Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 10:20 PM EDT

PDB ID	:	1JBQ
Title	:	STRUCTURE OF HUMAN CYSTATHIONINE BETA-SYNTHASE: A UNIQUE PYRIDOXAL 5'-PHOSPHATE DEPENDENT HEMEPROTEIN
Authors	:	Meier, M.; Janosik, M.; Kery, V.; Kraus, J.P.; Burkhard, P.
Deposited on	:	2001-06-06
Resolution	:	2.60 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:

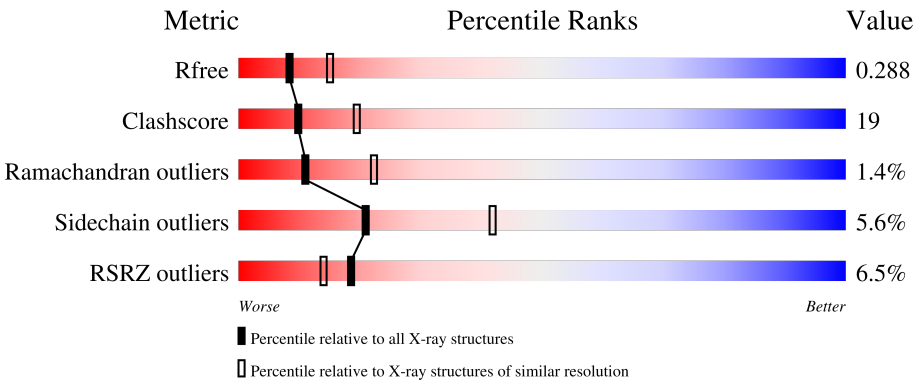
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	435	3%, 51%, 26%, •, 20%
1	B	435	8%, 51%, 26%, •, 20%
1	C	435	6%, 50%, 27%, •, 20%
1	D	435	6%, 50%, 27%, •, 20%
1	E	435	4%, 52%, 25%, •, 20%

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Mol	Chain	Length	Quality of chain
1	F	435	4% 53% 25% • 20%

2 Entry composition (i)

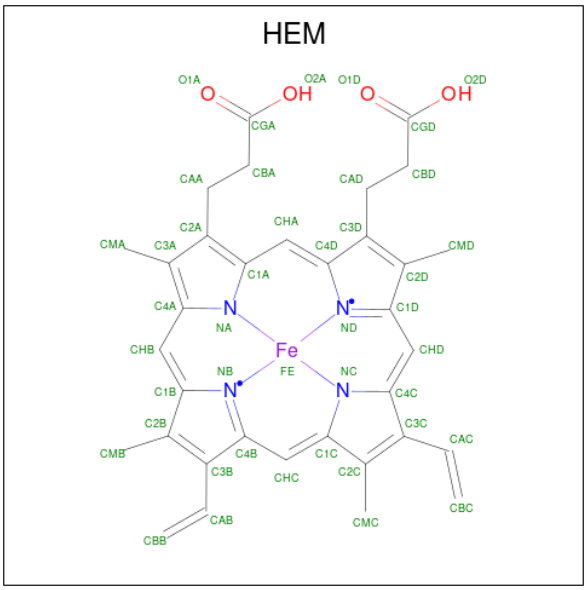
There are 4 unique types of molecules in this entry. The entry contains 16522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYSTATHIONINE BETA-SYNTHASE.

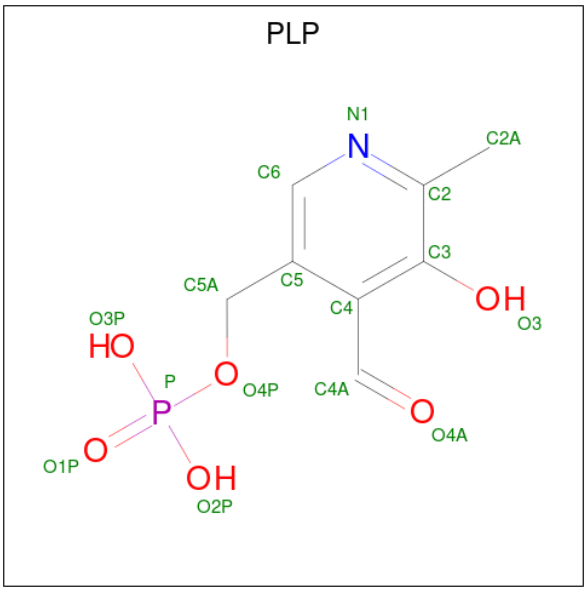
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	2667	1678	469	503	17	0	0	0
1	B	348	2667	1678	469	503	17	0	0	0
1	C	348	2667	1678	469	503	17	0	0	0
1	D	348	2667	1678	469	503	17	0	0	0
1	E	350	2685	1689	472	507	17	0	0	0
1	F	348	2667	1678	469	503	17	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	15	8	1	5	1	0	0
3	B	1	15	8	1	5	1	0	0
3	C	1	15	8	1	5	1	0	0
3	D	1	15	8	1	5	1	0	0
3	E	1	15	8	1	5	1	0	0
3	F	1	15	8	1	5	1	0	0

- Molecule 4 is water.

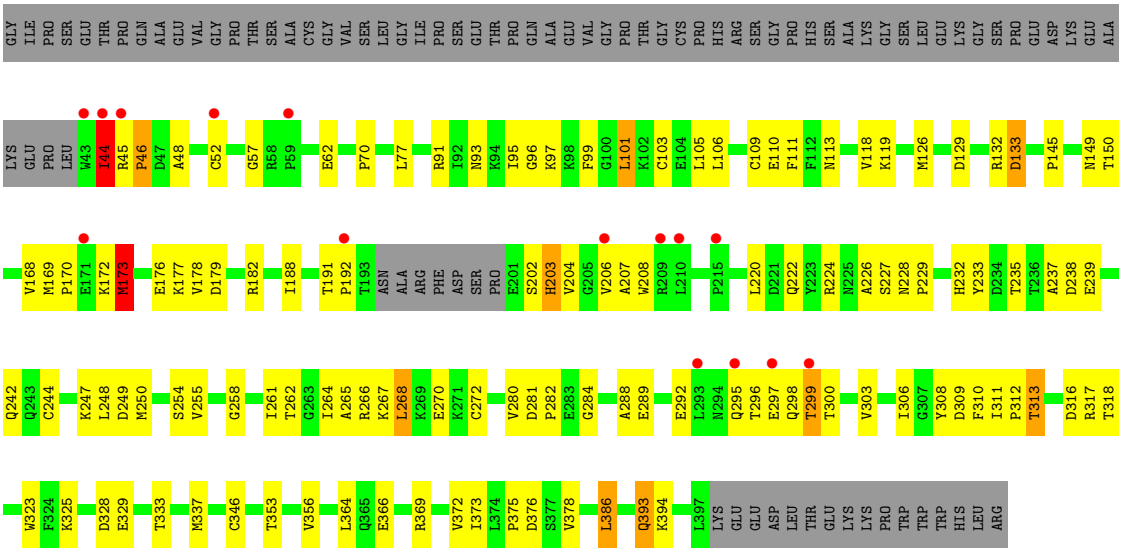
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	22	22	22	0	0
			Total	O		
4	B	30	30	30	0	0
			Total	O		
4	C	25	25	25	0	0
			Total	O		
4	D	24	24	24	0	0
			Total	O		
4	E	31	31	31	0	0
			Total	O		
4	F	22	22	22	0	0

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.

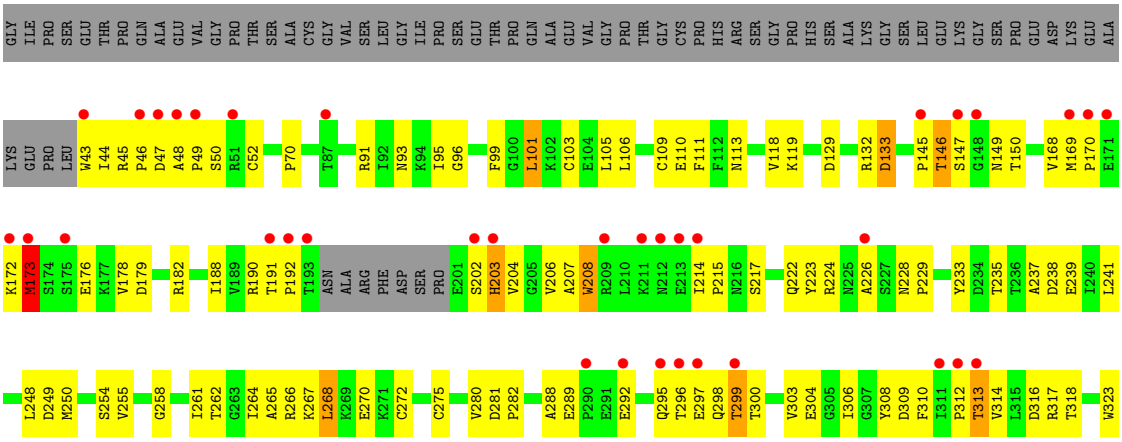
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

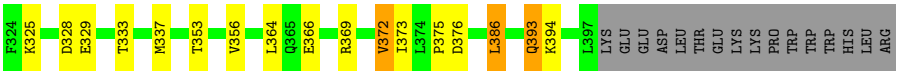
Chain A:



• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

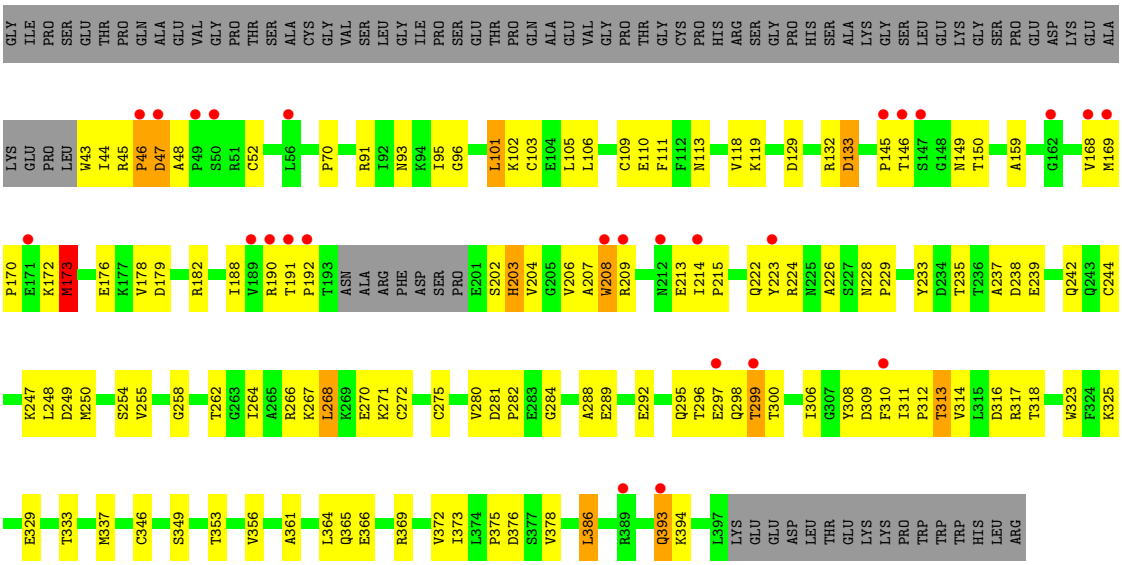
Chain B:





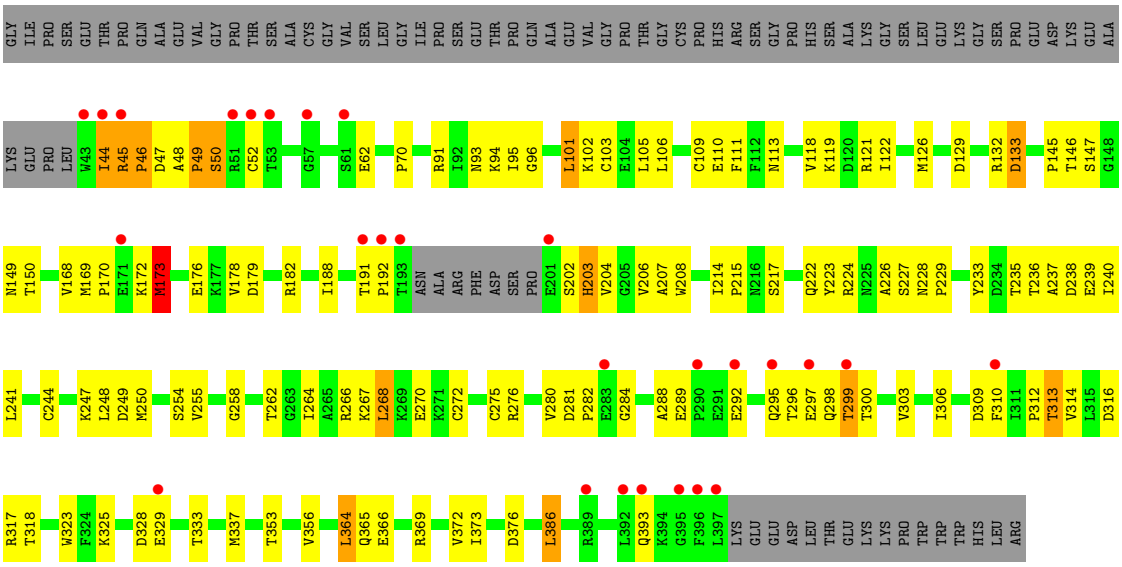
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain C:



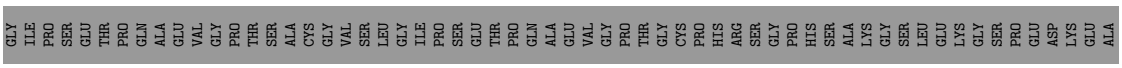
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

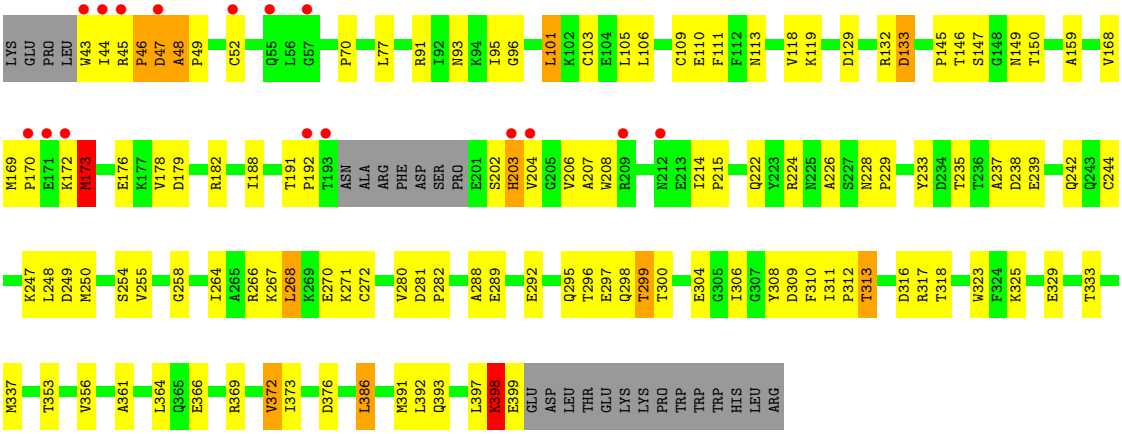
Chain D:



• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

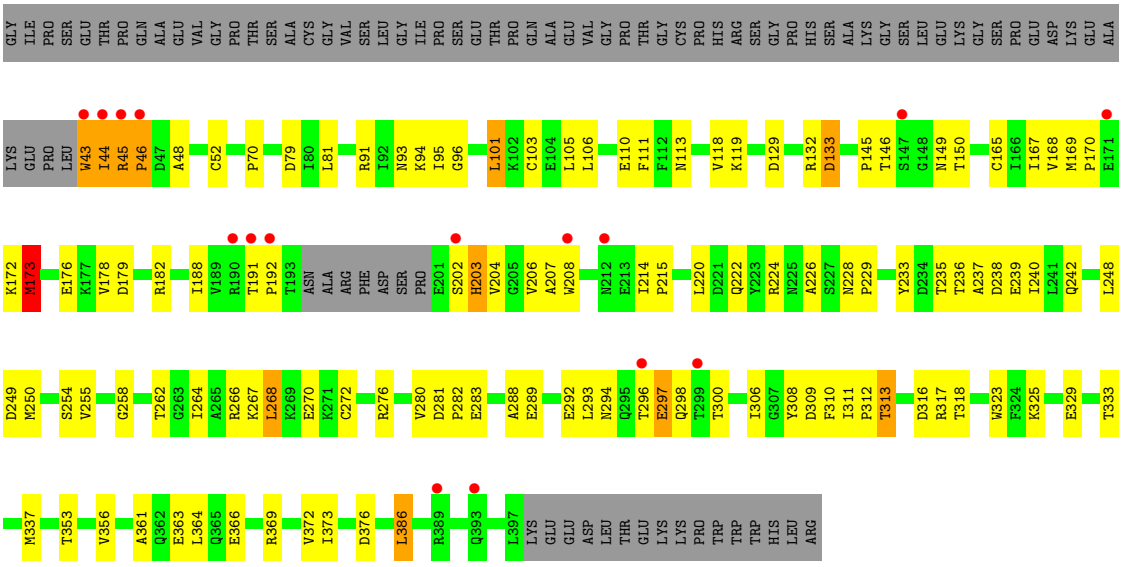
Chain E:





- Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	144.52Å 144.52Å 108.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.34 – 2.60 43.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.3 (43.34-2.60) 82.3 (43.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.296 0.250 , 0.288	Depositor DCC
R_{free} test set	3219 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.036 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16522	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7767e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PLP, HEM

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	0.39	0/2715	0.67	1/3672 (0.0%)
1	B	0.38	0/2715	0.65	0/3672
1	C	0.39	0/2715	0.65	0/3672
1	D	0.37	0/2715	0.66	1/3672 (0.0%)
1	E	0.38	0/2733	0.67	0/3695
1	F	0.38	0/2715	0.66	0/3672
All	All	0.38	0/16308	0.66	2/22055 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	ILE	N-CA-C	-8.54	87.93	111.00
1	D	44	ILE	N-CA-C	-7.01	92.06	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2667	0	2691	108	0
1	B	2667	0	2691	103	0
1	C	2667	0	2691	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2667	0	2691	114	0
1	E	2685	0	2710	96	0
1	F	2667	0	2691	107	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	1	0
3	E	15	0	7	1	0
3	F	15	0	7	1	0
4	A	22	0	0	4	0
4	B	30	0	0	2	0
4	C	25	0	0	6	0
4	D	24	0	0	7	0
4	E	31	0	0	2	0
4	F	22	0	0	0	0
All	All	16522	0	16387	628	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 19.

