Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 07:33 PM EDT

PDB ID	:	5TIA
Title	:	Crystal structure of human TDO in complex with Trp, Northeast Structural Genomics Consortium Target HR6161
Authors	:	Forouhar, F.; Lewis-Ballester, A.; Lew, S.; Karkashon, S.; Seetharaman, J.; Yeh, S.R.; Tong, L.
Deposited on	:	2016-10-01
Resolution	:	2.44 Å(reported)

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

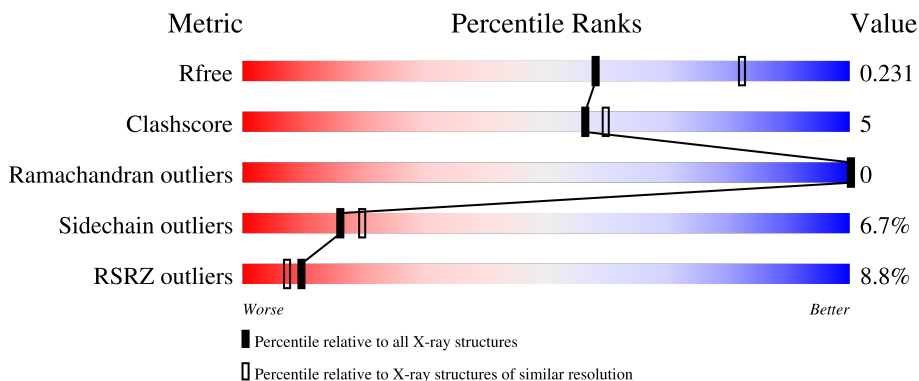|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1   Overall quality at a glance   ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		6.7%
RSRZ outliers		8.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	380	6% / 76% / 11% · 11%
1	B	380	5% / 75% / 11% · 12%
1	C	380	13% / 70% / 12% · 15%
1	D	380	7% / 78% / 12% · 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12061 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	337	Total	C	N	O	S	0	0	0
			2837	1822	500	504	11			
1	B	334	Total	C	N	O	S	0	0	0
			2803	1799	486	508	10			
1	C	323	Total	C	N	O	S	0	0	0
			2713	1749	472	482	10			
1	D	349	Total	C	N	O	S	0	0	0
			2942	1889	518	524	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

WORLDWIDE
PDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
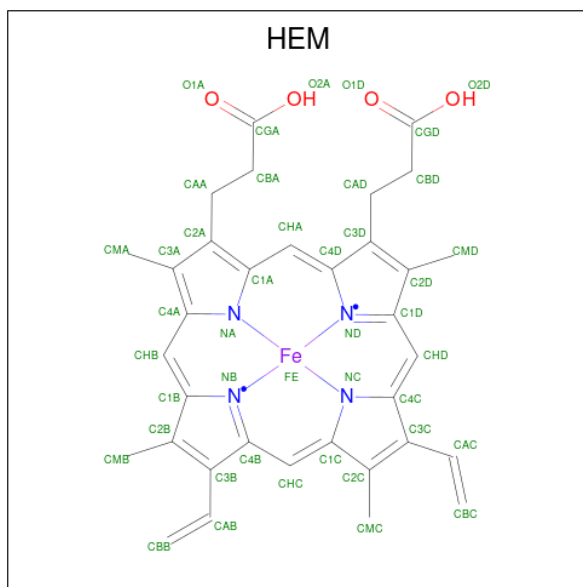
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).
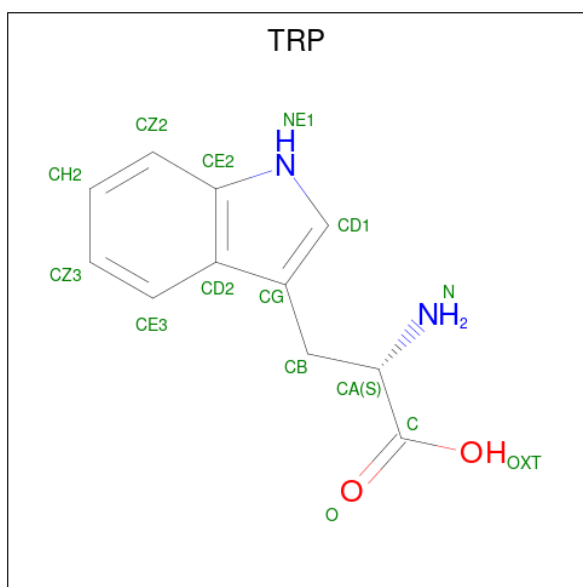
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		
4	B	127	Total	O	0	0
			127	127		
4	C	103	Total	O	0	0
			103	103		
4	D	142	Total	O	0	0
			142	142		

3 Residue-property plots ⓘ

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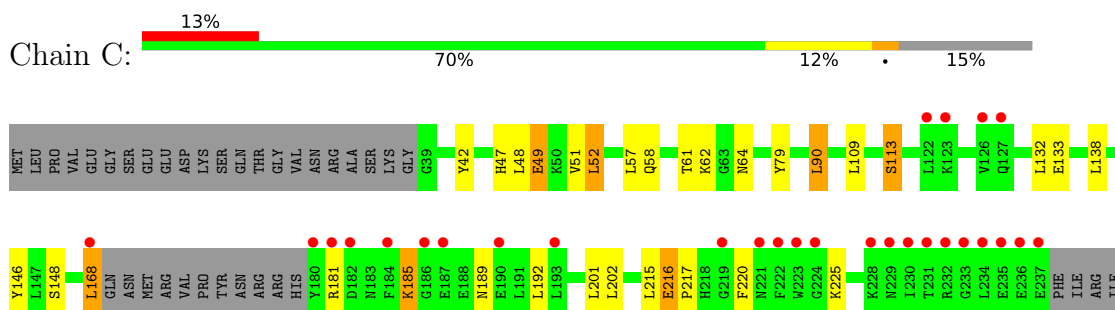
- Molecule 1: Tryptophan 2,3-dioxygenase
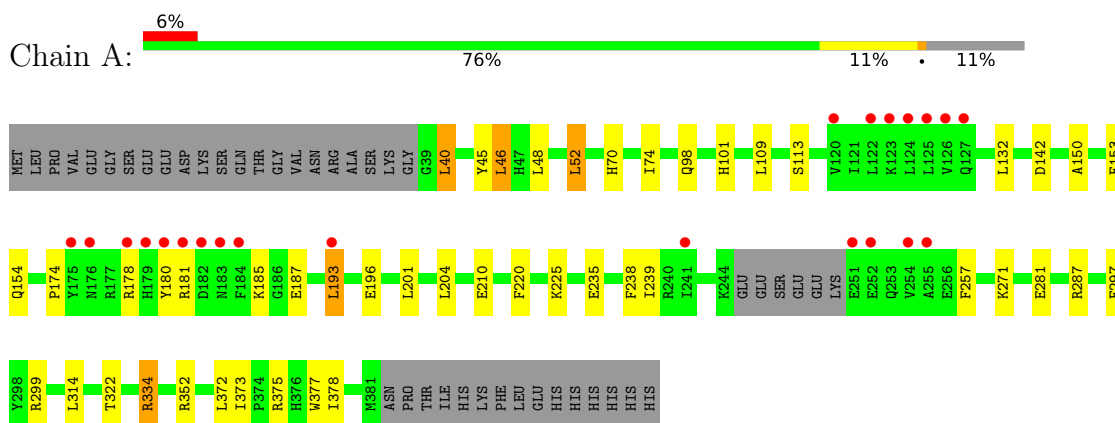
- Molecule 1: Tryptophan 2,3-dioxygenase

