



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:08 PM EDT

PDB ID : 3VR8 / pdb_00003vr8
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum*
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on : 2012-04-07
Resolution : 2.81 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

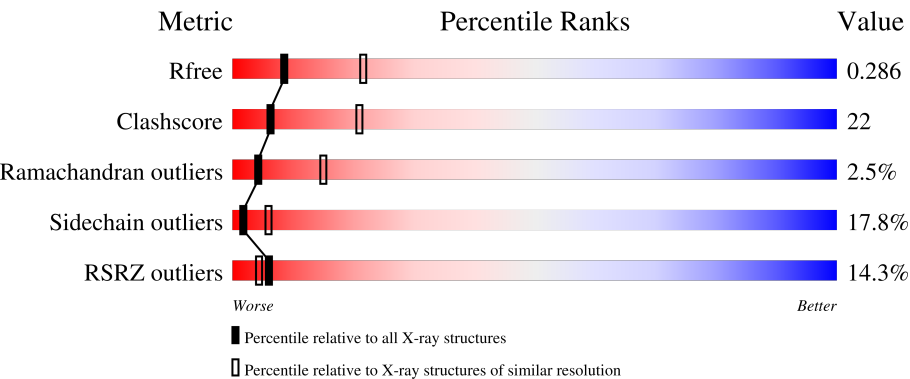
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	12% 49%38%7%5%
1	E	645	14% 46%41%8%5%
2	B	282	15% 45%33%9%12%
2	F	282	11% 42%36%9%12%

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Mol	Chain	Length	Quality of chain
3	C	188	
3	G	188	
4	D	156	
4	H	156	

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
5	MLI	A	701	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 18232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			
1	E	613	Total	C	N	O	S	0	0	0
			4758	2983	851	896	28			

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			
2	F	249	Total	C	N	O	S	0	0	0
			1973	1254	337	359	23			

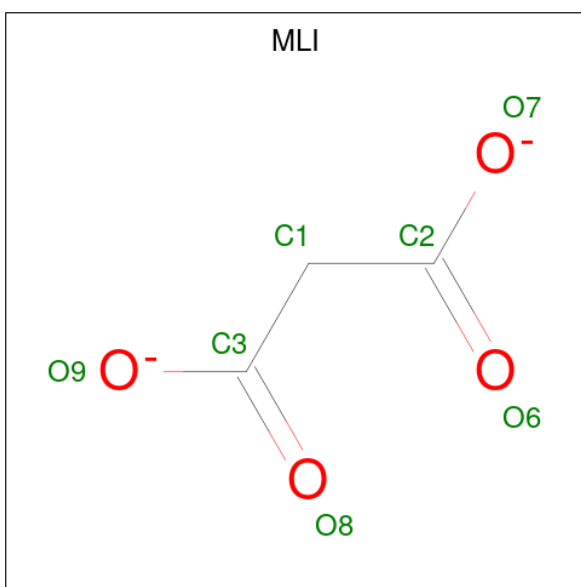
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	150	Total	C	N	O	S	0	0	0
			1195	798	201	190	6			

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

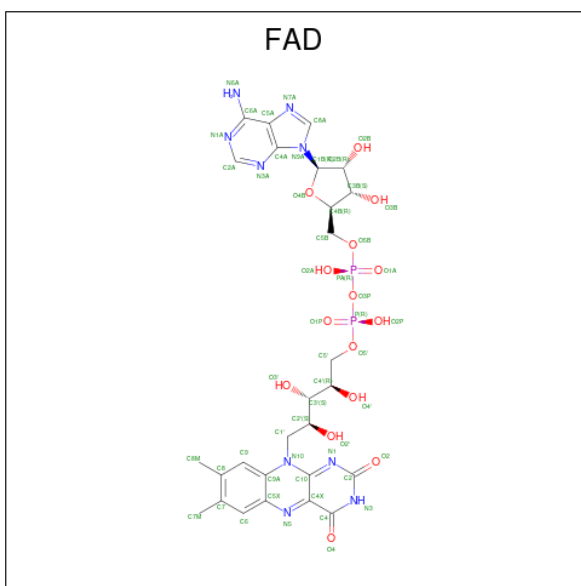
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			
4	H	129	Total	C	N	O	S	0	0	0
			994	658	165	166	5			

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



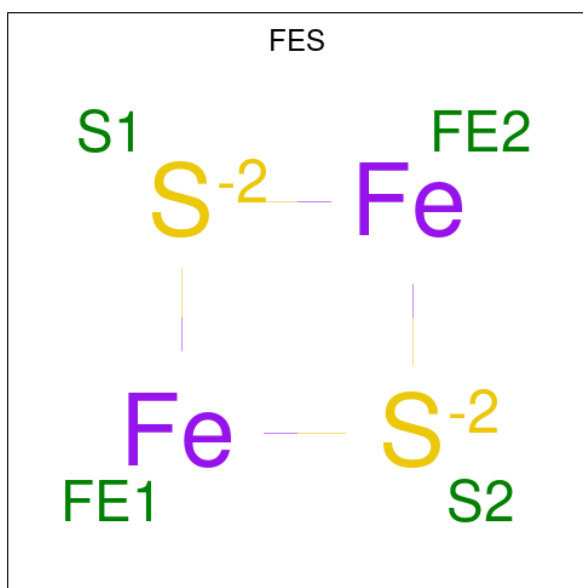
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 3 4	0	0
5	E	1	Total C O 7 3 4	0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



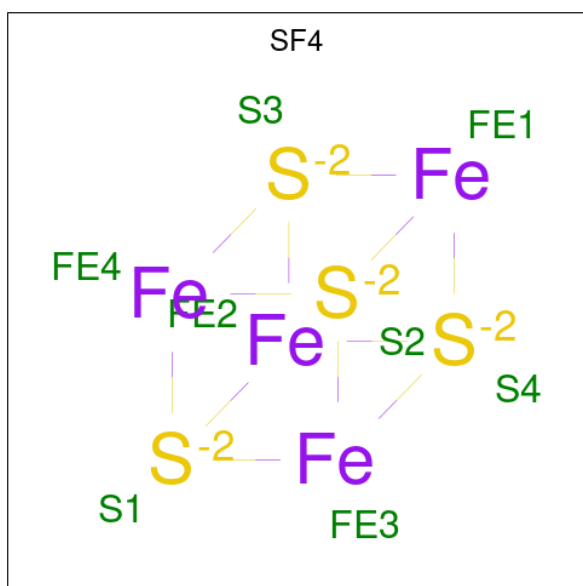
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
6	E	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



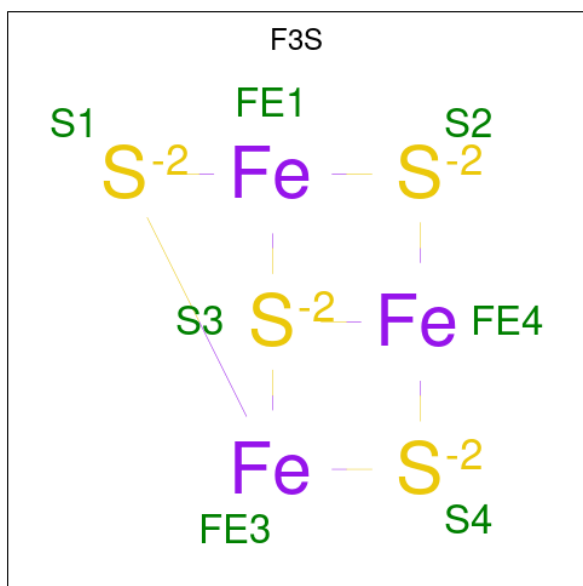
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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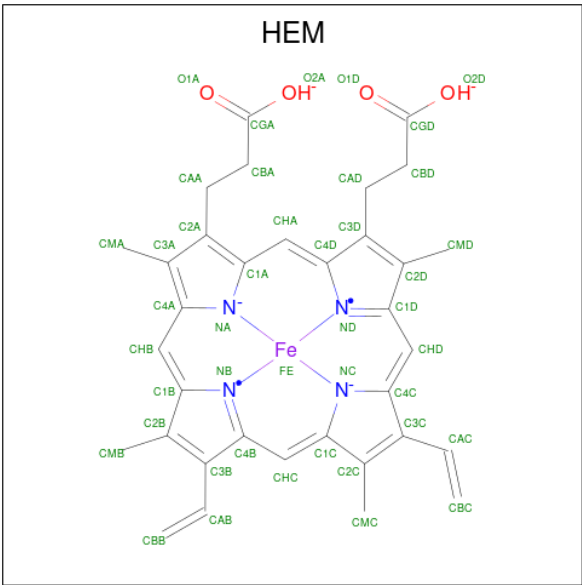
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



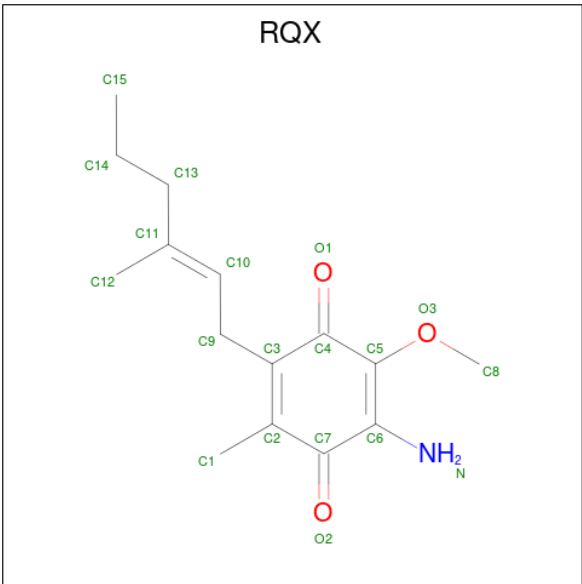
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is 2-amino-3-methoxy-6-methyl-5-[(2E)-3-methylhex-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: RQX) (formula: C₁₅H₂₁NO₃).



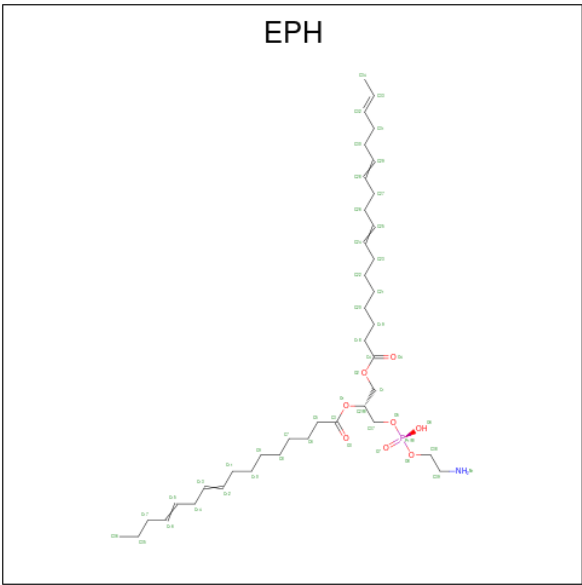
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			19	15	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	G	1	Total	C	N	O	0	0
			19	15	1	3		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).

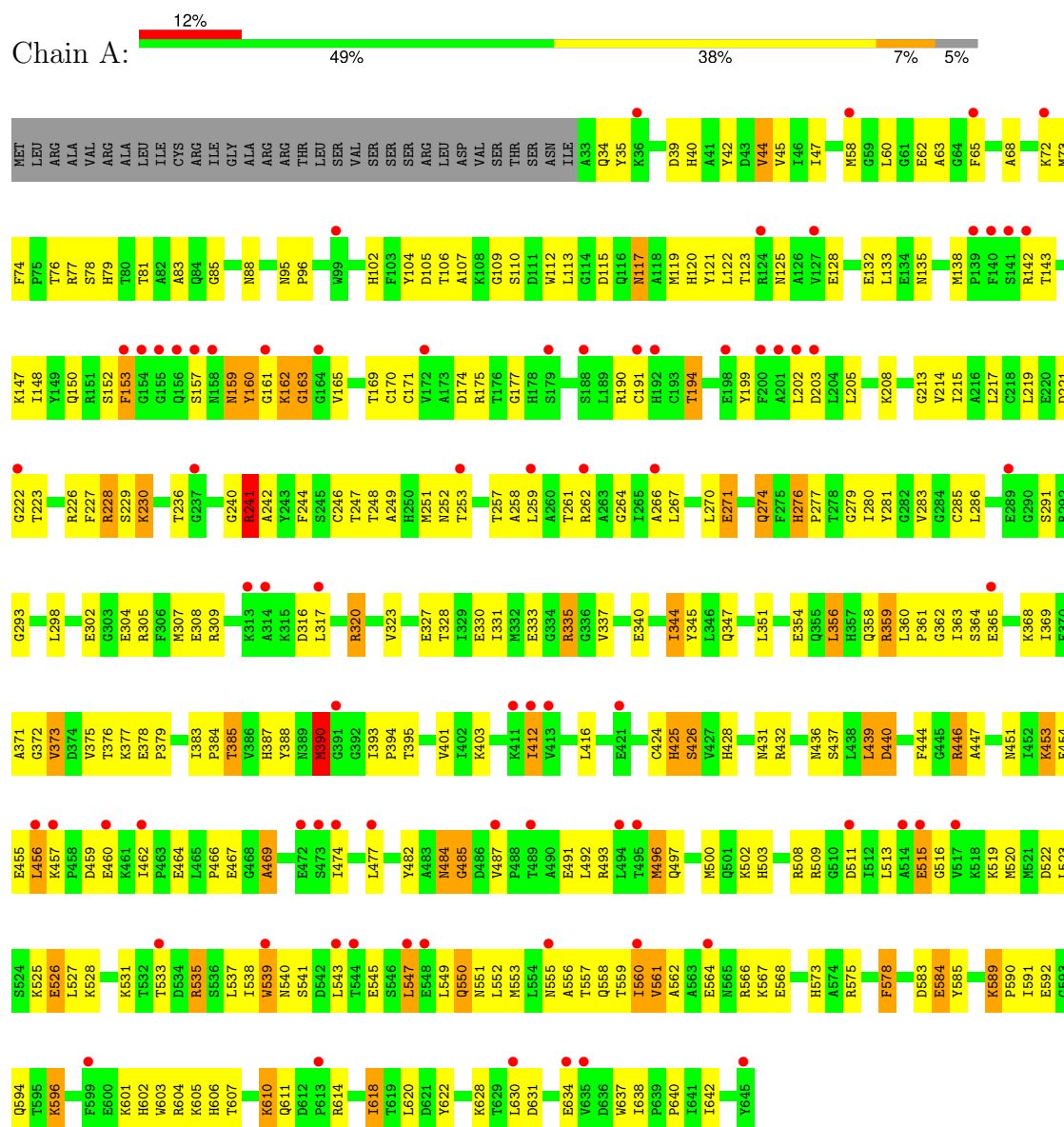


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

3 Residue-property plots

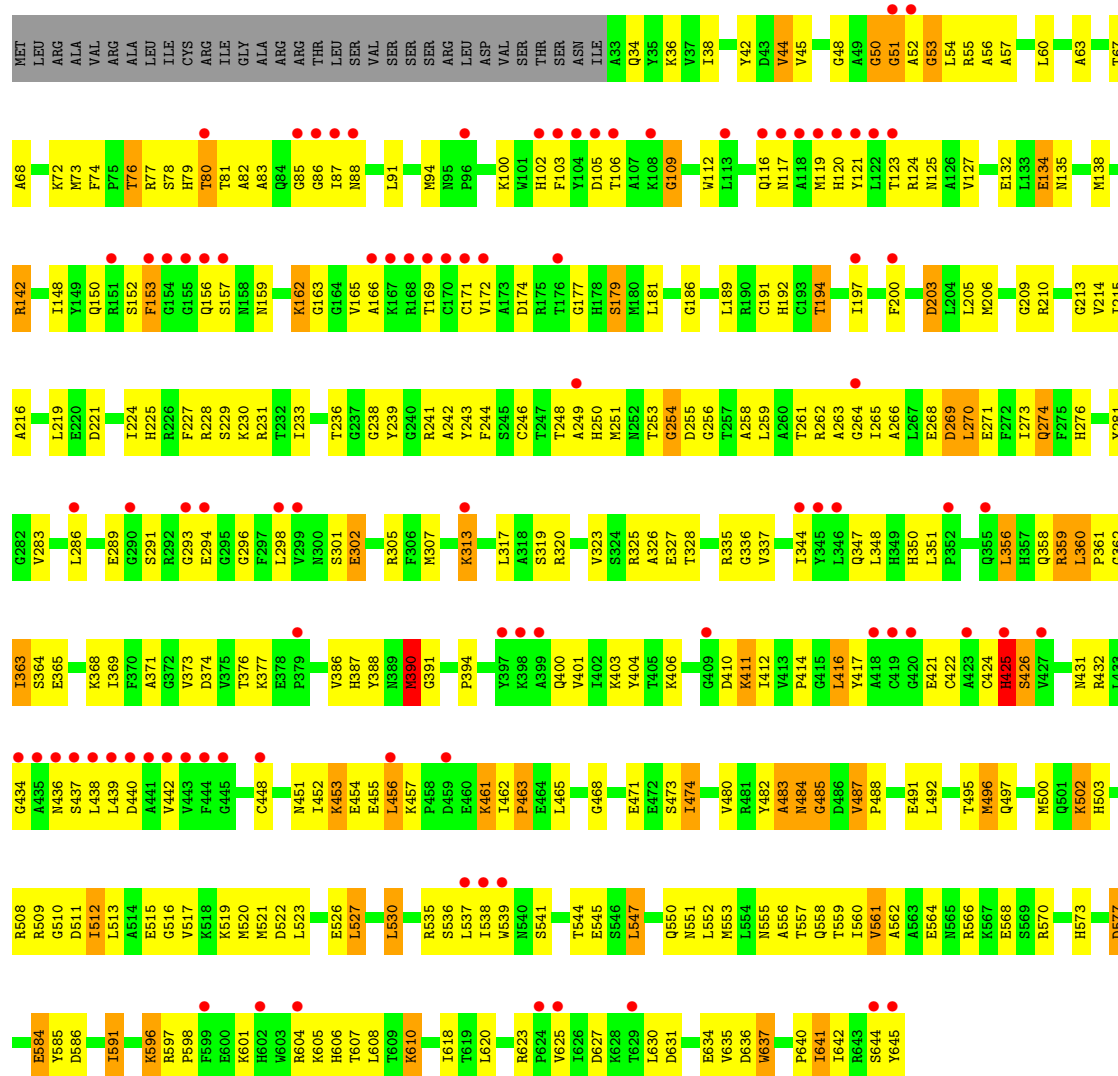
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Flavoprotein subunit of complex II

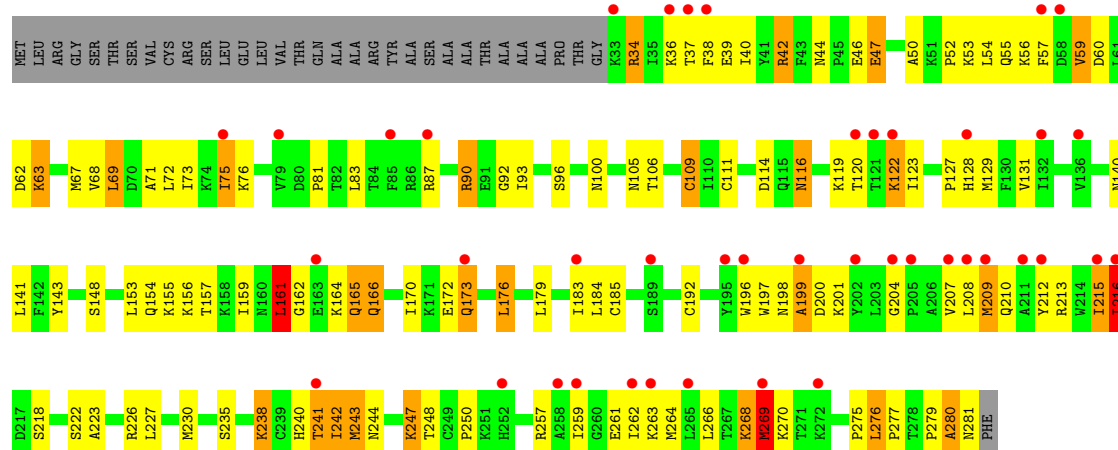


• Molecule 1: Flavoprotein subunit of complex II

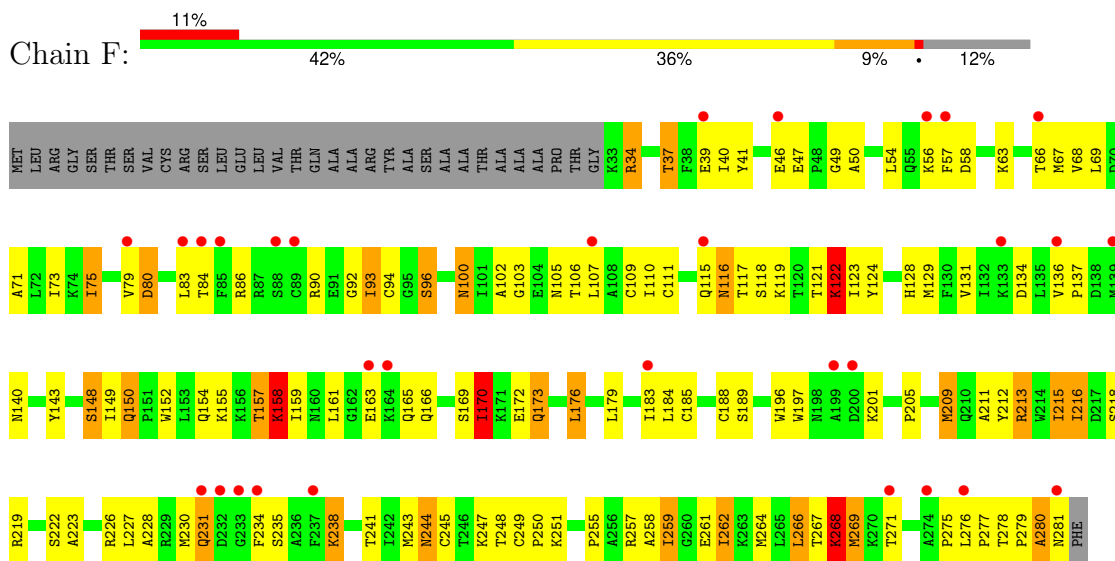




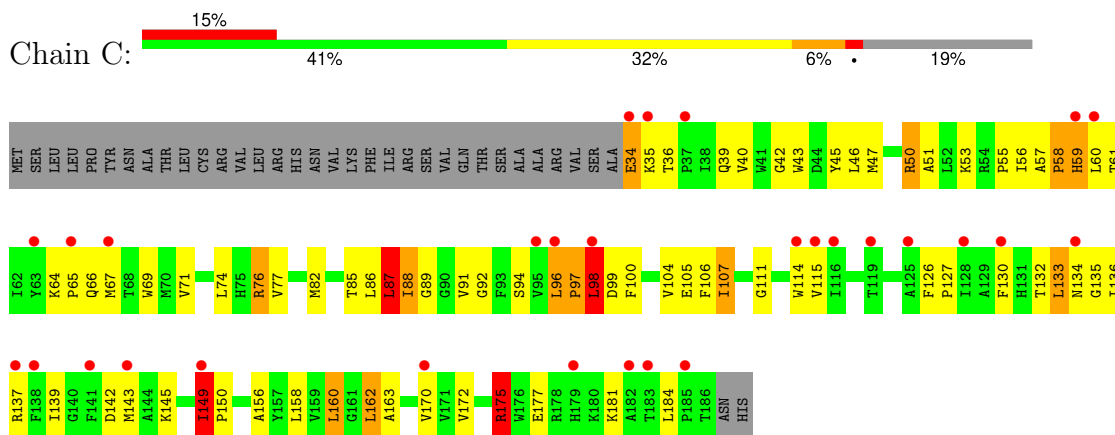
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase



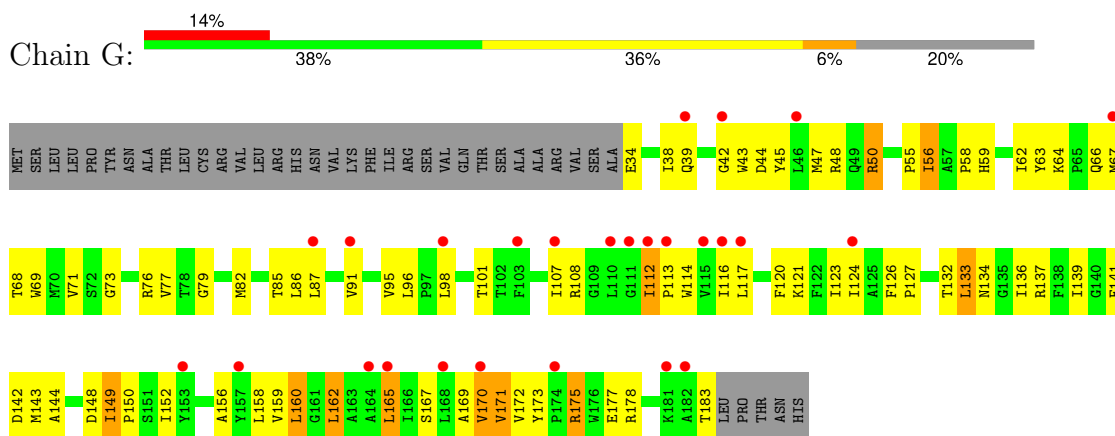
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase



- Molecule 3: Cytochrome b-large subunit

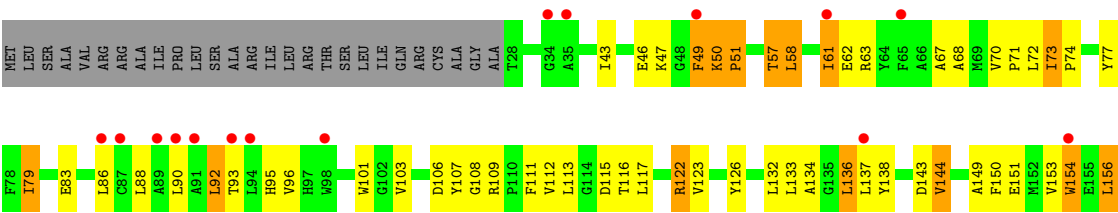


- Molecule 3: Cytochrome b-large subunit

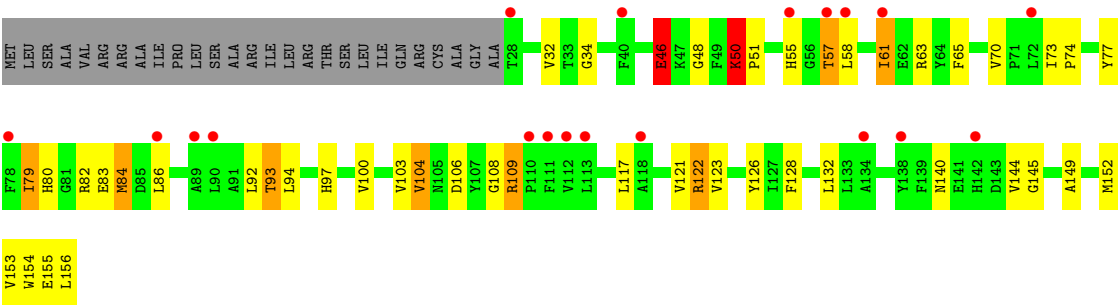


- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial





• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



V153
W154
E155
L156

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.71Å 129.09Å 221.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.81 48.56 – 2.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.56-2.81) 92.1 (48.56-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.297 0.223 , 0.286	Depositor DCC
R_{free} test set	4025 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, FAD, SF4, RQX, F3S, FES, HEM, EPH

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	0.79	1/4859 (0.0%)	1.09	12/6564 (0.2%)
1	E	0.80	1/4859 (0.0%)	1.11	17/6564 (0.3%)
2	B	0.87	0/2016	1.13	8/2723 (0.3%)
2	F	0.93	3/2016 (0.1%)	1.12	9/2723 (0.3%)
3	C	0.83	1/1255 (0.1%)	1.14	5/1709 (0.3%)
3	G	0.80	0/1232	1.01	0/1676
4	D	0.85	0/1026	1.11	2/1402 (0.1%)
4	H	0.80	0/1026	1.04	1/1402 (0.1%)
All	All	0.83	6/18289 (0.0%)	1.10	54/24763 (0.2%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	267	THR	CA-C	8.87	1.56	1.52
2	F	271	THR	CA-CB	5.72	1.60	1.53
1	A	412	ILE	CA-CB	5.67	1.59	1.54
1	E	194	THR	CA-CB	5.08	1.60	1.53
2	F	170	ILE	CA-CB	5.03	1.61	1.54
3	C	149	ILE	CA-CB	5.01	1.57	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	140	ASN	N-CA-C	8.27	121.33	111.33
2	F	269	MET	N-CA-C	7.66	120.46	110.43
1	A	373	VAL	N-CA-C	7.49	119.37	108.58
1	E	142	ARG	N-CA-C	7.49	121.80	109.06
1	A	425	HIS	N-CA-C	-7.29	104.36	113.18
1	E	238	GLY	N-CA-C	6.95	123.31	111.98
1	A	550	GLN	N-CA-C	-6.88	103.71	111.14
1	E	289	GLU	N-CA-C	-6.84	104.20	112.54
2	F	140	ASN	N-CA-C	6.60	119.47	111.82
1	E	268	GLU	N-CA-C	6.56	119.68	109.52
1	A	171	CYS	N-CA-C	6.54	119.14	108.55
3	C	40	VAL	N-CA-C	-6.13	105.16	110.74
1	A	276	HIS	CA-C-N	6.13	126.31	119.32
1	A	276	HIS	C-N-CA	6.13	126.31	119.32
3	C	106	PHE	N-CA-C	-6.12	105.91	113.19
1	A	248	THR	N-CA-C	6.11	118.22	110.33
2	B	204	GLY	CA-C-N	6.01	125.22	118.97
2	B	204	GLY	C-N-CA	6.01	125.22	118.97
2	B	207	VAL	N-CA-C	5.99	116.73	110.62
4	H	32	VAL	N-CA-C	5.88	118.23	109.17
2	F	122	LYS	N-CA-C	5.85	118.05	108.52
2	F	235	SER	N-CA-C	5.79	118.34	111.33
3	C	175	ARG	N-CA-C	-5.79	106.25	113.38
4	D	115	ASP	N-CA-C	5.76	118.30	111.33
2	B	270	LYS	N-CA-C	5.71	118.87	109.85
1	E	631	ASP	CA-C-N	5.70	126.97	119.84
1	E	631	ASP	C-N-CA	5.70	126.97	119.84
1	E	390	MET	N-CA-CB	5.67	118.95	110.22
2	F	96	SER	N-CA-C	5.63	117.50	111.36
1	E	425	HIS	N-CA-C	-5.62	106.28	113.02
1	A	578	PHE	CA-C-N	5.54	125.21	119.56
1	A	578	PHE	C-N-CA	5.54	125.21	119.56
1	A	390	MET	N-CA-CB	5.50	118.30	110.16
2	B	242	ILE	N-CA-C	5.50	116.13	110.36
1	E	191	CYS	N-CA-C	5.49	119.15	111.30
2	F	79	VAL	N-CA-C	5.45	117.91	111.09
1	E	248	THR	N-CA-C	5.43	116.93	110.19
1	A	142	ARG	N-CA-C	5.43	118.25	109.40
2	F	262	ILE	CB-CA-C	-5.40	104.95	112.02
1	E	487	VAL	N-CA-C	5.35	112.85	107.55
2	F	80	ASP	CA-C-N	-5.31	114.55	120.45
2	F	80	ASP	C-N-CA	-5.31	114.55	120.45
1	E	391	GLY	N-CA-C	5.30	118.16	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	216	ILE	N-CA-C	5.30	118.07	112.83
1	E	171	CYS	N-CA-C	5.28	116.55	108.52
4	D	73	ILE	N-CA-CB	5.27	114.56	110.45
1	E	416	LEU	N-CA-C	5.27	116.99	108.34
2	B	269	MET	N-CA-C	5.21	117.25	110.43
1	E	281	TYR	N-CA-C	5.15	116.70	111.14
1	A	560	ILE	N-CA-C	5.13	116.47	110.62
1	E	134	GLU	N-CA-C	-5.06	105.76	111.28
1	E	50	GLY	N-CA-C	-5.01	103.92	112.64
3	C	36	THR	CA-C-N	-5.00	113.50	119.05
3	C	36	THR	C-N-CA	-5.00	113.50	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	425	HIS	Peptide

5.2 Too-close contacts ⓘ

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	4758	0	4692	210	0
1	E	4758	0	4692	220	0
2	B	1973	0	1993	96	0
2	F	1973	0	1992	108	0
3	C	1217	0	1265	59	0
3	G	1195	0	1240	76	0
4	D	994	0	977	46	0
4	H	994	0	977	38	0
5	A	7	0	2	2	0
5	E	7	0	2	0	0
6	A	53	0	31	7	0
6	E	53	0	31	10	0
7	B	4	0	0	1	0
7	F	4	0	0	0	0
8	B	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	8	0	0	0	0
9	B	7	0	0	1	0
9	F	7	0	0	0	0
10	C	43	0	30	17	0
10	G	43	0	30	9	0
11	C	19	0	21	8	0
11	G	19	0	21	7	0
12	D	44	0	53	6	0
12	H	44	0	53	8	0
All	All	18232	0	18102	803	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 22.

