Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:36 PM BST

PDB ID	:	4PNX
Title	:	Crystal structure of the complex of lactoperoxidase with bromo methane at 2.41 angstrom resolution
Authors	:	Sirohi, H.V.; Tyagi, T.K.; Singh, A.K.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2014-02-22
Resolution	:	2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

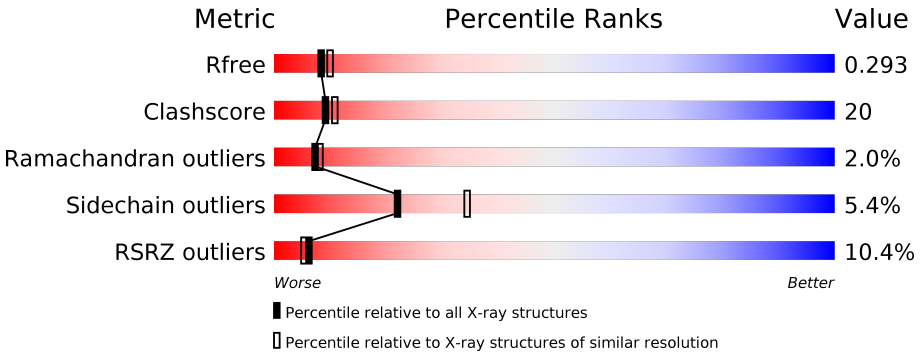
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 on 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	595	10%, 66%, 28%, 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BMM	A	607	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5000 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.

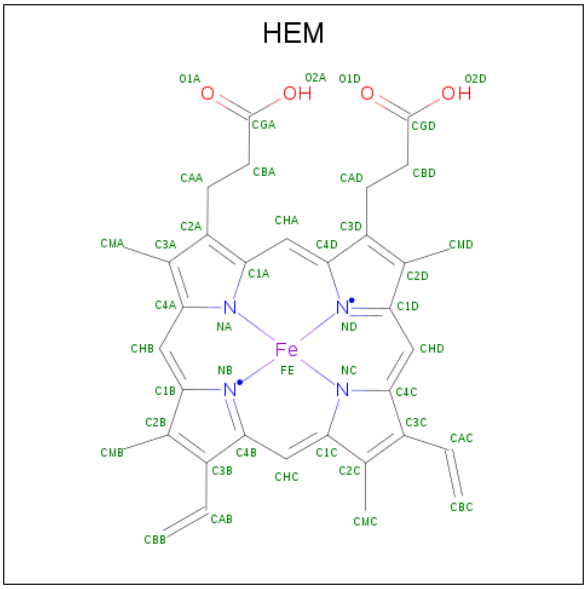
- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

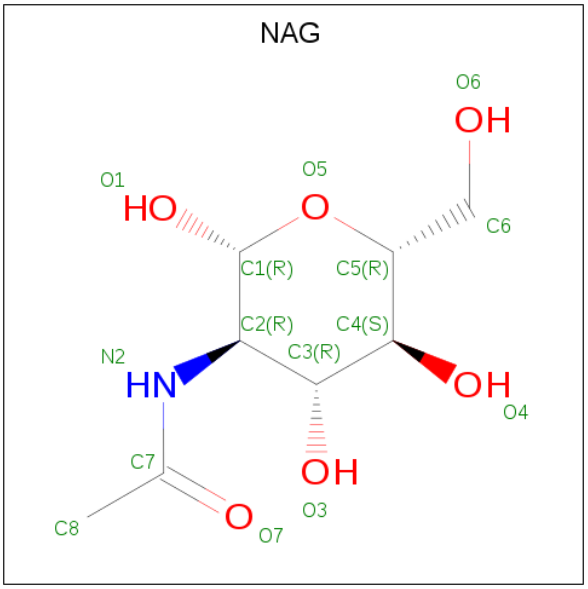
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



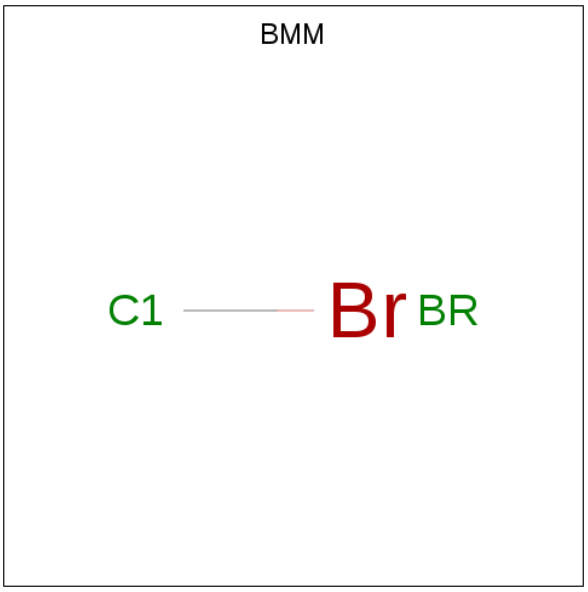
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BROMOMETHANE (three-letter code: BMM) (formula: CH_3Br).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Br	C	0	0
			2	1	1		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	I	0	0
			13	13		

- Molecule 7 is water.