- Molecule 1: Tryptophan 2,3-dioxygenase

• Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:
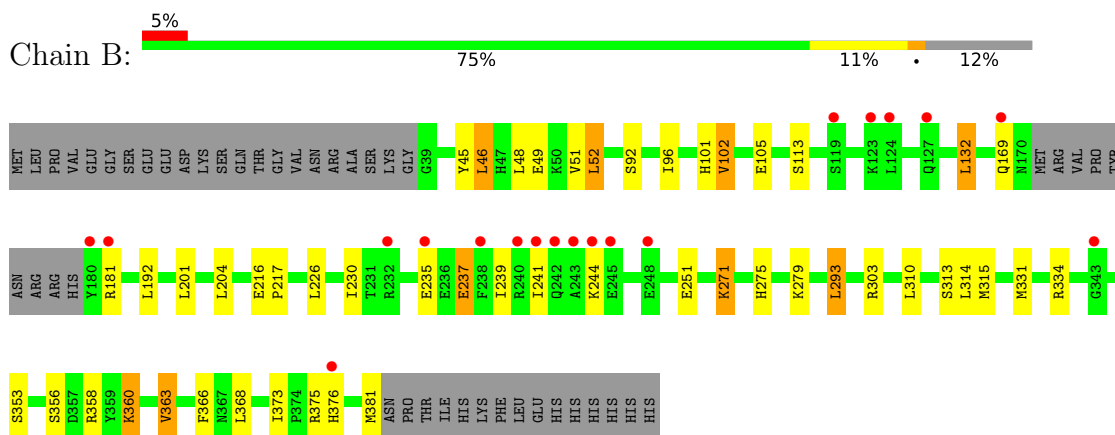
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.36Å 153.56Å 88.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.13 – 2.44 45.92 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.13-2.44) 99.3 (45.92-2.44)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.168 , 0.230 0.172 , 0.231	Depositor DCC
R_{free} test set	7379 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12061	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.40	0/2902	0.53	0/3904
1	B	0.41	1/2865 (0.0%)	0.53	0/3853
1	C	0.38	0/2777	0.50	0/3737
1	D	0.40	0/3011	0.55	1/4052 (0.0%)
All	All	0.40	1/11555 (0.0%)	0.53	1/15546 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	GLU	CD-OE2	6.51	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	MET	CG-SD-CE	-5.13	91.99	100.20

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	2837	0	2830	22	0
1	B	2803	0	2786	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2713	0	2703	32	0
1	D	2942	0	2926	28	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	30	0	18	0	0
3	B	30	0	18	1	0
3	C	30	0	18	0	0
3	D	30	0	18	1	0
4	A	102	0	0	1	0
4	B	127	0	0	3	0
4	C	103	0	0	2	0
4	D	142	0	0	3	0
All	All	12061	0	11437	115	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 5.

All (115) 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:A:150:ALA:HA	1:A:154:GLN:HE22	1.49	0.76
1:D:348:TYR:OH	1:D:352:ARG:NH1	2.25	0.69
1:D:96:ILE:HG22	1:D:102:VAL:HG13	1.75	0.68
1:A:220:PHE:O	1:A:225:LYS:NZ	2.25	0.67
1:A:299:ARG:HH22	1:A:375:ARG:HH22	1.42	0.67
1:C:380:LYS:HD3	1:C:380:LYS:H	1.58	0.67
1:D:68:ASP:HB3	1:D:135:MET:SD	2.36	0.66
2:D:401:HEM:HBC2	2:D:401:HEM:HHD	1.77	0.66
1:C:181:ARG:HG3	1:C:192:LEU:HD23	1.78	0.66
1:D:303:ARG:HD3	1:D:389:LEU:HA	1.80	0.63
1:C:375:ARG:NH1	4:C:501:HOH:O	2.32	0.62
1:B:315:MET:CE	1:D:334:ARG:HG3	2.32	0.59
1:C:133:GLU:HG3	1:C:331:MET:HE2	1.84	0.58
2:B:401:HEM:HBC2	2:B:401:HEM:HHD	1.86	0.58
1:A:98:GLN:NE2	4:A:501:HOH:O	2.37	0.57
1:B:315:MET:HE3	1:B:366:PHE:HA	1.87	0.57
1:B:105:GLU:OE1	3:B:403:TRP:N	2.38	0.57
1:B:51:VAL:HG12	1:B:52:LEU:HD13	1.86	0.57
1:A:299:ARG:HH22	1:A:375:ARG:NH2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD12	1:A:45:TYR:HB2	1.88	0.54
1:B:48:LEU:HB3	1:B:52:LEU:HD22	1.90	0.54
1:D:57:LEU:O	1:D:61:THR:HG23	2.07	0.54
1:D:369:SER:HA	1:D:372:LEU:HD13	1.88	0.54
1:C:373:ILE:HG13	1:C:377:TRP:HB2	1.89	0.54
1:A:352:ARG:HH11	1:C:356:SER:HA	1.73	0.54
1:C:47:HIS:ND1	1:C:49:GLU:OE1	2.42	0.53
1:D:342:THR:HG1	3:D:402:TRP:N	2.06	0.53
1:A:181:ARG:HH12	1:A:193:LEU:HD21	1.73	0.52
1:C:90:LEU:HD21	1:C:201:LEU:HD22	1.91	0.52
1:D:299:ARG:HH12	1:D:375:ARG:HH22	1.55	0.52
1:B:92:SER:O	1:B:96:ILE:HG12	2.10	0.52
1:C:360:LYS:HB3	1:C:363:VAL:HG13	1.90	0.52
1:C:334:ARG:HD2	4:C:579:HOH:O	2.10	0.52
1:B:356:SER:HB2	1:B:358:ARG:HH21	1.75	0.51
1:D:202:LEU:HD21	1:D:283:ARG:HB3	1.93	0.51
2:A:401:HEM:HBC2	2:A:401:HEM:HHD	1.93	0.50
1:B:216:GLU:H	1:B:216:GLU:CD	2.14	0.50
1:B:315:MET:HE2	1:D:334:ARG:HG3	1.93	0.50
1:B:315:MET:CE	1:B:366:PHE:HA	2.43	0.49
1:B:271:LYS:H	1:B:271:LYS:HD2	1.77	0.49
1:C:47:HIS:HA	1:C:49:GLU:OE1	2.13	0.49
1:C:51:VAL:HG12	1:C:52:LEU:HD13	1.95	0.48
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.72	0.48
1:C:64:ASN:OD1	1:C:146:TYR:OH	2.27	0.47
1:D:168:LEU:HD13	1:D:283:ARG:NH1	2.29	0.47
1:D:123:LYS:NZ	4:D:501:HOH:O	2.44	0.47
1:B:275:HIS:HB2	4:B:610:HOH:O	2.14	0.47
1:C:48:LEU:HB3	1:C:52:LEU:HD22	1.96	0.47
2:B:401:HEM:HHD	2:B:401:HEM:CBC	2.45	0.47
1:C:185:LYS:HA	1:C:189:ASN:HB2	1.96	0.47
1:B:334:ARG:HD2	4:B:593:HOH:O	2.13	0.47
1:C:57:LEU:O	1:C:61:THR:HG23	2.15	0.47
1:D:382:ASN:HB2	1:D:383:PRO:HD2	1.97	0.47
1:A:235:GLU:O	1:A:239:ILE:HG12	2.15	0.46
1:B:376:HIS:HB2	4:B:614:HOH:O	2.15	0.46
1:B:45:TYR:CD2	1:B:46:LEU:HD13	2.51	0.46
1:B:132:LEU:HB3	1:B:331:MET:CE	2.46	0.46
1:D:220:PHE:O	1:D:225:LYS:HE2	2.15	0.46
1:B:237:GLU:O	1:B:241:ILE:HG12	2.16	0.46
1:A:210:GLU:HG2	1:A:287:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HB3	1:A:52:LEU:HD22	1.97	0.46
1:B:235:GLU:O	1:B:239:ILE:HG12	2.16	0.46
1:C:42:TYR:HB2	1:D:154:GLN:HB2	1.98	0.46
1:A:109:LEU:O	1:A:113:SER:OG	2.26	0.45
1:C:202:LEU:HD21	1:C:283:ARG:HB3	1.98	0.45
1:A:45:TYR:CD2	1:A:46:LEU:HD13	2.51	0.45
1:C:220:PHE:CD2	1:C:385:ILE:HG13	2.51	0.45
1:A:334:ARG:O	1:A:334:ARG:HG3	2.16	0.45
1:B:358:ARG:HD2	1:B:358:ARG:H	1.82	0.45
1:D:58:GLN:O	1:D:62:LYS:HB2	2.17	0.45
1:B:315:MET:HE3	1:B:366:PHE:CA	2.47	0.45
2:B:401:HEM:HMB1	2:B:401:HEM:HBB2	1.99	0.44
1:A:142:ASP:OD1	1:C:375:ARG:NH2	2.50	0.44
1:D:216:GLU:HA	1:D:217:PRO:HD2	1.83	0.44
1:D:259:LYS:HD2	1:D:259:LYS:HA	1.75	0.44
1:D:45:TYR:CD2	1:D:46:LEU:HD13	2.53	0.44
1:D:194:LYS:HD2	1:D:194:LYS:HA	1.76	0.44
1:A:238:PHE:HB2	1:A:257:PHE:CZ	2.53	0.44
1:B:226:LEU:O	1:B:230:ILE:HG12	2.18	0.44
1:A:180:TYR:OH	1:A:196:GLU:OE2	2.36	0.43
1:C:380:LYS:HD3	1:C:380:LYS:N	2.30	0.43
1:C:385:ILE:HG22	1:C:389:LEU:HD23	2.00	0.43
1:D:123:LYS:O	1:D:127:GLN:HG2	2.18	0.43
1:D:334:ARG:HD2	4:D:580:HOH:O	2.18	0.43
1:C:58:GLN:O	1:C:62:LYS:HB2	2.19	0.43
1:C:293:LEU:HD13	1:C:368:LEU:HD22	2.00	0.43
1:B:244:LYS:HE2	1:B:244:LYS:HB3	1.90	0.43
1:B:303:ARG:HG2	1:C:391:HIS:HB2	2.01	0.43
2:A:401:HEM:HMB1	2:A:401:HEM:HBB2	2.02	0.42
1:B:96:ILE:HG22	1:B:102:VAL:HG13	2.01	0.42
1:B:192:LEU:HD12	1:B:192:LEU:HA	1.85	0.42
1:B:356:SER:OG	1:B:358:ARG:HD3	2.18	0.42
1:B:230:ILE:CD1	1:B:373:ILE:HG21	2.50	0.42
1:B:279:LYS:HB3	1:B:279:LYS:HE2	1.83	0.42
1:B:216:GLU:HA	1:B:217:PRO:HD3	1.80	0.42
1:A:70:HIS:CE1	1:A:74:ILE:HD13	2.54	0.42
1:D:179:HIS:CE1	1:D:181:ARG:HB2	2.55	0.42
1:C:79:TYR:CD1	2:C:401:HEM:HAC	2.55	0.42
2:D:401:HEM:HMB1	2:D:401:HEM:HBB2	2.01	0.42
2:D:401:HEM:HHD	2:D:401:HEM:CBC	2.49	0.41
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.76	0.41
1:A:299:ARG:HD3	1:C:138:LEU:HD13	2.03	0.41
1:B:293:LEU:HG	1:B:368:LEU:HD22	2.01	0.41
1:C:133:GLU:HG3	1:C:331:MET:CE	2.49	0.41
1:C:192:LEU:HD12	1:C:192:LEU:HA	1.89	0.41
1:D:59:SER:HB2	1:D:64:ASN:O	2.20	0.41
1:D:110:LYS:HE3	1:D:110:LYS:HB2	1.85	0.41
1:A:297:PHE:CG	1:A:378:ILE:HD12	2.56	0.41
1:B:360:LYS:O	1:B:363:VAL:HG22	2.21	0.41
1:C:216:GLU:HA	1:C:217:PRO:HD3	1.76	0.41
1:A:373:ILE:HD12	1:A:377:TRP:HB2	2.03	0.41
1:D:106:ARG:NH1	4:D:506:HOH:O	2.54	0.41
1:A:174:PRO:O	1:A:178:ARG:HG2	2.22	0.40
1:C:109:LEU:O	1:C:113:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	333/380 (88%)	324 (97%)	9 (3%)	0	100	100
1	B	330/380 (87%)	324 (98%)	6 (2%)	0	100	100
1	C	317/380 (83%)	310 (98%)	7 (2%)	0	100	100
1	D	345/380 (91%)	337 (98%)	8 (2%)	0	100	100
All	All	1325/1520 (87%)	1295 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	309/348 (89%)	292 (94%)	17 (6%)	21	28
1	B	306/348 (88%)	284 (93%)	22 (7%)	14	17
1	C	297/348 (85%)	274 (92%)	23 (8%)	13	15
1	D	321/348 (92%)	300 (94%)	21 (6%)	17	21
All	All	1233/1392 (89%)	1150 (93%)	83 (7%)	16	20

