Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 01:24 PM EDT

PDB ID	:	2NW7
Title	:	Crystal Structure of Tryptophan 2,3-dioxygenase (TDO) from Xanthomonas campestris in complex with ferric heme. Northeast Structural Genomics Target XcR13
Authors	:	Forouhar, F.; Anderson, J.L.R.; Mowat, C.G.; Hussain, A.; Bruckmann, C.; Thackray, S.J.; Seetharaman, J.; Tucker, T.; Ho, C.K.; Ma, L.C.; Cunningham, K.; Janjua, H.; Zhao, L.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Chapman, S.K.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2006-11-14
Resolution	:	2.70 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 (1)) were used in the production of this report:

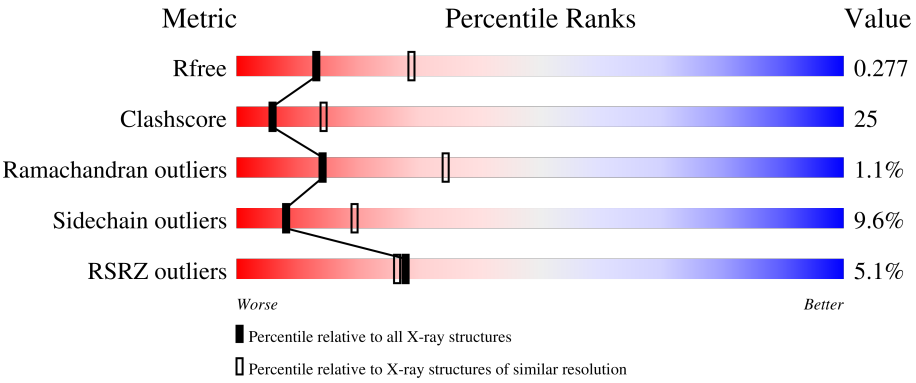
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	306	5% 40% 40% 5% 15%
1	B	306	3% 44% 36% · 15%

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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

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Mol	Chain	Length	Quality of chain
1	C	306	6% 45% 35% 15%
1	D	306	3% 44% 33% 8% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8957 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2158	1387	380	384	7			
1	B	259	Total	C	N	O	S	0	0	0
			2158	1387	380	384	7			
1	C	259	Total	C	N	O	S	0	0	0
			2158	1387	380	384	7			
1	D	260	Total	C	N	O	S	0	0	0
			2169	1393	384	385	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	LEU	-	cloning artifact	UNP Q8PDA8
A	300	GLU	-	cloning artifact	UNP Q8PDA8
A	301	HIS	-	cloning artifact	UNP Q8PDA8
A	302	HIS	-	cloning artifact	UNP Q8PDA8
A	303	HIS	-	cloning artifact	UNP Q8PDA8
A	304	HIS	-	cloning artifact	UNP Q8PDA8
A	305	HIS	-	cloning artifact	UNP Q8PDA8
A	306	HIS	-	cloning artifact	UNP Q8PDA8
B	299	LEU	-	cloning artifact	UNP Q8PDA8
B	300	GLU	-	cloning artifact	UNP Q8PDA8
B	301	HIS	-	cloning artifact	UNP Q8PDA8
B	302	HIS	-	cloning artifact	UNP Q8PDA8
B	303	HIS	-	cloning artifact	UNP Q8PDA8
B	304	HIS	-	cloning artifact	UNP Q8PDA8
B	305	HIS	-	cloning artifact	UNP Q8PDA8
B	306	HIS	-	cloning artifact	UNP Q8PDA8
C	299	LEU	-	cloning artifact	UNP Q8PDA8
C	300	GLU	-	cloning artifact	UNP Q8PDA8
C	301	HIS	-	cloning artifact	UNP Q8PDA8
C	302	HIS	-	cloning artifact	UNP Q8PDA8
C	303	HIS	-	cloning artifact	UNP Q8PDA8

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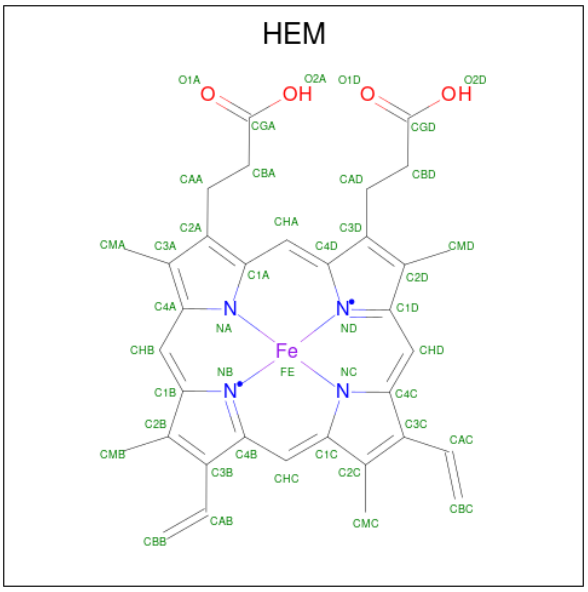
Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	cloning artifact	UNP Q8PDA8
C	305	HIS	-	cloning artifact	UNP Q8PDA8
C	306	HIS	-	cloning artifact	UNP Q8PDA8
D	299	LEU	-	cloning artifact	UNP Q8PDA8
D	300	GLU	-	cloning artifact	UNP Q8PDA8
D	301	HIS	-	cloning artifact	UNP Q8PDA8
D	302	HIS	-	cloning artifact	UNP Q8PDA8
D	303	HIS	-	cloning artifact	UNP Q8PDA8
D	304	HIS	-	cloning artifact	UNP Q8PDA8
D	305	HIS	-	cloning artifact	UNP Q8PDA8
D	306	HIS	-	cloning artifact	UNP Q8PDA8

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

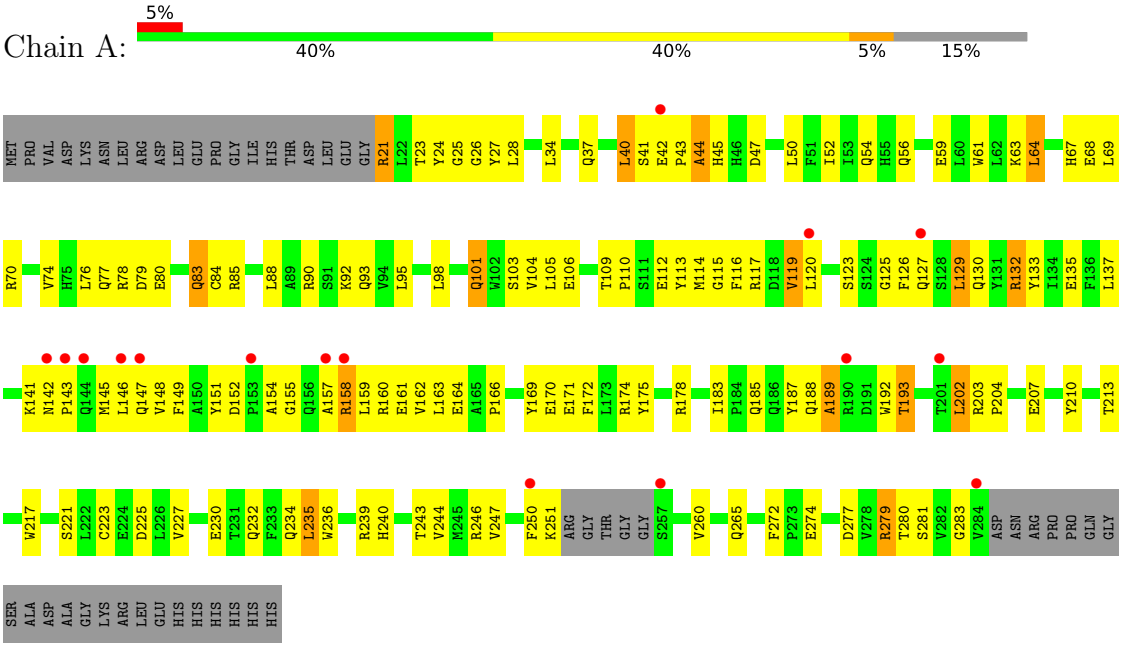
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0
3	B	44	Total O 44 44	0	0
3	C	37	Total O 37 37	0	0
3	D	33	Total O 33 33	0	0

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.

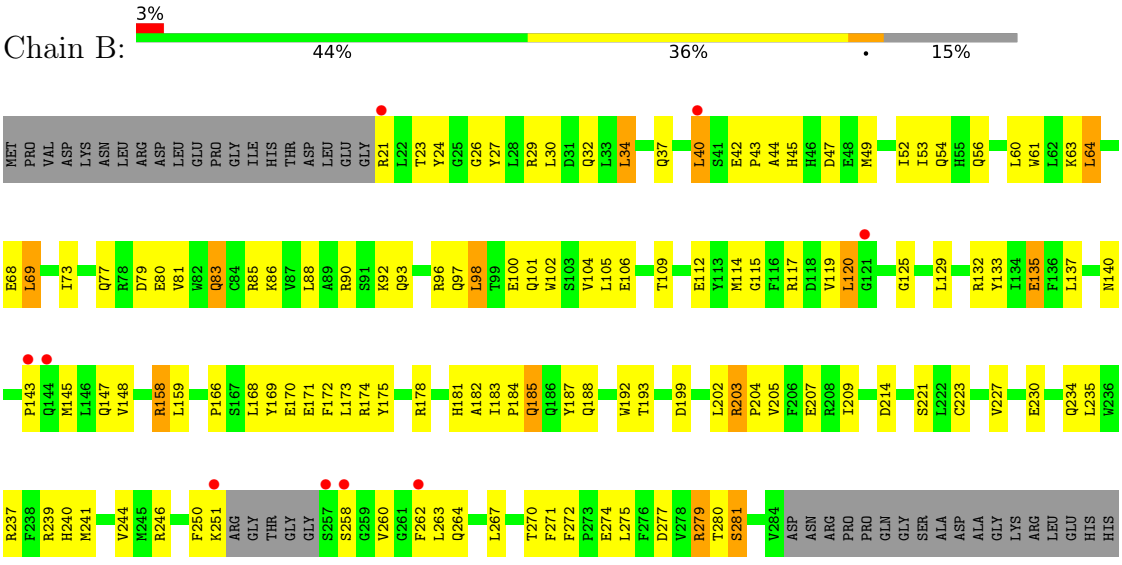
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



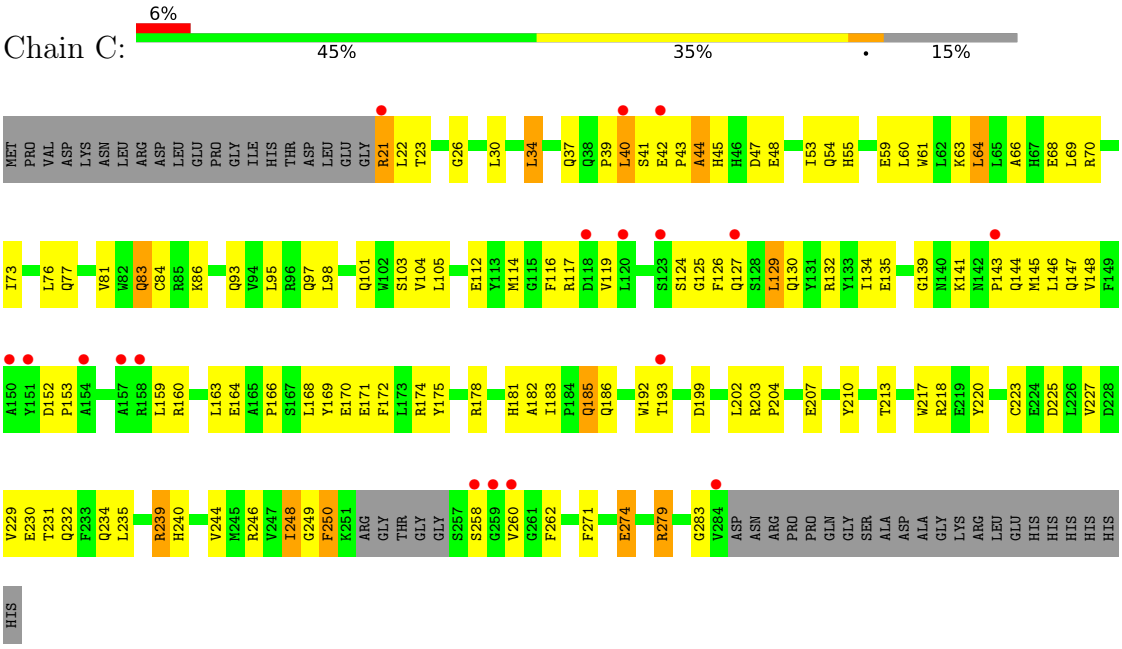
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain B:



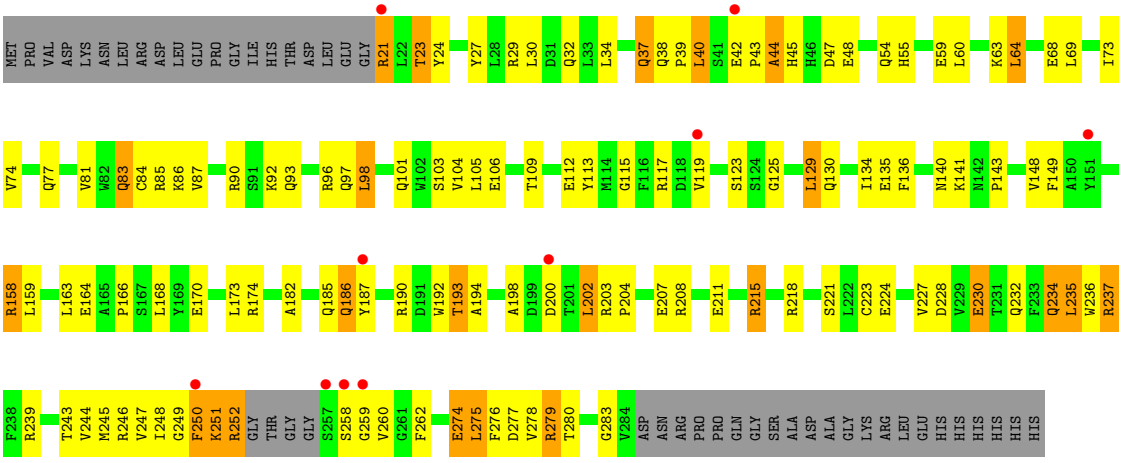
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain C:



• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.94Å 109.36Å 125.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 2.70 46.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	72.0 (46.43-2.70) 85.5 (46.43-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.263 0.273 , 0.277	Depositor DCC
R_{free} test set	3770 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8957	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 77.38 % 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 8.6044e-07. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/2213	0.60	0/2999
1	B	0.45	0/2213	0.59	0/2999
1	C	0.43	0/2213	0.58	0/2999
1	D	0.46	0/2224	0.60	0/3013
All	All	0.44	0/8863	0.59	0/12010

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2158	0	2117	133	0
1	B	2158	0	2117	118	0
1	C	2158	0	2117	116	0
1	D	2169	0	2130	119	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	9	0
2	D	43	0	30	9	0
3	A	28	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	0	5	0
3	C	37	0	0	2	0
3	D	33	0	0	2	0
All	All	8957	0	8601	436	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 25.