All (803) 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:E:79:HIS:NE2	6:E:702:FAD:HM81	1.16	1.41
1:A:79:HIS:NE2	6:A:702:FAD:C8M	1.84	1.38
1:E:79:HIS:NE2	6:E:702:FAD:C8M	1.84	1.37
1:A:79:HIS:NE2	6:A:702:FAD:HM82	0.90	1.21
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.07	1.18
2:F:34:ARG:HG2	2:F:34:ARG:HH21	1.14	1.12
3:C:149:ILE:HD13	3:C:149:ILE:H	1.05	1.09
2:F:268:LYS:HG2	2:F:269:MET:H	0.91	1.08
3:G:149:ILE:HD13	3:G:149:ILE:H	1.08	1.07
1:A:79:HIS:CD2	6:A:702:FAD:HM82	1.90	1.05
10:C:201:HEM:HHC	10:C:201:HEM:HBB2	1.40	1.03
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.40	1.03
2:F:268:LYS:HG2	2:F:269:MET:N	1.72	1.03
4:H:109:ARG:HG2	4:H:109:ARG:HH21	1.24	1.02
3:C:149:ILE:H	3:C:149:ILE:CD1	1.75	1.00
2:F:268:LYS:CG	2:F:269:MET:H	1.75	0.99
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.44	0.99
1:E:79:HIS:CD2	6:E:702:FAD:HM83	2.01	0.95
1:A:117:ASN:H	1:A:117:ASN:HD22	1.03	0.94
3:C:34:GLU:OE2	3:C:34:GLU:HA	1.65	0.94
3:G:76:ARG:HG2	10:G:201:HEM:O2D	1.69	0.93
4:D:50:LYS:N	4:D:51:PRO:HD2	1.83	0.92
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.54	0.91
1:A:280:ILE:HD12	1:A:285:CYS:HB2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:SER:HB2	2:F:46:GLU:OE1	1.70	0.90
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.05	0.89
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.07	0.89
1:A:120:HIS:HD2	1:A:630:LEU:H	1.19	0.89
3:C:133:LEU:O	3:C:136:ILE:HG13	1.73	0.89
4:D:151:GLU:HG2	12:D:201:EPH:O7	1.74	0.88
1:E:390:MET:HE3	1:E:431:ASN:HA	1.54	0.88
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.56	0.88
1:A:117:ASN:HD22	1:A:117:ASN:N	1.71	0.88
2:B:192:CYS:HG	9:B:303:F3S:FE4	0.85	0.88
1:E:480:VAL:CG2	1:E:550:GLN:HE22	1.87	0.87
3:G:149:ILE:H	3:G:149:ILE:CD1	1.83	0.87
1:A:120:HIS:CD2	1:A:630:LEU:HB2	2.10	0.87
3:G:132:THR:HG23	10:G:201:HEM:CAB	2.06	0.85
1:E:496:MET:HB2	1:E:520:MET:HE1	1.58	0.85
3:G:132:THR:HG23	10:G:201:HEM:HAB	1.56	0.85
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.20	0.85
2:F:37:THR:HB	2:F:58:ASP:OD2	1.76	0.85
3:C:114:TRP:HB2	3:C:175:ARG:HH11	1.42	0.85
1:E:78:SER:O	1:E:81:THR:HG22	1.77	0.84
1:E:480:VAL:HG21	1:E:550:GLN:NE2	1.93	0.84
1:E:541:SER:O	1:E:545:GLU:HG3	1.76	0.84
3:C:149:ILE:HD13	3:C:149:ILE:N	1.90	0.84
2:B:116:ASN:C	2:B:116:ASN:HD22	1.86	0.83
10:C:201:HEM:HBA1	10:C:201:HEM:HHA	1.60	0.83
4:H:50:LYS:H	4:H:51:PRO:HD3	1.43	0.83
1:A:509:ARG:HD2	1:A:511:ASP:OD2	1.79	0.82
1:E:480:VAL:HG21	1:E:550:GLN:HE22	1.42	0.82
2:B:36:LYS:HE3	2:B:119:LYS:O	1.79	0.82
1:A:304:GLU:OE2	1:A:309:ARG:HD3	1.80	0.82
2:B:179:LEU:HD23	2:B:213:ARG:HA	1.62	0.82
1:A:148:ILE:H	2:B:165:GLN:HE22	1.21	0.82
1:E:327:GLU:HG2	1:E:344:ILE:HD13	1.62	0.82
1:A:77:ARG:HD2	2:B:96:SER:OG	1.80	0.81
3:G:114:TRP:HB2	3:G:175:ARG:NH1	1.94	0.81
1:A:230:LYS:HD2	1:A:462:ILE:HA	1.60	0.81
1:A:117:ASN:H	1:A:117:ASN:ND2	1.78	0.81
3:C:114:TRP:HB2	3:C:175:ARG:NH1	1.96	0.80
3:G:133:LEU:O	3:G:136:ILE:HG13	1.82	0.80
1:A:73:MET:HE3	1:A:78:SER:HA	1.64	0.80
2:F:230:MET:HE3	2:F:262:ILE:HG21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ARG:HH12	11:C:202:RQX:C5	1.96	0.79
3:C:82:MET:HB2	10:C:201:HEM:HAC	1.63	0.79
1:E:120:HIS:HD2	1:E:630:LEU:HB2	1.46	0.79
10:C:201:HEM:HAA1	4:D:63:ARG:HH12	1.48	0.79
3:G:149:ILE:HD13	3:G:149:ILE:N	1.93	0.79
1:E:254:GLY:HA3	1:E:555:ASN:ND2	1.97	0.79
1:E:508:ARG:NH1	1:E:573:HIS:HD2	1.81	0.79
1:A:446:ARG:HG3	1:A:446:ARG:NH1	1.87	0.79
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.64	0.79
2:B:268:LYS:CG	2:B:269:MET:H	1.96	0.78
2:F:71:ALA:O	2:F:75:ILE:HG23	1.84	0.78
1:A:620:LEU:HD23	1:A:622:TYR:OH	1.83	0.78
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.66	0.77
1:E:480:VAL:CG2	1:E:550:GLN:NE2	2.46	0.77
3:C:135:GLY:O	3:C:139:ILE:HG13	1.84	0.77
1:E:500:MET:HE1	1:E:560:ILE:HB	1.66	0.77
1:A:492:LEU:HD11	1:A:526:GLU:HB2	1.65	0.77
1:A:589:LYS:HB3	1:A:590:PRO:HD2	1.67	0.77
1:A:320:ARG:HH12	5:A:701:MLI:C2	1.98	0.76
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.68	0.76
1:A:589:LYS:HB3	1:A:590:PRO:CD	2.16	0.76
1:E:508:ARG:HH11	1:E:573:HIS:CD2	2.04	0.76
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.69	0.75
1:E:503:HIS:HD2	1:E:512:ILE:O	1.70	0.74
1:A:541:SER:O	1:A:545:GLU:HG3	1.88	0.74
1:E:79:HIS:CE1	6:E:702:FAD:HM81	2.15	0.73
10:C:201:HEM:HHA	10:C:201:HEM:HBD1	1.71	0.73
4:H:109:ARG:HG2	4:H:109:ARG:NH2	1.98	0.73
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.70	0.73
1:E:159:ASN:HD22	1:E:163:GLY:HA3	1.54	0.73
2:F:34:ARG:HH21	2:F:34:ARG:CG	1.97	0.73
1:A:333:GLU:HB3	1:A:335:ARG:HH12	1.53	0.73
1:A:221:ASP:OD2	1:A:223:THR:OG1	2.06	0.73
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.23	0.73
1:E:42:TYR:O	1:E:229:SER:HA	1.89	0.73
1:E:274:GLN:HB2	1:E:390:MET:HE1	1.70	0.72
2:B:230:MET:HE1	2:B:262:ILE:HD13	1.72	0.72
1:E:291:SER:HB2	1:E:348:LEU:HD21	1.71	0.72
3:C:158:LEU:O	3:C:162:LEU:HB2	1.88	0.72
1:E:91:LEU:HD23	1:E:127:VAL:HG13	1.70	0.72
1:E:401:VAL:HG21	1:E:416:LEU:HG	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:584:GLU:OE2	1:E:604:ARG:NH1	2.23	0.72
2:F:34:ARG:HG2	2:F:34:ARG:NH2	1.94	0.72
3:C:76:ARG:HH11	3:C:76:ARG:HG3	1.55	0.71
2:F:86:ARG:NH1	2:F:137:PRO:HD2	2.06	0.71
1:E:557:THR:O	1:E:560:ILE:HG22	1.90	0.71
1:E:80:THR:HG22	1:E:181:LEU:HB2	1.73	0.71
4:H:50:LYS:N	4:H:51:PRO:HD3	2.04	0.71
4:D:101:TRP:CH2	4:D:122:ARG:HG2	2.25	0.71
3:C:76:ARG:HE	4:D:103:VAL:HG22	1.55	0.71
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.27	0.70
1:A:371:ALA:O	1:A:373:VAL:HG23	1.91	0.70
1:E:203:ASP:HB2	1:E:473:SER:OG	1.92	0.70
1:E:249:ALA:C	1:E:251:MET:H	2.00	0.69
1:E:627:ASP:HB3	1:E:637:TRP:CD1	2.27	0.69
1:A:307:MET:HE2	1:A:323:VAL:HG22	1.75	0.69
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.26	0.69
2:B:197:TRP:NE1	11:C:202:RQX:O1	2.21	0.69
3:C:149:ILE:HG12	3:C:150:PRO:HD3	1.74	0.69
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.27	0.69
1:E:262:ARG:HH12	1:E:551:ASN:HD21	1.40	0.69
1:E:135:ASN:ND2	2:F:161:LEU:O	2.25	0.69
1:A:228:ARG:HH11	1:A:464:GLU:HA	1.58	0.68
1:E:262:ARG:NH1	1:E:551:ASN:HD21	1.89	0.68
2:B:268:LYS:CG	2:B:269:MET:N	2.56	0.68
1:E:120:HIS:HD2	1:E:630:LEU:H	1.40	0.68
1:E:44:VAL:HG21	1:E:60:LEU:HD13	1.75	0.68
2:B:131:VAL:CG2	3:C:55:PRO:HG2	2.24	0.68
3:G:69:TRP:HE3	11:G:202:RQX:H1	1.60	0.67
3:G:175:ARG:HH22	3:G:178:ARG:NH2	1.92	0.67
2:F:124:TYR:CE1	3:G:62:ILE:HG21	2.30	0.67
2:B:71:ALA:O	2:B:75:ILE:HG23	1.93	0.67
4:H:92:LEU:HD21	12:H:201:EPH:H222	1.76	0.67
1:E:598:PRO:HG2	1:E:601:LYS:HD3	1.76	0.67
1:A:174:ASP:OD2	1:A:362:GLY:N	2.28	0.66
1:A:274:GLN:HB2	1:A:390:MET:HE1	1.77	0.66
2:B:172:GLU:OE2	2:B:275:PRO:HD2	1.95	0.66
2:F:155:LYS:NZ	2:F:219:ARG:O	2.29	0.66
2:F:122:LYS:N	2:F:122:LYS:HD3	2.12	0.66
1:E:527:LEU:HD11	1:E:553:MET:HG3	1.78	0.65
1:A:502:LYS:HD3	1:A:503:HIS:CE1	2.32	0.65
1:A:631:ASP:HB3	1:A:634:GLU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:170:VAL:HG11	12:H:201:EPH:H61	1.78	0.65
1:A:365:GLU:O	1:A:369:ILE:HG12	1.95	0.65
2:B:222:SER:O	2:B:223:ALA:C	2.40	0.65
1:E:103:PHE:HA	1:E:123:THR:HG21	1.78	0.65
1:A:277:PRO:HD3	1:A:320:ARG:HB3	1.79	0.64
1:A:446:ARG:HH11	1:A:446:ARG:CG	1.97	0.64
1:A:65:PHE:HE2	1:A:456:LEU:HD12	1.63	0.64
1:E:100:LYS:HD3	1:E:635:VAL:HG23	1.78	0.64
1:A:63:ALA:HB1	1:A:453:LYS:HD2	1.78	0.64
2:B:155:LYS:HD2	2:B:166:GLN:NE2	2.12	0.64
4:D:50:LYS:N	4:D:51:PRO:CD	2.59	0.64
2:F:268:LYS:CG	2:F:269:MET:N	2.41	0.64
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.79	0.64
3:G:126:PHE:HA	3:G:167:SER:OG	1.97	0.64
3:C:156:ALA:O	3:C:160:LEU:HB2	1.98	0.64
1:E:244:PHE:HA	1:E:497:GLN:HB3	1.80	0.64
3:C:82:MET:CB	10:C:201:HEM:HAC	2.27	0.64
3:G:114:TRP:HD1	3:G:175:ARG:HE	1.44	0.64
2:B:268:LYS:HG3	2:B:269:MET:H	1.62	0.64
1:E:105:ASP:OD2	1:E:157:SER:N	2.30	0.63
1:A:42:TYR:O	1:A:229:SER:HA	1.98	0.63
1:E:120:HIS:CD2	1:E:630:LEU:H	2.17	0.63
3:G:126:PHE:HB3	3:G:127:PRO:HD3	1.81	0.63
4:H:156:LEU:O	4:H:156:LEU:HD12	1.99	0.63
1:E:502:LYS:HD2	1:E:503:HIS:CE1	2.34	0.63
3:C:133:LEU:HD23	3:C:163:ALA:HB2	1.80	0.63
1:E:451:ASN:O	1:E:455:GLU:HG3	1.99	0.63
11:C:202:RQX:H20	4:D:107:TYR:CE2	2.33	0.62
1:E:48:GLY:HA2	6:E:702:FAD:H1B	1.81	0.62
2:F:92:GLY:O	2:F:251:LYS:NZ	2.33	0.62
1:A:105:ASP:OD2	1:A:157:SER:N	2.28	0.62
2:B:215:ILE:HG22	2:B:226:ARG:HD2	1.81	0.62
1:A:244:PHE:HA	1:A:497:GLN:HB3	1.81	0.62
4:D:72:LEU:HD21	4:D:88:LEU:HD23	1.80	0.62
1:A:159:ASN:O	1:A:161:GLY:N	2.32	0.62
2:F:150:GLN:HB3	2:F:152:TRP:CH2	2.35	0.62
2:F:258:ALA:O	2:F:262:ILE:HG13	1.99	0.62
4:D:154:TRP:HB3	12:D:201:EPH:H381	1.81	0.62
1:E:186:GLY:HA2	1:E:189:LEU:HD12	1.82	0.61
2:F:197:TRP:NE1	11:G:202:RQX:O1	2.25	0.61
4:D:93:THR:HA	4:D:132:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:215:ILE:HG22	2:F:226:ARG:HD2	1.82	0.61
1:E:77:ARG:HA	2:F:94:CYS:HB2	1.81	0.61
1:E:327:GLU:HG2	1:E:344:ILE:CD1	2.31	0.61
1:A:262:ARG:HH22	1:A:551:ASN:HD21	1.49	0.61
1:A:358:GLN:HG3	1:A:359:ARG:HE	1.66	0.61
1:E:320:ARG:NH1	1:E:434:GLY:HA2	2.16	0.61
3:C:74:LEU:HD23	3:C:130:PHE:CE1	2.35	0.60
1:A:34:GLN:HE21	1:A:35:TYR:H	1.49	0.60
4:H:109:ARG:HH21	4:H:109:ARG:CG	2.07	0.60
1:A:228:ARG:NH1	1:A:464:GLU:HA	2.17	0.60
1:E:73:MET:HE3	1:E:78:SER:HA	1.84	0.60
4:H:140:ASN:HD22	4:H:145:GLY:HA2	1.67	0.60
1:E:242:ALA:O	1:E:497:GLN:HA	2.00	0.60
2:F:183:ILE:HG13	2:F:185:CYS:HB3	1.83	0.60
1:E:496:MET:HE1	1:E:552:LEU:HB3	1.84	0.60
1:E:109:GLY:O	1:E:431:ASN:HB3	2.01	0.60
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.83	0.60
3:C:149:ILE:CD1	3:C:149:ILE:N	2.57	0.59
1:A:120:HIS:CD2	1:A:630:LEU:H	2.09	0.59
1:A:73:MET:SD	1:A:251:MET:HG2	2.42	0.59
2:B:39:GLU:OE1	2:B:54:LEU:HD13	2.01	0.59
1:E:264:GLY:O	1:E:403:LYS:NZ	2.31	0.59
1:E:44:VAL:HG22	1:E:67:THR:HG23	1.84	0.59
2:F:116:ASN:C	2:F:116:ASN:HD22	2.09	0.59
2:B:172:GLU:CD	2:B:275:PRO:HD2	2.28	0.59
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.83	0.59
1:A:484:ASN:O	1:A:485:GLY:O	2.19	0.59
1:A:492:LEU:HD11	1:A:526:GLU:CB	2.32	0.59
1:E:150:GLN:HA	1:E:169:THR:O	2.03	0.59
10:C:201:HEM:HHC	10:C:201:HEM:CBB	2.24	0.59
1:E:38:ILE:HG23	4:H:34:GLY:HA3	1.84	0.59
1:A:122:LEU:HG	1:A:439:LEU:HD12	1.85	0.59
1:A:281:TYR:HA	1:A:383:ILE:HG22	1.85	0.59
1:A:492:LEU:HB3	1:A:549:LEU:HD21	1.84	0.59
1:E:307:MET:HE2	1:E:323:VAL:HG22	1.83	0.59
1:A:72:LYS:HE3	1:A:251:MET:HG3	1.84	0.58
1:A:85:GLY:HA3	1:A:153:PHE:CZ	2.38	0.58
1:E:557:THR:O	1:E:561:VAL:HG13	2.03	0.58
3:G:112:ILE:HB	3:G:113:PRO:CD	2.33	0.58
1:A:241:ARG:HH22	2:B:90:ARG:NH2	2.01	0.58
1:E:52:ALA:O	1:E:53:GLY:C	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LEU:HD21	1:E:544:THR:HG21	1.84	0.58
4:D:43:ILE:O	4:D:46:GLU:HB3	2.03	0.58
1:A:247:THR:HG21	1:A:286:LEU:HD13	1.85	0.58
3:C:46:LEU:HD13	4:D:111:PHE:CD1	2.38	0.58
1:A:106:THR:HG22	1:A:119:MET:SD	2.43	0.58
1:E:112:TRP:CH2	1:E:641:ILE:HG13	2.39	0.58
1:A:148:ILE:N	2:B:165:GLN:HE22	1.99	0.58
1:A:249:ALA:C	1:A:251:MET:H	2.10	0.58
2:B:154:GLN:HG3	2:B:222:SER:OG	2.03	0.58
1:E:566:ARG:NH2	1:E:605:LYS:O	2.34	0.58
3:G:156:ALA:O	3:G:160:LEU:HB2	2.04	0.58
1:E:249:ALA:C	1:E:251:MET:N	2.61	0.58
1:A:253:THR:HG22	1:A:552:LEU:CD1	2.34	0.57
1:A:363:ILE:HG13	1:A:364:SER:N	2.18	0.57
1:A:451:ASN:O	1:A:455:GLU:HG3	2.04	0.57
1:E:159:ASN:HB2	1:E:163:GLY:CA	2.35	0.57
4:H:77:TYR:HA	12:H:201:EPH:H11	1.86	0.57
3:C:76:ARG:HG3	3:C:76:ARG:NH1	2.19	0.57
1:E:50:GLY:O	1:E:51:GLY:C	2.47	0.57
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.04	0.57
1:E:138:MET:HE2	1:E:172:VAL:HG23	1.86	0.57
1:E:495:THR:OG1	1:E:523:LEU:HD21	2.04	0.57
2:B:128:HIS:CD2	2:B:196:TRP:HB3	2.40	0.57
3:C:114:TRP:CB	3:C:175:ARG:HH11	2.17	0.57
1:A:83:ALA:HB3	1:A:177:GLY:CA	2.33	0.57
1:A:120:HIS:HD2	1:A:630:LEU:N	1.97	0.57
3:C:92:GLY:O	3:C:96:LEU:HB2	2.05	0.57
1:E:262:ARG:HH12	1:E:551:ASN:ND2	2.02	0.57
1:E:148:ILE:H	2:F:165:GLN:HE22	1.52	0.56
1:E:241:ARG:NH2	1:E:246:CYS:SG	2.77	0.56
1:E:400:GLN:HB3	1:E:412:ILE:HG23	1.87	0.56
2:F:116:ASN:ND2	2:F:118:SER:OG	2.39	0.56
1:A:135:ASN:O	2:B:153:LEU:HD23	2.05	0.56
2:B:268:LYS:HG3	2:B:269:MET:N	2.21	0.56
3:C:181:LYS:HA	3:C:184:LEU:HB3	1.86	0.56
2:F:227:LEU:CD2	2:F:266:LEU:HD13	2.35	0.56
1:A:522:ASP:O	1:A:525:LYS:HB2	2.04	0.56
1:E:72:LYS:HE2	1:E:251:MET:HG3	1.86	0.56
1:E:86:GLY:HA3	1:E:169:THR:CG2	2.36	0.56
1:A:369:ILE:HG22	2:B:67:MET:HE1	1.88	0.56
2:B:92:GLY:HA2	7:B:301:FES:S2	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:LEU:HD23	2:B:277:PRO:HD2	1.88	0.56
3:C:64:LYS:O	3:C:66:GLN:HG3	2.06	0.56
2:F:234:PHE:O	2:F:238:LYS:HB2	2.06	0.56
2:F:34:ARG:CG	2:F:34:ARG:NH2	2.64	0.56
4:H:109:ARG:CD	4:H:109:ARG:H	2.18	0.56
4:D:79:ILE:HG13	4:D:79:ILE:O	2.05	0.55
1:E:159:ASN:HB2	1:E:163:GLY:HA3	1.88	0.55
1:E:254:GLY:HA3	1:E:555:ASN:HD21	1.67	0.55
4:D:50:LYS:H	4:D:51:PRO:HD2	1.66	0.55
1:E:120:HIS:HD2	1:E:630:LEU:CB	2.16	0.55
2:B:36:LYS:NZ	2:B:114:ASP:HB3	2.22	0.55
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.41	0.55
1:E:262:ARG:NH1	1:E:551:ASN:ND2	2.53	0.55
1:E:439:LEU:C	1:E:439:LEU:HD13	2.31	0.55
2:B:116:ASN:C	2:B:116:ASN:ND2	2.58	0.55
4:H:108:GLY:O	4:H:122:ARG:NH2	2.40	0.55
1:A:327:GLU:O	1:A:331:ILE:HG12	2.07	0.55
2:B:198:ASN:C	2:B:200:ASP:H	2.15	0.55
1:A:132:GLU:HG2	2:B:161:LEU:HG	1.89	0.55
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.89	0.55
1:E:586:ASP:OD1	1:E:586:ASP:C	2.50	0.55
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.88	0.55
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.07	0.55
1:E:394:PRO:HA	1:E:424:CYS:O	2.05	0.55
2:B:153:LEU:HD21	2:B:166:GLN:HE22	1.73	0.54
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.43	0.54
1:A:249:ALA:HB3	1:A:252:ASN:HD22	1.72	0.54
1:E:231:ARG:NH1	1:E:456:LEU:HD23	2.21	0.54
10:G:201:HEM:HHA	10:G:201:HEM:HBA1	1.89	0.54
1:E:517:VAL:HG21	1:E:564:GLU:HG3	1.89	0.54
2:B:59:VAL:CG2	2:B:75:ILE:HG22	2.38	0.54
10:C:201:HEM:NC	4:D:95:HIS:CD2	2.74	0.54
3:G:114:TRP:HD1	3:G:175:ARG:NE	2.06	0.54
1:A:213:GLY:HA3	1:A:227:PHE:O	2.08	0.54
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.90	0.54
3:G:134:ASN:O	3:G:137:ARG:HB3	2.06	0.54
3:C:86:LEU:HD11	4:D:92:LEU:HD23	1.88	0.54
1:A:230:LYS:NZ	1:A:460:GLU:O	2.40	0.54
3:G:79:GLY:C	10:G:201:HEM:HMD1	2.33	0.54
3:G:79:GLY:O	10:G:201:HEM:HMD1	2.07	0.54
1:A:203:ASP:HA	1:A:259:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LEU:HD23	2:B:213:ARG:CA	2.35	0.54
3:C:82:MET:HE3	10:C:201:HEM:HAC	1.91	0.54
2:F:150:GLN:HE22	4:H:46:GLU:CG	2.20	0.54
3:G:64:LYS:O	3:G:66:GLN:HG3	2.07	0.53
1:A:508:ARG:NH1	1:A:573:HIS:HD2	2.06	0.53
1:A:327:GLU:OE2	1:A:384:PRO:HD3	2.08	0.53
1:A:496:MET:HE1	1:A:552:LEU:HB3	1.90	0.53
1:A:631:ASP:HB3	1:A:634:GLU:CB	2.37	0.53
1:E:452:ILE:O	1:E:453:LYS:C	2.51	0.53
1:E:77:ARG:HD2	2:F:96:SER:OG	2.08	0.53
2:B:179:LEU:CD2	2:B:216:ILE:HD11	2.39	0.53
2:B:223:ALA:O	2:B:227:LEU:HD12	2.09	0.53
2:F:67:MET:HE3	2:F:110:ILE:HA	1.91	0.53
3:G:42:GLY:O	3:G:45:TYR:HB3	2.08	0.53
2:B:198:ASN:O	2:B:200:ASP:N	2.42	0.53
10:C:201:HEM:HBA1	10:C:201:HEM:HBD1	1.89	0.53
1:A:230:LYS:HD2	1:A:462:ILE:CA	2.34	0.53
1:A:558:GLN:HA	1:A:618:ILE:HD13	1.91	0.52
2:B:47:GLU:HB3	2:B:50:ALA:HB2	1.91	0.52
4:D:71:PRO:O	4:D:74:PRO:HD2	2.10	0.52
1:E:233:ILE:HA	1:E:417:TYR:O	2.09	0.52
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.92	0.52
1:E:215:ILE:HA	1:E:225:HIS:O	2.08	0.52
2:F:179:LEU:HD11	2:F:257:ARG:HH22	1.74	0.52
1:A:47:ILE:HG22	1:A:236:THR:HG22	1.91	0.52
3:C:76:ARG:NH1	11:C:202:RQX:C5	2.69	0.52
1:E:541:SER:HB2	2:F:84:THR:HG23	1.92	0.52
3:G:169:ALA:O	3:G:173:TYR:HB3	2.08	0.52
2:B:183:ILE:HG13	2:B:185:CYS:HB3	1.91	0.52
1:E:258:ALA:O	1:E:259:LEU:C	2.52	0.52
1:A:121:TYR:O	1:A:125:ASN:OD1	2.27	0.52
1:E:432:ARG:HD2	1:E:437:SER:HB2	1.92	0.52
2:F:179:LEU:CD1	2:F:257:ARG:HH22	2.22	0.52
2:F:205:PRO:HA	2:F:259:ILE:HD11	1.90	0.52
3:G:82:MET:HB2	10:G:201:HEM:HAC	1.92	0.52
1:A:174:ASP:CB	1:A:361:PRO:HD2	2.28	0.52
4:D:101:TRP:HH2	4:D:122:ARG:HG2	1.75	0.52
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.90	0.52
4:H:84:MET:HA	4:H:84:MET:CE	2.40	0.52
1:E:206:MET:HG3	1:E:263:ALA:HB1	1.92	0.52
2:B:34:ARG:HD2	2:B:62:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:TYR:CE1	3:G:62:ILE:CG2	2.92	0.52
2:F:243:MET:HE3	3:G:141:PHE:CD1	2.45	0.52
3:G:76:ARG:NH2	4:H:106:ASP:OD2	2.43	0.52
1:A:117:ASN:O	1:A:120:HIS:HB3	2.09	0.52
10:C:201:HEM:HBC2	4:D:96:VAL:CG2	2.40	0.52
1:E:172:VAL:HG21	1:E:179:SER:HB3	1.91	0.52
1:E:401:VAL:CG2	1:E:416:LEU:HG	2.39	0.52
1:E:48:GLY:O	1:E:53:GLY:HA3	2.10	0.51
2:B:40:ILE:CD1	2:B:75:ILE:HD11	2.41	0.51
1:E:153:PHE:HD1	1:E:434:GLY:HA3	1.75	0.51
2:F:57:PHE:CG	2:F:75:ILE:HD12	2.45	0.51
2:F:172:GLU:OE2	2:F:275:PRO:HD2	2.10	0.51
3:G:120:PHE:O	3:G:124:ILE:HG13	2.09	0.51
2:B:198:ASN:C	2:B:200:ASP:N	2.67	0.51
2:B:230:MET:CE	2:B:262:ILE:HG21	2.41	0.51
1:E:347:GLN:HG2	1:E:350:HIS:ND1	2.25	0.51
3:G:76:ARG:NH1	11:G:202:RQX:O3	2.43	0.51
3:G:183:THR:HG23	3:G:183:THR:O	2.10	0.51
1:A:135:ASN:ND2	2:B:161:LEU:O	2.43	0.51
1:A:371:ALA:O	1:A:373:VAL:N	2.44	0.51
1:A:493:ARG:HB2	1:A:549:LEU:HD13	1.92	0.51
2:B:279:PRO:O	2:B:280:ALA:CB	2.58	0.51
1:E:301:SER:HB3	1:E:336:GLY:O	2.09	0.51
1:A:120:HIS:HD2	1:A:630:LEU:HB2	1.72	0.51
1:E:513:LEU:O	1:E:517:VAL:HG23	2.11	0.51
3:G:69:TRP:CE3	11:G:202:RQX:H1	2.42	0.51
4:H:144:VAL:HG11	4:H:152:MET:HE1	1.91	0.51
2:F:131:VAL:CG2	3:G:55:PRO:HG2	2.41	0.51
1:A:291:SER:HA	1:A:360:LEU:HD11	1.91	0.51
2:F:234:PHE:CD1	2:F:238:LYS:HG3	2.46	0.51
2:F:40:ILE:HG21	2:F:83:LEU:HD11	1.93	0.51
2:F:54:LEU:HD11	2:F:124:TYR:OH	2.10	0.51
1:A:591:ILE:HA	1:A:594:GLN:NE2	2.26	0.51
1:E:585:TYR:CZ	1:E:596:LYS:HD3	2.46	0.51
3:C:87:LEU:O	3:C:89:GLY:N	2.44	0.50
3:C:100:PHE:CE1	4:D:149:ALA:HA	2.46	0.50
4:D:88:LEU:O	4:D:92:LEU:HB2	2.11	0.50
4:D:153:VAL:O	4:D:156:LEU:HD12	2.11	0.50
1:A:159:ASN:O	1:A:160:TYR:C	2.54	0.50
2:B:240:HIS:C	2:B:241:THR:HG23	2.37	0.50
11:C:202:RQX:H20	4:D:107:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:92:GLY:HA2	2:F:109:CYS:SG	2.51	0.50
1:A:221:ASP:HA	1:A:538:ILE:HG12	1.92	0.50
1:A:378:GLU:HB3	1:A:379:PRO:CD	2.42	0.50
3:G:69:TRP:HE3	11:G:202:RQX:C1	2.24	0.50
1:E:120:HIS:HD2	1:E:630:LEU:N	2.08	0.50
1:E:356:LEU:HD12	1:E:360:LEU:HD12	1.93	0.50
2:B:36:LYS:NZ	2:B:114:ASP:O	2.44	0.50
2:B:38:PHE:O	2:B:56:LYS:HA	2.12	0.50
1:E:88:ASN:ND2	1:E:169:THR:OG1	2.45	0.50