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	46	LEU
1	A	52	LEU
1	A	101	HIS
1	A	132	LEU
1	A	153	PHE
1	A	185	LYS
1	A	187	GLU
1	A	193	LEU
1	A	201	LEU
1	A	204	LEU
1	A	271	LYS
1	A	281	GLU
1	A	314	LEU
1	A	322	THR
1	A	334	ARG
1	A	372	LEU
1	B	46	LEU
1	B	49	GLU
1	B	52	LEU
1	B	101	HIS
1	B	102	VAL
1	B	113	SER
1	B	132	LEU

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Mol	Chain	Res	Type
1	B	169	GLN
1	B	181	ARG
1	B	201	LEU
1	B	204	LEU
1	B	237	GLU
1	B	271	LYS
1	B	293	LEU
1	B	310	LEU
1	B	313	SER
1	B	314	LEU
1	B	353	SER
1	B	360	LYS
1	B	363	VAL
1	B	375	ARG
1	B	381	MET
1	C	49	GLU
1	C	52	LEU
1	C	90	LEU
1	C	113	SER
1	C	132	LEU
1	C	148	SER
1	C	168	LEU
1	C	185	LYS
1	C	215	LEU
1	C	216	GLU
1	C	225	LYS
1	C	265	LEU
1	C	271	LYS
1	C	310	LEU
1	C	313	SER
1	C	314	LEU
1	C	318	ASP
1	C	319	SER
1	C	352	ARG
1	C	363	VAL
1	C	373	ILE
1	C	380	LYS
1	C	386	HIS
1	D	46	LEU
1	D	62	LYS
1	D	102	VAL
1	D	119	SER

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Mol	Chain	Res	Type
1	D	127	GLN
1	D	132	LEU
1	D	168	LEU
1	D	169	GLN
1	D	187	GLU
1	D	201	LEU
1	D	204	LEU
1	D	230	ILE
1	D	239	ILE
1	D	259	LYS
1	D	276	LEU
1	D	277	LEU
1	D	314	LEU
1	D	322	THR
1	D	352	ARG
1	D	363	VAL
1	D	386	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	170	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	TRP	B	403	-	14,16,16	0.87	1 (7%)	16,22,22	1.12	2 (12%)
2	HEM	C	401	1	41,50,50	1.99	6 (14%)	45,82,82	1.77	7 (15%)
2	HEM	D	401	1	41,50,50	1.90	6 (14%)	45,82,82	1.80	8 (17%)
2	HEM	A	401	1	41,50,50	1.97	8 (19%)	45,82,82	1.73	8 (17%)
2	HEM	B	401	1	41,50,50	1.88	5 (12%)	45,82,82	1.79	10 (22%)
3	TRP	C	402	-	14,16,16	0.89	1 (7%)	16,22,22	1.23	2 (12%)
3	TRP	D	402	-	14,16,16	0.85	1 (7%)	16,22,22	1.12	2 (12%)
3	TRP	B	402	-	14,16,16	0.94	1 (7%)	16,22,22	1.18	2 (12%)
3	TRP	A	402	-	14,16,16	0.87	0	16,22,22	1.07	2 (12%)
3	TRP	C	403	-	14,16,16	0.82	1 (7%)	16,22,22	1.23	2 (12%)
3	TRP	A	403	-	14,16,16	0.79	1 (7%)	16,22,22	1.16	2 (12%)
3	TRP	D	403	-	14,16,16	0.83	0	16,22,22	1.04	2 (12%)

