Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 07:23 pm BST

PDB ID	:	5C2W / pdb_00005c2w
Title	:	Kuenenia stuttgartiensis Hydrazine Synthase Pressurized with 20 bar Xenon
Authors	:	Dietl, A.; Ferousi, C.; Maalcke, W.J.; Menzel, A.; de Vries, S.; Keltjens, J.T.; Jetten, M.S.M.; Kartal, B.; Barends, T.R.M.
Deposited on	:	2015-06-16
Resolution	:	3.20 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 (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:

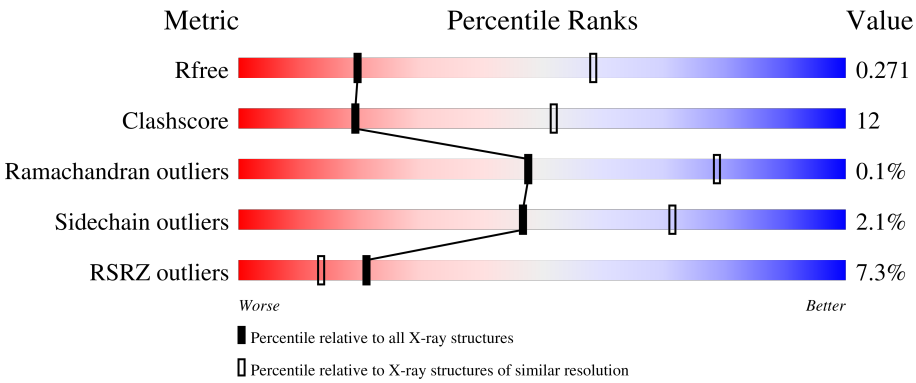
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 <=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	782	.% 83% 14% • •
1	D	782	5% 80% 18% • •
2	B	352	.% 78% 21% •
2	E	352	23% 60% 30% 9% •
3	C	314	3% 79% 21%

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Mol	Chain	Length	Quality of chain
3	F	314	20% 68% 30%

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	XE	D	901	-	-	-	X
5	CL	A	903[A]	-	-	X	-
8	HEC	A	908	X	-	-	-
8	HEC	C	404	X	-	-	-
8	HEC	C	405	X	-	-	-
8	HEC	D	907	X	-	-	-
8	HEC	D	908	X	-	-	-
8	HEC	F	404	X	-	-	-
8	HEC	F	405	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 23386 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 HYDRAZINE SYNTHASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	768	6081	3867	1045	1144	25	0	0	0
1	D	770	6087	3871	1044	1147	25	0	0	0

- Molecule 2 is a protein called HYDRAZINE SYNTHASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	352	2706	1697	464	531	14	0	1	0
2	E	352	2692	1688	459	531	14	0	1	0

- Molecule 3 is a protein called Hypothetical (Di heme) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	314	2457	1543	432	472	10	0	0	0
3	F	314	2443	1534	427	472	10	0	0	0

- Molecule 4 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Xe		
4	A	2	2	2	0	0
4	D	2	2	2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 2 2	0	1
5	D	1	Total Cl 1 1	0	0

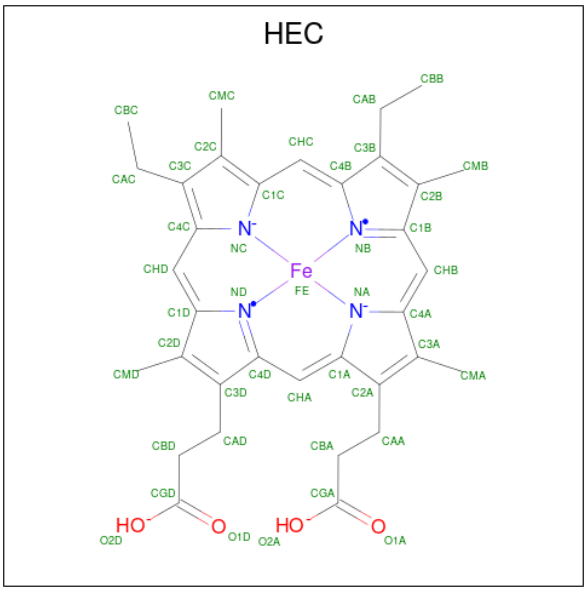
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	1	Total Ca 1 1	0	0
6	C	3	Total Ca 3 3	0	0
6	D	2	Total Ca 2 2	0	0
6	E	1	Total Ca 1 1	0	0
6	F	3	Total Ca 3 3	0	0

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

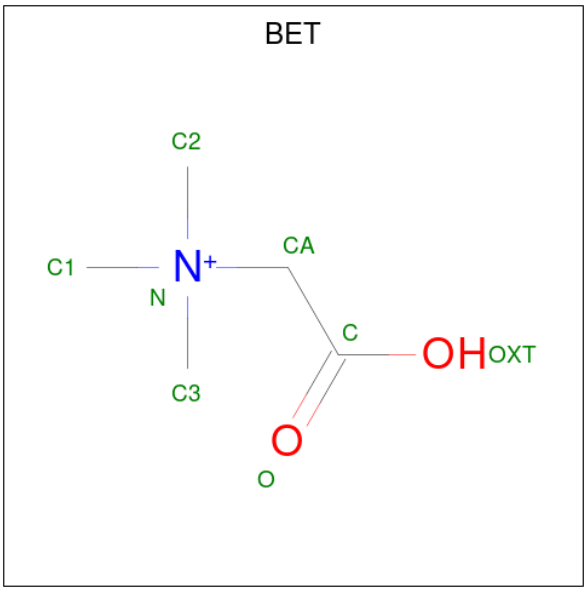
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0
7	D	1	Total Zn 1 1	0	0

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
8	F	1	43	34	1	4	4	0	0

- Molecule 9 is TRIMETHYL GLYCINE (CCD ID: BET) (formula: $C_5H_{12}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	8	5	1	2	0	0
9	A	1	8	5	1	2	0	0
9	A	1	8	5	1	2	0	0
9	B	1	8	5	1	2	0	0
9	C	1	8	5	1	2	0	0
9	D	1	8	5	1	2	0	0
9	E	1	8	5	1	2	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	B	1	1	1	0	0
10	E	1	1	1	0	0

- Molecule 11 is water.

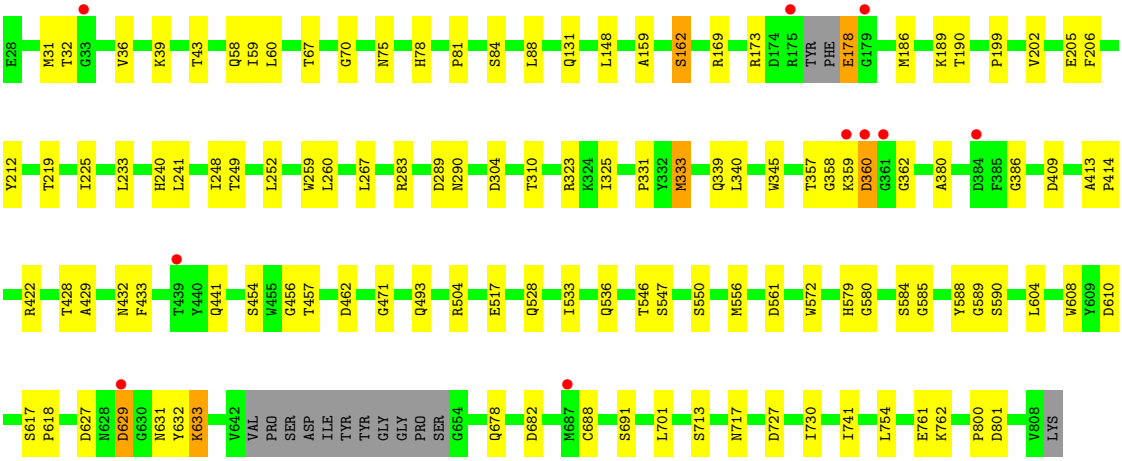
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	163	163	163	0	0
			Total	O		
11	B	59	59	59	0	0
			Total	O		
11	C	88	88	88	0	0
			Total	O		
11	D	112	112	112	0	0
			Total	O		
11	E	30	30	30	0	0
			Total	O		
11	F	45	45	45	0	0

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 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.

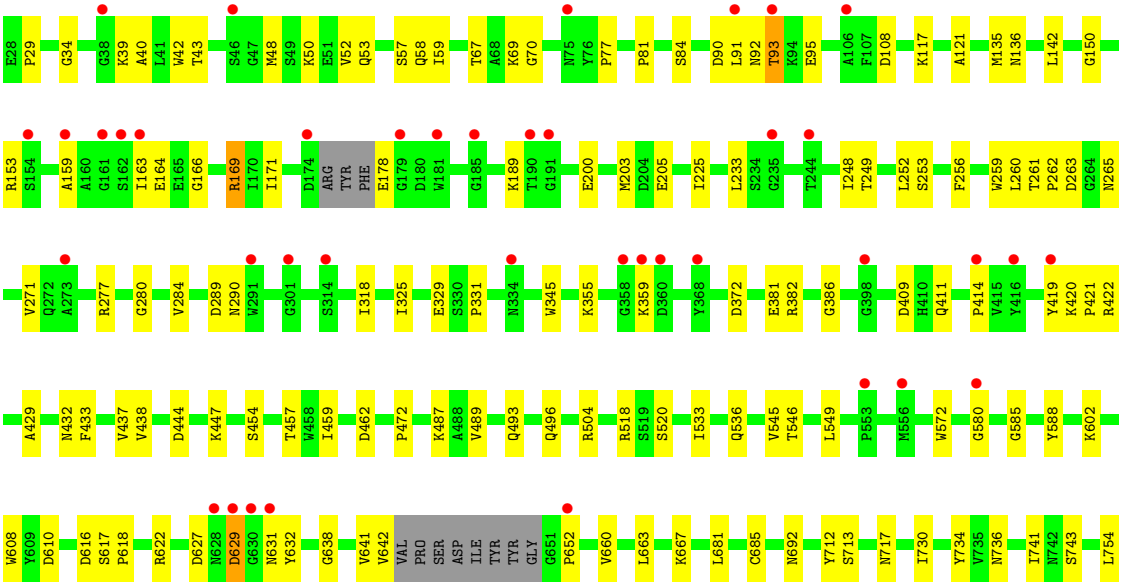
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

Chain A:



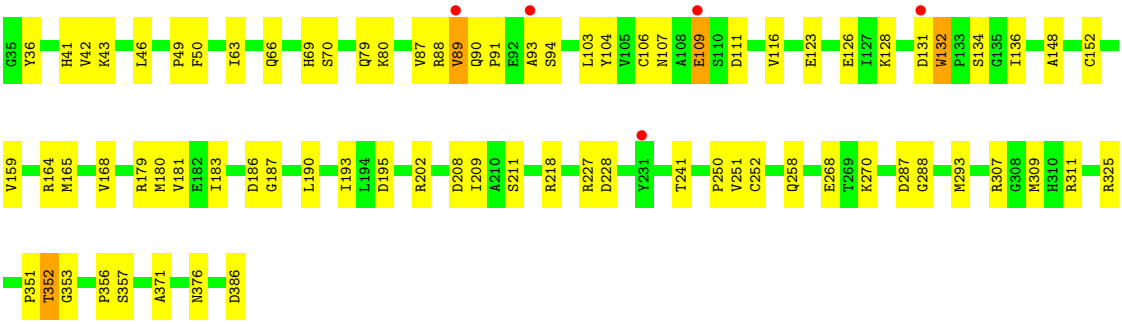
• Molecule 1: HYDRAZINE SYNTHASE ALPHA SUBUNIT

Chain D:



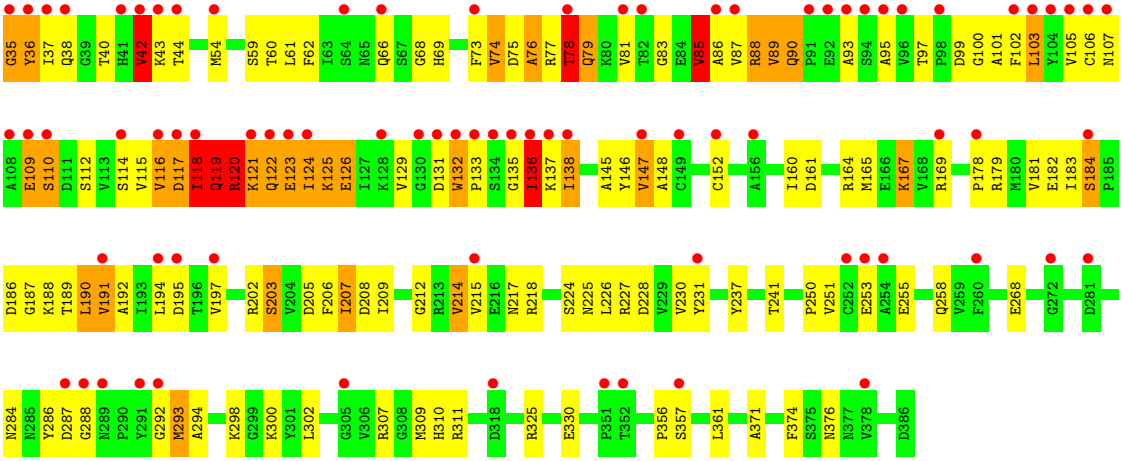
• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain B:



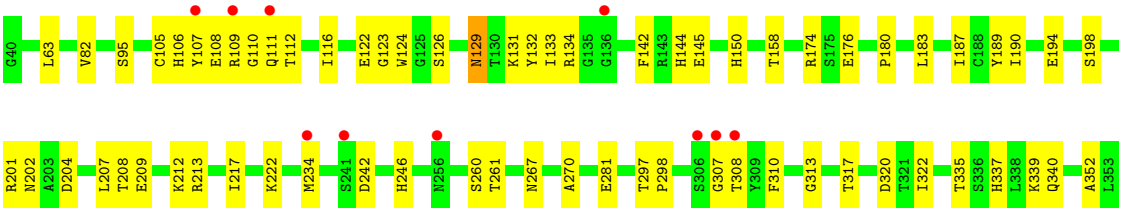
• Molecule 2: HYDRAZINE SYNTHASE BETA SUBUNIT

Chain E:



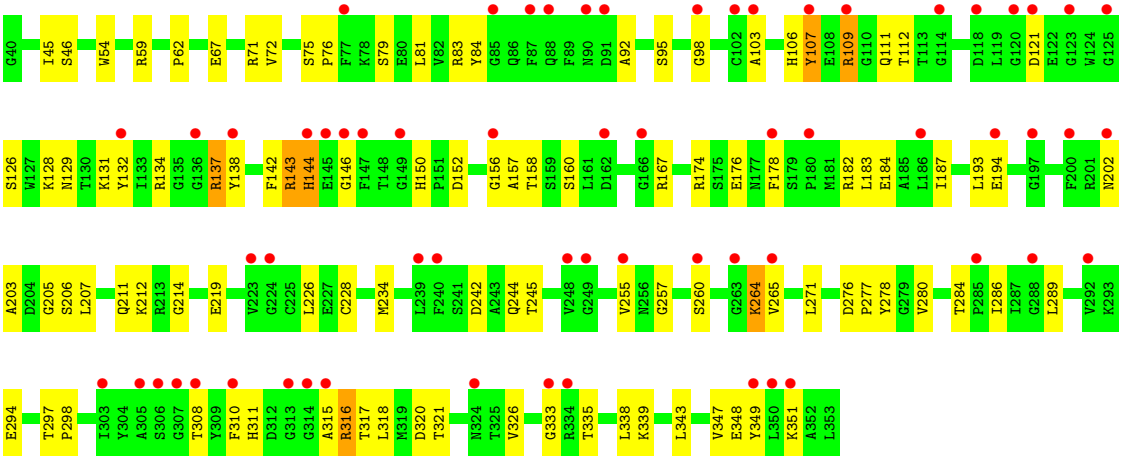
• Molecule 3: Hypothetical (Di heme) protein

Chain C:



• Molecule 3: Hypothetical (Di heme) protein

Chain F:


G40
I45
S46
W54
R59
P62
E67
R71
V72
S75
P76
F77
K78
S79
E80
L81
V82
R83
Y84
G85
Q86
F87
Q88
F89
N90
D91
A92
S95
G98
C102
A103
H106
Y107
E108
R109
G110
Q111
T112
T113
G114
D118
L119
G120
D121
E122
G123
W124
G125
S126
W127
K128
N129
T130
K131
Y132
I133
R134
G135
G136
R137
Y138
F142
R143
H144
E145
G146
F147
T148
G149
H150
P151
D152
G156
A157
T158
S159
S160
L161
D162
G166
R167
R174
S175
E176
N177
F178
S179
P180
M181
R182
L183
E184
A185
L186
I187
L193
E194
G197
F200
R201
N202
A203
D204
G205
S206
L207
Q211
K212
R213
G214
E219
V223
G224
C225
L226
E227
C228
M234
L239
F240
S241
D242
A243
Q244
T245
V248
G249
V255
N256
G257
S260
G263
K264
V265
L271
D276
P277
Y278
G279
V280
T284
P285
I286
I287
G288
L289
V292
K293
E294
T297
P298
I303
Y304
A305
S306
G307
T308
Y309
F310
H311
D312
G313
G314
A315
R316
T317
L318
M319
D320
T321
N324
T325
V326
G333
R334
T335
L338
K339
L343
V347
E348
Y349
L350
K351
A352
L353

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	464.12Å 464.12Å 145.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.50 – 3.20 48.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.50-3.20) 100.0 (48.50-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.231 , 0.267 0.237 , 0.271	Depositor DCC
R_{free} test set	4865 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	67.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23386	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: HEC, BET, CA, XE, CL, MG, ZN