All (628) 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:296:THR:HG22	1:E:298:GLN:H	1.30	0.94
1:A:296:THR:HG22	1:A:298:GLN:H	1.33	0.93
1:C:296:THR:HG22	1:C:298:GLN:H	1.32	0.92
1:D:296:THR:HG22	1:D:298:GLN:H	1.33	0.92
1:B:296:THR:HG22	1:B:298:GLN:H	1.33	0.91
1:C:129:ASP:HA	1:C:132:ARG:HH12	1.33	0.91
1:E:129:ASP:HA	1:E:132:ARG:HH12	1.35	0.90
1:B:129:ASP:HA	1:B:132:ARG:HH12	1.34	0.90
1:F:129:ASP:HA	1:F:132:ARG:HH12	1.37	0.90
1:D:129:ASP:HA	1:D:132:ARG:HH12	1.35	0.89
1:A:129:ASP:HA	1:A:132:ARG:HH12	1.35	0.89
1:F:43:TRP:NE1	1:F:45:ARG:HG3	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:LYS:HG3	1:E:399:GLU:H	1.40	0.86
1:D:224:ARG:HG2	1:D:313:THR:HG21	1.58	0.86
1:B:224:ARG:HG2	1:B:313:THR:HG21	1.58	0.85
1:C:129:ASP:HA	1:C:132:ARG:NH1	1.91	0.84
1:C:224:ARG:HG2	1:C:313:THR:HG21	1.59	0.84
1:B:224:ARG:HG2	1:B:313:THR:CG2	2.08	0.84
1:F:224:ARG:HG2	1:F:313:THR:CG2	2.09	0.83
1:E:191:THR:HG21	1:E:203:HIS:HA	1.61	0.82
1:A:129:ASP:HA	1:A:132:ARG:NH1	1.94	0.82
1:D:224:ARG:HG2	1:D:313:THR:CG2	2.08	0.82
1:B:191:THR:HG21	1:B:203:HIS:HA	1.62	0.82
1:B:129:ASP:HA	1:B:132:ARG:NH1	1.95	0.81
1:C:224:ARG:HG2	1:C:313:THR:CG2	2.10	0.81
1:E:129:ASP:HA	1:E:132:ARG:NH1	1.96	0.81
1:F:129:ASP:HA	1:F:132:ARG:NH1	1.96	0.81
1:C:191:THR:HG21	1:C:203:HIS:HA	1.62	0.81
1:D:191:THR:HG21	1:D:203:HIS:HA	1.61	0.81
1:F:224:ARG:HG2	1:F:313:THR:HG21	1.62	0.80
1:D:129:ASP:HA	1:D:132:ARG:NH1	1.95	0.80
1:E:224:ARG:HG2	1:E:313:THR:HG21	1.64	0.80
1:B:304:GLU:HG3	4:B:1017:HOH:O	1.82	0.80
1:F:191:THR:HG21	1:F:203:HIS:HA	1.62	0.79
1:A:191:THR:HG21	1:A:203:HIS:HA	1.64	0.79
1:A:224:ARG:HG2	1:A:313:THR:HG21	1.64	0.78
1:E:224:ARG:HG2	1:E:313:THR:CG2	2.14	0.78
1:A:224:ARG:HG2	1:A:313:THR:CG2	2.14	0.78
1:D:118:VAL:O	4:D:1022:HOH:O	2.01	0.77
1:C:316:ASP:OD2	1:C:318:THR:HB	1.85	0.76
1:C:310:PHE:HA	4:C:1003:HOH:O	1.84	0.76
1:A:44:ILE:HG22	1:A:45:ARG:N	2.02	0.75
1:A:316:ASP:OD2	1:A:318:THR:HB	1.86	0.75
1:C:393:GLN:HG3	1:C:394:LYS:N	2.01	0.75
1:E:46:PRO:O	1:E:313:THR:HG22	1.86	0.74
1:D:121:ARG:N	4:D:1022:HOH:O	2.20	0.74
1:A:46:PRO:O	1:A:313:THR:HG22	1.88	0.74
1:D:281:ASP:O	1:D:325:LYS:HA	1.88	0.73
1:E:271:LYS:HD2	4:E:1009:HOH:O	1.89	0.73
1:A:281:ASP:O	1:A:325:LYS:HA	1.89	0.72
1:F:297:GLU:HG3	1:F:298:GLN:H	1.52	0.72
1:C:281:ASP:O	1:C:325:LYS:HA	1.89	0.72
1:F:316:ASP:OD2	1:F:318:THR:HB	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:HD2	1:C:47:ASP:OD2	1.90	0.71
1:F:281:ASP:O	1:F:325:LYS:HA	1.91	0.71
1:B:281:ASP:O	1:B:325:LYS:HA	1.90	0.71
1:E:316:ASP:OD2	1:E:318:THR:HB	1.89	0.71
1:B:316:ASP:OD2	1:B:318:THR:HB	1.91	0.69
1:E:281:ASP:O	1:E:325:LYS:HA	1.92	0.69
1:F:266:ARG:O	1:F:270:GLU:HG3	1.93	0.69
1:A:44:ILE:CG2	1:A:45:ARG:N	2.56	0.69
1:C:266:ARG:O	1:C:270:GLU:HG3	1.92	0.69
1:A:44:ILE:CG2	1:A:45:ARG:H	2.06	0.69
1:B:145:PRO:O	1:B:146:THR:HB	1.91	0.69
1:F:43:TRP:CE2	1:F:45:ARG:HG3	2.27	0.68
1:A:118:VAL:HG11	4:A:1019:HOH:O	1.92	0.68
1:D:316:ASP:OD2	1:D:318:THR:HB	1.91	0.68
1:D:173:MET:HA	1:D:173:MET:CE	2.23	0.68
1:B:266:ARG:O	1:B:270:GLU:HG3	1.93	0.68
1:A:299:THR:HG22	1:A:300:THR:HG23	1.75	0.67
1:B:43:TRP:C	1:B:44:ILE:HD12	2.14	0.67
1:A:296:THR:HG22	1:A:297:GLU:N	2.10	0.67
1:F:283:GLU:HB3	1:F:296:THR:HG21	1.75	0.67
1:D:266:ARG:O	1:D:270:GLU:HG3	1.94	0.67
1:C:296:THR:HG22	1:C:297:GLU:N	2.10	0.67
1:A:266:ARG:O	1:A:270:GLU:HG3	1.96	0.66
1:F:48:ALA:O	1:F:313:THR:HB	1.95	0.66
1:E:299:THR:HG22	1:E:300:THR:HG23	1.75	0.66
1:E:296:THR:HG22	1:E:297:GLU:N	2.10	0.66
1:D:296:THR:HG22	1:D:297:GLU:N	2.11	0.66
1:B:296:THR:HG22	1:B:297:GLU:N	2.10	0.66
1:C:299:THR:HG22	1:C:300:THR:HG23	1.76	0.66
1:D:299:THR:HG22	1:D:300:THR:HG23	1.77	0.65
1:E:266:ARG:O	1:E:270:GLU:HG3	1.96	0.64
1:F:44:ILE:HG22	1:F:224:ARG:CD	2.27	0.64
1:F:173:MET:HA	1:F:173:MET:CE	2.28	0.64
1:F:296:THR:HG22	1:F:297:GLU:HG2	1.80	0.64
1:C:46:PRO:O	1:C:313:THR:HG22	1.97	0.64
1:B:299:THR:HG22	1:B:300:THR:HG23	1.78	0.63
1:A:44:ILE:HG22	1:A:45:ARG:H	1.64	0.62
1:C:179:ASP:HB3	1:D:386:LEU:HD13	1.81	0.62
1:F:46:PRO:O	1:F:313:THR:HG22	1.99	0.62
1:A:289:GLU:OE2	1:A:317:ARG:HB3	2.00	0.62
1:A:296:THR:HG21	1:A:298:GLN:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:MET:CE	1:E:173:MET:HA	2.30	0.61
1:F:353:THR:HG22	1:F:372:VAL:CG2	2.30	0.61
1:B:46:PRO:O	1:B:313:THR:HG22	2.00	0.61
1:A:179:ASP:HB3	1:B:386:LEU:HD13	1.82	0.61
1:C:233:TYR:CE1	1:C:267:LYS:HE3	2.36	0.61
1:E:296:THR:HG21	1:E:298:GLN:HG2	1.83	0.61
1:C:103:CYS:HB3	1:C:364:LEU:HB3	1.83	0.61
1:A:232:HIS:NE2	4:A:1020:HOH:O	2.29	0.61
1:E:91:ARG:HD2	1:E:93:ASN:OD1	2.02	0.60
1:D:91:ARG:HD2	1:D:93:ASN:OD1	2.02	0.60
1:B:91:ARG:HD2	1:B:93:ASN:OD1	2.00	0.60
1:B:296:THR:HG21	1:B:298:GLN:HG2	1.83	0.60
1:F:280:VAL:HG22	1:F:356:VAL:HG21	1.84	0.60
1:B:233:TYR:CE1	1:B:267:LYS:HE3	2.36	0.60
1:D:46:PRO:O	1:D:313:THR:HG22	2.02	0.60
1:D:121:ARG:HG2	4:D:1020:HOH:O	2.01	0.60
1:F:103:CYS:HB3	1:F:364:LEU:HB3	1.84	0.60
1:A:48:ALA:O	1:A:313:THR:HB	2.02	0.60
1:E:129:ASP:O	1:E:133:ASP:HB2	2.02	0.60
1:E:386:LEU:HD13	1:F:179:ASP:HB3	1.84	0.59
1:A:57:GLY:N	4:A:1022:HOH:O	2.34	0.59
1:C:223:TYR:HE1	4:C:1005:HOH:O	1.84	0.59
1:D:233:TYR:CE1	1:D:267:LYS:HE3	2.36	0.59
1:C:296:THR:HG21	1:C:298:GLN:HG2	1.83	0.59
1:D:353:THR:HG22	1:D:372:VAL:CG2	2.32	0.59
1:C:173:MET:HA	1:C:173:MET:CE	2.31	0.59
1:D:103:CYS:HB3	1:D:364:LEU:HB3	1.85	0.59
1:F:129:ASP:O	1:F:133:ASP:HB2	2.02	0.59
1:D:296:THR:HG21	1:D:298:GLN:HG2	1.84	0.59
1:A:393:GLN:HG3	1:A:394:LYS:N	2.18	0.59
1:A:353:THR:HG22	1:A:372:VAL:CG2	2.33	0.59
1:B:353:THR:HG22	1:B:372:VAL:HG22	1.83	0.59
1:A:103:CYS:HB3	1:A:364:LEU:HB3	1.85	0.59
1:E:103:CYS:HB3	1:E:364:LEU:HB3	1.85	0.59
1:E:179:ASP:HB3	1:F:386:LEU:HD13	1.84	0.59
1:E:310:PHE:O	1:E:312:PRO:HD3	2.03	0.59
1:B:310:PHE:O	1:B:312:PRO:HD3	2.03	0.58
1:B:353:THR:HG22	1:B:372:VAL:CG2	2.33	0.58
1:B:103:CYS:HB3	1:B:364:LEU:HB3	1.85	0.58
1:F:110:GLU:HG2	1:F:118:VAL:CB	2.34	0.58
1:D:353:THR:HG22	1:D:372:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:ND2	3:A:1001:PLP:H2A1	2.18	0.58
1:B:264:ILE:HG22	1:B:268:LEU:HD22	1.86	0.58
1:C:310:PHE:O	1:C:312:PRO:HD3	2.03	0.58
1:C:48:ALA:O	1:C:313:THR:HB	2.02	0.58
1:E:233:TYR:CE1	1:E:267:LYS:HE3	2.39	0.58
1:E:353:THR:HG22	1:E:372:VAL:CG2	2.34	0.58
1:C:281:ASP:OD2	1:C:282:PRO:HD2	2.03	0.58
1:C:353:THR:HG22	1:C:372:VAL:CG2	2.33	0.58
1:E:110:GLU:HG2	1:E:118:VAL:CB	2.33	0.58
1:A:353:THR:HG22	1:A:372:VAL:HG22	1.86	0.58
1:A:173:MET:HA	1:A:173:MET:CE	2.34	0.57
1:D:110:GLU:HG2	1:D:118:VAL:CB	2.34	0.57
1:D:237:ALA:HB2	1:D:264:ILE:HA	1.86	0.57
1:B:45:ARG:HH12	1:B:48:ALA:HA	1.70	0.57
1:E:119:LYS:HD2	1:E:150:THR:OG1	2.04	0.57
1:A:264:ILE:HG22	1:A:268:LEU:HD22	1.87	0.57
1:B:110:GLU:HG2	1:B:118:VAL:CB	2.34	0.57
1:B:237:ALA:HB2	1:B:264:ILE:HA	1.87	0.57
1:C:129:ASP:O	1:C:133:ASP:HB2	2.05	0.57
1:F:310:PHE:O	1:F:312:PRO:HD3	2.04	0.57
1:A:310:PHE:O	1:A:312:PRO:HD3	2.04	0.57
1:C:106:LEU:HD11	1:C:369:ARG:HD2	1.86	0.57
1:F:353:THR:HG22	1:F:372:VAL:HG22	1.85	0.57
1:C:95:ILE:HG23	1:C:337:MET:CE	2.35	0.56
1:E:237:ALA:HB2	1:E:264:ILE:HA	1.87	0.56
1:A:255:VAL:HG13	1:A:258:GLY:HA2	1.88	0.56
1:C:248:LEU:HD23	1:C:250:MET:H	1.69	0.56
1:C:296:THR:CG2	1:C:298:GLN:HG2	2.35	0.56
1:E:106:LEU:HD11	1:E:369:ARG:HD2	1.86	0.56
1:E:110:GLU:HG2	1:E:118:VAL:HB	1.88	0.56
1:F:149:ASN:ND2	3:F:1001:PLP:H2A1	2.19	0.56
1:B:296:THR:CG2	1:B:298:GLN:HG2	2.36	0.56
1:D:129:ASP:O	1:D:133:ASP:HB2	2.06	0.56
1:E:353:THR:HG22	1:E:372:VAL:HG22	1.86	0.56
1:C:264:ILE:HG22	1:C:268:LEU:HD22	1.86	0.56
1:D:149:ASN:ND2	3:D:1001:PLP:H2A1	2.20	0.56
1:E:296:THR:CG2	1:E:298:GLN:HG2	2.35	0.56
1:A:110:GLU:HG2	1:A:118:VAL:CB	2.35	0.56
1:D:172:LYS:HD2	1:D:172:LYS:N	2.21	0.56
1:F:172:LYS:HD2	1:F:172:LYS:N	2.21	0.56
1:E:281:ASP:OD2	1:E:282:PRO:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ASP:OD2	1:F:282:PRO:HD2	2.05	0.56
1:A:386:LEU:HD13	1:B:179:ASP:HB3	1.88	0.56
1:B:129:ASP:O	1:B:133:ASP:HB2	2.06	0.56
1:D:119:LYS:C	4:D:1022:HOH:O	2.43	0.56
1:C:110:GLU:HG2	1:C:118:VAL:CB	2.36	0.55
1:B:268:LEU:O	1:B:272:CYS:N	2.40	0.55
1:E:172:LYS:HD2	1:E:172:LYS:N	2.21	0.55
1:F:264:ILE:HG22	1:F:268:LEU:HD22	1.89	0.55
1:A:129:ASP:O	1:A:133:ASP:HB2	2.06	0.55
1:D:264:ILE:HG22	1:D:268:LEU:HD22	1.87	0.55
1:A:248:LEU:HD23	1:A:250:MET:H	1.72	0.55
1:F:91:ARG:HD2	1:F:93:ASN:OD1	2.07	0.55
1:B:172:LYS:N	1:B:172:LYS:HD2	2.21	0.55
1:F:106:LEU:HD11	1:F:369:ARG:HD2	1.88	0.55
1:A:172:LYS:HD2	1:A:172:LYS:N	2.22	0.55
1:B:173:MET:CE	1:B:173:MET:HA	2.36	0.55
1:D:296:THR:CG2	1:D:298:GLN:HG2	2.36	0.55
1:A:106:LEU:HD11	1:A:369:ARG:HD2	1.88	0.55
1:A:280:VAL:HG22	1:A:356:VAL:HG21	1.89	0.55
1:A:296:THR:CG2	1:A:298:GLN:HG2	2.36	0.55
1:C:119:LYS:HD2	1:C:150:THR:OG1	2.06	0.55
1:B:228:ASN:HB3	1:B:229:PRO:CD	2.37	0.55
1:F:235:THR:O	1:F:239:GLU:HG3	2.07	0.54
1:B:106:LEU:HD11	1:B:369:ARG:HD2	1.89	0.54
1:D:228:ASN:HB3	1:D:229:PRO:CD	2.37	0.54
1:C:172:LYS:HD2	1:C:172:LYS:N	2.22	0.54
1:C:353:THR:HG22	1:C:372:VAL:HG22	1.88	0.54
1:E:264:ILE:HG22	1:E:268:LEU:HD22	1.90	0.54
1:C:349:SER:HB3	4:C:1009:HOH:O	2.08	0.54
1:A:296:THR:HG22	1:A:297:GLU:H	1.73	0.54
1:A:233:TYR:CE1	1:A:267:LYS:HE3	2.42	0.54
1:E:149:ASN:ND2	3:E:1001:PLP:H2A1	2.22	0.54
1:D:310:PHE:O	1:D:312:PRO:HD3	2.06	0.54
1:A:228:ASN:HB3	1:A:229:PRO:CD	2.37	0.53
1:B:248:LEU:HD23	1:B:249:ASP:N	2.23	0.53
1:D:49:PRO:O	1:D:50:SER:O	2.26	0.53
1:C:237:ALA:HB2	1:C:264:ILE:HA	1.89	0.53
1:E:248:LEU:HD23	1:E:250:MET:H	1.72	0.53
1:B:95:ILE:HG23	1:B:337:MET:CE	2.38	0.53
1:D:296:THR:HG22	1:D:297:GLU:H	1.74	0.53
1:E:289:GLU:OE2	1:E:317:ARG:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LEU:HD23	1:F:250:MET:H	1.73	0.53
1:A:281:ASP:OD2	1:A:282:PRO:HD2	2.09	0.53
1:C:129:ASP:CA	1:C:132:ARG:HH12	2.14	0.53
1:D:235:THR:O	1:D:239:GLU:HG3	2.09	0.53
1:F:233:TYR:CE1	1:F:267:LYS:HE3	2.43	0.53
1:C:268:LEU:O	1:C:272:CYS:N	2.42	0.53
1:D:48:ALA:O	1:D:313:THR:HB	2.09	0.53
1:D:281:ASP:OD2	1:D:282:PRO:HD2	2.09	0.52
1:F:145:PRO:HB3	1:F:207:ALA:HB2	1.92	0.52
1:C:110:GLU:HG3	1:C:113:ASN:ND2	2.25	0.52
1:C:248:LEU:HD23	1:C:249:ASP:N	2.25	0.52
1:B:147:SER:HB3	1:B:169:MET:SD	2.49	0.52
1:E:296:THR:HG22	1:E:297:GLU:H	1.74	0.52
1:B:149:ASN:ND2	3:B:1001:PLP:H2A1	2.24	0.52
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.09	0.52
1:C:296:THR:HG22	1:C:297:GLU:H	1.72	0.52
1:C:149:ASN:ND2	3:C:1001:PLP:H2A1	2.25	0.52
1:C:255:VAL:HG13	1:C:258:GLY:HA2	1.90	0.52
1:F:119:LYS:HD2	1:F:150:THR:OG1	2.10	0.52
1:A:91:ARG:HD2	1:A:93:ASN:OD1	2.10	0.52
1:A:237:ALA:HB2	1:A:264:ILE:HA	1.92	0.52
1:B:248:LEU:HD23	1:B:250:MET:H	1.73	0.52
1:D:248:LEU:HD23	1:D:250:MET:H	1.74	0.52
1:F:110:GLU:HG2	1:F:118:VAL:HB	1.91	0.52
1:B:145:PRO:HB3	1:B:207:ALA:HB2	1.92	0.52
1:C:91:ARG:HD2	1:C:93:ASN:OD1	2.09	0.52
1:D:254:SER:HA	1:D:280:VAL:HB	1.92	0.52
1:B:203:HIS:CD2	1:B:204:VAL:HG23	2.45	0.52
1:B:296:THR:HG22	1:B:297:GLU:H	1.75	0.52
1:C:145:PRO:HB3	1:C:207:ALA:HB2	1.92	0.52
1:C:386:LEU:HD13	1:D:179:ASP:HB3	1.91	0.52
1:E:304:GLU:HG3	4:E:1016:HOH:O	2.09	0.52
1:C:329:GLU:O	1:C:333:THR:HG23	2.10	0.51
1:F:255:VAL:HG13	1:F:258:GLY:HA2	1.92	0.51
1:B:110:GLU:HG2	1:B:118:VAL:HB	1.92	0.51
1:C:228:ASN:HB3	1:C:229:PRO:CD	2.41	0.51
1:B:109:CYS:HB3	1:B:111:PHE:CE2	2.45	0.51
1:D:106:LEU:HD11	1:D:369:ARG:HD2	1.91	0.51
1:D:236:THR:O	1:D:240:ILE:HG13	2.11	0.51
1:F:224:ARG:HG2	1:F:313:THR:HG23	1.89	0.51
1:D:147:SER:HB3	1:D:169:MET:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:HIS:CD2	1:F:204:VAL:HG23	2.46	0.51
1:E:235:THR:O	1:E:239:GLU:HG3	2.11	0.51
1:E:95:ILE:HG23	1:E:337:MET:CE	2.40	0.51
1:A:203:HIS:CD2	1:A:204:VAL:HG23	2.46	0.51
1:B:254:SER:HA	1:B:280:VAL:HB	1.93	0.51
1:D:121:ARG:HB2	4:D:1022:HOH:O	2.11	0.51
1:E:398:LYS:HG3	1:E:399:GLU:N	2.18	0.51
1:A:268:LEU:O	1:A:272:CYS:N	2.41	0.51
1:B:376:ASP:HB2	4:B:1028:HOH:O	2.11	0.51
1:C:203:HIS:CD2	1:C:204:VAL:HG23	2.46	0.51
1:E:203:HIS:CD2	1:E:204:VAL:HG23	2.46	0.51
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.93	0.51
1:D:248:LEU:HD23	1:D:249:ASP:N	2.26	0.51
1:E:228:ASN:HB3	1:E:229:PRO:CD	2.40	0.51
1:E:268:LEU:O	1:E:272:CYS:N	2.41	0.51
1:B:329:GLU:O	1:B:333:THR:HG23	2.11	0.50
1:E:145:PRO:HB3	1:E:207:ALA:HB2	1.92	0.50
1:B:119:LYS:HD2	1:B:150:THR:OG1	2.11	0.50
1:F:95:ILE:HG23	1:F:337:MET:CE	2.41	0.50
1:A:95:ILE:HG23	1:A:337:MET:CE	2.41	0.50
1:D:119:LYS:HD2	1:D:150:THR:OG1	2.10	0.50
1:D:288:ALA:HA	1:D:323:TRP:CD2	2.46	0.50
1:D:329:GLU:O	1:D:333:THR:HG23	2.11	0.50
1:F:110:GLU:HG3	1:F:113:ASN:ND2	2.27	0.50
1:F:228:ASN:HB3	1:F:229:PRO:CD	2.41	0.50
1:F:296:THR:CG2	1:F:297:GLU:HG2	2.41	0.50
1:A:110:GLU:HG2	1:A:118:VAL:HG23	1.93	0.50
1:A:262:THR:HG23	1:A:316:ASP:HB3	1.93	0.50
1:E:254:SER:HA	1:E:280:VAL:HB	1.94	0.50
1:E:329:GLU:O	1:E:333:THR:HG23	2.12	0.50
1:C:132:ARG:NH1	1:C:132:ARG:HB3	2.27	0.50
1:D:203:HIS:CD2	1:D:204:VAL:HG23	2.46	0.50
1:F:296:THR:HG22	1:F:297:GLU:N	2.25	0.50
1:F:169:MET:HE2	1:F:188:ILE:HG23	1.94	0.50
1:F:268:LEU:O	1:F:272:CYS:N	2.43	0.50
1:C:150:THR:OG1	1:C:222:GLN:NE2	2.45	0.50
1:F:292:GLU:O	1:F:294:ASN:N	2.45	0.50
1:A:288:ALA:HA	1:A:323:TRP:CD2	2.46	0.49
1:D:110:GLU:HG2	1:D:118:VAL:HB	1.94	0.49
1:D:255:VAL:HG13	1:D:258:GLY:HA2	1.93	0.49
1:C:254:SER:HA	1:C:280:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLU:HG3	1:D:113:ASN:ND2	2.27	0.49
1:F:237:ALA:HB2	1:F:264:ILE:HA	1.94	0.49
1:E:255:VAL:HG13	1:E:258:GLY:HA2	1.93	0.49
1:D:147:SER:HB2	1:D:173:MET:CG	2.43	0.49
1:D:169:MET:HE2	1:D:188:ILE:HG23	1.93	0.49
1:F:288:ALA:HB3	1:F:294:ASN:HD21	1.77	0.49
1:D:45:ARG:HD2	1:D:47:ASP:OD1	2.12	0.49
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.13	0.49
1:B:178:VAL:O	1:B:182:ARG:HG3	2.13	0.49
1:B:280:VAL:HG22	1:B:356:VAL:HG21	1.94	0.49
1:B:393:GLN:HG3	1:B:394:LYS:N	2.26	0.49
1:D:110:GLU:HG2	1:D:118:VAL:HG23	1.94	0.49
1:A:329:GLU:O	1:A:333:THR:HG23	2.12	0.49
1:B:132:ARG:NH1	1:B:132:ARG:HB3	2.28	0.49
1:A:248:LEU:HD23	1:A:249:ASP:N	2.27	0.49
1:A:292:GLU:O	1:A:295:GLN:HG3	2.13	0.49
1:D:95:ILE:HG12	1:D:337:MET:CE	2.42	0.49
1:D:145:PRO:HB3	1:D:207:ALA:HB2	1.94	0.49