All (436) 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:D:105:LEU:HD23	1:D:243:THR:HG21	1.45	0.98
1:A:143:PRO:HG3	1:A:193:THR:HG22	1.43	0.97
1:C:250:PHE:HA	1:C:260:VAL:HG11	1.47	0.96
1:C:83:GLN:HE21	1:C:83:GLN:H	0.99	0.96
2:C:401:HEM:HBC2	2:C:401:HEM:HHD	1.45	0.96
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.45	0.96
1:A:250:PHE:HA	1:A:260:VAL:HG11	1.49	0.95
1:B:54:GLN:HG2	1:B:105:LEU:HD22	1.55	0.88
1:D:250:PHE:HA	1:D:260:VAL:HG11	1.53	0.87
1:B:83:GLN:H	1:B:83:GLN:HE21	1.23	0.87
1:A:101:GLN:O	1:A:104:VAL:HG12	1.77	0.84
1:A:279:ARG:HD3	1:C:246:ARG:O	1.80	0.81
1:B:100:GLU:HG3	1:C:97:GLN:HE22	1.45	0.81
1:B:45:HIS:HD2	1:B:47:ASP:H	1.26	0.81
1:A:42:GLU:HB2	1:A:43:PRO:HD3	1.63	0.81
1:D:42:GLU:HB2	1:D:43:PRO:HD3	1.61	0.81
1:B:23:THR:HG22	1:B:26:GLY:H	1.43	0.80
1:D:83:GLN:H	1:D:83:GLN:HE21	1.27	0.80
1:B:23:THR:HG23	1:C:127:GLN:HE22	1.47	0.79
1:D:29:ARG:HE	1:D:32:GLN:NE2	1.82	0.78
1:A:93:GLN:NE2	1:D:103:SER:HB3	1.99	0.77
1:C:73:ILE:O	1:C:77:GLN:HG3	1.84	0.77
1:B:29:ARG:HE	1:B:32:GLN:HE21	1.33	0.77
1:C:223:CYS:O	1:C:227:VAL:HG23	1.84	0.77
1:A:155:GLY:HA2	1:A:158:ARG:HE	1.49	0.76
1:A:235:LEU:HD11	1:C:239:ARG:HD3	1.66	0.76
1:C:83:GLN:HE21	1:C:83:GLN:N	1.81	0.76
1:D:105:LEU:HD21	2:D:401:HEM:HAB	1.67	0.76
1:B:73:ILE:O	1:B:77:GLN:HG3	1.86	0.76
1:B:29:ARG:HE	1:B:32:GLN:NE2	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:MET:O	1:C:148:VAL:HG22	1.86	0.75
1:C:42:GLU:HB2	1:C:43:PRO:HD3	1.67	0.75
1:C:178:ARG:HH11	1:C:178:ARG:HB2	1.51	0.75
1:C:105:LEU:HD21	2:C:401:HEM:HAB	1.70	0.74
1:A:105:LEU:HD21	2:A:401:HEM:HAB	1.68	0.73
2:D:401:HEM:HHA	2:D:401:HEM:HBA2	1.70	0.73
1:B:246:ARG:O	1:D:279:ARG:HD3	1.89	0.72
1:D:135:GLU:HG3	1:D:140:ASN:HB3	1.72	0.72
2:C:401:HEM:HBA2	2:C:401:HEM:HHA	1.70	0.72
1:B:93:GLN:NE2	1:C:103:SER:HB3	2.04	0.71
1:A:246:ARG:O	1:C:279:ARG:HD3	1.89	0.71
1:A:175:TYR:HA	1:A:178:ARG:NH1	2.06	0.71
1:B:240:HIS:O	1:B:244:VAL:HG23	1.91	0.70
1:C:45:HIS:HD2	1:C:47:ASP:H	1.40	0.70
1:B:239:ARG:HD3	1:D:235:LEU:HD11	1.72	0.70
1:A:74:VAL:HA	1:A:77:GLN:OE1	1.92	0.69
1:D:158:ARG:HG2	1:D:158:ARG:HH21	1.57	0.69
1:B:63:LYS:NZ	1:C:37:GLN:HE21	1.89	0.69
1:A:155:GLY:HA2	1:A:158:ARG:NE	2.08	0.69
1:B:105:LEU:HD21	2:B:401:HEM:HAB	1.76	0.69
1:B:49:MET:HB3	3:B:411:HOH:O	1.92	0.68
1:A:63:LYS:HZ3	1:D:37:GLN:HE21	1.40	0.68
1:D:92:LYS:HE2	1:D:228:ASP:HB2	1.75	0.68
1:B:241:MET:HE2	1:B:264:GLN:HA	1.75	0.68
1:D:203:ARG:O	1:D:207:GLU:HG3	1.94	0.68
1:A:203:ARG:NH1	1:A:277:ASP:HB3	2.09	0.68
1:C:83:GLN:H	1:C:83:GLN:NE2	1.83	0.68
1:B:63:LYS:HZ3	1:C:37:GLN:HE21	1.38	0.67
1:C:203:ARG:O	1:C:207:GLU:HG3	1.94	0.67
1:C:199:ASP:HB3	1:C:202:LEU:HD23	1.75	0.67
1:B:109:THR:OG1	1:B:112:GLU:HG3	1.94	0.67
1:A:141:LYS:HD2	1:A:163:LEU:HD12	1.75	0.67
1:C:86:LYS:HE3	3:C:431:HOH:O	1.95	0.67
1:B:239:ARG:HD2	3:B:432:HOH:O	1.94	0.66
1:A:88:LEU:O	1:A:92:LYS:HG3	1.94	0.66
1:A:243:THR:O	1:A:247:VAL:HG23	1.95	0.66
1:B:40:LEU:HD11	1:B:119:VAL:HB	1.75	0.66
1:D:101:GLN:O	1:D:104:VAL:HG12	1.95	0.66
1:A:127:GLN:HE22	1:D:23:THR:HG22	1.60	0.66
1:A:246:ARG:C	1:C:279:ARG:HD3	2.17	0.65
1:B:135:GLU:HG3	1:B:140:ASN:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PHE:HD1	1:D:251:LYS:H	1.43	0.65
1:A:80:GLU:HB3	1:A:83:GLN:NE2	2.11	0.65
1:A:230:GLU:O	1:A:234:GLN:HG2	1.97	0.64
1:B:203:ARG:HH21	1:B:203:ARG:HB2	1.62	0.64
1:A:63:LYS:NZ	1:D:37:GLN:HE21	1.96	0.64
1:B:203:ARG:O	1:B:207:GLU:HG3	1.97	0.64
1:A:109:THR:OG1	1:A:112:GLU:HG3	1.97	0.63
1:B:172:PHE:O	1:B:175:TYR:HB3	1.97	0.63
1:C:181:HIS:O	1:C:183:ILE:N	2.28	0.63
1:A:127:GLN:HE22	1:D:24:TYR:H	1.46	0.63
1:B:101:GLN:O	1:B:104:VAL:HG12	1.99	0.63
1:D:45:HIS:HD2	1:D:47:ASP:H	1.45	0.63
1:D:215:ARG:HH21	1:D:215:ARG:HG3	1.64	0.63
1:A:145:MET:O	1:A:148:VAL:HG22	1.99	0.62
1:A:21:ARG:NH1	1:A:21:ARG:HB2	2.14	0.62
1:A:27:TYR:HE1	1:D:40:LEU:HD22	1.64	0.62
1:D:141:LYS:HD2	1:D:163:LEU:HD12	1.82	0.62
1:B:86:LYS:HG3	3:B:428:HOH:O	1.99	0.62
1:B:175:TYR:HA	1:B:178:ARG:NH1	2.14	0.62
1:A:40:LEU:HD21	1:A:119:VAL:HB	1.80	0.62
1:A:23:THR:HG22	1:A:25:GLY:H	1.64	0.62
1:D:170:GLU:O	1:D:174:ARG:HG3	2.00	0.62
1:A:157:ALA:O	1:A:161:GLU:HG3	2.00	0.61
1:A:166:PRO:HG3	1:A:192:TRP:CE2	2.35	0.61
1:B:145:MET:O	1:B:148:VAL:HG22	2.00	0.61
1:C:30:LEU:HB3	1:C:34:LEU:HD22	1.83	0.61
1:B:83:GLN:H	1:B:83:GLN:NE2	1.95	0.61
1:A:37:GLN:HE21	1:D:63:LYS:NZ	1.98	0.61
1:A:63:LYS:NZ	1:D:37:GLN:NE2	2.49	0.61
1:C:116:PHE:O	1:C:119:VAL:HG22	2.00	0.61
1:A:126:PHE:HE2	1:A:148:VAL:HG11	1.64	0.60
1:D:113:TYR:CE1	1:D:117:ARG:HG3	2.36	0.60
1:D:125:GLY:HA3	2:D:401:HEM:C1D	2.36	0.60
1:A:170:GLU:O	1:A:174:ARG:HG2	2.02	0.60
1:C:30:LEU:O	1:C:34:LEU:HB2	2.02	0.60
1:A:23:THR:HB	1:A:26:GLY:H	1.65	0.60
1:A:127:GLN:NE2	1:D:24:TYR:HB3	2.16	0.60
1:D:198:ALA:HA	1:D:274:GLU:OE1	2.02	0.60
1:B:80:GLU:HB3	1:B:83:GLN:NE2	2.17	0.60
1:A:171:GLU:HA	1:A:174:ARG:HG3	1.85	0.59
1:A:166:PRO:HB2	1:A:171:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:THR:HG23	1:C:127:GLN:NE2	2.16	0.59
1:D:98:LEU:HB3	1:D:236:TRP:CD1	2.37	0.59
1:D:230:GLU:O	1:D:234:GLN:HG2	2.03	0.58
1:C:129:LEU:HD21	1:C:159:LEU:HG	1.85	0.58
1:B:45:HIS:CD2	1:B:47:ASP:H	2.13	0.58
1:A:279:ARG:HB3	1:C:248:ILE:O	2.04	0.58
1:A:21:ARG:HB2	1:A:21:ARG:HH11	1.67	0.58
1:A:127:GLN:NE2	1:D:23:THR:HG22	2.18	0.58
1:C:126:PHE:HE2	1:C:148:VAL:HG11	1.69	0.58
1:A:158:ARG:HG2	1:A:158:ARG:HH21	1.69	0.58
1:B:93:GLN:HE22	1:B:96:ARG:HH21	1.52	0.58
1:D:259:GLY:H	1:D:262:PHE:HB3	1.69	0.57
1:C:258:SER:HA	1:C:262:PHE:HB2	1.85	0.57
1:D:166:PRO:HG3	1:D:192:TRP:CE2	2.39	0.57
1:D:148:VAL:HG23	1:D:149:PHE:CD2	2.39	0.57
1:D:250:PHE:O	1:D:251:LYS:HB2	2.02	0.57
1:A:37:GLN:HE21	1:D:63:LYS:HZ3	1.52	0.57
1:A:123:SER:HB3	1:D:24:TYR:HB2	1.86	0.57
1:A:93:GLN:HE22	1:D:103:SER:HB3	1.68	0.56
1:B:40:LEU:CD1	1:B:119:VAL:HB	2.35	0.56
1:D:83:GLN:HE21	1:D:83:GLN:N	1.99	0.56
1:A:223:CYS:O	1:A:227:VAL:HG23	2.05	0.56
1:B:54:GLN:NE2	1:B:101:GLN:HG2	2.20	0.56
1:B:104:VAL:HG11	1:C:61:TRP:CH2	2.41	0.56
1:A:116:PHE:O	1:A:120:LEU:HD13	2.04	0.56
1:C:45:HIS:CD2	1:C:47:ASP:H	2.22	0.56
1:B:54:GLN:HE22	1:B:101:GLN:HG2	1.71	0.56
1:A:23:THR:HG22	1:A:25:GLY:N	2.21	0.55
1:B:81:VAL:HB	3:B:402:HOH:O	2.05	0.55
1:C:73:ILE:HG23	1:C:171:GLU:HG3	1.88	0.55
1:D:30:LEU:O	1:D:34:LEU:HB2	2.05	0.55
1:B:27:TYR:HE1	1:C:40:LEU:HD22	1.70	0.55
1:A:141:LYS:HE2	1:A:162:VAL:O	2.07	0.55
1:B:42:GLU:HB2	1:B:43:PRO:HD3	1.89	0.55
1:B:79:ASP:OD2	1:B:178:ARG:NH1	2.39	0.55
1:B:158:ARG:HG2	1:B:158:ARG:HH21	1.71	0.55
1:D:45:HIS:CD2	1:D:47:ASP:H	2.23	0.55
1:D:130:GLN:O	1:D:134:ILE:HG12	2.07	0.55
1:A:277:ASP:O	1:A:280:THR:HG22	2.07	0.55
1:B:241:MET:HG3	1:B:263:LEU:HB2	1.87	0.55
1:D:186:GLN:OE1	1:D:190:ARG:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:THR:O	1:C:235:LEU:HD13	2.07	0.55
2:C:401:HEM:HBA2	2:C:401:HEM:CHA	2.37	0.55
1:A:127:GLN:O	1:A:127:GLN:HG2	2.07	0.54
1:B:88:LEU:O	1:B:92:LYS:HG3	2.07	0.54
1:A:127:GLN:NE2	1:D:24:TYR:H	2.04	0.54
1:B:27:TYR:CE1	1:C:40:LEU:HD22	2.42	0.54
1:D:223:CYS:O	1:D:227:VAL:HG23	2.06	0.54
1:C:21:ARG:HB2	1:C:21:ARG:CZ	2.36	0.54
1:A:27:TYR:CE1	1:D:40:LEU:HD22	2.43	0.54
1:B:52:ILE:O	1:B:56:GLN:HG3	2.06	0.54
1:B:114:MET:SD	1:D:283:GLY:HA3	2.48	0.54
1:C:55:HIS:CE1	2:C:401:HEM:HMC1	2.43	0.54
1:D:29:ARG:HE	1:D:32:GLN:HE22	1.56	0.54
2:D:401:HEM:HBA2	2:D:401:HEM:CHA	2.37	0.54
1:B:83:GLN:HE21	1:B:83:GLN:N	2.00	0.54
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	1.89	0.53
1:B:53:ILE:HD12	1:C:64:LEU:HG	1.90	0.53
1:C:54:GLN:HG2	1:C:105:LEU:HD22	1.88	0.53
1:D:73:ILE:O	1:D:77:GLN:HG3	2.08	0.53
1:A:21:ARG:HG3	1:A:23:THR:H	1.73	0.53
1:B:23:THR:HG22	1:B:26:GLY:N	2.20	0.53
1:B:37:GLN:HE21	1:C:63:LYS:NZ	2.07	0.53
1:B:86:LYS:NZ	1:C:112:GLU:OE2	2.42	0.53
1:A:45:HIS:CE1	1:A:115:GLY:HA3	2.44	0.53
1:D:234:GLN:HE21	1:D:234:GLN:HA	1.72	0.53
1:B:47:ASP:OD2	1:B:112:GLU:HB3	2.09	0.53
1:A:40:LEU:HG	1:A:119:VAL:CG1	2.38	0.52
1:A:45:HIS:HD2	1:A:47:ASP:H	1.56	0.52
1:B:29:ARG:NE	1:B:32:GLN:NE2	2.56	0.52
1:D:81:VAL:O	1:D:85:ARG:HG3	2.09	0.52
1:A:155:GLY:CA	1:A:158:ARG:HE	2.21	0.52
1:B:85:ARG:CZ	1:B:221:SER:HB3	2.40	0.52
1:C:210:TYR:OH	1:C:279:ARG:NH1	2.42	0.52
1:A:37:GLN:NE2	1:D:63:LYS:NZ	2.58	0.52
1:B:258:SER:HA	1:B:262:PHE:HB2	1.92	0.52
1:C:240:HIS:O	1:C:244:VAL:HG23	2.08	0.52
1:B:93:GLN:O	1:B:97:GLN:HG2	2.09	0.52
1:C:170:GLU:O	1:C:174:ARG:HG3	2.10	0.52
1:B:205:VAL:O	1:B:209:ILE:HG13	2.10	0.52
1:D:245:MET:O	1:D:249:GLY:HA2	2.09	0.52
1:D:215:ARG:HG3	1:D:215:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:HB3	1:B:202:LEU:HD23	1.91	0.52
1:B:125:GLY:HA3	2:B:401:HEM:C1D	2.44	0.52
1:B:166:PRO:HG3	1:B:192:TRP:CE2	2.45	0.52
1:B:170:GLU:O	1:B:174:ARG:HG2	2.10	0.52
1:A:21:ARG:HH11	1:A:21:ARG:CB	2.23	0.51
1:C:114:MET:HG3	1:C:117:ARG:NH1	2.25	0.51
1:A:169:TYR:HB3	3:A:417:HOH:O	2.10	0.51
1:B:279:ARG:HD3	1:D:246:ARG:O	2.10	0.51
1:A:240:HIS:O	1:A:244:VAL:HG23	2.11	0.51
1:A:210:TYR:OH	1:A:279:ARG:NH1	2.35	0.51
1:B:45:HIS:CE1	1:B:115:GLY:HA3	2.46	0.51
1:A:95:LEU:HB3	1:A:232:GLN:HG2	1.93	0.51
1:A:54:GLN:OE1	1:A:104:VAL:HG13	2.10	0.51
1:A:283:GLY:HA3	1:C:114:MET:SD	2.51	0.51
1:D:258:SER:HA	1:D:262:PHE:HB2	1.92	0.51
1:A:61:TRP:CH2	1:D:104:VAL:HG11	2.46	0.51
1:A:98:LEU:HB3	1:A:236:TRP:CD1	2.46	0.51
1:C:59:GLU:HG3	1:C:130:GLN:HE21	1.76	0.51
1:C:203:ARG:N	1:C:204:PRO:HD2	2.26	0.51
1:A:37:GLN:NE2	1:D:63:LYS:HZ2	2.09	0.50
1:B:61:TRP:HB2	1:B:98:LEU:HD13	1.94	0.50
1:D:158:ARG:HG2	1:D:158:ARG:NH2	2.25	0.50
1:C:178:ARG:HB2	1:C:178:ARG:NH1	2.21	0.50
1:B:34:LEU:C	1:B:37:GLN:HE22	2.15	0.50
1:C:39:PRO:HA	1:C:48:GLU:OE2	2.12	0.50
1:C:21:ARG:HB2	1:C:21:ARG:NH1	2.27	0.49
1:A:114:MET:SD	1:C:283:GLY:HA3	2.52	0.49
1:A:141:LYS:HD2	1:A:163:LEU:HA	1.94	0.49
1:A:154:ALA:O	1:A:158:ARG:HD3	2.12	0.49
1:B:277:ASP:O	1:B:280:THR:HG22	2.13	0.49
1:D:164:GLU:O	1:D:192:TRP:HB2	2.13	0.49
1:B:246:ARG:C	1:D:279:ARG:HD3	2.33	0.49
