44
3:Z:211:VAL:HG11	3:Z:228:PHE:CD1	2.52	0.44
3:Z:400:ILE:HG23	3:Z:439:SER:HB3	1.99	0.44
1:B:217:SER:N	1:B:218:PRO:HD3	2.33	0.44
1:B:487:ASN:OD1	1:B:489:ILE:N	2.50	0.44
1:C:270:ILE:HD12	2:O:27:LEU:HD23	1.99	0.44
1:E:102:GLU:HB3	1:E:442:VAL:HG23	1.98	0.44
1:F:282:GLY:O	1:F:285:ARG:HB3	2.18	0.44
1:F:412:VAL:HG13	1:F:497:THR:HG22	2.00	0.44
1:G:414:GLY:O	1:G:417:VAL:HG12	2.17	0.44
1:H:522:THR:HG22	1:H:523:ASP:O	2.17	0.44
1:J:284:ARG:HD2	1:J:284:ARG:N	2.32	0.44
1:J:514:MET:O	1:J:517:THR:HG22	2.17	0.44
2:O:40:VAL:HG12	2:O:63:ASP:O	2.17	0.44
2:P:11:ILE:HD13	2:P:85:ILE:HD11	2.00	0.44
2:Q:11:ILE:O	2:Q:41:LEU:N	2.44	0.44
2:T:50:GLU:C	2:T:52:GLY:H	2.25	0.44
3:Z:397:PHE:C	3:Z:399:HIS:H	2.26	0.44
1:B:10:ASN:OD1	1:B:14:VAL:HG13	2.17	0.44
1:I:102:GLU:CD	1:I:442:VAL:HG22	2.43	0.44
1:J:217:SER:HA	1:J:320:ALA:O	2.18	0.44
1:M:25:ASP:HA	1:M:28:LYS:NZ	2.31	0.44
1:M:73:MET:O	1:M:77:VAL:HG12	2.18	0.44
1:M:185:ASP:OD1	1:M:382:GLY:N	2.45	0.44
2:O:49:LEU:C	2:O:50:GLU:HG3	2.43	0.44
1:B:105:LYS:HE2	1:I:110:GLY:C	2.43	0.44
1:C:230:ILE:HA	1:C:233:MET:HG2	1.99	0.44
1:F:325:ILE:HA	1:F:329:THR:O	2.18	0.44
1:I:385:THR:O	1:I:389:MET:HG3	2.17	0.44
1:J:18:ARG:NH1	1:J:18:ARG:HB2	2.32	0.44
1:N:342:ILE:HG13	1:N:343:GLN:N	2.33	0.44
1:A:188:ASP:OD1	1:A:188:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:CYS:SG	1:B:411:VAL:HG22	2.58	0.44
1:D:199:TYR:CE2	1:D:327:LYS:HA	2.53	0.44
1:G:39:VAL:HG13	1:G:49:ILE:HD13	2.00	0.44
1:G:270:ILE:HD13	2:R:27:LEU:HD21	2.00	0.44
1:I:102:GLU:CD	1:I:102:GLU:C	2.85	0.44
1:K:16:MET:HE3	1:K:520:MET:HE2	2.00	0.44
1:L:69:MET:HE1	1:M:41:ASP:HA	2.00	0.44
1:N:451:LEU:O	1:N:455:VAL:HG12	2.18	0.44
2:U:76:GLU:HG2	2:U:78:ILE:CD1	2.48	0.44
3:Z:125:ASP:OD1	3:Z:310:LYS:NZ	2.38	0.44
3:Z:287:HIS:ND1	3:Z:321:HIS:CD2	2.86	0.44
1:A:131:LEU:HD23	1:A:501:ARG:HB2	2.00	0.43
1:C:41:ASP:HB3	1:D:69:MET:SD	2.58	0.43
1:D:37:ASN:OD1	1:D:50:THR:O	2.36	0.43
1:F:7:LYS:O	1:F:8:PHE:HD1	2.00	0.43
1:H:339:GLU:HA	1:H:342:ILE:HD12	2.00	0.43
1:J:114:MET:SD	1:K:459:GLY:CA	3.06	0.43
1:K:102:GLU:HA	1:K:105:LYS:HG2	2.00	0.43
1:K:451:LEU:O	1:K:454:ILE:HG22	2.17	0.43
1:M:259:LEU:O	1:M:263:VAL:HG12	2.18	0.43
2:O:76:GLU:CD	2:O:83:VAL:HG23	2.43	0.43
2:O:94:ILE:HG22	2:P:4:ARG:HB3	2.00	0.43
2:T:2:ASN:OD1	2:T:2:ASN:C	2.60	0.43
1:A:98:ALA:O	1:A:101:THR:HG22	2.18	0.43
1:E:100:ILE:HD11	1:E:511:ALA:HA	2.00	0.43
1:E:289:LEU:HA	1:E:292:ILE:HG12	2.00	0.43
1:F:235:PRO:HA	1:F:238:GLU:CD	2.42	0.43
1:F:237:LEU:HA	1:F:240:VAL:HG12	2.00	0.43
1:G:403:THR:HG23	1:G:404:ARG:N	2.32	0.43
1:I:257:GLU:HA	1:I:261:THR:HG23	1.99	0.43
1:J:513:LEU:HD11	1:K:49:ILE:HD11	2.00	0.43
1:M:193:MET:HE1	1:M:371:LYS:CB	2.48	0.43
1:M:461:GLU:CD	1:M:463:SER:OG	2.62	0.43
2:Q:11:ILE:HD12	2:Q:42:ALA:HB3	1.99	0.43
2:R:55:LYS:HG3	2:R:56:PRO:HD2	2.00	0.43
2:T:78:ILE:HD13	2:T:83:VAL:HG21	2.00	0.43
1:D:24:ALA:C	1:D:28:LYS:HZ3	2.26	0.43
1:D:342:ILE:CG2	1:D:372:LEU:HD21	2.47	0.43
1:F:381:VAL:O	1:F:389:MET:HE1	2.18	0.43
1:H:519:CYS:SG	1:I:38:VAL:HG13	2.58	0.43
1:I:221:LEU:HD21	1:I:223:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:278:ALA:HB3	1:M:285:ARG:HH11	1.83	0.43
2:R:79:ASP:HB2	2:R:81:GLU:OE1	2.18	0.43
3:Z:277:ARG:HA	3:Z:277:ARG:NE	2.34	0.43
1:A:10:ASN:OD1	1:A:11:ASP:N	2.52	0.43
1:A:73:MET:HE1	1:G:47:PRO:HD2	2.00	0.43
1:B:234:LEU:O	1:B:238:GLU:HG2	2.18	0.43
1:B:450:PRO:O	1:B:454:ILE:HG13	2.18	0.43
1:C:455:VAL:HG21	1:C:465:VAL:HG11	1.99	0.43
1:D:152:ALA:HB1	1:D:158:VAL:HG21	2.01	0.43
1:F:386:GLU:O	1:F:390:LYS:HG2	2.19	0.43
1:F:423:ALA:O	1:F:444:LEU:HD11	2.19	0.43
1:G:281:PHE:HA	1:G:285:ARG:HD2	1.99	0.43
1:H:203:TYR:O	1:H:203:TYR:CD1	2.71	0.43
1:K:41:ASP:OD1	1:K:42:LYS:N	2.51	0.43
1:L:123:ALA:HB2	1:L:440:ILE:HD13	2.00	0.43
1:L:367:GLU:HG2	1:L:368:ARG:N	2.34	0.43
1:M:193:MET:SD	1:M:372:LEU:HD23	2.57	0.43
1:N:40:LEU:HD23	1:N:50:THR:HG22	1.99	0.43
3:Z:25:LEU:HG	3:Z:72:TYR:CE1	2.53	0.43
1:A:404:ARG:O	1:A:407:VAL:HG12	2.18	0.43
1:A:423:ALA:O	1:A:444:LEU:HD22	2.18	0.43
1:B:10:ASN:O	1:B:14:VAL:HG13	2.18	0.43
1:D:217:SER:N	1:D:218:PRO:HD3	2.33	0.43
1:F:125:THR:O	1:F:129:GLU:OE2	2.37	0.43
1:G:234:LEU:O	1:G:238:GLU:HG3	2.19	0.43
1:I:260:ALA:O	1:I:263:VAL:HG12	2.18	0.43
1:J:478:TYR:CE1	1:J:480:ALA:HA	2.54	0.43
1:M:284:ARG:HG3	1:M:364:LYS:HB3	2.00	0.43
1:M:349:ILE:HG21	1:M:369:VAL:HG13	2.00	0.43
1:N:6:VAL:HG12	1:N:8:PHE:CE1	2.54	0.43
2:T:88:GLU:HG2	2:T:89:SER:N	2.33	0.43
3:Z:380:PHE:O	3:Z:384:GLY:N	2.51	0.43
1:C:233:MET:HE2	1:C:237:LEU:HD11	2.01	0.43
1:D:49:ILE:HD12	1:E:513:LEU:CD2	2.49	0.43
1:D:252:GLU:OE1	1:D:252:GLU:N	2.51	0.43
1:D:404:ARG:O	1:D:407:VAL:HG12	2.19	0.43
1:E:384:ALA:CA	1:E:388:GLU:OE2	2.67	0.43
1:E:385:THR:O	1:E:388:GLU:HG2	2.18	0.43
1:I:16:MET:HE1	1:I:73:MET:HE3	2.01	0.43
1:I:359:ASP:OD1	1:I:362:ARG:NH1	2.50	0.43
1:I:428:ASP:O	1:I:429:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:GLU:O	1:J:191:GLU:OE1	2.37	0.43
1:L:514:MET:O	1:L:517:THR:HG22	2.18	0.43
1:M:111:MET:SD	1:M:435:ASP:OD1	2.77	0.43
1:N:42:LYS:HE3	1:N:44:PHE:HB2	2.01	0.43
2:O:4:ARG:HH22	2:U:96:GLU:CD	2.25	0.43
2:O:49:LEU:O	2:O:50:GLU:HG3	2.19	0.43
2:O:75:SER:OG	2:O:84:LEU:CD2	2.67	0.43
2:O:81:GLU:CD	2:O:82:GLU:O	2.62	0.43
2:Q:96:GLU:HB2	2:R:1:MET:CE	2.48	0.43
3:Z:42:ALA:HB1	3:Z:81:THR:HG23	1.99	0.43
3:Z:313:ARG:NH2	3:Z:342:MET:O	2.33	0.43
1:C:105:LYS:HD2	1:J:111:MET:CE	2.48	0.43
1:H:322:ARG:HG3	1:H:333:ILE:HD13	2.00	0.43
1:H:461:GLU:HG3	1:H:464:VAL:HG23	2.01	0.43
1:K:307:MET:CE	1:K:312:ALA:HA	2.49	0.43
1:L:305:ILE:O	1:L:305:ILE:HG22	2.19	0.43
2:O:48:ILE:HG22	2:O:48:ILE:O	2.19	0.43
2:O:76:GLU:OE2	2:O:83:VAL:HG23	2.18	0.43
2:R:40:VAL:HG11	2:R:60:LYS:O	2.18	0.43
3:Z:273:THR:O	3:Z:277:ARG:HG2	2.18	0.43
3:Z:304:THR:O	3:Z:308:HIS:HB2	2.19	0.43
1:A:496:PRO:O	1:A:499:VAL:HG12	2.17	0.43
1:B:39:VAL:HG23	1:C:517:THR:HG23	2.00	0.43
1:C:462:PRO:O	1:C:465:VAL:HG12	2.18	0.43
1:F:203:TYR:OH	1:G:305:ILE:HD11	2.18	0.43
1:G:48:THR:HG23	1:G:390:LYS:NZ	2.34	0.43
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.49	0.43
1:N:411:VAL:CG2	1:N:494:LEU:HD12	2.48	0.43
2:T:12:VAL:HG12	2:T:40:VAL:HA	2.00	0.43
2:U:6:LEU:HD23	2:U:6:LEU:H	1.82	0.43
3:Z:180:CYS:HB3	3:Z:184:TRP:CZ3	2.54	0.43
3:Z:371:MET:HE2	3:Z:375:ARG:C	2.44	0.43
1:B:305:ILE:HG13	1:B:305:ILE:O	2.19	0.43
1:F:213:VAL:HB	1:F:325:ILE:HG12	2.01	0.43
1:G:385:THR:N	1:G:388:GLU:OE2	2.52	0.43
1:K:405:ALA:O	1:K:408:GLU:HG2	2.19	0.43
1:N:58:ARG:HG2	1:N:58:ARG:HH11	1.84	0.43
2:O:92:LEU:HA	2:P:9:ARG:NH1	2.33	0.43
2:O:93:ALA:HB1	2:P:3:ILE:HG22	2.00	0.43
2:T:11:ILE:HD12	2:T:85:ILE:HG13	1.99	0.43
3:Z:325:MET:CG	3:Z:371:MET:SD	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:O	1:B:105:LYS:HB2	2.18	0.43
1:D:321:LYS:HD3	1:D:334:ASP:HB3	2.01	0.43
1:E:281:PHE:O	1:E:284:ARG:HG2	2.19	0.43
1:H:186:GLU:OE1	1:H:187:LEU:N	2.52	0.43
1:H:213:VAL:HG13	1:H:325:ILE:HB	2.01	0.43
1:H:216:GLU:HG3	1:H:322:ARG:NH1	2.33	0.43
1:F:7:LYS:C	1:F:8:PHE:CD1	2.97	0.42
1:I:383:ALA:H	1:I:389:MET:HE3	1.84	0.42
1:M:281:PHE:CE1	1:M:284:ARG:NH2	2.87	0.42
1:N:393:LYS:O	1:N:396:VAL:HG22	2.19	0.42
2:P:73:VAL:HG11	2:P:84:LEU:HD23	2.00	0.42
3:Z:105:LEU:HD13	3:Z:269:ALA:HB2	2.00	0.42
3:Z:325:MET:HE1	3:Z:376:MET:HG2	2.01	0.42
1:D:34:LYS:HE3	1:D:458:CYS:SG	2.59	0.42
1:D:363:GLU:HA	1:D:366:GLN:HG2	2.01	0.42
1:E:267:MET:SD	1:F:305:ILE:CD1	3.07	0.42
1:F:193:MET:SD	1:F:371:LYS:O	2.77	0.42
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.01	0.42
1:L:149:THR:O	1:L:154:SER:N	2.51	0.42
1:M:124:VAL:HG23	1:M:504:LEU:CD2	2.49	0.42
1:M:487:ASN:OD1	1:M:489:ILE:HG12	2.19	0.42
1:N:417:VAL:O	1:N:421:ARG:HG2	2.19	0.42
2:Q:96:GLU:C	2:R:1:MET:HE2	2.44	0.42
2:R:66:ILE:HD11	2:R:95:VAL:HG22	2.01	0.42
3:Z:132:TYR:CE2	3:Z:136:PHE:CE2	3.07	0.42
3:Z:443:ASP:HA	3:Z:446:GLN:NE2	2.34	0.42
1:C:3:ALA:O	1:C:524:LEU:HG	2.19	0.42
1:E:458:CYS:CB	1:E:460:GLU:OE1	2.68	0.42
1:F:278:ALA:HB3	1:F:285:ARG:HD2	2.01	0.42
1:F:284:ARG:HG3	1:F:288:MET:HE1	2.01	0.42
1:J:388:GLU:HA	1:J:391:GLU:CG	2.49	0.42
1:L:85:ALA:HB2	1:L:498:LYS:HG2	1.99	0.42
1:L:287:ALA:O	1:L:290:GLN:HG3	2.18	0.42
1:M:352:GLN:HB2	1:M:365:LEU:HD11	2.00	0.42
1:N:180:GLY:HA2	1:N:380:LYS:CG	2.50	0.42
1:N:362:ARG:NH2	1:N:363:GLU:OE2	2.44	0.42
3:Z:136:PHE:O	3:Z:137:ASP:C	2.62	0.42
1:B:236:VAL:O	1:B:240:VAL:HG23	2.19	0.42
1:B:260:ALA:O	1:B:264:VAL:HG23	2.19	0.42
1:E:199:TYR:CE1	1:E:205:ILE:HD11	2.54	0.42
1:F:165:ALA:O	1:F:169:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LEU:C	1:H:23:LEU:HD23	2.44	0.42
1:J:34:LYS:HE3	1:J:458:CYS:SG	2.60	0.42
1:J:192:GLY:N	1:J:375:GLY:HA3	2.35	0.42
1:K:139:SER:O	1:K:171:LYS:NZ	2.52	0.42
2:R:1:MET:HG3	2:R:2:ASN:O	2.19	0.42
2:T:4:ARG:NH2	2:T:5:PRO:O	2.52	0.42
3:Z:164:ILE:HG13	3:Z:391:THR:HG22	2.00	0.42
1:C:445:ARG:HG3	1:C:445:ARG:HH11	1.84	0.42
1:E:6:VAL:HG12	1:E:521:VAL:HG12	2.01	0.42
1:H:4:LYS:HB2	1:I:63:GLU:OE2	2.19	0.42
1:H:230:ILE:CD1	1:H:259:LEU:HB2	2.50	0.42
1:J:363:GLU:O	1:J:367:GLU:OE1	2.38	0.42
1:M:67:GLU:OE2	1:M:67:GLU:N	2.51	0.42
2:P:63:ASP:HB3	2:P:94:ILE:CD1	2.48	0.42
2:Q:2:ASN:OD1	2:Q:2:ASN:C	2.62	0.42
2:T:94:ILE:HG21	2:U:4:ARG:CZ	2.49	0.42
1:B:268:ARG:HD2	2:P:27:LEU:CD2	2.49	0.42
1:C:523:ASP:OD1	1:C:524:LEU:N	2.52	0.42
1:D:128:VAL:HG23	1:D:501:ARG:CG	2.49	0.42
1:E:385:THR:N	1:E:388:GLU:OE2	2.51	0.42
1:F:308:GLU:OE2	1:F:310:GLU:OE1	2.37	0.42
1:F:336:VAL:HG12	1:F:336:VAL:O	2.19	0.42
1:G:217:SER:HA	1:G:320:ALA:O	2.20	0.42
1:G:270:ILE:CD1	2:R:27:LEU:HD21	2.49	0.42
1:G:372:LEU:C	1:G:372:LEU:HD23	2.44	0.42
1:I:193:MET:HB2	1:I:295:LEU:CD2	2.49	0.42
1:K:58:ARG:HB2	1:K:58:ARG:NH1	2.34	0.42
1:M:461:GLU:CD	1:M:461:GLU:C	2.87	0.42
1:N:449:ALA:N	1:N:450:PRO:HD2	2.35	0.42
2:P:47:ARG:HH11	2:P:47:ARG:HG2	1.84	0.42
2:R:91:ILE:O	2:S:6:LEU:HD21	2.20	0.42
2:S:47:ARG:HH22	2:T:48:ILE:HG22	1.84	0.42
3:Z:141:VAL:HG13	3:Z:145:ALA:HB3	2.00	0.42
1:A:80:LYS:O	1:A:84:ALA:N	2.42	0.42
1:F:116:LEU:O	1:F:120:ILE:HG13	2.20	0.42
1:F:186:GLU:OE2	1:F:188:ASP:OD1	2.38	0.42
1:I:363:GLU:OE1	1:I:366:GLN:NE2	2.48	0.42
1:K:65:LYS:O	1:K:69:MET:HG3	2.20	0.42
1:L:217:SER:N	1:L:218:PRO:CD	2.82	0.42
1:M:30:THR:HG21	1:M:53:GLY:CA	2.49	0.42
1:N:194:GLN:HA	1:N:331:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:94:ILE:O	2:O:94:ILE:HG23	2.20	0.42
1:A:16:MET:HE1	1:A:70:GLY:N	2.35	0.42
1:A:36:ARG:HD2	1:B:518:GLU:OE1	2.20	0.42
1:B:54:VAL:HG13	1:B:58:ARG:HH22	1.85	0.42
1:D:65:LYS:O	1:D:69:MET:HG2	2.20	0.42
1:D:366:GLN:HA	1:D:369:VAL:HG22	2.00	0.42
1:D:460:GLU:OE1	1:D:460:GLU:N	2.48	0.42
1:E:292:ILE:HG13	1:E:293:ALA:N	2.35	0.42
1:F:23:LEU:HD12	1:F:60:ILE:HG13	2.01	0.42
1:G:152:ALA:CB	1:G:158:VAL:HG21	2.50	0.42
1:G:183:LEU:HD11	1:G:384:ALA:HB2	2.01	0.42
1:G:232:GLU:CB	1:G:309:LEU:HD23	2.48	0.42
1:G:412:VAL:HG12	1:G:413:ALA:N	2.35	0.42
1:I:433:ASN:OD1	1:I:434:GLU:N	2.43	0.42
1:K:233:MET:HB2	1:K:309:LEU:HD13	2.02	0.42
1:L:180:GLY:HA2	1:L:381:VAL:O	2.20	0.42
1:M:69:MET:HE1	1:N:41:ASP:CG	2.44	0.42
1:M:178:GLU:OE2	1:M:380:LYS:HE3	2.20	0.42
2:Q:92:LEU:HA	2:R:9:ARG:HE	1.84	0.42
2:U:10:VAL:O	2:U:85:ILE:HD12	2.18	0.42
3:Z:50:SER:CB	3:Z:69:ALA:H	2.32	0.42
3:Z:309:CYS:SG	3:Z:322:THR:HA	2.60	0.42
1:A:229:ASN:OD1	1:A:229:ASN:O	2.37	0.42
1:A:462:PRO:O	1:A:465:VAL:HG12	2.20	0.42
1:A:492:GLY:C	1:A:494:LEU:HD12	2.45	0.42
1:F:238:GLU:O	1:F:242:LYS:N	2.41	0.42
1:H:3:ALA:O	1:H:524:LEU:N	2.40	0.42
1:I:429:LEU:HB3	1:I:440:ILE:CD1	2.49	0.42
1:J:18:ARG:HB2	1:J:18:ARG:HH11	1.85	0.42
1:K:287:ALA:O	1:K:290:GLN:HG3	2.20	0.42
1:L:124:VAL:HG13	1:L:504:LEU:CD2	2.50	0.42
1:L:283:ASP:OD1	1:L:284:ARG:HD2	2.20	0.42
1:L:338:GLU:O	1:L:342:ILE:HD12	2.20	0.42
1:N:48:THR:O	1:N:48:THR:HG23	2.20	0.42
3:Z:128:VAL:HG22	3:Z:355:GLN:HE21	1.85	0.42
1:D:145:ALA:O	1:D:149:THR:HG23	2.20	0.42
1:E:183:LEU:HD11	1:E:384:ALA:HB2	2.01	0.42
1:E:353:ILE:HG13	1:E:365:LEU:HB3	2.01	0.42
1:G:144:ILE:HD11	1:G:403:THR:OG1	2.19	0.42
1:G:290:GLN:NE2	1:G:294:THR:OG1	2.53	0.42
1:I:217:SER:HA	1:I:320:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:462:PRO:O	1:I:465:VAL:HG12	2.20	0.42
1:I:496:PRO:O	1:I:499:VAL:HG22	2.20	0.42
1:J:358:SER:C	1:J:359:ASP:OD1	2.62	0.42
1:M:180:GLY:N	1:M:381:VAL:O	2.52	0.42
3:Z:109:MET:HA	3:Z:113:GLN:HG3	2.02	0.42
3:Z:194:GLU:CG	3:Z:195:PRO:HD3	2.49	0.42
3:Z:448:TYR:HA	3:Z:449:PRO:HD3	1.73	0.42
1:B:14:VAL:HG23	1:B:15:LYS:N	2.34	0.41
1:D:223:ALA:HA	1:D:301:ILE:HG22	2.02	0.41