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	0.27	0/6259	0.73	2/8503 (0.0%)
1	D	0.28	0/6266	0.76	2/8514 (0.0%)
2	B	0.31	0/2758	0.80	2/3752 (0.1%)
2	E	0.66	6/2744 (0.2%)	1.30	45/3737 (1.2%)
3	C	0.29	0/2522	0.76	3/3421 (0.1%)
3	F	0.33	0/2508	0.86	9/3406 (0.3%)
All	All	0.36	6/23057 (0.0%)	0.85	63/31333 (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
2	E	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	89	VAL	CA-CB	6.18	1.60	1.54
2	E	117	ASP	N-CA	5.74	1.53	1.46
2	E	136	ILE	CA-CB	-5.62	1.46	1.54
2	E	119	GLN	CA-C	5.40	1.60	1.52
2	E	119	GLN	N-CA	5.20	1.52	1.46
2	E	122	GLN	CA-C	5.12	1.59	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	79	GLN	N-CA-C	17.10	135.39	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	90	GLN	CB-CA-C	-11.45	103.07	111.20
2	E	85	VAL	N-CA-C	10.57	125.12	108.85
2	E	120	ARG	CA-CB-CG	9.49	133.08	114.10
1	D	93	THR	N-CA-C	-9.46	100.31	112.23
2	E	121	LYS	CA-C-N	9.09	137.30	122.39
2	E	121	LYS	C-N-CA	9.09	137.30	122.39
2	E	136	ILE	N-CA-C	9.08	128.22	109.34
2	E	117	ASP	N-CA-C	8.93	120.47	107.88
2	E	120	ARG	N-CA-C	8.31	128.49	110.80
2	E	120	ARG	N-CA-CB	-7.94	97.07	110.49
2	E	132	TRP	CA-C-N	-7.90	111.61	119.90
2	E	132	TRP	C-N-CA	-7.90	111.61	119.90
2	E	42	VAL	N-CA-C	7.80	119.13	107.51
3	F	143	ARG	CB-CA-C	-7.67	105.61	116.34
2	E	76	ALA	N-CA-C	7.55	120.61	111.40
2	E	78	THR	N-CA-C	7.34	120.34	111.82
2	E	120	ARG	CA-C-N	7.13	133.69	122.93
2	E	120	ARG	C-N-CA	7.13	133.69	122.93
3	F	276	ASP	CA-C-N	7.04	127.35	119.32
3	F	276	ASP	C-N-CA	7.04	127.35	119.32
2	E	119	GLN	N-CA-C	6.63	124.93	110.80
2	E	136	ILE	CB-CA-C	-6.62	100.43	111.29
2	E	123	GLU	N-CA-C	6.58	119.19	108.26
2	E	118	ILE	CA-C-N	6.57	134.09	121.54
2	E	118	ILE	C-N-CA	6.57	134.09	121.54
3	C	198	SER	CA-C-N	6.32	126.45	119.87
3	C	198	SER	C-N-CA	6.32	126.45	119.87
1	D	166	GLY	N-CA-C	6.22	118.25	110.29
2	E	36	TYR	CA-C-N	6.21	129.07	120.49
2	E	36	TYR	C-N-CA	6.21	129.07	120.49
2	B	132	TRP	CA-C-N	-6.20	113.14	119.83
2	B	132	TRP	C-N-CA	-6.20	113.14	119.83
2	E	184	SER	CA-C-N	6.17	126.35	119.32
2	E	184	SER	C-N-CA	6.17	126.35	119.32
3	F	143	ARG	N-CA-C	5.96	116.83	108.00
2	E	147	VAL	N-CA-C	5.85	116.30	107.75
3	F	107	TYR	CA-CB-CG	5.82	124.37	113.90
3	F	333	GLY	N-CA-C	-5.81	106.43	111.95
1	A	471	GLY	CA-C-N	5.81	125.42	119.56
1	A	471	GLY	C-N-CA	5.81	125.42	119.56
2	E	100	GLY	N-CA-C	-5.77	104.02	114.46
2	E	79	GLN	CB-CA-C	-5.75	99.65	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	110	SER	N-CA-C	-5.67	106.33	113.20
2	E	124	ILE	N-CA-C	5.64	116.42	110.72
2	E	124	ILE	CB-CA-C	-5.60	104.50	112.22
2	E	43	LYS	N-CA-C	5.51	118.46	109.59
2	E	119	GLN	CB-CG-CD	5.43	121.83	112.60
2	E	203	SER	N-CA-C	5.41	117.48	109.69
3	F	205	GLY	N-CA-C	-5.40	108.27	114.69
2	E	184	SER	N-CA-C	5.35	121.63	109.81
3	F	310	PHE	CB-CA-C	-5.35	109.42	115.79
2	E	109	GLU	N-CA-C	5.33	119.78	113.28
2	E	90	GLN	N-CA-C	5.31	123.11	111.53
2	E	79	GLN	CA-C-N	5.29	131.30	121.62
2	E	79	GLN	C-N-CA	5.29	131.30	121.62
2	E	35	GLY	CA-C-N	-5.27	114.19	122.73
2	E	35	GLY	C-N-CA	-5.27	114.19	122.73
3	F	144	HIS	N-CA-C	-5.26	105.08	112.12
3	C	310	PHE	CB-CA-C	-5.23	108.99	115.89
2	E	189	THR	N-CA-C	5.20	116.90	108.26
2	E	116	VAL	CA-C-O	-5.11	116.31	121.67
2	E	125	LYS	CA-CB-CG	5.05	124.21	114.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	118	ILE	Peptide
2	E	119	GLN	Peptide
2	E	120	ARG	Peptide
2	E	42	VAL	Peptide
2	E	78	THR	Peptide