1:B:251:LYS:CE	1:D:280:THR:HG21	2.42	0.49
1:C:59:GLU:HG3	1:C:130:GLN:NE2	2.28	0.49
1:A:126:PHE:CZ	1:A:145:MET:SD	3.06	0.48
1:B:207:GLU:OE2	1:B:281:SER:HB2	2.13	0.48
1:C:23:THR:HB	1:C:26:GLY:H	1.78	0.48
1:D:54:GLN:OE1	1:D:104:VAL:HG13	2.12	0.48
1:B:199:ASP:CG	1:B:202:LEU:HD23	2.34	0.48
1:C:130:GLN:O	1:C:134:ILE:HG12	2.13	0.48
1:A:93:GLN:OE1	1:A:93:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:N	1:B:204:PRO:HD2	2.28	0.48
1:C:76:LEU:HG	1:C:84:CYS:SG	2.53	0.48
1:C:132:ARG:HH21	1:C:135:GLU:HG2	1.79	0.48
1:A:183:ILE:HG22	1:A:187:TYR:HD2	1.79	0.48
1:C:163:LEU:O	1:C:193:THR:HA	2.12	0.48
1:A:85:ARG:CZ	1:A:221:SER:HB3	2.44	0.48
1:D:74:VAL:HA	1:D:77:GLN:OE1	2.14	0.48
1:B:60:LEU:HD12	1:C:60:LEU:HD12	1.95	0.48
1:A:50:LEU:HD22	1:D:90:ARG:CZ	2.44	0.48
1:C:169:TYR:OH	1:C:274:GLU:HG3	2.13	0.48
1:A:203:ARG:HH21	1:A:203:ARG:HB2	1.79	0.47
1:A:213:THR:O	1:A:217:TRP:N	2.47	0.47
1:B:169:TYR:O	1:B:172:PHE:HB3	2.14	0.47
1:A:203:ARG:HB2	1:A:203:ARG:NH2	2.29	0.47
1:B:40:LEU:HD11	1:B:119:VAL:O	2.14	0.47
1:A:68:GLU:CD	1:A:90:ARG:HD2	2.35	0.47
1:D:40:LEU:H	1:D:40:LEU:CD2	2.27	0.47
1:C:160:ARG:HG3	1:C:160:ARG:HH11	1.79	0.47
1:A:43:PRO:O	1:A:44:ALA:HB3	2.14	0.47
1:B:109:THR:HG22	1:D:224:GLU:OE1	2.14	0.47
1:B:184:PRO:HB2	1:B:187:TYR:CE2	2.50	0.47
1:B:230:GLU:OE2	1:B:270:THR:HA	2.15	0.47
1:D:43:PRO:O	1:D:44:ALA:HB3	2.14	0.47
1:C:43:PRO:HD2	3:C:411:HOH:O	2.13	0.47
1:C:81:VAL:HG21	1:C:218:ARG:HD3	1.95	0.47
1:D:207:GLU:O	1:D:211:GLU:HG3	2.14	0.47
1:B:250:PHE:HA	1:B:260:VAL:HG11	1.95	0.47
1:C:172:PHE:O	1:C:175:TYR:HB3	2.14	0.47
1:C:248:ILE:HG22	1:C:249:GLY:N	2.29	0.47
1:D:39:PRO:HA	1:D:48:GLU:OE2	2.14	0.47
1:A:40:LEU:HD11	1:A:119:VAL:O	2.15	0.47
1:A:106:GLU:OE2	1:A:239:ARG:NH1	2.48	0.47
1:C:59:GLU:OE1	1:C:130:GLN:NE2	2.41	0.47
1:C:225:ASP:O	1:C:229:VAL:HG23	2.15	0.47
1:D:40:LEU:H	1:D:40:LEU:HD23	1.80	0.47
1:D:237:ARG:HG3	3:D:428:HOH:O	2.15	0.47
1:A:145:MET:O	1:A:145:MET:HG3	2.15	0.46
1:D:277:ASP:O	1:D:280:THR:HG22	2.15	0.46
1:B:171:GLU:OE2	1:B:171:GLU:HA	2.16	0.46
1:C:146:LEU:HD11	1:C:163:LEU:CD2	2.46	0.46
1:B:143:PRO:HG3	1:B:193:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:TYR:HA	1:C:178:ARG:NH1	2.30	0.46
1:D:136:PHE:CD2	1:D:159:LEU:HD22	2.50	0.46
1:A:52:ILE:O	1:A:56:GLN:HG3	2.15	0.46
1:A:158:ARG:HG2	1:A:158:ARG:NH2	2.31	0.46
1:A:265:GLN:HG3	3:A:406:HOH:O	2.16	0.46
1:C:230:GLU:O	1:C:234:GLN:HG2	2.15	0.46
1:B:54:GLN:CD	1:B:105:LEU:HB2	2.36	0.46
1:B:185:GLN:HE21	1:B:185:GLN:HB3	1.57	0.46
1:A:125:GLY:HA3	2:A:401:HEM:C1D	2.50	0.46
1:A:59:GLU:HG3	1:A:130:GLN:NE2	2.30	0.46
1:B:64:LEU:HG	1:C:53:ILE:HD12	1.98	0.46
1:C:93:GLN:HA	1:C:93:GLN:OE1	2.15	0.46
1:C:143:PRO:C	1:C:145:MET:H	2.19	0.46
1:A:40:LEU:CD2	1:A:119:VAL:HB	2.45	0.45
1:B:30:LEU:HB3	1:B:34:LEU:HD23	1.97	0.45
1:C:139:GLY:O	1:C:141:LYS:HG2	2.16	0.45
1:D:190:ARG:HH22	1:D:194:ALA:HB3	1.80	0.45
2:D:401:HEM:HHD	2:D:401:HEM:CBC	2.30	0.45
1:B:133:TYR:HD1	1:B:159:LEU:HD23	1.81	0.45
1:A:110:PRO:HD2	1:C:210:TYR:HE1	1.81	0.45
1:B:234:GLN:HE22	1:B:267:LEU:HA	1.80	0.45
1:B:45:HIS:HD2	1:B:47:ASP:N	2.05	0.45
1:C:66:ALA:HB2	1:C:134:ILE:HD11	1.98	0.45
1:A:154:ALA:O	1:A:158:ARG:NE	2.49	0.45
1:B:112:GLU:OE2	1:C:86:LYS:NZ	2.45	0.45
1:C:40:LEU:CD2	1:C:40:LEU:H	2.30	0.45
1:A:63:LYS:HB2	1:A:130:GLN:OE1	2.17	0.45
1:A:112:GLU:OE2	1:D:86:LYS:NZ	2.50	0.45
1:A:160:ARG:O	1:A:164:GLU:HG3	2.17	0.45
1:D:45:HIS:CE1	1:D:115:GLY:HA3	2.52	0.45
1:A:132:ARG:HD3	1:A:145:MET:CG	2.48	0.44
1:A:24:TYR:HB2	1:D:123:SER:HB3	1.99	0.44
1:C:40:LEU:HD21	1:C:119:VAL:HG23	1.98	0.44
1:D:29:ARG:HE	1:D:32:GLN:HE21	1.59	0.44
1:D:143:PRO:HG3	1:D:193:THR:HG23	1.99	0.44
1:A:78:ARG:O	1:A:79:ASP:HB2	2.18	0.44
1:A:126:PHE:CE2	1:A:148:VAL:HG11	2.49	0.44
2:A:401:HEM:HHD	2:A:401:HEM:CBC	2.48	0.44
1:C:124:SER:C	1:C:126:PHE:H	2.20	0.44
1:D:274:GLU:H	1:D:274:GLU:HG2	1.45	0.44
1:C:126:PHE:CZ	1:C:145:MET:SD	3.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLN:O	1:D:97:GLN:HG2	2.18	0.44
1:A:28:LEU:HD13	1:D:55:HIS:HB3	1.99	0.44
1:D:59:GLU:HG3	1:D:130:GLN:HE21	1.82	0.44
1:D:106:GLU:OE2	1:D:239:ARG:NH1	2.50	0.44
1:A:23:THR:HB	1:A:26:GLY:N	2.32	0.44
1:A:133:TYR:O	1:A:137:LEU:HB2	2.18	0.44
1:A:169:TYR:O	1:A:172:PHE:HB3	2.18	0.44
1:B:100:GLU:HG3	1:C:97:GLN:NE2	2.23	0.44
1:C:40:LEU:H	1:C:40:LEU:HD23	1.83	0.44
1:D:276:PHE:O	1:D:279:ARG:HB2	2.17	0.44
1:A:109:THR:HG21	1:C:220:TYR:OH	2.18	0.44
1:A:132:ARG:HH21	1:A:135:GLU:HG2	1.83	0.44
1:A:135:GLU:OE1	1:A:135:GLU:HA	2.18	0.44
1:A:146:LEU:HD11	1:A:163:LEU:HD22	2.00	0.44
1:B:171:GLU:HA	1:B:174:ARG:HG3	1.99	0.44
1:C:160:ARG:O	1:C:164:GLU:HG3	2.18	0.44
1:A:63:LYS:HZ2	1:D:37:GLN:NE2	2.15	0.43
1:A:202:LEU:HD13	1:A:202:LEU:HA	1.73	0.43
1:B:101:GLN:O	1:B:101:GLN:HG2	2.18	0.43
1:A:151:TYR:CE2	1:A:152:ASP:HB2	2.53	0.43
1:C:40:LEU:HD11	1:C:119:VAL:O	2.18	0.43
1:C:185:GLN:HE21	1:C:185:GLN:HB3	1.61	0.43
1:A:64:LEU:O	1:A:67:HIS:HB3	2.18	0.43
1:B:234:GLN:HA	1:B:234:GLN:NE2	2.33	0.43
1:B:102:TRP:O	1:B:106:GLU:HG3	2.19	0.43
1:A:132:ARG:HD3	1:A:145:MET:HG2	1.99	0.43
1:B:170:GLU:O	1:B:174:ARG:CG	2.65	0.43
1:D:275:LEU:O	1:D:278:VAL:HG12	2.18	0.43
1:A:50:LEU:HD22	1:D:90:ARG:NE	2.34	0.43
1:B:40:LEU:CG	1:B:119:VAL:HB	2.49	0.43
1:B:188:GLN:HG2	3:B:435:HOH:O	2.19	0.43
1:B:43:PRO:O	1:B:44:ALA:HB3	2.19	0.43
1:C:125:GLY:HA3	2:C:401:HEM:C1D	2.54	0.43
1:A:129:LEU:HD12	1:A:149:PHE:CG	2.54	0.43
1:B:37:GLN:HE21	1:C:63:LYS:HZ3	1.65	0.43
1:B:42:GLU:CB	1:B:43:PRO:HD3	2.48	0.43
1:C:213:THR:O	1:C:217:TRP:N	2.52	0.43
1:D:84:CYS:O	1:D:87:VAL:HG22	2.19	0.43
1:A:41:SER:O	1:A:44:ALA:N	2.52	0.42
1:A:113:TYR:O	1:A:117:ARG:HB2	2.20	0.42
1:A:188:GLN:O	1:A:189:ALA:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HG23	1:B:171:GLU:HG3	2.01	0.42
1:D:21:ARG:CB	1:D:21:ARG:HH11	2.31	0.42
1:A:23:THR:HG22	1:A:24:TYR:N	2.34	0.42
1:B:68:GLU:CD	1:B:90:ARG:HD2	2.40	0.42
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.85	0.42
2:C:401:HEM:HHD	2:C:401:HEM:CBC	2.30	0.42
1:B:223:CYS:O	1:B:227:VAL:HG23	2.20	0.42
1:D:109:THR:OG1	1:D:112:GLU:HG3	2.19	0.42
1:D:203:ARG:N	1:D:204:PRO:HD2	2.35	0.42
1:B:135:GLU:CG	1:B:140:ASN:HD22	2.33	0.42
1:B:199:ASP:CB	1:B:202:LEU:HD23	2.50	0.42
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.82	0.42
1:B:37:GLN:HB2	1:C:63:LYS:HZ3	1.83	0.42
1:A:40:LEU:HD22	1:D:27:TYR:HE1	1.84	0.42
1:A:250:PHE:O	1:A:251:LYS:C	2.58	0.42
1:C:47:ASP:OD2	1:C:112:GLU:HB3	2.20	0.42
1:C:101:GLN:O	1:C:104:VAL:HG12	2.19	0.42
1:C:166:PRO:HG3	1:C:192:TRP:CE2	2.55	0.42
1:C:178:ARG:HH11	1:C:178:ARG:CB	2.26	0.42
1:A:40:LEU:HG	1:A:119:VAL:HG12	2.02	0.42
1:B:181:HIS:O	1:B:183:ILE:N	2.53	0.42
1:C:41:SER:O	1:C:44:ALA:N	2.53	0.42
1:C:64:LEU:HD22	1:C:68:GLU:HG2	2.02	0.42
1:C:97:GLN:O	1:C:101:GLN:HB2	2.20	0.42
1:A:101:GLN:HA	1:D:97:GLN:OE1	2.20	0.41
1:A:142:ASN:O	1:A:145:MET:HB3	2.20	0.41
1:D:38:GLN:HA	1:D:38:GLN:NE2	2.34	0.41
1:D:259:GLY:O	1:D:262:PHE:HB3	2.20	0.41
1:C:59:GLU:CG	1:C:130:GLN:HE21	2.33	0.41
1:C:230:GLU:CD	1:C:271:PHE:H	2.24	0.41
1:D:60:LEU:HD23	1:D:60:LEU:HA	1.86	0.41
1:A:103:SER:HB3	1:D:93:GLN:NE2	2.35	0.41
1:B:117:ARG:O	1:B:120:LEU:HB2	2.21	0.41
1:C:274:GLU:H	1:C:274:GLU:HG2	1.33	0.41
1:D:158:ARG:NH2	1:D:158:ARG:CG	2.83	0.41
1:D:247:VAL:HG12	1:D:248:ILE:HG23	2.00	0.41
1:A:203:ARG:N	1:A:204:PRO:HD2	2.36	0.41
1:C:124:SER:C	1:C:126:PHE:N	2.74	0.41
1:C:152:ASP:HA	1:C:153:PRO:HD2	1.91	0.41
1:C:244:VAL:HG22	2:C:401:HEM:C1B	2.56	0.41
1:D:239:ARG:HD2	3:D:421:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PHE:CE1	1:D:252:ARG:HB3	2.55	0.41
1:B:69:LEU:HD23	1:B:137:LEU:HD22	2.02	0.41
1:D:218:ARG:O	1:D:221:SER:HB2	2.20	0.41
1:D:259:GLY:H	1:D:262:PHE:CB	2.31	0.41
1:C:83:GLN:O	1:C:86:LYS:HB3	2.20	0.41
1:D:38:GLN:HA	1:D:38:GLN:HE21	1.86	0.41
1:D:129:LEU:HD21	1:D:159:LEU:HG	2.03	0.41
1:D:190:ARG:NH2	1:D:194:ALA:HB3	2.35	0.41
1:D:200:ASP:C	1:D:202:LEU:H	2.24	0.41
1:B:24:TYR:HB3	1:C:127:GLN:HB3	2.02	0.41
1:B:230:GLU:CD	1:B:271:PHE:H	2.24	0.41
1:C:22:LEU:HD22	1:C:22:LEU:N	2.36	0.41
1:C:95:LEU:HB3	1:C:232:GLN:HG2	2.02	0.41
2:C:401:HEM:HHA	2:C:401:HEM:CBA	2.46	0.41
1:D:64:LEU:HD22	1:D:68:GLU:HG2	2.03	0.41
1:D:96:ARG:HA	1:D:232:GLN:NE2	2.36	0.41
1:D:202:LEU:HD13	1:D:202:LEU:HA	1.88	0.41
1:D:244:VAL:HG22	2:D:401:HEM:C1B	2.56	0.41
1:A:70:ARG:NH2	3:A:414:HOH:O	2.54	0.40
1:B:21:ARG:NH1	1:B:21:ARG:HB2	2.36	0.40
1:D:166:PRO:HG3	1:D:192:TRP:CD2	2.56	0.40
1:A:204:PRO:HA	1:A:207:GLU:OE1	2.21	0.40
1:B:175:TYR:HA	1:B:178:ARG:HH12	1.86	0.40
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.94	0.40
1:C:95:LEU:HB3	1:C:232:GLN:CG	2.51	0.40
2:D:401:HEM:HBC2	2:D:401:HEM:CHD	2.28	0.40
1:A:85:ARG:HH21	1:A:225:ASP:CG	2.20	0.40
1:B:40:LEU:HD21	1:B:119:VAL:HG23	2.04	0.40
1:C:126:PHE:CE2	1:C:148:VAL:HG11	2.54	0.40
1:C:143:PRO:HG3	1:C:193:THR:HG23	2.04	0.40
1:C:250:PHE:CA	1:C:260:VAL:HG11	2.35	0.40
1:A:40:LEU:HD22	1:D:27:TYR:CE1	2.57	0.40
1:B:166:PRO:HG3	1:B:192:TRP:CD2	2.57	0.40
2:D:401:HEM:HHA	2:D:401:HEM:CBA	2.46	0.40
1:A:76:LEU:HG	1:A:84:CYS:SG	2.62	0.40
1:D:21:ARG:HB2	1:D:21:ARG:NH1	2.36	0.40
1:D:186:GLN:HG3	1:D:187:TYR:N	2.35	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	255/306 (83%)	241 (94%)	12 (5%)	2 (1%)	19	43
1	B	255/306 (83%)	242 (95%)	12 (5%)	1 (0%)	34	60
1	C	255/306 (83%)	237 (93%)	14 (6%)	4 (2%)	9	24
1	D	256/306 (84%)	233 (91%)	19 (7%)	4 (2%)	9	24
All	All	1021/1224 (83%)	953 (93%)	57 (6%)	11 (1%)	14	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	ALA
1	D	251	LYS
1	C	144	GLN
1	C	248	ILE
1	B	182	ALA
1	A	44	ALA
1	A	189	ALA
1	C	44	ALA
1	D	44	ALA
1	D	182	ALA
1	D	119	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	229/267 (86%)	208 (91%)	21 (9%)	9 21
1	B	229/267 (86%)	206 (90%)	23 (10%)	7 18
1	C	229/267 (86%)	212 (93%)	17 (7%)	13 32
1	D	230/267 (86%)	203 (88%)	27 (12%)	5 12
All	All	917/1068 (86%)	829 (90%)	88 (10%)	8 19