1:D:70:PRO:HG2	1:D:238:ASP:HB3	1.95	0.49
1:A:110:GLU:HG3	1:A:113:ASN:ND2	2.28	0.49
1:C:43:TRP:HA	1:C:208:TRP:CE2	2.47	0.48
1:C:110:GLU:HG2	1:C:118:VAL:HB	1.95	0.48
1:F:44:ILE:HG22	1:F:224:ARG:HD2	1.94	0.48
1:A:110:GLU:HG2	1:A:118:VAL:HB	1.95	0.48
1:C:289:GLU:OE2	1:C:317:ARG:HB3	2.12	0.48
1:D:147:SER:CB	1:D:173:MET:HG2	2.43	0.48
1:F:132:ARG:NH1	1:F:132:ARG:HB3	2.28	0.48
1:D:129:ASP:CA	1:D:132:ARG:HH12	2.18	0.48
1:F:276:ARG:CZ	1:F:363:GLU:OE2	2.62	0.48
1:A:169:MET:HE2	1:A:188:ILE:HG23	1.95	0.48
1:D:254:SER:HB2	1:D:306:ILE:HG21	1.95	0.48
1:A:109:CYS:HB3	1:A:111:PHE:CE2	2.49	0.48
1:A:145:PRO:HB3	1:A:207:ALA:HB2	1.95	0.48
1:B:44:ILE:HD12	1:B:44:ILE:N	2.29	0.48
1:B:254:SER:HB2	1:B:306:ILE:HG21	1.95	0.48
1:E:296:THR:HG21	1:E:298:GLN:CG	2.43	0.48
1:B:110:GLU:HG3	1:B:113:ASN:ND2	2.29	0.48
1:C:271:LYS:NZ	4:C:1019:HOH:O	2.39	0.48
1:D:109:CYS:HB3	1:D:111:PHE:CE2	2.49	0.48
1:D:264:ILE:CD1	1:D:373:ILE:HD11	2.43	0.48
1:E:168:VAL:HG12	1:E:203:HIS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:LEU:HD23	1:E:249:ASP:N	2.28	0.48
1:D:173:MET:HA	1:D:173:MET:HE2	1.96	0.48
1:E:132:ARG:NH1	1:E:132:ARG:HB3	2.28	0.48
1:A:254:SER:HA	1:A:280:VAL:HB	1.96	0.48
1:C:169:MET:HE2	1:C:188:ILE:HG23	1.94	0.48
1:E:280:VAL:HG22	1:E:356:VAL:HG21	1.96	0.48
1:B:110:GLU:HG2	1:B:118:VAL:HG23	1.96	0.47
1:C:296:THR:HG21	1:C:298:GLN:CG	2.43	0.47
1:A:129:ASP:CA	1:A:132:ARG:HH12	2.18	0.47
1:B:296:THR:CG2	1:B:297:GLU:N	2.77	0.47
1:E:173:MET:HA	1:E:173:MET:HE3	1.96	0.47
1:B:223:TYR:O	1:B:314:VAL:HG13	2.14	0.47
1:C:288:ALA:HA	1:C:323:TRP:CD2	2.49	0.47
1:C:292:GLU:O	1:C:295:GLN:HG3	2.15	0.47
1:D:280:VAL:HG22	1:D:356:VAL:HG21	1.97	0.47
1:A:296:THR:CG2	1:A:297:GLU:N	2.77	0.47
1:C:296:THR:CG2	1:C:297:GLU:N	2.77	0.47
1:F:264:ILE:CD1	1:F:373:ILE:HD11	2.44	0.47
1:A:132:ARG:NH1	1:A:132:ARG:HB3	2.29	0.47
1:C:110:GLU:HG2	1:C:118:VAL:HG23	1.96	0.47
1:D:289:GLU:OE2	1:D:317:ARG:HB3	2.14	0.47
1:B:235:THR:O	1:B:239:GLU:HG3	2.14	0.47
1:B:292:GLU:O	1:B:295:GLN:HG3	2.15	0.47
1:C:45:ARG:HG3	1:C:45:ARG:O	2.14	0.47
1:D:132:ARG:NH1	1:D:132:ARG:HB3	2.29	0.47
1:F:248:LEU:HD23	1:F:249:ASP:N	2.29	0.47
1:A:254:SER:HB2	1:A:306:ILE:HG21	1.96	0.47
1:C:375:PRO:HD2	4:C:1009:HOH:O	2.15	0.47
1:E:288:ALA:HA	1:E:323:TRP:CD2	2.50	0.47
1:F:178:VAL:O	1:F:182:ARG:HG3	2.15	0.47
1:B:48:ALA:O	1:B:313:THR:HB	2.14	0.47
1:B:264:ILE:CD1	1:B:373:ILE:HD11	2.45	0.47
1:D:168:VAL:HG12	1:D:203:HIS:HB2	1.97	0.47
1:B:150:THR:OG1	1:B:222:GLN:NE2	2.48	0.47
1:C:224:ARG:HG2	1:C:313:THR:HG23	1.94	0.47
1:E:296:THR:CG2	1:E:297:GLU:N	2.77	0.47
1:F:297:GLU:CG	1:F:298:GLN:H	2.22	0.47
1:D:268:LEU:O	1:D:272:CYS:N	2.44	0.46
1:F:43:TRP:HE1	1:F:45:ARG:HG3	1.72	0.46
1:B:224:ARG:HG2	1:B:313:THR:HG23	1.92	0.46
1:C:52:CYS:HA	2:C:501:HEM:C1A	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:HG21	1:F:224:ARG:CZ	2.45	0.46
1:F:95:ILE:HG12	1:F:337:MET:HE3	1.96	0.46
1:B:147:SER:HB3	1:B:169:MET:CB	2.45	0.46
1:C:159:ALA:O	1:D:94:LYS:NZ	2.48	0.46
1:C:254:SER:HB2	1:C:306:ILE:HG21	1.96	0.46
1:E:44:ILE:HG22	1:E:224:ARG:HD2	1.97	0.46
1:D:147:SER:HB2	1:D:173:MET:HG3	1.96	0.46
1:D:224:ARG:HG2	1:D:313:THR:HG23	1.93	0.46
1:F:150:THR:OG1	1:F:222:GLN:NE2	2.48	0.46
1:B:296:THR:HG21	1:B:298:GLN:CG	2.44	0.46
1:E:366:GLU:H	1:E:366:GLU:HG2	1.52	0.46
1:F:168:VAL:HG12	1:F:203:HIS:HB2	1.97	0.46
1:A:226:ALA:HA	2:A:501:HEM:HMD2	1.98	0.46
1:C:284:GLY:HA2	1:C:298:GLN:O	2.16	0.46
1:D:296:THR:HG21	1:D:298:GLN:CG	2.45	0.46
1:E:52:CYS:HA	2:E:501:HEM:C1A	2.50	0.46
1:F:297:GLU:HG3	1:F:298:GLN:N	2.25	0.46
1:A:296:THR:HG21	1:A:298:GLN:CG	2.45	0.46
1:C:353:THR:CG2	1:C:372:VAL:HG22	2.46	0.46
1:E:111:PHE:HB3	1:E:376:ASP:C	2.36	0.46
1:F:173:MET:HA	1:F:173:MET:HE2	1.95	0.46
1:F:276:ARG:NH1	1:F:363:GLU:OE2	2.49	0.46
1:A:178:VAL:O	1:A:182:ARG:HG3	2.15	0.46
1:C:96:GLY:O	1:C:101:LEU:HB2	2.16	0.46
1:C:111:PHE:HB3	1:C:376:ASP:C	2.37	0.46
1:E:110:GLU:HG3	1:E:113:ASN:ND2	2.31	0.46
1:F:329:GLU:O	1:F:333:THR:HG23	2.15	0.46
1:E:202:SER:O	1:E:206:VAL:HG23	2.16	0.46
1:F:70:PRO:HG2	1:F:238:ASP:HB3	1.98	0.46
1:F:353:THR:CG2	1:F:372:VAL:HG22	2.46	0.46
1:B:366:GLU:H	1:B:366:GLU:HG2	1.54	0.45
1:E:292:GLU:O	1:E:295:GLN:HG3	2.16	0.45
1:C:280:VAL:HG22	1:C:356:VAL:HG21	1.98	0.45
1:C:366:GLU:H	1:C:366:GLU:HG2	1.57	0.45
1:D:95:ILE:HG12	1:D:337:MET:HE3	1.98	0.45
1:D:150:THR:OG1	1:D:222:GLN:NE2	2.50	0.45
1:F:289:GLU:OE2	1:F:317:ARG:HD3	2.16	0.45
1:A:264:ILE:CD1	1:A:373:ILE:HD11	2.46	0.45
1:B:52:CYS:HA	2:B:501:HEM:C1A	2.51	0.45
1:D:145:PRO:O	1:D:146:THR:HB	2.17	0.45
1:E:70:PRO:HG2	1:E:238:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:LYS:HG3	1:E:149:ASN:HB2	1.97	0.45
1:E:391:MET:HB3	1:E:397:LEU:HB2	1.99	0.45
1:D:178:VAL:O	1:D:182:ARG:HG3	2.16	0.45
1:A:52:CYS:HA	2:A:501:HEM:C1A	2.52	0.45
1:C:132:ARG:HB3	1:C:132:ARG:CZ	2.46	0.45
1:C:178:VAL:O	1:C:182:ARG:HG3	2.17	0.45
1:D:111:PHE:HB3	1:D:376:ASP:C	2.36	0.45
1:A:119:LYS:HG3	1:A:149:ASN:HB2	1.99	0.45
1:D:70:PRO:HG3	1:D:235:THR:HA	1.98	0.45
1:A:235:THR:O	1:A:239:GLU:HG3	2.16	0.45
1:B:70:PRO:HG2	1:B:238:ASP:HB3	1.99	0.45
1:B:288:ALA:HA	1:B:323:TRP:CD2	2.52	0.45
1:D:96:GLY:O	1:D:101:LEU:HB2	2.16	0.45
1:D:292:GLU:O	1:D:295:GLN:HG3	2.17	0.45
1:D:353:THR:CG2	1:D:372:VAL:HG22	2.46	0.45
1:F:254:SER:HA	1:F:280:VAL:HB	1.99	0.45
1:B:262:THR:HG23	1:B:316:ASP:HB3	1.99	0.45
1:B:353:THR:CG2	1:B:372:VAL:HG22	2.46	0.45
1:C:119:LYS:HG3	1:C:149:ASN:HB2	1.98	0.45
1:E:70:PRO:HG3	1:E:235:THR:HA	1.99	0.45
1:F:298:GLN:HG3	1:F:300:THR:O	2.17	0.45
1:D:202:SER:O	1:D:206:VAL:HG23	2.17	0.45
1:E:169:MET:HE2	1:E:188:ILE:HG23	1.98	0.45
1:E:178:VAL:O	1:E:182:ARG:HG3	2.17	0.45
1:C:264:ILE:CD1	1:C:373:ILE:HD11	2.47	0.45
1:C:168:VAL:HG12	1:C:203:HIS:HB2	1.99	0.44
1:D:122:ILE:N	4:D:1022:HOH:O	2.26	0.44
1:E:48:ALA:HA	1:E:49:PRO:HD2	1.79	0.44
1:F:236:THR:O	1:F:240:ILE:HG13	2.17	0.44
1:F:296:THR:CG2	1:F:297:GLU:N	2.80	0.44
1:C:70:PRO:HG3	1:C:235:THR:HA	1.99	0.44
1:E:264:ILE:CD1	1:E:373:ILE:HD11	2.47	0.44
1:E:353:THR:CG2	1:E:372:VAL:HG22	2.48	0.44
1:F:111:PHE:HB3	1:F:376:ASP:C	2.37	0.44
1:F:262:THR:HG23	1:F:316:ASP:HB3	2.00	0.44
1:B:147:SER:OG	1:B:173:MET:CG	2.65	0.44
1:F:52:CYS:HA	2:F:501:HEM:C1A	2.52	0.44
1:F:95:ILE:HG12	1:F:337:MET:CE	2.47	0.44
1:A:111:PHE:HB3	1:A:376:ASP:C	2.37	0.44
1:C:361:ALA:O	1:C:364:LEU:HB2	2.18	0.44
1:D:52:CYS:HA	2:D:501:HEM:C1A	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:HG23	1:D:316:ASP:HB3	1.99	0.44
1:E:43:TRP:O	1:E:44:ILE:HG12	2.16	0.44
1:F:96:GLY:O	1:F:101:LEU:HB2	2.17	0.44
1:A:168:VAL:HG12	1:A:203:HIS:HB2	1.99	0.44
1:B:169:MET:HE2	1:B:188:ILE:HG23	1.99	0.44
1:C:235:THR:O	1:C:239:GLU:HG3	2.17	0.44
1:C:262:THR:HG23	1:C:316:ASP:HB3	1.99	0.44
1:B:168:VAL:HG12	1:B:203:HIS:HB2	1.99	0.44
1:B:308:TYR:HD2	1:B:310:PHE:O	2.01	0.44
1:F:110:GLU:CG	1:F:118:VAL:HA	2.48	0.44
1:F:254:SER:HB2	1:F:306:ILE:HG21	1.99	0.44
1:B:132:ARG:HB3	1:B:132:ARG:CZ	2.47	0.44
1:C:214:ILE:HA	1:C:215:PRO:HD3	1.91	0.44
1:D:110:GLU:CG	1:D:118:VAL:HA	2.48	0.44
1:F:145:PRO:O	1:F:146:THR:HB	2.18	0.44
1:A:70:PRO:HG2	1:A:238:ASP:HB3	2.00	0.44
1:F:226:ALA:HA	2:F:501:HEM:HMD2	1.99	0.44
1:C:95:ILE:HG23	1:C:337:MET:HE3	1.99	0.44
1:E:109:CYS:HB3	1:E:111:PHE:CE2	2.53	0.44
1:E:150:THR:OG1	1:E:222:GLN:NE2	2.51	0.44
1:F:311:ILE:CD1	1:F:317:ARG:NH1	2.81	0.44
1:A:77:LEU:HD12	1:A:77:LEU:N	2.32	0.43
1:A:132:ARG:HB3	1:A:132:ARG:CZ	2.47	0.43
1:A:353:THR:CG2	1:A:372:VAL:HG22	2.47	0.43
1:C:209:ARG:O	1:C:213:GLU:HG3	2.18	0.43
1:C:271:LYS:HE3	4:C:1014:HOH:O	2.18	0.43
1:D:95:ILE:HG23	1:D:337:MET:CE	2.47	0.43
1:F:110:GLU:HG2	1:F:118:VAL:HG23	2.00	0.43
1:D:295:GLN:O	1:D:296:THR:OG1	2.34	0.43
1:E:47:ASP:O	1:E:48:ALA:HB3	2.18	0.43
1:E:254:SER:HB2	1:E:306:ILE:HG21	1.99	0.43
1:F:119:LYS:HG3	1:F:149:ASN:HB2	2.00	0.43
1:A:70:PRO:HG3	1:A:235:THR:HA	1.99	0.43
1:C:308:TYR:HD2	1:C:310:PHE:O	2.02	0.43
1:F:220:LEU:HD23	1:F:220:LEU:HA	1.79	0.43
1:A:202:SER:O	1:A:206:VAL:HG23	2.18	0.43
1:B:248:LEU:HD22	1:B:275:CYS:SG	2.58	0.43
1:C:70:PRO:HG2	1:C:238:ASP:HB3	2.00	0.43
1:D:296:THR:CG2	1:D:297:GLU:N	2.77	0.43
1:E:311:ILE:HD13	1:E:317:ARG:CZ	2.49	0.43
1:E:397:LEU:HD22	1:E:398:LYS:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:LEU:HD12	1:F:101:LEU:HA	1.90	0.43
1:F:129:ASP:CA	1:F:132:ARG:HH12	2.19	0.43
1:F:288:ALA:HA	1:F:323:TRP:CD2	2.53	0.43
1:B:214:ILE:HA	1:B:215:PRO:HD3	1.89	0.43
1:D:44:ILE:O	1:D:45:ARG:O	2.37	0.43
1:D:132:ARG:HB3	1:D:132:ARG:CZ	2.48	0.43
1:A:96:GLY:O	1:A:101:LEU:HB2	2.18	0.43
1:A:308:TYR:HD2	1:A:310:PHE:O	2.02	0.43
1:C:202:SER:O	1:C:206:VAL:HG23	2.18	0.43
1:B:289:GLU:OE2	1:B:317:ARG:HB3	2.18	0.43
1:C:44:ILE:O	1:C:45:ARG:C	2.57	0.43
1:C:109:CYS:HB3	1:C:111:PHE:CE2	2.54	0.43
1:D:119:LYS:HG3	1:D:149:ASN:HB2	1.99	0.43
1:F:132:ARG:HB3	1:F:132:ARG:CZ	2.48	0.43
1:A:95:ILE:HG12	1:A:337:MET:CE	2.48	0.43
1:C:223:TYR:O	1:C:314:VAL:HG13	2.19	0.43
1:D:241:LEU:HD21	1:D:268:LEU:HD12	2.01	0.43
1:E:132:ARG:HB3	1:E:132:ARG:CZ	2.49	0.43
1:F:311:ILE:HD13	1:F:317:ARG:NH1	2.33	0.43
1:B:111:PHE:HB3	1:B:376:ASP:C	2.40	0.43
1:B:303:VAL:HG22	1:B:328:ASP:OD2	2.19	0.43
1:C:226:ALA:HA	2:C:501:HEM:HMD2	2.01	0.43
1:B:96:GLY:O	1:B:101:LEU:HB2	2.19	0.42
1:B:110:GLU:CG	1:B:118:VAL:HA	2.49	0.42
1:B:202:SER:O	1:B:206:VAL:HG23	2.19	0.42
1:D:226:ALA:HA	2:D:501:HEM:HMD2	2.00	0.42
1:F:366:GLU:H	1:F:366:GLU:HG2	1.56	0.42
1:A:126:MET:HG2	1:A:227:SER:HB2	2.01	0.42
1:B:70:PRO:HG3	1:B:235:THR:HA	2.02	0.42
1:B:119:LYS:HG3	1:B:149:ASN:HB2	2.00	0.42
1:C:311:ILE:HD13	1:C:317:ARG:CZ	2.48	0.42
1:D:62:GLU:O	2:D:501:HEM:HMB1	2.19	0.42
1:A:44:ILE:HD12	1:A:44:ILE:HA	1.66	0.42
1:A:110:GLU:CG	1:A:118:VAL:HA	2.49	0.42
1:B:373:ILE:O	1:B:375:PRO:HD3	2.19	0.42
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.88	0.42
1:E:244:CYS:HB3	1:E:247:LYS:O	2.20	0.42
1:A:95:ILE:O	1:A:99:PHE:HD1	2.03	0.42
1:A:311:ILE:HD13	1:A:317:ARG:CZ	2.49	0.42
1:B:95:ILE:HG12	1:B:337:MET:CE	2.49	0.42
1:F:44:ILE:HG22	1:F:224:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:HD13	1:F:44:ILE:HA	1.65	0.42
1:A:110:GLU:HG2	1:A:118:VAL:CG2	2.49	0.42
1:D:126:MET:HG2	1:D:227:SER:HB2	2.00	0.42
1:E:96:GLY:O	1:E:101:LEU:HB2	2.19	0.42
1:F:70:PRO:HG3	1:F:235:THR:HA	2.01	0.42
1:C:95:ILE:HG12	1:C:337:MET:CE	2.49	0.42
1:C:110:GLU:CG	1:C:118:VAL:HA	2.50	0.42
1:A:233:TYR:CD1	1:A:267:LYS:HB2	2.54	0.42
1:A:150:THR:OG1	1:A:222:GLN:NE2	2.53	0.42
1:A:229:PRO:O	2:A:501:HEM:HBC1	2.20	0.42
1:A:244:CYS:HB3	1:A:247:LYS:O	2.20	0.42
1:D:121:ARG:CA	4:D:1022:HOH:O	2.65	0.42
1:D:233:TYR:CD1	1:D:267:LYS:HB2	2.55	0.42
1:D:366:GLU:H	1:D:366:GLU:HG2	1.55	0.42
1:E:77:LEU:N	1:E:77:LEU:HD12	2.35	0.42
1:A:295:GLN:O	1:A:296:THR:OG1	2.35	0.42
1:A:346:CYS:O	1:A:378:VAL:CG1	2.68	0.42
1:B:43:TRP:HD1	1:B:208:TRP:CE3	2.37	0.42
1:B:44:ILE:N	1:B:44:ILE:CD1	2.83	0.42
1:C:311:ILE:CD1	1:C:317:ARG:NH1	2.83	0.42
1:D:110:GLU:HG2	1:D:118:VAL:CG2	2.49	0.42
1:B:241:LEU:HD21	1:B:268:LEU:HD12	2.02	0.41
1:E:147:SER:HB2	1:E:173:MET:CG	2.50	0.41
1:F:308:TYR:HD2	1:F:310:PHE:O	2.02	0.41
1:A:173:MET:HE3	1:A:177:LYS:NZ	2.35	0.41
1:B:190:ARG:NH1	1:B:190:ARG:HG3	2.35	0.41
1:C:173:MET:HA	1:C:173:MET:HE2	2.02	0.41
1:F:79:ASP:OD1	1:F:81:LEU:N	2.53	0.41
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.84	0.41
1:D:223:TYR:O	1:D:314:VAL:HG13	2.20	0.41
1:E:110:GLU:CG	1:E:118:VAL:HA	2.50	0.41
1:E:311:ILE:CD1	1:E:317:ARG:NH1	2.83	0.41
1:F:202:SER:O	1:F:206:VAL:HG23	2.20	0.41
1:B:110:GLU:HG2	1:B:118:VAL:CG2	2.51	0.41
1:F:45:ARG:O	1:F:224:ARG:HD2	2.20	0.41
1:F:311:ILE:HD13	1:F:317:ARG:CZ	2.50	0.41
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.90	0.41
1:E:129:ASP:CA	1:E:132:ARG:HH12	2.19	0.41
1:E:392:LEU:HD23	1:E:397:LEU:O	2.21	0.41
1:A:224:ARG:HG2	1:A:313:THR:HG23	1.98	0.41
1:C:102:LYS:NZ	1:C:365:GLN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:O	1:A:265:ALA:CB	2.69	0.41
1:A:373:ILE:O	1:A:375:PRO:HD3	2.21	0.41
1:D:147:SER:CB	1:D:173:MET:CG	2.99	0.41
1:F:45:ARG:HE	1:F:45:ARG:HB2	1.30	0.41
1:A:62:GLU:O	2:A:501:HEM:HMB1	2.21	0.41
1:A:95:ILE:HG12	1:A:337:MET:HE3	2.02	0.41
1:A:97:LYS:HG2	4:A:1006:HOH:O	2.21	0.41
1:A:366:GLU:H	1:A:366:GLU:HG2	1.60	0.41
1:B:95:ILE:O	1:B:99:PHE:HD1	2.04	0.41
1:B:226:ALA:HA	2:B:501:HEM:HMD2	2.02	0.41
1:C:145:PRO:O	1:C:146:THR:HB	2.21	0.41
1:C:248:LEU:HD22	1:C:275:CYS:SG	2.61	0.41
1:C:346:CYS:O	1:C:378:VAL:CG1	2.69	0.41
1:D:102:LYS:HE3	1:D:365:GLN:HA	2.02	0.41
1:D:214:ILE:HB	1:D:217:SER:OG	2.20	0.41
1:E:308:TYR:HD2	1:E:310:PHE:O	2.02	0.41
1:F:165:CYS:SG	1:F:167:ILE:CD1	3.09	0.41
1:E:214:ILE:HA	1:E:215:PRO:HD3	1.89	0.41
1:C:110:GLU:HG2	1:C:118:VAL:HA	2.02	0.40
1:E:159:ALA:O	1:F:94:LYS:NZ	2.51	0.40
1:A:311:ILE:CD1	1:A:317:ARG:NH1	2.85	0.40
1:B:295:GLN:O	1:B:296:THR:OG1	2.34	0.40
1:C:101:LEU:HD12	1:C:101:LEU:HA	1.86	0.40
1:D:272:CYS:O	1:D:275:CYS:HB2	2.22	0.40
1:E:145:PRO:O	1:E:146:THR:HB	2.21	0.40
1:E:361:ALA:O	1:E:364:LEU:HB2	2.22	0.40
1:A:303:VAL:HG22	1:A:328:ASP:OD2	2.21	0.40
1:C:244:CYS:HB3	1:C:247:LYS:O	2.22	0.40
1:D:284:GLY:HA2	1:D:298:GLN:O	2.22	0.40
1:F:214:ILE:HA	1:F:215:PRO:HD3	1.91	0.40
1:F:361:ALA:O	1:F:364:LEU:HB2	2.21	0.40
1:D:244:CYS:HB3	1:D:247:LYS:O	2.21	0.40
1:E:110:GLU:HG2	1:E:118:VAL:HG23	2.03	0.40
1:E:226:ALA:HA	2:E:501:HEM:HMD2	2.02	0.40
1:A:284:GLY:HA2	1:A:298:GLN:O	2.21	0.40
1:B:110:GLU:HG2	1:B:118:VAL:HA	2.04	0.40
1:B:214:ILE:HB	1:B:217:SER:OG	2.21	0.40
1:B:261:ILE:O	1:B:265:ALA:CB	2.70	0.40
1:C:190:ARG:NH1	1:C:190:ARG:HG3	2.37	0.40
1:D:214:ILE:HA	1:D:215:PRO:HD3	1.90	0.40
1:D:303:VAL:HG22	1:D:328:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:ALA:HA	2:F:501:HEM:CMD	2.52	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	344/435 (79%)	325 (94%)	16 (5%)	3 (1%)	17	35
1	B	344/435 (79%)	319 (93%)	19 (6%)	6 (2%)	9	18
1	C	344/435 (79%)	323 (94%)	18 (5%)	3 (1%)	17	35
1	D	344/435 (79%)	319 (93%)	19 (6%)	6 (2%)	9	18
1	E	346/435 (80%)	321 (93%)	19 (6%)	6 (2%)	9	18
1	F	344/435 (79%)	322 (94%)	17 (5%)	5 (2%)	10	21
All	All	2066/2610 (79%)	1929 (93%)	108 (5%)	29 (1%)	11	22