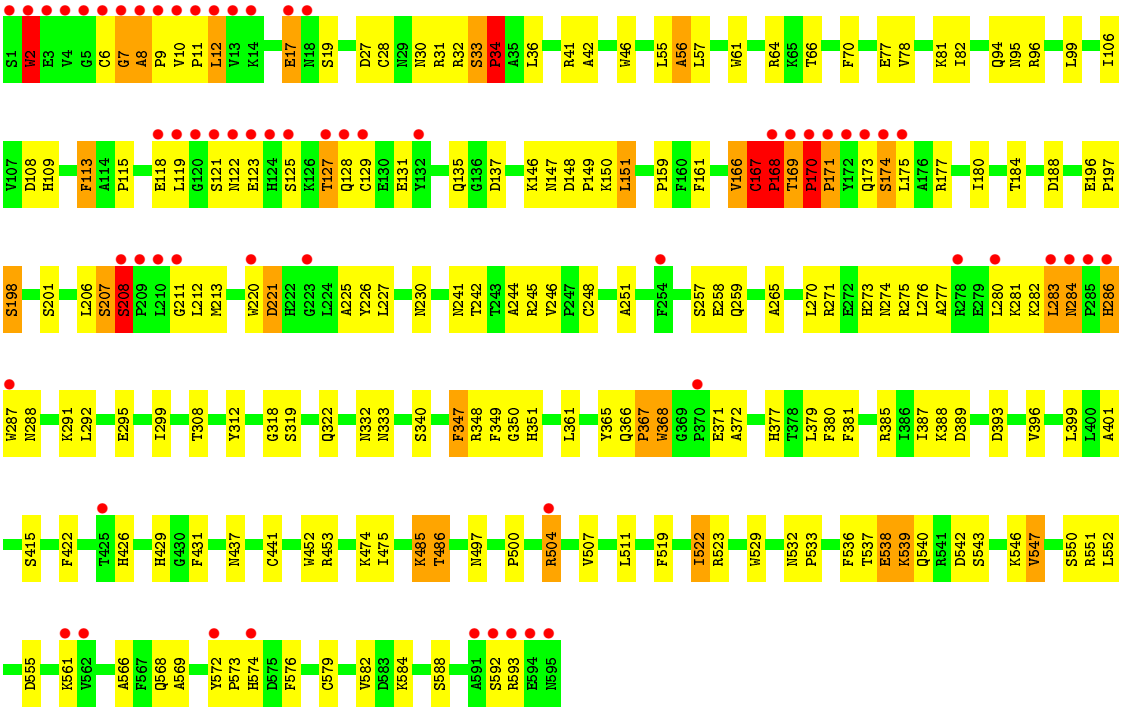
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	111	Total	O	0	0
			111	111		

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: Lactoperoxidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.74Å 80.38Å 73.18Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	71.15 – 2.41 34.99 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.0 (71.15-2.41) 99.0 (34.99-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.299 0.225 , 0.293	Depositor DCC
R_{free} test set	1192 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5000	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SEP, CA, BMM, HEM, IOD

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	0.85	2/4891 (0.0%)	0.98	32/6634 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CD	25.35	1.83	1.47
1	A	34	PRO	N-CD	23.72	1.81	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	SER	N-CA-CB	-13.31	90.54	110.50
1	A	168	PRO	CA-N-CD	-12.64	93.81	111.50
1	A	34	PRO	CA-N-CD	-11.02	96.08	111.50
1	A	113	PHE	CB-CA-C	10.10	130.59	110.40
1	A	485	LYS	CB-CA-C	-9.68	91.04	110.40
1	A	547	VAL	CB-CA-C	-9.68	93.01	111.40
1	A	283	LEU	CB-CA-C	9.67	128.58	110.20
1	A	208	SER	N-CA-CB	-9.57	96.14	110.50
1	A	34	PRO	N-CA-CB	9.30	114.46	103.30
1	A	2	TRP	N-CA-C	-9.23	86.07	111.00
1	A	2	TRP	CB-CA-C	-9.08	92.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	579	CYS	CB-CA-C	8.62	127.63	110.40
1	A	113	PHE	N-CA-C	-7.84	89.82	111.00
1	A	167	CYS	N-CA-C	-7.52	90.70	111.00
1	A	170	PRO	N-CA-C	6.87	129.97	112.10
1	A	426	HIS	N-CA-CB	6.71	122.68	110.60
1	A	426	HIS	N-CA-C	-6.48	93.49	111.00
1	A	168	PRO	N-CA-C	-6.42	95.41	112.10
1	A	7	GLY	N-CA-C	-6.32	97.29	113.10
1	A	118	GLU	N-CA-C	5.83	126.75	111.00
1	A	368	TRP	CB-CA-C	5.79	121.98	110.40
1	A	137	ASP	CB-CA-C	-5.75	98.89	110.40
1	A	221	ASP	CA-C-N	-5.53	105.03	117.20
1	A	504	ARG	CB-CA-C	-5.52	99.35	110.40
1	A	453	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	486	THR	N-CA-CB	5.45	120.65	110.30
1	A	207	SER	C-N-CA	5.35	135.09	121.70
1	A	6	CYS	N-CA-C	-5.26	96.79	111.00
1	A	174	SER	N-CA-C	5.26	125.19	111.00
1	A	33	SER	C-N-CD	-5.24	109.08	120.60
1	A	151	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	170	PRO	C-N-CD	-5.08	109.41	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	Peptide
1	A	170	PRO	Peptide
1	A	2	TRP	Peptide
1	A	206	LEU	Mainchain
1	A	7	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4692	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	43	0	30	16	0
4	A	56	0	52	10	0
5	A	2	0	0	3	0
6	A	13	0	0	2	0
7	A	111	0	0	15	0
All	All	5000	0	4774	192	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 20.