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	34	LEU
1	A	40	LEU
1	A	64	LEU
1	A	69	LEU
1	A	83	GLN
1	A	101	GLN
1	A	119	VAL
1	A	129	LEU
1	A	132	ARG
1	A	147	GLN
1	A	158	ARG
1	A	159	LEU
1	A	185	GLN
1	A	193	THR
1	A	202	LEU
1	A	235	LEU
1	A	272	PHE
1	A	274	GLU
1	A	279	ARG
1	A	281	SER
1	B	34	LEU
1	B	40	LEU
1	B	64	LEU
1	B	69	LEU
1	B	83	GLN
1	B	98	LEU
1	B	120	LEU
1	B	129	LEU
1	B	132	ARG
1	B	135	GLU
1	B	147	GLN
1	B	158	ARG

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Mol	Chain	Res	Type
1	B	168	LEU
1	B	173	LEU
1	B	185	GLN
1	B	203	ARG
1	B	214	ASP
1	B	237	ARG
1	B	272	PHE
1	B	274	GLU
1	B	275	LEU
1	B	279	ARG
1	B	281	SER
1	C	21	ARG
1	C	34	LEU
1	C	40	LEU
1	C	64	LEU
1	C	69	LEU
1	C	70	ARG
1	C	83	GLN
1	C	98	LEU
1	C	129	LEU
1	C	147	GLN
1	C	168	LEU
1	C	185	GLN
1	C	186	GLN
1	C	239	ARG
1	C	250	PHE
1	C	274	GLU
1	C	279	ARG
1	D	21	ARG
1	D	23	THR
1	D	37	GLN
1	D	40	LEU
1	D	64	LEU
1	D	69	LEU
1	D	83	GLN
1	D	98	LEU
1	D	129	LEU
1	D	158	ARG
1	D	168	LEU
1	D	173	LEU
1	D	185	GLN
1	D	186	GLN

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Mol	Chain	Res	Type
1	D	193	THR
1	D	202	LEU
1	D	208	ARG
1	D	215	ARG
1	D	230	GLU
1	D	234	GLN
1	D	235	LEU
1	D	237	ARG
1	D	250	PHE
1	D	252	ARG
1	D	274	GLU
1	D	275	LEU
1	D	279	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLN
1	A	38	GLN
1	A	45	HIS
1	A	83	GLN
1	A	127	GLN
1	A	156	GLN
1	A	185	GLN
1	A	188	GLN
1	A	234	GLN
1	A	240	HIS
1	A	264	GLN
1	B	32	GLN
1	B	37	GLN
1	B	38	GLN
1	B	45	HIS
1	B	83	GLN
1	B	140	ASN
1	B	185	GLN
1	B	234	GLN
1	B	240	HIS
1	C	32	GLN
1	C	37	GLN
1	C	38	GLN
1	C	45	HIS

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Mol	Chain	Res	Type
1	C	83	GLN
1	C	97	GLN
1	C	156	GLN
1	C	185	GLN
1	C	188	GLN
1	C	234	GLN
1	D	32	GLN
1	D	37	GLN
1	D	38	GLN
1	D	45	HIS
1	D	83	GLN
1	D	127	GLN
1	D	140	ASN
1	D	147	GLN
1	D	185	GLN
1	D	188	GLN
1	D	232	GLN
1	D	234	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)

4 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	$\#\|Z\| > 2$
2	HEM	C	401	1	41,50,50	1.47	8 (19%)	45,82,82	1.87	10 (22%)
2	HEM	B	401	1	41,50,50	1.48	9 (21%)	45,82,82	1.86	10 (22%)
2	HEM	D	401	1	41,50,50	1.45	8 (19%)	45,82,82	1.86	10 (22%)
2	HEM	A	401	1	41,50,50	1.48	9 (21%)	45,82,82	1.86	10 (22%)

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
2	HEM	C	401	1	-	12/12/54/54	-
2	HEM	B	401	1	-	9/12/54/54	-
2	HEM	D	401	1	-	12/12/54/54	-
2	HEM	A	401	1	-	9/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3C-CAC	-2.94	1.41	1.47
2	D	401	HEM	C3C-CAC	-2.93	1.41	1.47
2	A	401	HEM	C3C-CAC	-2.92	1.41	1.47
2	B	401	HEM	C3C-CAC	-2.91	1.41	1.47
2	A	401	HEM	FE-NB	2.77	2.10	1.96
2	B	401	HEM	FE-NB	2.68	2.10	1.96
2	C	401	HEM	CMB-C2B	2.67	1.56	1.50
2	A	401	HEM	CMB-C2B	2.67	1.56	1.50
2	B	401	HEM	CMB-C2B	2.65	1.56	1.50
2	D	401	HEM	CMB-C2B	2.64	1.56	1.50
2	D	401	HEM	C2C-C1C	2.46	1.48	1.42
2	A	401	HEM	C2C-C1C	2.43	1.48	1.42
2	D	401	HEM	C1B-NB	-2.41	1.36	1.40
2	B	401	HEM	C2C-C1C	2.41	1.48	1.42
2	C	401	HEM	C2C-C1C	2.40	1.48	1.42
2	B	401	HEM	CBB-CAB	2.39	1.42	1.30
2	C	401	HEM	CBB-CAB	2.39	1.42	1.30
2	D	401	HEM	CBB-CAB	2.39	1.42	1.30
2	C	401	HEM	C1B-NB	-2.38	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	CBB-CAB	2.38	1.42	1.30
2	A	401	HEM	C1B-NB	-2.37	1.36	1.40
2	B	401	HEM	C1B-NB	-2.35	1.36	1.40
2	B	401	HEM	CHA-C4D	2.27	1.40	1.35
2	A	401	HEM	CHA-C4D	2.26	1.40	1.35
2	C	401	HEM	CHA-C4D	2.25	1.40	1.35
2	D	401	HEM	CHA-C4D	2.25	1.40	1.35
2	C	401	HEM	O1A-CGA	2.23	1.29	1.22
2	B	401	HEM	O1A-CGA	2.23	1.29	1.22
2	A	401	HEM	O1A-CGA	2.22	1.29	1.22
2	D	401	HEM	O1A-CGA	2.21	1.29	1.22
2	C	401	HEM	CHB-C1B	2.17	1.40	1.35
2	D	401	HEM	CHB-C1B	2.17	1.40	1.35
2	B	401	HEM	CHB-C1B	2.17	1.40	1.35
2	A	401	HEM	CHB-C1B	2.17	1.40	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HEM	CBA-CAA-C2A	5.75	122.43	112.62
2	C	401	HEM	CBA-CAA-C2A	5.75	122.42	112.62
2	A	401	HEM	CBA-CAA-C2A	5.74	122.42	112.62
2	B	401	HEM	CBA-CAA-C2A	5.74	122.41	112.62
2	D	401	HEM	CAD-CBD-CGD	4.20	122.63	113.60
2	A	401	HEM	CAD-CBD-CGD	4.18	122.59	113.60
2	B	401	HEM	CAD-CBD-CGD	4.18	122.59	113.60
2	C	401	HEM	CAD-CBD-CGD	4.17	122.58	113.60
2	C	401	HEM	C4C-CHD-C1D	3.77	127.54	122.56
2	D	401	HEM	C4C-CHD-C1D	3.77	127.54	122.56
2	A	401	HEM	C4C-CHD-C1D	3.75	127.51	122.56
2	B	401	HEM	C4C-CHD-C1D	3.74	127.49	122.56
2	C	401	HEM	C4B-C3B-C2B	-3.60	104.25	107.11
2	B	401	HEM	C4B-C3B-C2B	-3.57	104.28	107.11
2	A	401	HEM	C4B-C3B-C2B	-3.56	104.29	107.11
2	D	401	HEM	C4B-C3B-C2B	-3.55	104.30	107.11
2	C	401	HEM	CBD-CAD-C3D	3.36	121.95	112.63
2	A	401	HEM	CBD-CAD-C3D	3.34	121.91	112.63
2	B	401	HEM	CBD-CAD-C3D	3.34	121.91	112.63
2	D	401	HEM	CBD-CAD-C3D	3.34	121.91	112.63
2	B	401	HEM	C4B-CHC-C1C	3.17	126.74	122.56
2	A	401	HEM	C4B-CHC-C1C	3.16	126.73	122.56
2	C	401	HEM	C4B-CHC-C1C	3.16	126.73	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HEM	C4B-CHC-C1C	3.15	126.71	122.56
2	C	401	HEM	C2C-C3C-C4C	-2.64	105.06	106.90
2	A	401	HEM	C2C-C3C-C4C	-2.64	105.06	106.90
2	B	401	HEM	C2C-C3C-C4C	-2.62	105.07	106.90
2	D	401	HEM	C2C-C3C-C4C	-2.59	105.09	106.90
2	A	401	HEM	CAA-CBA-CGA	2.57	120.95	113.76
2	B	401	HEM	CAA-CBA-CGA	2.56	120.94	113.76
2	D	401	HEM	CAA-CBA-CGA	2.56	120.94	113.76
2	C	401	HEM	CAA-CBA-CGA	2.56	120.92	113.76
2	D	401	HEM	O2D-CGD-CBD	2.34	121.55	114.03
2	A	401	HEM	O2D-CGD-CBD	2.34	121.53	114.03
2	C	401	HEM	O2D-CGD-CBD	2.33	121.53	114.03
2	B	401	HEM	O2D-CGD-CBD	2.33	121.51	114.03
2	C	401	HEM	O1D-CGD-CBD	-2.25	115.85	123.08
2	B	401	HEM	O1D-CGD-CBD	-2.25	115.87	123.08
2	D	401	HEM	O1D-CGD-CBD	-2.24	115.87	123.08
2	A	401	HEM	O1D-CGD-CBD	-2.24	115.88	123.08