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	6081	0	5782	81	0
1	D	6087	0	5784	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2706	0	2675	54	0
2	E	2692	0	2642	183	0
3	C	2457	0	2324	49	0
3	F	2443	0	2290	90	0
4	A	2	0	0	1	0
4	D	2	0	0	0	0
5	A	2	0	0	3	0
5	D	1	0	0	1	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	0	0
6	F	3	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	86	0	60	3	0
8	C	86	0	59	5	0
8	D	86	0	60	6	0
8	F	86	0	59	7	0
9	A	24	0	33	0	0
9	B	8	0	11	0	0
9	C	8	0	11	0	0
9	D	8	0	11	0	0
9	E	8	0	11	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
11	A	163	0	0	2	0
11	B	59	0	0	2	0
11	C	88	0	0	6	0
11	D	112	0	0	4	0
11	E	30	0	0	1	0
11	F	45	0	0	5	0
All	All	23386	0	21812	523	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 (523) 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)
3:F:228:CYS:SG	8:F:405:HEC:CAC	2.02	1.47
3:C:105:CYS:SG	8:C:404:HEC:CAC	2.04	1.46
2:E:120:ARG:HD3	2:E:122:GLN:H	1.00	1.09
2:E:88:ARG:HD2	2:E:110:SER:HB2	1.34	1.09
3:C:107:TYR:HD2	3:C:108:GLU:H	1.14	0.92
2:E:120:ARG:HD3	2:E:122:GLN:N	1.84	0.92
2:E:182:GLU:HG2	2:E:230:VAL:HA	1.50	0.92
3:C:105:CYS:SG	8:C:404:HEC:C3C	2.57	0.92
2:E:88:ARG:NH2	2:E:109:GLU:OE1	2.04	0.91
2:E:118:ILE:HB	2:E:119:GLN:HG2	1.51	0.90
3:F:228:CYS:SG	8:F:405:HEC:C3C	2.59	0.90
2:E:36:TYR:HH	2:E:40:THR:HG1	1.03	0.90
1:A:359:LYS:HG3	1:A:360:ASP:H	1.37	0.89
2:E:88:ARG:HG2	2:E:89:VAL:H	1.37	0.88
2:E:120:ARG:NH2	2:E:122:GLN:OE1	2.09	0.84
2:E:136:ILE:HG21	2:E:147:VAL:HA	1.61	0.82
2:E:120:ARG:HG3	2:E:121:LYS:H	1.43	0.81
2:E:88:ARG:HG2	2:E:89:VAL:N	1.95	0.81
1:D:163:ILE:HG13	3:F:62:PRO:HD2	1.63	0.81
2:E:88:ARG:CZ	2:E:107:ASN:HB2	2.10	0.80
3:F:107:TYR:CE2	3:F:111:GLN:HB2	2.17	0.80
3:F:107:TYR:HE2	3:F:111:GLN:HB2	1.45	0.80
2:E:183:ILE:HG13	2:E:190:LEU:HD22	1.63	0.80
1:D:92:ASN:CG	1:D:93:THR:H	1.90	0.79
2:B:36:TYR:H	2:B:69:HIS:HE2	1.31	0.79
2:E:69:HIS:CE1	2:E:89:VAL:HG23	2.17	0.78
2:E:120:ARG:CD	2:E:122:GLN:H	1.90	0.78
2:B:90:GLN:HB3	2:B:109:GLU:HG2	1.66	0.77
2:E:145:ALA:HB3	2:E:160:ILE:HB	1.66	0.77
1:D:429:ALA:HB3	1:D:433:PHE:HB3	1.67	0.76
1:A:359:LYS:CG	1:A:360:ASP:H	1.99	0.75
2:E:135:GLY:O	2:E:136:ILE:HG23	1.86	0.75
2:E:88:ARG:NH2	2:E:89:VAL:O	2.20	0.75
2:E:288:GLY:H	2:E:309:MET:HG2	1.52	0.74
2:E:125:LYS:HD2	2:E:126:GLU:N	2.02	0.74
2:E:88:ARG:HH22	2:E:109:GLU:H	1.36	0.74
2:E:183:ILE:HD12	2:E:191:VAL:H	1.51	0.74
3:F:109:ARG:HG2	3:F:109:ARG:HH11	1.53	0.73
2:E:120:ARG:CG	2:E:121:LYS:H	1.97	0.73
3:C:307:GLY:O	11:C:501:HOH:O	2.06	0.73
1:D:608:TRP:NE1	1:D:610:ASP:O	2.21	0.73
2:E:88:ARG:HD2	2:E:110:SER:CB	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:GLU:C	2:E:183:ILE:HD13	2.15	0.72
2:E:125:LYS:HD2	2:E:126:GLU:H	1.55	0.72
2:E:38:GLN:HB2	2:E:90:GLN:NE2	2.06	0.71
2:E:36:TYR:OH	2:E:42:VAL:N	2.23	0.71
2:E:119:GLN:CG	2:E:120:ARG:HB3	2.21	0.71
2:B:288:GLY:H	2:B:309:MET:HG2	1.56	0.70
2:E:77:ARG:N	2:E:79:GLN:HE22	1.89	0.70
2:E:101:ALA:HA	2:E:118:ILE:HD11	1.72	0.70
2:E:88:ARG:NH1	2:E:110:SER:H	1.88	0.70
2:E:62:PHE:HD1	2:E:73:PHE:CE1	2.10	0.70
1:D:150:GLY:HA2	1:D:200:GLU:HG3	1.74	0.70
3:F:71:ARG:HH21	3:F:184:GLU:HG3	1.57	0.70
3:C:122:GLU:OE2	11:C:502:HOH:O	2.09	0.69
2:E:66:GLN:HG3	2:E:90:GLN:HG2	1.74	0.69
1:A:422:ARG:NH1	3:C:95:SER:O	2.25	0.69
1:D:438:VAL:O	3:F:167:ARG:NH2	2.26	0.69
2:E:85:VAL:HB	2:E:121:LYS:HE2	1.74	0.69
1:D:642:VAL:HG12	1:D:652:PRO:HG3	1.74	0.69
1:D:58:GLN:HG2	1:D:90:ASP:OD1	1.93	0.68
2:E:74:VAL:HG12	2:E:79:GLN:HG2	1.74	0.68
2:E:119:GLN:HG3	2:E:120:ARG:HG2	1.74	0.68
2:E:78:THR:H	2:E:79:GLN:NE2	1.92	0.68
3:F:111:GLN:HB3	3:F:132:TYR:CE1	2.29	0.67
3:F:131:LYS:NZ	3:F:143:ARG:O	2.19	0.67
1:A:173:ARG:NH2	1:A:178:GLU:OE2	2.27	0.67
2:E:101:ALA:HA	2:E:118:ILE:CD1	2.24	0.67
2:E:190:LEU:HB3	2:E:207:ILE:HB	1.75	0.67
2:E:136:ILE:HG22	2:E:181:VAL:HG22	1.77	0.67
3:C:129:ASN:ND2	11:C:505:HOH:O	2.28	0.66
1:A:422:ARG:HB2	3:C:176:GLU:HB2	1.76	0.66
2:B:307:ARG:HE	2:B:357:SER:HB3	1.61	0.66
1:A:386:GLY:HA2	1:A:409:ASP:HB2	1.77	0.65
3:C:109:ARG:HG2	3:C:109:ARG:HH11	1.61	0.65
1:D:159:ALA:HB3	1:D:420:LYS:HD2	1.79	0.65
3:F:131:LYS:NZ	11:F:505:HOH:O	2.29	0.65
1:D:280:GLY:O	1:D:518:ARG:NH1	2.29	0.65
2:E:136:ILE:HG21	2:E:147:VAL:CA	2.25	0.65
1:A:429:ALA:HB3	1:A:433:PHE:HB3	1.78	0.64
3:F:137:ARG:NH2	3:F:194:GLU:OE2	2.31	0.64
2:E:40:THR:HG22	3:F:193:LEU:HA	1.77	0.64
2:E:118:ILE:HG22	2:E:119:GLN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ASP:OD1	1:D:411:GLN:NE2	2.31	0.63
2:B:250:PRO:O	2:B:258:GLN:NE2	2.31	0.63
2:E:87:VAL:HG11	2:E:105:VAL:HG21	1.79	0.63
1:A:589:GLY:N	5:A:903[B]:CL:CL	2.64	0.63
2:E:36:TYR:HE2	2:E:40:THR:O	1.82	0.63
2:B:195:ASP:OD1	2:B:202:ARG:NH1	2.32	0.63
2:E:119:GLN:HG3	2:E:120:ARG:HB3	1.79	0.63
2:B:126:GLU:OE1	2:B:128:LYS:NZ	2.29	0.63
2:E:85:VAL:HG23	2:E:121:LYS:HG3	1.81	0.62
2:E:202:ARG:HD2	2:E:224:SER:HA	1.81	0.62
1:A:588:TYR:HB3	5:A:903[A]:CL:CL	2.38	0.61
1:D:386:GLY:HA2	1:D:409:ASP:HB2	1.82	0.61
2:E:97:THR:OG1	2:E:102:PHE:N	2.32	0.61
2:E:138:ILE:HB	2:E:145:ALA:HA	1.83	0.61
1:A:590:SER:OG	5:A:903[A]:CL:CL	2.55	0.61
2:E:120:ARG:HE	2:E:122:GLN:HB3	1.66	0.60
1:D:225:ILE:HG13	1:D:233:LEU:HB2	1.83	0.60
1:D:622:ARG:HD2	1:D:638:GLY:HA3	1.82	0.60
1:A:713:SER:O	1:A:717:ASN:ND2	2.28	0.60
1:D:39:LYS:HD2	1:D:40:ALA:N	2.17	0.60
1:D:248:ILE:HG13	1:D:249:THR:HG23	1.83	0.60
1:D:496:GLN:NE2	11:D:1004:HOH:O	2.35	0.60
1:D:265:ASN:OD1	1:D:290:ASN:ND2	2.35	0.60
3:C:107:TYR:OH	11:C:503:HOH:O	2.16	0.59
2:E:169:ARG:HH22	2:E:212:GLY:HA3	1.67	0.59
2:E:73:PHE:CE1	2:E:121:LYS:HE3	2.38	0.59
1:D:271:VAL:HG22	1:D:284:VAL:HG22	1.85	0.59
2:E:119:GLN:HG3	2:E:120:ARG:CG	2.32	0.59
2:E:136:ILE:HG22	2:E:181:VAL:CG2	2.32	0.59
2:E:207:ILE:HD13	2:E:214:VAL:HG12	1.84	0.58
3:F:129:ASN:ND2	11:F:507:HOH:O	2.35	0.58
1:D:422:ARG:HB3	3:F:176:GLU:HB2	1.85	0.58
1:A:536:GLN:HG2	1:A:546:THR:HB	1.84	0.58
3:F:265:VAL:HB	3:F:271:LEU:HD12	1.86	0.58
2:E:112:SER:HA	2:E:129:VAL:HG22	1.86	0.58
3:F:132:TYR:CE2	3:F:134:ARG:HB2	2.38	0.58
1:D:29:PRO:HA	1:D:40:ALA:HB2	1.86	0.57
3:F:207:LEU:HB2	3:F:212:LYS:HG3	1.85	0.57
1:D:741:ILE:HG12	1:D:755:SER:HB3	1.86	0.57
3:F:75:SER:HB2	3:F:184:GLU:OE2	2.04	0.57
1:D:536:GLN:HG2	1:D:546:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:ILE:HB	2:E:146:TYR:O	2.05	0.57
2:E:59:SER:O	2:E:76:ALA:N	2.38	0.57
3:C:63:LEU:HD21	3:C:180:PRO:HG3	1.86	0.57
3:C:222:LYS:HE2	3:C:337:HIS:CD2	2.39	0.57
1:A:75:ASN:ND2	11:A:1006:HOH:O	2.37	0.56
2:B:218:ARG:NH1	2:B:268:GLU:O	2.35	0.56
3:C:242:ASP:OD2	3:C:246:HIS:NE2	2.38	0.56
2:B:79:GLN:C	2:B:80:LYS:HD3	2.31	0.56
3:C:107:TYR:HD2	3:C:108:GLU:N	1.95	0.56
3:C:339:LYS:HG3	3:C:340:GLN:H	1.70	0.56
1:D:736:ASN:HD22	1:D:743:SER:HA	1.70	0.56
2:E:137:LYS:HD2	2:E:181:VAL:O	2.04	0.56
2:E:186:ASP:OD1	2:E:187:GLY:N	2.38	0.56
2:E:206:PHE:O	2:E:215:VAL:N	2.39	0.56
1:D:92:ASN:CG	1:D:93:THR:N	2.63	0.56
3:F:202:ASN:OD1	3:F:203:ALA:N	2.39	0.56
1:A:688:CYS:SG	8:A:908:HEC:C2C	2.79	0.56
1:D:203:MET:O	1:D:496:GLN:NE2	2.38	0.56
3:C:107:TYR:CD2	3:C:109:ARG:HG3	2.41	0.56
2:E:287:ASP:OD1	2:E:311:ARG:NH2	2.37	0.56
1:D:622:ARG:NH2	1:D:667:LYS:O	2.39	0.55
2:E:191:VAL:HA	2:E:205:ASP:O	2.05	0.55
2:B:88:ARG:NE	2:B:126:GLU:OE2	2.40	0.55
2:E:81:VAL:HG12	2:E:83:GLY:H	1.70	0.55
2:E:88:ARG:CD	2:E:110:SER:HB2	2.22	0.55
2:E:102:PHE:HA	2:E:117:ASP:HB3	1.88	0.55
2:E:89:VAL:HG22	2:E:109:GLU:OE2	2.06	0.55
1:D:169:ARG:HH21	1:D:171:ILE:HD11	1.72	0.55
2:E:75:ASP:CG	2:E:79:GLN:HE21	2.13	0.55
2:B:90:GLN:HB3	2:B:109:GLU:CG	2.37	0.55
3:C:145:GLU:OE1	3:C:150:HIS:NE2	2.32	0.55
2:B:111:ASP:OD2	2:B:131:ASP:HA	2.06	0.55
2:B:183:ILE:HG12	2:B:190:LEU:HD23	1.88	0.55
1:D:90:ASP:HB3	1:D:95:GLU:OE2	2.06	0.55
2:E:228:ASP:HB2	2:E:292:GLY:HA2	1.88	0.55
2:E:250:PRO:O	2:E:258:GLN:NE2	2.40	0.55
1:A:67:THR:HB	1:A:70:GLY:H	1.70	0.54
1:A:169:ARG:HB3	1:A:186:MET:HE2	1.89	0.54
1:D:422:ARG:NH1	3:F:95:SER:O	2.40	0.54
3:F:214:GLY:HA3	3:F:349:TYR:HB2	1.89	0.54
3:C:187:ILE:HA	3:C:190:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:TYR:HE1	2:E:42:VAL:O	1.90	0.54
3:C:116:ILE:HD11	3:C:308:THR:HG21	1.88	0.54
2:B:287:ASP:OD1	2:B:311:ARG:NH2	2.39	0.54
2:E:78:THR:H	2:E:79:GLN:HE22	1.54	0.54
1:D:42:TRP:HA	1:D:48:MET:SD	2.48	0.54
1:A:32:THR:OG1	2:B:309:MET:O	2.22	0.54
2:E:79:GLN:N	2:E:79:GLN:OE1	2.41	0.54
2:E:106:CYS:SG	2:E:133:PRO:HB2	2.47	0.54
2:E:208:ASP:O	2:E:212:GLY:N	2.41	0.54
3:C:132:TYR:CE2	3:C:134:ARG:HB2	2.42	0.54
1:D:325:ILE:HD11	1:D:345:TRP:HE3	1.73	0.54
1:A:31:MET:O	2:B:311:ARG:NH1	2.40	0.54
2:E:119:GLN:NE2	2:E:120:ARG:HG2	2.22	0.54
1:D:329:GLU:OE2	1:D:355:LYS:NZ	2.27	0.53
1:D:493:GLN:HB2	1:D:533:ILE:HG13	1.90	0.53
3:C:82:VAL:HG23	3:C:189:TYR:HA	1.90	0.53
2:E:105:VAL:HB	2:E:114:SER:HB2	1.91	0.53
2:E:101:ALA:O	2:E:117:ASP:HB2	2.08	0.53
1:A:359:LYS:CG	1:A:360:ASP:N	2.67	0.53
1:A:762:LYS:NZ	2:E:330:GLU:OE2	2.38	0.53
2:B:179:ARG:NH1	3:C:107:TYR:OH	2.42	0.53
3:F:255:VAL:HA	3:F:264:LYS:HG3	1.91	0.53
1:A:283:ARG:NH2	1:A:304:ASP:OD1	2.42	0.53
2:B:46:LEU:HD13	2:B:376:ASN:HD21	1.74	0.53
3:F:128:LYS:NZ	8:F:404:HEC:O2D	2.42	0.53
1:A:631:ASN:ND2	11:A:1009:HOH:O	2.41	0.53
2:E:90:GLN:HB2	2:E:109:GLU:OE1	2.09	0.53
1:A:604:LEU:HD13	2:B:250:PRO:HG3	1.89	0.52
3:C:107:TYR:CE2	3:C:109:ARG:HG3	2.44	0.52
2:E:120:ARG:CG	2:E:121:LYS:N	2.69	0.52
1:A:691:SER:OG	2:E:325:ARG:NH1	2.42	0.52
1:A:741:ILE:HG13	1:A:754:LEU:HB3	1.91	0.52
2:E:88:ARG:CZ	2:E:110:SER:H	2.22	0.52
1:D:345:TRP:O	2:E:284:ASN:ND2	2.42	0.52
2:E:131:ASP:OD1	2:E:132:TRP:N	2.43	0.52
3:F:109:ARG:HH11	3:F:109:ARG:CG	2.23	0.52
1:D:52:VAL:HG11	1:D:419:TYR:HB2	1.92	0.52
2:B:208:ASP:HB3	2:B:211:SER:HB3	1.92	0.52
3:C:322:ILE:HG23	3:C:335:THR:HG21	1.91	0.52
2:E:62:PHE:CD1	2:E:73:PHE:CE1	2.97	0.52
2:E:195:ASP:OD2	2:E:227:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:CYS:SG	11:C:574:HOH:O	2.59	0.52
3:F:318:LEU:O	3:F:321:THR:OG1	2.24	0.52
2:E:118:ILE:CB	2:E:119:GLN:HG2	2.34	0.51
1:D:520:SER:O	1:D:712:TYR:OH	2.25	0.51
2:E:38:GLN:NE2	3:F:109:ARG:HA	2.26	0.51
2:E:93:ALA:CB	2:E:135:GLY:HA2	2.41	0.51
2:E:38:GLN:HE21	3:F:109:ARG:HA	1.75	0.51
3:C:201:ARG:HD3	3:C:352:ALA:HB1	1.92	0.51
1:D:205:GLU:OE1	1:D:253:SER:OG	2.23	0.51
2:E:184:SER:HB3	2:E:231:TYR:HE2	1.76	0.51
2:B:148:ALA:HB2	2:B:181:VAL:HG13	1.93	0.51
3:C:317:THR:OG1	3:C:320:ASP:OD2	2.27	0.51
2:E:181:VAL:HG12	2:E:192:ALA:HB2	1.93	0.51
1:D:762:LYS:O	1:D:762:LYS:HG3	2.11	0.50
2:E:117:ASP:C	2:E:119:GLN:HE21	2.19	0.50
3:F:311:HIS:ND1	8:F:405:HEC:O2D	2.38	0.50
1:A:678:GLN:NE2	1:A:682:ASP:OD1	2.44	0.50
2:B:90:GLN:CB	2:B:109:GLU:HG2	2.40	0.50
2:E:60:THR:HA	2:E:75:ASP:HA	1.93	0.50
2:E:69:HIS:CD2	2:E:90:GLN:H	2.29	0.50
2:E:88:ARG:HH22	2:E:109:GLU:N	2.05	0.50
2:B:227:ARG:NH2	11:B:509:HOH:O	2.44	0.50
2:E:78:THR:N	2:E:79:GLN:NE2	2.58	0.50
3:F:81:LEU:HA	3:F:84:TYR:HD2	1.76	0.50
1:D:135:MET:HE2	1:D:142:LEU:HD23	1.93	0.50
1:A:248:ILE:HG13	1:A:249:THR:HG23	1.93	0.50
1:A:462:ASP:O	1:A:585:GLY:HA2	2.12	0.50
1:A:608:TRP:NE1	1:A:610:ASP:O	2.42	0.50
1:D:770:LEU:HD21	8:D:908:HEC:HBC2	1.94	0.50
2:E:120:ARG:HH12	2:E:124:ILE:HD12	1.76	0.50
2:E:169:ARG:NH2	2:E:212:GLY:HA3	2.26	0.50
1:D:260:LEU:HD13	1:D:421:PRO:HG2	1.93	0.50
1:D:277:ARG:HG3	8:D:907:HEC:O1D	2.12	0.50
1:D:444:ASP:OD1	1:D:447:LYS:N	2.44	0.49
1:D:457:THR:O	1:D:580:GLY:HA2	2.12	0.49
2:E:152:CYS:SG	3:F:107:TYR:OH	2.70	0.49
1:A:432:ASN:ND2	1:A:454:SER:OG	2.39	0.49
2:B:42:VAL:HG11	3:C:82:VAL:HG11	1.94	0.49
3:C:202:ASN:ND2	3:C:207:LEU:O	2.43	0.49
3:F:150:HIS:CD2	3:F:156:GLY:H	2.30	0.49
2:B:104:TYR:HB3	2:B:136:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:206:SER:HA	3:F:234:MET:HE1	1.95	0.49
3:F:317:THR:OG1	3:F:320:ASP:OD2	2.26	0.49
3:F:335:THR:HA	3:F:338:LEU:HD13	1.95	0.49
1:A:547:SER:OG	1:A:617:SER:OG	2.26	0.49
1:A:340:LEU:HB2	1:A:357:THR:HG22	1.95	0.49
1:D:34:GLY:HA3	1:D:39:LYS:O	2.12	0.49
1:D:57:SER:O	1:D:91:LEU:HG	2.13	0.49
2:E:75:ASP:C	2:E:79:GLN:NE2	2.71	0.49
2:E:115:VAL:HG11	2:E:165:MET:SD	2.51	0.49
2:E:241:THR:HG23	2:E:293:MET:SD	2.53	0.49