1:A:78:SER:O	1:A:81:THR:HG22	2.11	0.50
2:B:39:GLU:HB2	2:B:122:LYS:HB3	1.94	0.50
1:E:106:THR:HG22	1:E:119:MET:SD	2.51	0.50
1:E:253:THR:HG22	1:E:552:LEU:HD11	1.92	0.50
3:G:139:ILE:HG22	3:G:143:MET:HE3	1.94	0.50
1:A:270:LEU:HD12	1:A:558:GLN:HB3	1.93	0.49
2:B:238:LYS:O	2:B:240:HIS:HD2	1.95	0.49
2:F:131:VAL:HG22	3:G:55:PRO:O	2.12	0.49
2:F:173:GLN:O	2:F:176:LEU:HB2	2.12	0.49
3:G:121:LYS:HB3	3:G:171:VAL:HG22	1.94	0.49
1:E:635:VAL:HG22	1:E:636:ASP:H	1.77	0.49
2:F:244:ASN:HD21	3:G:66:GLN:NE2	2.10	0.49
4:H:140:ASN:ND2	4:H:145:GLY:HA2	2.26	0.49
1:A:222:GLY:O	1:A:537:LEU:HD13	2.12	0.49
1:A:242:ALA:HA	1:A:496:MET:CE	2.43	0.49
1:A:557:THR:O	1:A:560:ILE:HG22	2.11	0.49
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.48	0.49
1:E:294:GLU:OE1	1:E:359:ARG:HG2	2.12	0.49
1:E:566:ARG:NH1	1:E:568:GLU:OE2	2.44	0.49
2:F:102:ALA:HA	2:F:122:LYS:HE2	1.95	0.49
1:A:246:CYS:O	2:B:90:ARG:NH2	2.46	0.49
1:A:520:MET:HG2	1:A:560:ILE:HG21	1.95	0.49
2:F:100:ASN:C	2:F:100:ASN:HD22	2.21	0.49
1:A:58:MET:HA	1:A:191:CYS:SG	2.53	0.49
1:E:241:ARG:HH11	1:E:250:HIS:CE1	2.31	0.49
1:A:246:CYS:HA	1:A:385:THR:HG22	1.95	0.49
1:A:508:ARG:NH1	1:A:573:HIS:CD2	2.81	0.49
1:A:73:MET:CE	1:A:78:SER:HA	2.40	0.48
1:E:221:ASP:HA	1:E:538:ILE:HG12	1.94	0.48
2:F:47:GLU:HB3	2:F:50:ALA:HB2	1.95	0.48
2:B:263:LYS:NZ	3:C:142:ASP:OD1	2.44	0.48
1:E:547:LEU:HD12	1:E:547:LEU:HA	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:TYR:CZ	3:G:62:ILE:HG21	2.48	0.48
1:A:253:THR:HG22	1:A:552:LEU:HD11	1.95	0.48
1:E:320:ARG:HH11	1:E:434:GLY:HA2	1.78	0.48
1:E:606:HIS:CD2	1:E:623:ARG:NH1	2.81	0.48
2:F:68:VAL:HG23	2:F:111:CYS:O	2.12	0.48
2:F:122:LYS:N	2:F:122:LYS:CD	2.75	0.48
4:H:50:LYS:N	4:H:51:PRO:CD	2.75	0.48
1:A:199:TYR:HA	1:A:217:LEU:O	2.14	0.48
3:G:62:ILE:HD12	3:G:63:TYR:N	2.29	0.48
3:G:95:VAL:HG13	3:G:96:LEU:HD12	1.95	0.48
1:A:45:VAL:HG22	1:A:68:ALA:HB3	1.95	0.48
2:F:150:GLN:HA	2:F:152:TRP:CZ3	2.48	0.48
4:D:126:TYR:H	4:D:126:TYR:HD1	1.62	0.48
1:E:276:HIS:NE2	1:E:320:ARG:NH2	2.62	0.48
2:F:244:ASN:ND2	3:G:66:GLN:NE2	2.62	0.48
1:A:249:ALA:C	1:A:251:MET:N	2.72	0.48
1:A:276:HIS:O	1:A:384:PRO:HA	2.13	0.48
1:A:527:LEU:HD11	1:A:553:MET:HG3	1.96	0.48
11:C:202:RQX:H3	11:C:202:RQX:H9	1.50	0.48
4:D:136:LEU:O	4:D:137:LEU:C	2.55	0.48
1:E:72:LYS:NZ	1:E:255:ASP:OD2	2.44	0.48
1:E:200:PHE:O	1:E:216:ALA:HB1	2.14	0.48
1:A:242:ALA:HA	1:A:496:MET:HE3	1.96	0.48
2:B:179:LEU:HG	2:B:209:MET:HE2	1.96	0.48
2:F:100:ASN:C	2:F:100:ASN:ND2	2.72	0.48
2:F:155:LYS:HD2	2:F:166:GLN:NE2	2.29	0.48
2:B:250:PRO:HD2	8:B:302:SF4:S3	2.54	0.48
4:D:113:LEU:HD22	4:D:117:LEU:HD22	1.96	0.48
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.96	0.48
1:E:492:LEU:HD23	1:E:530:LEU:HD12	1.95	0.48
2:F:86:ARG:HH11	2:F:137:PRO:HD2	1.77	0.48
2:F:179:LEU:CD2	2:F:216:ILE:HD11	2.44	0.48
1:A:477:LEU:HD12	1:A:543:LEU:HD11	1.96	0.47
2:B:155:LYS:HD2	2:B:166:GLN:HE21	1.77	0.47
2:B:208:LEU:HD13	2:B:259:ILE:HG12	1.96	0.47
1:E:294:GLU:CD	1:E:359:ARG:HG2	2.39	0.47
2:B:244:ASN:ND2	3:C:66:GLN:NE2	2.61	0.47
2:F:40:ILE:HG22	2:F:41:TYR:O	2.14	0.47
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.97	0.47
10:C:201:HEM:HBA1	10:C:201:HEM:CHA	2.35	0.47
1:E:484:ASN:O	1:E:485:GLY:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:520:MET:HE3	1:E:553:MET:HE1	1.95	0.47
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.45	0.47
3:G:114:TRP:HB2	3:G:175:ARG:CZ	2.44	0.47
1:A:85:GLY:HA3	1:A:153:PHE:HZ	1.80	0.47
1:A:244:PHE:CA	1:A:497:GLN:HB3	2.44	0.47
1:A:378:GLU:HB3	1:A:379:PRO:HD2	1.96	0.47
1:E:410:ASP:C	1:E:411:LYS:HG2	2.40	0.47
1:E:561:VAL:CG2	1:E:618:ILE:HG21	2.44	0.47
1:A:394:PRO:O	1:A:395:THR:HG22	2.14	0.47
1:E:138:MET:HE2	1:E:172:VAL:CG2	2.44	0.47
1:E:517:VAL:O	1:E:521:MET:HG2	2.14	0.47
1:E:519:LYS:O	1:E:522:ASP:HB2	2.14	0.47
2:F:150:GLN:HB3	2:F:152:TRP:CZ2	2.49	0.47
3:G:148:ASP:OD2	3:G:150:PRO:HD2	2.13	0.47
1:A:121:TYR:CD1	1:A:121:TYR:C	2.93	0.47
3:C:76:ARG:HA	10:C:201:HEM:O2D	2.15	0.47
1:E:156:GLN:HB3	1:E:166:ALA:HB3	1.97	0.47
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.27	0.47
4:H:149:ALA:O	4:H:153:VAL:HG23	2.14	0.47
1:A:107:ALA:O	1:A:110:SER:OG	2.31	0.47
2:B:179:LEU:CD1	2:B:257:ARG:HH22	2.28	0.47
4:D:108:GLY:HA2	4:D:113:LEU:HD11	1.97	0.47
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.97	0.47
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.96	0.47
1:A:270:LEU:HD12	1:A:558:GLN:CB	2.45	0.47
2:B:179:LEU:HD22	2:B:216:ILE:HD11	1.96	0.47
1:E:80:THR:CG2	1:E:181:LEU:HB2	2.42	0.47
1:E:121:TYR:HB2	1:E:630:LEU:HD11	1.95	0.47
1:E:462:ILE:O	1:E:463:PRO:C	2.57	0.47
1:E:471:GLU:HA	1:E:474:ILE:HG23	1.95	0.47
1:A:424:CYS:C	1:A:426:SER:H	2.21	0.47
2:B:268:LYS:HG2	2:B:269:MET:H	1.74	0.47
3:C:76:ARG:NH1	3:C:76:ARG:CG	2.77	0.47
4:D:126:TYR:N	4:D:126:TYR:CD1	2.83	0.47
1:E:492:LEU:HD12	1:E:523:LEU:HD23	1.97	0.47
1:A:102:HIS:CE1	1:A:123:THR:HG22	2.50	0.46
1:A:401:VAL:HG21	1:A:416:LEU:HG	1.97	0.46
1:A:432:ARG:NE	1:A:437:SER:HB2	2.30	0.46
2:F:245:CYS:HB2	2:F:255:PRO:HG2	1.97	0.46
2:F:264:MET:SD	3:G:143:MET:HG2	2.55	0.46
2:B:238:LYS:HE3	4:D:106:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ASN:HB2	1:E:163:GLY:N	2.29	0.46
1:A:115:ASP:HB3	1:A:117:ASN:HD21	1.81	0.46
1:A:159:ASN:O	1:A:162:LYS:N	2.48	0.46
2:B:179:LEU:HD11	2:B:257:ARG:HH22	1.79	0.46
3:C:105:GLU:C	3:C:107:ILE:H	2.23	0.46
11:C:202:RQX:H15	4:D:107:TYR:CE2	2.50	0.46
1:E:132:GLU:HG2	2:F:161:LEU:HG	1.97	0.46
2:F:172:GLU:CD	2:F:275:PRO:HD2	2.39	0.46
2:F:197:TRP:HZ2	11:G:202:RQX:H11	1.81	0.46
2:B:72:LEU:HD23	2:B:72:LEU:HA	1.77	0.46
3:C:35:LYS:HB3	3:C:39:GLN:HB3	1.97	0.46
1:E:213:GLY:HA3	1:E:227:PHE:O	2.15	0.46
1:A:78:SER:OG	6:A:702:FAD:O3B	2.19	0.46
1:A:500:MET:HE1	1:A:556:ALA:O	2.16	0.46
2:F:169:SER:O	2:F:170:ILE:C	2.58	0.46
1:A:267:LEU:HD12	1:A:270:LEU:HD11	1.98	0.46
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.28	0.46
1:E:482:TYR:O	1:E:483:ALA:C	2.59	0.46
1:A:122:LEU:HD11	1:A:440:ASP:HA	1.97	0.46
10:C:201:HEM:CAA	4:D:63:ARG:HH12	2.23	0.46
1:E:74:PHE:CE2	1:E:76:THR:HB	2.51	0.46
1:E:552:LEU:O	1:E:556:ALA:N	2.43	0.46
1:A:466:PRO:O	1:A:469:ALA:HB2	2.16	0.46
1:A:585:TYR:CE1	1:A:596:LYS:HA	2.50	0.46
1:E:313:LYS:HB2	1:E:645:TYR:O	2.15	0.46
1:A:274:GLN:HB3	1:A:388:TYR:HB3	1.97	0.46
1:A:293:GLY:HA2	1:A:317:LEU:HD11	1.98	0.46
1:A:511:ASP:O	1:A:515:GLU:HB2	2.15	0.46
1:E:404:TYR:HB3	1:E:608:LEU:HD11	1.98	0.46
1:E:610:LYS:O	1:E:618:ILE:HA	2.14	0.46
1:A:276:HIS:HB2	1:A:387:HIS:CG	2.51	0.46
1:E:296:GLY:HA3	1:E:348:LEU:HD23	1.98	0.46
1:E:320:ARG:NH1	1:E:432:ARG:NH2	2.64	0.46
2:F:100:ASN:HD21	2:F:103:GLY:HA2	1.81	0.46
3:G:58:PRO:HB2	3:G:62:ILE:HG12	1.98	0.46
1:A:42:TYR:CD2	1:A:68:ALA:HB2	2.51	0.45
1:A:482:TYR:CE2	1:A:535:ARG:HG2	2.50	0.45
2:B:39:GLU:HA	2:B:55:GLN:O	2.15	0.45
2:B:68:VAL:HG23	2:B:111:CYS:O	2.16	0.45
4:D:67:ALA:HA	4:D:70:VAL:HG23	1.98	0.45
1:E:266:ALA:HB2	1:E:610:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:124:ILE:HG23	12:H:201:EPH:H272	1.97	0.45
1:A:113:LEU:O	1:A:606:HIS:HE1	1.99	0.45
2:B:44:ASN:HD22	2:B:47:GLU:HB2	1.81	0.45
1:A:264:GLY:O	1:A:403:LYS:NZ	2.50	0.45
1:A:279:GLY:HA3	1:A:385:THR:OG1	2.16	0.45
2:B:244:ASN:HD21	3:C:66:GLN:NE2	2.15	0.45
3:C:86:LEU:CD1	4:D:92:LEU:HD23	2.47	0.45
1:E:457:LYS:HA	1:E:457:LYS:HD3	1.62	0.45
4:D:143:ASP:OD2	4:D:144:VAL:HG22	2.15	0.45
1:A:541:SER:HB3	2:B:76:LYS:NZ	2.32	0.45
2:B:90:ARG:C	2:B:90:ARG:HD2	2.41	0.45
3:C:82:MET:HE3	10:C:201:HEM:CAC	2.47	0.45
1:E:570:ARG:HH22	1:E:604:ARG:HG3	1.81	0.45
1:A:502:LYS:HD3	1:A:503:HIS:HE1	1.78	0.45
1:A:540:ASN:HB3	1:A:543:LEU:HB3	1.98	0.45
1:E:243:TYR:CD2	1:E:386:VAL:HG21	2.52	0.45
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.98	0.45
2:F:80:ASP:OD2	2:F:80:ASP:C	2.60	0.45
3:G:126:PHE:HB3	3:G:127:PRO:CD	2.44	0.45
3:G:149:ILE:CD1	3:G:149:ILE:N	2.62	0.45
1:A:503:HIS:CD2	1:A:516:GLY:CA	3.00	0.45
2:B:83:LEU:HD12	2:B:83:LEU:HA	1.76	0.45
1:A:65:PHE:CE2	1:A:456:LEU:HD12	2.47	0.45
1:A:133:LEU:HD13	1:A:138:MET:SD	2.57	0.45
1:A:148:ILE:HG13	2:B:165:GLN:NE2	2.31	0.45
1:E:45:VAL:HG21	1:E:227:PHE:HB3	1.98	0.45
1:E:85:GLY:N	6:E:702:FAD:O4	2.50	0.45
1:E:152:SER:O	1:E:293:GLY:HA3	2.17	0.45
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.17	0.45
3:G:112:ILE:HB	3:G:113:PRO:HD3	1.98	0.45
1:A:40:HIS:HB3	1:A:42:TYR:HE1	1.81	0.45
1:A:276:HIS:ND1	1:A:277:PRO:HD2	2.32	0.45
1:A:344:ILE:HG12	1:A:345:TYR:N	2.32	0.45
4:D:68:ALA:O	4:D:71:PRO:HD2	2.17	0.45
1:E:174:ASP:OD2	1:E:362:GLY:N	2.49	0.45
1:E:488:PRO:HB2	1:E:491:GLU:HG3	1.99	0.45
2:B:141:LEU:HD21	2:B:199:ALA:O	2.17	0.45
4:D:49:PHE:C	4:D:51:PRO:HD2	2.41	0.45
1:E:480:VAL:HG22	1:E:550:GLN:NE2	2.29	0.45
2:F:84:THR:HB	2:F:134:ASP:HB2	1.98	0.45
2:F:279:PRO:O	2:F:280:ALA:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:CD	1:A:462:ILE:HA	2.39	0.44
1:E:325:ARG:O	1:E:326:ALA:C	2.60	0.44
1:E:468:GLY:O	1:E:471:GLU:HB2	2.17	0.44
1:E:509:ARG:HA	1:E:577:ASP:OD2	2.16	0.44
1:A:88:ASN:ND2	1:A:169:THR:OG1	2.51	0.44
2:B:59:VAL:HG21	2:B:75:ILE:HG22	1.98	0.44
4:D:77:TYR:HA	12:D:201:EPH:H11	1.98	0.44
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.98	0.44
1:E:461:LYS:HB3	1:E:461:LYS:HE2	1.61	0.44
2:F:209:MET:HE3	2:F:258:ALA:CB	2.47	0.44
3:G:76:ARG:HE	4:H:103:VAL:HG22	1.82	0.44
1:A:333:GLU:HB3	1:A:335:ARG:NH1	2.27	0.44
1:E:570:ARG:NH2	1:E:604:ARG:HG3	2.33	0.44
3:G:112:ILE:HD12	3:G:117:LEU:HG	1.99	0.44
4:H:55:HIS:O	4:H:55:HIS:CG	2.71	0.44
1:A:109:GLY:O	1:A:431:ASN:HB3	2.16	0.44
1:A:190:ARG:O	1:A:190:ARG:HG2	2.16	0.44
1:A:566:ARG:HB3	1:A:573:HIS:CE1	2.53	0.44
1:E:86:GLY:HA3	1:E:169:THR:HG22	1.99	0.44
3:G:47:MET:HE1	3:G:50:ARG:NH1	2.32	0.44
3:G:121:LYS:HB3	3:G:171:VAL:CG2	2.47	0.44
1:A:611:GLN:HG3	1:A:618:ILE:HG12	1.99	0.44
2:B:42:ARG:O	2:B:52:PRO:HA	2.17	0.44
1:E:116:GLN:HA	1:E:119:MET:HE3	1.99	0.44
4:H:57:THR:O	4:H:61:ILE:HG23	2.18	0.44
2:B:196:TRP:CZ3	3:C:59:HIS:HB2	2.52	0.44
3:C:114:TRP:HB2	3:C:175:ARG:CZ	2.48	0.44
1:E:496:MET:HB2	1:E:520:MET:CE	2.38	0.44
2:F:150:GLN:HE22	4:H:46:GLU:HG3	1.82	0.44
3:G:76:ARG:HH21	4:H:103:VAL:HA	1.82	0.44
2:B:60:ASP:OD2	2:B:63:LYS:HE2	2.17	0.44
2:B:116:ASN:ND2	2:B:119:LYS:H	2.16	0.44
3:C:86:LEU:HD22	4:D:136:LEU:HD11	1.98	0.44
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.48	0.44
2:F:157:THR:O	2:F:158:LYS:C	2.60	0.44
3:G:165:LEU:HD22	3:G:165:LEU:HA	1.92	0.44
1:A:117:ASN:N	1:A:117:ASN:ND2	2.45	0.44
1:A:128:GLU:HG2	2:B:162:GLY:HA3	2.00	0.44
1:A:262:ARG:HH12	1:A:551:ASN:ND2	2.15	0.44
1:A:584:GLU:HG3	1:A:602:HIS:CE1	2.53	0.44
6:A:702:FAD:H1'1	6:A:702:FAD:H9	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:ARG:HG3	3:C:51:ALA:N	2.33	0.44
1:A:47:ILE:HD11	1:A:214:VAL:HG21	2.00	0.43
1:A:104:TYR:HD1	1:A:638:ILE:HD13	1.83	0.43
1:A:202:LEU:HB2	1:A:215:ILE:HG23	1.99	0.43
1:A:568:GLU:O	1:A:575:ARG:HG2	2.18	0.43
2:F:228:ALA:HA	2:F:231:GLN:CG	2.48	0.43
3:G:114:TRP:CD1	3:G:175:ARG:NE	2.86	0.43
3:G:143:MET:O	3:G:144:ALA:HB3	2.18	0.43
1:A:562:ALA:HB1	1:A:607:THR:HG21	2.00	0.43
1:E:124:ARG:HD2	1:E:634:GLU:OE2	2.18	0.43
1:E:363:ILE:HG13	1:E:364:SER:N	2.34	0.43
2:F:39:GLU:HB2	2:F:122:LYS:HB3	1.99	0.43
2:F:148:SER:HB3	3:G:38:ILE:HD13	2.01	0.43
4:D:126:TYR:HD1	4:D:126:TYR:N	2.16	0.43
1:A:74:PHE:CD1	2:B:143:TYR:CE2	3.06	0.43
1:E:74:PHE:CD1	2:F:143:TYR:CZ	3.06	0.43
1:E:79:HIS:O	1:E:80:THR:C	2.61	0.43
3:G:85:THR:HG21	12:H:201:EPH:H271	2.01	0.43
3:G:114:TRP:HB2	3:G:175:ARG:HH11	1.80	0.43
4:H:79:ILE:C	4:H:80:HIS:HD2	2.27	0.43
4:D:58:LEU:O	4:D:62:GLU:HG2	2.19	0.43
1:E:286:LEU:HA	1:E:286:LEU:HD12	1.76	0.43
2:F:188:CYS:SG	2:F:189:SER:N	2.92	0.43
1:A:428:HIS:CE1	1:A:432:ARG:HG3	2.54	0.43
1:E:448:CYS:O	1:E:452:ILE:HG13	2.18	0.43
2:B:92:GLY:HA2	2:B:109:CYS:SG	2.59	0.43
3:C:86:LEU:HD23	3:C:86:LEU:HA	1.84	0.43
3:G:158:LEU:O	3:G:162:LEU:HB2	2.18	0.43
2:B:264:MET:SD	3:C:143:MET:HG2	2.59	0.43
1:E:209:GLY:O	1:E:414:PRO:HD2	2.18	0.43
4:H:155:GLU:HB2	12:H:201:EPH:N1	2.34	0.43
1:E:74:PHE:CE1	2:F:143:TYR:CD1	3.07	0.42
1:E:374:ASP:OD1	1:E:376:THR:OG1	2.29	0.42
2:F:222:SER:O	2:F:223:ALA:C	2.62	0.42
2:B:247:LYS:O	2:B:247:LYS:HG3	2.16	0.42
2:F:39:GLU:HG2	2:F:56:LYS:HG3	2.00	0.42
2:F:67:MET:HG3	2:F:109:CYS:O	2.18	0.42
2:F:107:LEU:HD11	2:F:183:ILE:HD11	2.00	0.42
1:A:42:TYR:HE2	1:A:194:THR:CG2	2.32	0.42
1:A:320:ARG:NH1	5:A:701:MLI:C2	2.74	0.42
2:B:172:GLU:OE2	2:B:275:PRO:CD	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HD23	1:A:376:THR:HG22	2.01	0.42
2:B:242:ILE:O	2:B:243:MET:HB2	2.18	0.42
3:C:71:VAL:HG13	3:C:130:PHE:HZ	1.84	0.42
3:C:126:PHE:O	3:C:127:PRO:C	2.62	0.42
1:E:210:ARG:CZ	1:E:414:PRO:HB3	2.49	0.42
1:E:537:LEU:HD23	1:E:537:LEU:HA	1.90	0.42
2:F:243:MET:HB3	3:G:152:ILE:HD13	2.01	0.42
3:G:43:TRP:O	3:G:44:ASP:C	2.59	0.42
4:H:84:MET:HA	4:H:84:MET:HE2	2.01	0.42
1:A:162:LYS:H	1:A:162:LYS:HG2	1.68	0.42
1:A:305:ARG:NH2	1:A:316:ASP:OD1	2.49	0.42
1:A:547:LEU:O	1:A:550:GLN:HB2	2.19	0.42
1:A:603:TRP:O	1:A:605:LYS:N	2.52	0.42
1:E:38:ILE:CG2	4:H:34:GLY:HA3	2.46	0.42
1:E:153:PHE:C	1:E:317:LEU:HD22	2.44	0.42
1:E:606:HIS:HD2	1:E:623:ARG:NH1	2.18	0.42
3:G:162:LEU:HA	3:G:162:LEU:HD22	1.75	0.42
4:H:93:THR:HA	4:H:132:LEU:HD23	2.02	0.42
1:A:95:ASN:HB2	1:A:96:PRO:HD2	2.02	0.42
1:A:242:ALA:HB2	1:A:552:LEU:HD22	2.01	0.42
11:G:202:RQX:H1	11:G:202:RQX:H9	1.82	0.42
4:H:65:PHE:CZ	4:H:94:LEU:HD23	2.55	0.42
1:A:148:ILE:HG21	1:A:170:CYS:HB3	2.01	0.42
1:A:614:ARG:CZ	1:A:614:ARG:HB3	2.49	0.42
3:C:43:TRP:CZ2	3:C:47:MET:HE3	2.54	0.42
4:H:77:TYR:O	12:H:201:EPH:H371	2.19	0.42
2:B:69:LEU:O	2:B:73:ILE:HG13	2.19	0.42
4:D:137:LEU:O	4:D:138:TYR:C	2.63	0.42
1:E:54:LEU:O	1:E:55:ARG:C	2.60	0.42
2:F:249:CYS:HA	2:F:250:PRO:HD2	1.81	0.42
1:A:567:LYS:HB3	1:A:578:PHE:CD1	2.55	0.42
1:E:390:MET:SD	1:E:390:MET:N	2.93	0.42
1:E:519:LYS:O	1:E:523:LEU:HD12	2.19	0.42
1:A:267:LEU:HA	1:A:394:PRO:HD3	2.02	0.42
1:E:510:GLY:H	1:E:577:ASP:CG	2.27	0.42
6:E:702:FAD:H9	6:E:702:FAD:H1'1	1.81	0.42
3:G:47:MET:HE2	3:G:47:MET:HA	2.01	0.42
3:G:112:ILE:H	3:G:112:ILE:HG13	1.73	0.42
1:A:333:GLU:CB	1:A:335:ARG:HH12	2.29	0.41
4:D:92:LEU:HD21	12:D:201:EPH:H222	2.02	0.41
1:E:73:MET:CE	1:E:78:SER:HA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:GLU:HB2	1:E:148:ILE:HD11	2.02	0.41
2:F:149:ILE:HG21	2:F:211:ALA:HB2	2.01	0.41
1:A:508:ARG:HH11	1:A:573:HIS:CD2	2.37	0.41
3:C:57:ALA:HA	3:C:58:PRO:HD2	1.89	0.41
3:C:134:ASN:O	3:C:137:ARG:HB3	2.20	0.41
4:D:57:THR:O	4:D:61:ILE:HG23	2.20	0.41
1:E:77:ARG:HD3	2:F:94:CYS:O	2.19	0.41
1:E:83:ALA:HA	6:E:702:FAD:C6	2.50	0.41
1:E:302:GLU:HG2	1:E:335:ARG:HG2	2.01	0.41
1:E:371:ALA:O	1:E:373:VAL:HG23	2.20	0.41
3:G:69:TRP:O	3:G:73:GLY:N	2.51	0.41
2:B:54:LEU:HD23	2:B:54:LEU:HA	1.79	0.41
2:B:244:ASN:OD1	3:C:69:TRP:HB3	2.19	0.41
1:E:72:LYS:HD3	6:E:702:FAD:C5A	2.50	0.41
2:F:105:ASN:O	2:F:106:THR:HB	2.21	0.41
2:F:230:MET:HE3	2:F:262:ILE:CG2	2.44	0.41
1:A:150:GLN:HA	1:A:169:THR:O	2.20	0.41
1:A:271:GLU:OE2	1:A:562:ALA:HB1	2.20	0.41
2:F:93:ILE:HD13	2:F:93:ILE:O	2.20	0.41
2:F:213:ARG:O	2:F:213:ARG:HD3	2.21	0.41
3:G:76:ARG:CG	10:G:201:HEM:O2D	2.55	0.41
3:C:97:PRO:O	3:C:98:LEU:C	2.64	0.41
3:C:170:VAL:HG11	12:D:201:EPH:H61	2.01	0.41
1:E:56:ALA:O	1:E:57:ALA:C	2.64	0.41
1:E:512:ILE:H	1:E:512:ILE:HG13	1.65	0.41
4:H:97:HIS:HE1	4:H:126:TYR:CE2	2.39	0.41
1:A:240:GLY:O	1:A:242:ALA:N	2.53	0.41
2:B:40:ILE:HD12	2:B:57:PHE:CD1	2.56	0.41
11:C:202:RQX:H6	4:D:106:ASP:OD2	2.20	0.41
1:E:215:ILE:HD11	1:E:224:ILE:HG21	2.01	0.41
1:E:228:ARG:NH1	1:E:463:PRO:O	2.53	0.41
1:E:239:TYR:OH	1:E:270:LEU:HD22	2.20	0.41
4:H:104:VAL:HG13	4:H:121:VAL:HG12	2.02	0.41
1:A:253:THR:HG22	1:A:552:LEU:HD12	2.03	0.41
1:A:258:ALA:O	1:A:262:ARG:HB2	2.20	0.41
1:A:584:GLU:OE2	1:A:584:GLU:N	2.54	0.41
2:F:75:ILE:HD13	2:F:75:ILE:HG21	1.80	0.41
2:F:86:ARG:CZ	2:F:136:VAL:HG13	2.51	0.41
4:H:154:TRP:CE2	12:H:201:EPH:H52	2.55	0.41
1:A:393:ILE:CG2	1:A:401:VAL:HG13	2.51	0.41
2:B:173:GLN:O	2:B:176:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:LYS:HE2	2:B:268:LYS:HB3	1.33	0.41
3:C:42:GLY:O	3:C:45:TYR:HB3	2.21	0.41
1:E:162:LYS:H	1:E:162:LYS:HG2	1.69	0.41
1:E:325:ARG:O	1:E:328:THR:N	2.52	0.41
1:E:553:MET:HA	1:E:553:MET:HE3	2.02	0.41
4:H:70:VAL:O	4:H:74:PRO:HD2	2.19	0.41
1:A:219:LEU:H	1:A:219:LEU:HD12	1.85	0.41
10:C:201:HEM:HHA	10:C:201:HEM:CBA	2.41	0.41
1:E:270:LEU:HD12	1:E:558:GLN:HB3	2.02	0.41
1:E:363:ILE:HG13	1:E:364:SER:H	1.86	0.41
1:E:465:LEU:HD23	1:E:465:LEU:HA	1.91	0.41
3:G:133:LEU:O	3:G:136:ILE:N	2.54	0.41
3:G:142:ASP:OD2	4:H:63:ARG:NH1	2.53	0.41
2:B:212:TYR:O	2:B:216:ILE:HG13	2.21	0.41
1:E:231:ARG:HH11	1:E:456:LEU:HD23	1.86	0.41
1:A:560:ILE:O	1:A:560:ILE:HG13	2.20	0.40
1:E:523:LEU:HA	1:E:526:GLU:HB2	2.02	0.40
1:A:276:HIS:CG	1:A:286:LEU:HD11	2.56	0.40
1:A:388:TYR:CZ	1:A:432:ARG:HD2	2.57	0.40
2:F:209:MET:HE3	2:F:258:ALA:HB2	2.02	0.40
1:A:557:THR:O	1:A:561:VAL:HG13	2.21	0.40
4:D:133:LEU:O	4:D:134:ALA:C	2.63	0.40
1:E:45:VAL:HG22	1:E:68:ALA:HB3	2.03	0.40
1:E:102:HIS:CE1	1:E:123:THR:HG22	2.56	0.40
1:E:269:ASP:O	1:E:271:GLU:N	2.54	0.40
1:E:270:LEU:O	1:E:559:THR:HG23	2.21	0.40
1:E:365:GLU:OE1	1:E:369:ILE:HD11	2.21	0.40
1:E:438:LEU:O	1:E:442:VAL:HG23	2.22	0.40
1:E:516:GLY:O	1:E:520:MET:HB2	2.21	0.40
2:F:268:LYS:HB3	2:F:268:LYS:HE2	1.38	0.40
1:A:78:SER:OG	6:A:702:FAD:C3B	2.68	0.40
1:A:561:VAL:HG11	1:A:618:ILE:HD12	2.04	0.40
1:E:276:HIS:HD2	1:E:387:HIS:CD2	2.39	0.40
2:F:244:ASN:HD21	3:G:66:GLN:HE21	1.68	0.40
1:A:162:LYS:O	1:A:163:GLY:O	2.38	0.40
1:A:262:ARG:HH22	1:A:551:ASN:ND2	2.18	0.40
1:A:555:ASN:O	1:A:559:THR:OG1	2.29	0.40
1:E:79:HIS:O	1:E:82:ALA:N	2.42	0.40
1:E:461:LYS:H	1:E:461:LYS:HG2	1.68	0.40
2:F:128:HIS:O	2:F:128:HIS:ND1	2.54	0.40
2:F:128:HIS:HA	3:G:56:ILE:HG23	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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	611/645 (95%)	531 (87%)	68 (11%)	12 (2%)	6	19
1	E	611/645 (95%)	540 (88%)	56 (9%)	15 (2%)	4	15
2	B	247/282 (88%)	214 (87%)	26 (10%)	7 (3%)	4	13
2	F	247/282 (88%)	206 (83%)	33 (13%)	8 (3%)	3	10
3	C	151/188 (80%)	127 (84%)	18 (12%)	6 (4%)	2	7
3	G	148/188 (79%)	127 (86%)	18 (12%)	3 (2%)	6	19
4	D	127/156 (81%)	109 (86%)	16 (13%)	2 (2%)	7	24
4	H	127/156 (81%)	105 (83%)	18 (14%)	4 (3%)	3	11
All	All	2269/2542 (89%)	1959 (86%)	253 (11%)	57 (2%)	4	15