1:E:232:GLU:C	1:E:233:MET:HE2	2.45	0.41
1:G:7:LYS:HG3	1:G:66:PHE:HE2	1.85	0.41
1:G:477:GLY:HA3	1:G:488:MET:HE2	2.02	0.41
1:I:263:VAL:HG13	1:I:264:VAL:N	2.35	0.41
1:J:2:ALA:O	1:J:3:ALA:HB3	2.20	0.41
1:J:388:GLU:O	1:J:391:GLU:HG3	2.20	0.41
1:M:89:THR:HG23	1:M:90:THR:N	2.35	0.41
1:M:225:LYS:HG3	1:M:226:LYS:N	2.34	0.41
1:N:193:MET:SD	1:N:371:LYS:HB3	2.60	0.41
2:S:76:GLU:OE1	2:S:76:GLU:N	2.53	0.41
2:T:12:VAL:CG2	2:T:86:MET:HE1	2.47	0.41
2:U:66:ILE:HG22	2:U:93:ALA:HB3	2.01	0.41
1:B:295:LEU:O	1:B:337:GLY:N	2.47	0.41
1:D:12:ALA:O	1:D:520:MET:HE1	2.20	0.41
1:D:16:MET:HE1	1:D:514:MET:HG2	2.00	0.41
1:D:280:GLY:O	1:D:285:ARG:NH2	2.47	0.41
1:D:385:THR:O	1:D:389:MET:N	2.52	0.41
1:F:187:LEU:HD21	1:F:189:VAL:HG23	2.01	0.41
1:H:22:VAL:HG11	1:H:62:LEU:HD11	2.02	0.41
1:H:197:ARG:HG2	1:H:197:ARG:HH11	1.85	0.41
1:J:114:MET:HG2	1:J:117:LYS:NZ	2.35	0.41
1:J:397:GLU:C	1:J:401:HIS:HD1	2.24	0.41
1:J:421:ARG:HG2	1:J:421:ARG:HH11	1.85	0.41
1:J:465:VAL:HG13	1:J:466:ALA:N	2.35	0.41
1:K:187:LEU:O	1:K:187:LEU:HD12	2.20	0.41
1:K:223:ALA:HB1	1:K:227:ILE:CD1	2.51	0.41
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.60	0.41
1:L:445:ARG:NE	1:L:445:ARG:HA	2.35	0.41
1:L:521:VAL:O	1:M:41:ASP:HB2	2.20	0.41
1:M:267:MET:HE2	1:M:271:VAL:HB	2.02	0.41
1:M:468:THR:HG21	1:M:485:TYR:CE2	2.56	0.41
1:M:477:GLY:HA3	1:M:488:MET:HE2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:123:ALA:HB2	1:N:440:ILE:HD13	2.02	0.41
2:O:75:SER:OG	2:O:84:LEU:HD23	2.20	0.41
2:O:81:GLU:OE2	2:O:82:GLU:O	2.37	0.41
2:P:7:HIS:HB2	2:P:46:GLY:O	2.20	0.41
3:Z:251:PHE:CD1	3:Z:258:VAL:HG22	2.55	0.41
1:A:125:THR:O	1:A:128:VAL:HG12	2.20	0.41
1:A:162:ILE:HG21	1:A:403:THR:HG21	2.01	0.41
1:B:461:GLU:OE2	1:J:463:SER:HB3	2.20	0.41
1:C:397:GLU:OE2	1:C:397:GLU:HA	2.20	0.41
1:D:12:ALA:HB1	1:D:520:MET:SD	2.61	0.41
1:F:97:GLN:O	1:F:100:ILE:HG22	2.21	0.41
1:F:240:VAL:O	1:F:244:GLY:N	2.47	0.41
1:G:252:GLU:HG3	1:G:285:ARG:NH1	2.35	0.41
1:H:140:ASP:OD1	1:H:141:SER:N	2.53	0.41
1:I:432:GLN:OE1	1:I:436:GLN:OE1	2.39	0.41
1:K:333:ILE:N	1:K:333:ILE:HD12	2.34	0.41
1:N:37:ASN:ND2	1:N:49:ILE:HD11	2.34	0.41
1:N:162:ILE:O	1:N:166:MET:HG3	2.19	0.41
2:S:64:ILE:O	2:S:94:ILE:HD12	2.21	0.41
3:Z:109:MET:HA	3:Z:113:GLN:CG	2.50	0.41
3:Z:123:MET:HG2	3:Z:307:VAL:HG21	2.01	0.41
1:A:130:GLU:O	1:A:134:LEU:HD23	2.20	0.41
1:G:286:LYS:HD3	1:G:286:LYS:C	2.45	0.41
1:H:3:ALA:HB1	1:I:63:GLU:HG3	2.03	0.41
1:I:328:ASP:OD1	1:I:329:THR:N	2.53	0.41
1:J:111:MET:HE2	1:J:111:MET:N	2.35	0.41
1:J:190:VAL:O	1:J:376:VAL:N	2.47	0.41
1:J:287:ALA:O	1:J:290:GLN:HG3	2.21	0.41
1:K:185:ASP:OD2	1:K:380:LYS:O	2.38	0.41
1:L:153:ASN:CG	1:L:395:ARG:HH22	2.29	0.41
1:M:155:ASP:HB3	1:M:158:VAL:HG22	2.03	0.41
1:N:193:MET:N	1:N:332:ILE:O	2.38	0.41
1:N:426:LEU:HD11	1:N:429:LEU:HD22	2.02	0.41
2:O:6:LEU:HD21	2:U:91:ILE:HG22	2.02	0.41
2:R:40:VAL:HG12	2:R:63:ASP:O	2.21	0.41
3:Z:137:ASP:HB3	3:Z:314:LEU:O	2.20	0.41
3:Z:239:GLU:OE1	3:Z:243:ARG:NE	2.54	0.41
3:Z:264:GLY:O	3:Z:268:GLY:N	2.52	0.41
1:A:12:ALA:O	1:A:520:MET:HE1	2.20	0.41
1:B:351:GLN:HA	1:B:354:GLU:OE1	2.20	0.41
1:C:41:ASP:OD1	1:C:41:ASP:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:LEU:HD23	1:C:400:LEU:C	2.45	0.41
1:C:488:MET:HE3	1:C:493:ILE:HG21	2.02	0.41
1:D:365:LEU:HD23	1:D:368:ARG:NH2	2.35	0.41
1:F:60:ILE:HA	1:G:4:LYS:NZ	2.35	0.41
1:F:186:GLU:OE2	1:F:187:LEU:C	2.64	0.41
1:H:364:LYS:CG	1:H:365:LEU:HD22	2.49	0.41
1:J:49:ILE:O	1:J:49:ILE:CG2	2.68	0.41
1:K:16:MET:HE2	1:K:520:MET:SD	2.60	0.41
1:M:217:SER:N	1:M:218:PRO:CD	2.83	0.41
2:O:10:VAL:HG23	2:O:86:MET:SD	2.60	0.41
2:O:65:VAL:HB	2:O:91:ILE:HG23	2.03	0.41
2:U:71:TYR:OH	3:Z:431:LYS:HB2	2.20	0.41
1:B:73:MET:SD	1:B:74:VAL:N	2.94	0.41
1:C:39:VAL:HG23	1:D:517:THR:HG23	2.02	0.41
1:D:61:GLU:OE2	1:E:2:ALA:O	2.38	0.41
1:G:152:ALA:O	1:G:153:ASN:HB2	2.20	0.41
1:G:385:THR:HG22	1:G:386:GLU:N	2.35	0.41
1:H:41:ASP:OD2	1:N:523:ASP:N	2.52	0.41
1:I:13:ARG:HG2	1:I:104:LEU:HD12	2.02	0.41
1:K:284:ARG:HD2	1:K:284:ARG:N	2.35	0.41
1:L:371:LYS:HA	1:L:371:LYS:HE3	2.03	0.41
1:M:141:SER:O	1:M:145:ALA:N	2.47	0.41
1:N:291:ASP:OD1	1:N:345:ARG:NE	2.52	0.41
2:O:70:GLY:O	2:O:73:VAL:HG12	2.21	0.41
2:O:86:MET:SD	2:O:86:MET:N	2.94	0.41
3:Z:109:MET:HG3	3:Z:303:TYR:CE2	2.55	0.41
1:F:235:PRO:HA	1:F:238:GLU:OE1	2.20	0.41
1:J:271:VAL:HG12	1:J:273:VAL:CG2	2.50	0.41
1:K:338:GLU:O	1:K:342:ILE:HD12	2.20	0.41
1:N:140:ASP:OD1	1:N:141:SER:N	2.53	0.41
1:N:411:VAL:HG21	1:N:494:LEU:HD12	2.02	0.41
2:U:2:ASN:OD1	2:U:2:ASN:C	2.63	0.41
3:Z:377:PRO:HA	3:Z:380:PHE:CD2	2.56	0.41
1:A:16:MET:SD	1:A:70:GLY:HA2	2.61	0.41
1:A:105:LYS:HE3	1:H:111:MET:HE1	2.02	0.41
1:A:321:LYS:NZ	1:A:334:ASP:OD2	2.50	0.41
1:B:179:ASP:HA	1:B:389:MET:CE	2.50	0.41
1:B:346:VAL:HG13	1:B:369:VAL:HG23	2.02	0.41
1:B:440:ILE:HG23	1:B:441:LYS:N	2.36	0.41
1:C:31:LEU:HD12	1:C:90:THR:HG22	2.02	0.41
1:E:53:GLY:HA3	1:E:90:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:ILE:HD13	1:G:261:THR:HG21	2.02	0.41
1:G:237:LEU:HD22	2:R:26:VAL:CG2	2.50	0.41
1:G:336:VAL:O	1:G:336:VAL:CG1	2.69	0.41
1:I:90:THR:HG1	6:I:2002:ADP:PB	2.38	0.41
1:I:392:LYS:O	1:I:396:VAL:HG23	2.20	0.41
1:K:48:THR:O	1:K:49:ILE:HG22	2.21	0.41
1:M:249:ILE:HD13	1:M:259:LEU:HD21	2.03	0.41
2:P:16:GLU:OE2	2:P:17:VAL:O	2.39	0.41
2:Q:50:GLU:OE1	2:Q:50:GLU:O	2.39	0.41
3:Z:24:VAL:HB	3:Z:85:TYR:HB2	2.03	0.41
3:Z:109:MET:HE1	3:Z:123:MET:HB2	2.01	0.41
3:Z:122:LYS:HA	3:Z:302:GLY:O	2.21	0.41
3:Z:234:ALA:CB	3:Z:239:GLU:OE1	2.69	0.41
1:A:40:LEU:HD23	1:B:521:VAL:CG2	2.51	0.41
1:A:169:VAL:HG21	1:A:175:ILE:HD11	2.02	0.41
1:A:230:ILE:HA	1:A:233:MET:CE	2.51	0.41
1:A:383:ALA:HB3	1:A:389:MET:CE	2.50	0.41
1:A:479:ASN:HD22	1:A:491:MET:CE	2.34	0.41
1:B:16:MET:SD	1:B:70:GLY:HA2	2.61	0.41
1:B:73:MET:HE2	1:B:514:MET:HB2	2.03	0.41
1:C:193:MET:HG3	1:C:295:LEU:HD23	2.03	0.41
1:C:307:MET:HE3	1:C:307:MET:HA	2.02	0.41
1:C:404:ARG:O	1:C:408:GLU:OE1	2.39	0.41
1:E:152:ALA:HB2	1:E:158:VAL:HG21	2.01	0.41
1:F:193:MET:O	1:F:331:THR:HA	2.21	0.41
1:G:6:VAL:HG12	1:G:521:VAL:HG12	2.03	0.41
1:H:24:ALA:HA	1:H:27:VAL:HG12	2.03	0.41
1:I:36:ARG:HH11	1:I:36:ARG:HG2	1.86	0.41
1:I:97:GLN:O	1:I:101:THR:HG22	2.21	0.41
1:I:325:ILE:HG13	1:I:330:THR:HG23	2.03	0.41
1:J:48:THR:O	1:J:49:ILE:HG22	2.21	0.41
1:K:17:LEU:HD23	1:K:17:LEU:C	2.45	0.41
1:K:293:ALA:O	1:K:297:GLY:N	2.54	0.41
1:L:49:ILE:HG23	1:L:49:ILE:O	2.19	0.41
1:M:117:LYS:HG3	1:M:512:GLY:HA2	2.02	0.41
1:M:231:ARG:O	1:M:231:ARG:HD2	2.20	0.41
1:M:349:ILE:CG2	1:M:369:VAL:HG13	2.51	0.41
1:N:31:LEU:HD23	1:N:31:LEU:C	2.46	0.41
2:O:68:ASN:O	2:O:90:ASP:OD1	2.38	0.41
2:P:11:ILE:CG2	2:P:42:ALA:HB3	2.50	0.41
2:P:94:ILE:CG2	2:Q:4:ARG:CG	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:11:ILE:HG12	2:Q:85:ILE:CD1	2.51	0.41
2:R:5:PRO:HB2	2:R:9:ARG:CB	2.51	0.41
2:R:16:GLU:OE1	2:R:17:VAL:N	2.53	0.41
2:T:66:ILE:N	2:T:93:ALA:O	2.45	0.41
2:U:4:ARG:O	2:U:4:ARG:HG3	2.20	0.41
3:Z:68:ASP:OD1	3:Z:68:ASP:O	2.39	0.41
3:Z:123:MET:SD	3:Z:307:VAL:HG11	2.61	0.41
3:Z:294:VAL:HG23	3:Z:295:THR:N	2.35	0.41
3:Z:325:MET:HB3	3:Z:367:ILE:CG2	2.51	0.41
3:Z:372:ASN:HB2	3:Z:440:PHE:CG	2.56	0.41
3:Z:385:ASN:C	3:Z:385:ASN:OD1	2.64	0.41
1:A:194:GLN:O	1:A:371:LYS:HE3	2.21	0.41
1:C:126:ALA:HB1	1:C:426:LEU:HD11	2.03	0.41
1:D:125:THR:O	1:D:128:VAL:HG12	2.21	0.41
1:D:414:GLY:O	1:D:417:VAL:HG12	2.21	0.41
1:E:28:LYS:HE3	1:E:453:GLN:NE2	2.36	0.41
1:E:194:GLN:NE2	1:E:195:PHE:O	2.54	0.41
1:H:522:THR:CB	1:I:41:ASP:OD2	2.67	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.21	0.41
1:M:258:ALA:O	1:M:261:THR:OG1	2.39	0.41
1:A:179:ASP:HA	1:A:381:VAL:HG12	2.03	0.40
1:A:215:LEU:HD12	1:A:246:PRO:CB	2.51	0.40
1:A:234:LEU:HD22	2:Q:26:VAL:HG11	2.03	0.40
1:A:384:ALA:HB3	1:A:388:GLU:OE2	2.21	0.40
1:B:41:ASP:OD1	1:B:42:LYS:N	2.54	0.40
1:B:257:GLU:CD	1:B:258:ALA:N	2.79	0.40
1:C:74:VAL:O	1:C:77:VAL:HG12	2.20	0.40
1:D:326:ASN:CG	1:D:327:LYS:N	2.79	0.40
1:E:338:GLU:O	1:E:342:ILE:HG12	2.21	0.40
1:E:513:LEU:HD23	1:E:513:LEU:C	2.47	0.40
1:H:124:VAL:HG22	1:H:504:LEU:HD21	2.04	0.40
1:J:332:ILE:H	1:J:332:ILE:HD12	1.85	0.40
1:K:142:LYS:O	1:K:146:GLN:NE2	2.54	0.40
1:K:217:SER:N	1:K:218:PRO:CD	2.84	0.40
1:K:367:GLU:O	1:K:371:LYS:N	2.49	0.40
1:L:97:GLN:O	1:L:101:THR:HG23	2.20	0.40
1:L:449:ALA:N	1:L:450:PRO:CD	2.84	0.40
1:N:12:ALA:HB1	1:N:520:MET:HE3	2.02	0.40
2:Q:14:ARG:NH1	2:Q:17:VAL:HG22	2.36	0.40
3:Z:6:ARG:O	3:Z:70:LEU:HD11	2.21	0.40
1:C:291:ASP:OD2	1:C:368:ARG:NH1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:ASN:HB2	1:C:491:MET:HE1	2.03	0.40
1:D:58:ARG:HH11	1:D:58:ARG:CB	2.34	0.40
1:D:130:GLU:OE2	1:D:133:ALA:HB3	2.20	0.40
1:D:152:ALA:CB	1:D:158:VAL:HG21	2.51	0.40
1:D:386:GLU:OE2	1:E:76:GLU:CD	2.64	0.40
1:E:224:ASP:O	1:E:225:LYS:HG2	2.21	0.40
1:G:150:ILE:CD1	1:G:493:ILE:HD13	2.51	0.40
1:I:207:LYS:N	1:I:208:PRO:CD	2.84	0.40
1:J:40:LEU:HB2	1:J:48:THR:OG1	2.22	0.40
1:J:455:VAL:HG23	1:J:462:PRO:HB3	2.03	0.40
1:L:419:LEU:HD21	1:L:500:THR:CG2	2.51	0.40
1:L:504:LEU:HD23	1:L:504:LEU:C	2.46	0.40
2:O:88:GLU:HG2	2:O:89:SER:N	2.36	0.40
2:P:14:ARG:NH2	2:P:84:LEU:HD21	2.37	0.40
2:S:7:HIS:HB3	2:S:45:ASN:OD1	2.21	0.40
1:C:178:GLU:OE2	1:C:380:LYS:HG2	2.22	0.40
1:E:225:LYS:HD2	1:E:225:LYS:HA	1.89	0.40
1:F:326:ASN:N	1:F:329:THR:O	2.38	0.40
1:F:359:ASP:OD1	1:F:362:ARG:NH1	2.54	0.40
1:H:462:PRO:O	1:H:465:VAL:HG12	2.22	0.40
1:I:165:ALA:HB1	1:I:175:ILE:HD13	2.02	0.40
1:I:217:SER:N	1:I:218:PRO:CD	2.85	0.40
1:J:169:VAL:HG21	1:J:377:ALA:HB2	2.03	0.40
1:L:106:ALA:HB1	1:L:111:MET:CE	2.52	0.40
2:U:78:ILE:O	2:U:81:GLU:N	2.52	0.40
3:Z:383:LEU:CD2	3:Z:385:ASN:OD1	2.70	0.40
1:A:63:GLU:CD	1:A:64:ASP:N	2.80	0.40
1:C:13:ARG:NH1	1:C:107:VAL:HG11	2.36	0.40
1:D:301:ILE:HD12	1:D:301:ILE:HA	1.99	0.40
1:F:47:PRO:HB2	1:G:73:MET:HE1	2.03	0.40
1:H:65:LYS:HB3	1:H:522:THR:HG21	2.04	0.40
1:H:207:LYS:N	1:H:208:PRO:CD	2.85	0.40
1:H:332:ILE:O	1:H:332:ILE:HG23	2.20	0.40
1:H:465:VAL:HG13	1:H:466:ALA:N	2.35	0.40
1:I:461:GLU:HG3	1:I:464:VAL:HG23	2.02	0.40
1:J:179:ASP:OD2	1:J:179:ASP:C	2.64	0.40
1:K:190:VAL:HG22	1:K:191:GLU:N	2.36	0.40
1:L:435:ASP:O	1:L:438:VAL:HG22	2.21	0.40
1:N:213:VAL:HG13	1:N:213:VAL:O	2.22	0.40
1:N:321:LYS:NZ	1:N:334:ASP:OD2	2.40	0.40
2:Q:93:ALA:HB1	2:R:3:ILE:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:96:ASP:OD2	3:Z:277:ARG:NH2	2.45	0.40
3:Z:190:ILE:HB	3:Z:228:PHE:CD1	2.57	0.40
3:Z:296:SER:HB3	3:Z:298:GLN:OE1	2.21	0.40
3:Z:383:LEU:HG	3:Z:385:ASN:OD1	2.22	0.40
1:B:73:MET:SD	1:B:510:VAL:CG1	3.10	0.40
1:C:248:LEU:HD22	1:C:323:VAL:HG11	2.02	0.40
1:C:339:GLU:O	1:C:342:ILE:HG22	2.21	0.40
1:E:433:ASN:CG	1:E:436:GLN:OE1	2.64	0.40
1:F:25:ASP:OD2	1:G:8:PHE:CZ	2.75	0.40
1:J:350:ARG:HA	1:J:353:ILE:HD12	2.03	0.40
1:M:263:VAL:HG13	1:M:264:VAL:H	1.85	0.40
1:M:284:ARG:O	1:M:288:MET:HG2	2.21	0.40
1:N:56:VAL:HG13	1:N:57:ALA:N	2.36	0.40
1:N:363:GLU:OE1	1:N:366:GLN:NE2	2.46	0.40
2:O:66:ILE:HG23	2:O:92:LEU:HB2	2.03	0.40
2:Q:7:HIS:C	2:Q:9:ARG:H	2.30	0.40
2:Q:65:VAL:HB	2:Q:91:ILE:HG23	2.02	0.40
2:S:79:ASP:OD1	2:S:81:GLU:HB3	2.21	0.40
3:Z:93:ASN:HD21	3:Z:100:MET:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	522/547 (95%)	509 (98%)	12 (2%)	1 (0%)	43 77
1	B	522/547 (95%)	509 (98%)	13 (2%)	0	100 100
1	C	522/547 (95%)	509 (98%)	12 (2%)	1 (0%)	43 77
1	D	522/547 (95%)	509 (98%)	13 (2%)	0	100 100
1	E	522/547 (95%)	506 (97%)	15 (3%)	1 (0%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	522/547 (95%)	512 (98%)	10 (2%)	0	100	100
1	G	522/547 (95%)	511 (98%)	11 (2%)	0	100	100
1	H	521/547 (95%)	501 (96%)	20 (4%)	0	100	100
1	I	521/547 (95%)	501 (96%)	19 (4%)	1 (0%)	43	77
1	J	521/547 (95%)	491 (94%)	28 (5%)	2 (0%)	30	66
1	K	521/547 (95%)	491 (94%)	28 (5%)	2 (0%)	30	66
1	L	521/547 (95%)	492 (94%)	28 (5%)	1 (0%)	43	77
1	M	521/547 (95%)	499 (96%)	22 (4%)	0	100	100
1	N	521/547 (95%)	509 (98%)	12 (2%)	0	100	100
2	O	95/97 (98%)	82 (86%)	11 (12%)	2 (2%)	5	30
2	P	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	5	30
2	Q	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	30
2	R	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	5	30
2	S	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	30
2	T	95/97 (98%)	83 (87%)	10 (10%)	2 (2%)	5	30
2	U	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	30
3	Z	457/466 (98%)	395 (86%)	57 (12%)	5 (1%)	11	45
All	All	8423/8803 (96%)	8031 (95%)	364 (4%)	28 (0%)	37	71