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C2B-C3B-CAB-CBB
2	A	401	HEM	C2D-C3D-CAD-CBD
2	A	401	HEM	C4D-C3D-CAD-CBD
2	B	401	HEM	C2B-C3B-CAB-CBB
2	B	401	HEM	C2D-C3D-CAD-CBD
2	B	401	HEM	C4D-C3D-CAD-CBD
2	C	401	HEM	C1A-C2A-CAA-CBA
2	C	401	HEM	C3A-C2A-CAA-CBA
2	C	401	HEM	C2B-C3B-CAB-CBB
2	C	401	HEM	C2D-C3D-CAD-CBD
2	D	401	HEM	C1A-C2A-CAA-CBA
2	D	401	HEM	C3A-C2A-CAA-CBA
2	D	401	HEM	C2B-C3B-CAB-CBB
2	D	401	HEM	C2D-C3D-CAD-CBD
2	C	401	HEM	C4D-C3D-CAD-CBD
2	D	401	HEM	C4D-C3D-CAD-CBD
2	C	401	HEM	C3D-CAD-CBD-CGD
2	D	401	HEM	C3D-CAD-CBD-CGD
2	C	401	HEM	C2A-CAA-CBA-CGA
2	D	401	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
2	A	401	HEM	C4B-C3B-CAB-CBB
2	B	401	HEM	C4B-C3B-CAB-CBB
2	C	401	HEM	C4B-C3B-CAB-CBB
2	D	401	HEM	C4B-C3B-CAB-CBB
2	A	401	HEM	C3D-CAD-CBD-CGD
2	B	401	HEM	C3D-CAD-CBD-CGD
2	C	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O1A
2	A	401	HEM	CAA-CBA-CGA-O2A
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	C	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
2	A	401	HEM	CAD-CBD-CGD-O2D
2	B	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O2D
2	D	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D
2	D	401	HEM	CAD-CBD-CGD-O1D
2	A	401	HEM	CAD-CBD-CGD-O1D
2	B	401	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

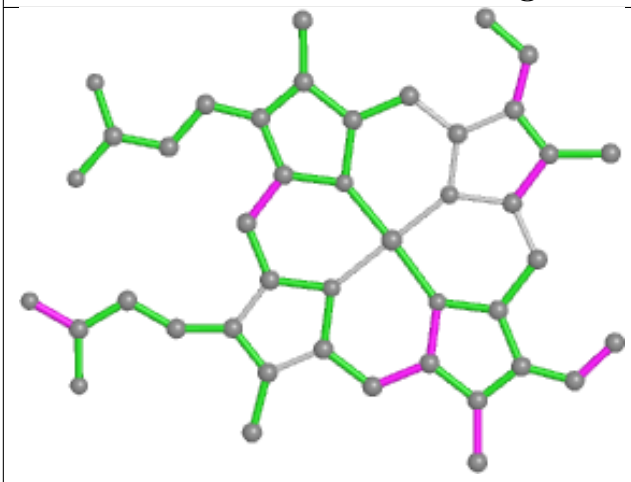
4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HEM	9	0
2	B	401	HEM	2	0
2	D	401	HEM	9	0
2	A	401	HEM	4	0

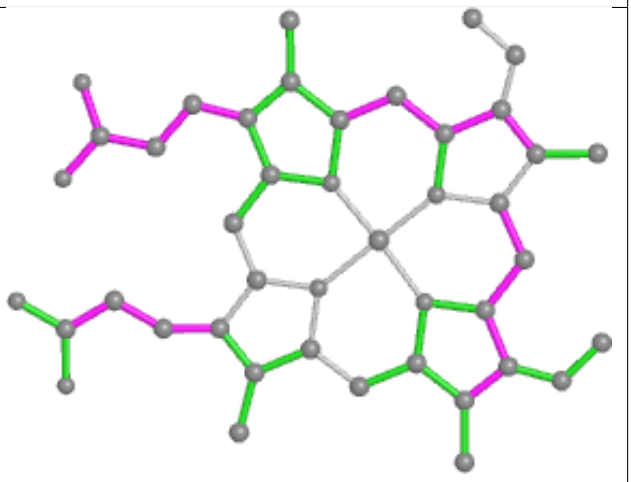
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