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	SER
1	B	146	THR
1	B	173	MET
1	C	173	MET
1	D	45	ARG
1	D	50	SER
1	D	173	MET
1	E	173	MET
1	F	173	MET
1	A	170	PRO
1	A	173	MET

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Mol	Chain	Res	Type
1	A	192	PRO
1	B	170	PRO
1	B	192	PRO
1	C	192	PRO
1	D	170	PRO
1	D	192	PRO
1	E	170	PRO
1	E	192	PRO
1	F	170	PRO
1	F	192	PRO
1	F	293	LEU
1	C	170	PRO
1	E	47	ASP
1	E	398	LYS
1	F	297	GLU
1	B	49	PRO
1	D	49	PRO
1	E	48	ALA

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	288/362 (80%)	272 (94%)	16 (6%)	21	42
1	B	288/362 (80%)	273 (95%)	15 (5%)	23	46
1	C	288/362 (80%)	272 (94%)	16 (6%)	21	42
1	D	288/362 (80%)	272 (94%)	16 (6%)	21	42
1	E	290/362 (80%)	272 (94%)	18 (6%)	18	37
1	F	288/362 (80%)	272 (94%)	16 (6%)	21	42
All	All	1730/2172 (80%)	1633 (94%)	97 (6%)	21	42

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	46	PRO
1	A	101	LEU
1	A	105	LEU
1	A	133	ASP
1	A	173	MET
1	A	176	GLU
1	A	203	HIS
1	A	208	TRP
1	A	242	GLN
1	A	268	LEU
1	A	299	THR
1	A	309	ASP
1	A	313	THR
1	A	386	LEU
1	A	393	GLN
1	B	47	ASP
1	B	101	LEU
1	B	105	LEU
1	B	133	ASP
1	B	173	MET
1	B	176	GLU
1	B	203	HIS
1	B	208	TRP
1	B	268	LEU
1	B	299	THR
1	B	309	ASP
1	B	313	THR
1	B	372	VAL
1	B	386	LEU
1	B	393	GLN
1	C	46	PRO
1	C	47	ASP
1	C	101	LEU
1	C	105	LEU
1	C	133	ASP
1	C	173	MET
1	C	176	GLU
1	C	203	HIS
1	C	208	TRP
1	C	242	GLN
1	C	268	LEU
1	C	299	THR

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Mol	Chain	Res	Type
1	C	309	ASP
1	C	313	THR
1	C	386	LEU
1	C	393	GLN
1	D	46	PRO
1	D	101	LEU
1	D	105	LEU
1	D	133	ASP
1	D	173	MET
1	D	176	GLU
1	D	203	HIS
1	D	208	TRP
1	D	268	LEU
1	D	276	ARG
1	D	299	THR
1	D	309	ASP
1	D	313	THR
1	D	364	LEU
1	D	386	LEU
1	D	393	GLN
1	E	45	ARG
1	E	46	PRO
1	E	101	LEU
1	E	105	LEU
1	E	133	ASP
1	E	173	MET
1	E	176	GLU
1	E	203	HIS
1	E	208	TRP
1	E	242	GLN
1	E	268	LEU
1	E	299	THR
1	E	309	ASP
1	E	313	THR
1	E	372	VAL
1	E	386	LEU
1	E	393	GLN
1	E	398	LYS
1	F	43	TRP
1	F	44	ILE
1	F	45	ARG
1	F	46	PRO

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Mol	Chain	Res	Type
1	F	101	LEU
1	F	105	LEU
1	F	133	ASP
1	F	173	MET
1	F	176	GLU
1	F	203	HIS
1	F	208	TRP
1	F	242	GLN
1	F	268	LEU
1	F	309	ASP
1	F	313	THR
1	F	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	222	GLN
1	A	242	GLN
1	B	203	HIS
1	B	222	GLN
1	B	242	GLN
1	B	341	GLN
1	C	203	HIS
1	C	222	GLN
1	C	242	GLN
1	C	341	GLN
1	D	203	HIS
1	D	222	GLN
1	D	242	GLN
1	D	341	GLN
1	E	203	HIS
1	E	222	GLN
1	E	242	GLN
1	E	393	GLN
1	F	203	HIS
1	F	222	GLN
1	F	242	GLN
1	F	294	ASN
1	F	295	GLN
1	F	393	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
3	PLP	F	1001	1	15,15,16	1.28	2 (13%)	20,22,23	1.13	2 (10%)
3	PLP	C	1001	1	15,15,16	1.21	0	20,22,23	1.11	2 (10%)
2	HEM	B	501	1	41,50,50	1.75	7 (17%)	45,82,82	1.32	7 (15%)
3	PLP	E	1001	1	15,15,16	1.51	1 (6%)	20,22,23	1.10	1 (5%)
2	HEM	D	501	1	41,50,50	1.76	7 (17%)	45,82,82	1.33	7 (15%)
2	HEM	C	501	1	41,50,50	1.75	9 (21%)	45,82,82	1.35	7 (15%)
2	HEM	E	501	1	41,50,50	1.75	8 (19%)	45,82,82	1.38	6 (13%)
2	HEM	A	501	1	41,50,50	1.79	9 (21%)	45,82,82	1.34	7 (15%)
3	PLP	B	1001	1	15,15,16	1.24	1 (6%)	20,22,23	1.11	1 (5%)
2	HEM	F	501	1	41,50,50	1.76	8 (19%)	45,82,82	1.38	6 (13%)
3	PLP	D	1001	1	15,15,16	1.26	1 (6%)	20,22,23	1.11	1 (5%)
3	PLP	A	1001	1	15,15,16	1.29	2 (13%)	20,22,23	1.16	1 (5%)