1:D:419:TYR:OH	3:F:59:ARG:NH1	2.46	0.49
1:D:734:TYR:HE1	8:D:908:HEC:HBA2	1.78	0.49
3:F:219:GLU:HG2	3:F:226:LEU:HD21	1.94	0.49
2:E:38:GLN:HB2	2:E:90:GLN:HE22	1.78	0.49
2:E:117:ASP:CG	2:E:119:GLN:NE2	2.71	0.49
2:E:218:ARG:NH1	2:E:268:GLU:O	2.38	0.49
3:F:107:TYR:CB	3:F:109:ARG:H	2.26	0.49
1:D:77:PRO:HB3	1:D:256:PHE:CG	2.47	0.48
1:D:90:ASP:OD2	1:D:92:ASN:ND2	2.46	0.48
2:E:191:VAL:HG13	2:E:231:TYR:OH	2.14	0.48
3:F:71:ARG:NH2	3:F:184:GLU:HG3	2.27	0.48
3:F:245:THR:HG22	3:F:294:GLU:HB3	1.96	0.48
2:B:41:HIS:CD2	3:C:194:GLU:HG3	2.49	0.48
2:B:94:SER:HB2	2:B:103:LEU:HD11	1.94	0.48
3:F:59:ARG:NH2	3:F:176:GLU:OE2	2.38	0.48
2:E:286:TYR:O	2:E:311:ARG:NH2	2.47	0.48
2:E:119:GLN:CB	2:E:120:ARG:HB3	2.43	0.48
1:D:169:ARG:HE	1:D:171:ILE:HD11	1.78	0.48
1:D:432:ASN:HA	1:D:454:SER:HB3	1.95	0.48
2:E:119:GLN:CG	2:E:120:ARG:HG2	2.43	0.48
2:E:294:ALA:HB1	2:E:361:LEU:HG	1.95	0.48
2:B:352:THR:HG22	2:B:353:GLY:H	1.79	0.48
2:E:202:ARG:NH1	2:E:225:ASN:H	2.12	0.48
1:A:225:ILE:HG13	1:A:233:LEU:HB2	1.95	0.48
3:C:142:PHE:HB2	3:C:158:THR:HB	1.95	0.48
2:E:36:TYR:CD1	2:E:37:ILE:N	2.82	0.47
2:E:74:VAL:HG12	2:E:79:GLN:CG	2.44	0.47
2:E:376:ASN:HD21	3:F:83:ARG:NH2	2.12	0.47
1:A:58:GLN:HB3	1:A:88:LEU:HD11	1.95	0.47
1:A:504:ARG:HD3	1:A:800:PRO:HB3	1.96	0.47
8:D:908:HEC:HBD2	8:D:908:HEC:HHA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:ARG:NH1	2:E:110:SER:N	2.60	0.47
3:F:106:HIS:CD2	8:F:404:HEC:NB	2.82	0.47
3:F:137:ARG:NH2	3:F:138:TYR:OH	2.48	0.47
1:A:357:THR:HA	1:A:358:GLY:HA3	1.44	0.47
1:D:67:THR:HB	1:D:70:GLY:H	1.80	0.47
2:E:187:GLY:O	2:E:209:ILE:HD12	2.13	0.47
3:F:111:GLN:O	3:F:132:TYR:HA	2.14	0.47
8:A:908:HEC:HBC3	8:A:908:HEC:HHD	1.94	0.47
3:C:209:GLU:O	3:C:213:ARG:HB2	2.14	0.47
2:E:85:VAL:HB	2:E:121:LYS:CE	2.43	0.47
2:E:109:GLU:HA	11:E:511:HOH:O	2.14	0.47
2:E:117:ASP:OD1	2:E:118:ILE:HG12	2.13	0.47
1:A:240:HIS:CD2	1:A:241:LEU:HG	2.49	0.47
2:E:119:GLN:HG3	2:E:120:ARG:CB	2.43	0.47
3:C:131:LYS:HB3	8:C:404:HEC:HBA1	1.97	0.47
2:E:182:GLU:O	2:E:183:ILE:HD13	2.15	0.47
1:A:688:CYS:SG	8:A:908:HEC:C4C	2.89	0.47
2:E:183:ILE:CG1	2:E:190:LEU:HD22	2.41	0.47
1:A:289:ASP:OD1	1:A:290:ASN:N	2.48	0.46
1:D:261:THR:OG1	1:D:263:ASP:OD1	2.31	0.46
3:C:106:HIS:HA	3:C:112:THR:HA	1.97	0.46
1:D:81:PRO:HB2	1:D:84:SER:OG	2.15	0.46
2:E:88:ARG:NH2	2:E:109:GLU:H	2.07	0.46
1:A:259:TRP:N	1:A:267:LEU:O	2.48	0.46
1:A:339:GLN:HB3	1:A:357:THR:O	2.15	0.46
3:C:110:GLY:HA2	3:C:133:ILE:HD11	1.98	0.46
2:E:307:ARG:NE	2:E:357:SER:OG	2.41	0.46
3:F:316:ARG:H	3:F:316:ARG:HG2	1.50	0.46
1:A:60:LEU:O	1:A:413:ALA:N	2.43	0.46
3:C:208:THR:O	3:C:212:LYS:HG3	2.16	0.46
1:D:289:ASP:OD1	1:D:290:ASN:N	2.48	0.46
1:D:504:ARG:NH2	1:D:801:ASP:O	2.48	0.46
2:E:116:VAL:HA	2:E:120:ARG:NH1	2.31	0.46
2:B:50:PHE:HB2	2:B:66:GLN:HB2	1.98	0.46
1:D:462:ASP:O	1:D:585:GLY:HA2	2.16	0.46
3:F:142:PHE:HB2	3:F:158:THR:HB	1.98	0.46
1:A:206:PHE:CZ	1:A:333:MET:HE1	2.51	0.46
1:A:504:ARG:NH1	1:A:801:ASP:O	2.45	0.46
2:E:109:GLU:OE1	2:E:109:GLU:N	2.40	0.46
1:A:169:ARG:HA	1:A:186:MET:HG2	1.98	0.46
1:D:795:ASP:OD2	11:D:1001:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ARG:HA	2:B:356:PRO:HD2	1.97	0.45
1:D:472:PRO:HB2	1:D:730:ILE:HD13	1.98	0.45
1:D:760:ARG:NE	1:D:762:LYS:O	2.47	0.45
2:E:40:THR:HG22	3:F:193:LEU:CA	2.46	0.45
1:A:78:HIS:ND1	1:A:212:TYR:OH	2.39	0.45
1:A:131:GLN:HE22	1:A:148:LEU:H	1.64	0.45
2:B:88:ARG:HB2	2:B:107:ASN:CG	2.41	0.45
2:B:159:VAL:HG23	2:B:168:VAL:HB	1.98	0.45
2:E:119:GLN:CD	2:E:120:ARG:HG2	2.42	0.45
1:A:761:GLU:CD	1:A:761:GLU:H	2.23	0.45
1:D:741:ILE:HG13	1:D:754:LEU:HB3	1.99	0.45
2:E:54:MET:HG3	2:E:61:LEU:HD23	1.98	0.45
2:E:251:VAL:HG12	11:F:504:HOH:O	2.16	0.45
1:A:81:PRO:HB2	1:A:84:SER:OG	2.16	0.45
1:D:588:TYR:HB3	5:D:903:CL:CL	2.53	0.45
1:A:627:ASP:HB3	1:A:633:LYS:HD3	1.99	0.45
2:B:70:SER:HA	2:B:87:VAL:HG22	1.99	0.45
2:B:325:ARG:HD3	1:D:692:ASN:HA	1.99	0.45
2:E:37:ILE:HD11	2:E:44:THR:HG23	1.99	0.45
3:F:207:LEU:HB3	3:F:211:GLN:HB2	1.97	0.45
1:A:362:GLY:HA3	1:A:380:ALA:O	2.17	0.45
3:F:134:ARG:NH1	3:F:194:GLU:O	2.37	0.45
1:A:162:SER:OG	1:A:189:LYS:HB3	2.16	0.45
1:A:608:TRP:CE3	3:C:123:GLY:HA2	2.52	0.45
2:B:93:ALA:HB3	2:B:106:CYS:HB2	1.99	0.45
3:F:228:CYS:HA	3:F:242:ASP:HB2	1.99	0.45
1:A:190:THR:HG1	1:A:219:THR:HG1	1.57	0.45
1:A:493:GLN:HB2	1:A:533:ILE:HG13	1.98	0.45
1:D:549:LEU:HD21	1:D:663:LEU:HA	1.99	0.45
2:E:121:LYS:HD2	2:E:121:LYS:HA	1.71	0.45
1:A:43:THR:O	1:A:422:ARG:NH2	2.50	0.45
2:E:69:HIS:CG	2:E:89:VAL:HA	2.51	0.45
2:E:203:SER:HB3	2:E:217:ASN:OD1	2.16	0.44
3:C:123:GLY:O	3:C:126:SER:OG	2.27	0.44
1:D:627:ASP:OD2	1:D:631:ASN:HB2	2.18	0.44
3:F:315:ALA:HB2	3:F:326:VAL:HG21	1.99	0.44
1:A:173:ARG:HB3	1:A:441:GLN:NE2	2.33	0.44
2:E:190:LEU:HD12	2:E:207:ILE:HG13	1.98	0.44
3:F:126:SER:HB3	3:F:289:LEU:O	2.18	0.44
3:C:260:SER:OG	3:C:261:THR:N	2.47	0.44
1:D:43:THR:O	1:D:422:ARG:NH2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:760:ARG:NH2	8:D:908:HEC:O2A	2.47	0.44
3:F:297:THR:HA	3:F:298:PRO:HD3	1.79	0.44
3:C:106:HIS:CD2	8:C:404:HEC:NB	2.86	0.44
3:C:111:GLN:HB3	3:C:132:TYR:CE1	2.52	0.44
1:D:153:ARG:NH1	11:D:1020:HOH:O	2.50	0.44
1:D:169:ARG:HG3	3:F:67:GLU:OE2	2.17	0.44
1:D:382:ARG:HA	1:D:382:ARG:HD3	1.55	0.44
2:E:81:VAL:HG12	2:E:83:GLY:N	2.32	0.44
3:F:45:ILE:HG23	3:F:46:SER:H	1.83	0.44
2:E:93:ALA:HB3	2:E:135:GLY:HA2	2.00	0.44
2:B:228:ASP:HB3	2:B:293:MET:HE2	2.00	0.44
2:E:93:ALA:HB3	2:E:106:CYS:HB3	2.00	0.44
3:F:112:THR:HB	3:F:131:LYS:O	2.18	0.44
2:B:241:THR:HG23	2:B:293:MET:SD	2.57	0.44
1:D:259:TRP:CG	1:D:260:LEU:H	2.36	0.44
3:F:178:PHE:HA	3:F:182:ARG:HH12	1.82	0.44
2:E:85:VAL:HG21	2:E:122:GLN:N	2.33	0.43
2:E:160:ILE:HG12	2:E:167:LYS:HA	1.99	0.43
1:A:331:PRO:HB2	1:D:331:PRO:HB3	1.99	0.43
1:A:428:THR:HB	1:A:579:HIS:HE1	1.81	0.43
1:A:629:ASP:OD1	1:A:629:ASP:N	2.51	0.43
2:B:116:VAL:HA	2:B:123:GLU:HA	2.00	0.43
1:A:310:THR:O	1:A:333:MET:HG3	2.19	0.43
3:F:59:ARG:HH21	3:F:176:GLU:CD	2.25	0.43
3:F:143:ARG:HB3	3:F:144:HIS:H	1.54	0.43
2:B:164:ARG:NH2	11:B:512:HOH:O	2.51	0.43
1:D:53:GLN:NE2	1:D:372:ASP:OD1	2.51	0.43
1:D:489:VAL:HG22	1:D:536:GLN:O	2.18	0.43
2:E:36:TYR:CE2	2:E:40:THR:O	2.68	0.43
1:A:159:ALA:HB1	1:A:162:SER:O	2.19	0.43
1:D:117:LYS:HA	1:D:136:ASN:HA	2.01	0.43
1:D:432:ASN:ND2	11:D:1015:HOH:O	2.47	0.43
2:E:102:PHE:CD1	2:E:117:ASP:HB3	2.54	0.43
2:E:133:PRO:HA	2:E:148:ALA:O	2.19	0.43
2:E:183:ILE:HG22	2:E:184:SER:N	2.34	0.43
2:E:253[B]:GLU:HA	3:F:174:ARG:HG3	2.01	0.43
1:A:259:TRP:CG	1:A:260:LEU:H	2.36	0.43
1:A:561:ASP:O	1:A:632:TYR:N	2.42	0.43
2:B:187:GLY:O	2:B:209:ILE:HD12	2.19	0.43
1:D:713:SER:O	1:D:717:ASN:ND2	2.38	0.43
2:E:374:PHE:HB3	3:F:54:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:107:TYR:HB3	3:F:109:ARG:H	1.83	0.43
3:F:244:GLN:OE1	3:F:244:GLN:N	2.52	0.43
1:A:633:LYS:HD2	1:A:633:LYS:HA	1.88	0.43
2:E:42:VAL:HG13	3:F:79:SER:HB2	2.00	0.43
3:F:143:ARG:NH2	8:F:404:HEC:O2D	2.51	0.43
1:A:428:THR:HB	1:A:579:HIS:CE1	2.53	0.43
1:D:252:LEU:HD12	1:D:572:TRP:CZ2	2.54	0.43
2:E:69:HIS:ND1	2:E:89:VAL:HA	2.34	0.43
3:F:75:SER:HB3	3:F:76:PRO:HD2	2.00	0.43
1:D:163:ILE:HD13	1:D:420:LYS:HE2	2.00	0.43
2:E:137:LYS:HD3	2:E:182:GLU:OE1	2.19	0.43
2:E:293:MET:HE2	2:E:302:LEU:HD11	2.01	0.43
3:F:284:THR:HG21	3:F:308:THR:HG21	2.01	0.42
2:B:69:HIS:CE1	2:B:89:VAL:HG12	2.54	0.42
2:B:356:PRO:HA	2:B:371:ALA:O	2.19	0.42
1:D:617:SER:HA	1:D:618:PRO:HD3	1.87	0.42
1:A:556:MET:HE3	1:A:556:MET:HB2	1.81	0.42
2:B:132:TRP:CH2	3:C:109:ARG:HD3	2.54	0.42
3:C:183:LEU:O	3:C:187:ILE:HG12	2.19	0.42
3:F:72:VAL:O	3:F:160:SER:HB2	2.20	0.42
1:A:727:ASP:HB3	1:A:730:ILE:HG13	2.02	0.42
1:D:359:LYS:HA	1:D:359:LYS:HD2	1.72	0.42
1:A:59:ILE:HG22	1:A:414:PRO:HA	2.02	0.42
2:B:180:MET:HB3	2:B:193:ILE:HD11	2.02	0.42
1:D:189:LYS:HE3	1:D:189:LYS:HB2	1.87	0.42
2:E:298:LYS:HD3	2:E:300:LYS:HE2	2.02	0.42
2:B:252:CYS:O	3:C:174:ARG:NE	2.52	0.42
1:D:629:ASP:OD1	1:D:629:ASP:N	2.52	0.42
2:E:184:SER:HB3	2:E:231:TYR:CE2	2.55	0.42
3:C:107:TYR:CD2	3:C:108:GLU:N	2.75	0.42
1:D:437:VAL:HG13	3:F:121:ASP:HA	2.02	0.42
1:D:459:ILE:HB	1:D:545:VAL:HG23	2.00	0.42
2:E:42:VAL:CG1	3:F:79:SER:HB2	2.50	0.42
2:E:120:ARG:HH22	2:E:124:ILE:HD12	1.85	0.42
2:E:179:ARG:O	2:E:179:ARG:HG3	2.19	0.42
3:F:339:LYS:O	3:F:343:LEU:HG	2.19	0.42
1:A:325:ILE:HD11	1:A:345:TRP:HE3	1.85	0.42
2:B:250:PRO:HB3	3:C:124:TRP:CZ3	2.55	0.42
2:B:251:VAL:HG12	11:C:511:HOH:O	2.19	0.42
3:C:297:THR:HA	3:C:298:PRO:HD3	1.81	0.42
1:D:641:VAL:HA	1:D:660:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:THR:CG2	3:F:193:LEU:HD23	2.50	0.42
2:E:85:VAL:HB	2:E:121:LYS:CD	2.50	0.42
2:E:85:VAL:HG13	2:E:86:ALA:N	2.35	0.42
2:E:118:ILE:HD12	2:E:118:ILE:HG23	1.58	0.42
2:E:161:ASP:HB3	2:E:164:ARG:HB3	2.02	0.42
2:E:118:ILE:C	2:E:119:GLN:HG2	2.45	0.42
2:E:146:TYR:OH	2:E:209:ILE:HG23	2.20	0.42
3:F:103:ALA:HA	3:F:107:TYR:O	2.19	0.42
3:F:183:LEU:O	3:F:187:ILE:HG12	2.20	0.42
1:A:617:SER:HA	1:A:618:PRO:HD3	1.90	0.41
2:E:95:ALA:O	2:E:103:LEU:HA	2.20	0.41
3:F:128:LYS:HG3	8:F:404:HEC:O2D	2.20	0.41
1:A:190:THR:OG1	1:A:219:THR:OG1	2.22	0.41
1:D:381:GLU:O	1:D:382:ARG:NH1	2.53	0.41
2:E:97:THR:HG23	2:E:102:PHE:O	2.20	0.41
1:A:31:MET:SD	1:A:323:ARG:NH2	2.93	0.41
3:C:267:ASN:HB3	3:C:270:ALA:HB3	2.02	0.41
3:C:308:THR:HG22	3:C:313:GLY:CA	2.50	0.41
1:D:602:LYS:HG2	3:F:278:TYR:CZ	2.55	0.41
2:E:88:ARG:NH1	2:E:107:ASN:HB2	2.34	0.41
3:F:257:GLY:O	3:F:260:SER:OG	2.37	0.41
1:A:131:GLN:NE2	1:A:148:LEU:H	2.18	0.41
1:A:584:SER:HB2	1:A:590:SER:HB3	2.02	0.41
2:B:91:PRO:HA	2:B:106:CYS:O	2.20	0.41
3:C:144:HIS:ND1	8:C:404:HEC:O2D	2.39	0.41
1:D:121:ALA:HB2	1:D:153:ARG:HA	2.02	0.41
2:E:178:PRO:HB3	2:E:194:LEU:HD23	2.02	0.41
2:E:237:TYR:CE1	2:E:268:GLU:HG2	2.55	0.41
2:E:253[B]:GLU:HB3	2:E:255:GLU:OE1	2.19	0.41
3:F:134:ARG:HD2	3:F:194:GLU:O	2.20	0.41
4:A:902:XE:XE	2:B:351:PRO:HG3	2.98	0.41
1:D:159:ALA:O	1:D:420:LYS:NZ	2.37	0.41
1:A:199:PRO:HG2	1:A:202:VAL:HG21	2.02	0.41
2:E:310:HIS:HA	2:E:356:PRO:HD2	2.02	0.41
3:F:348:GLU:O	3:F:351:LYS:HB2	2.21	0.41
3:F:146:GLY:C	3:F:157:ALA:HB2	2.46	0.41
2:B:386:ASP:N	2:B:386:ASP:OD1	2.54	0.41
1:D:163:ILE:HG13	3:F:62:PRO:CD	2.41	0.41
2:E:136:ILE:HG23	2:E:148:ALA:H	1.85	0.41
2:B:49:PRO:HB3	2:B:63:ILE:CG2	2.51	0.41
1:D:487:LYS:HB3	1:D:632:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:GLY:HA3	2:E:68:GLY:C	2.46	0.41
2:E:36:TYR:CE1	2:E:42:VAL:C	2.99	0.41
3:F:320:ASP:O	11:F:501:HOH:O	2.21	0.41
3:F:347:VAL:HG13	3:F:351:LYS:NZ	2.35	0.41
1:A:252:LEU:HD12	1:A:572:TRP:CZ2	2.56	0.40
1:A:456:GLY:N	1:A:550:SER:OG	2.54	0.40
1:D:59:ILE:HA	1:D:414:PRO:HA	2.03	0.40
1:D:608:TRP:HD1	1:D:616:ASP:OD2	2.05	0.40
3:F:150:HIS:HD2	3:F:156:GLY:H	1.69	0.40
3:F:228:CYS:O	3:F:242:ASP:HB2	2.20	0.40
1:D:277:ARG:NH1	8:D:907:HEC:O2D	2.53	0.40
1:D:681:LEU:O	1:D:685:CYS:HB2	2.21	0.40
2:E:136:ILE:CG2	2:E:146:TYR:O	2.69	0.40
3:F:92:ALA:O	3:F:98:GLY:HA2	2.21	0.40
3:F:112:THR:HG21	11:F:519:HOH:O	2.22	0.40
1:A:205:GLU:HA	1:A:528:GLN:NE2	2.36	0.40
1:A:457:THR:O	1:A:580:GLY:HA2	2.22	0.40
1:A:678:GLN:HG2	1:A:701:LEU:HG	2.03	0.40
2:B:134:SER:OG	2:B:179:ARG:O	2.18	0.40
2:B:165:MET:HE3	2:B:165:MET:HB2	2.02	0.40
2:E:99:ASP:OD1	2:E:99:ASP:N	2.52	0.40
3:F:277:PRO:HA	3:F:286:ILE:HD11	2.02	0.40
1:D:262:PRO:HD3	1:D:318:ILE:HD12	2.03	0.40
1:D:432:ASN:HD22	1:D:454:SER:HB3	1.85	0.40
3:F:81:LEU:O	3:F:84:TYR:HB2	2.22	0.40
1:D:252:LEU:HD23	1:D:252:LEU:HA	1.94	0.40
2:E:118:ILE:HB	2:E:119:GLN:CG	2.37	0.40
2:E:122:GLN:OE1	2:E:123:GLU:N	2.54	0.40
2:E:183:ILE:HG22	2:E:184:SER:H	1.86	0.40
2:E:356:PRO:HA	2:E:371:ALA:O	2.21	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	762/782 (97%)	728 (96%)	34 (4%)	0	100	100
1	D	764/782 (98%)	740 (97%)	24 (3%)	0	100	100
2	B	351/352 (100%)	344 (98%)	7 (2%)	0	100	100
2	E	351/352 (100%)	332 (95%)	16 (5%)	3 (1%)	14	47
3	C	312/314 (99%)	296 (95%)	16 (5%)	0	100	100
3	F	312/314 (99%)	294 (94%)	18 (6%)	0	100	100
All	All	2852/2896 (98%)	2734 (96%)	115 (4%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	118	ILE
2	E	136	ILE
2	E	119	GLN