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	7	HIS
2	P	7	HIS
2	Q	7	HIS
2	R	7	HIS
2	S	7	HIS
2	T	7	HIS
2	U	7	HIS
3	Z	422	PRO
3	Z	449	PRO
1	L	217	SER
2	T	8	ASP
1	I	85	ALA
1	J	217	SER
2	O	8	ASP

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Mol	Chain	Res	Type
2	R	8	ASP
2	S	8	ASP
2	U	8	ASP
3	Z	50	SER
3	Z	404	VAL
1	K	49	ILE
1	K	217	SER
2	P	8	ASP
2	Q	8	ASP
1	J	3	ALA
3	Z	457	VAL
1	C	336	VAL
1	A	336	VAL
1	E	336	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/414 (98%)	404 (100%)	0	100	100
1	B	404/414 (98%)	404 (100%)	0	100	100
1	C	404/414 (98%)	404 (100%)	0	100	100
1	D	404/414 (98%)	404 (100%)	0	100	100
1	E	404/414 (98%)	404 (100%)	0	100	100
1	F	404/414 (98%)	404 (100%)	0	100	100
1	G	404/414 (98%)	404 (100%)	0	100	100
1	H	402/414 (97%)	402 (100%)	0	100	100
1	I	402/414 (97%)	402 (100%)	0	100	100
1	J	402/414 (97%)	402 (100%)	0	100	100
1	K	402/414 (97%)	402 (100%)	0	100	100
1	L	402/414 (97%)	402 (100%)	0	100	100
1	M	402/414 (97%)	402 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	402/414 (97%)	402 (100%)	0	100	100
2	O	80/80 (100%)	80 (100%)	0	100	100
2	P	80/80 (100%)	80 (100%)	0	100	100
2	Q	80/80 (100%)	80 (100%)	0	100	100
2	R	80/80 (100%)	80 (100%)	0	100	100
2	S	80/80 (100%)	80 (100%)	0	100	100
2	T	80/80 (100%)	80 (100%)	0	100	100
2	U	80/80 (100%)	80 (100%)	0	100	100
3	Z	348/354 (98%)	348 (100%)	0	100	100
All	All	6550/6710 (98%)	6550 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	ASN
1	A	343	GLN
1	B	194	GLN
1	C	194	GLN
1	C	366	GLN
1	C	401	HIS
1	C	453	GLN
1	C	457	ASN
1	D	153	ASN
1	D	194	GLN
1	D	401	HIS
1	D	467	ASN
1	D	475	ASN
1	D	505	GLN
1	E	97	GLN
1	E	319	GLN
1	E	326	ASN
1	F	112	ASN
1	F	194	GLN
1	F	229	ASN
1	F	326	ASN
1	F	348	GLN
1	F	366	GLN

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Mol	Chain	Res	Type
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	153	ASN
1	G	319	GLN
1	G	326	ASN
1	G	432	GLN
1	G	436	GLN
1	G	457	ASN
1	H	37	ASN
1	H	184	GLN
1	H	432	GLN
1	H	453	GLN
1	I	194	GLN
1	I	351	GLN
1	I	401	HIS
1	I	436	GLN
1	I	437	ASN
1	I	453	GLN
1	J	37	ASN
1	J	265	ASN
1	J	352	GLN
1	J	453	GLN
1	K	82	ASN
1	K	265	ASN
1	K	352	GLN
1	L	82	ASN
1	L	194	GLN
1	L	352	GLN
1	M	505	GLN
1	N	82	ASN
1	N	184	GLN
1	N	453	GLN
2	O	68	ASN
2	R	68	ASN
2	S	2	ASN
3	Z	93	ASN
3	Z	321	HIS
3	Z	387	ASN
3	Z	430	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 21 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	J	601	5,7	27,29,29	1.32	4 (14%)	42,45,45	2.06	12 (28%)
4	AF3	B	602	6	0,3,3	-	-	-		
6	ADP	M	2003	5,7	27,29,29	1.66	6 (22%)	42,45,45	2.20	13 (30%)
6	ADP	G	602	5,4	27,29,29	1.33	4 (14%)	42,45,45	1.99	11 (26%)
6	ADP	I	2002	5,7	27,29,29	1.39	4 (14%)	42,45,45	2.38	9 (21%)
6	ADP	D	601	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.00	11 (26%)
6	ADP	E	603	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.00	11 (26%)
6	ADP	A	603	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.11	13 (30%)
4	AF3	A	601	6	0,3,3	-	-	-		
6	ADP	L	603	5,7	27,29,29	1.33	4 (14%)	42,45,45	2.03	11 (26%)
6	ADP	F	603	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.05	12 (28%)
6	ADP	H	2002	5,7	27,29,29	1.33	4 (14%)	42,45,45	2.07	11 (26%)
4	AF3	F	601	1,6	0,3,3	-	-	-		
4	AF3	E	601	1,6	0,3,3	-	-	-		
6	ADP	K	602	5,7	27,29,29	1.33	4 (14%)	42,45,45	2.08	12 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	N	601	5,7	27,29,29	1.31	4 (14%)	42,45,45	2.06	12 (28%)
4	AF3	G	601	6	0,3,3	-	-	-		
4	AF3	D	602	6	0,3,3	-	-	-		
6	ADP	C	603	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.11	13 (30%)
6	ADP	B	603	5,4	27,29,29	1.32	4 (14%)	42,45,45	2.13	11 (26%)
4	AF3	C	602	1,6	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	G	602	5,4	-	0/16/32/32	0/3/3/3
6	ADP	I	2002	5,7	1/1/6/6	4/16/32/32	0/3/3/3
6	ADP	J	601	5,7	-	3/16/32/32	0/3/3/3
6	ADP	L	603	5,7	-	4/16/32/32	0/3/3/3
6	ADP	D	601	5,4	-	0/16/32/32	0/3/3/3
6	ADP	K	602	5,7	-	2/16/32/32	0/3/3/3
6	ADP	E	603	5,4	-	4/16/32/32	0/3/3/3
6	ADP	N	601	5,7	-	3/16/32/32	0/3/3/3
6	ADP	A	603	5,4	-	3/16/32/32	0/3/3/3
6	ADP	C	603	5,4	-	0/16/32/32	0/3/3/3
6	ADP	F	603	5,4	-	3/16/32/32	0/3/3/3
6	ADP	B	603	5,4	-	0/16/32/32	0/3/3/3
6	ADP	H	2002	5,7	-	1/16/32/32	0/3/3/3
6	ADP	M	2003	5,7	1/1/6/6	3/16/32/32	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2002	ADP	C5-C4	4.38	1.47	1.39
6	H	2002	ADP	C5-C4	4.32	1.47	1.39
6	L	603	ADP	C5-C4	4.30	1.47	1.39
6	M	2003	ADP	C5-C4	4.26	1.47	1.39
6	K	602	ADP	C5-C4	4.24	1.46	1.39
6	G	602	ADP	C5-C4	4.23	1.46	1.39
6	E	603	ADP	C5-C4	4.23	1.46	1.39
6	A	603	ADP	C5-C4	4.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	603	ADP	C5-C4	4.22	1.46	1.39
6	J	601	ADP	C5-C4	4.17	1.46	1.39
6	D	601	ADP	C5-C4	4.15	1.46	1.39
6	N	601	ADP	C5-C4	4.15	1.46	1.39
6	B	603	ADP	C5-C4	4.15	1.46	1.39
6	F	603	ADP	C5-C4	4.15	1.46	1.39
6	M	2003	ADP	O4'-C4'	-4.10	1.35	1.45
6	M	2003	ADP	C3'-C4'	-3.03	1.45	1.53
6	J	601	ADP	C5-C6	2.58	1.48	1.41
6	L	603	ADP	C5-C6	2.57	1.48	1.41
6	F	603	ADP	C5-C6	2.56	1.48	1.41
6	K	602	ADP	C5-C6	2.54	1.48	1.41
6	M	2003	ADP	C5-C6	2.54	1.48	1.41
6	C	603	ADP	C5-C6	2.53	1.48	1.41
6	G	602	ADP	C5-C6	2.53	1.48	1.41
6	A	603	ADP	C5-C6	2.52	1.48	1.41
6	I	2002	ADP	C5-C6	2.51	1.48	1.41
6	D	601	ADP	C5-C6	2.50	1.48	1.41
6	B	603	ADP	C5-C6	2.49	1.48	1.41
6	N	601	ADP	C5-C6	2.48	1.48	1.41
6	I	2002	ADP	C5-N7	-2.48	1.34	1.39
6	D	601	ADP	C8-N7	2.47	1.36	1.31
6	E	603	ADP	C5-C6	2.46	1.47	1.41
6	H	2002	ADP	C5-C6	2.46	1.47	1.41
6	H	2002	ADP	C5-N7	-2.46	1.34	1.39
6	F	603	ADP	C8-N7	2.44	1.36	1.31
6	B	603	ADP	C8-N7	2.42	1.36	1.31
6	K	602	ADP	C8-N7	2.42	1.36	1.31
6	L	603	ADP	C8-N7	2.42	1.36	1.31
6	J	601	ADP	C8-N7	2.41	1.36	1.31
6	G	602	ADP	C8-N7	2.38	1.36	1.31
6	E	603	ADP	C5-N7	-2.37	1.34	1.39
6	A	603	ADP	C5-N7	-2.37	1.34	1.39
6	B	603	ADP	C5-N7	-2.36	1.34	1.39
6	M	2003	ADP	C8-N7	2.36	1.36	1.31
6	N	601	ADP	C5-N7	-2.36	1.34	1.39
6	A	603	ADP	C8-N7	2.35	1.36	1.31
6	C	603	ADP	C8-N7	2.35	1.36	1.31
6	N	601	ADP	C8-N7	2.33	1.36	1.31
6	H	2002	ADP	C8-N7	2.33	1.36	1.31
6	C	603	ADP	C5-N7	-2.33	1.34	1.39
6	G	602	ADP	C5-N7	-2.33	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	2003	ADP	C5-N7	-2.32	1.34	1.39
6	K	602	ADP	C5-N7	-2.32	1.34	1.39
6	D	601	ADP	C5-N7	-2.32	1.34	1.39
6	E	603	ADP	C8-N7	2.30	1.36	1.31
6	I	2002	ADP	C8-N7	2.30	1.36	1.31
6	F	603	ADP	C5-N7	-2.30	1.34	1.39
6	J	601	ADP	C5-N7	-2.29	1.34	1.39
6	L	603	ADP	C5-N7	-2.29	1.34	1.39

