



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:11 PM UTC

PDB ID : 4PNX / pdb_00004pnx
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

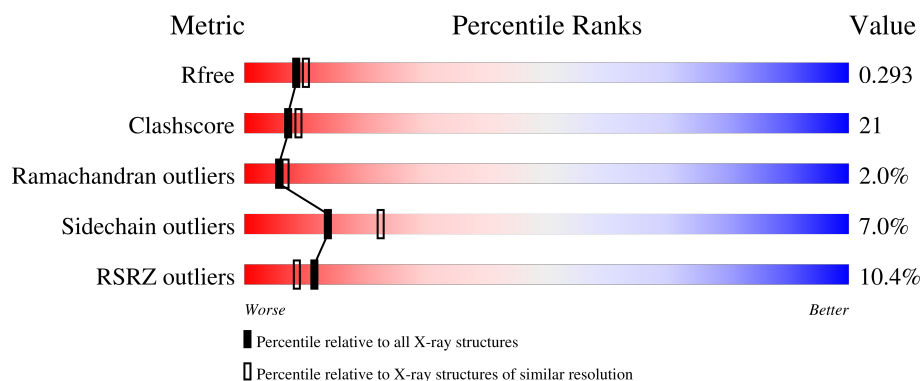
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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 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 $\leq 5\%$. 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	

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 [i](#)

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.

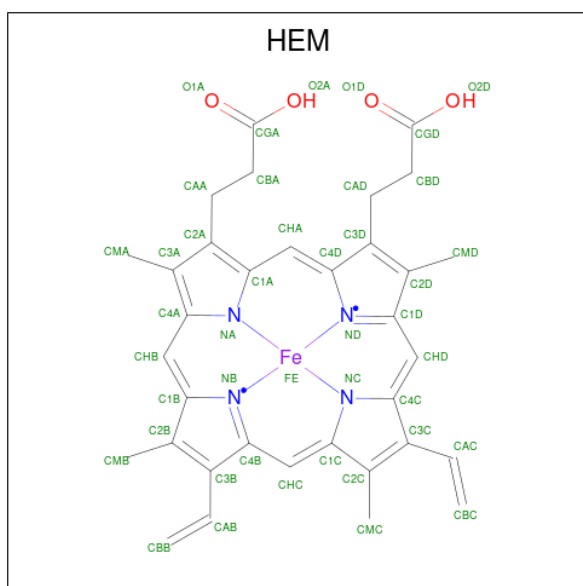
- Molecule 1 is a protein called Lactoperoxidase.

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 (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

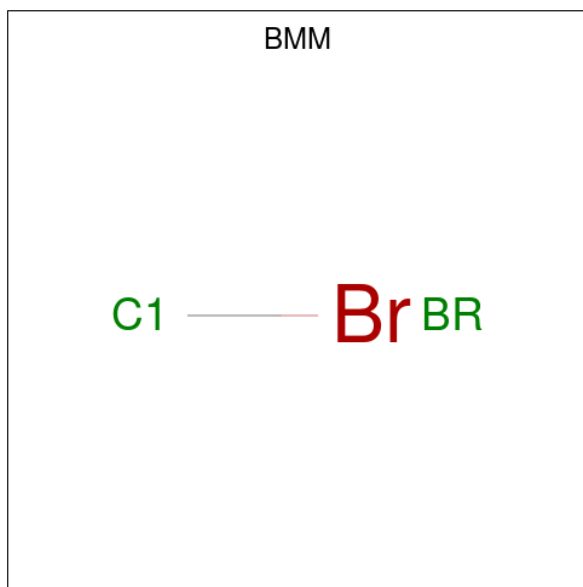


- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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 (CCD ID: 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 (CCD ID: IOD) (formula: I).