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	TYR
1	A	163	GLY
1	A	372	GLY
1	A	485	GLY
2	B	161	LEU
3	C	97	PRO
3	C	98	LEU
4	D	47	LYS
1	E	485	GLY
1	E	591	ILE
2	F	158	LYS
2	F	280	ALA
3	G	98	LEU
4	H	50	LYS

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Mol	Chain	Res	Type
1	A	539	TRP
2	B	109	CYS
2	B	243	MET
2	B	280	ALA
3	C	111	GLY
1	E	51	GLY
1	E	269	ASP
1	E	305	ARG
1	E	426	SER
2	F	268	LYS
3	G	48	ARG
4	H	48	GLY
4	H	82	ARG
1	A	159	ASN
1	A	241	ARG
1	A	330	GLU
1	A	469	ALA
1	A	592	GLU
3	C	58	PRO
4	D	51	PRO
1	E	63	ALA
1	E	109	GLY
1	E	254	GLY
1	E	270	LEU
1	E	463	PRO
2	F	213	ARG
1	A	604	ARG
2	B	218	SER
1	E	539	TRP
2	F	49	GLY
2	F	116	ASN
2	F	218	SER
4	H	46	GLU
2	B	199	ALA
3	C	87	LEU
1	E	125	ASN
2	F	277	PRO
1	E	483	ALA
3	G	123	ILE
2	B	81	PRO
3	C	88	ILE
1	A	589	LYS

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Mol	Chain	Res	Type
1	E	53	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	498/526 (95%)	419 (84%)	79 (16%)	2	8
1	E	498/526 (95%)	423 (85%)	75 (15%)	3	9
2	B	219/242 (90%)	173 (79%)	46 (21%)	1	3
2	F	219/242 (90%)	176 (80%)	43 (20%)	1	4
3	C	127/158 (80%)	98 (77%)	29 (23%)	1	3
3	G	124/158 (78%)	99 (80%)	25 (20%)	1	4
4	D	96/119 (81%)	76 (79%)	20 (21%)	1	4
4	H	96/119 (81%)	79 (82%)	17 (18%)	2	6
All	All	1877/2090 (90%)	1543 (82%)	334 (18%)	2	6

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	62	GLU
1	A	76	THR
1	A	117	ASN
1	A	143	THR
1	A	147	LYS
1	A	152	SER
1	A	153	PHE
1	A	162	LYS
1	A	165	VAL
1	A	175	ARG
1	A	194	THR
1	A	205	LEU
1	A	208	LYS

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Mol	Chain	Res	Type
1	A	228	ARG
1	A	230	LYS
1	A	241	ARG
1	A	257	THR
1	A	261	THR
1	A	271	GLU
1	A	274	GLN
1	A	283	VAL
1	A	298	LEU
1	A	302	GLU
1	A	308	GLU
1	A	320	ARG
1	A	328	THR
1	A	335	ARG
1	A	337	VAL
1	A	340	GLU
1	A	344	ILE
1	A	347	GLN
1	A	351	LEU
1	A	354	GLU
1	A	356	LEU
1	A	359	ARG
1	A	368	LYS
1	A	375	VAL
1	A	377	LYS
1	A	385	THR
1	A	390	MET
1	A	412	ILE
1	A	425	HIS
1	A	426	SER
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP
1	A	446	ARG
1	A	453	LYS
1	A	454	GLU
1	A	456	LEU
1	A	457	LYS
1	A	459	ASP
1	A	467	GLU
1	A	474	ILE
1	A	484	ASN

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Mol	Chain	Res	Type
1	A	487	VAL
1	A	491	GLU
1	A	496	MET
1	A	515	GLU
1	A	519	LYS
1	A	523	LEU
1	A	526	GLU
1	A	528	LYS
1	A	531	LYS
1	A	533	THR
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	561	VAL
1	A	583	ASP
1	A	584	GLU
1	A	596	LYS
1	A	601	LYS
1	A	610	LYS
1	A	618	ILE
1	A	628	LYS
1	A	637	TRP
1	A	642	ILE
2	B	34	ARG
2	B	37	THR
2	B	42	ARG
2	B	46	GLU
2	B	47	GLU
2	B	53	LYS
2	B	59	VAL
2	B	63	LYS
2	B	69	LEU
2	B	75	ILE
2	B	87	ARG
2	B	90	ARG
2	B	93	ILE
2	B	100	ASN
2	B	106	THR
2	B	116	ASN
2	B	120	THR
2	B	122	LYS
2	B	123	ILE

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Mol	Chain	Res	Type
2	B	129	MET
2	B	148	SER
2	B	156	LYS
2	B	157	THR
2	B	159	ILE
2	B	161	LEU
2	B	164	LYS
2	B	165	GLN
2	B	166	GLN
2	B	170	ILE
2	B	173	GLN
2	B	176	LEU
2	B	184	LEU
2	B	209	MET
2	B	210	GLN
2	B	215	ILE
2	B	216	ILE
2	B	235	SER
2	B	238	LYS
2	B	241	THR
2	B	247	LYS
2	B	248	THR
2	B	266	LEU
2	B	268	LYS
2	B	269	MET
2	B	276	LEU
2	B	281	ASN
3	C	34	GLU
3	C	50	ARG
3	C	53	LYS
3	C	56	ILE
3	C	59	HIS
3	C	60	LEU
3	C	61	THR
3	C	67	MET
3	C	76	ARG
3	C	77	VAL
3	C	85	THR
3	C	87	LEU
3	C	88	ILE
3	C	91	VAL
3	C	94	SER

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Mol	Chain	Res	Type
3	C	96	LEU
3	C	98	LEU
3	C	99	ASP
3	C	104	VAL
3	C	107	ILE
3	C	115	VAL
3	C	133	LEU
3	C	145	LYS
3	C	149	ILE
3	C	160	LEU
3	C	162	LEU
3	C	172	VAL
3	C	175	ARG
3	C	177	GLU
4	D	49	PHE
4	D	50	LYS
4	D	57	THR
4	D	58	LEU
4	D	61	ILE
4	D	73	ILE
4	D	79	ILE
4	D	83	GLU
4	D	86	LEU
4	D	90	LEU
4	D	92	LEU
4	D	109	ARG
4	D	112	VAL
4	D	116	THR
4	D	122	ARG
4	D	123	VAL
4	D	136	LEU
4	D	144	VAL
4	D	154	TRP
4	D	156	LEU
1	E	34	GLN
1	E	36	LYS
1	E	44	VAL
1	E	76	THR
1	E	80	THR
1	E	87	ILE
1	E	94	MET
1	E	117	ASN

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Mol	Chain	Res	Type
1	E	142	ARG
1	E	153	PHE
1	E	162	LYS
1	E	165	VAL
1	E	179	SER
1	E	192	HIS
1	E	194	THR
1	E	197	ILE
1	E	203	ASP
1	E	205	LEU
1	E	214	VAL
1	E	230	LYS
1	E	261	THR
1	E	265	ILE
1	E	273	ILE
1	E	274	GLN
1	E	283	VAL
1	E	298	LEU
1	E	302	GLU
1	E	313	LYS
1	E	319	SER
1	E	337	VAL
1	E	351	LEU
1	E	356	LEU
1	E	358	GLN
1	E	359	ARG
1	E	360	LEU
1	E	363	ILE
1	E	368	LYS
1	E	377	LYS
1	E	390	MET
1	E	406	LYS
1	E	411	LYS
1	E	422	CYS
1	E	425	HIS
1	E	426	SER
1	E	436	ASN
1	E	440	ASP
1	E	453	LYS
1	E	454	GLU
1	E	456	LEU
1	E	461	LYS

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Mol	Chain	Res	Type
1	E	474	ILE
1	E	484	ASN
1	E	487	VAL
1	E	496	MET
1	E	502	LYS
1	E	511	ASP
1	E	512	ILE
1	E	515	GLU
1	E	527	LEU
1	E	530	LEU
1	E	535	ARG
1	E	547	LEU
1	E	561	VAL
1	E	577	ASP
1	E	584	GLU
1	E	591	ILE
1	E	596	LYS
1	E	597	ARG
1	E	610	LYS
1	E	620	LEU
1	E	625	VAL
1	E	637	TRP
1	E	641	ILE
1	E	642	ILE
1	E	644	SER
2	F	34	ARG
2	F	37	THR
2	F	63	LYS
2	F	66	THR
2	F	69	LEU
2	F	73	ILE
2	F	75	ILE
2	F	90	ARG
2	F	93	ILE
2	F	100	ASN
2	F	115	GLN
2	F	117	THR
2	F	119	LYS
2	F	121	THR
2	F	122	LYS
2	F	123	ILE
2	F	129	MET

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Mol	Chain	Res	Type
2	F	148	SER
2	F	150	GLN
2	F	154	GLN
2	F	157	THR
2	F	158	LYS
2	F	159	ILE
2	F	163	GLU
2	F	170	ILE
2	F	173	GLN
2	F	176	LEU
2	F	184	LEU
2	F	209	MET
2	F	215	ILE
2	F	216	ILE
2	F	231	GLN
2	F	238	LYS
2	F	241	THR
2	F	244	ASN
2	F	247	LYS
2	F	248	THR
2	F	259	ILE
2	F	266	LEU
2	F	268	LYS
2	F	276	LEU
2	F	278	THR
2	F	281	ASN
3	G	34	GLU
3	G	50	ARG
3	G	56	ILE
3	G	59	HIS
3	G	67	MET
3	G	68	THR
3	G	71	VAL
3	G	77	VAL
3	G	91	VAL
3	G	101	THR
3	G	107	ILE
3	G	108	ARG
3	G	112	ILE
3	G	116	ILE
3	G	133	LEU
3	G	149	ILE

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Mol	Chain	Res	Type
3	G	159	VAL
3	G	160	LEU
3	G	162	LEU
3	G	165	LEU
3	G	170	VAL
3	G	171	VAL
3	G	172	VAL
3	G	175	ARG
3	G	177	GLU
4	H	46	GLU
4	H	50	LYS
4	H	57	THR
4	H	58	LEU
4	H	61	ILE
4	H	73	ILE
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	93	THR
4	H	100	VAL
4	H	104	VAL
4	H	109	ARG
4	H	117	LEU
4	H	122	ARG
4	H	123	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	150	GLN
1	A	252	ASN
1	A	349	HIS
1	A	355	GLN
1	A	389	ASN
1	A	428	HIS
1	A	431	ASN

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Mol	Chain	Res	Type
1	A	436	ASN
1	A	451	ASN
1	A	497	GLN
1	A	503	HIS
1	A	550	GLN
1	A	551	ASN
1	A	565	ASN
1	A	573	HIS
1	A	594	GLN
1	A	606	HIS
2	B	44	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	112	ASN
2	B	115	GLN
2	B	116	ASN
2	B	145	GLN
2	B	165	GLN
2	B	166	GLN
2	B	173	GLN
2	B	210	GLN
2	B	240	HIS
2	B	281	ASN
3	C	66	GLN
4	D	140	ASN
4	D	142	HIS
1	E	88	ASN
1	E	95	ASN
1	E	117	ASN
1	E	120	HIS
1	E	125	ASN
1	E	150	GLN
1	E	156	GLN
1	E	159	ASN
1	E	274	GLN
1	E	355	GLN
1	E	431	ASN
1	E	436	ASN
1	E	451	ASN
1	E	497	GLN
1	E	503	HIS

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Mol	Chain	Res	Type
1	E	550	GLN
1	E	551	ASN
1	E	555	ASN
1	E	573	HIS
1	E	606	HIS
2	F	100	ASN
2	F	105	ASN
2	F	112	ASN
2	F	116	ASN
2	F	145	GLN
2	F	150	GLN
2	F	165	GLN
2	F	166	GLN
2	F	168	GLN
2	F	244	ASN
2	F	281	ASN
3	G	66	GLN
4	H	140	ASN

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](#)

16 ligands are modelled in this entry.