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	2002	ADP	C5-C4-N3	-6.98	117.64	126.75
6	I	2002	ADP	C2'-C1'-N9	6.75	130.39	113.30
6	H	2002	ADP	C5-C4-N3	-6.45	118.33	126.75
6	A	603	ADP	C5-C4-N3	-6.31	118.51	126.75
6	K	602	ADP	C5-C4-N3	-6.23	118.62	126.75
6	N	601	ADP	C5-C4-N3	-6.18	118.68	126.75
6	L	603	ADP	C5-C4-N3	-6.17	118.70	126.75
6	F	603	ADP	C5-C4-N3	-6.16	118.71	126.75
6	M	2003	ADP	C5-C4-N3	-6.14	118.74	126.75
6	C	603	ADP	C5-C4-N3	-6.13	118.75	126.75
6	J	601	ADP	C5-C4-N3	-6.11	118.78	126.75
6	E	603	ADP	C5-C4-N3	-6.06	118.84	126.75
6	G	602	ADP	C5-C4-N3	-6.05	118.86	126.75
6	B	603	ADP	C5-C4-N3	-6.03	118.88	126.75
6	D	601	ADP	C5-C4-N3	-6.02	118.89	126.75
6	I	2002	ADP	N3-C4-N9	5.46	136.07	127.08
6	H	2002	ADP	N3-C4-N9	5.02	135.35	127.08
6	N	601	ADP	N3-C4-N9	4.88	135.13	127.08
6	A	603	ADP	N3-C4-N9	4.87	135.11	127.08
6	E	603	ADP	N3-C4-N9	4.85	135.07	127.08
6	M	2003	ADP	N3-C4-N9	4.84	135.05	127.08
6	C	603	ADP	N3-C4-N9	4.82	135.03	127.08
6	K	602	ADP	N3-C4-N9	4.78	134.96	127.08
6	G	602	ADP	N3-C4-N9	4.77	134.95	127.08
6	L	603	ADP	N3-C4-N9	4.77	134.95	127.08
6	F	603	ADP	N3-C4-N9	4.74	134.89	127.08
6	B	603	ADP	N3-C4-N9	4.71	134.84	127.08
6	J	601	ADP	N3-C4-N9	4.66	134.76	127.08
6	D	601	ADP	N3-C4-N9	4.63	134.71	127.08
6	B	603	ADP	PA-O3A-PB	-4.61	117.00	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	603	ADP	PA-O3A-PB	-4.46	117.51	132.83
6	M	2003	ADP	PA-O3A-PB	-4.35	117.92	132.83
6	I	2002	ADP	C2-N3-C4	4.32	121.95	111.75
6	M	2003	ADP	C4'-O4'-C1'	-4.24	100.12	109.47
6	H	2002	ADP	PA-O3A-PB	-4.22	118.34	132.83
6	I	2002	ADP	PA-O3A-PB	-4.18	118.50	132.83
6	N	601	ADP	PA-O3A-PB	-4.13	118.65	132.83
6	J	601	ADP	PA-O3A-PB	-4.09	118.80	132.83
6	F	603	ADP	C2-N3-C4	4.08	121.40	111.75
6	H	2002	ADP	C2-N3-C4	4.08	121.40	111.75
6	K	602	ADP	C2-N3-C4	4.05	121.33	111.75
6	A	603	ADP	C2-N3-C4	4.04	121.29	111.75
6	J	601	ADP	C2-N3-C4	4.03	121.27	111.75
6	C	603	ADP	C2-N3-C4	4.02	121.25	111.75
6	N	601	ADP	C2-N3-C4	4.02	121.25	111.75
6	L	603	ADP	C2-N3-C4	4.02	121.24	111.75
6	D	601	ADP	C2-N3-C4	4.02	121.24	111.75
6	M	2003	ADP	C2-N3-C4	3.99	121.19	111.75
6	G	602	ADP	C2-N3-C4	3.97	121.12	111.75
6	B	603	ADP	C2-N3-C4	3.96	121.11	111.75
6	L	603	ADP	PA-O3A-PB	-3.96	119.23	132.83
6	K	602	ADP	PA-O3A-PB	-3.95	119.27	132.83
6	E	603	ADP	C2-N3-C4	3.95	121.08	111.75
6	E	603	ADP	PA-O3A-PB	-3.73	120.03	132.83
6	G	602	ADP	PA-O3A-PB	-3.71	120.09	132.83
6	A	603	ADP	PA-O3A-PB	-3.68	120.20	132.83
6	F	603	ADP	N3-C2-N1	-3.65	122.90	128.60
6	D	601	ADP	N3-C2-N1	-3.62	122.94	128.60
6	B	603	ADP	N3-C2-N1	-3.60	122.97	128.60
6	K	602	ADP	N3-C2-N1	-3.59	122.99	128.60
6	C	603	ADP	N3-C2-N1	-3.57	123.03	128.60
6	G	602	ADP	N3-C2-N1	-3.56	123.03	128.60
6	J	601	ADP	N3-C2-N1	-3.56	123.03	128.60
6	B	603	ADP	O4'-C1'-N9	3.56	115.08	108.06
6	L	603	ADP	N3-C2-N1	-3.56	123.04	128.60
6	H	2002	ADP	N3-C2-N1	-3.55	123.05	128.60
6	E	603	ADP	N3-C2-N1	-3.54	123.06	128.60
6	N	601	ADP	N3-C2-N1	-3.54	123.07	128.60
6	M	2003	ADP	N3-C2-N1	-3.54	123.07	128.60
6	I	2002	ADP	N3-C2-N1	-3.53	123.08	128.60
6	A	603	ADP	N3-C2-N1	-3.53	123.09	128.60
6	F	603	ADP	C4-C5-N7	-3.43	106.44	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	601	ADP	C4-C5-N7	-3.43	106.44	110.62
6	B	603	ADP	C4-C5-N7	-3.40	106.47	110.62
6	K	602	ADP	C4-C5-N7	-3.40	106.48	110.62
6	L	603	ADP	C4-C5-N7	-3.35	106.54	110.62
6	A	603	ADP	C4-C5-N7	-3.34	106.55	110.62
6	D	601	ADP	C4-C5-N7	-3.33	106.56	110.62
6	G	602	ADP	C4-C5-N7	-3.28	106.63	110.62
6	M	2003	ADP	C4-C5-N7	-3.27	106.64	110.62
6	C	603	ADP	C4-C5-N7	-3.22	106.70	110.62
6	D	601	ADP	PA-O3A-PB	-3.20	121.83	132.83
6	N	601	ADP	C4-C5-N7	-3.20	106.72	110.62
6	H	2002	ADP	C4-C5-N7	-3.13	106.80	110.62
6	I	2002	ADP	C4-C5-N7	-3.12	106.82	110.62
6	F	603	ADP	PA-O3A-PB	-3.11	122.14	132.83
6	E	603	ADP	C4-C5-N7	-3.11	106.83	110.62
6	B	603	ADP	C5-N7-C8	3.07	107.87	103.51
6	F	603	ADP	C5-N7-C8	3.05	107.84	103.51
6	M	2003	ADP	C2'-C3'-C4'	-3.03	96.76	102.64
6	K	602	ADP	C5-N7-C8	3.03	107.81	103.51
6	J	601	ADP	C5-N7-C8	3.01	107.79	103.51
6	B	603	ADP	C4-N9-C8	3.00	108.97	105.73
6	A	603	ADP	C5-N7-C8	2.99	107.76	103.51
6	L	603	ADP	C5-N7-C8	2.97	107.73	103.51
6	D	601	ADP	C5-N7-C8	2.96	107.72	103.51
6	A	603	ADP	O4'-C1'-C2'	-2.95	100.21	106.64
6	G	602	ADP	C4-N9-C8	2.95	108.92	105.73
6	G	602	ADP	C5-N7-C8	2.94	107.69	103.51
6	E	603	ADP	C4-N9-C8	2.94	108.91	105.73
6	F	603	ADP	C4-N9-C8	2.93	108.90	105.73
6	M	2003	ADP	C5-N7-C8	2.92	107.66	103.51
6	N	601	ADP	C5-N7-C8	2.91	107.64	103.51
6	N	601	ADP	C4-N9-C8	2.90	108.87	105.73
6	M	2003	ADP	C4-N9-C8	2.89	108.86	105.73
6	C	603	ADP	C5-N7-C8	2.89	107.62	103.51
6	C	603	ADP	C4-N9-C8	2.87	108.84	105.73
6	D	601	ADP	C4-N9-C8	2.87	108.84	105.73
6	A	603	ADP	O4'-C1'-N9	2.87	113.71	108.06
6	J	601	ADP	C4-N9-C8	2.83	108.80	105.73
6	H	2002	ADP	O4'-C1'-N9	2.83	113.63	108.06
6	I	2002	ADP	C5-N7-C8	2.82	107.52	103.51
6	E	603	ADP	C5-N7-C8	2.81	107.51	103.51
6	H	2002	ADP	C5-N7-C8	2.80	107.49	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	603	ADP	O4'-C1'-N9	2.78	113.54	108.06
6	L	603	ADP	C4-N9-C8	2.78	108.74	105.73
6	K	602	ADP	C4-N9-C8	2.76	108.72	105.73
6	K	602	ADP	O4'-C1'-N9	2.67	113.31	108.06
6	A	603	ADP	C4-N9-C8	2.65	108.60	105.73
6	K	602	ADP	O4'-C1'-C2'	-2.64	100.89	106.64
6	C	603	ADP	O4'-C1'-N9	2.62	113.23	108.06
6	C	603	ADP	O4'-C1'-C2'	-2.58	101.01	106.64
6	B	603	ADP	N9-C8-N7	-2.57	110.40	113.91
6	F	603	ADP	N9-C8-N7	-2.54	110.44	113.91
6	D	601	ADP	N9-C8-N7	-2.49	110.50	113.91
6	J	601	ADP	N9-C8-N7	-2.48	110.52	113.91
6	L	603	ADP	O4'-C1'-C2'	-2.46	101.28	106.64
6	J	601	ADP	O4'-C1'-C2'	-2.45	101.29	106.64
6	G	602	ADP	N9-C8-N7	-2.45	110.56	113.91
6	N	601	ADP	N9-C8-N7	-2.43	110.59	113.91
6	K	602	ADP	N9-C8-N7	-2.43	110.59	113.91
6	N	601	ADP	O4'-C1'-C2'	-2.42	101.36	106.64
6	H	2002	ADP	C4-N9-C8	2.41	108.34	105.73
6	M	2003	ADP	N9-C8-N7	-2.40	110.63	113.91
6	C	603	ADP	N9-C8-N7	-2.40	110.64	113.91
6	D	601	ADP	C6-C5-N7	2.39	136.47	132.02
6	L	603	ADP	N9-C8-N7	-2.38	110.65	113.91
6	J	601	ADP	C6-C5-N7	2.38	136.45	132.02
6	F	603	ADP	C6-C5-N7	2.37	136.44	132.02
6	E	603	ADP	N9-C8-N7	-2.37	110.67	113.91
6	C	603	ADP	C4'-O4'-C1'	-2.36	104.27	109.47
6	D	601	ADP	O4'-C1'-N9	2.35	112.70	108.06
6	M	2003	ADP	O4'-C4'-C3'	2.35	109.76	105.11
6	A	603	ADP	N9-C8-N7	-2.34	110.72	113.91
6	F	603	ADP	O4'-C1'-C2'	-2.31	101.59	106.64
6	H	2002	ADP	O4'-C1'-C2'	-2.31	101.61	106.64
6	B	603	ADP	C6-C5-N7	2.30	136.31	132.02
6	K	602	ADP	C6-C5-N7	2.29	136.28	132.02
6	L	603	ADP	C6-C5-N7	2.27	136.25	132.02
6	N	601	ADP	O4'-C1'-N9	2.26	112.52	108.06
6	C	603	ADP	C6-C5-N7	2.22	136.16	132.02
6	G	602	ADP	C6-C5-N7	2.22	136.15	132.02
6	M	2003	ADP	C6-C5-N7	2.21	136.13	132.02
6	I	2002	ADP	C4-N9-C8	2.17	108.08	105.73
6	J	601	ADP	O4'-C1'-N9	2.15	112.30	108.06
6	A	603	ADP	C6-C5-N7	2.15	136.03	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	601	ADP	C6-C5-N7	2.15	136.02	132.02
6	E	603	ADP	C6-C5-N7	2.11	135.94	132.02
6	G	602	ADP	O3B-PB-O2B	2.10	115.65	107.64
6	H	2002	ADP	N9-C8-N7	-2.08	111.06	113.91
6	A	603	ADP	C4'-O4'-C1'	-2.07	104.91	109.47
6	E	603	ADP	O4'-C1'-N9	2.02	112.03	108.06

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	2002	ADP	C1'
6	M	2003	ADP	C4'

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	603	ADP	PA-O3A-PB-O2B
6	E	603	ADP	C3'-C4'-C5'-O5'
6	F	603	ADP	PA-O3A-PB-O2B
6	A	603	ADP	O4'-C4'-C5'-O5'
6	E	603	ADP	O4'-C4'-C5'-O5'
6	E	603	ADP	C4'-C5'-O5'-PA
6	M	2003	ADP	C4'-C5'-O5'-PA
6	M	2003	ADP	O4'-C4'-C5'-O5'
6	A	603	ADP	PA-O3A-PB-O2B
6	A	603	ADP	C3'-C4'-C5'-O5'
6	J	601	ADP	PB-O3A-PA-O2A
6	K	602	ADP	PB-O3A-PA-O2A
6	L	603	ADP	PB-O3A-PA-O2A
6	N	601	ADP	PB-O3A-PA-O2A
6	F	603	ADP	C5'-O5'-PA-O1A
6	L	603	ADP	C3'-C4'-C5'-O5'
6	I	2002	ADP	C3'-C4'-C5'-O5'
6	J	601	ADP	C3'-C4'-C5'-O5'
6	N	601	ADP	C3'-C4'-C5'-O5'
6	H	2002	ADP	PB-O3A-PA-O2A
6	I	2002	ADP	PB-O3A-PA-O2A
6	M	2003	ADP	PB-O3A-PA-O2A
6	J	601	ADP	PB-O3A-PA-O1A
6	L	603	ADP	PB-O3A-PA-O1A
6	F	603	ADP	C5'-O5'-PA-O3A
6	L	603	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	I	2002	ADP	PB-O3A-PA-O1A
6	K	602	ADP	PB-O3A-PA-O1A
6	N	601	ADP	PB-O3A-PA-O1A
6	I	2002	ADP	O4'-C1'-N9-C8

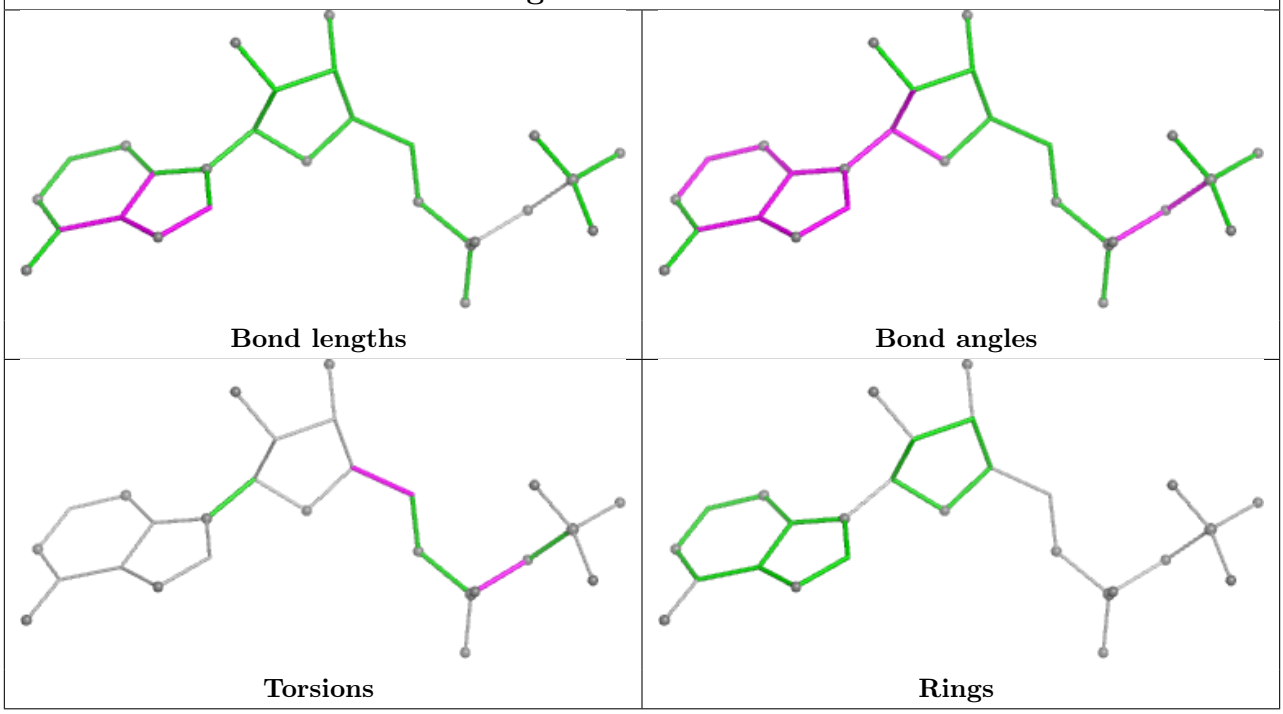
There are no ring outliers.