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	TRP	B	403	-	-	0/7/8/8	0/2/2/2
2	HEM	C	401	1	-	4/12/54/54	-
2	HEM	D	401	1	-	2/12/54/54	-
2	HEM	A	401	1	-	2/12/54/54	-
2	HEM	B	401	1	-	2/12/54/54	-
3	TRP	C	402	-	-	3/7/8/8	0/2/2/2
3	TRP	D	402	-	-	1/7/8/8	0/2/2/2
3	TRP	B	402	-	-	2/7/8/8	0/2/2/2
3	TRP	A	402	-	-	1/7/8/8	0/2/2/2
3	TRP	C	403	-	-	0/7/8/8	0/2/2/2
3	TRP	A	403	-	-	0/7/8/8	0/2/2/2
3	TRP	D	403	-	-	0/7/8/8	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C3D-C2D	7.64	1.53	1.36
2	B	401	HEM	C3D-C2D	7.57	1.52	1.36
2	A	401	HEM	C3D-C2D	7.54	1.52	1.36
2	D	401	HEM	C3D-C2D	7.15	1.51	1.36
2	A	401	HEM	C3C-C2C	-5.37	1.32	1.40
2	C	401	HEM	C3C-C2C	-4.81	1.33	1.40
2	D	401	HEM	C3C-C2C	-4.75	1.33	1.40
2	B	401	HEM	C3C-C2C	-4.37	1.34	1.40
2	D	401	HEM	C3C-CAC	3.76	1.55	1.47
2	C	401	HEM	FE-ND	3.73	2.15	1.96
2	C	401	HEM	C3C-CAC	3.38	1.54	1.47
2	C	401	HEM	CAB-C3B	3.26	1.56	1.47
2	D	401	HEM	CAB-C3B	3.24	1.56	1.47
2	A	401	HEM	CAB-C3B	3.10	1.55	1.47
2	A	401	HEM	C3C-CAC	3.08	1.54	1.47
2	B	401	HEM	CAB-C3B	3.01	1.55	1.47
2	B	401	HEM	C3C-CAC	2.94	1.53	1.47
2	B	401	HEM	FE-ND	2.88	2.11	1.96
2	D	401	HEM	FE-ND	2.67	2.10	1.96
2	A	401	HEM	CAA-C2A	2.36	1.55	1.52
2	A	401	HEM	FE-NB	2.29	2.08	1.96
2	A	401	HEM	FE-ND	2.28	2.08	1.96
3	B	403	TRP	OXT-C	-2.25	1.23	1.30
3	C	402	TRP	OXT-C	-2.22	1.23	1.30
2	D	401	HEM	CMB-C2B	2.21	1.55	1.50
3	B	402	TRP	OXT-C	-2.21	1.23	1.30
2	C	401	HEM	CAA-C2A	2.20	1.55	1.52
3	D	402	TRP	OXT-C	-2.16	1.23	1.30
2	A	401	HEM	CMB-C2B	2.09	1.55	1.50
3	A	403	TRP	OXT-C	-2.05	1.23	1.30
3	C	403	TRP	OXT-C	-2.04	1.23	1.30

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	HEM	C4D-ND-C1D	6.07	111.34	105.07
2	A	401	HEM	C4D-ND-C1D	5.78	111.05	105.07
2	B	401	HEM	C4D-ND-C1D	5.64	110.90	105.07
2	D	401	HEM	C4D-ND-C1D	5.42	110.68	105.07
2	D	401	HEM	C4C-CHD-C1D	4.41	128.38	122.56
2	A	401	HEM	CBD-CAD-C3D	-4.34	100.58	112.63
2	D	401	HEM	CBD-CAD-C3D	-4.27	100.77	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	HEM	C4B-CHC-C1C	3.93	127.74	122.56
2	B	401	HEM	CBD-CAD-C3D	-3.83	101.99	112.63
2	D	401	HEM	CBA-CAA-C2A	-3.80	106.14	112.62
2	B	401	HEM	C4C-CHD-C1D	3.69	127.43	122.56
2	C	401	HEM	CBD-CAD-C3D	-3.46	103.00	112.63
2	A	401	HEM	C4C-CHD-C1D	3.41	127.06	122.56
3	C	402	TRP	OXT-C-O	-3.12	117.01	124.09
2	C	401	HEM	CBA-CAA-C2A	-3.10	107.32	112.62
2	A	401	HEM	C1B-NB-C4B	3.10	108.27	105.07
2	B	401	HEM	C1B-NB-C4B	2.92	108.09	105.07
3	B	402	TRP	OXT-C-O	-2.86	117.59	124.09
2	C	401	HEM	C1B-NB-C4B	2.77	107.94	105.07
2	B	401	HEM	CMA-C3A-C4A	-2.73	124.26	128.46
3	A	403	TRP	OXT-C-O	-2.68	118.01	124.09
3	C	403	TRP	OXT-C-CA	2.65	122.41	113.38
3	D	402	TRP	OXT-C-O	-2.63	118.11	124.09
2	D	401	HEM	CMD-C2D-C1D	2.63	129.05	125.04
2	B	401	HEM	C3B-C2B-C1B	2.59	108.41	106.49
3	C	403	TRP	OXT-C-O	-2.57	118.26	124.09
2	A	401	HEM	C4B-CHC-C1C	2.56	125.93	122.56
3	B	403	TRP	OXT-C-O	-2.49	118.43	124.09
2	B	401	HEM	C2C-C3C-C4C	2.46	108.62	106.90
2	A	401	HEM	C3B-C2B-C1B	2.45	108.31	106.49
3	A	403	TRP	OXT-C-CA	2.40	121.57	113.38
2	B	401	HEM	CHA-C4D-ND	2.36	127.30	124.38
2	D	401	HEM	CAD-C3D-C4D	2.35	128.76	124.66
3	C	402	TRP	OXT-C-CA	2.34	121.34	113.38
2	C	401	HEM	C3B-C2B-C1B	2.22	108.13	106.49
3	D	403	TRP	OXT-C-O	-2.21	119.06	124.09
3	D	402	TRP	OXT-C-CA	2.21	120.92	113.38
2	D	401	HEM	C4B-CHC-C1C	2.21	125.47	122.56
2	D	401	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
3	B	403	TRP	OXT-C-CA	2.12	120.61	113.38
3	A	402	TRP	OXT-C-O	-2.12	119.28	124.09
2	A	401	HEM	CMD-C2D-C1D	2.12	128.26	125.04
2	A	401	HEM	C4A-C3A-C2A	2.09	108.45	107.00
2	C	401	HEM	C3C-C4C-NC	-2.09	107.00	110.94
2	B	401	HEM	C4A-C3A-C2A	2.08	108.44	107.00
2	B	401	HEM	CHD-C1D-ND	2.05	126.66	124.43
3	B	402	TRP	OXT-C-CA	2.02	120.26	113.38
3	D	403	TRP	OXT-C-CA	2.01	120.23	113.38
3	A	402	TRP	OXT-C-CA	2.01	120.22	113.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	TRP	CA-CB-CG-CD1
3	B	402	TRP	CA-CB-CG-CD1
3	C	402	TRP	CA-CB-CG-CD1
3	D	402	TRP	CA-CB-CG-CD1
2	A	401	HEM	CAA-CBA-CGA-O1A
2	D	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O1A
2	C	401	HEM	CAA-CBA-CGA-O2A
3	B	402	TRP	O-C-CA-N
2	A	401	HEM	CAA-CBA-CGA-O2A
3	C	402	TRP	OXT-C-CA-CB
2	B	401	HEM	CAA-CBA-CGA-O1A
2	B	401	HEM	CAA-CBA-CGA-O2A
2	D	401	HEM	CAA-CBA-CGA-O2A
3	C	402	TRP	O-C-CA-CB
2	C	401	HEM	CAD-CBD-CGD-O2D
2	C	401	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.
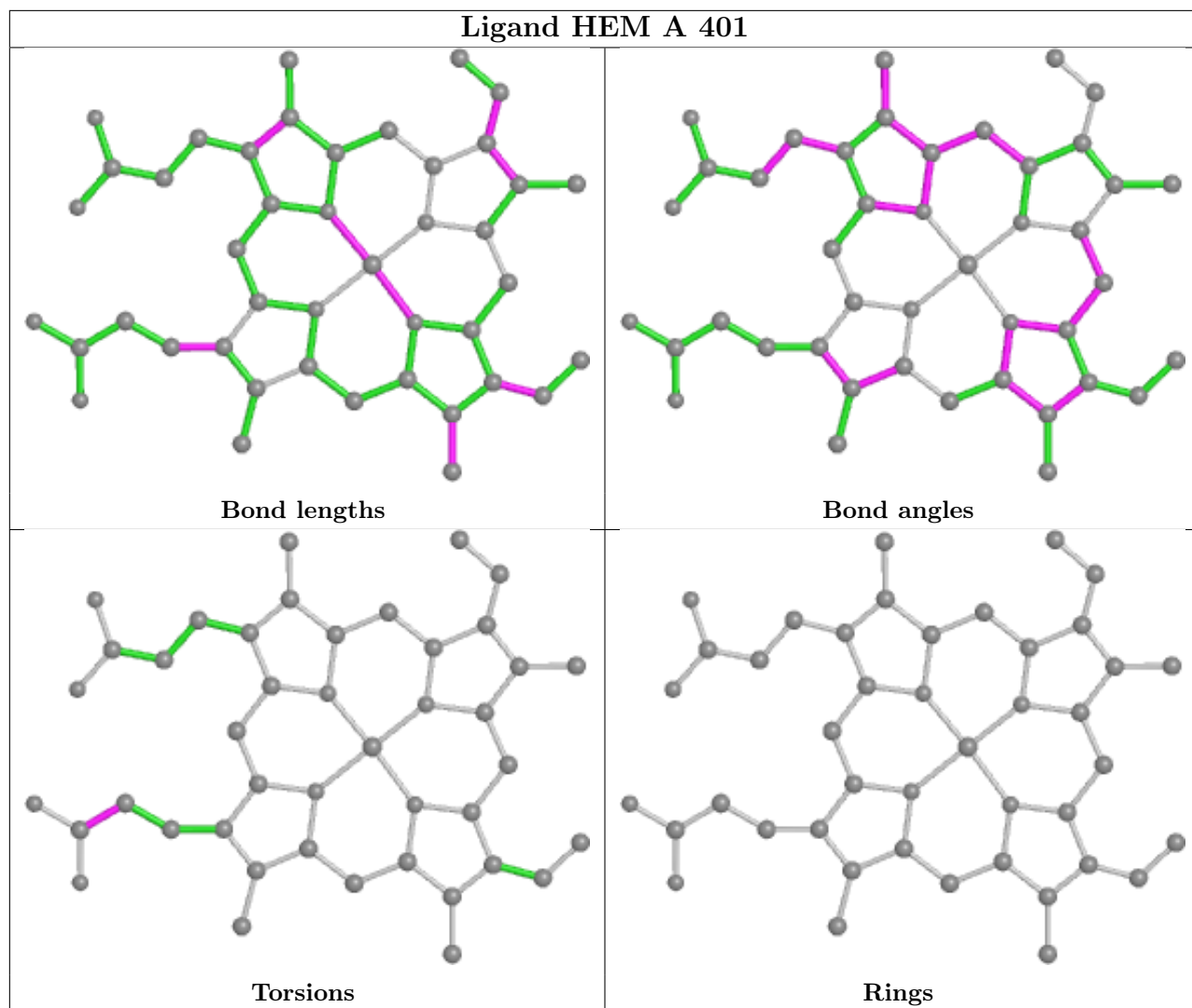
6 monomers are involved in 12 short contacts:

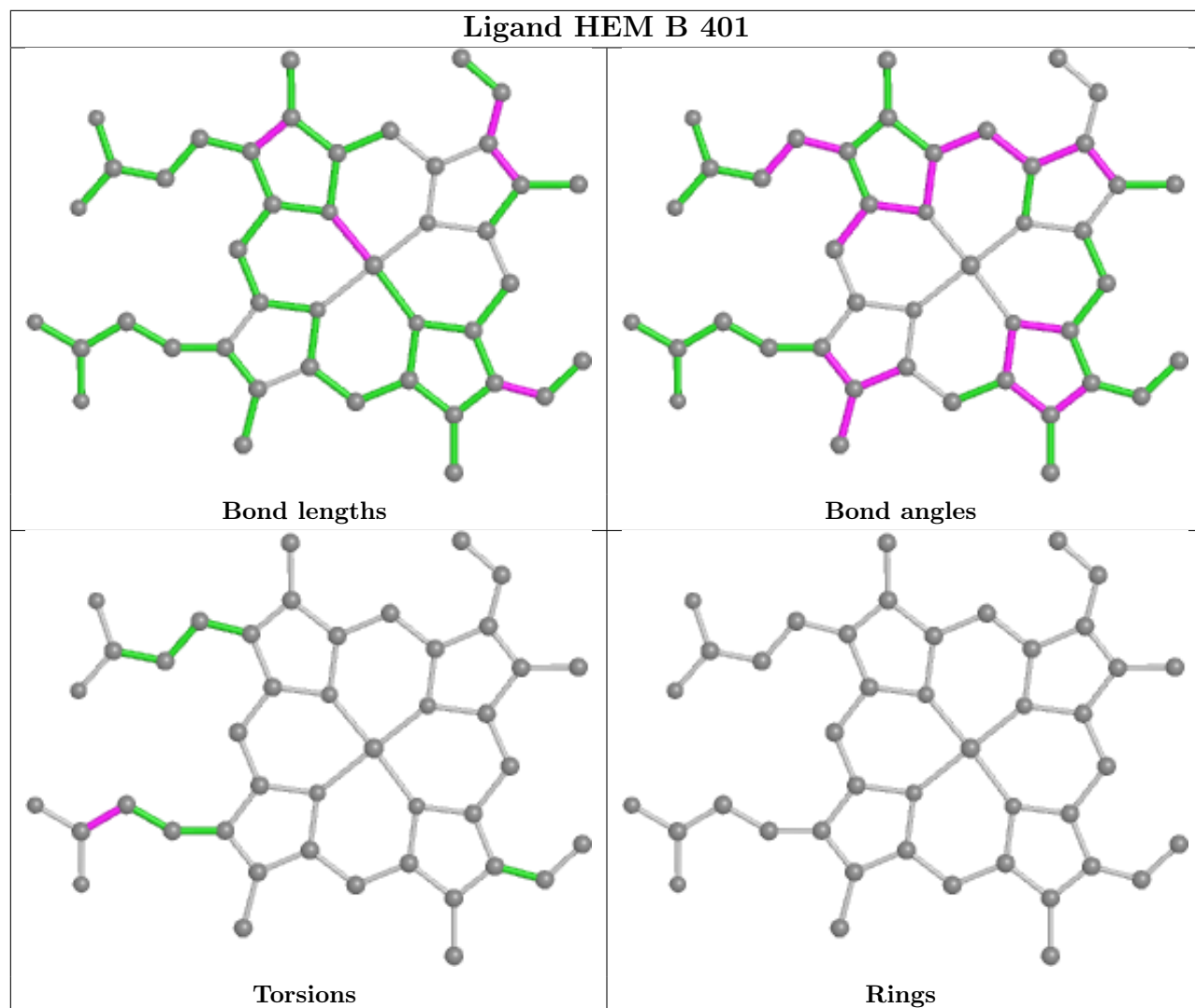| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	TRP	1	0
2	C	401	HEM	2	0
2	D	401	HEM	3	0
2	A	401	HEM	2	0
2	B	401	HEM	3	0
3	D	402	TRP	1	0

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 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 401