All (192) 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:168:PRO:N	1:A:168:PRO:CD	1.83	1.37
1:A:34:PRO:N	1:A:34:PRO:CD	1.81	1.34
1:A:108:ASP:OD1	3:A:602:HEM:HMD3	1.14	1.24
1:A:258:GLU:OE2	3:A:602:HEM:HMB1	1.39	1.23
1:A:108:ASP:CG	3:A:602:HEM:HMD3	1.59	1.21
1:A:108:ASP:OD1	3:A:602:HEM:CMD	1.98	1.10
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.33	1.08
1:A:30:ASN:O	1:A:33:SER:O	1.71	1.08
1:A:108:ASP:OD2	3:A:602:HEM:CMD	2.07	1.03
1:A:108:ASP:CG	3:A:602:HEM:CMD	2.26	1.03
1:A:95:ASN:ND2	4:A:603:NAG:C1	2.22	1.02
1:A:95:ASN:HD22	4:A:603:NAG:C1	1.71	1.02
1:A:283:LEU:C	1:A:284:ASN:HD22	1.64	1.01
1:A:108:ASP:OD2	3:A:602:HEM:HMD2	1.61	1.01
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.46	0.98
1:A:30:ASN:HB3	1:A:33:SER:O	1.65	0.97
1:A:241:ASN:ND2	1:A:244:ALA:HB3	1.90	0.86
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.07	0.84
1:A:547:VAL:HG23	1:A:547:VAL:O	1.76	0.84
1:A:319:SER:HB3	1:A:504:ARG:HH12	1.42	0.84
1:A:284:ASN:N	1:A:284:ASN:HD22	1.70	0.83
1:A:241:ASN:HD21	1:A:244:ALA:CB	1.93	0.81
1:A:33:SER:HB3	1:A:36:LEU:HD12	1.62	0.80
1:A:258:GLU:CD	3:A:602:HEM:HMB1	2.01	0.80
1:A:318:GLY:HA3	1:A:504:ARG:O	1.82	0.78
1:A:17:GLU:HB3	1:A:31:ARG:CD	2.13	0.77
1:A:318:GLY:CA	1:A:504:ARG:O	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:O	1:A:12:LEU:HB2	1.88	0.73
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.20	0.73
1:A:241:ASN:HD21	1:A:244:ALA:HB2	1.54	0.73
1:A:108:ASP:OD2	3:A:602:HEM:HMD3	1.80	0.73
1:A:33:SER:C	1:A:34:PRO:CD	2.57	0.73
1:A:284:ASN:N	1:A:284:ASN:ND2	2.30	0.72
1:A:319:SER:HB3	1:A:504:ARG:NH1	2.04	0.72
1:A:561:LYS:HD2	1:A:576:PHE:HB3	1.71	0.71
1:A:17:GLU:HB3	1:A:31:ARG:HD3	1.72	0.71
1:A:241:ASN:ND2	1:A:244:ALA:CB	2.52	0.71
1:A:241:ASN:ND2	4:A:605:NAG:C1	2.53	0.71
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.21	0.71
1:A:295:GLU:O	1:A:299:ILE:HG13	1.91	0.70
1:A:242:THR:O	1:A:245:ARG:HG3	1.92	0.69
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.90	0.69
1:A:149:PRO:HG2	6:A:619:IOD:I	2.64	0.68
1:A:422:PHE:CD1	1:A:429:HIS:CE1	2.83	0.67
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.19	0.66
1:A:283:LEU:C	1:A:284:ASN:ND2	2.45	0.66
1:A:167:CYS:CB	1:A:168:PRO:CD	2.74	0.66
1:A:95:ASN:ND2	4:A:603:NAG:C2	2.58	0.65
1:A:95:ASN:HD21	4:A:603:NAG:C2	2.10	0.65
1:A:275:ARG:HH11	1:A:555:ASP:CB	2.10	0.65
1:A:286:HIS:N	1:A:286:HIS:ND1	2.39	0.65
1:A:257:SER:O	1:A:381:PHE:HA	1.96	0.65
1:A:128:GLN:HB2	7:A:752:HOH:O	1.96	0.64
1:A:207:SER:O	1:A:208:SER:HB3	1.97	0.63
1:A:108:ASP:OD1	3:A:602:HEM:C2D	2.51	0.63
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.46	0.63
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.36	0.61
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.36	0.61
1:A:95:ASN:HB3	1:A:96:ARG:NH1	2.16	0.61
1:A:286:HIS:HE2	1:A:592:SER:HB3	1.66	0.60
1:A:56:ALA:HB2	1:A:177:ARG:HB2	1.83	0.60
1:A:127:THR:O	1:A:131:GLU:HB2	2.00	0.60
1:A:30:ASN:CB	1:A:33:SER:O	2.47	0.60
1:A:129:CYS:HB3	1:A:161:PHE:CZ	2.37	0.59
1:A:166:VAL:HG13	1:A:180:ILE:HG12	1.83	0.59
1:A:225:ALA:O	1:A:271:ARG:NH2	2.32	0.59
1:A:258:GLU:OE1	3:A:602:HEM:CMB	2.51	0.59
1:A:547:VAL:O	1:A:547:VAL:CG2	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	1:A:347:PHE:HB3	2.04	0.58
1:A:284:ASN:OD1	1:A:287:TRP:CZ2	2.56	0.58
1:A:109:HIS:NE2	5:A:607:BMM:C1	2.67	0.58
1:A:281:LYS:C	1:A:283:LEU:H	2.05	0.58
1:A:220:TRP:HB3	7:A:785:HOH:O	2.04	0.57
1:A:258:GLU:O	1:A:380:PHE:HA	2.04	0.57
1:A:2:TRP:CD1	1:A:175:LEU:HD11	2.39	0.57
1:A:32:ARG:CB	7:A:801:HOH:O	2.52	0.57
1:A:551:ARG:NH2	1:A:555:ASP:OD1	2.29	0.56
1:A:42:ALA:HB2	1:A:166:VAL:HG21	1.87	0.56
1:A:55:LEU:O	1:A:56:ALA:HB2	2.05	0.55
1:A:10:VAL:HG13	1:A:10:VAL:O	2.05	0.55
1:A:146:LYS:HG2	1:A:147:ASN:ND2	2.22	0.55
1:A:368:TRP:O	1:A:372:ALA:HB2	2.06	0.55
1:A:56:ALA:CB	1:A:177:ARG:HB2	2.38	0.54
1:A:167:CYS:O	1:A:168:PRO:O	2.25	0.54
1:A:241:ASN:OD1	1:A:241:ASN:C	2.44	0.54
1:A:220:TRP:CB	7:A:785:HOH:O	2.55	0.54
1:A:422:PHE:HB2	1:A:429:HIS:CD2	2.44	0.53
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.89	0.53
3:A:602:HEM:CMB	3:A:602:HEM:HBB2	2.38	0.53
1:A:207:SER:O	1:A:208:SER:CB	2.56	0.53
1:A:211:GLY:C	7:A:757:HOH:O	2.47	0.53
1:A:275:ARG:HH11	1:A:555:ASP:HB2	1.72	0.53
1:A:568:GLN:HB2	7:A:717:HOH:O	2.10	0.52
1:A:27:ASP:O	1:A:28:CYS:HB2	2.10	0.52
1:A:385:ARG:O	1:A:389:ASP:HB3	2.09	0.52
1:A:574:HIS:O	1:A:574:HIS:CG	2.62	0.52
1:A:348:ARG:HD3	1:A:437:ASN:ND2	2.25	0.51
1:A:258:GLU:CD	3:A:602:HEM:CMB	2.76	0.51
1:A:543:SER:O	1:A:546:LYS:HB2	2.10	0.51