15 monomers are involved in 17 short contacts:

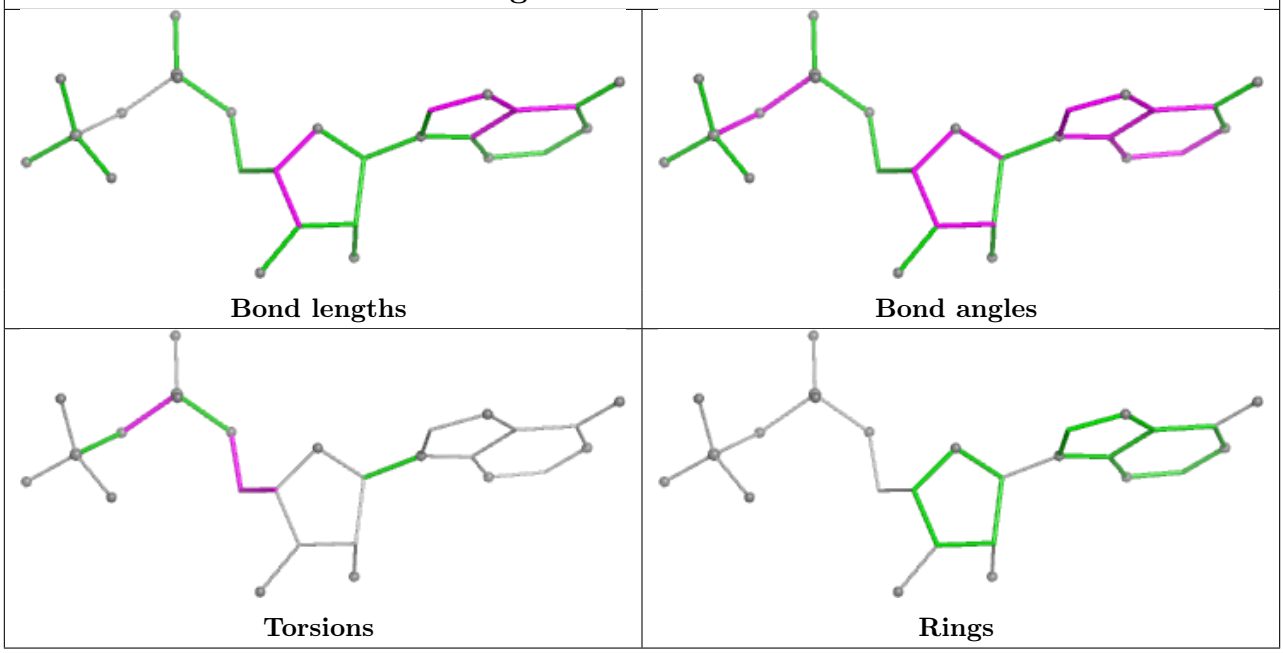
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	AF3	1	0
6	M	2003	ADP	1	0
6	I	2002	ADP	2	0
6	E	603	ADP	1	0
6	A	603	ADP	1	0
4	A	601	AF3	3	0
6	F	603	ADP	2	0
6	H	2002	ADP	1	0
4	F	601	AF3	1	0
4	E	601	AF3	1	0
4	G	601	AF3	2	0
4	D	602	AF3	2	0
6	C	603	ADP	1	0
6	B	603	ADP	1	0
4	C	602	AF3	2	0

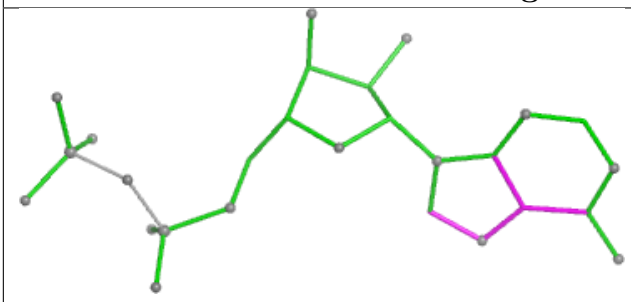
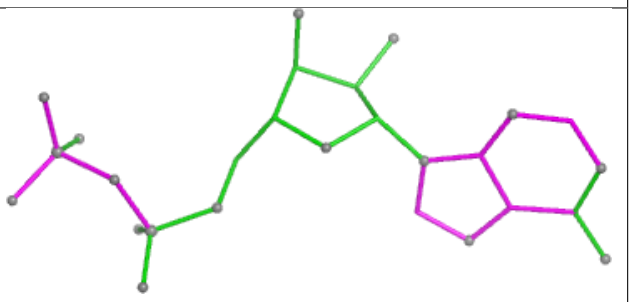
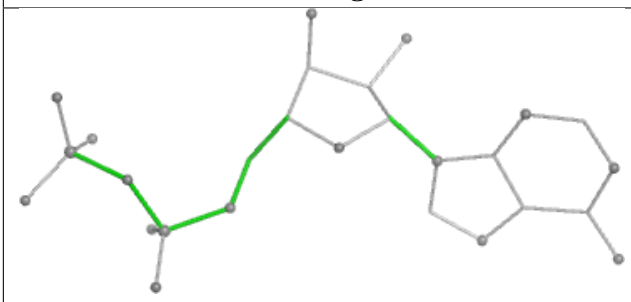
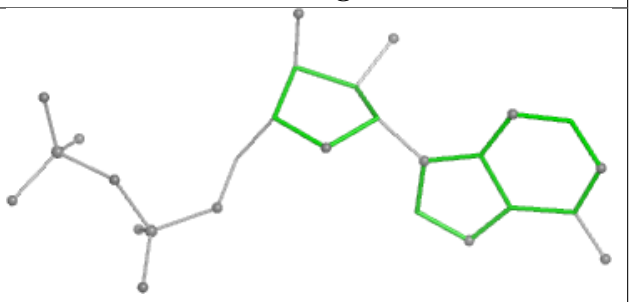
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

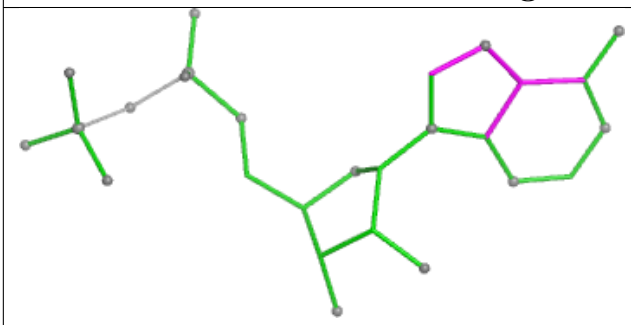
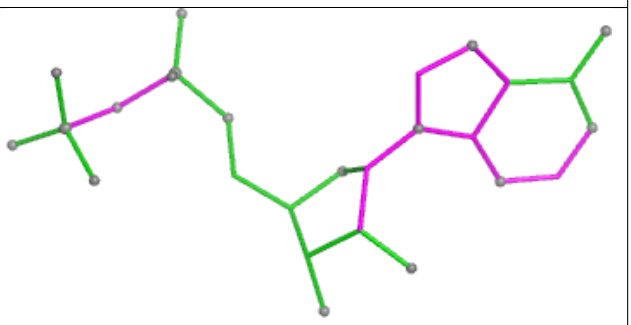
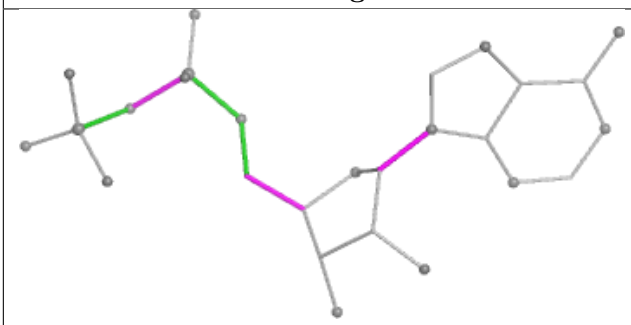
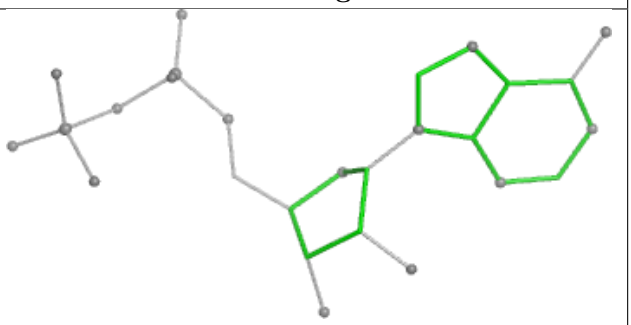
Ligand ADP J 601



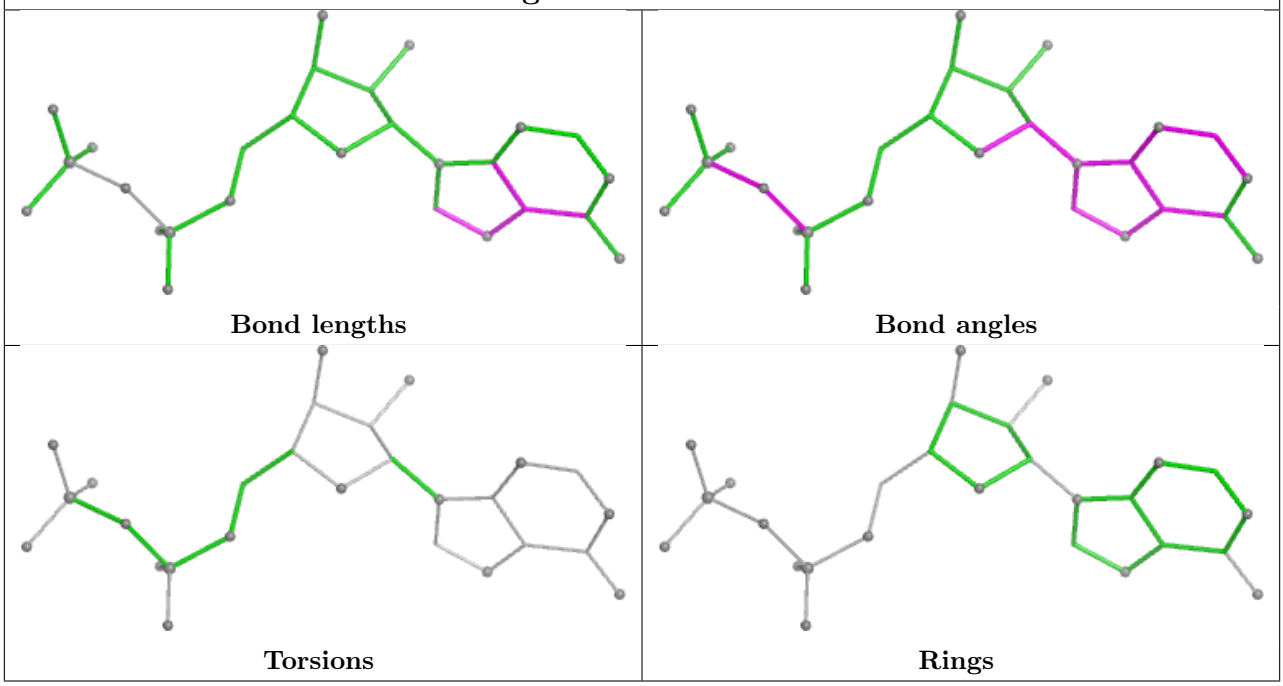
Ligand ADP M 2003



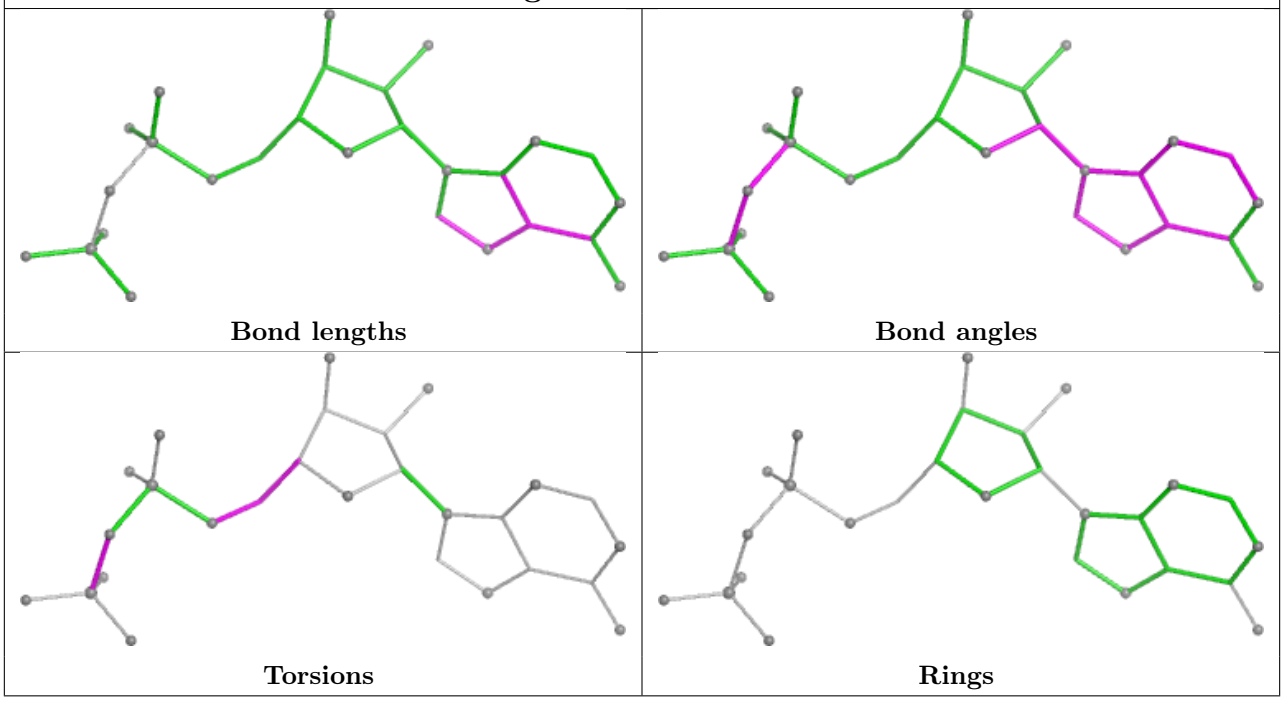
Ligand ADP G 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP I 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings

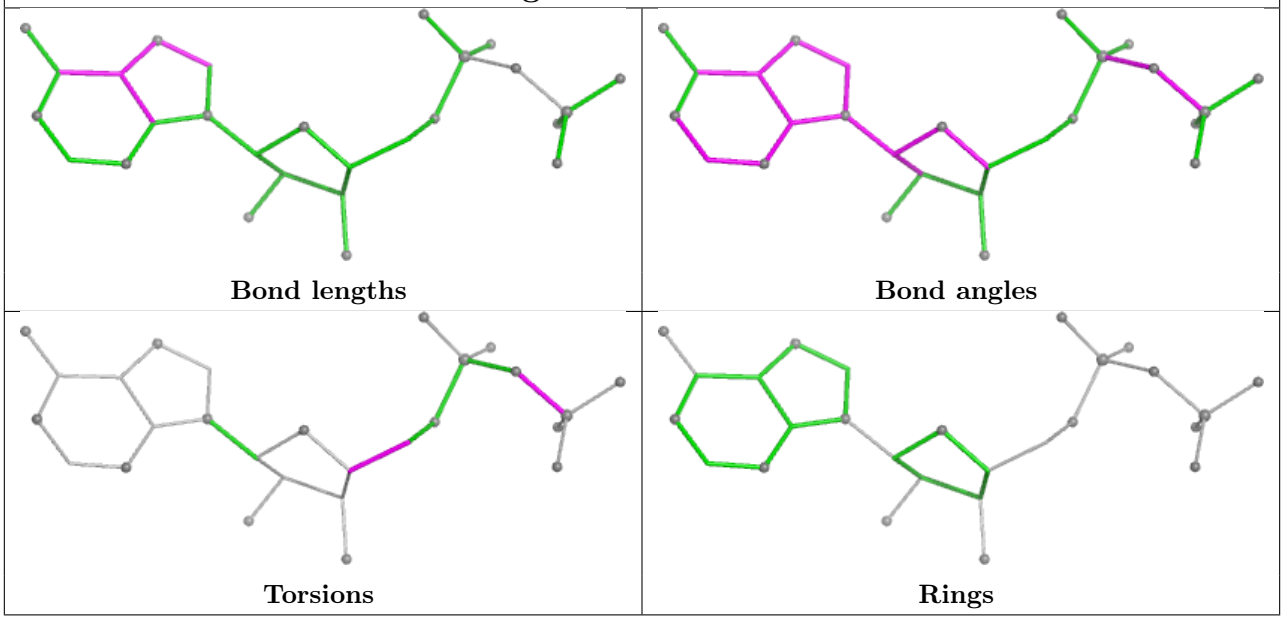
Ligand ADP D 601



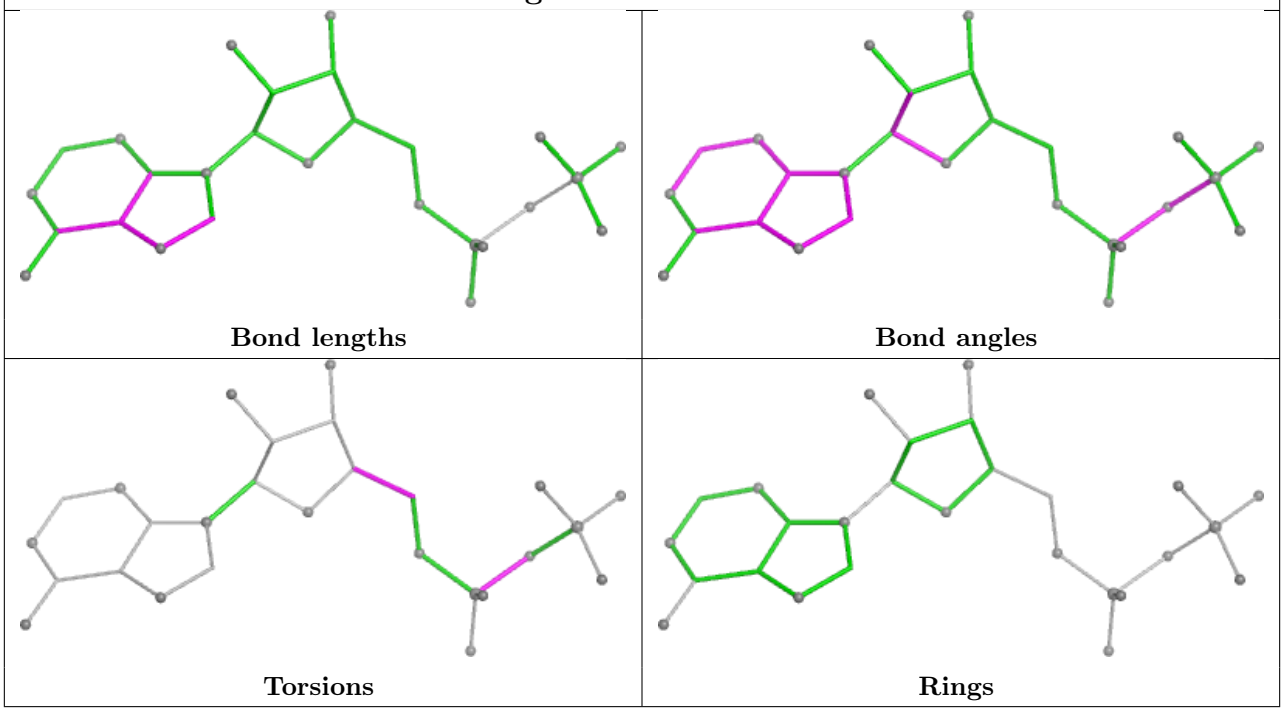
Ligand ADP E 603

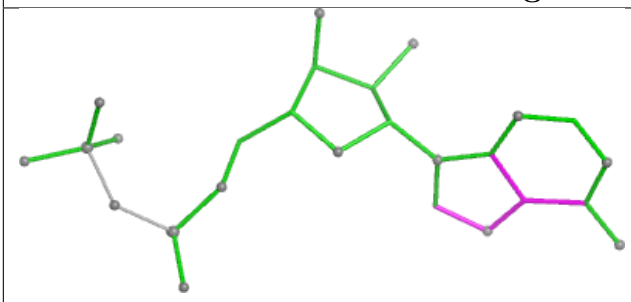
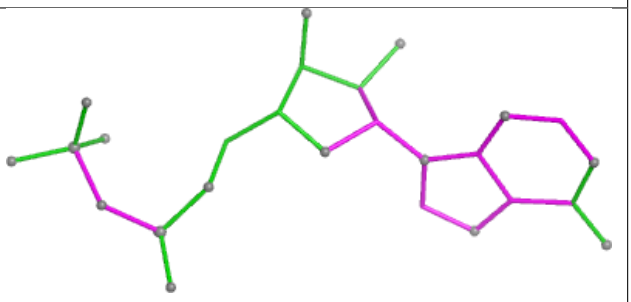
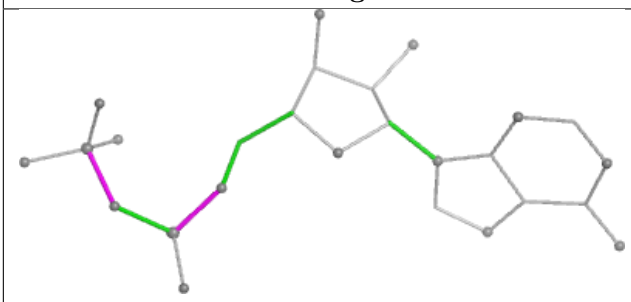
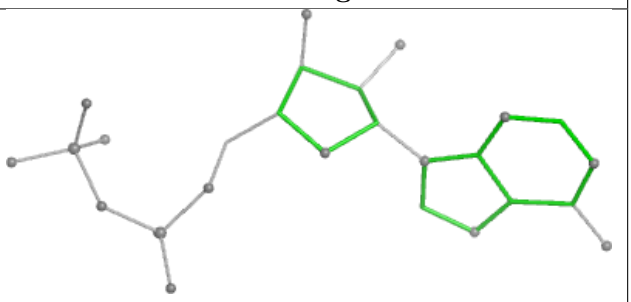