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
3	PLP	F	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	B	501	1	-	4/12/54/54	-
3	PLP	E	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	D	501	1	-	4/12/54/54	-
2	HEM	C	501	1	-	4/12/54/54	-
2	HEM	E	501	1	-	4/12/54/54	-
2	HEM	A	501	1	-	4/12/54/54	-
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	F	501	1	-	4/12/54/54	-
3	PLP	D	1001	1	-	0/6/6/8	0/1/1/1
3	PLP	A	1001	1	-	0/6/6/8	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CBB-CAB	4.97	1.54	1.30
2	D	501	HEM	CBB-CAB	4.95	1.54	1.30
2	A	501	HEM	CBB-CAB	4.91	1.54	1.30
2	C	501	HEM	CBB-CAB	4.89	1.54	1.30
2	E	501	HEM	CBB-CAB	4.85	1.54	1.30
2	F	501	HEM	CBB-CAB	4.80	1.54	1.30
2	E	501	HEM	C3C-CAC	4.48	1.57	1.47
2	C	501	HEM	C3C-CAC	4.36	1.56	1.47
2	A	501	HEM	C3C-CAC	4.33	1.56	1.47
2	D	501	HEM	C3C-CAC	4.24	1.56	1.47
2	F	501	HEM	C3C-CAC	4.17	1.56	1.47
3	E	1001	PLP	C3-C2	-4.14	1.36	1.40
2	B	501	HEM	C3C-CAC	3.80	1.55	1.47
2	A	501	HEM	CBC-CAC	3.72	1.54	1.29
2	D	501	HEM	CBC-CAC	3.63	1.53	1.29
2	F	501	HEM	CBC-CAC	3.61	1.53	1.29
2	E	501	HEM	CBC-CAC	3.60	1.53	1.29
2	C	501	HEM	CBC-CAC	3.60	1.53	1.29
2	B	501	HEM	CBC-CAC	3.51	1.52	1.29
2	B	501	HEM	C3C-C2C	-3.29	1.35	1.40
2	F	501	HEM	C3C-C2C	-3.27	1.35	1.40
2	A	501	HEM	CAB-C3B	3.18	1.56	1.47
2	F	501	HEM	CAB-C3B	3.03	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CAB-C3B	2.87	1.55	1.47
2	E	501	HEM	CAB-C3B	2.77	1.55	1.47
2	D	501	HEM	CAB-C3B	2.65	1.54	1.47
2	A	501	HEM	C3C-C2C	-2.60	1.36	1.40
2	C	501	HEM	CAB-C3B	2.56	1.54	1.47
2	E	501	HEM	C2C-C1C	2.37	1.47	1.42
2	F	501	HEM	C2C-C1C	2.36	1.47	1.42
2	A	501	HEM	C2C-C1C	2.34	1.47	1.42
2	D	501	HEM	C3C-C2C	-2.32	1.37	1.40
2	D	501	HEM	C2C-C1C	2.30	1.47	1.42
3	F	1001	PLP	C3-C2	-2.29	1.38	1.40
2	E	501	HEM	C3C-C2C	-2.27	1.37	1.40
2	D	501	HEM	O2A-CGA	-2.27	1.23	1.30
3	D	1001	PLP	C3-C2	-2.25	1.38	1.40
2	A	501	HEM	O1A-CGA	2.23	1.29	1.22
2	B	501	HEM	C2C-C1C	2.23	1.47	1.42
2	B	501	HEM	O2A-CGA	-2.22	1.23	1.30
3	A	1001	PLP	C3-C2	-2.22	1.38	1.40
3	F	1001	PLP	P-O3P	-2.22	1.46	1.54
3	B	1001	PLP	P-O3P	-2.21	1.46	1.54
2	E	501	HEM	O1A-CGA	2.19	1.29	1.22
3	A	1001	PLP	C2-N1	2.19	1.38	1.33
2	C	501	HEM	O1A-CGA	2.17	1.29	1.22
2	F	501	HEM	CBD-CAD	2.15	1.58	1.52
2	A	501	HEM	C4A-CHB	-2.15	1.35	1.41
2	C	501	HEM	CBD-CAD	2.13	1.58	1.52
2	F	501	HEM	O2A-CGA	-2.13	1.23	1.30
2	C	501	HEM	C2C-C1C	2.12	1.47	1.42
2	E	501	HEM	CMC-C2C	2.11	1.56	1.51
2	C	501	HEM	O2A-CGA	-2.10	1.23	1.30
2	C	501	HEM	CMC-C2C	2.04	1.56	1.51
2	A	501	HEM	CMC-C2C	2.01	1.56	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	HEM	C4C-CHD-C1D	4.23	128.13	122.56
2	E	501	HEM	C4C-CHD-C1D	4.08	127.95	122.56
2	A	501	HEM	C4C-CHD-C1D	3.98	127.82	122.56
2	D	501	HEM	C4C-CHD-C1D	3.98	127.81	122.56
2	B	501	HEM	C4C-CHD-C1D	3.89	127.70	122.56
2	C	501	HEM	C4C-CHD-C1D	3.89	127.69	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	HEM	CMC-C2C-C3C	3.45	131.13	124.68
2	D	501	HEM	CMC-C2C-C3C	3.31	130.87	124.68
2	C	501	HEM	CMC-C2C-C3C	3.26	130.78	124.68
2	A	501	HEM	CMC-C2C-C3C	3.23	130.72	124.68
2	E	501	HEM	C4B-CHC-C1C	3.09	126.63	122.56
2	F	501	HEM	CMC-C2C-C3C	3.08	130.43	124.68
2	B	501	HEM	CMC-C2C-C3C	3.02	130.33	124.68
2	A	501	HEM	C4B-CHC-C1C	2.98	126.50	122.56
2	F	501	HEM	C4B-CHC-C1C	2.96	126.46	122.56
2	B	501	HEM	C4B-CHC-C1C	2.95	126.45	122.56
2	C	501	HEM	C4B-CHC-C1C	2.84	126.31	122.56
2	D	501	HEM	C4B-CHC-C1C	2.83	126.29	122.56
2	C	501	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
2	F	501	HEM	CMA-C3A-C4A	-2.80	124.17	128.46
2	D	501	HEM	CMA-C3A-C4A	-2.76	124.23	128.46
2	F	501	HEM	O1A-CGA-CBA	-2.72	114.33	123.08
2	B	501	HEM	CMA-C3A-C4A	-2.72	124.28	128.46
2	E	501	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
3	B	1001	PLP	O3P-P-O1P	2.63	120.96	110.68
2	A	501	HEM	O1A-CGA-CBA	-2.59	114.77	123.08
2	E	501	HEM	O1A-CGA-CBA	-2.58	114.79	123.08
2	C	501	HEM	O1A-CGA-CBA	-2.58	114.81	123.08
2	B	501	HEM	O1A-CGA-CBA	-2.55	114.89	123.08
3	C	1001	PLP	O3P-P-O1P	2.54	120.61	110.68
3	E	1001	PLP	O3P-P-O1P	2.53	120.60	110.68
3	F	1001	PLP	O3P-P-O1P	2.53	120.58	110.68
2	A	501	HEM	CBB-CAB-C3B	-2.52	115.09	127.62
2	C	501	HEM	CBB-CAB-C3B	-2.52	115.11	127.62
3	A	1001	PLP	O3P-P-O1P	2.51	120.53	110.68
2	E	501	HEM	CBB-CAB-C3B	-2.50	115.16	127.62
3	D	1001	PLP	O3P-P-O1P	2.50	120.49	110.68
2	F	501	HEM	CBB-CAB-C3B	-2.46	115.38	127.62
2	D	501	HEM	O1A-CGA-CBA	-2.42	115.31	123.08
2	B	501	HEM	CBB-CAB-C3B	-2.39	115.75	127.62
2	A	501	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
2	D	501	HEM	CBB-CAB-C3B	-2.36	115.89	127.62
2	A	501	HEM	CBA-CAA-C2A	2.20	116.37	112.62
2	D	501	HEM	CBA-CAA-C2A	2.12	116.24	112.62
3	C	1001	PLP	O4P-C5A-C5	2.11	113.37	109.35
2	B	501	HEM	CBA-CAA-C2A	2.08	116.17	112.62
2	C	501	HEM	CBA-CAA-C2A	2.04	116.11	112.62
3	F	1001	PLP	C5-C6-N1	-2.01	120.48	123.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C2B-C3B-CAB-CBB
2	D	501	HEM	C2B-C3B-CAB-CBB
2	E	501	HEM	C2B-C3B-CAB-CBB
2	F	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAA-CBA-CGA-O2A
2	C	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAA-CBA-CGA-O1A
2	F	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	F	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
2	E	501	HEM	C4B-C3B-CAB-CBB
2	F	501	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1001	PLP	1	0
3	C	1001	PLP	1	0
2	B	501	HEM	2	0
3	E	1001	PLP	1	0
2	D	501	HEM	3	0
2	C	501	HEM	2	0
2	E	501	HEM	2	0
2	A	501	HEM	4	0
3	B	1001	PLP	1	0
2	F	501	HEM	3	0
3	D	1001	PLP	1	0

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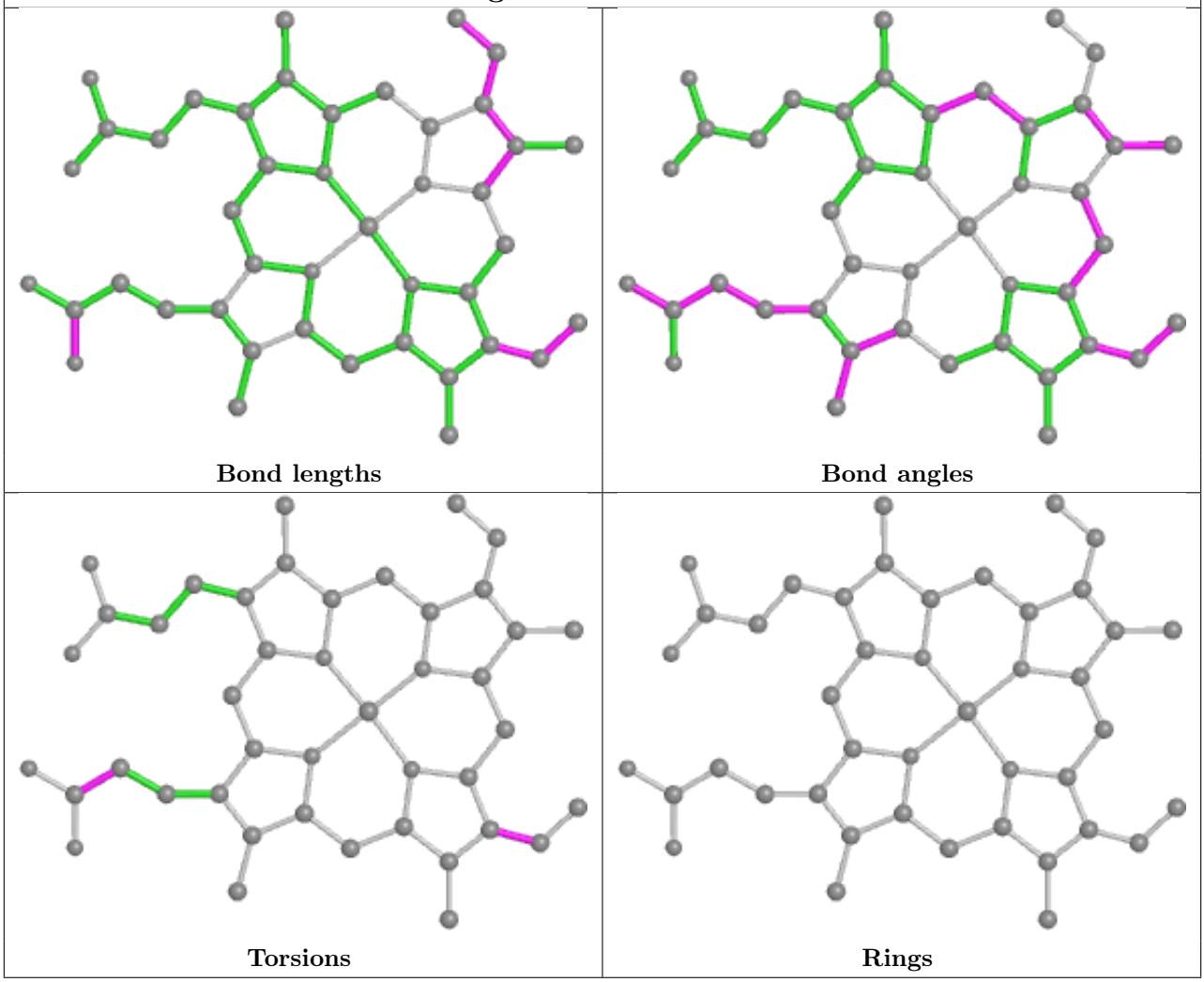
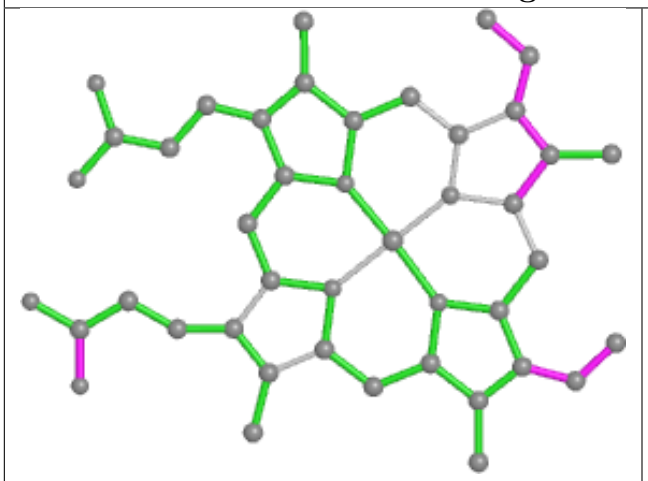
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PLP	1	0

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.