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.23	0.51
1:A:61:TRP:O	1:A:135:GLN:NE2	2.35	0.51
1:A:248:CYS:HB3	1:A:257:SER:OG	2.11	0.51
1:A:275:ARG:NH1	1:A:555:ASP:OD2	2.44	0.51
1:A:211:GLY:HA2	7:A:757:HOH:O	2.11	0.51
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.76	0.50
1:A:532:ASN:HD22	1:A:533:PRO:HD2	1.76	0.50
1:A:122:ASN:O	1:A:122:ASN:OD1	2.30	0.50
1:A:197:PRO:HD2	1:A:198:SEP:O2P	2.12	0.50
1:A:241:ASN:OD1	1:A:241:ASN:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:CG	4:A:605:NAG:C1	2.81	0.49
1:A:64:ARG:NH2	7:A:792:HOH:O	2.44	0.49
1:A:318:GLY:HA2	1:A:504:ARG:O	2.11	0.49
1:A:30:ASN:C	1:A:33:SER:O	2.49	0.49
1:A:361:LEU:CD1	1:A:401:ALA:HB3	2.42	0.49
1:A:551:ARG:NH1	1:A:582:VAL:O	2.46	0.48
1:A:281:LYS:C	1:A:283:LEU:N	2.67	0.48
1:A:78:VAL:HG13	1:A:82:ILE:HD12	1.95	0.48
1:A:365:TYR:HD1	1:A:401:ALA:HB2	1.78	0.48
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.49	0.47
1:A:33:SER:CA	1:A:34:PRO:CD	2.93	0.47
1:A:348:ARG:HG2	1:A:351:HIS:CE1	2.49	0.47
1:A:196:GLU:HB3	1:A:198:SEP:O2P	2.15	0.47
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.44	0.47
1:A:169:THR:H	1:A:170:PRO:CD	2.27	0.47
1:A:281:LYS:HD3	1:A:292:LEU:HD11	1.97	0.47
1:A:32:ARG:HB3	7:A:801:HOH:O	2.12	0.47
1:A:258:GLU:HG3	5:A:607:BMM:BR	2.70	0.47
1:A:332:ASN:ND2	4:A:606:NAG:C1	2.78	0.46
1:A:277:ALA:O	1:A:280:LEU:HB2	2.14	0.46
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.98	0.46
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.98	0.46
1:A:500:PRO:HD2	7:A:713:HOH:O	2.15	0.46
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.51	0.46
1:A:148:ASP:OD1	1:A:150:LYS:HB2	2.16	0.46
1:A:94:GLN:O	1:A:569:ALA:CB	2.64	0.46
1:A:273:HIS:HD2	1:A:274:ASN:OD1	1.99	0.45
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.51	0.45
1:A:246:VAL:HG11	1:A:387:ILE:HD13	1.96	0.45
1:A:350:GLY:HA3	3:A:602:HEM:CBC	2.46	0.45
1:A:538:GLU:HB3	1:A:539:LYS:HZ2	1.80	0.45
1:A:452:TRP:HH2	6:A:608:IOD:I	2.69	0.45
1:A:106:ILE:HD11	1:A:265:ALA:HB3	1.99	0.45
1:A:348:ARG:NH2	3:A:602:HEM:HAD1	2.31	0.45
1:A:119:LEU:HD22	1:A:170:PRO:HA	1.97	0.45
1:A:287:TRP:HB3	1:A:291:LYS:HB3	1.99	0.45
1:A:57:LEU:HD22	1:A:61:TRP:CD1	2.52	0.45
1:A:291:LYS:O	1:A:295:GLU:HB2	2.17	0.45
1:A:241:ASN:HD21	4:A:605:NAG:C1	2.27	0.45
1:A:66:THR:HB	1:A:70:PHE:O	2.17	0.45
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:OD1	1:A:230:ASN:C	2.54	0.44
1:A:113:PHE:CZ	1:A:115:PRO:HB3	2.52	0.44
1:A:507:VAL:HB	1:A:511:LEU:HB2	1.99	0.44
1:A:56:ALA:HB2	1:A:177:ARG:CB	2.46	0.44
1:A:32:ARG:HB2	7:A:801:HOH:O	2.15	0.44
1:A:241:ASN:O	1:A:241:ASN:CG	2.55	0.44
1:A:396:VAL:HA	1:A:399:LEU:HD12	2.01	0.43
1:A:366:GLN:OE1	1:A:367:PRO:HD2	2.17	0.43
1:A:572:TYR:HA	1:A:573:PRO:HA	1.69	0.43
1:A:212:LEU:N	7:A:757:HOH:O	2.50	0.43
1:A:551:ARG:HD3	1:A:584:LYS:CA	2.32	0.43
1:A:276:LEU:HD22	1:A:299:ILE:HD12	2.01	0.43
1:A:211:GLY:CA	7:A:757:HOH:O	2.66	0.43
1:A:109:HIS:CE1	5:A:607:BMM:C1	3.01	0.43
3:A:602:HEM:HBC2	3:A:602:HEM:HMC2	2.00	0.42
1:A:95:ASN:HB3	1:A:96:ARG:HH12	1.83	0.42
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.98	0.42
1:A:551:ARG:HE	1:A:555:ASP:CG	2.23	0.42
1:A:227:LEU:CD1	1:A:251:ALA:HB2	2.49	0.42
1:A:196:GLU:HB3	1:A:198:SEP:O1P	2.20	0.42
1:A:259:GLN:HA	1:A:379:LEU:O	2.20	0.42
1:A:291:LYS:HE2	7:A:796:HOH:O	2.19	0.42
1:A:10:VAL:HG23	1:A:41:ARG:HH22	1.84	0.42
1:A:94:GLN:O	1:A:569:ALA:HB3	2.20	0.41
1:A:286:HIS:HE2	1:A:592:SER:CB	2.33	0.41
1:A:17:GLU:HB3	1:A:31:ARG:HD2	2.01	0.41
1:A:308:THR:HA	1:A:312:TYR:HB3	2.03	0.41
1:A:332:ASN:CG	4:A:606:NAG:C1	2.89	0.41
1:A:537:THR:H	1:A:540:GLN:HB2	1.85	0.41
1:A:536:PHE:HB3	1:A:540:GLN:HB2	2.01	0.41
1:A:123:GLU:HG2	1:A:125:SER:OG	2.21	0.41
1:A:108:ASP:OD2	1:A:347:PHE:CD2	2.74	0.40
1:A:167:CYS:C	1:A:168:PRO:O	2.54	0.40
1:A:66:THR:HB	1:A:70:PHE:N	2.36	0.40
1:A:213:MET:HB3	1:A:270:LEU:HD11	2.02	0.40
1:A:30:ASN:O	1:A:33:SER:C	2.53	0.40
1:A:129:CYS:CB	1:A:161:PHE:CZ	3.04	0.40
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.39	0.40
1:A:333:ASN:ND2	7:A:801:HOH:O	2.52	0.40
1:A:593:ARG:HA	1:A:593:ARG:HD2	1.85	0.40
1:A:95:ASN:HD21	4:A:603:NAG:C7	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HG2	1:A:431:PHE:CE2	2.57	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	592/595 (100%)	527 (89%)	53 (9%)	12 (2%)	7 8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ALA
1	A	167	CYS
1	A	169	THR
1	A	171	PRO
1	A	208	SER
1	A	34	PRO
1	A	367	PRO
1	A	173	GLN
1	A	282	LYS
1	A	12	LEU
1	A	485	LYS
1	A	8	ALA