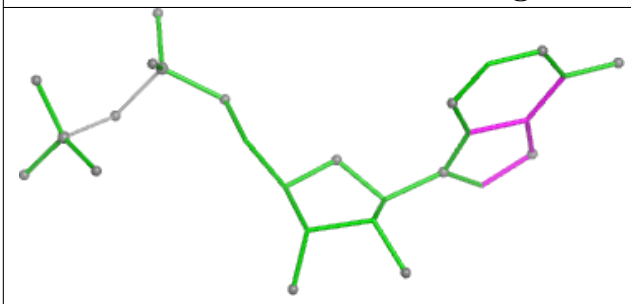
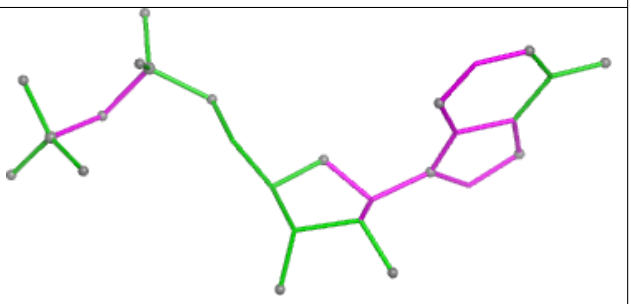
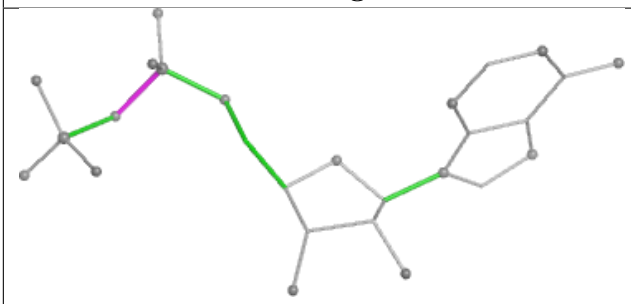
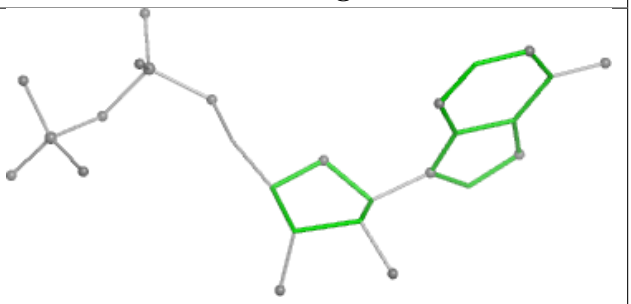
Ligand ADP A 603



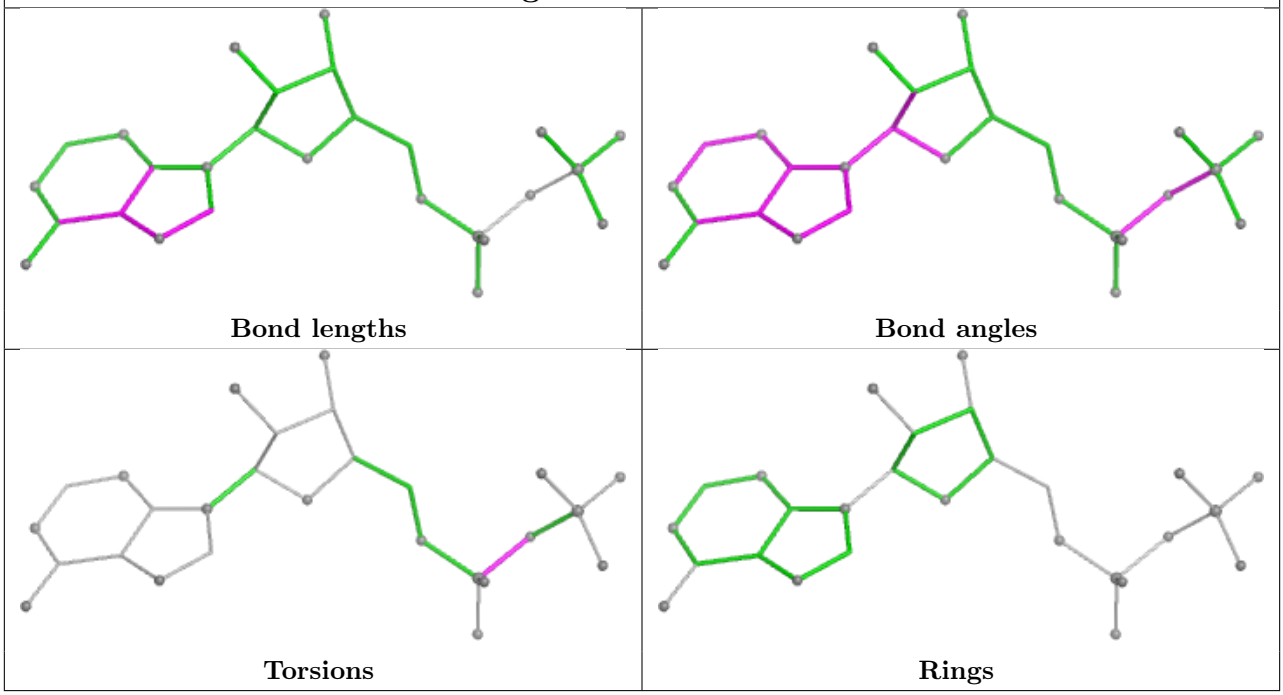
Ligand ADP L 603



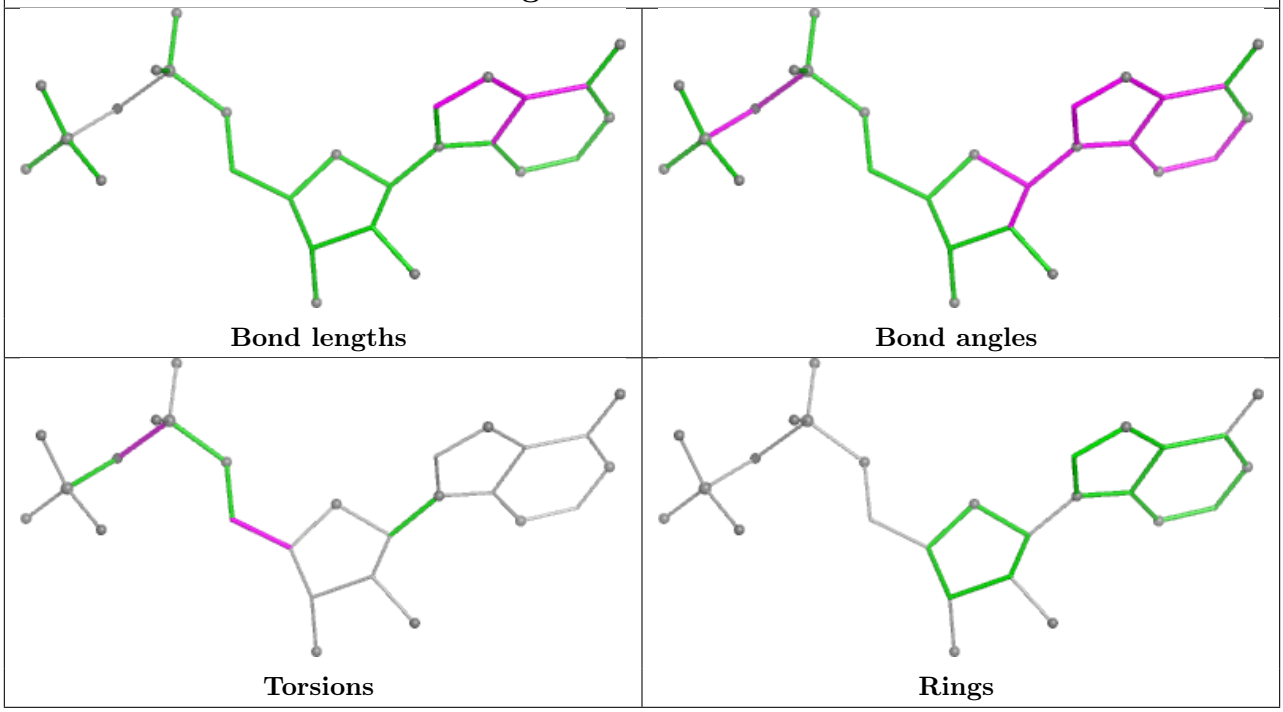
Ligand ADP F 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

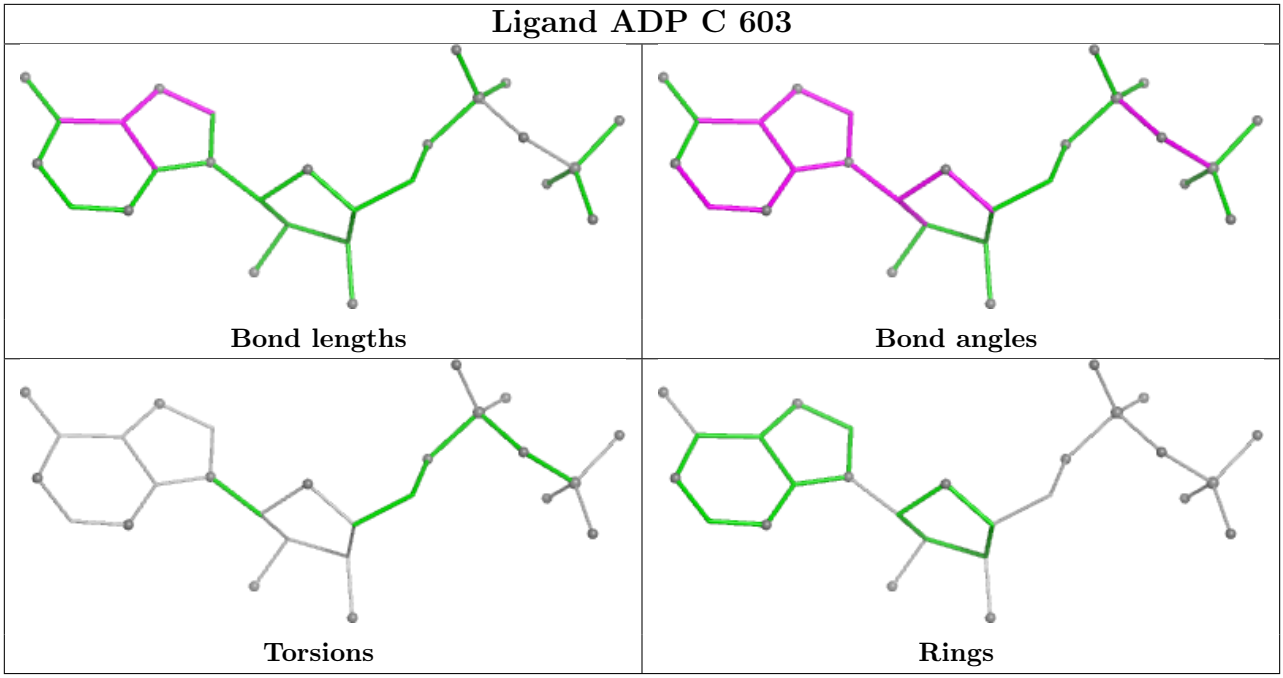
Ligand ADP H 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings

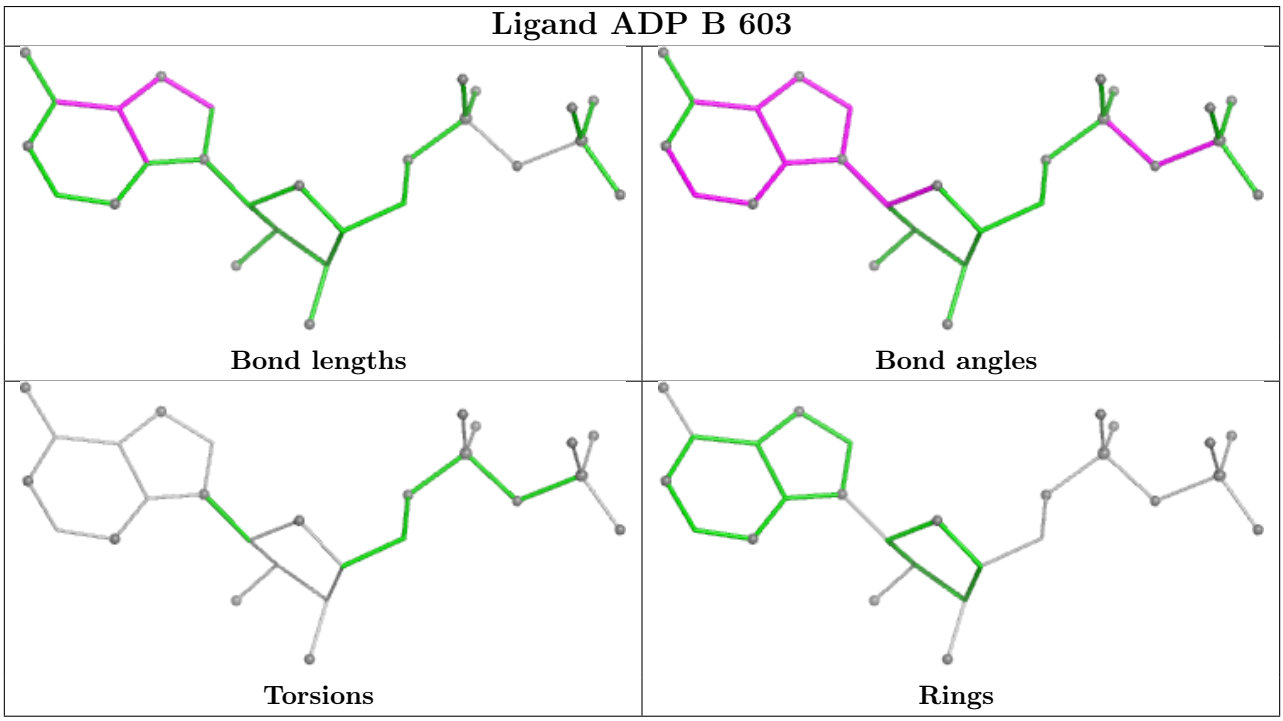
Ligand ADP K 602



Ligand ADP N 601







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

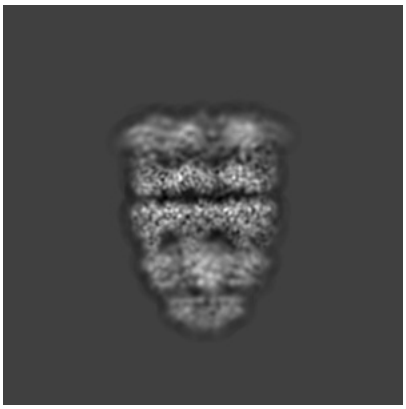
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-15944. These allow visual inspection of the internal detail of the map and identification of artifacts.