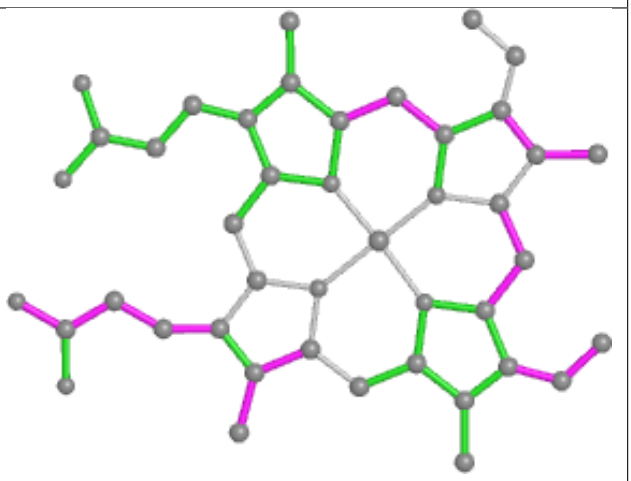
Ligand HEM B 501



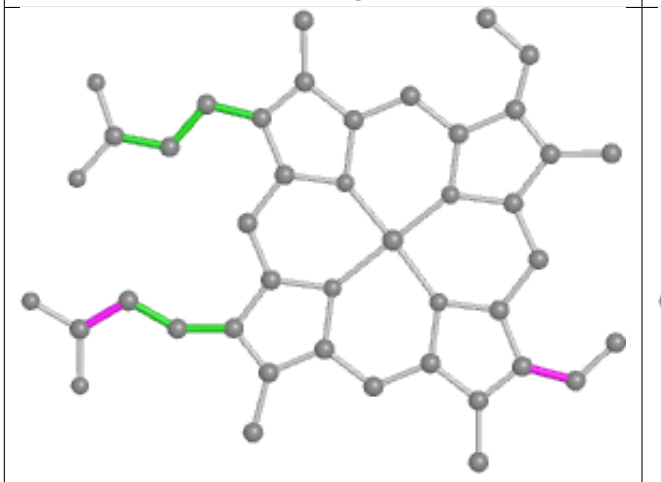
Ligand HEM D 501



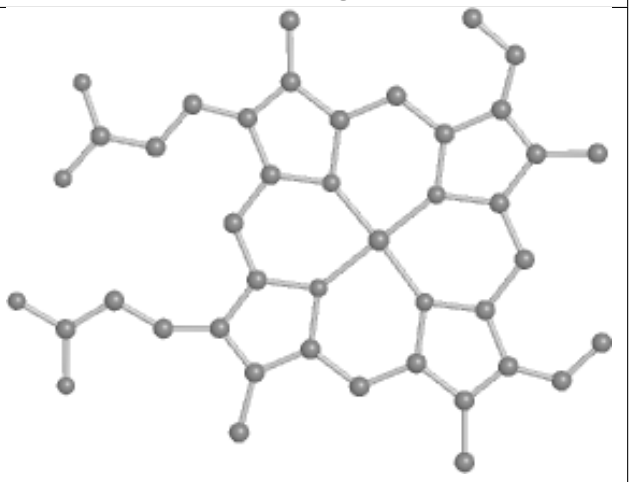
Bond lengths



Bond angles

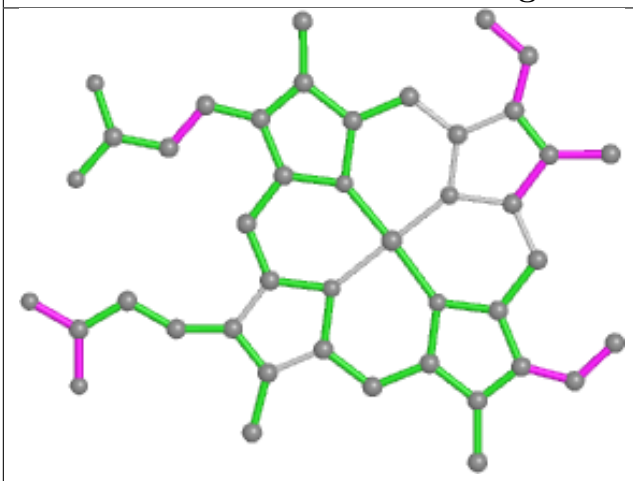


Torsions

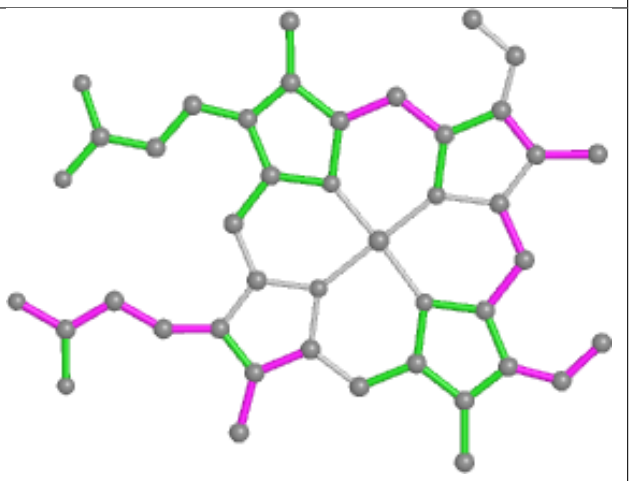


Rings

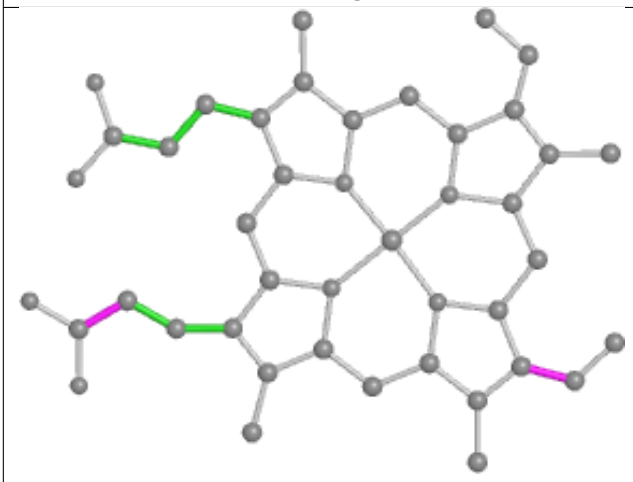
Ligand HEM C 501



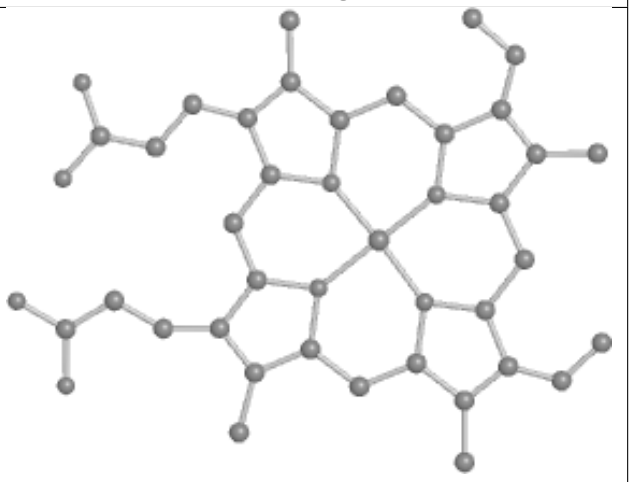
Bond lengths



Bond angles

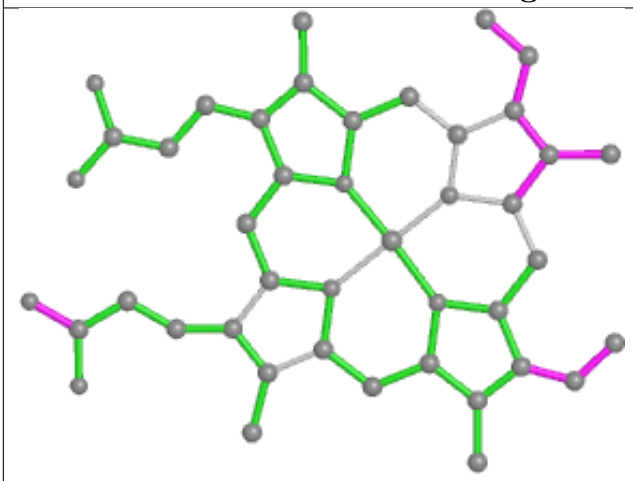


Torsions

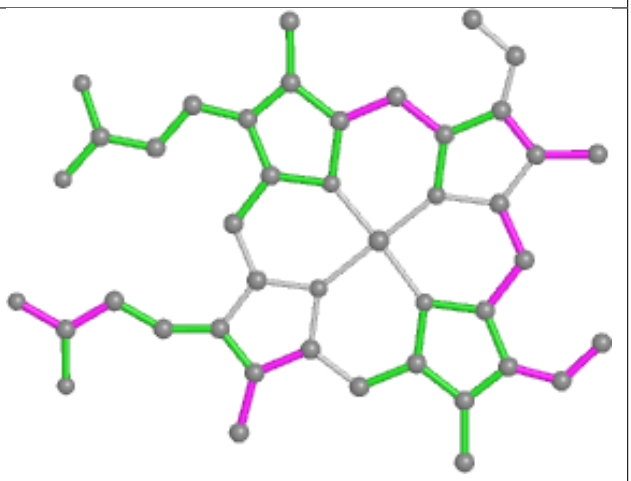


Rings

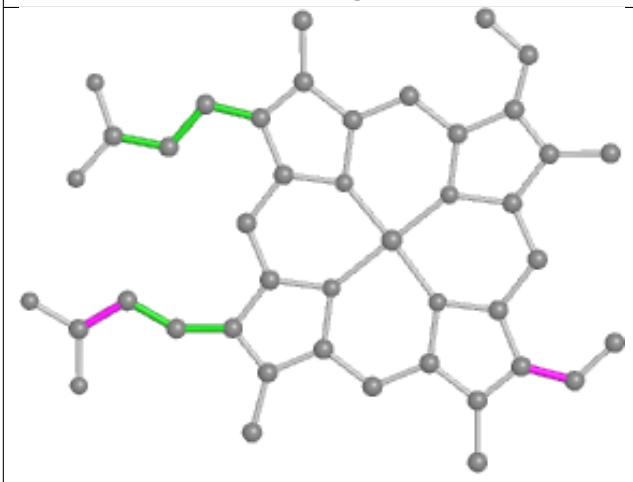
Ligand HEM E 501



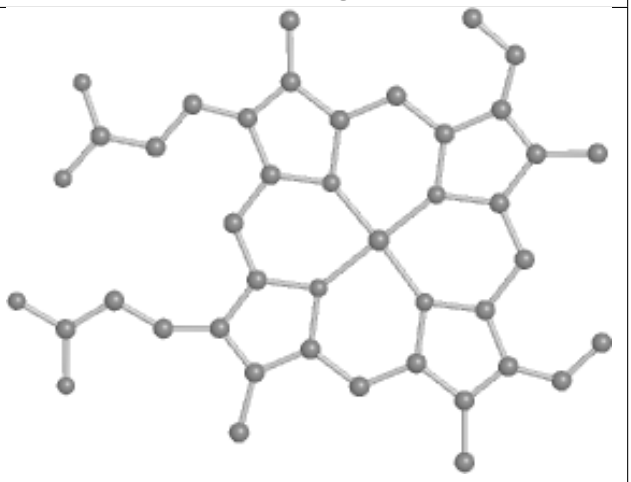
Bond lengths



Bond angles

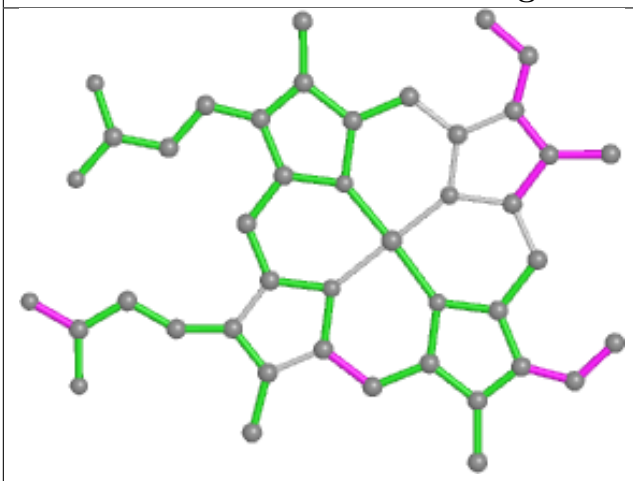


Torsions

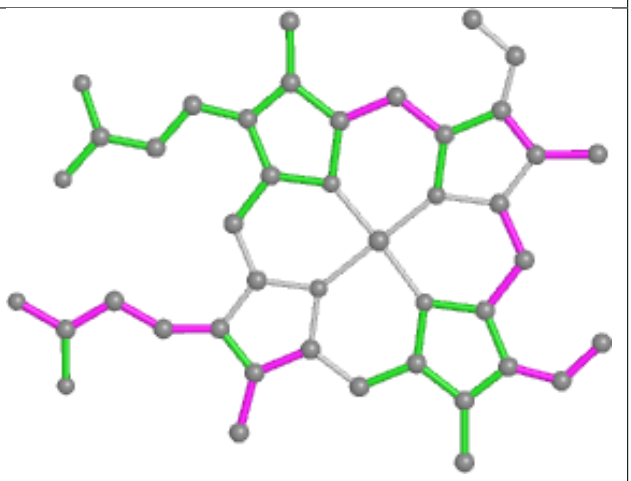


Rings

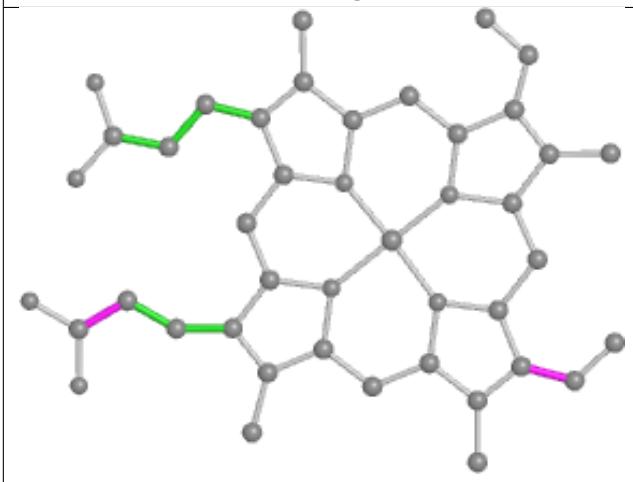
Ligand HEM A 501



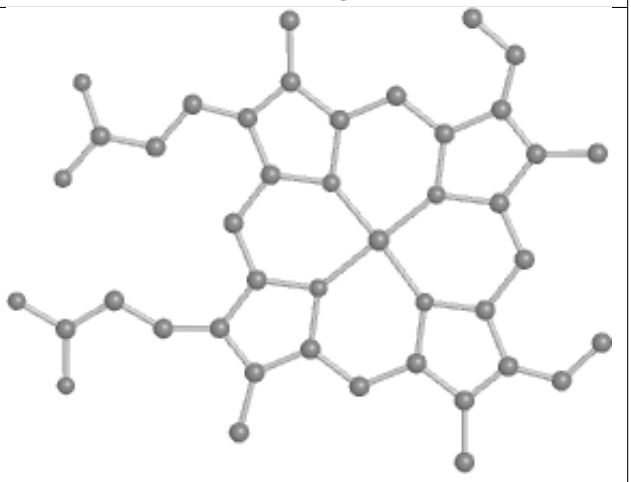
Bond lengths



Bond angles

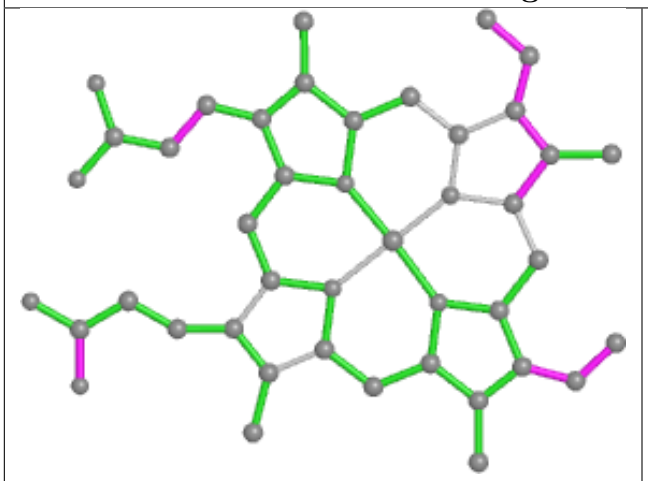


Torsions

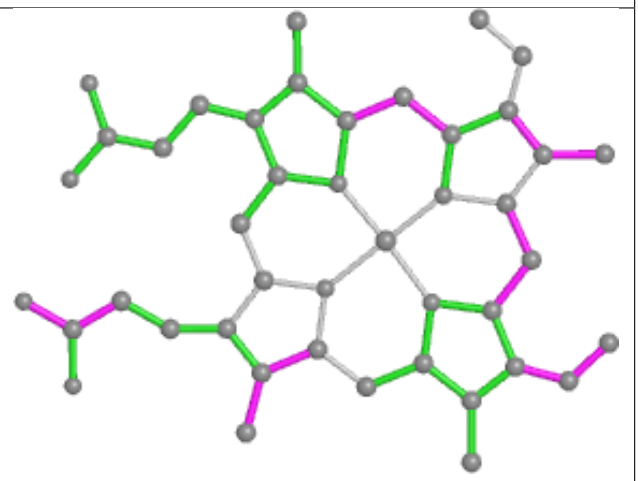


Rings

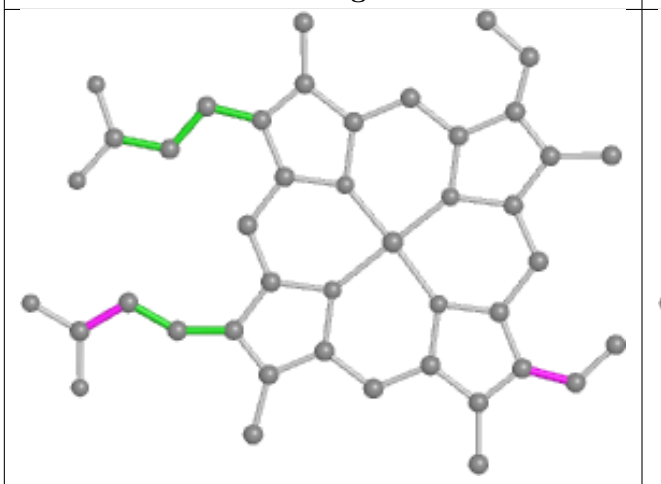
Ligand HEM F 501



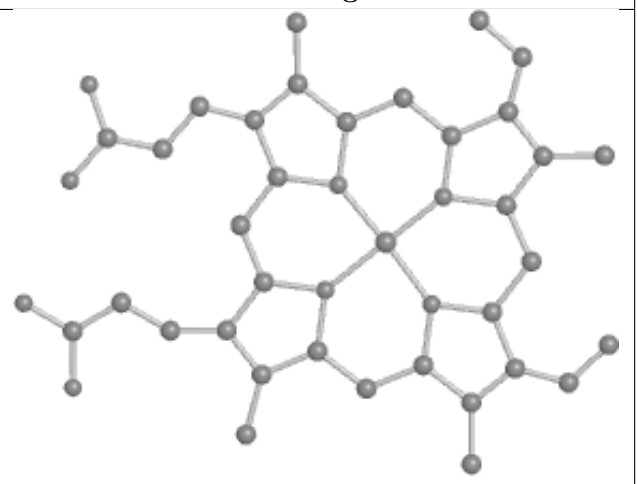
Bond lengths



Bond angles



Torsions



Rings

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	348/435 (80%)	0.21	15 (4%)	35	28	12, 32, 66, 85	0
1	B	348/435 (80%)	0.61	36 (10%)	6	4	9, 35, 75, 94	0
1	C	348/435 (80%)	0.44	26 (7%)	14	10	15, 36, 72, 87	0
1	D	348/435 (80%)	0.46	27 (7%)	13	9	17, 39, 76, 92	0
1	E	350/435 (80%)	0.15	16 (4%)	32	26	9, 27, 67, 90	0
1	F	348/435 (80%)	0.08	16 (4%)	32	26	9, 26, 67, 89	0
All	All	2090/2610 (80%)	0.32	136 (6%)	18	14	9, 33, 72, 94	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	THR	9.7
1	E	193	THR	6.7
1	B	43	TRP	6.3
1	F	147	SER	6.3
1	D	392	LEU	6.1
1	D	43	TRP	5.9
1	C	212	ASN	5.9
1	B	297	GLU	5.6
1	D	44	ILE	5.4
1	C	208	TRP	5.3
1	B	170	PRO	5.2
1	B	46	PRO	5.1
1	B	192	PRO	5.1
1	D	191	THR	5.1
1	B	212	ASN	5.1
1	A	299	THR	5.0
1	D	53	THR	4.9
1	B	191	THR	4.9
1	D	52	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	47	ASP	4.6
1	E	170	PRO	4.5
1	B	311	ILE	4.5
1	E	172	LYS	4.5
1	B	299	THR	4.3
1	D	193	THR	4.2
1	B	202	SER	4.2
1	E	43	TRP	4.2
1	E	192	PRO	4.2
1	C	192	PRO	4.2
1	C	50	SER	4.1
1	A	43	TRP	4.1
1	B	226	ALA	4.1
1	B	214	ILE	4.1
1	B	147	SER	4.0
1	B	171	GLU	4.0
1	F	43	TRP	4.0
1	B	313	THR	4.0
1	F	192	PRO	3.9
1	D	292	GLU	3.9
1	C	46	PRO	3.9
1	F	389	ARG	3.8
1	D	192	PRO	3.8
1	E	44	ILE	3.8
1	C	389	ARG	3.7
1	E	171	GLU	3.7
1	D	171	GLU	3.7
1	C	297	GLU	3.7
1	A	192	PRO	3.6
1	C	49	PRO	3.6
1	E	57	GLY	3.6
1	A	44	ILE	3.6
1	F	208	TRP	3.5
1	B	209	ARG	3.5
1	A	295	GLN	3.5
1	B	169	MET	3.3
1	C	191	THR	3.3
1	B	213	GLU	3.3
1	B	175	SER	3.3
1	D	299	THR	3.3
1	A	171	GLU	3.3
1	D	297	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	191	THR	3.3
1	F	46	PRO	3.3
1	D	397	LEU	3.2
1	A	45	ARG	3.2
1	B	312	PRO	3.2
1	C	393	GLN	3.2
1	E	203	HIS	3.2
1	B	49	PRO	3.2
1	F	45	ARG	3.1
1	D	396	PHE	3.0
1	F	190	ARG	3.0
1	C	190	ARG	3.0
1	A	209	ARG	3.0
1	D	393	GLN	3.0
1	C	299	THR	3.0
1	B	203	HIS	2.9
1	E	212	ASN	2.9
1	A	297	GLU	2.9
1	E	204	VAL	2.9
1	D	51	ARG	2.9
1	B	172	LYS	2.8
1	C	171	GLU	2.8
1	C	223	TYR	2.8
1	B	290	PRO	2.8
1	A	59	PRO	2.8
1	D	295	GLN	2.7
1	B	296	THR	2.7
1	E	45	ARG	2.7
1	D	57	GLY	2.7
1	C	147	SER	2.6
1	B	148	GLY	2.6
1	C	214	ILE	2.6
1	F	171	GLU	2.6
1	D	389	ARG	2.5
1	D	45	ARG	2.5
1	B	211	LYS	2.5
1	B	48	ALA	2.5
1	F	44	ILE	2.5
1	E	52	CYS	2.5
1	B	295	GLN	2.4
1	C	168	VAL	2.4
1	F	202	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	52	CYS	2.4
1	E	55	GLN	2.4
1	F	299	THR	2.4
1	A	293	LEU	2.3
1	A	215	PRO	2.3
1	B	47	ASP	2.3
1	E	209	ARG	2.3
1	E	47	ASP	2.3
1	C	189	VAL	2.3
1	C	162	GLY	2.3
1	A	206	VAL	2.3
1	D	201	GLU	2.3
1	A	210	LEU	2.3
1	D	290	PRO	2.2
1	F	212	ASN	2.2
1	D	283	GLU	2.2
1	C	56	LEU	2.2
1	C	145	PRO	2.2
1	B	51	ARG	2.1
1	D	310	PHE	2.1
1	D	395	GLY	2.1
1	B	173	MET	2.1
1	C	169	MET	2.1
1	C	209	ARG	2.1
1	C	310	PHE	2.1
1	D	61	SER	2.1
1	F	393	GLN	2.1
1	B	87	THR	2.1
1	F	296	THR	2.1
1	C	146	THR	2.1
1	B	292	GLU	2.0
1	B	145	PRO	2.0
1	D	329	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