Bond lengths

Bond angles

Torsions

Rings
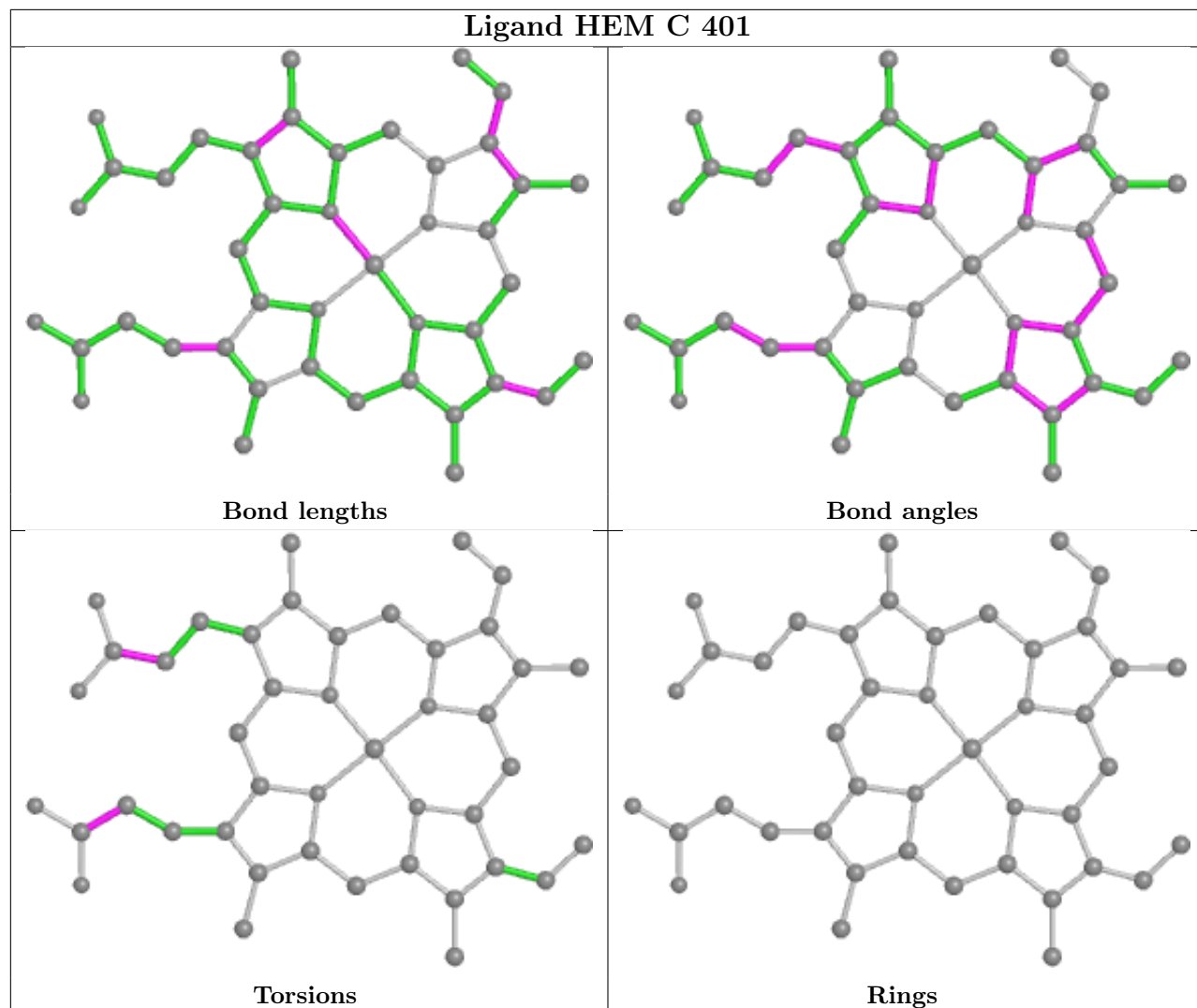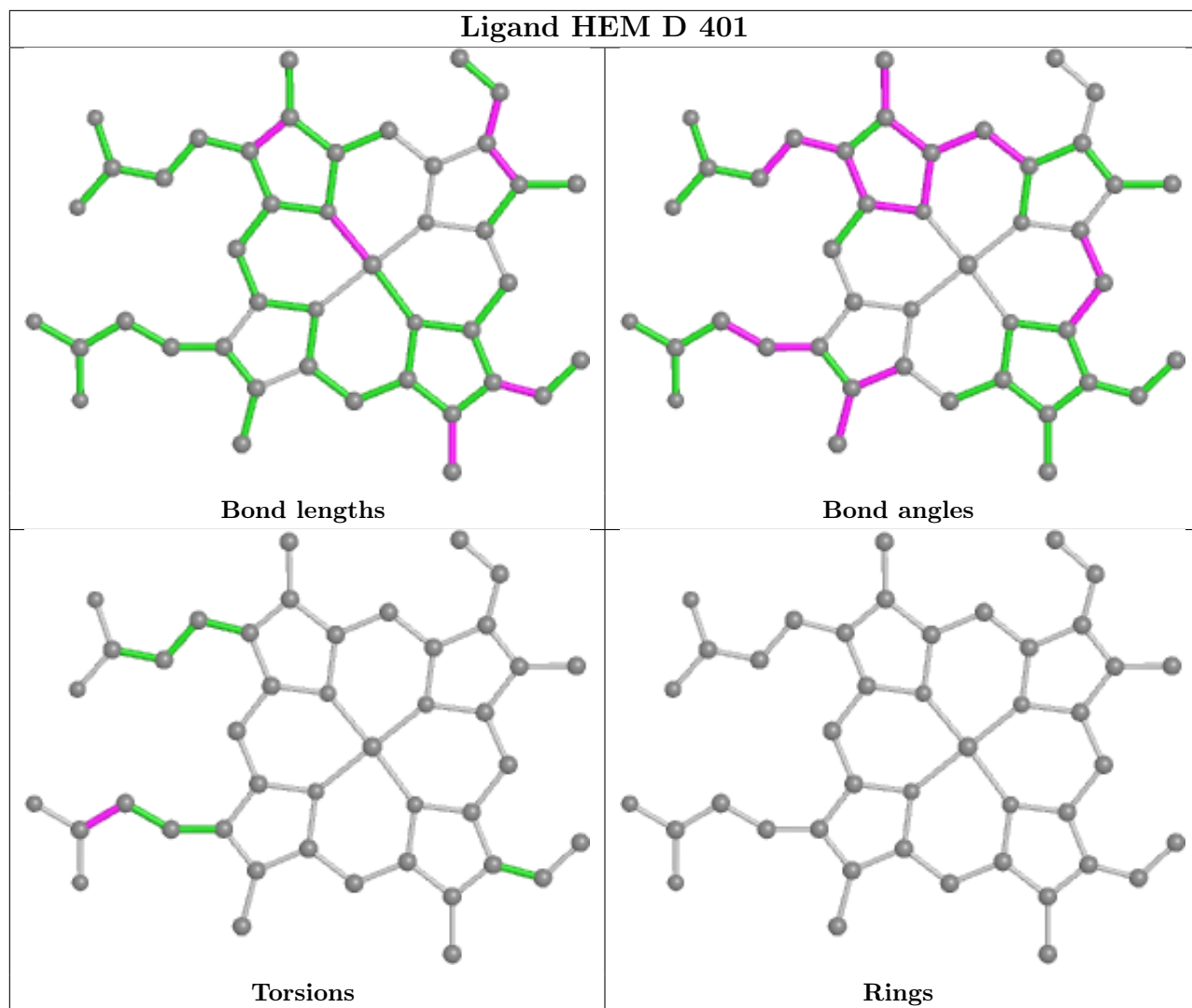
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data   ⓘ