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 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	641/653 (98%)	632 (99%)	9 (1%)	59	77
1	D	642/653 (98%)	635 (99%)	7 (1%)	65	79
2	B	303/302 (100%)	297 (98%)	6 (2%)	48	72
2	E	300/302 (99%)	283 (94%)	17 (6%)	18	51
3	C	262/264 (99%)	257 (98%)	5 (2%)	50	73
3	F	259/264 (98%)	253 (98%)	6 (2%)	44	70
All	All	2407/2438 (99%)	2357 (98%)	50 (2%)	47	71

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	39	LYS
1	A	162	SER
1	A	178	GLU
1	A	333	MET
1	A	360	ASP
1	A	517	GLU
1	A	629	ASP
1	A	633	LYS
2	B	43	LYS
2	B	89	VAL
2	B	109	GLU
2	B	186	ASP
2	B	270	LYS
2	B	352	THR
3	C	129	ASN
3	C	204	ASP
3	C	217	ILE
3	C	234	MET
3	C	281	GLU
1	D	50	LYS
1	D	69	LYS
1	D	164	GLU
1	D	169	ARG
1	D	178	GLU
1	D	629	ASP
1	D	762	LYS
2	E	74	VAL
2	E	85	VAL
2	E	88	ARG
2	E	103	LEU
2	E	120	ARG
2	E	126	GLU
2	E	136	ILE
2	E	138	ILE
2	E	167	LYS
2	E	188	LYS
2	E	190	LEU
2	E	191	VAL
2	E	197	VAL
2	E	207	ILE
2	E	214	VAL
2	E	226	LEU

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Mol	Chain	Res	Type
2	E	293	MET
3	F	109	ARG
3	F	137	ARG
3	F	152	ASP
3	F	264	LYS
3	F	280	VAL
3	F	316	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	131	GLN
1	A	207	HIS
1	A	213	ASN
1	A	272	GLN
1	A	441	GLN
1	A	475	HIS
1	A	528	GLN
2	B	41	HIS
2	B	107	ASN
2	B	376	ASN
3	C	327	ASN
3	C	337	HIS
3	C	340	GLN
3	C	344	GLN
1	D	136	ASN
1	D	184	HIS
1	D	207	HIS
1	D	208	ASN
1	D	213	ASN
1	D	290	ASN
1	D	410	HIS
1	D	432	ASN
1	D	441	GLN
1	D	496	GLN
1	D	536	GLN
1	D	631	ASN
1	D	668	GLN
1	D	678	GLN
1	D	736	ASN
2	E	51	HIS

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Mol	Chain	Res	Type
2	E	65	ASN
2	E	79	GLN
2	E	119	GLN
2	E	289	ASN
3	F	150	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 38 ligands modelled in this entry, 23 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
9	BET	B	403	-	7,7,7	2.52	1 (14%)	10,10,10	1.98	2 (20%)
9	BET	A	909	-	7,7,7	2.55	1 (14%)	10,10,10	1.87	2 (20%)
8	HEC	A	908	1	50,50,50	1.77	6 (12%)	68,82,82	1.43	7 (10%)
8	HEC	A	907	1,7	50,50,50	1.86	5 (10%)	68,82,82	1.37	5 (7%)
8	HEC	D	907	1,7	50,50,50	1.84	5 (10%)	68,82,82	1.40	5 (7%)
8	HEC	D	908	1	50,50,50	1.81	5 (10%)	68,82,82	1.42	6 (8%)
9	BET	A	911	-	7,7,7	2.51	1 (14%)	10,10,10	1.93	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BET	D	909	-	7,7,7	2.57	1 (14%)	10,10,10	1.94	2 (20%)
9	BET	A	910	-	7,7,7	2.53	1 (14%)	10,10,10	1.95	2 (20%)
8	HEC	F	404	11,3	50,50,50	1.79	6 (12%)	68,82,82	1.35	5 (7%)
8	HEC	C	405	3	50,50,50	1.80	6 (12%)	68,82,82	1.37	5 (7%)
9	BET	E	403	-	7,7,7	2.47	1 (14%)	10,10,10	1.96	2 (20%)
9	BET	C	406	-	7,7,7	2.54	1 (14%)	10,10,10	1.87	2 (20%)
8	HEC	C	404	11,3	50,50,50	1.80	6 (12%)	68,82,82	1.36	5 (7%)
8	HEC	F	405	3	50,50,50	1.83	5 (10%)	68,82,82	1.33	6 (8%)