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

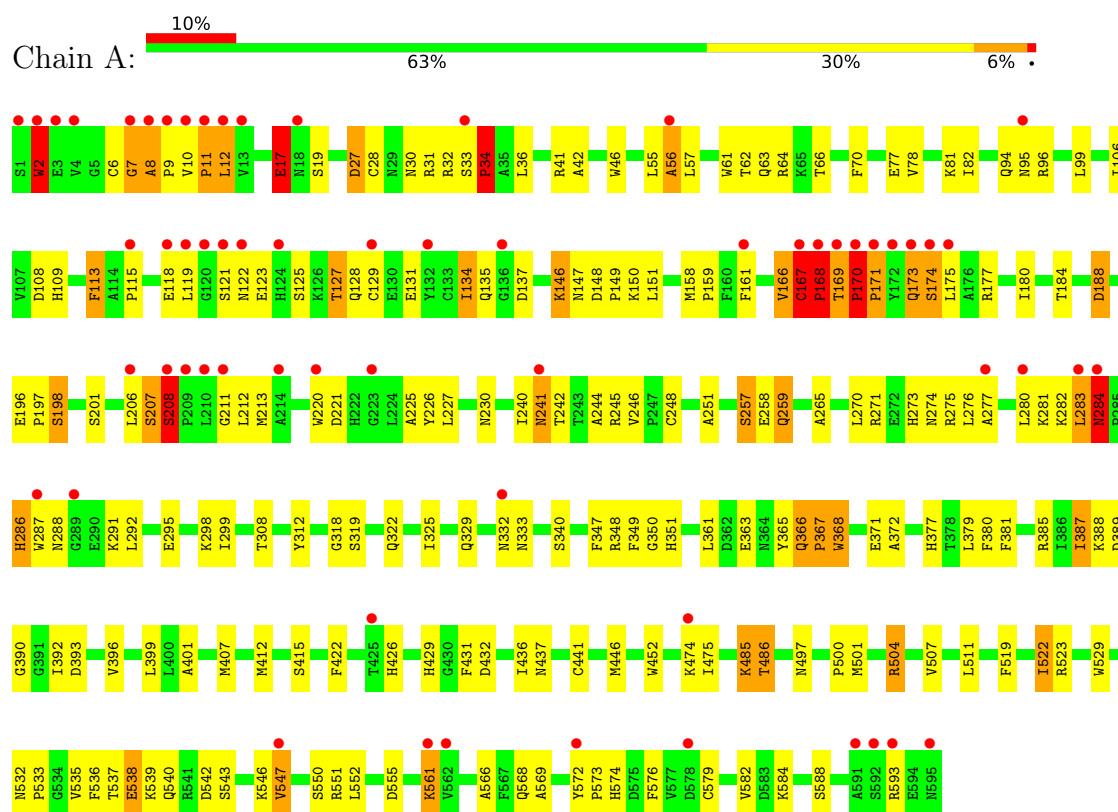
- Molecule 7 is water.

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



4 Data and refinement statistics

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 71.15 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.0 (71.15-2.41) 98.9 (71.15-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.09%)	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 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BMM, CA, NAG, SEP, IOD, 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	0.99	3/4891 (0.1%)	1.29	53/6634 (0.8%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CD	25.42	1.83	1.47
1	A	34	PRO	N-CD	23.79	1.81	1.47
1	A	170	PRO	CA-C	5.28	1.57	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	TRP	N-CA-C	-16.59	86.07	109.95
1	A	170	PRO	N-CA-C	15.80	129.97	110.70
1	A	168	PRO	CA-N-CD	-13.00	93.81	112.00
1	A	121	SER	N-CA-CB	-12.76	90.54	110.44
1	A	118	GLU	N-CA-C	12.55	126.75	112.57
1	A	113	PHE	N-CA-C	-12.21	89.82	108.99
1	A	547	VAL	CB-CA-C	-11.40	93.01	111.59
1	A	34	PRO	CA-N-CD	-11.37	96.08	112.00
1	A	34	PRO	N-CA-CB	10.67	114.46	103.25
1	A	2	TRP	CB-CA-C	-10.08	92.23	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	VAL	N-CA-C	9.84	122.65	109.37
1	A	485	LYS	CB-CA-C	-9.74	91.04	110.42
1	A	113	PHE	CB-CA-C	9.70	130.59	109.94
1	A	174	SER	N-CA-C	9.41	125.19	112.68
1	A	426	HIS	N-CA-C	-9.16	93.49	109.06
1	A	283	LEU	CB-CA-C	9.12	128.58	110.42
1	A	504	ARG	CB-CA-C	-8.83	99.35	111.89
1	A	170	PRO	CB-CA-C	-8.68	100.33	110.92
1	A	167	CYS	N-CA-C	-8.65	90.70	109.81
1	A	579	CYS	CB-CA-C	8.65	127.63	110.42
1	A	168	PRO	N-CA-C	-8.28	95.41	112.47
1	A	368	TRP	CB-CA-C	8.09	121.98	109.84
1	A	208	SER	N-CA-CB	-7.99	96.14	110.37
1	A	368	TRP	N-CA-C	-7.88	98.66	110.24
1	A	121	SER	N-CA-C	7.23	122.19	113.23
1	A	6	CYS	N-CA-C	-7.13	96.79	108.41
1	A	137	ASP	CB-CA-C	-7.13	98.89	110.08
1	A	390	GLY	N-CA-C	6.80	122.57	114.48
1	A	7	GLY	N-CA-C	-6.71	97.29	113.18
1	A	426	HIS	N-CA-CB	6.45	122.68	111.13
1	A	188	ASP	CB-CA-C	6.36	119.70	109.27
1	A	170	PRO	CA-C-N	6.22	127.62	119.84
1	A	170	PRO	C-N-CA	6.22	127.62	119.84
1	A	2	TRP	CA-C-N	5.95	131.67	121.86
1	A	2	TRP	C-N-CA	5.95	131.67	121.86
1	A	486	THR	N-CA-CB	5.78	120.65	110.37
1	A	27	ASP	CB-CA-C	-5.74	100.94	109.90
1	A	134	ILE	N-CA-C	5.65	114.88	106.85
1	A	436	ILE	N-CA-C	5.59	116.33	110.62
1	A	485	LYS	N-CA-C	5.56	122.64	110.80
1	A	363	GLU	N-CA-C	5.49	118.78	111.75
1	A	11	PRO	N-CA-CB	5.47	106.62	102.36
1	A	207	SER	CA-C-N	5.45	135.09	121.80
1	A	207	SER	C-N-CA	5.45	135.09	121.80
1	A	283	LEU	N-CA-C	-5.40	99.31	110.80
1	A	17	GLU	N-CA-C	-5.22	105.03	111.40
1	A	412	MET	N-CA-C	5.15	117.88	111.24
1	A	173	GLN	N-CA-C	5.13	121.73	110.80
1	A	284	ASN	N-CA-C	5.13	120.32	108.93
1	A	329	GLN	N-CA-C	-5.13	106.96	114.39
1	A	366	GLN	CA-C-N	5.08	126.19	119.84
1	A	366	GLN	C-N-CA	5.08	126.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	GLN	N-CA-C	-5.04	101.41	109.07