6.1   Protein, DNA and RNA chains   ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	337/380 (88%)	0.01	22 (6%)	18	15	32, 48, 88, 129	0
1	B	334/380 (87%)	0.07	19 (5%)	23	20	31, 46, 87, 125	0
1	C	323/380 (85%)	0.48	49 (15%)	2	1	32, 53, 104, 134	0
1	D	349/380 (91%)	0.18	28 (8%)	12	9	32, 47, 95, 158	0
All	All	1343/1520 (88%)	0.18	118 (8%)	10	7	31, 48, 93, 158	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	385	ILE	7.7
1	D	383	PRO	5.8
1	C	384	THR	5.3
1	B	169	GLN	4.8
1	C	385	ILE	4.7
1	D	384	THR	4.6
1	C	383	PRO	4.5
1	D	248	GLU	4.3
1	C	180	TYR	4.1
1	C	271	LYS	4.1
1	C	182	ASP	4.0
1	C	275	HIS	4.0
1	A	193	LEU	4.0
1	B	181	ARG	3.9
1	C	232	ARG	3.8
1	A	180	TYR	3.8
1	C	193	LEU	3.7
1	D	388	PHE	3.7
1	D	255	ALA	3.6
1	C	181	ARG	3.5
1	D	386	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	231	THR	3.4
1	C	219	GLY	3.3
1	C	224	GLY	3.3
1	D	254	VAL	3.3
1	B	241	ILE	3.3
1	A	254	VAL	3.2
1	B	244	LYS	3.1
1	A	241	ILE	3.1
1	D	389	LEU	3.0
1	C	386	HIS	3.0
1	C	221	ASN	3.0
1	C	258	GLN	3.0
1	A	251	GLU	2.9
1	C	277	LEU	2.9
1	C	279	LYS	2.9
1	D	218	HIS	2.9
1	B	376	HIS	2.9
1	A	252	GLU	2.8
1	C	272	ARG	2.8
1	B	235	GLU	2.8
1	B	232	ARG	2.8
1	D	124	LEU	2.8
1	A	179	HIS	2.8
1	D	123	LYS	2.7
1	C	123	LYS	2.7
1	D	126	VAL	2.7
1	A	182	ASP	2.7
1	D	250	LYS	2.6
1	C	236	GLU	2.6
1	A	123	LYS	2.6
1	C	273	HIS	2.6
1	D	251	GLU	2.6
1	C	229	ASN	2.6
1	D	125	LEU	2.6
1	C	230	ILE	2.6
1	C	257	PHE	2.6
1	A	175	TYR	2.6
1	C	387	LYS	2.5
1	C	276	LEU	2.5
1	B	180	TYR	2.5
1	C	344	GLY	2.5
1	C	233	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	275	HIS	2.5
1	C	274	GLU	2.5
1	C	278	SER	2.4
1	C	127	GLN	2.4
1	A	125	LEU	2.4
1	C	190	GLU	2.4
1	B	127	GLN	2.4
1	D	253	GLN	2.4
1	D	122	LEU	2.4
1	A	183	ASN	2.4
1	B	238	PHE	2.3
1	D	257	PHE	2.3
1	C	234	LEU	2.3
1	C	223	TRP	2.3
1	B	240	ARG	2.3
1	A	127	GLN	2.3
1	C	235	GLU	2.3
1	C	228	LYS	2.3
1	C	382	ASN	2.3
1	C	377	TRP	2.3
1	D	135	MET	2.3
1	D	259	LYS	2.2
1	C	122	LEU	2.2