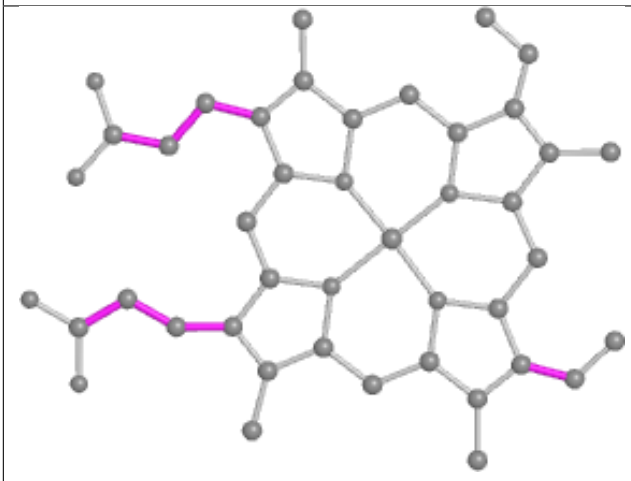
Ligand HEM C 401



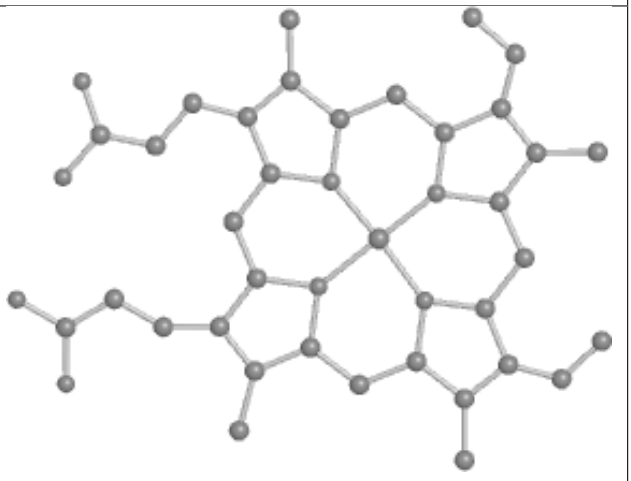
Bond lengths



Bond angles

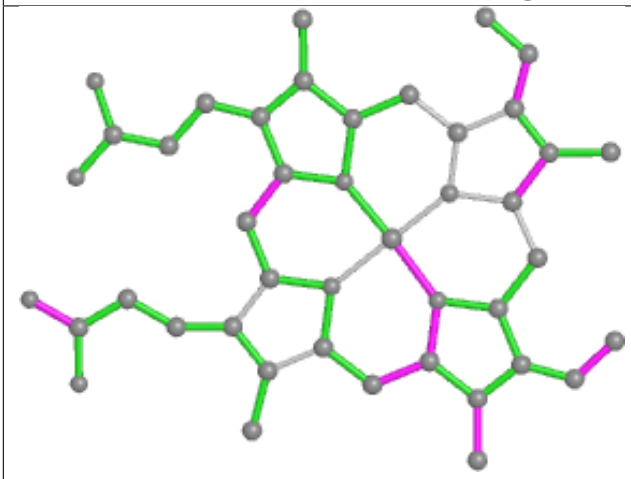


Torsions

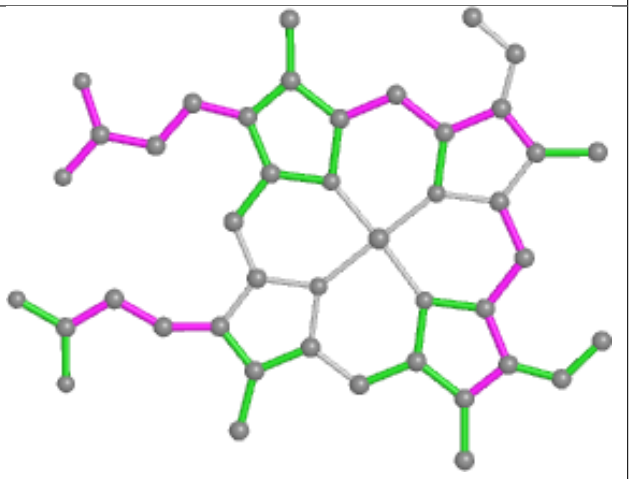


Rings

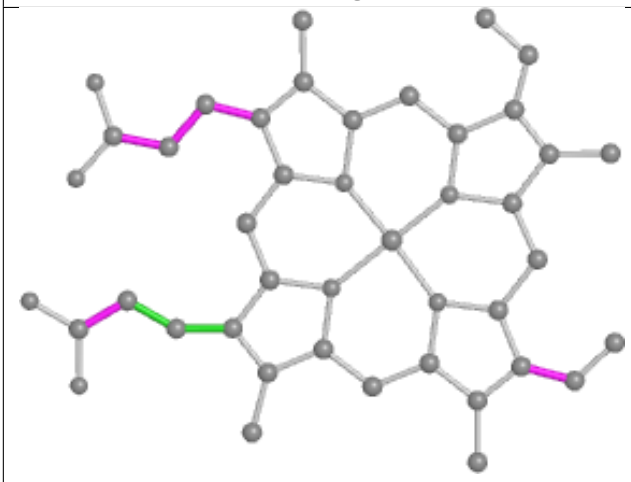
Ligand HEM B 401



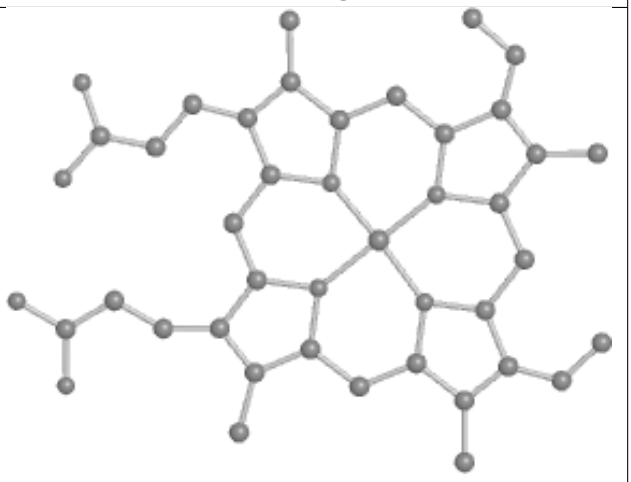
Bond lengths



Bond angles

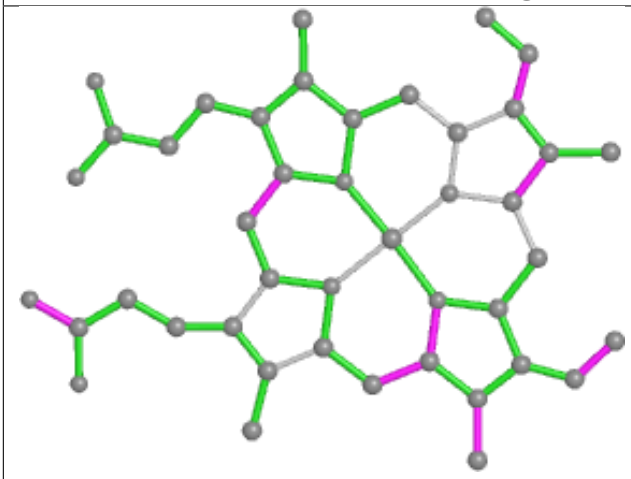


Torsions

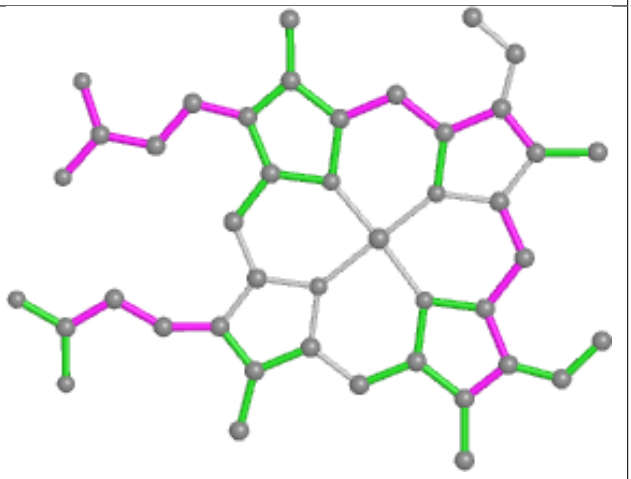


Rings

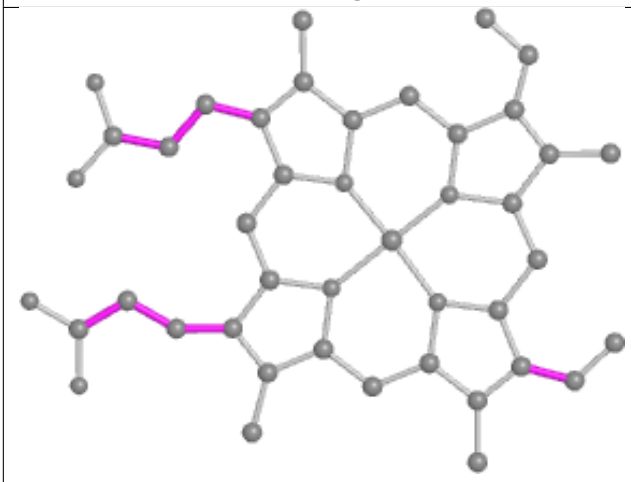
Ligand HEM D 401



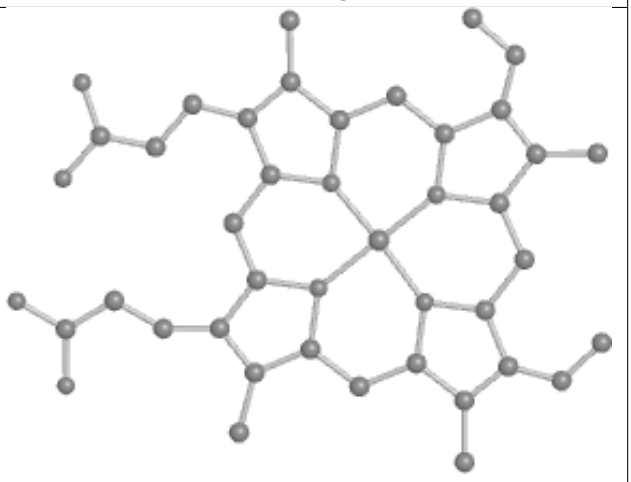
Bond lengths



Bond angles

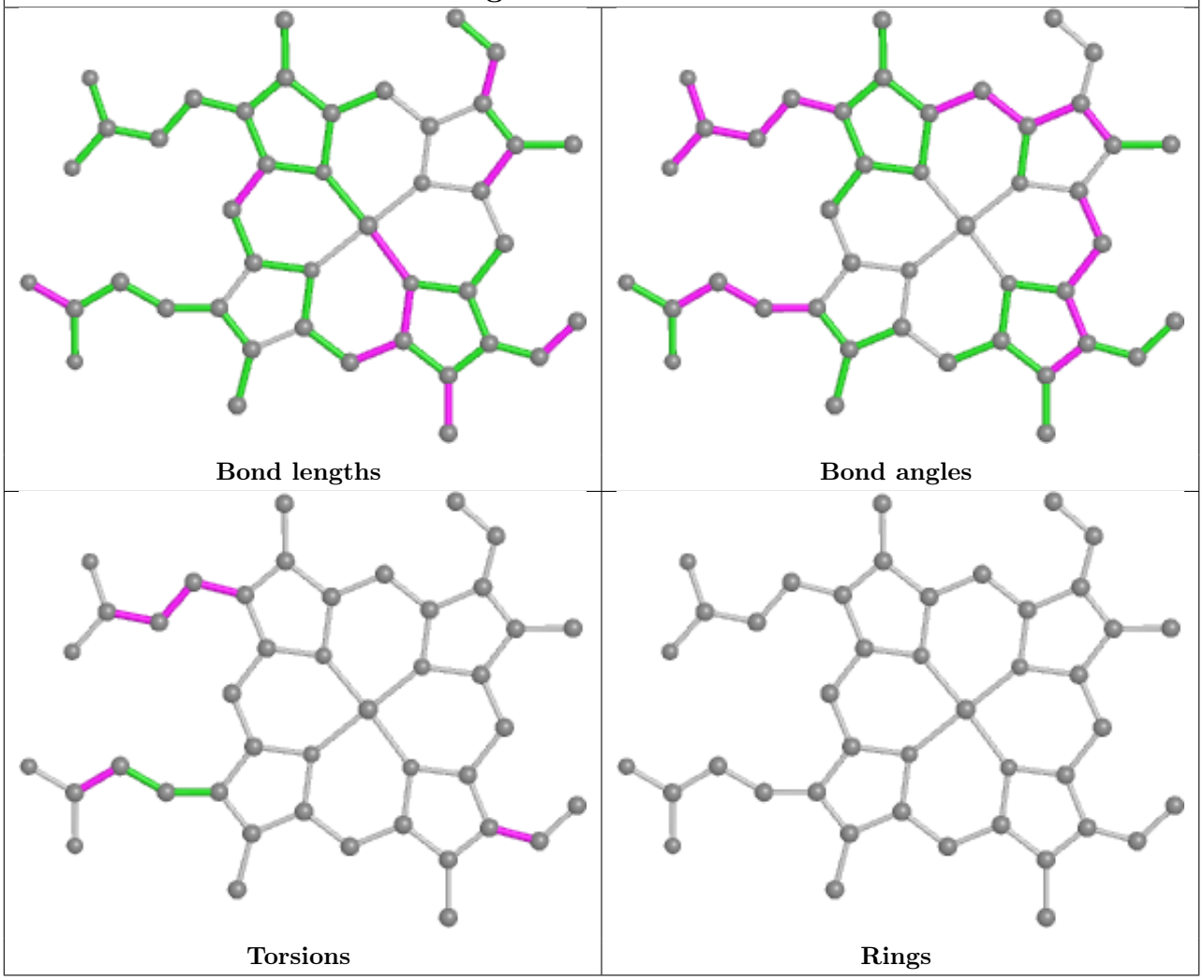


Torsions



Rings

Ligand HEM A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	259/306 (84%)	0.31	16 (6%)	20	19	18, 35, 61, 78	0
1	B	259/306 (84%)	0.03	9 (3%)	44	44	16, 30, 53, 63	0
1	C	259/306 (84%)	0.33	18 (6%)	16	15	16, 36, 62, 71	0
1	D	260/306 (84%)	0.11	10 (3%)	40	39	18, 29, 52, 63	0
All	All	1037/1224 (84%)	0.20	53 (5%)	28	26	16, 32, 58, 78	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	LEU	5.6
1	D	257	SER	4.7
1	A	127	GLN	4.6
1	C	42	GLU	4.4
1	D	119	VAL	4.2
1	A	143	PRO	4.1
1	C	154	ALA	3.9
1	D	42	GLU	3.7
1	D	259	GLY	3.7
1	C	259	GLY	3.6
1	D	21	ARG	3.6
1	C	258	SER	3.5
1	B	257	SER	3.3
1	C	157	ALA	3.3
1	B	40	LEU	3.3
1	C	284	VAL	3.3
1	B	251	LYS	3.2
1	A	158	ARG	3.1
1	A	144	GLN	3.1
1	A	257	SER	3.1
1	B	258	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	42	GLU	2.9
1	B	144	GLN	2.9
1	A	284	VAL	2.8
1	C	21	ARG	2.8
1	A	157	ALA	2.7
1	C	150	ALA	2.7
1	B	262	PHE	2.6
1	C	158	ARG	2.6
1	C	260	VAL	2.6
1	D	258	SER	2.6
1	A	120	LEU	2.5
1	C	143	PRO	2.4
1	B	143	PRO	2.4
1	A	250	PHE	2.4
1	D	151	TYR	2.4
1	C	123	SER	2.4
1	D	250	PHE	2.4
1	A	190	ARG	2.3
1	C	127	GLN	2.3
1	D	187	TYR	2.2
1	A	147	GLN	2.2
1	C	40	LEU	2.2
1	A	153	PRO	2.2
1	C	193	THR	2.2
1	C	120	LEU	2.1
1	C	118	ASP	2.1
1	A	142	ASN	2.1
1	B	21	ARG	2.0
1	B	121	GLY	2.0
1	C	151	TYR	2.0
1	D	200	ASP	2.0
1	A	201	THR	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)

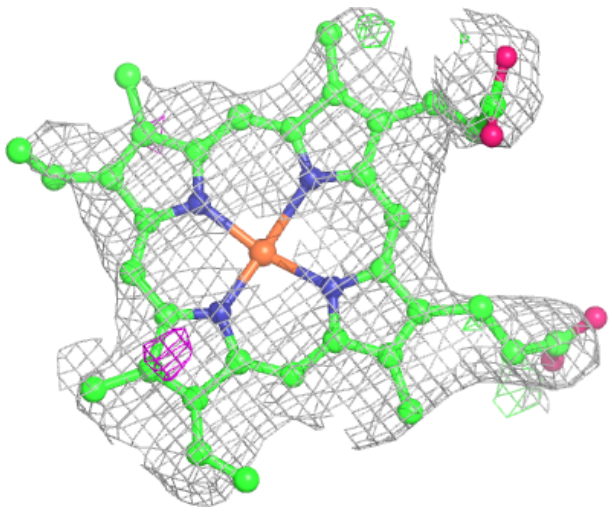
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