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	517/517 (100%)	489 (95%)	28 (5%)	22 34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	19	SER
1	A	127	THR
1	A	151	LEU
1	A	166	VAL
1	A	168	PRO
1	A	174	SER
1	A	201	SER
1	A	284	ASN
1	A	286	HIS
1	A	288	ASN
1	A	322	GLN
1	A	347	PHE
1	A	371	GLU
1	A	388	LYS
1	A	393	ASP
1	A	415	SER
1	A	441	CYS
1	A	474	LYS
1	A	475	ILE
1	A	486	THR
1	A	522	ILE
1	A	538	GLU
1	A	539	LYS
1	A	542	ASP
1	A	550	SER
1	A	552	LEU
1	A	588	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	122	ASN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	284	ASN
1	A	288	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	532	ASN
1	A	558	HIS
1	A	570	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	SEP	A	198	1	8,9,10	1.74	1 (12%)	8,12,14	1.96	2 (25%)

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
1	SEP	A	198	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.65	1.62	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	O3P-P-OG	4.44	118.54	106.73
1	A	198	SEP	OG-CB-CA	2.79	110.86	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	198	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 14 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	604	1	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
4	NAG	A	605	-	14,14,15	0.47	0	17,19,21	1.60	2 (11%)
3	HEM	A	602	1	27,50,50	2.19	6 (22%)	17,82,82	1.43	3 (17%)
4	NAG	A	606	-	14,14,15	0.58	0	17,19,21	2.59	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BMM	A	607	-	0,1,1	0.00	-	-		
4	NAG	A	603	-	14,14,15	0.58	0	17,19,21	1.78	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
4	NAG	A	603	-	-	2/6/23/26	0/1/1/1
3	HEM	A	602	1	-	0/6/54/54	-
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	606	-	-	0/6/23/26	0/1/1/1
4	NAG	A	605	-	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3B-C2B	-5.99	1.32	1.40
3	A	602	HEM	C3D-C2D	4.62	1.51	1.37
3	A	602	HEM	C3B-CAB	4.20	1.56	1.47
3	A	602	HEM	C3C-CAC	3.33	1.54	1.47
3	A	602	HEM	C3C-C2C	-3.31	1.35	1.40
3	A	602	HEM	CAA-C2A	2.17	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	NAG	C1-O5-C5	6.63	121.17	112.19
4	A	606	NAG	C1-O5-C5	6.20	120.59	112.19
4	A	605	NAG	C1-O5-C5	5.83	120.10	112.19
4	A	606	NAG	O5-C5-C6	4.38	114.06	107.20
4	A	606	NAG	C3-C4-C5	4.30	117.90	110.24
4	A	606	NAG	C4-C3-C2	4.23	117.22	111.02
3	A	602	HEM	CBA-CAA-C2A	-4.04	105.04	112.49
3	A	602	HEM	CBD-CAD-C3D	-2.63	107.64	112.48
3	A	602	HEM	CMC-C2C-C3C	2.34	129.05	124.68
4	A	604	NAG	O7-C7-N2	2.21	126.02	121.95
4	A	605	NAG	C6-C5-C4	-2.13	108.00	113.00
4	A	606	NAG	C2-N2-C7	2.10	125.89	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6