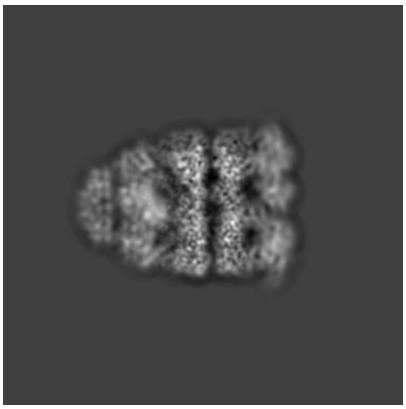
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

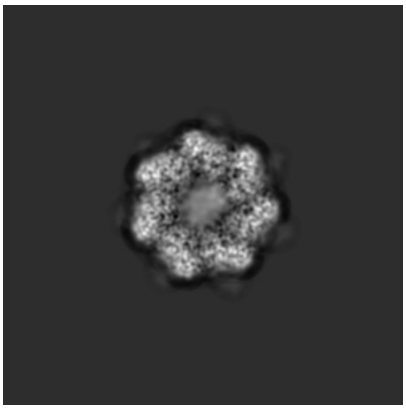
6.1.1 Primary map



X

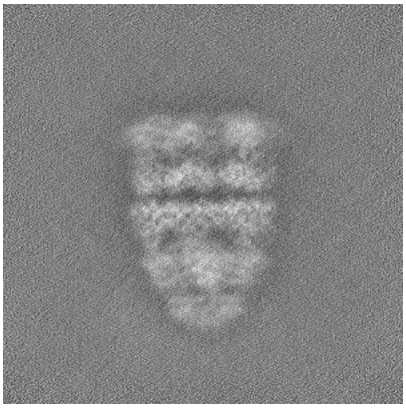


Y

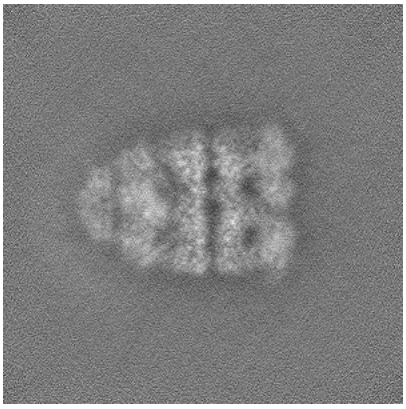


Z

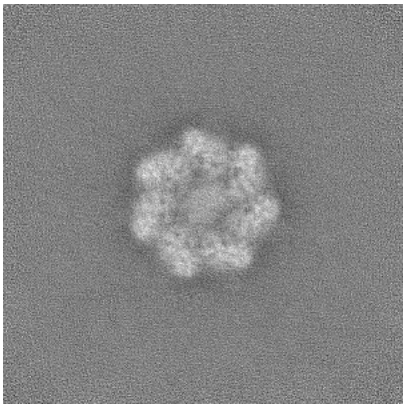
6.1.2 Raw map



X



Y



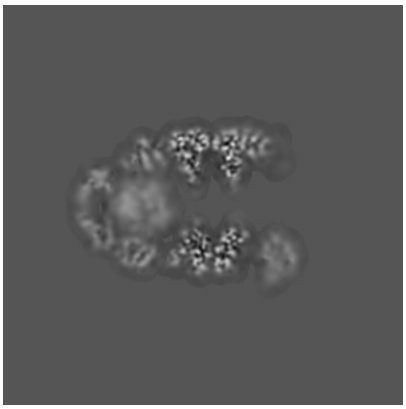
Z

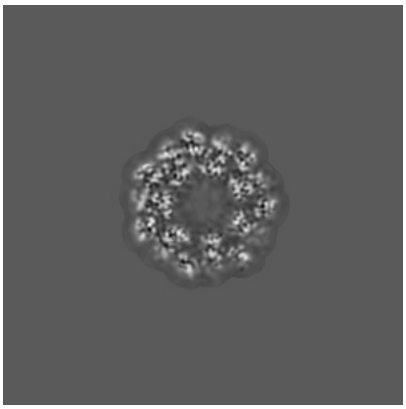
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

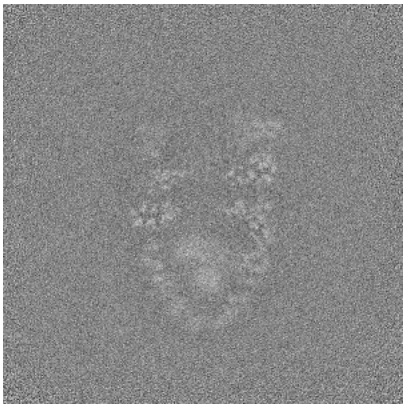
6.2.1 Primary map

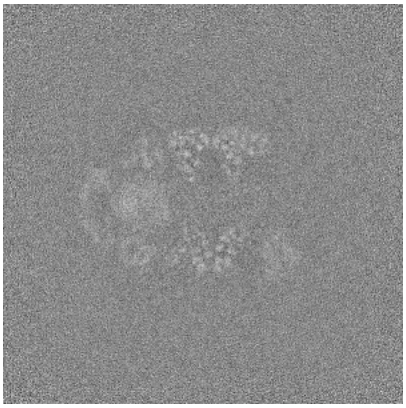
X Index: 224

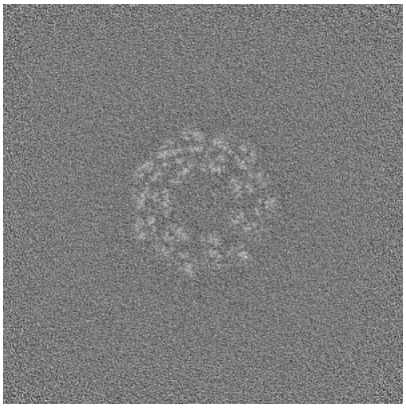

Y Index: 224


Z Index: 224

6.2.2 Raw map


X Index: 224

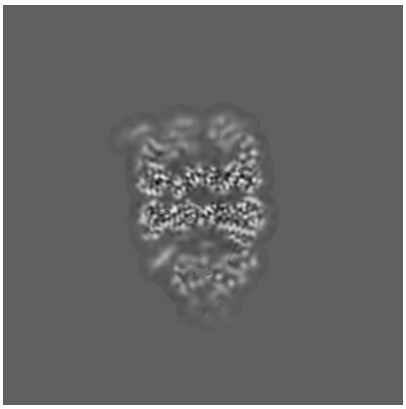

Y Index: 224


Z Index: 224

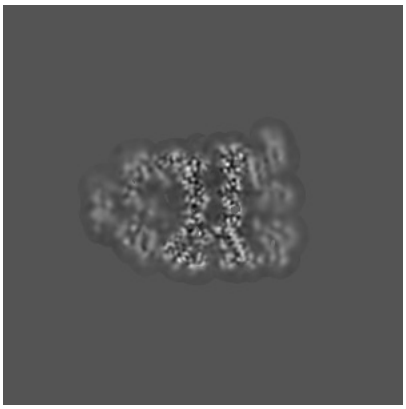
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

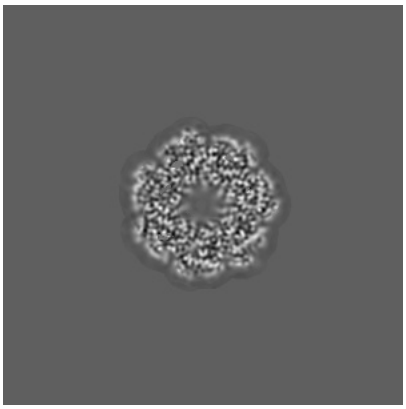
6.3.1 Primary map



X Index: 268

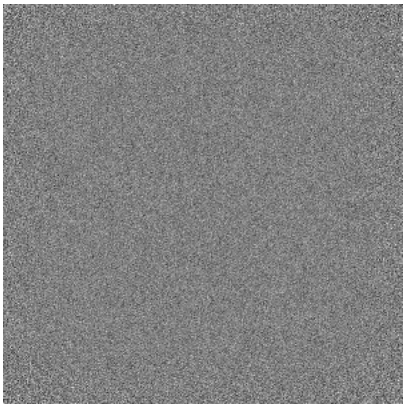


Y Index: 266

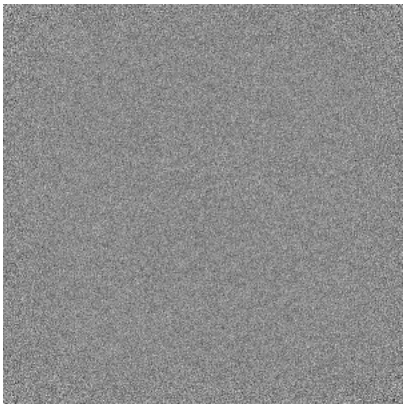


Z Index: 218

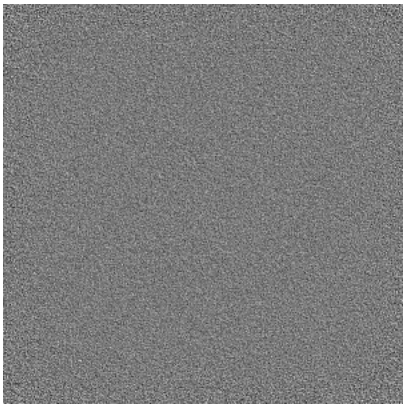
6.3.2 Raw map



X Index: 0



Y Index: 0

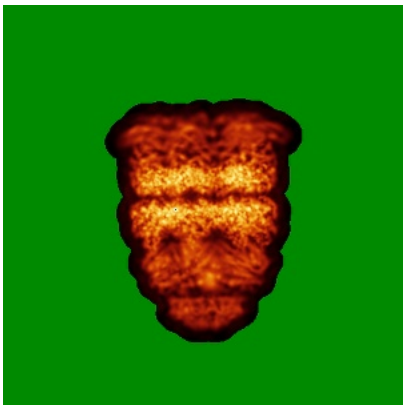


Z Index: 0

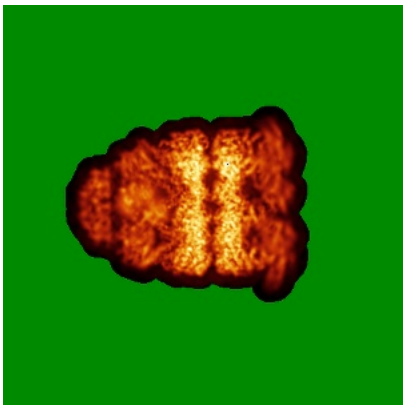
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

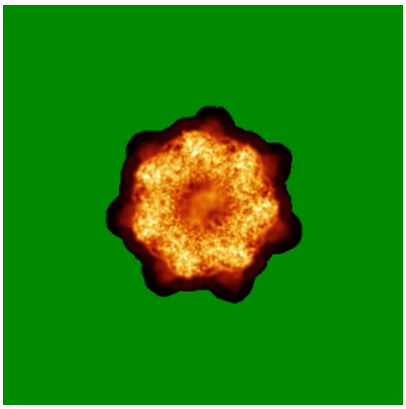
6.4.1 Primary map



X

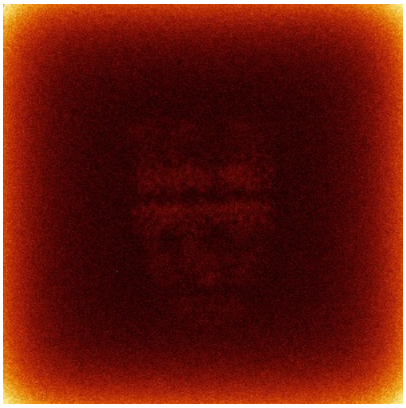


Y

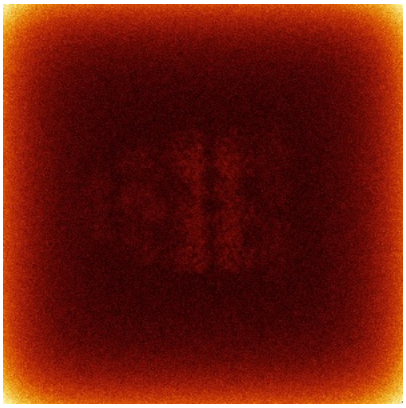


Z

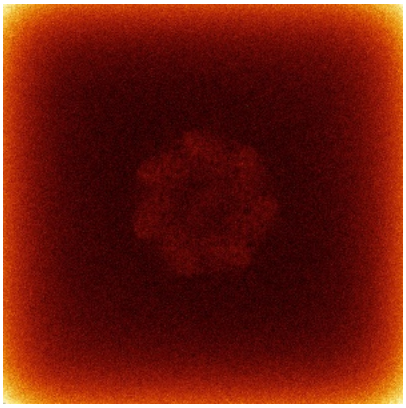
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

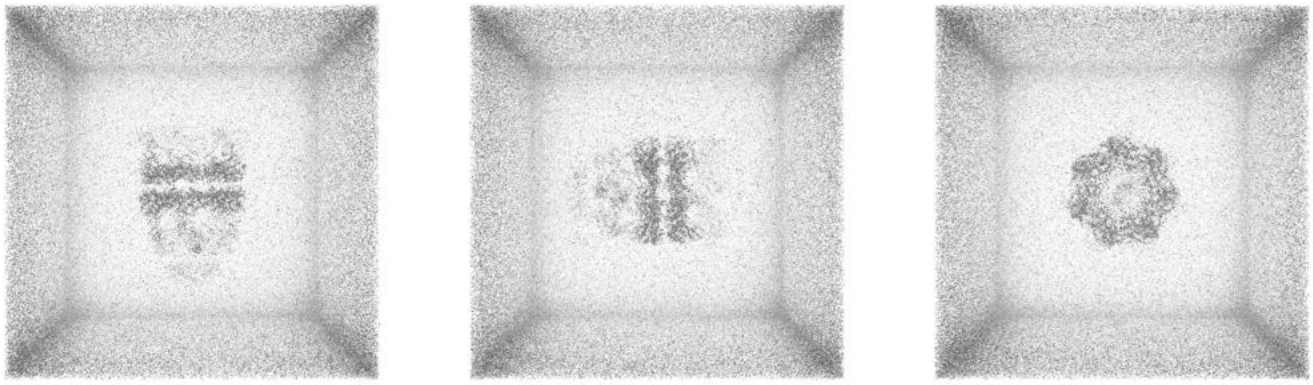
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

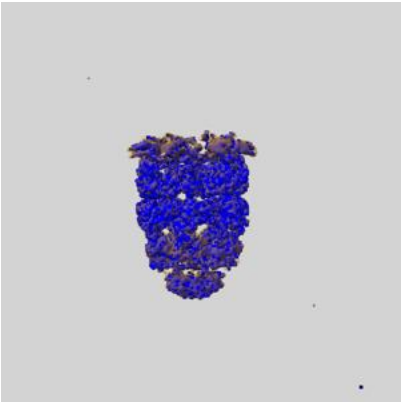
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

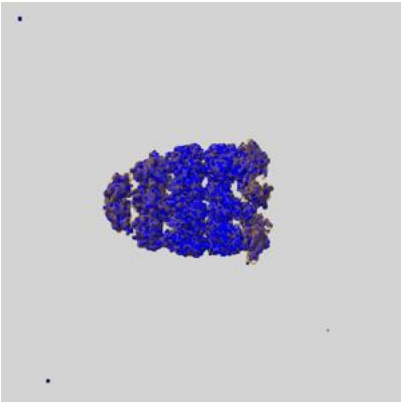
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

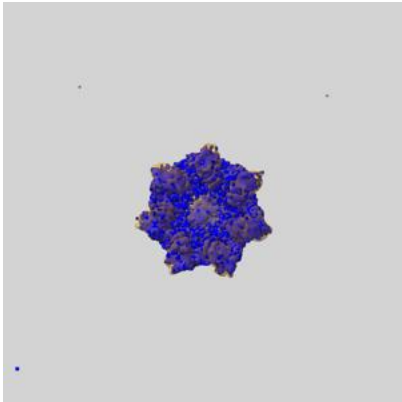
6.6.1 emd_15944_msk_1.map (i)



X



Y

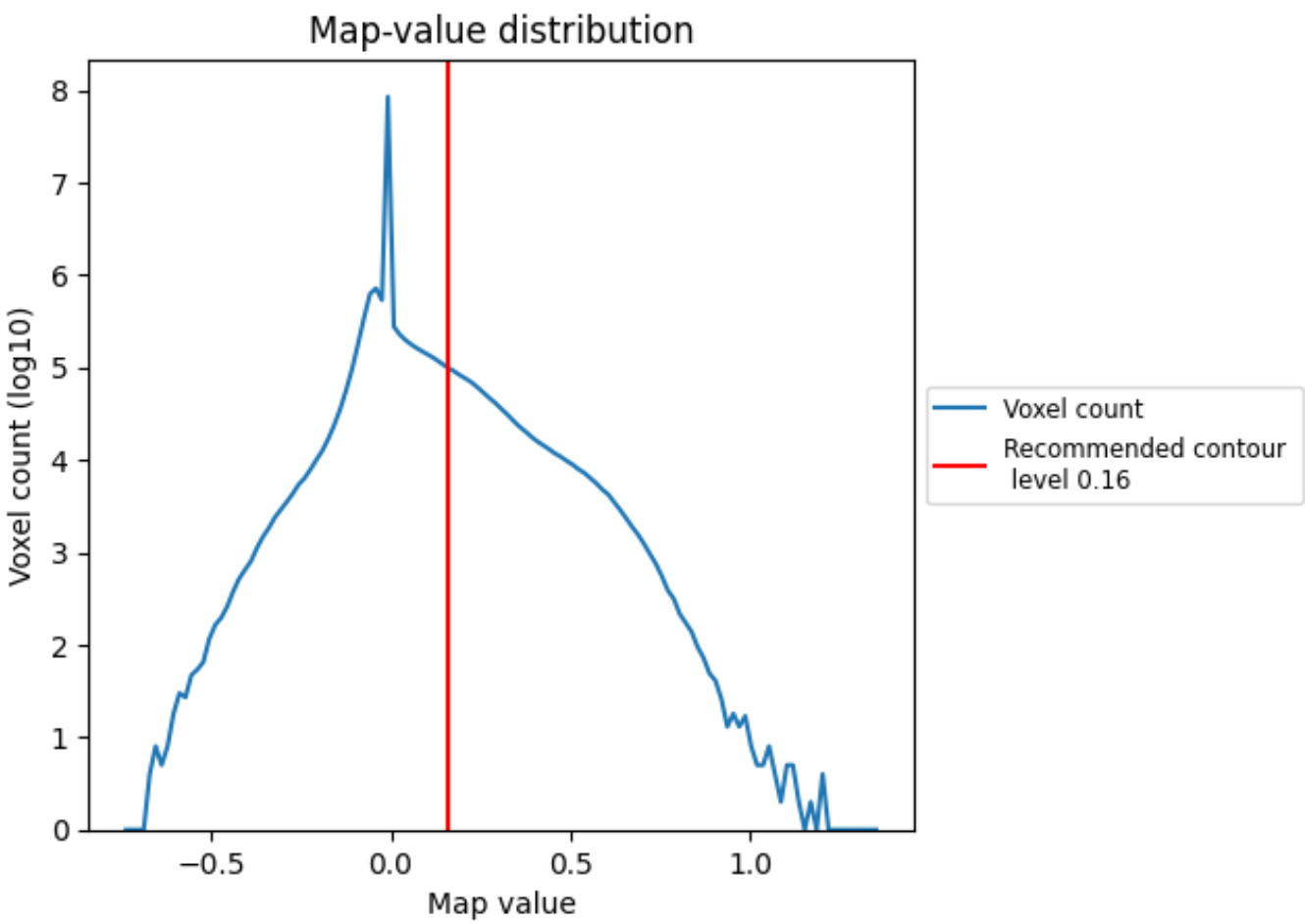


Z

7 Map analysis (i)

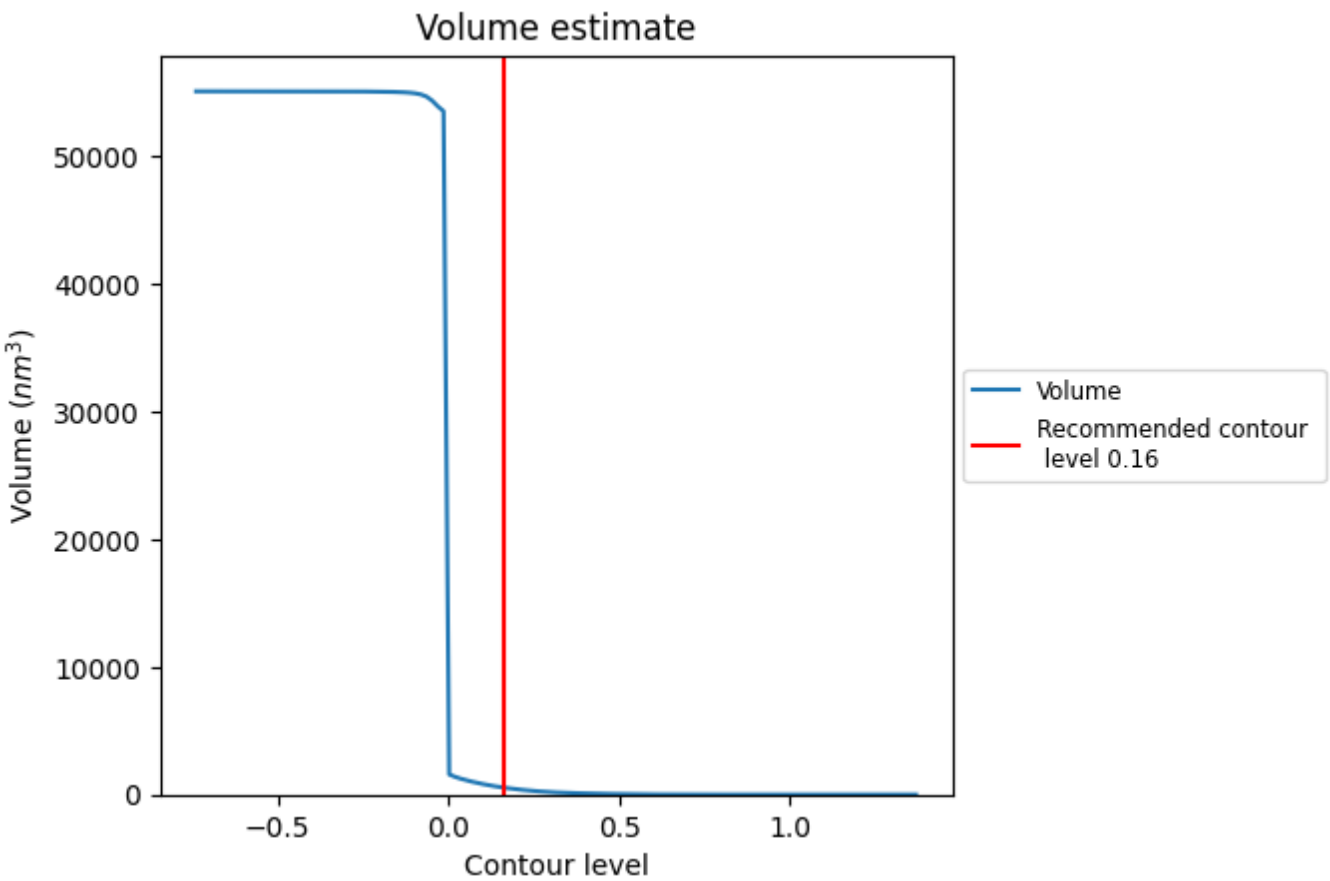
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