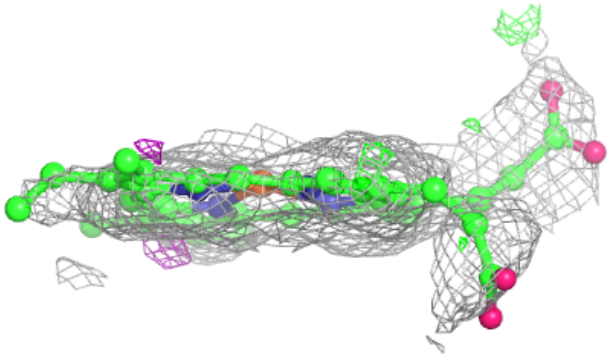
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	C	401	43/43	0.86	0.27	45,52,61,64	0
2	HEM	B	401	43/43	0.90	0.21	25,36,41,44	0
2	HEM	A	401	43/43	0.90	0.22	32,42,48,52	0
2	HEM	D	401	43/43	0.90	0.25	30,39,50,56	0

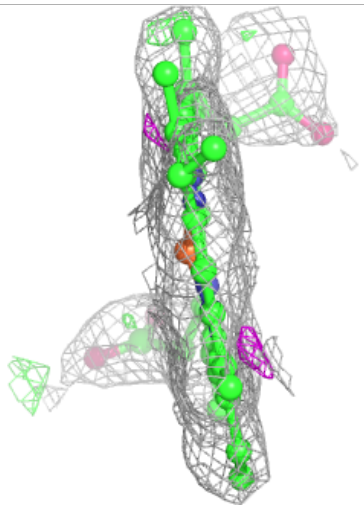
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM C 401:

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

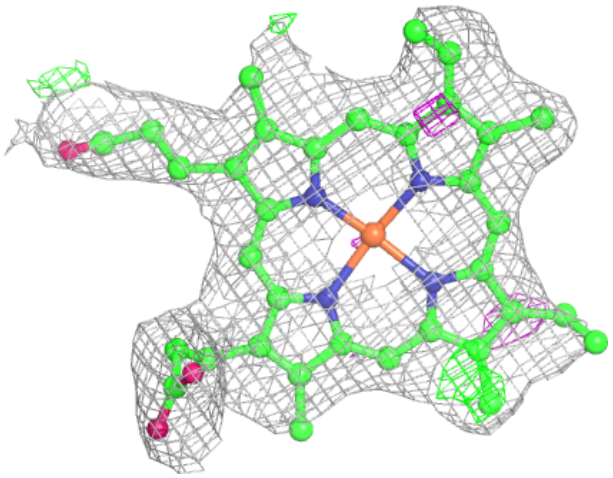


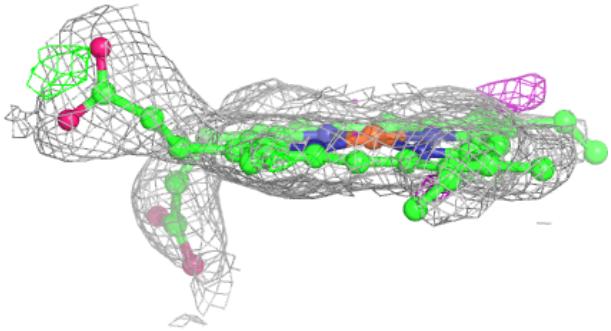


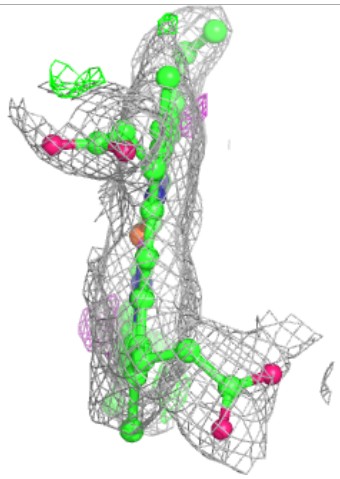


Electron density around HEM B 401:

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

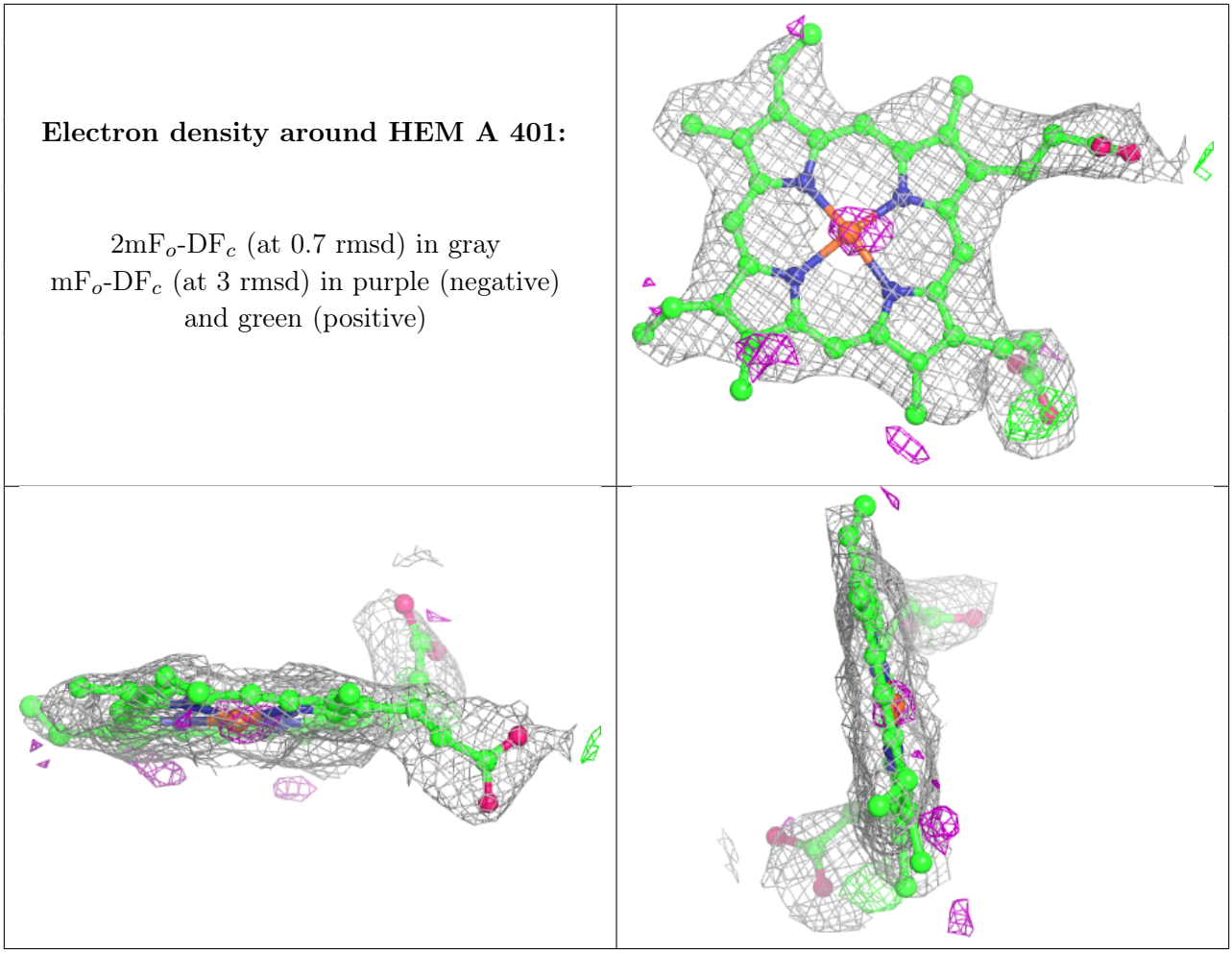






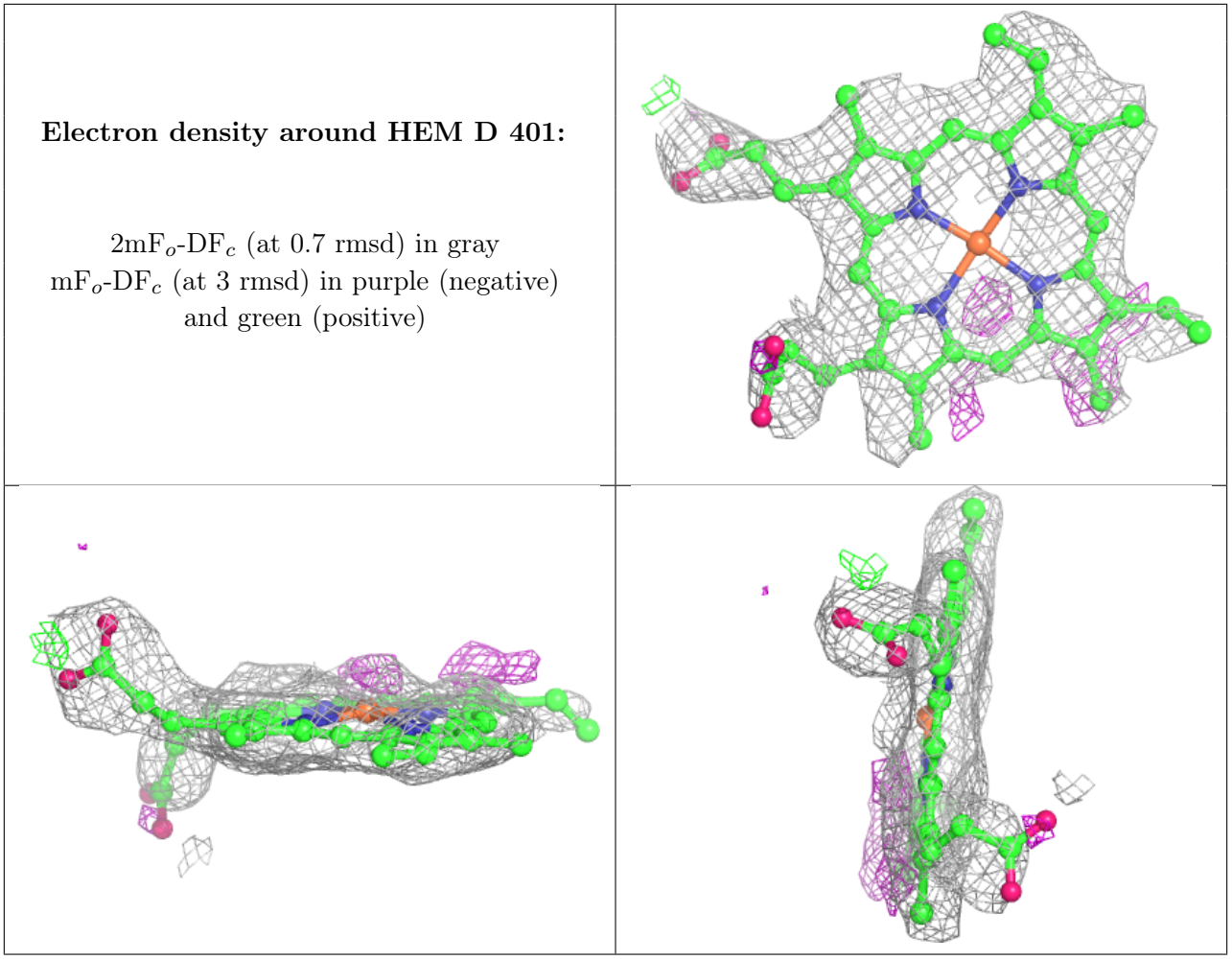
Electron density around HEM A 401:

$2mF_o$-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 401:

$2mF_o$-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.