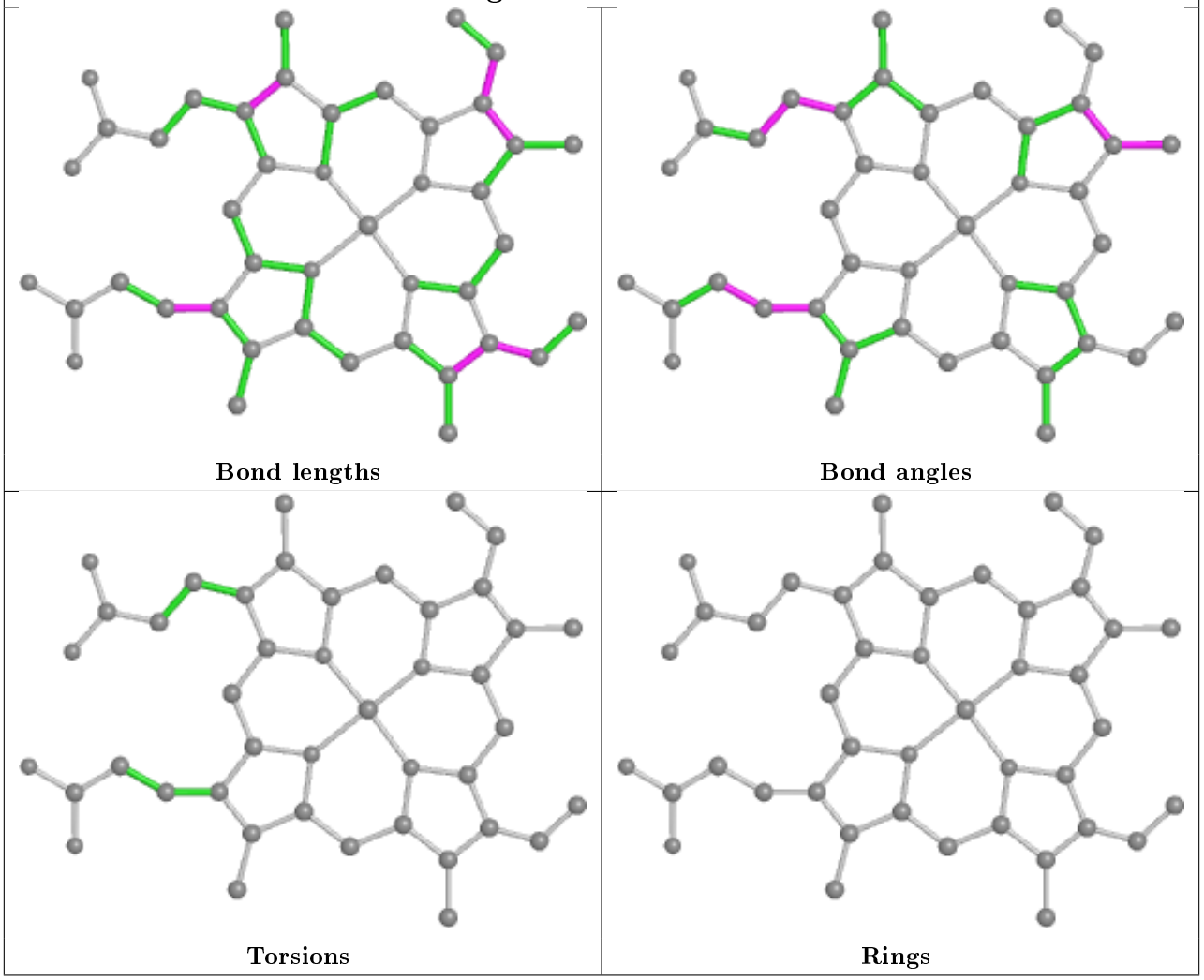
There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	NAG	3	0
3	A	602	HEM	16	0
4	A	606	NAG	2	0
5	A	607	BMM	3	0
4	A	603	NAG	5	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 A 602