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	$\# Z > 2$
12	EPH	H	201	-	43,43,48	1.91	9 (20%)	46,48,53	2.42	5 (10%)
12	EPH	D	201	-	43,43,48	1.91	9 (20%)	46,48,53	2.48	6 (13%)
5	MLI	A	701	-	6,6,6	4.70	2 (33%)	7,7,7	1.32	0
11	RQX	C	202	-	19,19,19	2.18	3 (15%)	19,26,26	2.83	6 (31%)
7	FES	B	301	2	0,4,4	-	-	-	-	-
9	F3S	F	303	2	0,9,9	-	-	-	-	-
10	HEM	C	201	4,3	50,50,50	1.86	10 (20%)	67,82,82	1.41	6 (8%)
6	FAD	E	702	-	58,58,58	1.25	6 (10%)	85,89,89	1.87	22 (25%)
9	F3S	B	303	2	0,9,9	-	-	-	-	-
8	SF4	B	302	2	0,12,12	-	-	-	-	-
10	HEM	G	201	4,3	50,50,50	1.87	9 (18%)	67,82,82	1.40	7 (10%)
11	RQX	G	202	-	19,19,19	2.47	2 (10%)	19,26,26	2.33	5 (26%)
8	SF4	F	302	2	0,12,12	-	-	-	-	-
7	FES	F	301	2	0,4,4	-	-	-	-	-
5	MLI	E	701	-	6,6,6	4.57	1 (16%)	7,7,7	1.70	1 (14%)
6	FAD	A	702	-	58,58,58	1.24	7 (12%)	85,89,89	1.92	25 (29%)

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
12	EPH	H	201	-	-	24/47/47/52	-
12	EPH	D	201	-	-	28/47/47/52	-
5	MLI	A	701	-	-	2/4/4/4	-
11	RQX	C	202	-	-	6/10/34/34	0/1/1/1
7	FES	B	301	2	-	-	0/1/1/1
9	F3S	F	303	2	-	-	0/3/3/3
10	HEM	C	201	4,3	-	8/14/54/54	-
6	FAD	E	702	-	-	12/34/50/50	0/6/6/6
9	F3S	B	303	2	-	-	0/3/3/3
8	SF4	B	302	2	-	-	0/6/5/5
10	HEM	G	201	4,3	-	12/14/54/54	-
11	RQX	G	202	-	-	6/10/34/34	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	F	301	2	-	-	0/1/1/1
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	A	702	-	-	11/34/50/50	0/6/6/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	MLI	C1-C2	-10.97	1.34	1.51
5	E	701	MLI	C1-C2	-10.75	1.34	1.51
11	G	202	RQX	C3-C2	8.13	1.49	1.35
10	G	201	HEM	C3D-C2D	7.65	1.53	1.36
10	C	201	HEM	C3D-C2D	7.61	1.53	1.36
12	D	201	EPH	C29-C28	7.11	1.72	1.31
12	H	201	EPH	C29-C28	6.93	1.71	1.31
11	C	202	RQX	C3-C2	6.74	1.47	1.35
10	C	201	HEM	FE-ND	5.71	2.12	1.94
11	G	202	RQX	C6-C5	5.33	1.50	1.40
11	C	202	RQX	C6-C5	5.20	1.50	1.40
10	G	201	HEM	FE-NA	5.10	2.12	1.95
10	G	201	HEM	FE-ND	4.56	2.08	1.94
6	E	702	FAD	C4X-N5	4.56	1.40	1.30
12	D	201	EPH	C18-C4	-4.05	1.38	1.50
12	H	201	EPH	C25-C24	4.00	1.54	1.31
6	A	702	FAD	C4X-N5	3.90	1.39	1.30
12	H	201	EPH	C13-C12	3.89	1.53	1.31
12	D	201	EPH	C13-C12	3.82	1.53	1.31
12	H	201	EPH	C18-C4	-3.81	1.39	1.50
12	D	201	EPH	C25-C24	3.70	1.52	1.31
12	D	201	EPH	C15-C16	3.43	1.54	1.29
6	A	702	FAD	P-O3P	3.34	1.63	1.59
12	H	201	EPH	C15-C16	3.32	1.53	1.29
12	H	201	EPH	P1-O7	3.15	1.61	1.50
12	D	201	EPH	C27-C28	-3.04	1.33	1.50
6	A	702	FAD	C2A-N3A	3.03	1.39	1.33
6	A	702	FAD	C2A-N1A	2.99	1.39	1.33
12	H	201	EPH	C27-C28	-2.97	1.33	1.50
10	C	201	HEM	CAC-C3C	2.94	1.55	1.47
12	D	201	EPH	P1-O7	2.85	1.60	1.50
10	G	201	HEM	FE-NB	2.85	2.03	1.94
6	E	702	FAD	C2A-N3A	2.76	1.38	1.33
10	G	201	HEM	CAB-C3B	2.75	1.54	1.47
10	C	201	HEM	FE-NB	2.70	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	201	HEM	CAB-C3B	2.66	1.54	1.47
12	H	201	EPH	C26-C25	2.65	1.64	1.50
12	D	201	EPH	C26-C25	2.64	1.64	1.50
5	A	701	MLI	C1-C3	-2.55	1.47	1.51
6	E	702	FAD	C5A-N7A	-2.41	1.34	1.39
10	G	201	HEM	CAC-C3C	2.38	1.53	1.47
10	C	201	HEM	FE-NC	2.38	2.03	1.95
6	E	702	FAD	O4B-C4B	-2.30	1.39	1.45
10	G	201	HEM	CMC-C2C	2.29	1.55	1.50
11	C	202	RQX	C3-C4	2.28	1.52	1.46
6	E	702	FAD	C10-N1	2.28	1.37	1.33
10	C	201	HEM	CAD-C3D	2.27	1.57	1.51
10	C	201	HEM	CMC-C2C	2.22	1.55	1.50
6	A	702	FAD	C9A-N10	-2.22	1.37	1.41
10	G	201	HEM	CAD-C3D	2.17	1.56	1.51
12	H	201	EPH	C10-C11	-2.14	1.43	1.52
6	A	702	FAD	C4X-C10	-2.13	1.37	1.44
6	A	702	FAD	C10-N1	2.12	1.37	1.33
10	C	201	HEM	C3B-C2B	-2.08	1.32	1.37
10	C	201	HEM	CMB-C2B	2.08	1.55	1.50
10	G	201	HEM	CMB-C2B	2.08	1.55	1.50
6	E	702	FAD	C2A-N1A	2.02	1.37	1.33
12	D	201	EPH	C5-C3	2.01	1.56	1.50

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C27-C26-C25	12.90	145.13	112.73
12	D	201	EPH	C27-C26-C25	12.29	143.60	112.73
11	C	202	RQX	C9-C3-C4	7.09	126.75	118.52
12	D	201	EPH	C2-O1-C3	6.27	132.81	117.80
11	C	202	RQX	C9-C3-C2	-6.25	114.17	124.89
6	E	702	FAD	N3A-C2A-N1A	-5.93	119.60	128.58
11	G	202	RQX	C9-C3-C4	5.78	125.23	118.52
6	A	702	FAD	N3A-C2A-N1A	-5.76	119.87	128.58
12	H	201	EPH	C15-C14-C13	5.51	139.16	112.02
12	D	201	EPH	C15-C14-C13	5.51	139.13	112.02
11	C	202	RQX	C1-C2-C3	-5.49	115.42	124.45
6	E	702	FAD	C5A-C4A-N3A	-5.26	119.47	126.72
6	A	702	FAD	C4'-C3'-C2'	-5.18	104.95	113.57
10	C	201	HEM	CAD-C3D-C4D	5.03	133.47	124.70
10	G	201	HEM	CAD-C3D-C4D	4.79	133.04	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	202	RQX	C9-C3-C2	-4.59	117.02	124.89
10	G	201	HEM	C4D-ND-C1D	4.52	110.56	105.21
6	E	702	FAD	O2'-C2'-C3'	-4.30	99.19	109.25
10	C	201	HEM	C4D-ND-C1D	4.25	110.24	105.21
6	A	702	FAD	N9A-C8A-N7A	-4.07	108.16	113.94
6	A	702	FAD	C5A-C4A-N3A	-3.90	121.35	126.72
6	E	702	FAD	C2A-N3A-C4A	3.84	121.22	111.83
6	E	702	FAD	C9A-C5X-N5	-3.67	118.56	122.45
6	A	702	FAD	C4-C4X-N5	3.56	123.13	118.21
11	G	202	RQX	C1-C2-C3	-3.56	118.59	124.45
12	H	201	EPH	C2-O1-C3	3.56	126.31	117.80
6	E	702	FAD	N9A-C8A-N7A	-3.50	108.97	113.94
6	E	702	FAD	C5A-N7A-C8A	3.49	108.93	103.45
12	D	201	EPH	C14-C15-C16	3.39	152.22	123.74
6	A	702	FAD	C5A-N7A-C8A	3.37	108.74	103.45
6	A	702	FAD	C10-C4X-N5	-3.31	118.04	124.81
6	A	702	FAD	C4-N3-C2	-3.31	119.77	125.64
6	A	702	FAD	C2A-N3A-C4A	3.28	119.83	111.83
10	G	201	HEM	CHC-C4B-NB	3.20	127.87	124.42
6	E	702	FAD	N3A-C4A-N9A	3.19	132.60	127.17
6	A	702	FAD	C4X-C10-N10	3.14	120.97	116.48
11	G	202	RQX	C3-C2-C7	3.12	121.63	119.17
12	H	201	EPH	C14-C15-C16	3.11	149.90	123.74
5	E	701	MLI	C3-C1-C2	3.11	123.92	112.95
6	A	702	FAD	O3'-C3'-C4'	3.10	115.98	108.93
6	A	702	FAD	O3B-C3B-C4B	-3.02	102.42	111.08
6	E	702	FAD	C4-C4X-N5	3.01	122.36	118.21
6	A	702	FAD	C9A-C5X-N5	-3.00	119.28	122.45
6	E	702	FAD	C10-C4X-N5	-2.99	118.70	124.81
6	A	702	FAD	O2-C2-N1	-2.93	116.94	121.80
11	C	202	RQX	C12-C11-C13	2.82	120.11	115.23
10	C	201	HEM	CBD-CAD-C3D	2.80	120.27	112.53
6	E	702	FAD	C1'-C2'-C3'	2.79	117.23	109.66
6	A	702	FAD	O2'-C2'-C3'	-2.76	102.80	109.25
12	H	201	EPH	O2-C4-C18	2.76	120.24	111.83
6	A	702	FAD	N3A-C4A-N9A	2.69	131.74	127.17
10	C	201	HEM	C4D-C3D-C2D	-2.68	102.99	106.89
6	E	702	FAD	C8M-C8-C9	-2.65	114.90	119.57
6	A	702	FAD	C4A-N9A-C8A	2.64	108.52	105.74
6	E	702	FAD	C5X-C9A-N10	2.63	120.35	117.97
6	E	702	FAD	C4A-C5A-N7A	-2.62	107.58	110.58
10	G	201	HEM	CAD-C3D-C2D	-2.61	122.98	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	C4X-C4-N3	2.58	119.81	113.25
6	A	702	FAD	C4A-C5A-N7A	-2.54	107.68	110.58
11	C	202	RQX	C7-C6-N	2.53	120.79	114.40
10	G	201	HEM	CBD-CAD-C3D	2.52	119.51	112.53
6	E	702	FAD	C4-N3-C2	-2.48	121.24	125.64
11	G	202	RQX	C10-C9-C3	2.47	118.16	112.08
6	E	702	FAD	O2A-PA-O3P	2.40	113.75	107.27
10	G	201	HEM	C4C-C3C-C2C	2.33	108.83	106.81
10	C	201	HEM	CAD-C3D-C2D	-2.31	123.54	127.87
12	D	201	EPH	O2-C4-C18	2.30	118.85	111.83
6	E	702	FAD	C4X-C10-N10	2.29	119.77	116.48
12	D	201	EPH	C30-C29-C28	-2.25	112.86	126.42
11	C	202	RQX	C1-C2-C7	2.24	124.60	116.93
6	E	702	FAD	C6A-C5A-C4A	2.24	120.24	117.18
6	E	702	FAD	C4'-C3'-C2'	-2.24	109.84	113.57
6	E	702	FAD	C5X-N5-C4X	2.22	121.68	118.09
6	A	702	FAD	O2-C2-N3	2.21	122.83	118.58
6	A	702	FAD	C5X-N5-C4X	2.18	121.61	118.09
6	A	702	FAD	O2B-C2B-C3B	2.13	118.64	111.82
10	C	201	HEM	O2D-CGD-CBD	2.11	120.66	114.00
6	E	702	FAD	C6-C5X-N5	2.05	121.85	118.44
6	E	702	FAD	O4B-C1B-C2B	-2.05	102.23	106.62
6	A	702	FAD	C1'-C2'-C3'	2.04	115.18	109.66
6	A	702	FAD	C10-N1-C2	2.03	121.23	116.85
6	A	702	FAD	O4-C4-C4X	-2.02	121.19	126.53
10	G	201	HEM	C4D-C3D-C2D	-2.00	103.98	106.89

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	C1'-C2'-C3'-O3'
6	A	702	FAD	C1'-C2'-C3'-C4'
6	A	702	FAD	O2'-C2'-C3'-O3'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	C3'-C4'-C5'-O5'
6	E	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	C5'-O5'-P-O2P
6	E	702	FAD	C5'-O5'-P-O3P
10	C	201	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
10	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD
10	G	201	HEM	C1A-C2A-CAA-CBA
10	G	201	HEM	C2B-C3B-CAB-CBB
10	G	201	HEM	C2C-C3C-CAC-CBC
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
10	G	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	C37-C2-O1-C3
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	C37-O5-P1-O6
12	D	201	EPH	C37-O5-P1-O8
12	D	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O2-C1-C2-O1
12	H	201	EPH	C25-C26-C27-C28
12	H	201	EPH	C14-C15-C16-C17
12	H	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O8-C38-C39-N1
11	G	202	RQX	C11-C13-C14-C15
6	A	702	FAD	O2'-C2'-C3'-C4'
12	D	201	EPH	C23-C24-C25-C26
12	D	201	EPH	C18-C4-O2-C1
11	C	202	RQX	C11-C13-C14-C15
12	D	201	EPH	C27-C28-C29-C30
12	D	201	EPH	C11-C12-C13-C14
12	D	201	EPH	O4-C4-O2-C1
10	C	201	HEM	C1A-C2A-CAA-CBA
10	C	201	HEM	C3D-CAD-CBD-CGD
12	H	201	EPH	C5-C6-C7-C8
12	D	201	EPH	C18-C19-C20-C21
12	H	201	EPH	C18-C19-C20-C21
12	H	201	EPH	C20-C21-C22-C23
12	H	201	EPH	C7-C8-C9-C10
12	H	201	EPH	C23-C24-C25-C26
12	H	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C6-C7-C8-C9
10	G	201	HEM	C3A-C2A-CAA-CBA
12	H	201	EPH	C28-C29-C30-C31
12	D	201	EPH	C5-C3-O1-C2
10	C	201	HEM	C4C-C3C-CAC-CBC
10	G	201	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
10	G	201	HEM	C4C-C3C-CAC-CBC
6	A	702	FAD	C3'-C4'-C5'-O5'
12	D	201	EPH	C5-C6-C7-C8
12	D	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C3-C5-C6-C7
12	D	201	EPH	C1-C2-C37-O5
11	C	202	RQX	C12-C11-C13-C14
12	D	201	EPH	C14-C15-C16-C17
12	D	201	EPH	O1-C2-C37-O5
12	H	201	EPH	O1-C2-C37-O5
12	H	201	EPH	C21-C22-C23-C24
12	H	201	EPH	C13-C14-C15-C16
11	G	202	RQX	C12-C11-C13-C14
11	C	202	RQX	C10-C11-C13-C14
11	G	202	RQX	C10-C11-C13-C14
6	A	702	FAD	PA-O3P-P-O5'
6	E	702	FAD	PA-O3P-P-O5'
12	D	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C1-C2-C37-O5
11	G	202	RQX	C2-C3-C9-C10
10	C	201	HEM	C4B-C3B-CAB-CBB
11	C	202	RQX	C4-C3-C9-C10
11	G	202	RQX	C4-C3-C9-C10
12	D	201	EPH	C7-C8-C9-C10
10	C	201	HEM	C3A-C2A-CAA-CBA
6	A	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	N10-C1'-C2'-C3'
12	D	201	EPH	C26-C27-C28-C29
12	H	201	EPH	C26-C27-C28-C29
12	H	201	EPH	O2-C1-C2-C37
11	C	202	RQX	C4-C5-O3-C8
6	E	702	FAD	C5B-O5B-PA-O1A
6	E	702	FAD	C5'-O5'-P-O1P
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	C38-O8-P1-O6
12	H	201	EPH	C38-O8-P1-O5
12	H	201	EPH	C38-O8-P1-O6
12	H	201	EPH	C3-C5-C6-C7
5	A	701	MLI	C2-C1-C3-O8
5	A	701	MLI	C2-C1-C3-O9
10	G	201	HEM	CAA-CBA-CGA-O1A
12	H	201	EPH	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
10	G	201	HEM	CAA-CBA-CGA-O2A
12	D	201	EPH	C12-C13-C14-C15
11	G	202	RQX	C4-C5-O3-C8
12	H	201	EPH	C11-C12-C13-C14
12	D	201	EPH	C11-C10-C9-C8
11	C	202	RQX	C2-C3-C9-C10
12	D	201	EPH	C22-C23-C24-C25
12	H	201	EPH	C24-C25-C26-C27
6	A	702	FAD	P-O3P-PA-O1A
6	E	702	FAD	P-O3P-PA-O1A
6	E	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	N10-C1'-C2'-O2'
10	G	201	HEM	CAD-CBD-CGD-O2D
6	E	702	FAD	O4B-C4B-C5B-O5B

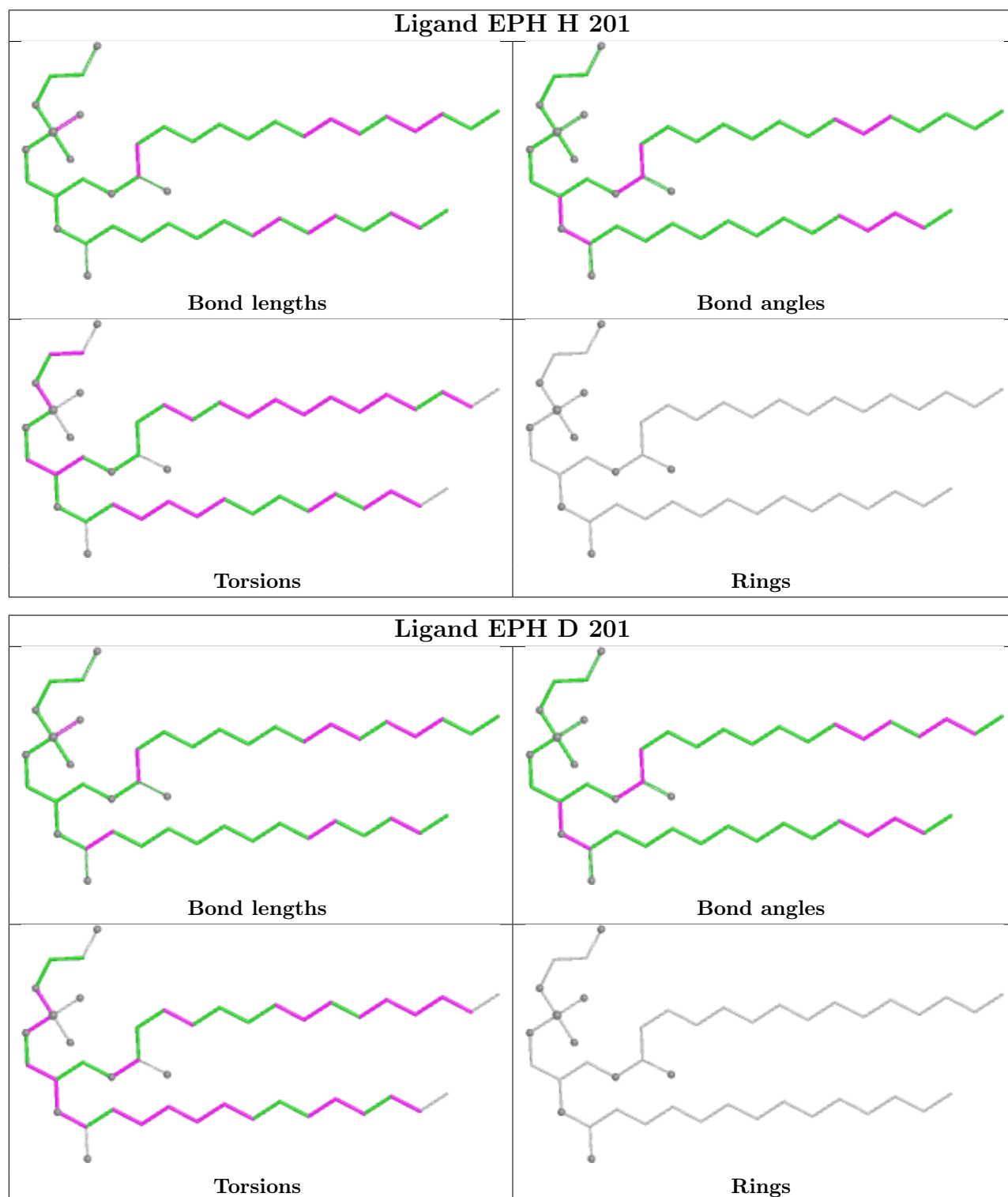
There are no ring outliers.

12 monomers are involved in 77 short contacts:

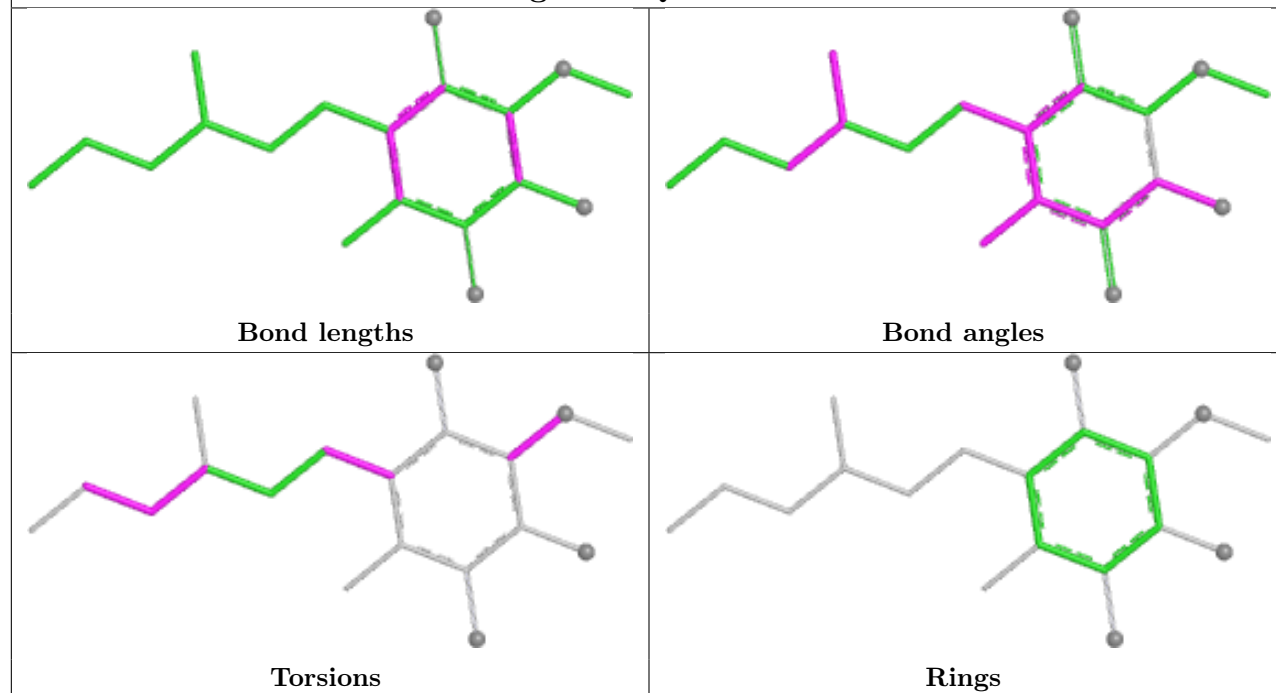
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	201	EPH	8	0
12	D	201	EPH	6	0
5	A	701	MLI	2	0
11	C	202	RQX	8	0
7	B	301	FES	1	0
10	C	201	HEM	17	0
6	E	702	FAD	10	0
9	B	303	F3S	1	0
8	B	302	SF4	1	0
10	G	201	HEM	9	0
11	G	202	RQX	7	0
6	A	702	FAD	7	0

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 than 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.