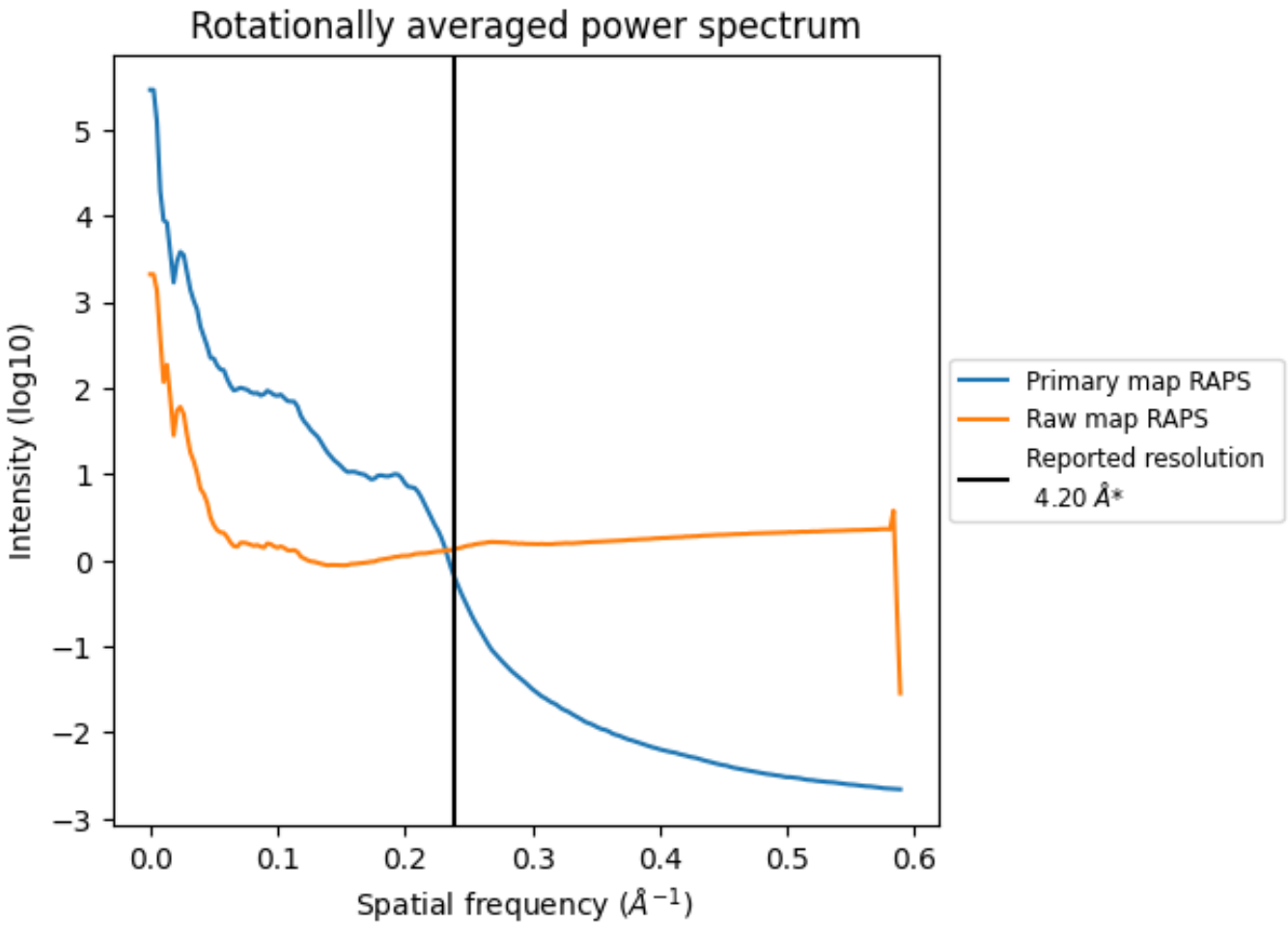
7.2 Volume estimate (i)



The volume at the recommended contour level is 555 nm^3; this corresponds to an approximate mass of 501 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

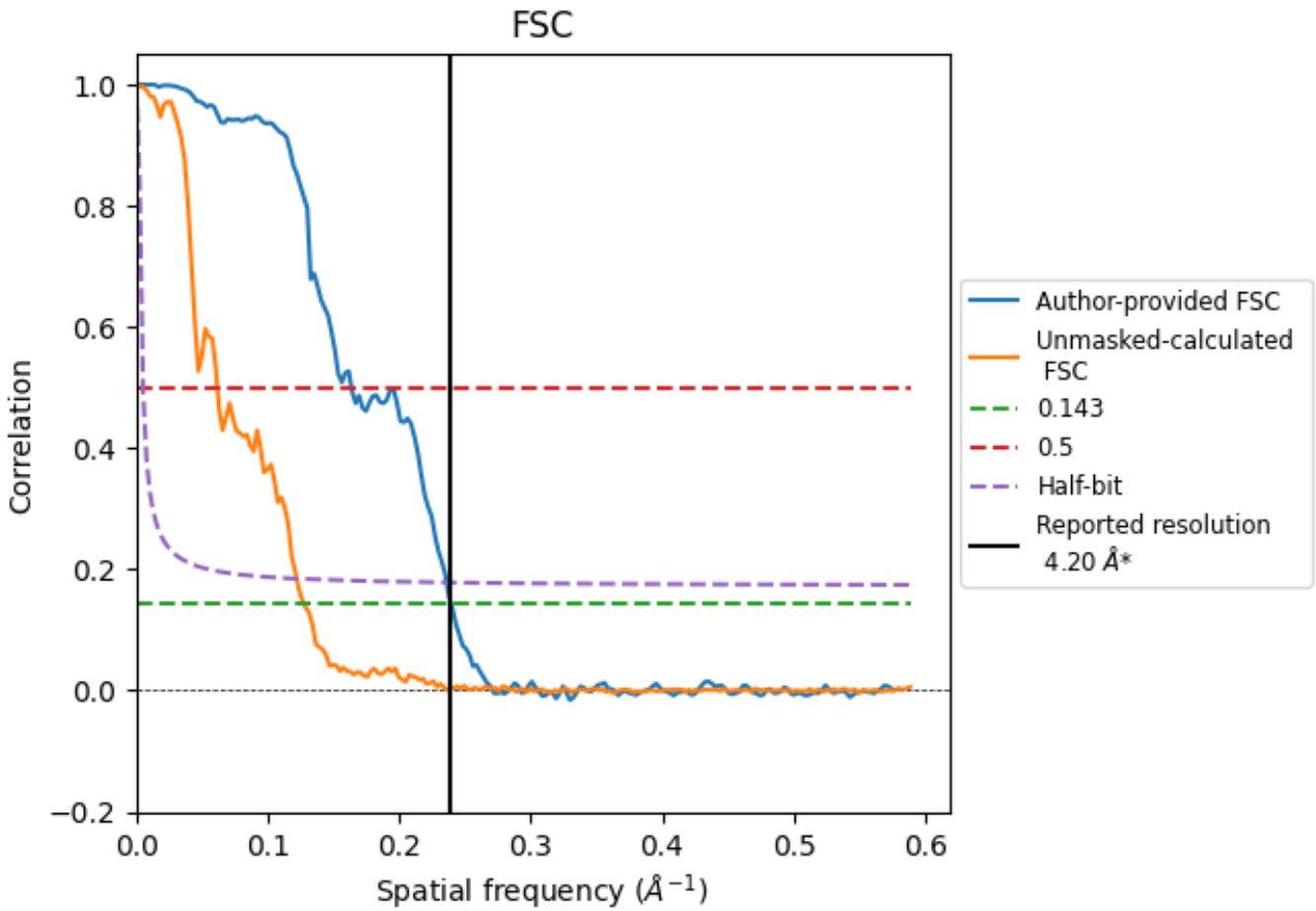


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

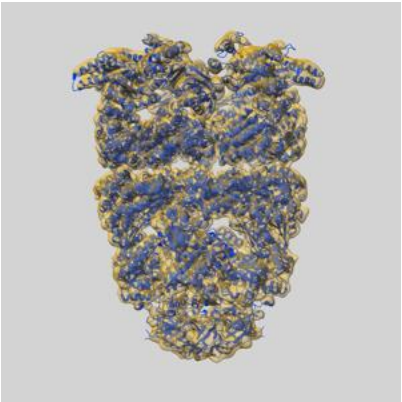
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.11	4.24
Unmasked-calculated*	7.84	16.21	8.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.84 differs from the reported value 4.2 by more than 10 %

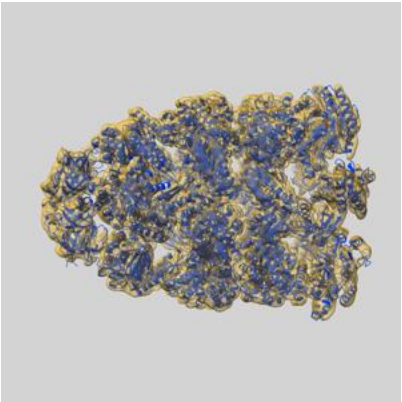
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-15944 and PDB model 8BAA. Per-residue inclusion information can be found in section 3 on page 9.

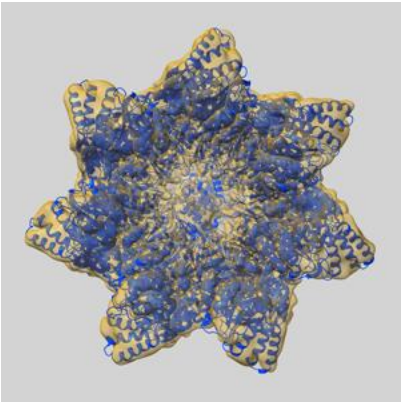
9.1 Map-model overlay (i)



X



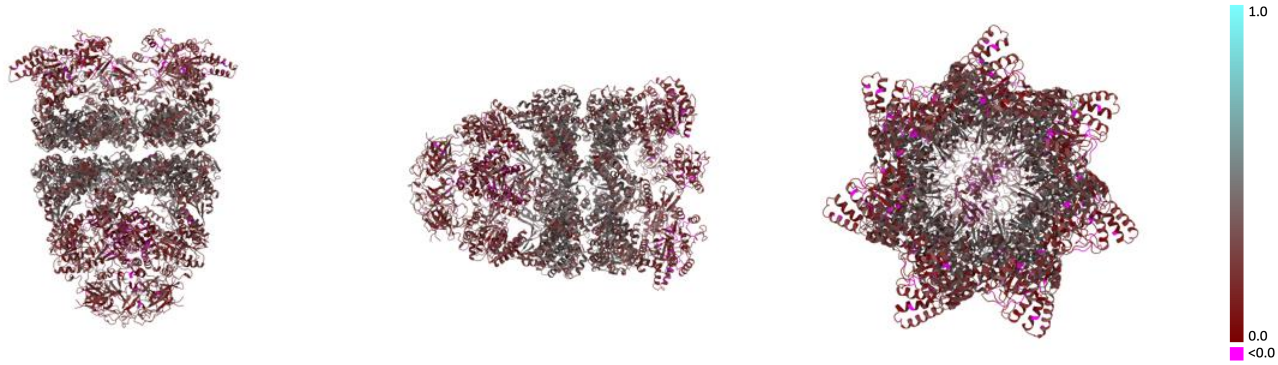
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

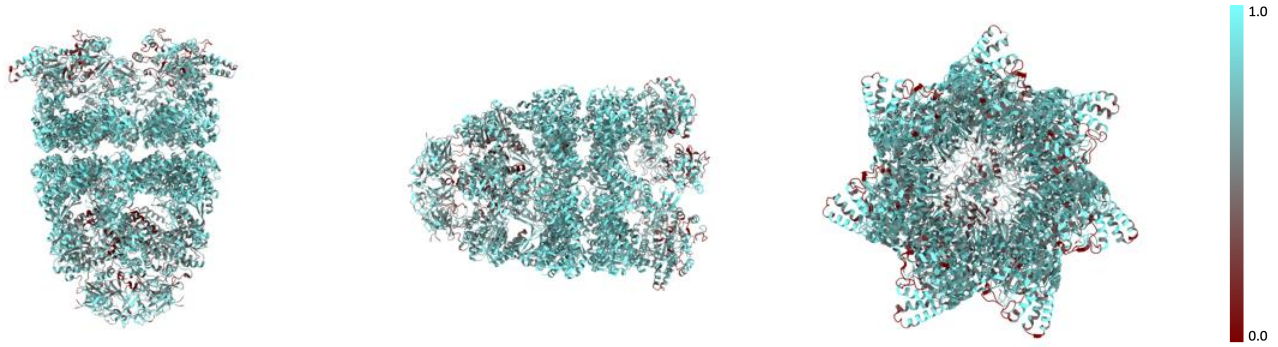
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

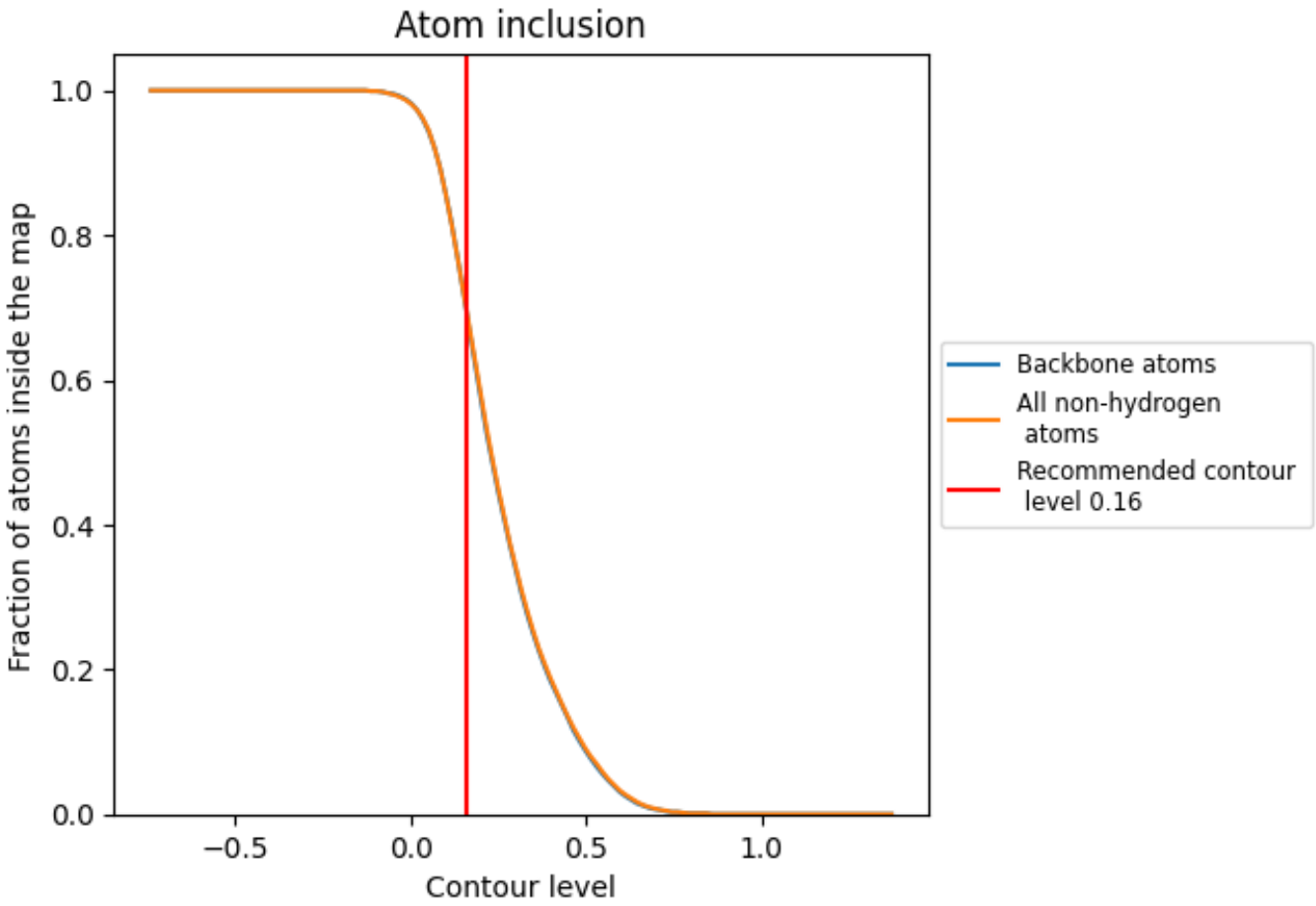
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.2730
A	0.7520	0.3160
B	0.7380	0.3120
C	0.7560	0.3180
D	0.7400	0.3140
E	0.7200	0.3050
F	0.7160	0.3030
G	0.7640	0.3160
H	0.6950	0.2700
I	0.6960	0.2680
J	0.7030	0.2720
K	0.7070	0.2680
L	0.7020	0.2760
M	0.7100	0.2740
N	0.7000	0.2730
O	0.5450	0.2060
P	0.6190	0.2320
Q	0.5480	0.2240
R	0.6040	0.2140
S	0.6550	0.2070
T	0.6690	0.2200
U	0.6040	0.2200
Z	0.5870	0.0540