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	594/595 (99%)	0.52	62 (10%) 6 5	14, 35, 72, 103	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	13.0
1	A	12	LEU	9.4
1	A	1	SER	8.8
1	A	120	GLY	8.6
1	A	170	PRO	7.9
1	A	121	SER	7.9
1	A	7	GLY	7.6
1	A	122	ASN	6.8
1	A	172	TYR	6.4
1	A	124	HIS	6.2
1	A	174	SER	5.8
1	A	171	PRO	5.7
1	A	4	VAL	5.6
1	A	119	LEU	5.6
1	A	173	GLN	5.6
1	A	132	TYR	5.1
1	A	595	ASN	5.1
1	A	175	LEU	4.8
1	A	118	GLU	4.5
1	A	8	ALA	4.5
1	A	125	SER	4.4
1	A	210	LEU	4.3
1	A	11	PRO	4.1
1	A	123	GLU	4.1
1	A	6	CYS	4.1
1	A	287	TRP	4.0
1	A	594	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	10	VAL	3.9
1	A	591	ALA	3.8
1	A	129	CYS	3.8
1	A	574	HIS	3.7
1	A	13	VAL	3.6
1	A	9	PRO	3.5
1	A	425	THR	3.5
1	A	18	ASN	3.4
1	A	17	GLU	3.4
1	A	169	THR	3.3
1	A	3	GLU	3.2
1	A	223	GLY	3.1
1	A	209	PRO	3.1
1	A	504	ARG	3.0
1	A	280	LEU	2.9
1	A	128	GLN	2.9
1	A	278	ARG	2.8
1	A	592	SER	2.8
1	A	562	VAL	2.8
1	A	593	ARG	2.7
1	A	168	PRO	2.7
1	A	561	LYS	2.6
1	A	284	ASN	2.6
1	A	5	GLY	2.5
1	A	208	SER	2.5
1	A	254	PHE	2.5
1	A	211	GLY	2.3
1	A	127	THR	2.3
1	A	286	HIS	2.3
1	A	220	TRP	2.3
1	A	370	PRO	2.3
1	A	285	PRO	2.3
1	A	283	LEU	2.3
1	A	572	TYR	2.2
1	A	14	LYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	A	198	10/11	0.82	0.23	41,43,53,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