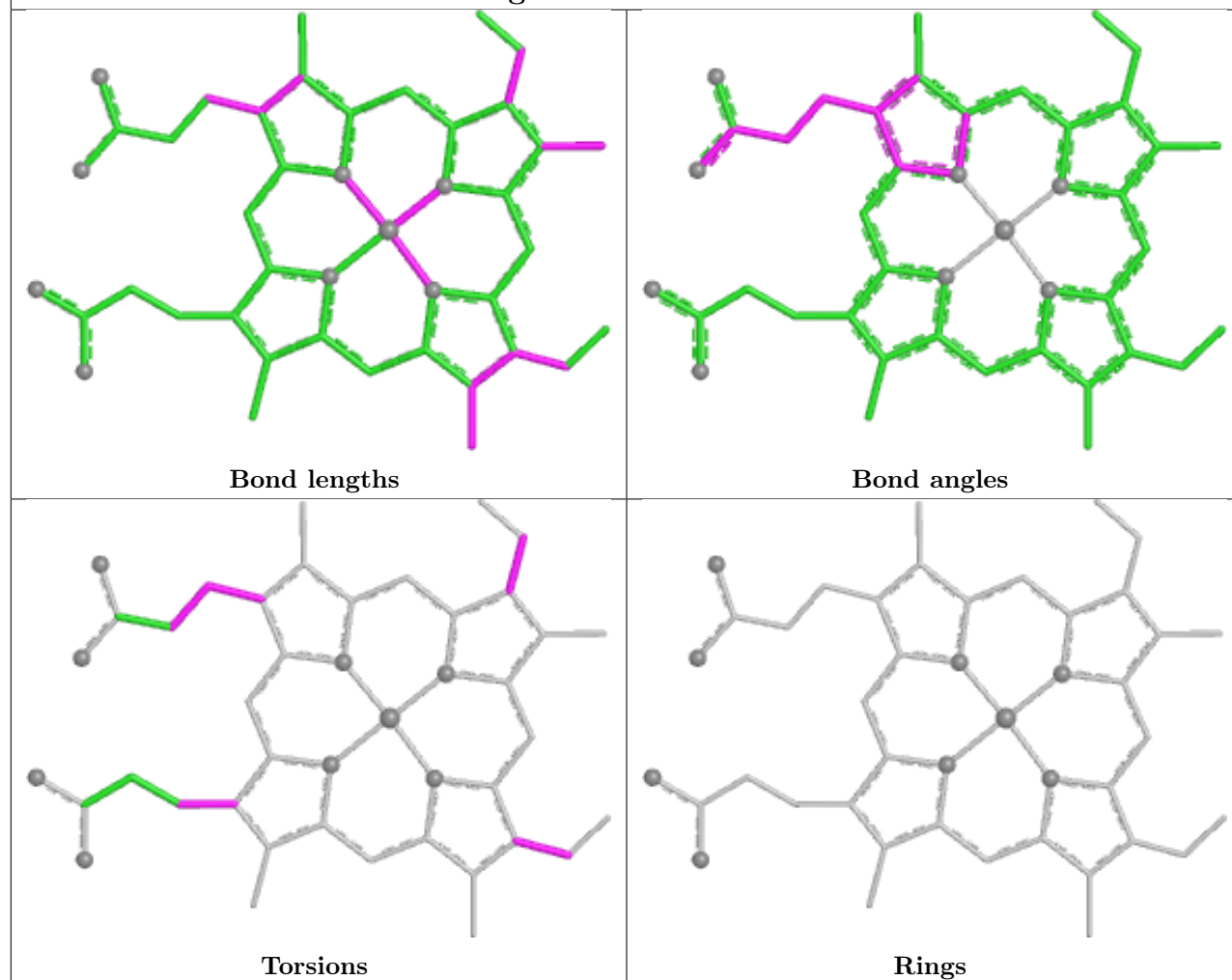
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

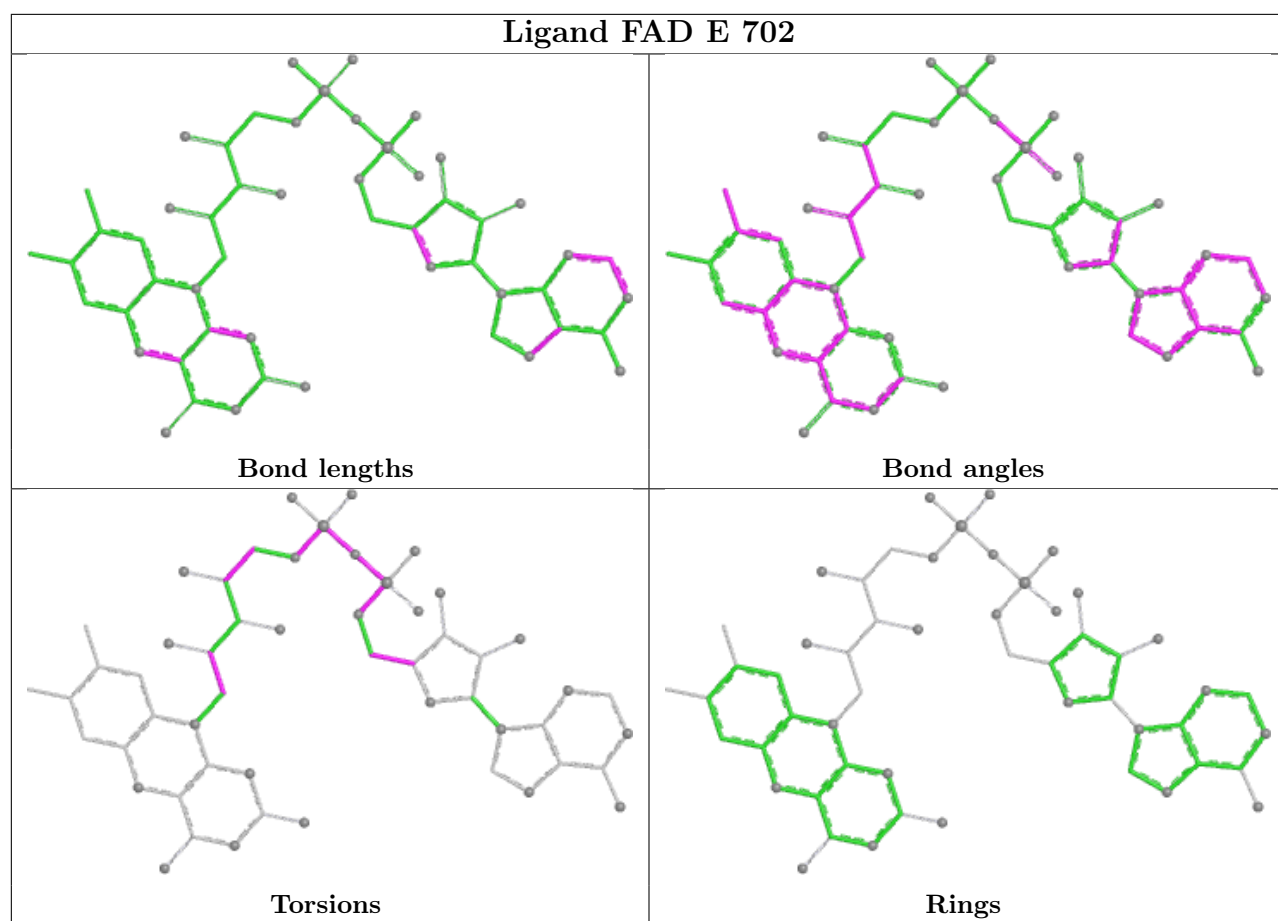


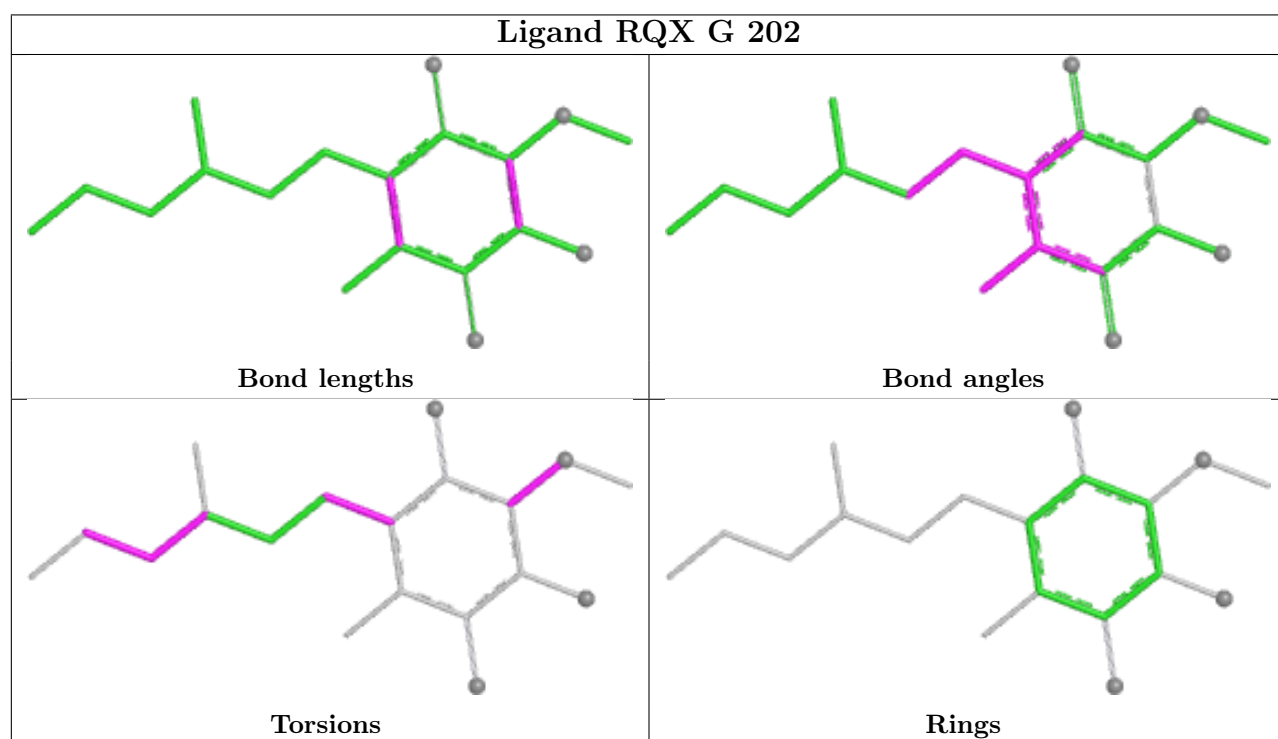
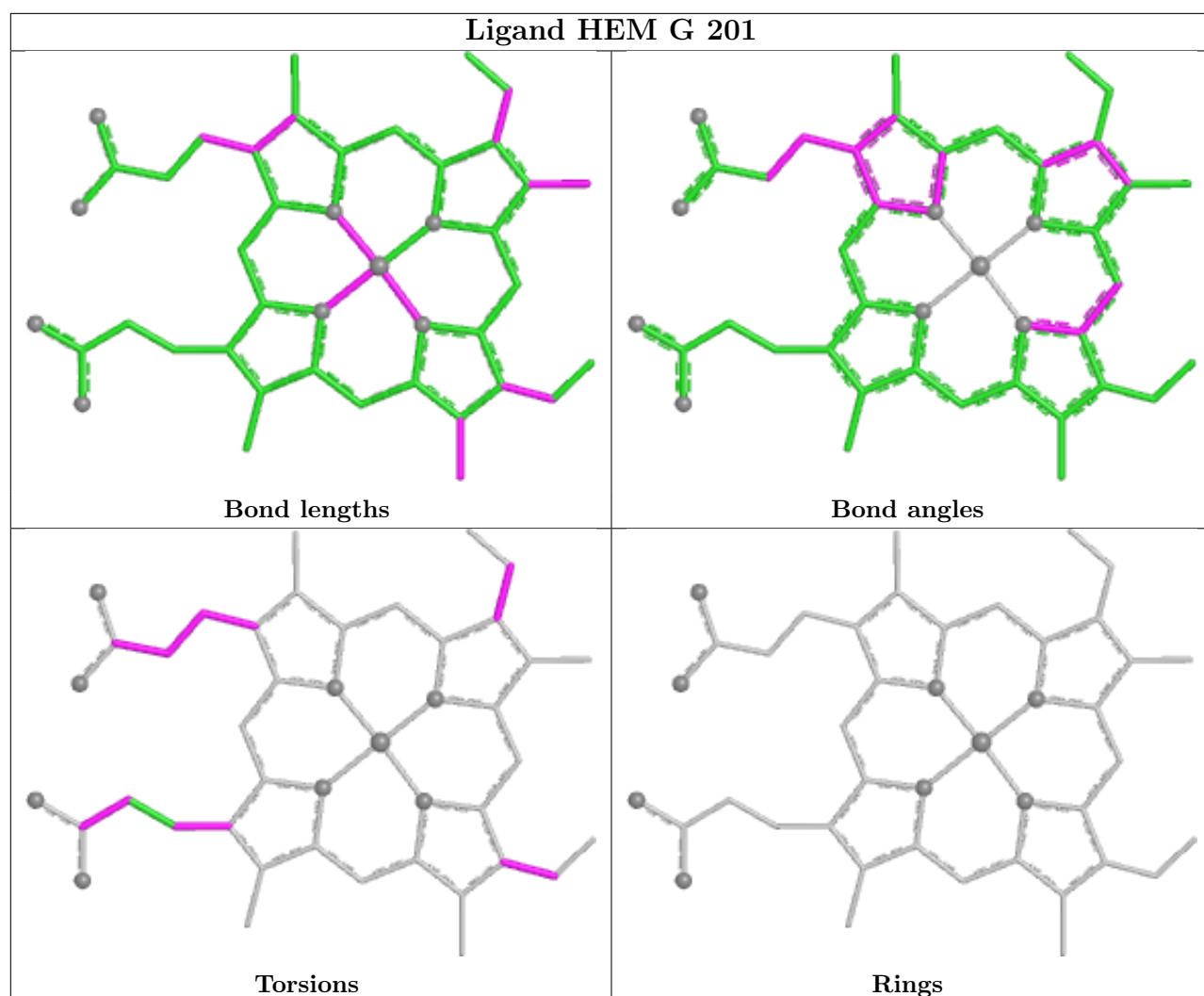
Ligand RQX C 202