1	C	186	GLY	2.2
1	D	238	PHE	2.2
1	A	176	ASN	2.2
1	A	120	VAL	2.2
1	D	271	LYS	2.2
1	A	181	ARG	2.2
1	A	126	VAL	2.2
1	A	255	ALA	2.2
1	A	178	ARG	2.2
1	B	245	GLU	2.2
1	B	123	LYS	2.1
1	B	243	ALA	2.1
1	A	124	LEU	2.1
1	A	122	LEU	2.1
1	C	267	LEU	2.1
1	C	126	VAL	2.1
1	D	121	ILE	2.1
1	A	184	PHE	2.1
1	C	184	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	131	ILE	2.1
1	C	168	LEU	2.1
1	B	242	GLN	2.1
1	C	237	GLU	2.0
1	C	389	LEU	2.0
1	D	252	GLU	2.0
1	C	187	GLU	2.0
1	B	119	SER	2.0
1	B	124	LEU	2.0
1	D	249	GLU	2.0
1	B	343	GLY	2.0
1	C	222	PHE	2.0
1	B	248	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	TRP	C	402	15/15	0.95	0.14	46,51,58,60	0
3	TRP	C	403	15/15	0.95	0.14	37,51,58,60	0
3	TRP	B	403	15/15	0.96	0.11	35,41,51,56	0
2	HEM	C	401	43/43	0.96	0.13	29,43,57,59	0
3	TRP	A	402	15/15	0.96	0.13	41,51,58,58	0
2	HEM	A	401	43/43	0.97	0.13	30,48,61,64	0
2	HEM	B	401	43/43	0.97	0.12	30,40,45,47	0
3	TRP	A	403	15/15	0.97	0.11	30,45,55,63	0
3	TRP	B	402	15/15	0.98	0.12	32,45,49,51	0
2	HEM	D	401	43/43	0.98	0.14	29,40,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	TRP	D	402	15/15	0.98	0.13	32,39,45,46	0
3	TRP	D	403	15/15	0.98	0.15	35,41,70,71	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.
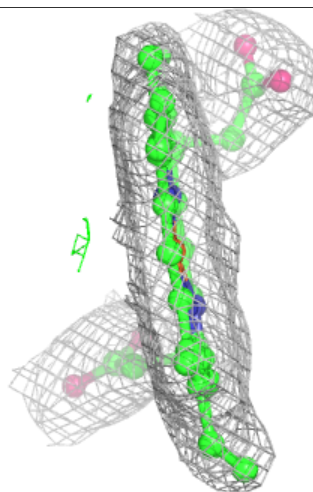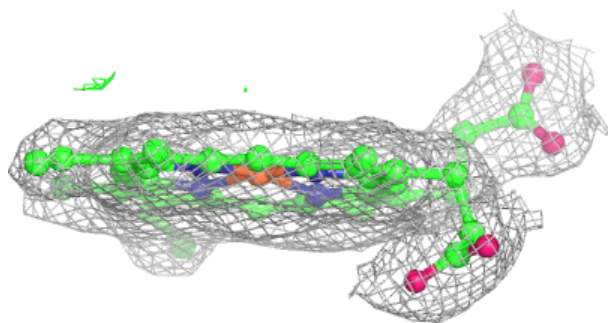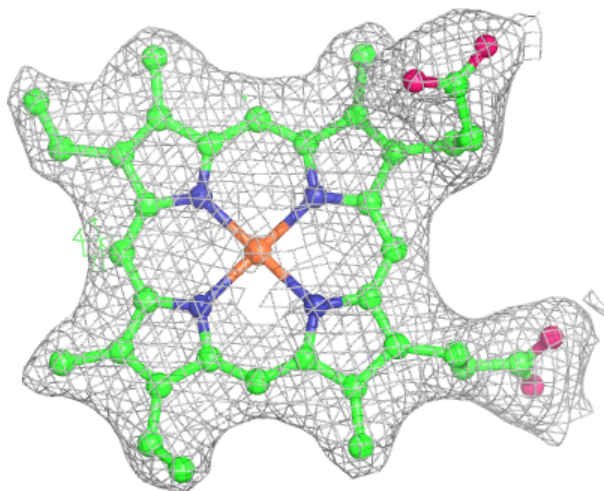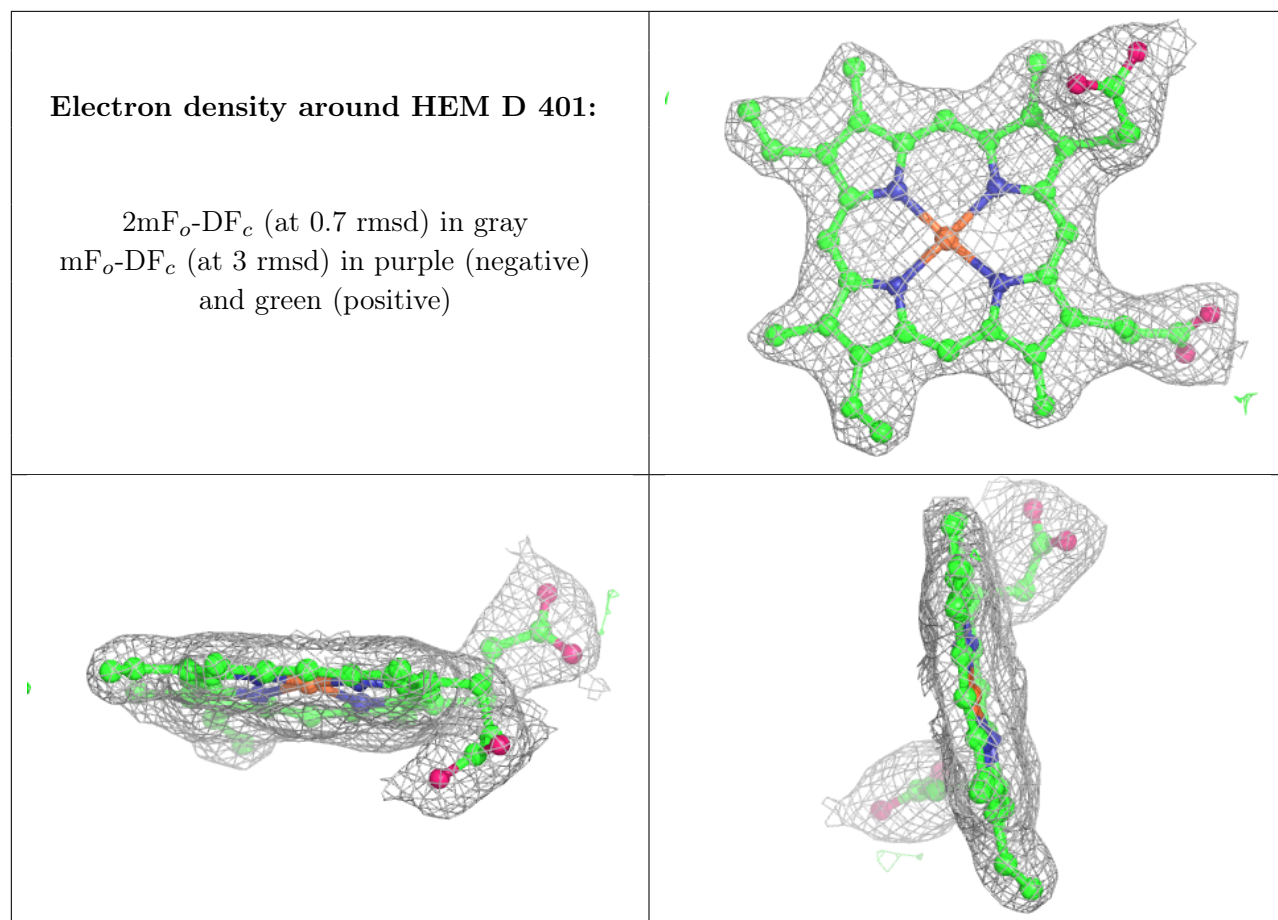
Electron density around HEM C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
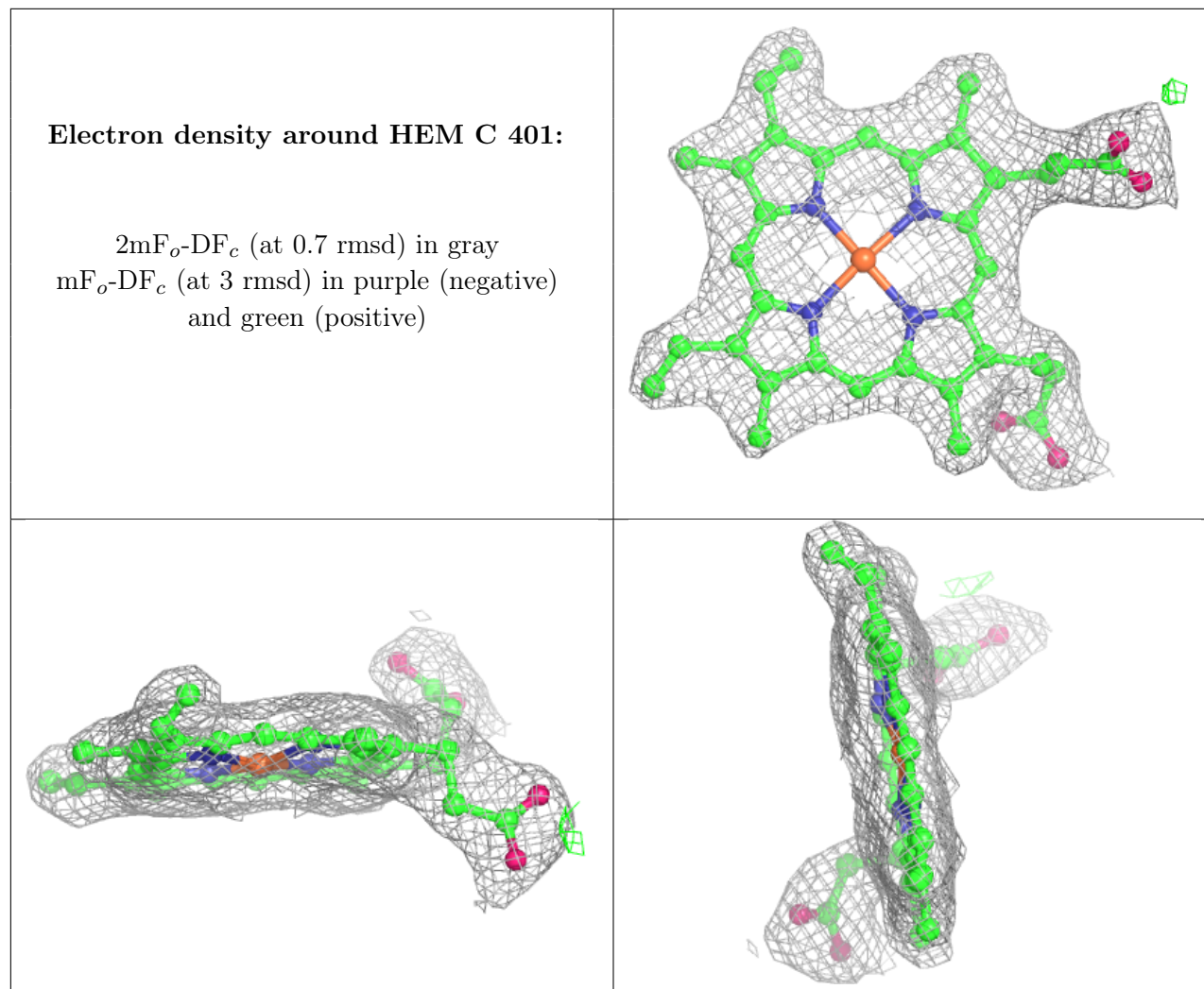
Electron density around HEM A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
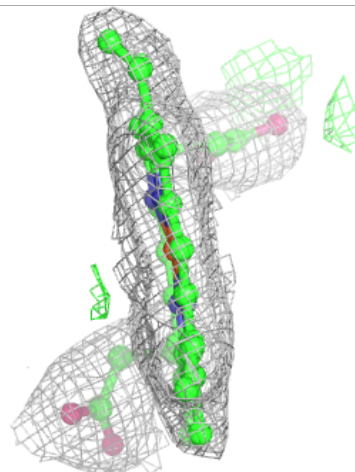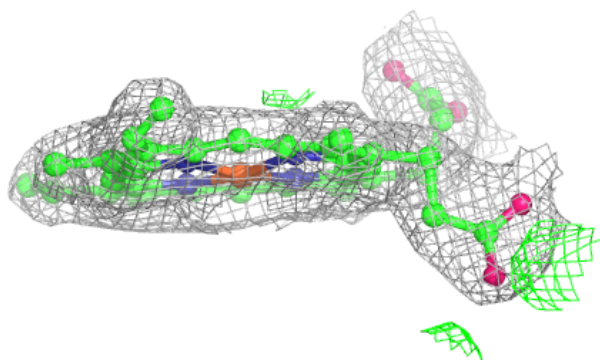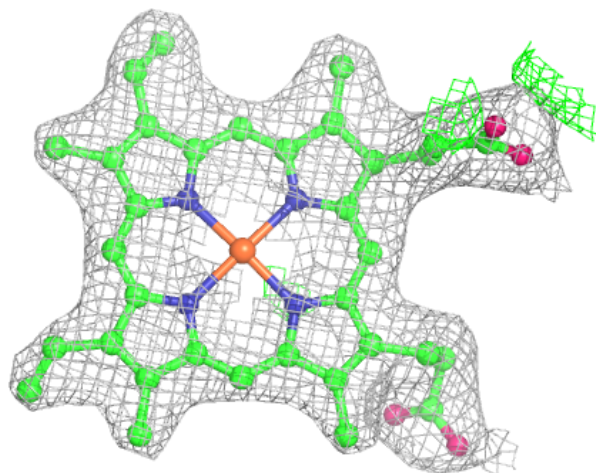
Electron density around HEM B 401:

$2mF_o$-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 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 ⓘ

There are no such residues in this entry.