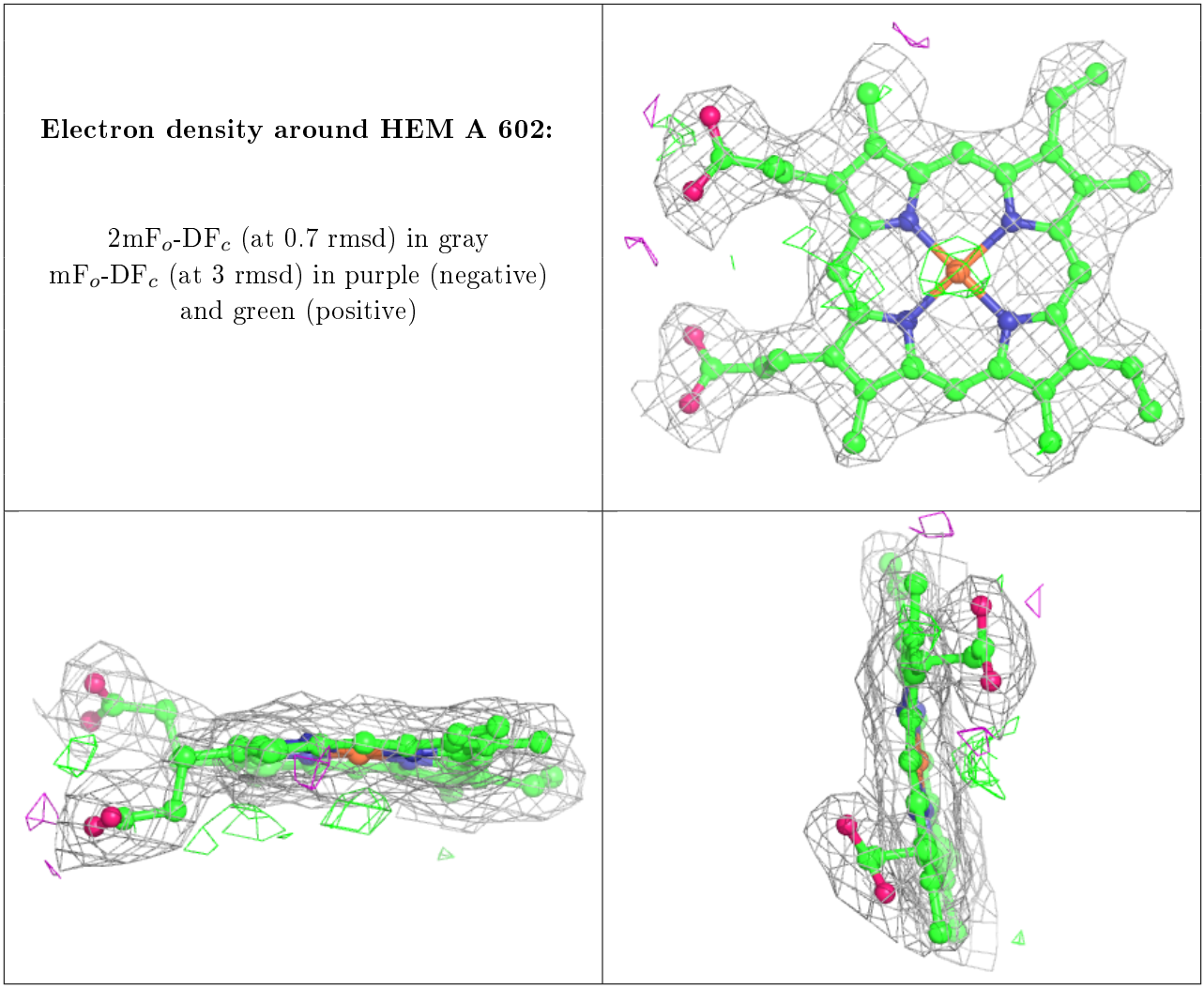
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	NAG	A	603	14/15	0.71	0.33	51,57,59,60	0
4	NAG	A	606	14/15	0.81	0.25	46,52,58,59	0
4	NAG	A	604	14/15	0.86	0.19	51,59,61,62	0
4	NAG	A	605	14/15	0.90	0.15	47,49,53,54	0
6	IOD	A	620	1/1	0.94	0.09	98,98,98,98	0
6	IOD	A	609	1/1	0.95	0.07	53,53,53,53	0
6	IOD	A	616	1/1	0.96	0.11	91,91,91,91	0
6	IOD	A	614	1/1	0.96	0.08	69,69,69,69	0
6	IOD	A	611	1/1	0.96	0.04	57,57,57,57	0
3	HEM	A	602	43/43	0.97	0.19	11,18,22,24	0
6	IOD	A	612	1/1	0.97	0.04	62,62,62,62	0
6	IOD	A	613	1/1	0.97	0.04	59,59,59,59	0
6	IOD	A	615	1/1	0.98	0.10	101,101,101,101	0
6	IOD	A	610	1/1	0.98	0.05	50,50,50,50	0
5	BMM	A	607	2/2	0.98	0.20	26,26,26,31	0
6	IOD	A	618	1/1	0.98	0.11	95,95,95,95	0
2	CA	A	601	1/1	0.99	0.09	26,26,26,26	0
6	IOD	A	617	1/1	0.99	0.05	96,96,96,96	0
6	IOD	A	619	1/1	0.99	0.11	97,97,97,97	0
6	IOD	A	608	1/1	1.00	0.04	32,32,32,32	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 A 602:

$2mF_o$-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.