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
9	BET	B	403	-	-	5/5/5/5	-
9	BET	A	909	-	-	5/5/5/5	-
8	HEC	A	908	1	1/1/3/7	4/14/54/54	-
8	HEC	D	907	1,7	1/1/3/7	4/14/54/54	-
8	HEC	D	908	1	1/1/3/7	6/14/54/54	-
8	HEC	A	907	1,7	-	4/14/54/54	-
9	BET	A	911	-	-	5/5/5/5	-
9	BET	D	909	-	-	5/5/5/5	-
9	BET	A	910	-	-	5/5/5/5	-
8	HEC	F	404	11,3	1/1/3/7	2/14/54/54	-
8	HEC	C	405	3	1/1/3/7	2/14/54/54	-
9	BET	E	403	-	-	5/5/5/5	-
9	BET	C	406	-	-	5/5/5/5	-
8	HEC	C	404	11,3	1/1/3/7	4/14/54/54	-
8	HEC	F	405	3	1/1/3/7	0/14/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	404	HEC	C3D-C2D	8.15	1.54	1.36
8	C	405	HEC	C3D-C2D	8.09	1.53	1.36
8	D	908	HEC	C3D-C2D	8.08	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	405	HEC	C3D-C2D	8.08	1.53	1.36
8	D	907	HEC	C3D-C2D	8.03	1.53	1.36
8	C	404	HEC	C3D-C2D	8.03	1.53	1.36
8	A	908	HEC	C3D-C2D	8.02	1.53	1.36
8	A	907	HEC	C3D-C2D	7.99	1.53	1.36
9	D	909	BET	CA-C	6.17	1.63	1.52
9	C	406	BET	CA-C	6.16	1.62	1.52
9	A	909	BET	CA-C	6.15	1.62	1.52
9	B	403	BET	CA-C	6.10	1.62	1.52
9	A	911	BET	CA-C	6.07	1.62	1.52
9	A	910	BET	CA-C	6.06	1.62	1.52
9	E	403	BET	CA-C	5.98	1.62	1.52
8	F	405	HEC	FE-ND	5.34	2.11	1.94
8	D	907	HEC	FE-ND	5.03	2.10	1.94
8	A	907	HEC	FE-ND	4.93	2.10	1.94
8	C	405	HEC	FE-NB	4.67	2.09	1.94
8	F	404	HEC	FE-NB	4.40	2.08	1.94
8	A	907	HEC	FE-NB	4.39	2.08	1.94
8	D	908	HEC	FE-NB	4.26	2.08	1.94
8	D	908	HEC	FE-ND	4.23	2.08	1.94
8	C	404	HEC	FE-ND	4.20	2.07	1.94
8	A	908	HEC	FE-ND	3.98	2.07	1.94
8	C	404	HEC	FE-NB	3.95	2.07	1.94
8	C	405	HEC	FE-ND	3.84	2.06	1.94
8	A	908	HEC	FE-NB	3.83	2.06	1.94
8	D	907	HEC	FE-NB	3.78	2.06	1.94
8	D	908	HEC	FE-NC	3.66	2.07	1.95
8	C	404	HEC	FE-NC	3.57	2.07	1.95
8	F	404	HEC	FE-ND	3.52	2.05	1.94
8	F	405	HEC	FE-NB	3.50	2.05	1.94
8	A	907	HEC	FE-NC	3.48	2.06	1.95
8	D	907	HEC	FE-NC	3.47	2.06	1.95
8	A	908	HEC	FE-NC	3.46	2.06	1.95
8	F	405	HEC	FE-NA	3.40	2.06	1.95
8	A	907	HEC	FE-NA	3.30	2.06	1.95
8	F	404	HEC	FE-NC	3.30	2.06	1.95
8	D	907	HEC	FE-NA	3.18	2.05	1.95
8	C	404	HEC	FE-NA	2.99	2.05	1.95
8	C	405	HEC	FE-NA	2.92	2.05	1.95
8	F	404	HEC	FE-NA	2.84	2.04	1.95
8	C	405	HEC	FE-NC	2.84	2.04	1.95
8	A	908	HEC	FE-NA	2.77	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	908	HEC	FE-NA	2.50	2.03	1.95
8	F	405	HEC	FE-NC	2.49	2.03	1.95
8	A	908	HEC	CMC-C2C	2.03	1.55	1.50
8	F	404	HEC	CMB-C2B	2.03	1.55	1.50
8	C	404	HEC	CMA-C3A	2.01	1.55	1.50
8	C	405	HEC	CMB-C2B	2.01	1.55	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	404	HEC	C1D-ND-C4D	6.57	111.86	105.07
8	D	908	HEC	C1D-ND-C4D	6.57	111.86	105.07
8	F	404	HEC	C1D-ND-C4D	6.37	111.66	105.07
8	A	908	HEC	C1D-ND-C4D	6.37	111.65	105.07
8	C	405	HEC	C1D-ND-C4D	6.28	111.56	105.07
8	F	405	HEC	C1D-ND-C4D	6.08	111.35	105.07
8	D	907	HEC	C1D-ND-C4D	5.92	111.19	105.07
8	A	907	HEC	C1D-ND-C4D	5.89	111.15	105.07
9	B	403	BET	C-CA-N	-4.83	109.70	116.34
9	E	403	BET	C-CA-N	-4.80	109.74	116.34
9	A	910	BET	C-CA-N	-4.76	109.79	116.34
9	A	911	BET	C-CA-N	-4.76	109.80	116.34
9	D	909	BET	C-CA-N	-4.72	109.85	116.34
9	C	406	BET	C-CA-N	-4.53	110.11	116.34
9	A	909	BET	C-CA-N	-4.52	110.12	116.34
9	A	909	BET	OXT-C-O	3.33	131.59	123.30
9	E	403	BET	OXT-C-O	3.31	131.56	123.30
9	A	910	BET	OXT-C-O	3.30	131.52	123.30
9	C	406	BET	OXT-C-O	3.30	131.51	123.30
9	B	403	BET	OXT-C-O	3.29	131.50	123.30
9	A	911	BET	OXT-C-O	3.29	131.50	123.30
9	D	909	BET	OXT-C-O	3.28	131.46	123.30
8	D	908	HEC	CAD-C3D-C4D	2.95	129.81	124.66
8	D	907	HEC	C4B-NB-C1B	2.80	107.97	105.07
8	A	907	HEC	C4B-NB-C1B	2.75	107.92	105.07
8	C	405	HEC	C4A-NA-C1A	2.74	108.03	105.35
8	D	908	HEC	C4A-NA-C1A	2.69	107.98	105.35
8	A	908	HEC	C4C-NC-C1C	2.67	107.97	105.35
8	C	405	HEC	C4B-NB-C1B	2.67	107.83	105.07
8	A	908	HEC	C4A-NA-C1A	2.67	107.96	105.35
8	C	405	HEC	C4C-NC-C1C	2.64	107.93	105.35
8	F	405	HEC	C4B-NB-C1B	2.63	107.79	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	907	HEC	C4A-NA-C1A	2.61	107.91	105.35
8	F	405	HEC	C4A-NA-C1A	2.59	107.89	105.35
8	A	908	HEC	C4B-NB-C1B	2.58	107.74	105.07
8	C	404	HEC	C4B-NB-C1B	2.58	107.74	105.07
8	A	907	HEC	C4C-NC-C1C	2.53	107.82	105.35
8	F	404	HEC	C4B-NB-C1B	2.48	107.64	105.07
8	F	405	HEC	C4C-NC-C1C	2.47	107.76	105.35
8	D	908	HEC	C2A-C1A-NA	-2.46	107.92	110.32
8	D	907	HEC	C4C-NC-C1C	2.46	107.76	105.35
8	C	404	HEC	C4A-NA-C1A	2.45	107.74	105.35
8	A	907	HEC	C4A-NA-C1A	2.44	107.74	105.35
8	C	405	HEC	C2A-C1A-NA	-2.43	107.95	110.32
8	D	908	HEC	C4B-NB-C1B	2.43	107.59	105.07
8	A	908	HEC	C2A-C1A-NA	-2.42	107.97	110.32
8	F	405	HEC	C2A-C1A-NA	-2.41	107.98	110.32
8	C	404	HEC	C4C-NC-C1C	2.41	107.71	105.35
8	F	404	HEC	C4A-NA-C1A	2.40	107.70	105.35
8	F	404	HEC	C4C-NC-C1C	2.35	107.65	105.35
8	D	907	HEC	C2A-C1A-NA	-2.33	108.05	110.32
8	F	404	HEC	C2A-C1A-NA	-2.16	108.22	110.32
8	A	908	HEC	C3C-C4C-NC	-2.15	107.74	110.15
8	C	404	HEC	C2A-C1A-NA	-2.15	108.23	110.32
8	A	908	HEC	CAD-CBD-CGD	-2.06	109.17	113.60
8	A	907	HEC	C2A-C1A-NA	-2.05	108.33	110.32
8	D	908	HEC	C4C-NC-C1C	2.05	107.36	105.35
8	F	405	HEC	C3C-C4C-NC	-2.04	107.87	110.15

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	908	HEC	NA
8	C	404	HEC	NA
8	C	405	HEC	NA
8	D	907	HEC	NA
8	D	908	HEC	NA
8	F	404	HEC	NA
8	F	405	HEC	NA

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	909	BET	C-CA-N-C2

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Mol	Chain	Res	Type	Atoms
9	A	909	BET	O-C-CA-N
9	A	909	BET	OXT-C-CA-N
9	A	910	BET	O-C-CA-N
9	A	910	BET	OXT-C-CA-N
9	A	911	BET	O-C-CA-N
9	A	911	BET	OXT-C-CA-N
9	B	403	BET	O-C-CA-N
9	B	403	BET	OXT-C-CA-N
9	C	406	BET	O-C-CA-N
9	C	406	BET	OXT-C-CA-N
9	D	909	BET	O-C-CA-N
9	D	909	BET	OXT-C-CA-N
9	E	403	BET	O-C-CA-N
9	E	403	BET	OXT-C-CA-N
9	E	403	BET	C-CA-N-C1
9	A	910	BET	C-CA-N-C1
9	A	911	BET	C-CA-N-C1
9	B	403	BET	C-CA-N-C1
9	B	403	BET	C-CA-N-C3
9	C	406	BET	C-CA-N-C2
9	D	909	BET	C-CA-N-C1
9	D	909	BET	C-CA-N-C3
9	E	403	BET	C-CA-N-C2
9	A	909	BET	C-CA-N-C1
8	D	908	HEC	C4D-C3D-CAD-CBD
9	A	909	BET	C-CA-N-C3
9	A	910	BET	C-CA-N-C2
9	A	910	BET	C-CA-N-C3
9	A	911	BET	C-CA-N-C2
9	A	911	BET	C-CA-N-C3
9	B	403	BET	C-CA-N-C2
9	C	406	BET	C-CA-N-C1
9	D	909	BET	C-CA-N-C2
9	E	403	BET	C-CA-N-C3
8	D	908	HEC	C2D-C3D-CAD-CBD
9	C	406	BET	C-CA-N-C3
8	A	908	HEC	C2C-C3C-CAC-CBC
8	F	404	HEC	C2D-C3D-CAD-CBD
8	F	404	HEC	C4D-C3D-CAD-CBD
8	A	908	HEC	C4C-C3C-CAC-CBC
8	D	908	HEC	C2C-C3C-CAC-CBC
8	D	907	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
8	C	404	HEC	C1A-C2A-CAA-CBA
8	D	907	HEC	C2D-C3D-CAD-CBD
8	C	404	HEC	CAD-CBD-CGD-O2D
8	C	405	HEC	CAD-CBD-CGD-O2D
8	D	907	HEC	CAA-CBA-CGA-O2A
8	C	404	HEC	C3A-C2A-CAA-CBA
8	A	907	HEC	CAA-CBA-CGA-O1A
8	A	907	HEC	CAD-CBD-CGD-O2D
8	C	404	HEC	CAD-CBD-CGD-O1D
8	C	405	HEC	CAD-CBD-CGD-O1D
8	A	907	HEC	CAD-CBD-CGD-O1D
8	A	907	HEC	CAA-CBA-CGA-O2A
8	A	908	HEC	CAD-CBD-CGD-O2D
8	D	908	HEC	CAD-CBD-CGD-O2D
8	D	908	HEC	CAA-CBA-CGA-O2A
8	D	907	HEC	C4D-C3D-CAD-CBD
8	A	908	HEC	CAD-CBD-CGD-O1D
8	D	908	HEC	CAD-CBD-CGD-O1D

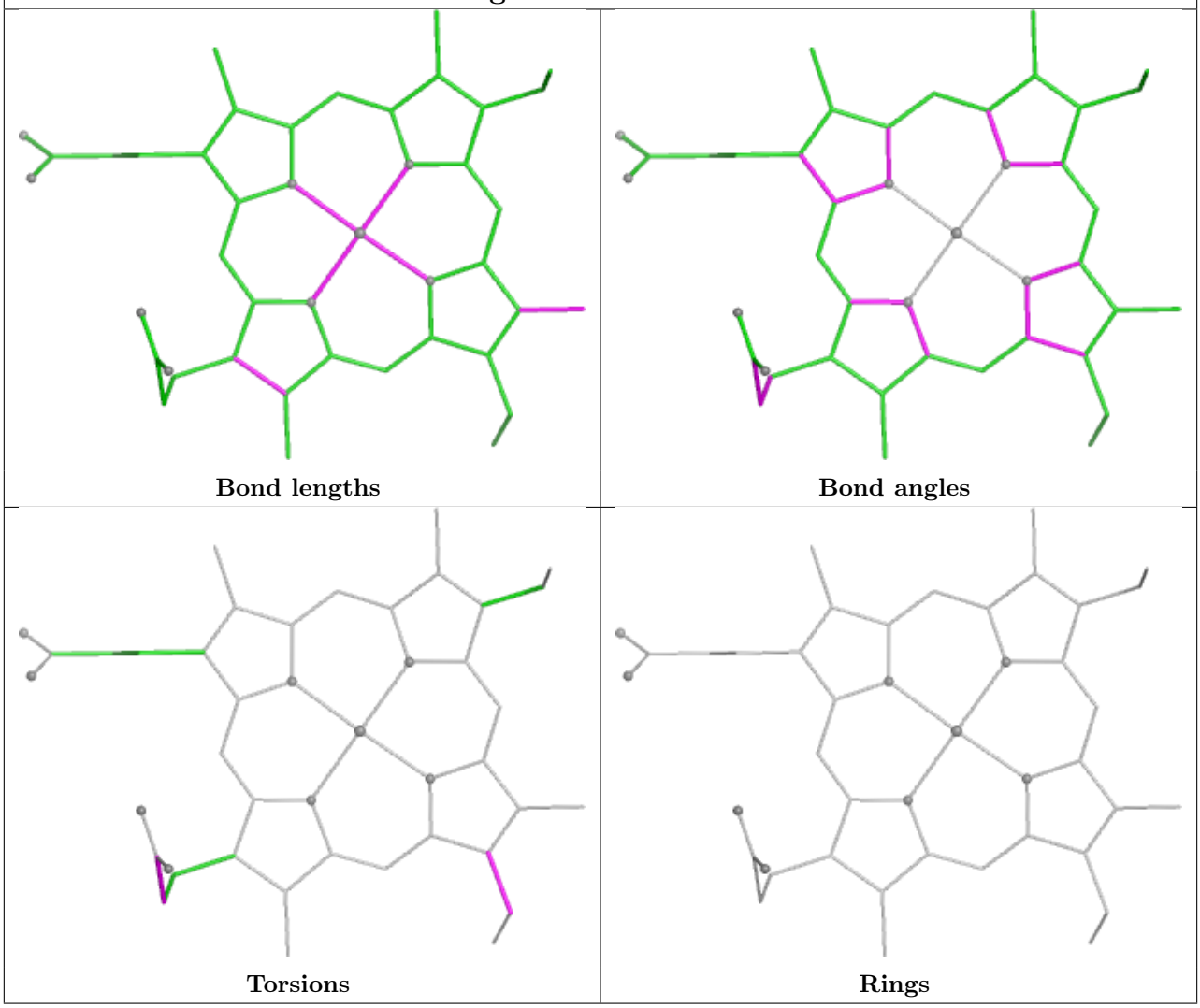
There are no ring outliers.

6 monomers are involved in 21 short contacts:

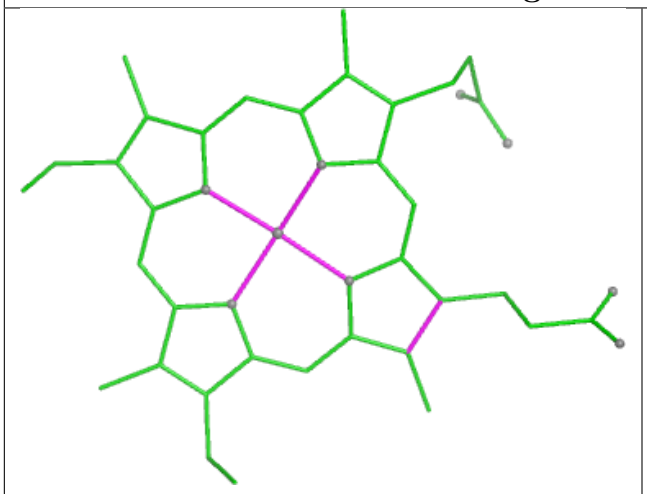
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	908	HEC	3	0
8	D	907	HEC	2	0
8	D	908	HEC	4	0
8	F	404	HEC	4	0
8	C	404	HEC	5	0
8	F	405	HEC	3	0

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.