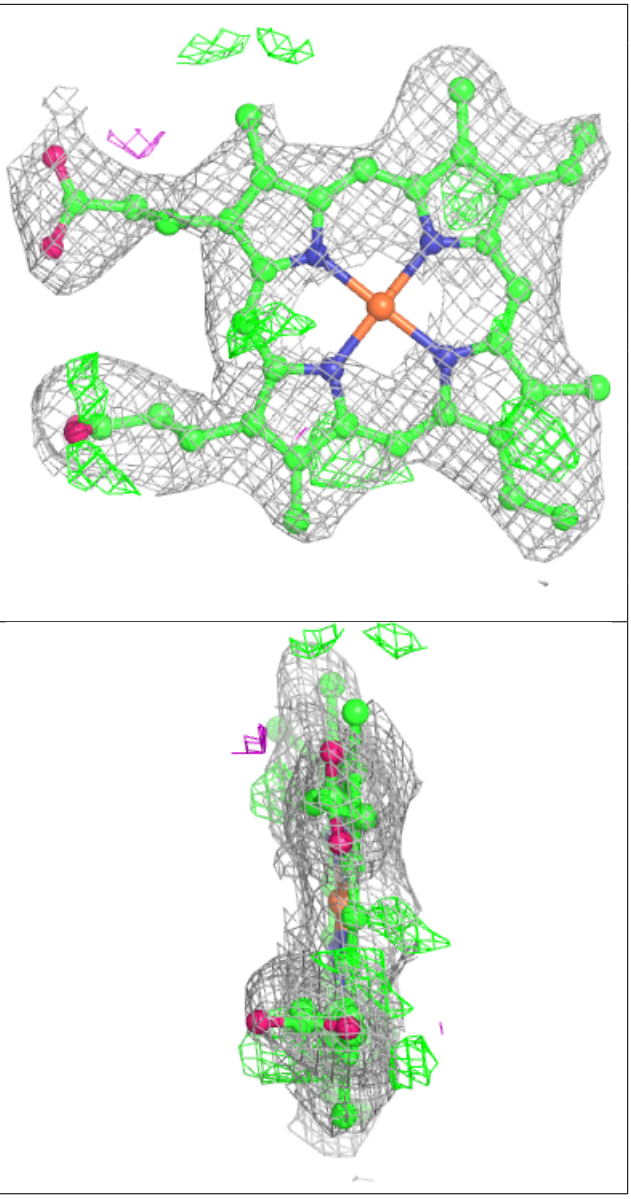
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	501	43/43	0.89	0.20	17,38,45,48	0
2	HEM	C	501	43/43	0.90	0.26	17,37,49,61	0
2	HEM	A	501	43/43	0.91	0.18	5,31,43,52	0
2	HEM	D	501	43/43	0.91	0.26	17,45,54,64	0
2	HEM	F	501	43/43	0.94	0.17	5,25,40,51	0
3	PLP	B	1001	15/16	0.94	0.18	2,15,25,26	0
2	HEM	E	501	43/43	0.95	0.15	8,27,42,48	0
3	PLP	C	1001	15/16	0.95	0.17	11,22,25,28	0
3	PLP	D	1001	15/16	0.95	0.15	15,22,31,32	0
3	PLP	A	1001	15/16	0.96	0.14	2,19,29,30	0
3	PLP	E	1001	15/16	0.97	0.16	2,12,18,23	0
3	PLP	F	1001	15/16	0.97	0.15	4,11,17,25	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.

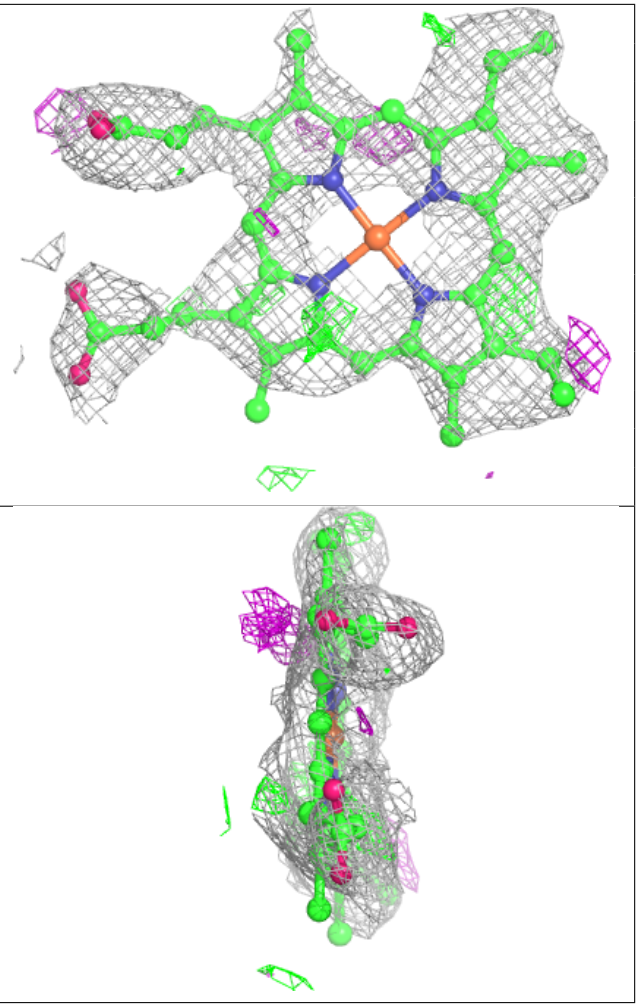
Electron density around HEM B 501:

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



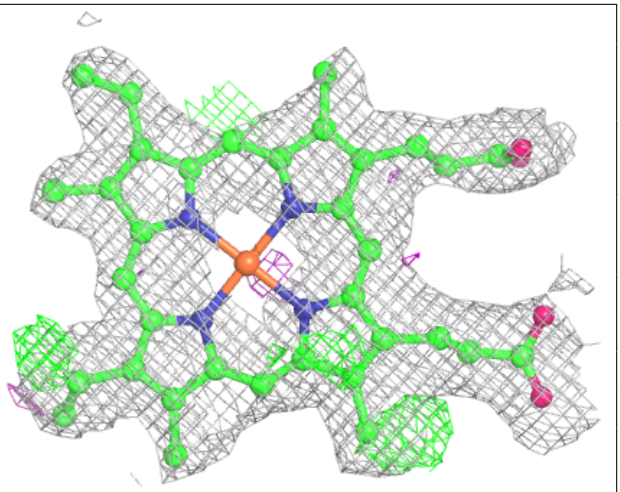
Electron density around HEM C 501:

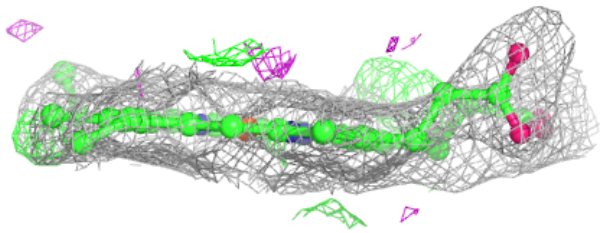
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

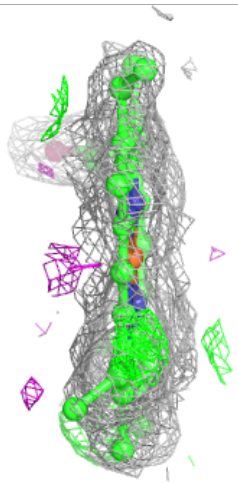


Electron density around HEM A 501:

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

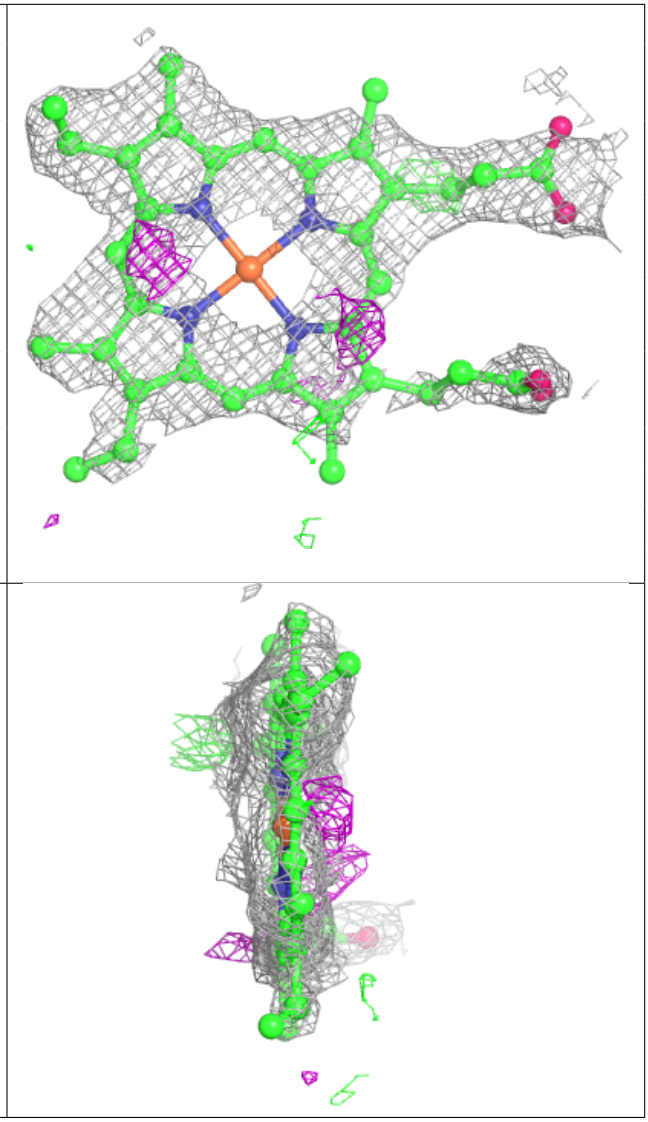






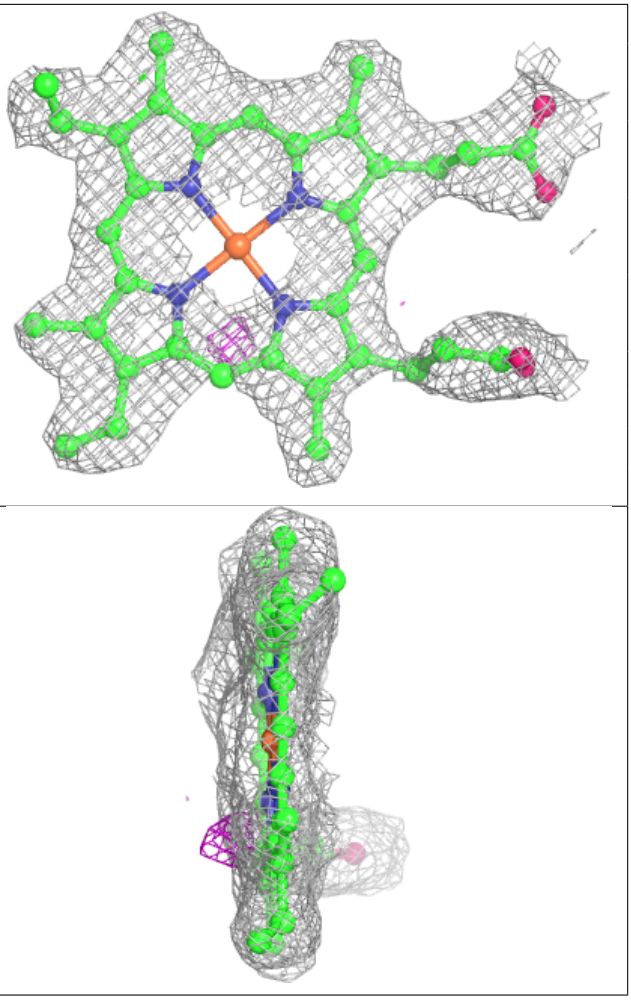
Electron density around HEM D 501:

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



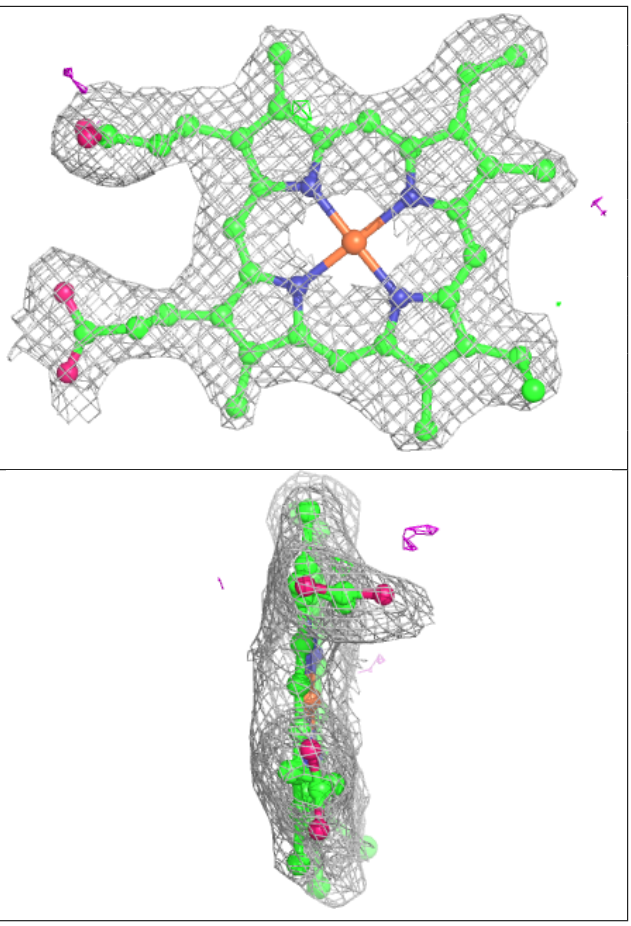
Electron density around HEM F 501:

$2mF_o$-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 E 501:

$2mF_o$-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.