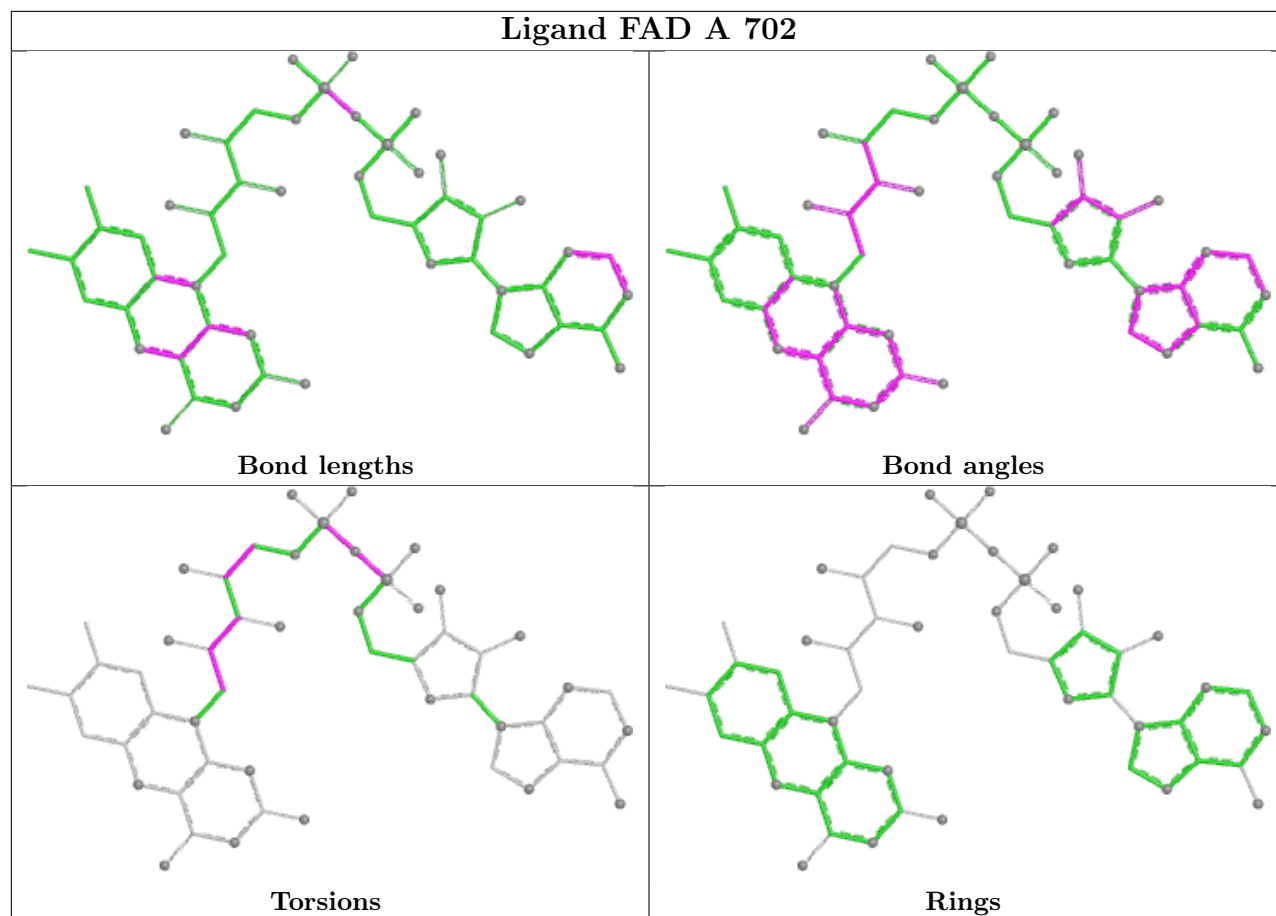


Ligand HEM C 201









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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/645 (95%)	0.57	76 (12%) 8 6	71, 96, 118, 136	0
1	E	613/645 (95%)	0.64	90 (14%) 6 4	70, 90, 112, 126	0
2	B	249/282 (88%)	0.67	42 (16%) 4 3	72, 89, 117, 137	0
2	F	249/282 (88%)	0.46	30 (12%) 9 6	67, 86, 109, 120	0
3	C	153/188 (81%)	0.86	29 (18%) 3 2	78, 97, 142, 162	0
3	G	150/188 (79%)	0.79	26 (17%) 4 3	77, 100, 151, 156	0
4	D	129/156 (82%)	0.69	15 (11%) 9 7	89, 101, 129, 142	0
4	H	129/156 (82%)	0.62	19 (14%) 6 4	86, 103, 133, 146	0
All	All	2285/2542 (89%)	0.63	327 (14%) 6 4	67, 94, 124, 162	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	8.3
4	D	90	LEU	8.0
1	E	86	GLY	7.9
1	E	103	PHE	7.8
1	E	444	PHE	7.8
1	A	200	PHE	7.7
1	E	88	ASN	7.7
1	E	122	LEU	7.4
1	E	440	ASP	7.4
1	E	441	ALA	7.3
1	E	538	ILE	7.1
1	E	427	VAL	6.7
1	A	544	THR	6.7
3	C	182	ALA	6.4
1	E	537	LEU	6.3
1	E	156	GLN	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	425	HIS	6.2
1	E	118	ALA	6.2
3	G	107	ILE	6.1
4	D	65	PHE	6.0
1	E	123	THR	6.0
2	B	199	ALA	6.0
1	E	153	PHE	6.0
1	E	155	GLY	5.9
1	E	435	ALA	5.8
1	E	423	ALA	5.8
4	D	87	CYS	5.7
4	H	78	PHE	5.7
1	A	472	GLU	5.7
1	A	161	GLY	5.5
1	E	172	VAL	5.5
3	G	115	VAL	5.3
2	B	163	GLU	5.3
3	C	183	THR	5.3
1	E	644	SER	5.3
1	A	547	LEU	5.2
1	E	119	MET	5.1
1	E	419	CYS	5.1
1	E	102	HIS	5.0
1	A	317	LEU	5.0
3	C	34	GLU	5.0
2	B	121	THR	4.9
2	B	208	LEU	4.9
4	D	86	LEU	4.9
2	F	83	LEU	4.8
1	E	420	GLY	4.8
2	B	204	GLY	4.8
1	A	155	GLY	4.8
1	E	438	LEU	4.7
1	E	176	THR	4.7
1	E	87	ILE	4.7
1	E	599	PHE	4.7
2	F	46	GLU	4.7
1	E	51	GLY	4.6
1	E	539	TRP	4.6
3	G	116	ILE	4.5
1	E	418	ALA	4.4
1	E	52	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	548	GLU	4.4
2	F	84	THR	4.4
1	E	171	CYS	4.4
2	B	262	ILE	4.4
1	E	434	GLY	4.3
1	E	352	PRO	4.3
2	F	163	GLU	4.3
1	E	448	CYS	4.3
3	C	115	VAL	4.2
1	A	517	VAL	4.2
2	B	136	VAL	4.2
3	G	110	LEU	4.2
3	C	119	THR	4.2
1	E	117	ASN	4.2
2	F	234	PHE	4.1
1	A	514	ALA	4.0
2	F	57	PHE	4.0
3	G	113	PRO	4.0
1	A	645	TYR	4.0
2	B	37	THR	3.9
1	E	170	CYS	3.9
3	G	111	GLY	3.8
3	C	95	VAL	3.8
2	F	199	ALA	3.8
1	A	313	LYS	3.7
4	D	93	THR	3.7
3	C	143	MET	3.7
3	C	138	PHE	3.7
3	G	67	MET	3.7
2	B	241	THR	3.7
1	E	443	VAL	3.6
1	E	624	PRO	3.6
1	E	120	HIS	3.6
3	G	153	TYR	3.6
2	B	265	LEU	3.6
1	E	293	GLY	3.6
2	B	212	TYR	3.6
1	E	166	ALA	3.5
1	E	625	VAL	3.5
1	E	439	LEU	3.5
4	D	35	ALA	3.5
1	E	299	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	3.5
1	A	262	ARG	3.5
4	H	61	ILE	3.4
4	D	91	ALA	3.4
1	A	533	THR	3.4
1	A	202	LEU	3.4
1	A	477	LEU	3.3
1	A	560	ILE	3.3
1	A	539	TRP	3.3
4	H	90	LEU	3.3
1	A	289	GLU	3.3
3	C	179	HIS	3.3
3	G	168	LEU	3.3
1	E	445	GLY	3.3
1	A	365	GLU	3.3
1	A	141	SER	3.3
1	E	645	TYR	3.2
2	B	205	PRO	3.2
2	B	132	ILE	3.2
4	H	118	ALA	3.2
1	E	604	ARG	3.2
1	A	473	SER	3.2
4	D	89	ALA	3.2
2	B	120	THR	3.2
1	A	511	ASP	3.2
1	E	197	ILE	3.2
1	A	201	ALA	3.2
1	E	629	THR	3.2
1	A	139	PRO	3.2
2	F	232	ASP	3.1
2	F	274	ALA	3.1
1	E	85	GLY	3.1
1	A	613	PRO	3.1
1	E	397	TYR	3.1
1	E	151	ARG	3.1
2	F	237	PHE	3.1
3	G	174	PRO	3.1
4	D	94	LEU	3.1
1	E	157	SER	3.1
1	E	355	GLN	3.1
3	C	137	ARG	3.1
1	A	543	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	634	GLU	3.1
1	A	253	THR	3.1
2	B	85	PHE	3.0
2	F	200	ASP	3.0
2	B	33	LYS	3.0
2	B	36	LYS	3.0
2	B	122	LYS	3.0
1	A	172	VAL	3.0
4	H	55	HIS	3.0
2	B	195	TYR	3.0
1	A	474	ILE	3.0
1	A	494	LEU	3.0
1	A	515	GLU	3.0
1	E	436	ASN	3.0
3	G	46	LEU	3.0
1	A	421	GLU	3.0
1	E	169	THR	3.0
1	A	72	LYS	3.0
1	A	237	GLY	2.9
2	F	88	SER	2.9
4	D	49	PHE	2.9
4	H	112	VAL	2.9
1	E	456	LEU	2.9
1	A	153	PHE	2.9
2	B	272	LYS	2.9
2	B	173	GLN	2.9
1	E	96	PRO	2.9
3	G	103	PHE	2.9
2	F	66	THR	2.9
4	H	28	THR	2.9
3	G	42	GLY	2.8
2	B	207	VAL	2.8
2	B	259	ILE	2.8
1	E	116	GLN	2.8
1	E	294	GLU	2.8
1	E	104	TYR	2.8
1	E	399	ALA	2.8
1	A	158	ASN	2.8
2	B	209	MET	2.8
3	C	59	HIS	2.8
2	F	139	MET	2.8
3	G	181	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	564	GLU	2.7
1	A	314	ALA	2.7
1	A	412	ILE	2.7
1	E	344	ILE	2.7
1	E	345	TYR	2.7
3	C	134	ASN	2.7
1	A	203	ASP	2.7
1	E	459	ASP	2.7
1	A	157	SER	2.7
1	A	179	SER	2.7
4	D	98	TRP	2.7
4	D	154	TRP	2.7
4	H	142	HIS	2.7
1	E	264	GLY	2.7
2	F	231	GLN	2.7
1	A	413	VAL	2.7
4	H	58	LEU	2.7
1	E	121	TYR	2.6
3	C	65	PRO	2.6
1	A	156	GLN	2.6
2	F	107	LEU	2.6
3	C	96	LEU	2.6
3	C	125	ALA	2.6
3	G	157	TYR	2.6
4	H	138	TYR	2.6
1	A	391	GLY	2.6
1	E	379	PRO	2.6
2	B	38	PHE	2.6
3	C	63	TYR	2.6
2	B	57	PHE	2.6
2	B	202	TYR	2.6
2	F	56	LYS	2.6
1	A	630	LEU	2.6
3	C	98	LEU	2.6
1	E	398	LYS	2.5
2	B	269	MET	2.5
2	F	183	ILE	2.5
2	B	252	HIS	2.5
1	A	36	LYS	2.5
1	A	222	GLY	2.5
2	B	183	ILE	2.5
4	H	57	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	105	ASP	2.5
4	H	86	LEU	2.5
1	A	142	ARG	2.5
4	H	113	LEU	2.4
3	C	149	ILE	2.4
1	A	188	SER	2.4
2	B	87	ARG	2.4
1	A	259	LEU	2.4
2	B	196	TRP	2.4
1	E	80	THR	2.4
2	B	215	ILE	2.4
4	D	61	ILE	2.4
3	G	112	ILE	2.4
1	A	164	GLY	2.4
2	B	79	VAL	2.4
2	F	233	GLY	2.4
2	F	89	CYS	2.4
2	F	85	PHE	2.4
2	B	211	ALA	2.4
3	G	164	ALA	2.4
4	H	134	ALA	2.4
1	A	58	MET	2.4
2	F	281	ASN	2.3
2	B	189	SER	2.3
3	C	67	MET	2.3
3	G	165	LEU	2.3
3	C	128	ILE	2.3
2	B	263	LYS	2.3
2	F	133	LYS	2.3
2	F	164	LYS	2.3
1	A	124	ARG	2.3
1	E	442	VAL	2.3
1	E	409	GLY	2.3
1	A	65	PHE	2.3
4	H	111	PHE	2.3
1	A	198	GLU	2.3
3	G	87	LEU	2.3
3	G	117	LEU	2.3
1	E	106	THR	2.3
2	B	75	ILE	2.3
4	D	34	GLY	2.3
1	A	140	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	346	LEU	2.3
3	G	39	GLN	2.3
3	G	98	LEU	2.3
1	A	99	TRP	2.3
1	E	200	PHE	2.3
4	H	40	PHE	2.3
3	C	35	LYS	2.3
1	A	555	ASN	2.2
1	E	168	ARG	2.2
1	A	191	CYS	2.2
1	E	290	GLY	2.2
2	B	258	ALA	2.2
1	E	113	LEU	2.2
1	E	167	LYS	2.2
3	C	60	LEU	2.2
1	A	462	ILE	2.2
2	F	115	GLN	2.2
2	B	58	ASP	2.2
1	A	489	THR	2.2
2	B	216	ILE	2.2
4	D	137	LEU	2.2
4	H	72	LEU	2.2
2	F	39	GLU	2.2
3	G	182	ALA	2.2
1	A	487	VAL	2.2
3	G	91	VAL	2.2
2	B	128	HIS	2.1
1	A	411	LYS	2.1
1	E	154	GLY	2.1
3	C	130	PHE	2.1
1	A	460	GLU	2.1
1	A	127	VAL	2.1
1	A	635	VAL	2.1
3	C	37	PRO	2.1
3	C	170	VAL	2.1
2	F	271	THR	2.1
1	A	456	LEU	2.1
3	C	114	TRP	2.1
1	E	249	ALA	2.1
3	C	116	ILE	2.1
1	E	602	HIS	2.1
1	A	457	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	437	SER	2.1
1	E	313	LYS	2.1
2	F	79	VAL	2.1
2	F	136	VAL	2.1
3	G	170	VAL	2.1
1	A	266	ALA	2.1
4	H	110	PRO	2.0
2	F	276	LEU	2.0
1	A	599	PHE	2.0
3	C	141	PHE	2.0
1	A	495	THR	2.0
3	G	124	ILE	2.0
4	H	89	ALA	2.0
1	A	192	HIS	2.0
1	E	286	LEU	2.0
1	E	298	LEU	2.0
1	E	108	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

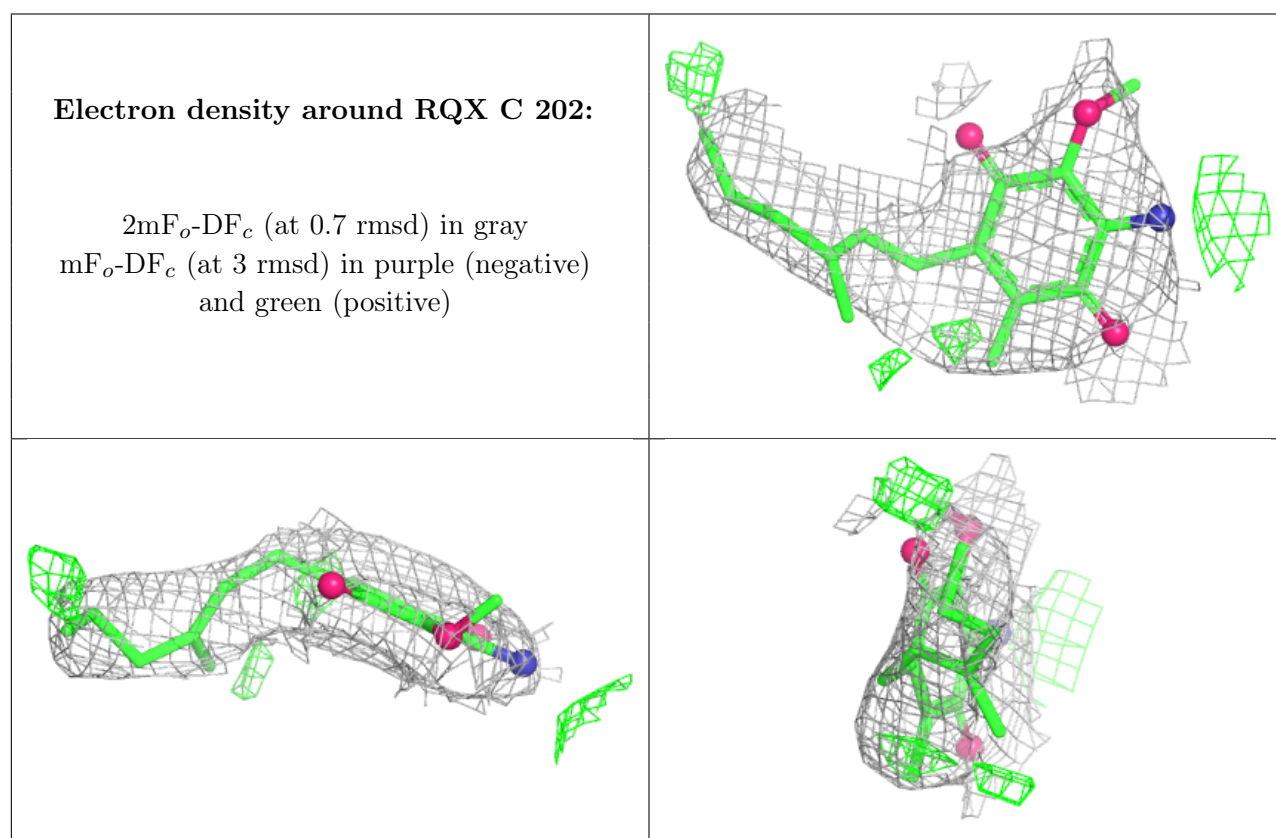
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	RQX	C	202	19/19	0.75	0.27	113,116,119,119	0
11	RQX	G	202	19/19	0.80	0.24	120,125,127,127	0
12	EPH	H	201	44/49	0.89	0.20	97,113,134,135	0
5	MLI	A	701	7/7	0.92	0.09	102,103,106,106	0
12	EPH	D	201	44/49	0.93	0.16	94,102,121,122	0
6	FAD	A	702	53/53	0.93	0.11	77,83,87,89	0

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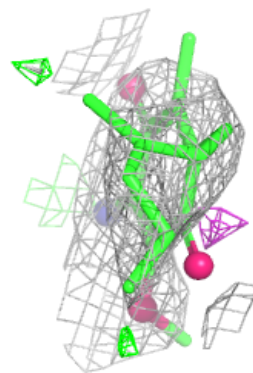
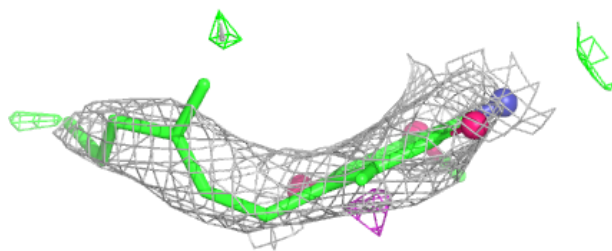
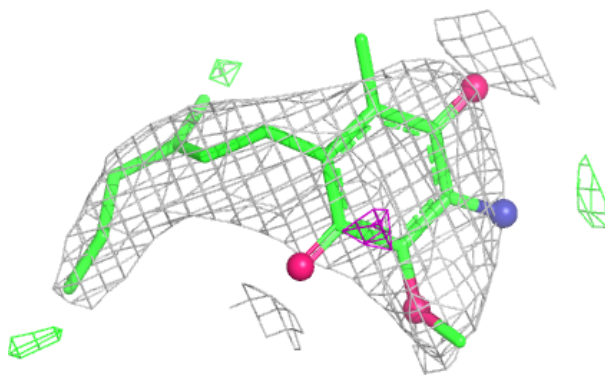
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	HEM	C	201	43/43	0.95	0.12	89,93,96,98	0
6	FAD	E	702	53/53	0.96	0.08	63,79,88,89	0
5	MLI	E	701	7/7	0.96	0.06	92,93,93,93	0
9	F3S	B	303	7/7	0.98	0.05	83,85,86,87	0
10	HEM	G	201	43/43	0.98	0.08	92,97,103,106	0
7	FES	F	301	4/4	0.99	0.07	60,66,68,75	0
9	F3S	F	303	7/7	0.99	0.04	82,83,84,87	0
8	SF4	F	302	8/8	1.00	0.04	57,61,64,65	0
7	FES	B	301	4/4	1.00	0.05	70,70,72,78	0
8	SF4	B	302	8/8	1.00	0.03	63,66,68,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



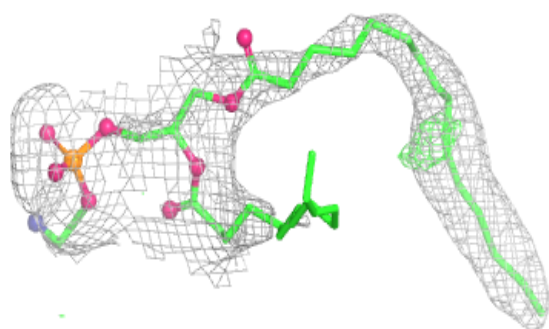
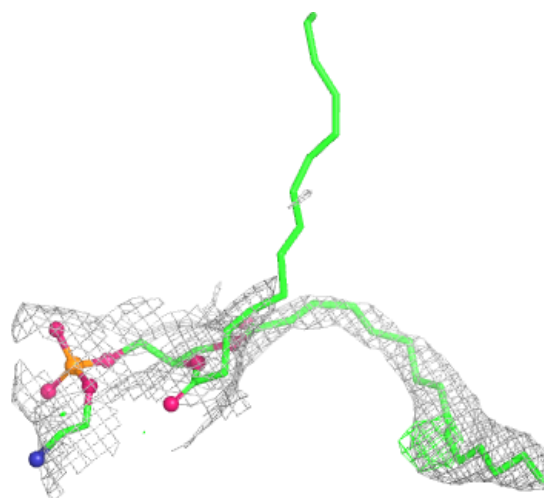
Electron density around RQX G 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



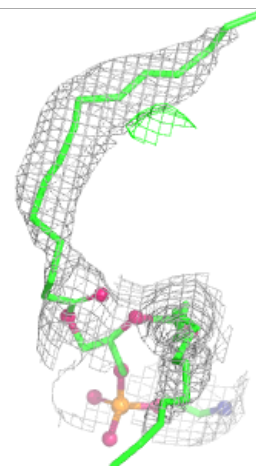
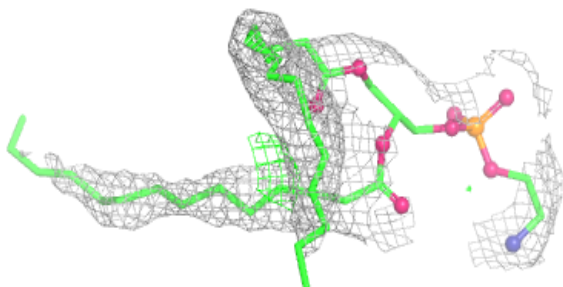
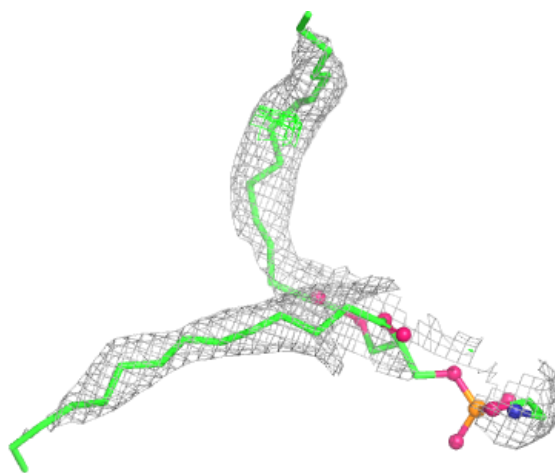
Electron density around EPH H 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



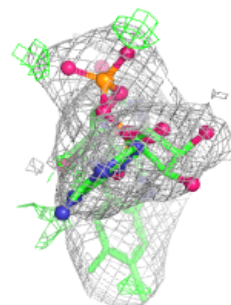
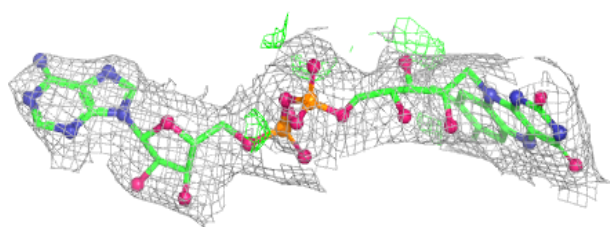
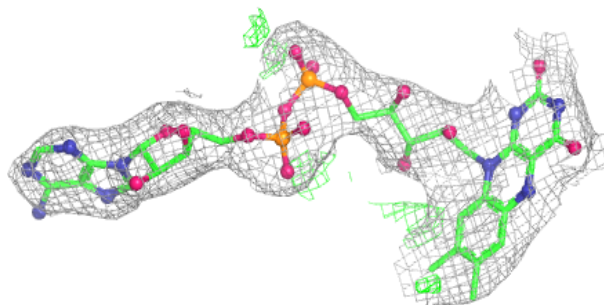
Electron density around EPH D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



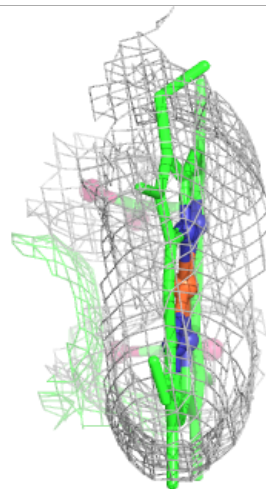
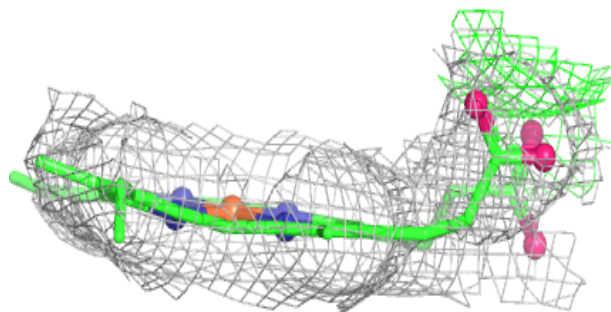
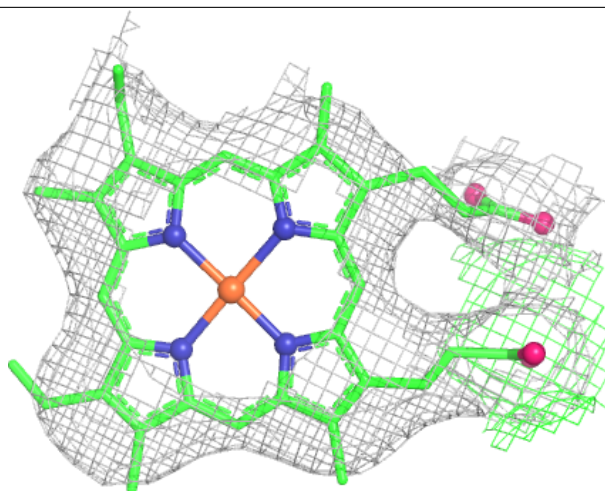
Electron density around FAD A 702:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



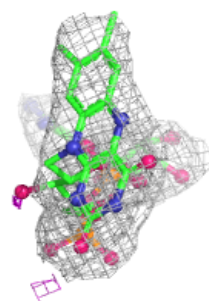
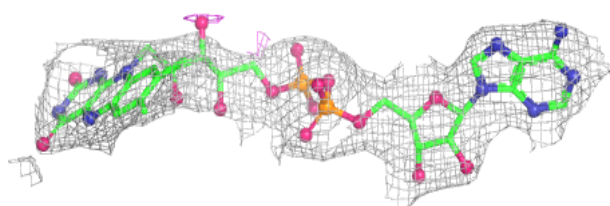
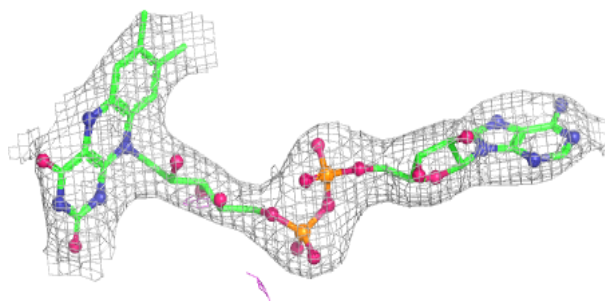
Electron density around HEM C 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

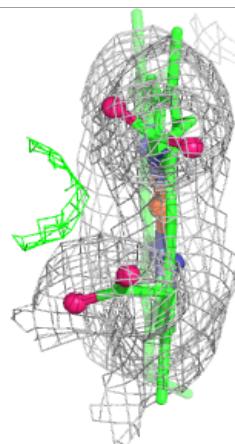
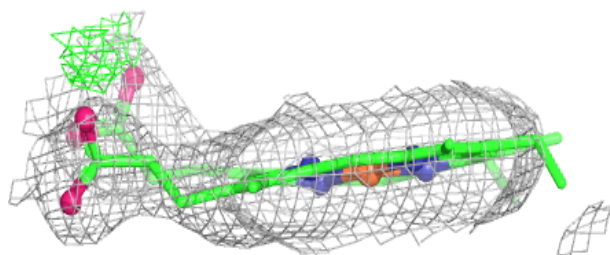
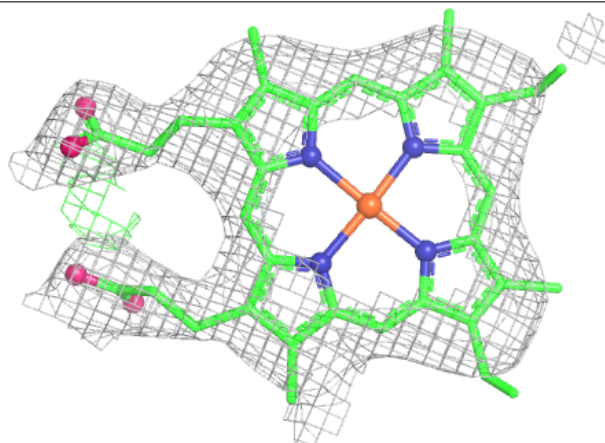


Electron density around FAD E 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HEM G 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.