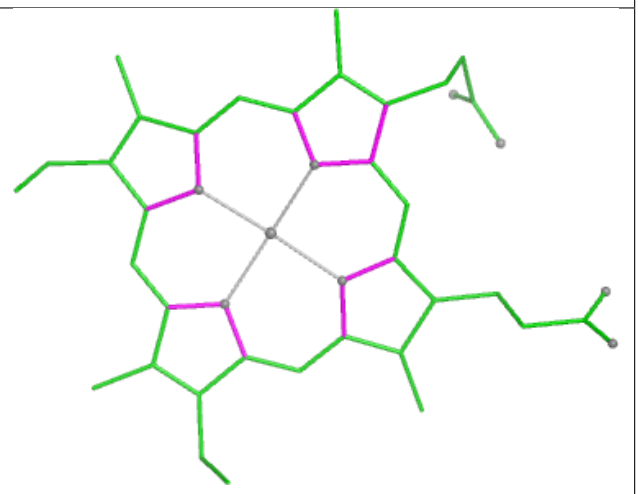
Ligand HEC A 908



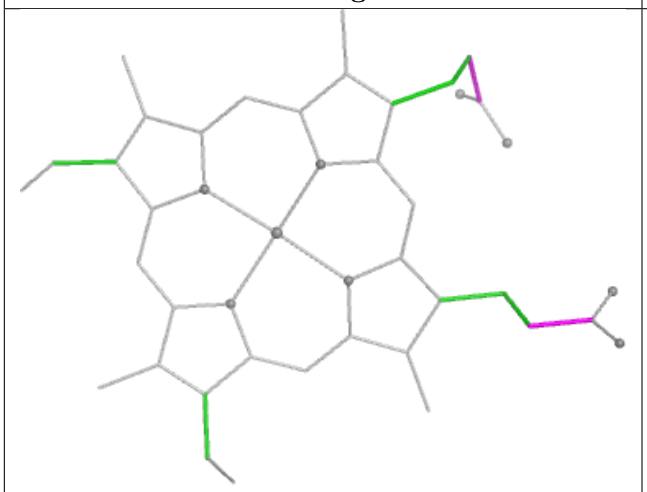
Ligand HEC A 907



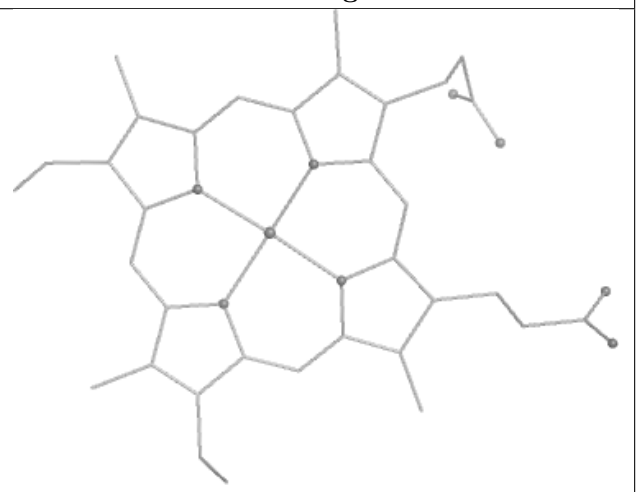
Bond lengths



Bond angles

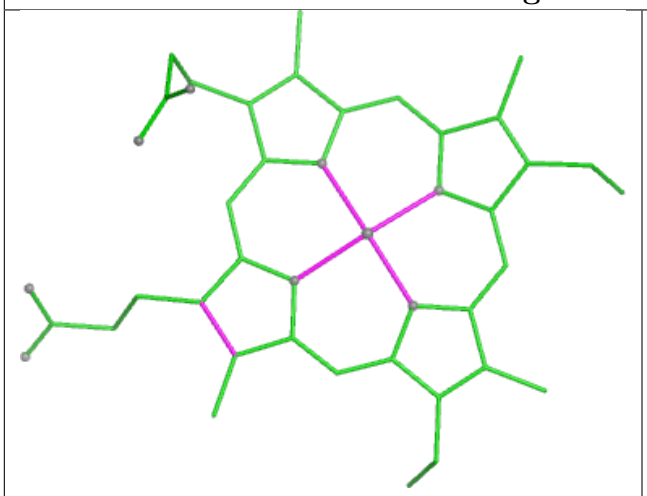


Torsions

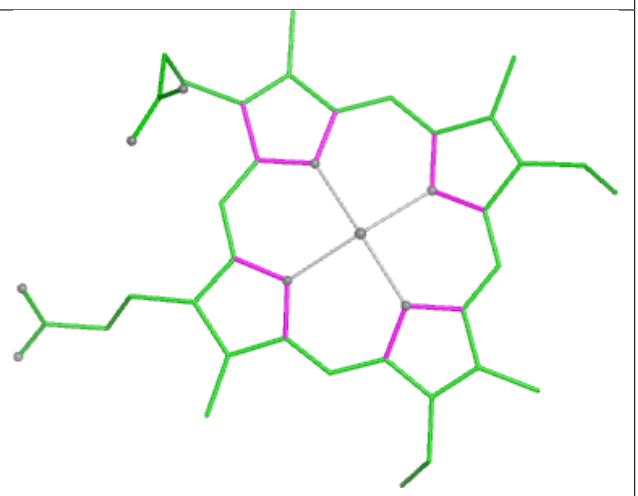


Rings

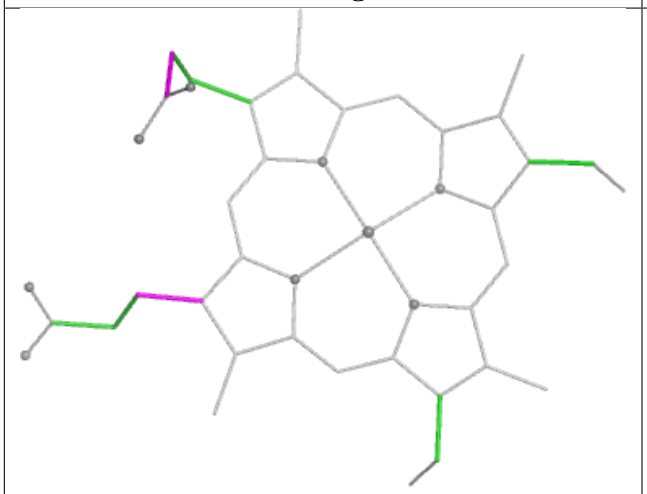
Ligand HEC D 907



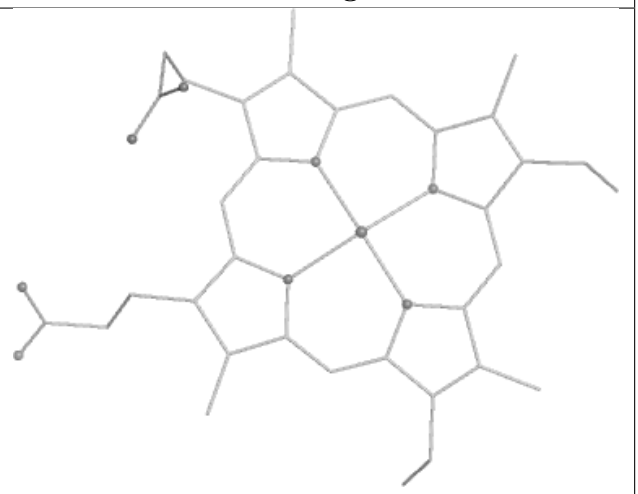
Bond lengths



Bond angles

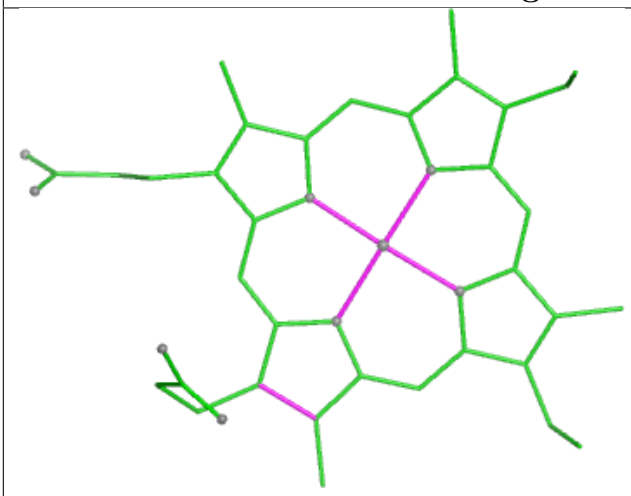


Torsions

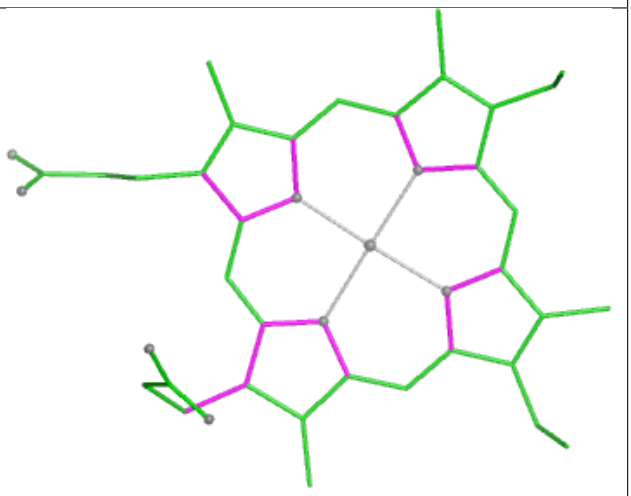


Rings

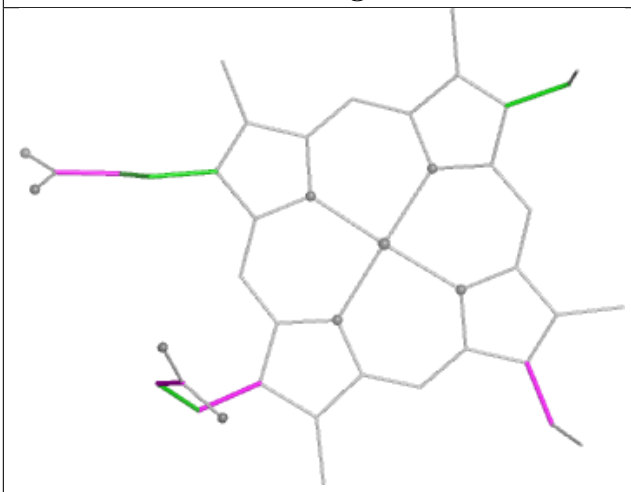
Ligand HEC D 908



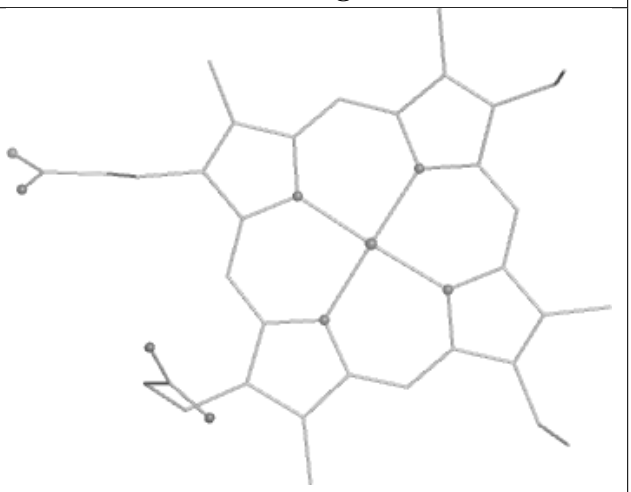
Bond lengths



Bond angles

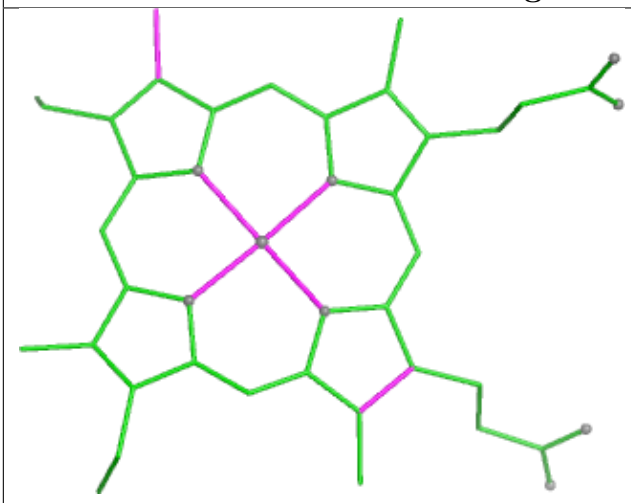


Torsions

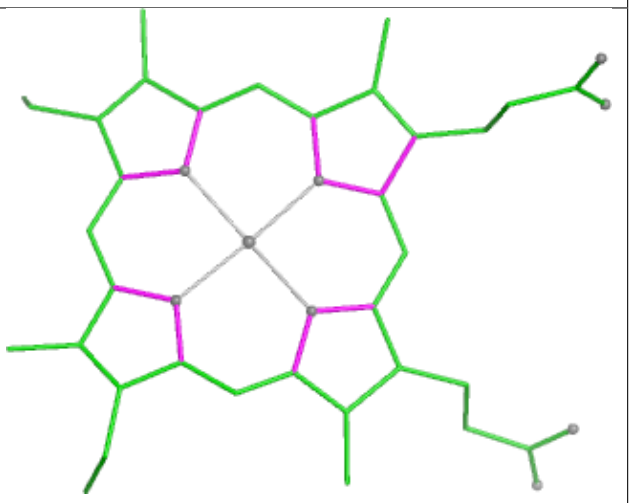


Rings

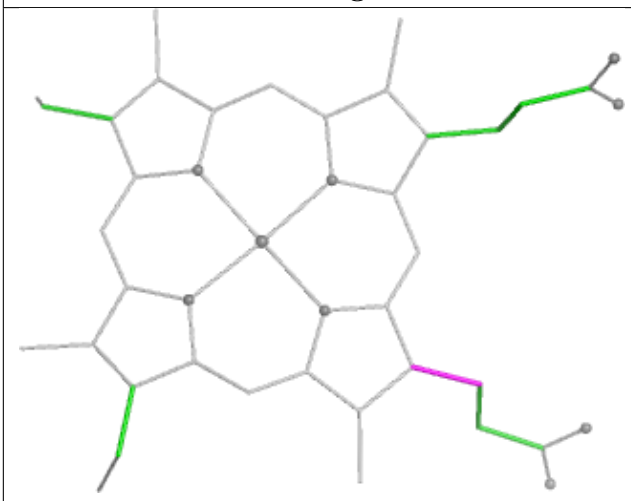
Ligand HEC F 404



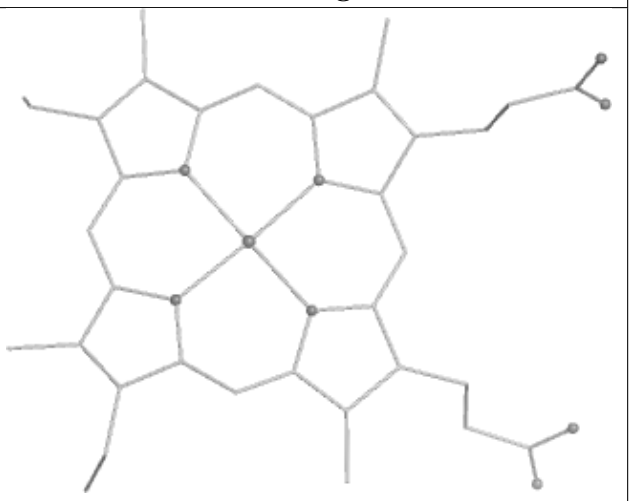
Bond lengths



Bond angles

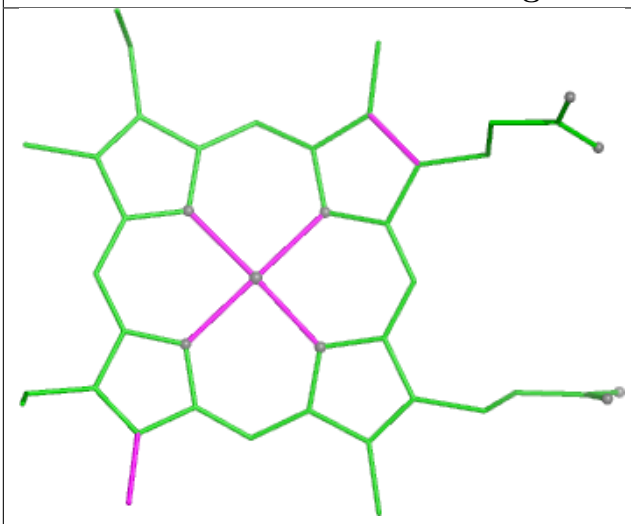


Torsions

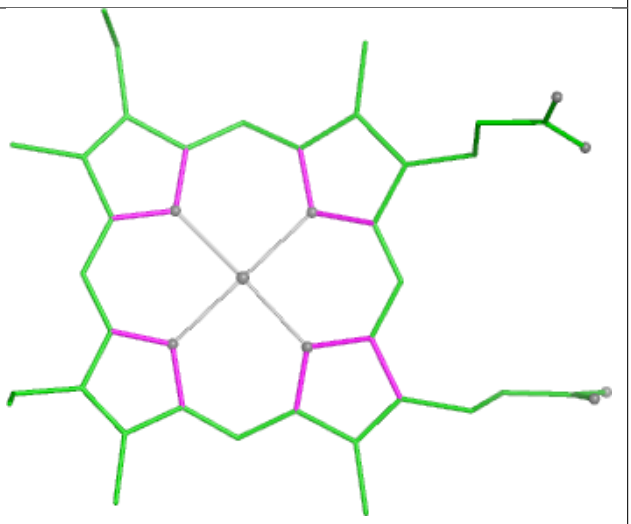


Rings

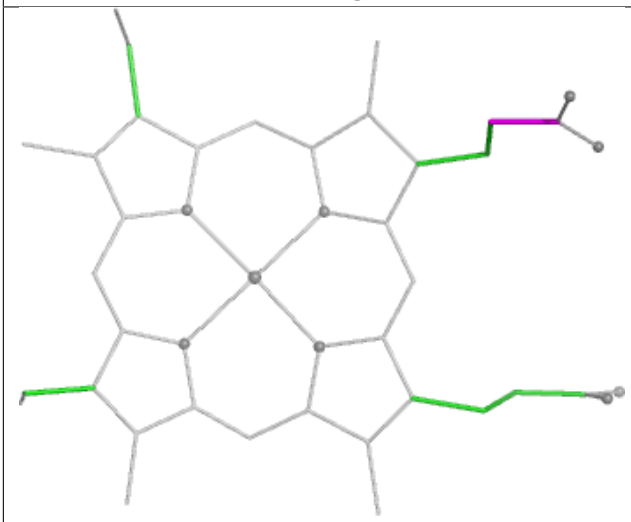
Ligand HEC C 405



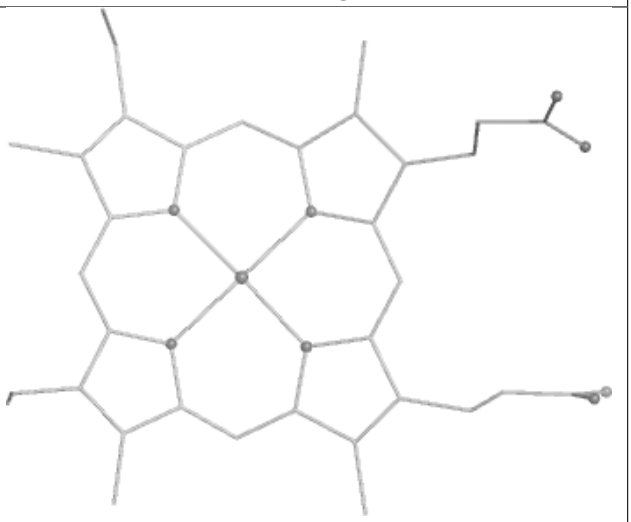
Bond lengths



Bond angles

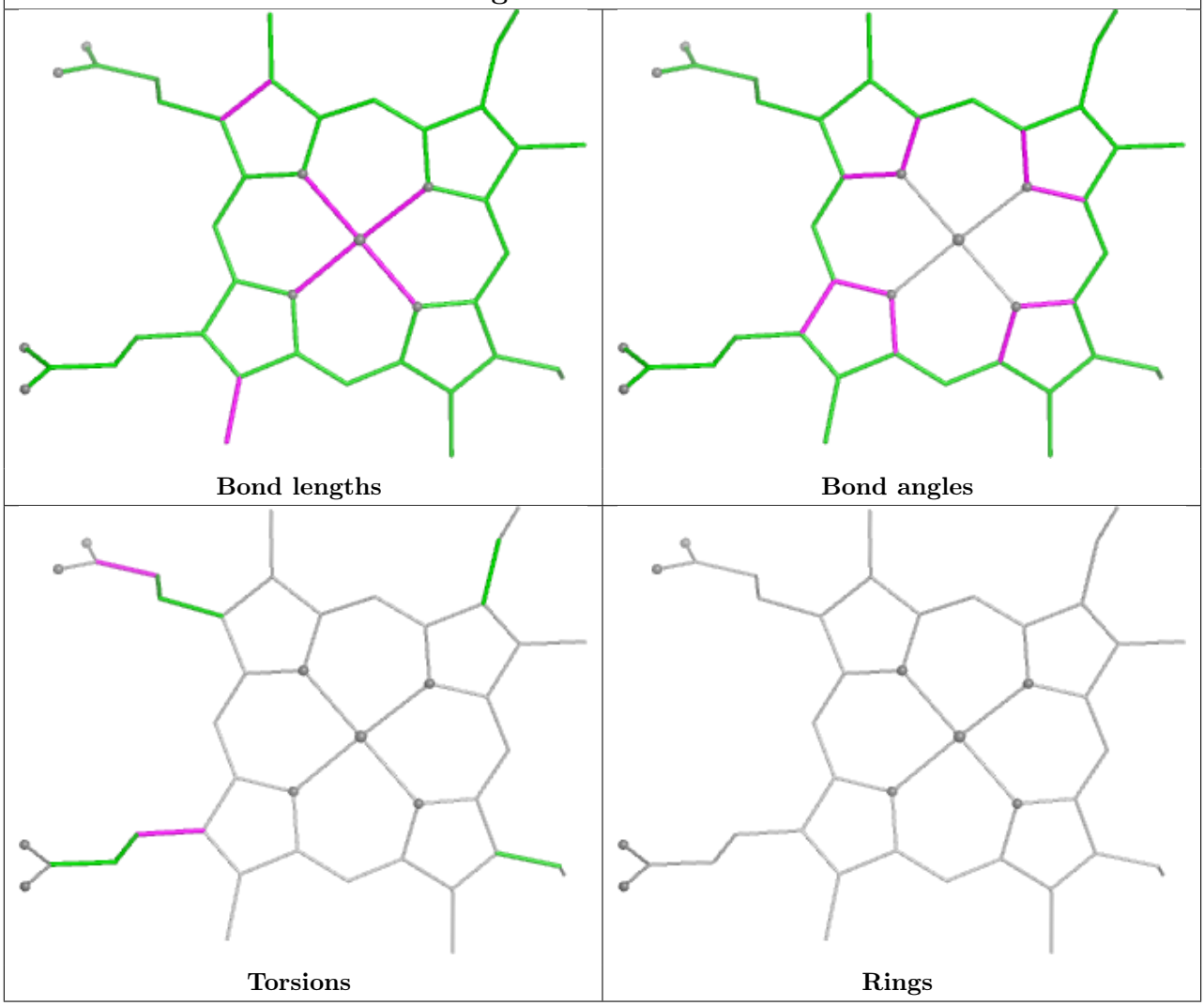


Torsions

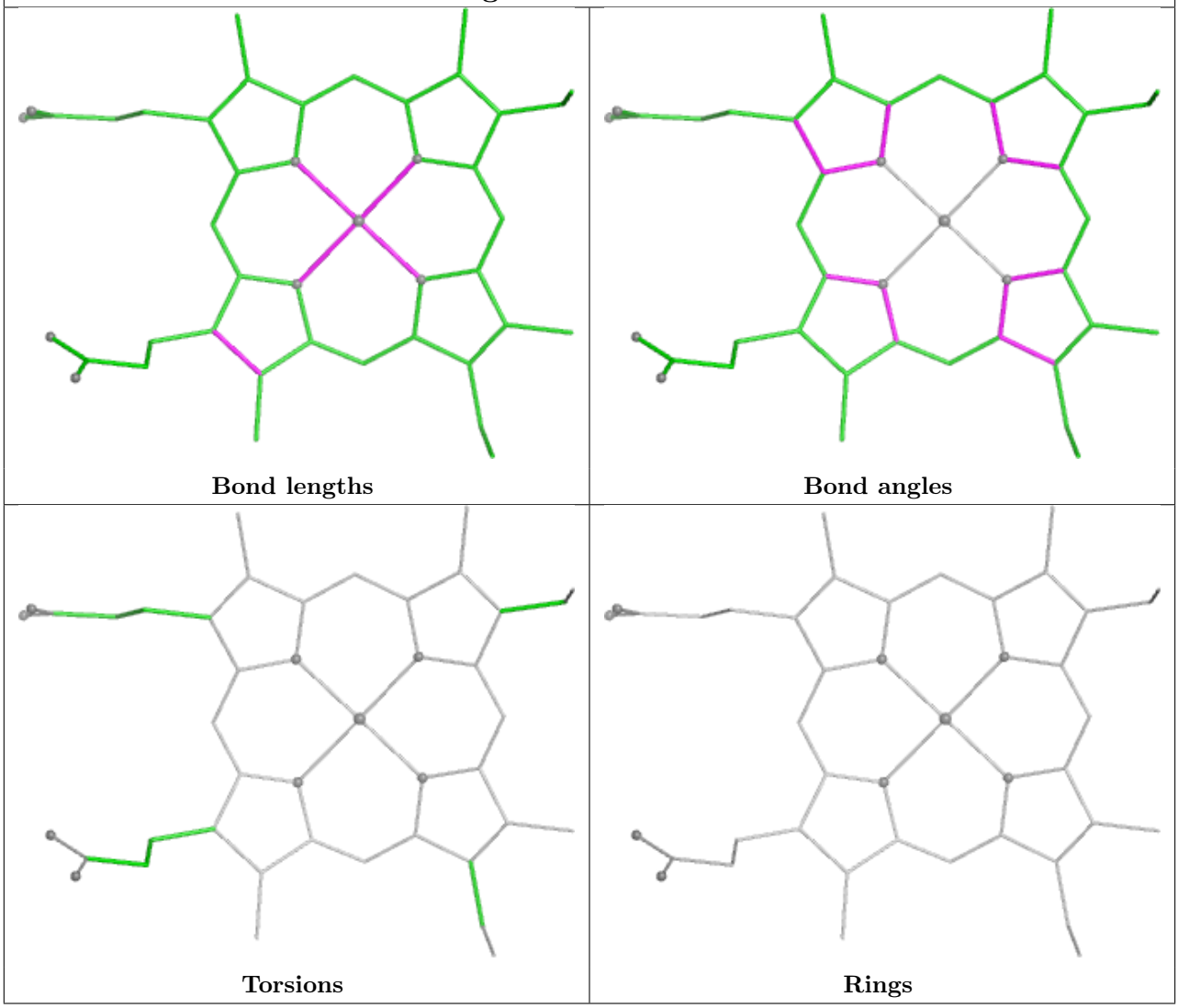


Rings

Ligand HEC C 404



Ligand HEC F 405



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	768/782 (98%)	0.27	10 (1%) 75 55	35, 60, 83, 111	0
1	D	770/782 (98%)	0.70	40 (5%) 33 21	42, 70, 94, 113	0
2	B	352/352 (100%)	0.54	5 (1%) 73 54	30, 65, 85, 102	1 (0%)
2	E	352/352 (100%)	1.38	81 (23%) 2 2	31, 90, 117, 136	1 (0%)
3	C	314/314 (100%)	0.49	10 (3%) 50 31	41, 63, 85, 95	0
3	F	314/314 (100%)	1.38	63 (20%) 3 2	60, 86, 105, 116	0
All	All	2870/2896 (99%)	0.70	209 (7%) 21 13	30, 70, 100, 136	2 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	35	GLY	6.0
3	F	307	GLY	5.3
2	B	109	GLU	5.2
3	F	107	TYR	4.4
2	E	134	SER	4.3
3	C	107	TYR	4.2
1	A	361	GLY	4.2
2	E	38	GLN	3.9
2	E	37	ILE	3.9
3	C	308	THR	3.9
3	F	263	GLY	3.9
2	E	131	ASP	3.9
1	D	191	GLY	3.6
2	E	135	GLY	3.6
2	E	95	ALA	3.6
2	E	94	SER	3.6
3	F	308	THR	3.6
2	E	36	TYR	3.5
3	F	149	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
3	F	103	ALA	3.5
2	E	132	TRP	3.5
2	E	121	LYS	3.4
2	E	91	PRO	3.3
2	E	42	VAL	3.3
3	F	194	GLU	3.3
2	E	106	CYS	3.3
1	D	628	ASN	3.3
1	D	181	TRP	3.2
3	C	234	MET	3.1
2	E	114	SER	3.0
2	E	118	ILE	3.0
2	E	41	HIS	3.0
2	E	288	GLY	3.0
3	F	223	VAL	3.0
1	D	580	GLY	2.9
3	F	120	GLY	2.9
2	E	136	ILE	2.9
3	F	180	PRO	2.9
1	D	416	TYR	2.9
2	E	122	GLN	2.9
3	F	77	PHE	2.9
2	B	131	ASP	2.8
3	F	87	PHE	2.8
2	E	98	PRO	2.8
1	D	244	THR	2.8
2	E	252	CYS	2.8
2	E	43	LYS	2.8
2	E	281	ASP	2.8
3	F	121	ASP	2.8
3	F	156	GLY	2.8
1	D	154	SER	2.7
2	E	254	ALA	2.7
2	E	272	GLY	2.7
1	A	360	ASP	2.7
2	E	93	ALA	2.7
1	D	629	ASP	2.7
1	D	235	GLY	2.6
2	E	149	CYS	2.6
3	C	306	SER	2.6
1	A	33	GLY	2.6
3	F	313	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	359	LYS	2.6
3	F	138	TYR	2.6
2	E	351	PRO	2.6
3	F	285	PRO	2.6
2	E	117	ASP	2.6
2	E	318	ASP	2.6
2	E	305	GLY	2.6
2	E	105	VAL	2.6
2	E	128	LYS	2.6
1	A	439	THR	2.6
2	E	130	GLY	2.5
2	E	73	PHE	2.5
2	E	110	SER	2.5
2	E	116	VAL	2.5
2	E	86	ALA	2.5
1	D	190	THR	2.5
2	E	82	THR	2.5
1	D	398	GLY	2.5
3	F	123	GLY	2.5
3	F	249	GLY	2.5
3	F	162	ASP	2.5
1	A	175	ARG	2.5
2	E	291	TYR	2.5
3	C	109	ARG	2.5
1	D	179	GLY	2.5
3	F	305	ALA	2.5
3	F	240	PHE	2.5
3	F	144	HIS	2.5
3	C	307	GLY	2.5
3	F	125	GLY	2.5
2	E	378	VAL	2.5
3	C	111	GLN	2.5
3	F	145	GLU	2.4
1	D	161	GLY	2.4
2	E	156	ALA	2.4
2	E	137	LYS	2.4
2	E	352	THR	2.4
2	E	124	ILE	2.4
2	E	104	TYR	2.4
2	E	231	TYR	2.4
2	E	108	ALA	2.4
3	F	303	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	194	LEU	2.4
2	E	147	VAL	2.4
1	D	358	GLY	2.4
3	F	202	ASN	2.4
1	D	291	TRP	2.4
1	D	652	PRO	2.4
3	F	333	GLY	2.3
1	D	334	ASN	2.3
2	E	138	ILE	2.3
2	E	152	CYS	2.3
2	E	103	LEU	2.3
2	E	66	GLN	2.3
3	F	248	VAL	2.3
3	F	292	VAL	2.3
3	F	114	GLY	2.3
3	F	136	GLY	2.3
3	F	288	GLY	2.3
2	B	93	ALA	2.3
3	F	102	CYS	2.3
3	F	132	TYR	2.3
1	D	75	ASN	2.3
3	F	118	ASP	2.3
2	E	133	PRO	2.3
2	E	357	SER	2.3
1	D	419	TYR	2.3
3	C	256	ASN	2.3
2	E	287	ASP	2.3
2	E	253[A]	GLU	2.3
3	F	255	VAL	2.3
1	D	163	ILE	2.3
1	D	38	GLY	2.3
3	F	146	GLY	2.3
3	F	166	GLY	2.3
3	F	147	PHE	2.3
1	D	159	ALA	2.2
1	D	273	ALA	2.2
3	F	186	LEU	2.2
3	F	310	PHE	2.2
1	D	631	ASN	2.2
2	E	96	VAL	2.2
2	E	197	VAL	2.2
1	D	174	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	360	ASP	2.2
1	D	414	PRO	2.2
1	D	556	MET	2.2
3	F	98	GLY	2.2
3	F	314	GLY	2.2
1	D	93	THR	2.2
2	E	64	SER	2.2
1	A	629	ASP	2.2
2	E	178	PRO	2.2
1	D	368	TYR	2.2
2	E	81	VAL	2.2
2	E	215	VAL	2.2
1	D	162	SER	2.2
1	D	106	ALA	2.2
2	E	44	THR	2.2
1	D	46	SER	2.2
1	A	687	MET	2.2
2	E	109	GLU	2.2
1	D	553	PRO	2.2
3	F	85	GLY	2.2
3	F	109	ARG	2.2
3	F	334	ARG	2.2
3	F	91	ASP	2.2
3	F	178	PHE	2.2
2	E	87	VAL	2.1
2	E	123	GLU	2.1
3	F	315	ALA	2.1
1	D	630	GLY	2.1
2	E	260	PHE	2.1
2	B	89	VAL	2.1
2	B	231	TYR	2.1
1	D	185	GLY	2.1
1	D	314	SER	2.1
3	C	136	GLY	2.1
3	C	241	SER	2.1
2	E	107	ASN	2.1
3	F	324	ASN	2.1
3	F	265	VAL	2.1
3	F	88	GLN	2.1
1	D	301	GLY	2.1
3	F	197	GLY	2.1
3	F	200	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	260	SER	2.1
3	F	306	SER	2.1
2	E	289	ASN	2.1
3	F	351	LYS	2.1
2	E	54	MET	2.1
3	F	349	TYR	2.1
3	F	90	ASN	2.1
2	E	169	ARG	2.1
2	E	292	GLY	2.1
3	F	224	GLY	2.1
2	E	102	PHE	2.1
1	D	91	LEU	2.0
1	A	384	ASP	2.0
2	E	195	ASP	2.0
1	D	359	LYS	2.0
2	E	92	GLU	2.0
2	E	191	VAL	2.0
3	F	350	LEU	2.0
2	E	184	SER	2.0
2	E	78	THR	2.0
1	A	179	GLY	2.0
3	F	239	LEU	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
4	XE	D	901	1/1	0.72	0.54	250,250,250,250	0

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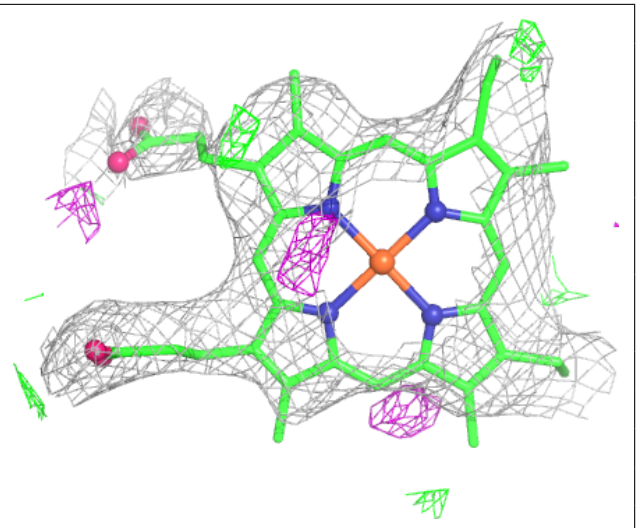
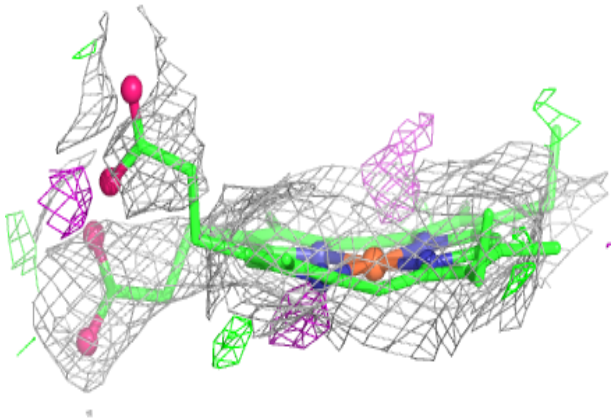
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	BET	D	909	8/8	0.83	0.23	76,85,90,93	0
9	BET	A	911	8/8	0.85	0.18	68,75,85,90	0
9	BET	C	406	8/8	0.88	0.16	58,70,75,78	0
9	BET	A	909	8/8	0.88	0.20	40,72,83,91	0
6	CA	F	401	1/1	0.89	0.12	91,91,91,91	0
6	CA	C	403	1/1	0.90	0.10	54,54,54,54	0
5	CL	D	903	1/1	0.90	0.12	61,61,61,61	0
9	BET	A	910	8/8	0.91	0.15	68,71,78,85	0
8	HEC	F	405	43/43	0.92	0.17	62,90,103,105	0
9	BET	B	403	8/8	0.92	0.17	40,46,59,70	0
6	CA	C	401	1/1	0.92	0.09	57,57,57,57	0
6	CA	F	403	1/1	0.92	0.07	73,73,73,73	0
4	XE	D	902	1/1	0.93	0.21	178,178,178,178	0
6	CA	F	402	1/1	0.93	0.08	82,82,82,82	0
6	CA	A	905	1/1	0.93	0.07	80,80,80,80	0
5	CL	A	903[A]	1/1	0.93	0.27	17,17,17,17	1
5	CL	A	903[B]	1/1	0.93	0.27	39,39,39,39	1
9	BET	E	403	8/8	0.93	0.14	58,69,81,81	0
10	MG	E	401	1/1	0.94	0.11	53,53,53,53	0
8	HEC	F	404	43/43	0.95	0.16	52,77,99,100	0
4	XE	A	901	1/1	0.96	0.12	127,127,127,127	0
6	CA	B	402	1/1	0.96	0.07	68,68,68,68	0
6	CA	E	402	1/1	0.96	0.08	90,90,90,90	0
8	HEC	C	405	43/43	0.96	0.11	48,69,77,82	0
10	MG	B	401	1/1	0.96	0.09	30,30,30,30	0
8	HEC	D	907	43/43	0.96	0.12	41,62,80,82	0
8	HEC	A	907	43/43	0.97	0.09	31,45,55,56	0
8	HEC	C	404	43/43	0.97	0.11	37,52,69,77	0
6	CA	A	904	1/1	0.97	0.06	75,75,75,75	0
8	HEC	D	908	43/43	0.98	0.09	35,54,67,77	0
6	CA	C	402	1/1	0.98	0.05	70,70,70,70	0
8	HEC	A	908	43/43	0.98	0.09	39,57,68,71	0
4	XE	A	902	1/1	0.98	0.04	81,81,81,81	0
6	CA	D	904	1/1	0.98	0.04	70,70,70,70	0
6	CA	D	905	1/1	0.98	0.05	84,84,84,84	0
7	ZN	A	906	1/1	0.99	0.05	54,54,54,54	0
7	ZN	D	906	1/1	1.00	0.05	55,55,55,55	0

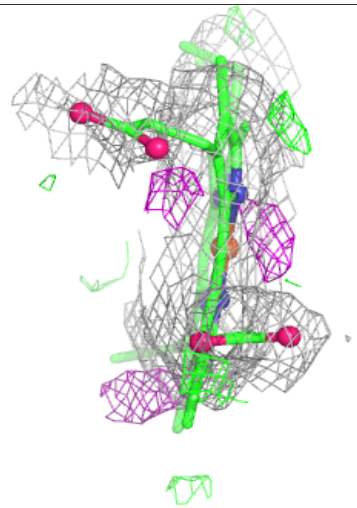
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC F 405:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

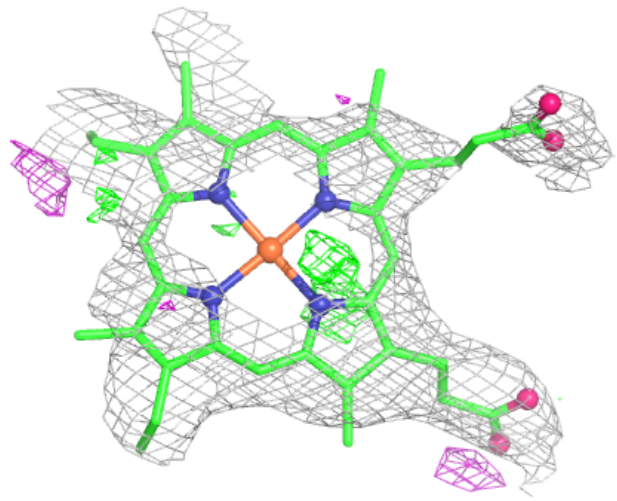


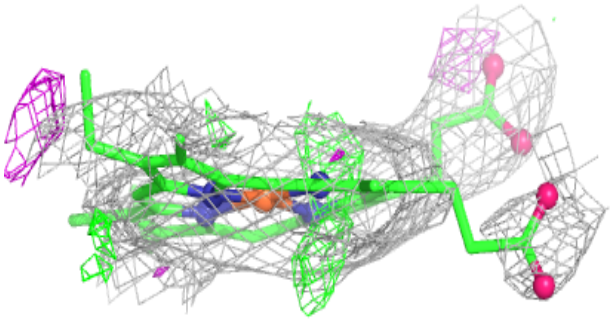


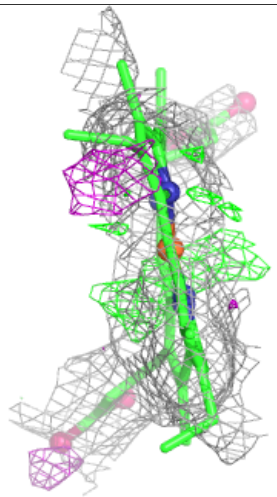


Electron density around HEC F 404:

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

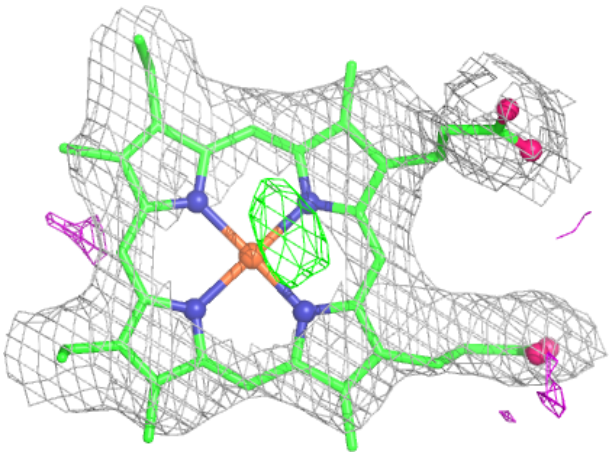


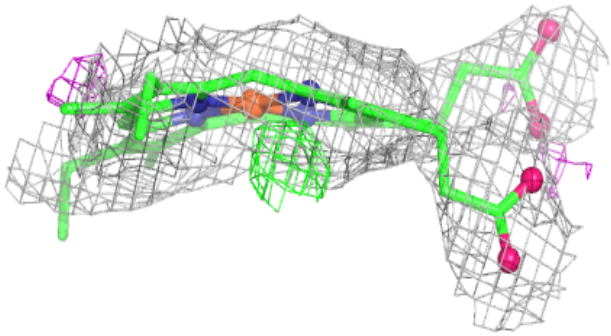


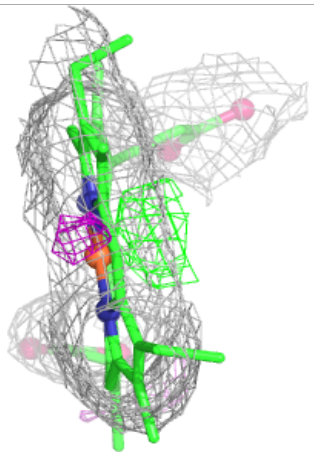


Electron density around HEC C 405:

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

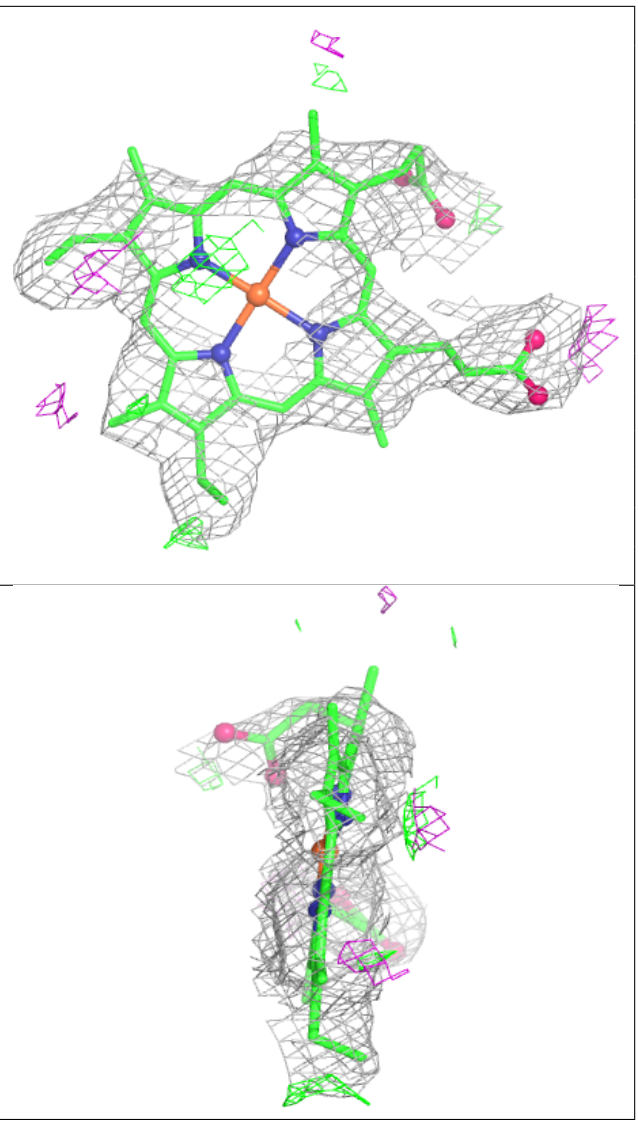






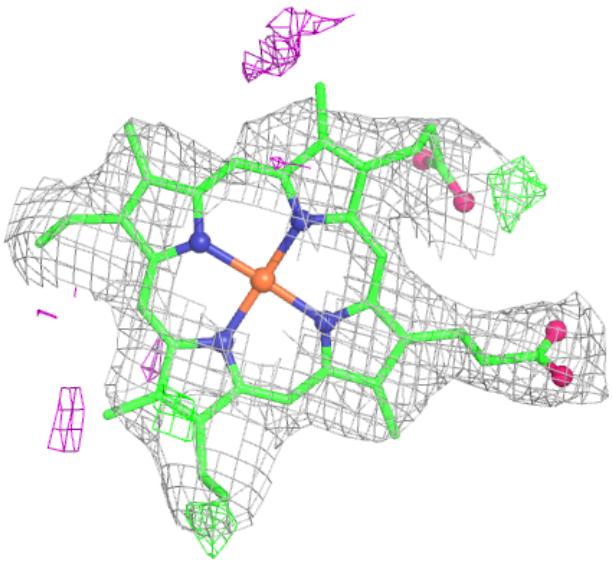
Electron density around HEC D 907:

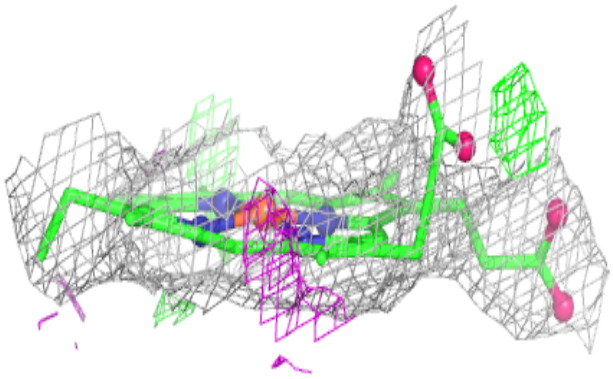
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

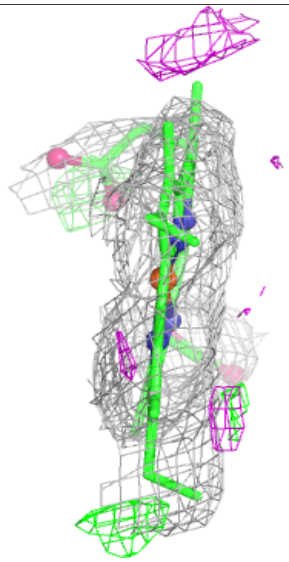


Electron density around HEC A 907:

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

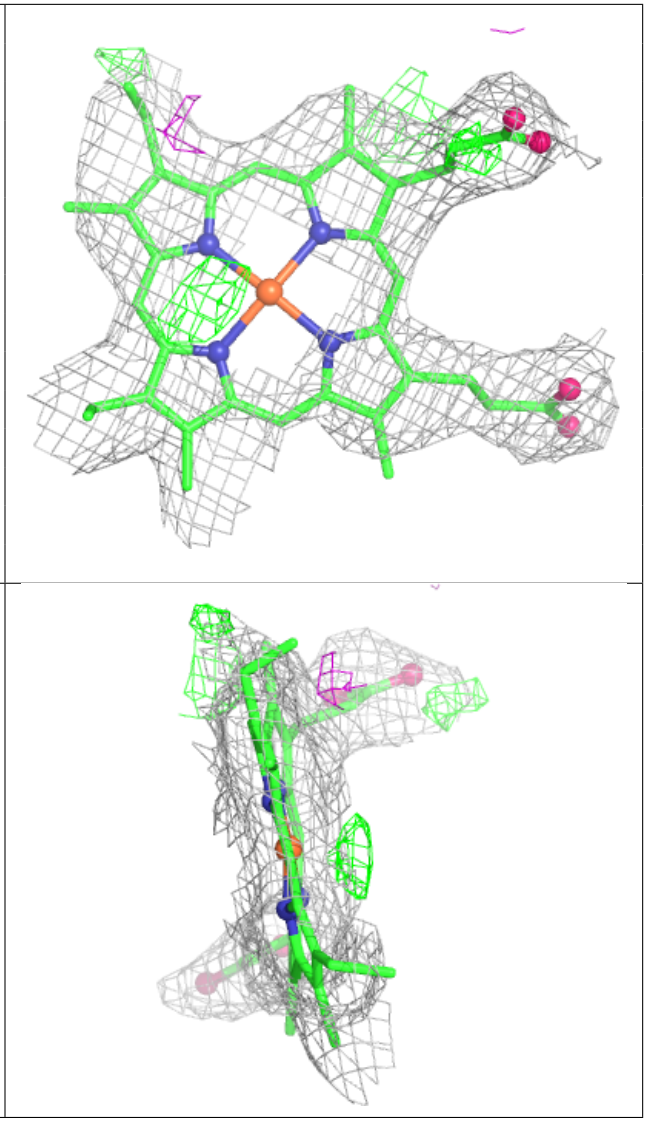






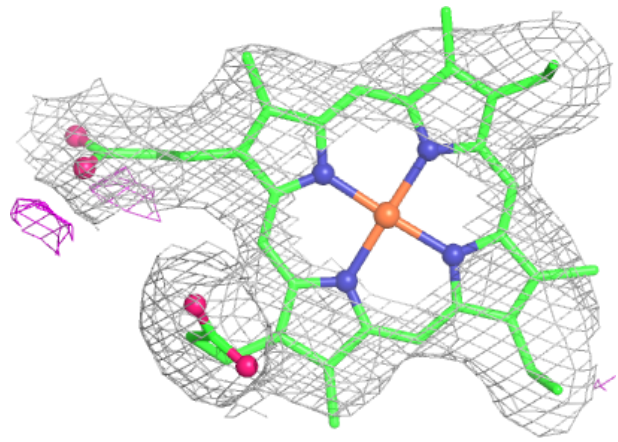
Electron density around HEC C 404:

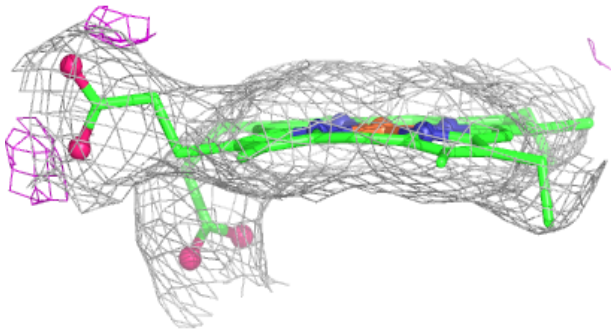
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

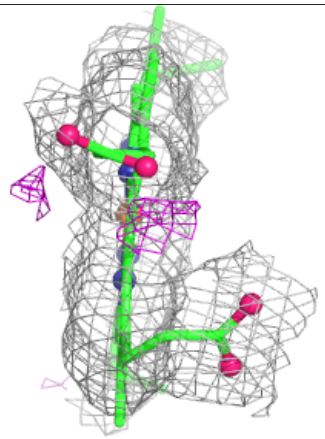


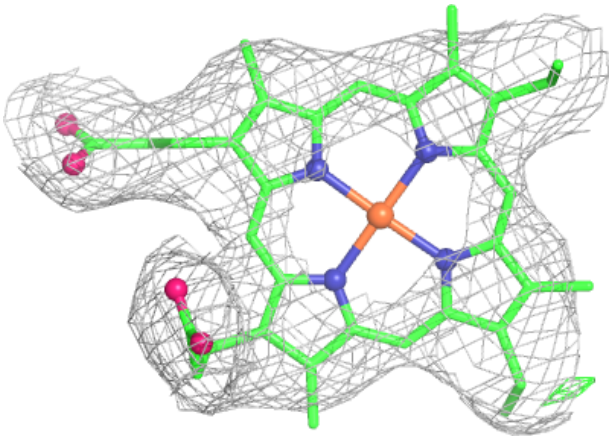
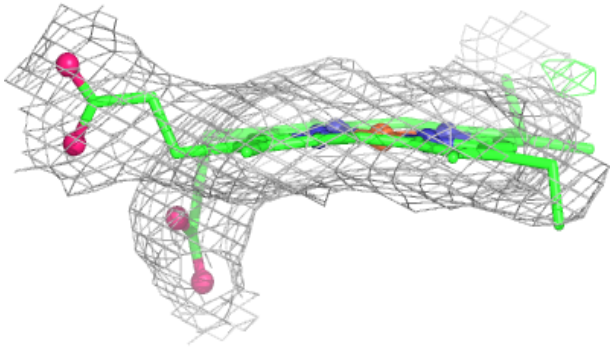
Electron density around HEC D 908:

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







Electron density around HEC A 908: 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.