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

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	197	0
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	199	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 21.

All (199) 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:108:ASP:CG	3:A:602:HEM:HMD1	1.39	1.46
1:A:168:PRO:N	1:A:168:PRO:CD	1.83	1.37
1:A:34:PRO:CD	1:A:34:PRO:N	1.81	1.34
1:A:108:ASP:OD2	3:A:602:HEM:HMD1	1.23	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:OE2	3:A:602:HEM:HMB1	1.39	1.23
1:A:108:ASP:OD1	3:A:602:HEM:CMD	1.98	1.11
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:CG	3:A:602:HEM:CMD	2.26	1.07
1:A:283:LEU:C	1:A:284:ASN:HD22	1.64	1.06
1:A:108:ASP:OD2	3:A:602:HEM:CMD	2.07	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:108:ASP:OD1	3:A:602:HEM:HMD1	1.58	1.02
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:286:HIS:H	1:A:286:HIS:HD1	1.15	0.92
1:A:241:ASN:ND2	1:A:244:ALA:HB3	1.90	0.86
1:A:258:GLU:CD	3:A:602:HEM:HMB1	2.01	0.85
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.07	0.84
1:A:547:VAL:O	1:A:547:VAL:HG23	1.76	0.84
1:A:319:SER:HB3	1:A:504:ARG:HH12	1.42	0.84
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: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:33:SER:C	1:A:34:PRO:CD	2.57	0.77
1:A:318:GLY:CA	1:A:504:ARG:O	2.35	0.74
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: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:284:ASN:HD22	1:A:284:ASN:N	1.70	0.71
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:283:LEU:C	1:A:284:ASN:ND2	2.45	0.68
1:A:149:PRO:HG2	6:A:619:IOD:I	2.64	0.68
1:A:286:HIS:HD1	1:A:286:HIS:N	1.89	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PHE:CD1	1:A:429:HIS:CE1	2.83	0.67
1:A:108:ASP:OD1	3:A:602:HEM:HMD2	1.91	0.67
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.19	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:257:SER:O	1:A:381:PHE:HA	1.96	0.65
1:A:275:ARG:HH11	1:A:555:ASP:CB	2.10	0.65
1:A:128:GLN:HB2	7:A:752:HOH:O	1.96	0.64
1:A:108:ASP:OD1	3:A:602:HEM:C2D	2.51	0.63
1:A:207:SER:O	1:A:208:SER:HB3	1.97	0.63
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.46	0.63
1:A:281:LYS:C	1:A:283:LEU:H	2.05	0.62
1:A:519:PHE:CD1	1:A:522:ILE:HD11	2.36	0.61
1:A:95:ASN:HB3	1:A:96:ARG:NH1	2.16	0.61
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.36	0.61
1:A:56:ALA:HB2	1:A:177:ARG:HB2	1.83	0.60
1:A:30:ASN:CB	1:A:33:SER:O	2.47	0.60
1:A:127:THR:O	1:A:131:GLU:HB2	2.00	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:241:ASN:OD1	1:A:241:ASN:C	2.44	0.59
1:A:258:GLU:CD	3:A:602:HEM:CMB	2.76	0.59
1:A:547:VAL:O	1:A:547:VAL:CG2	2.49	0.59
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:211:GLY:C	7:A:757:HOH:O	2.47	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:10:VAL:HG13	1:A:10:VAL:O	2.05	0.55
1:A:30:ASN:C	1:A:33:SER:O	2.49	0.55
1:A:55:LEU:O	1:A:56:ALA:HB2	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

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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	0.54
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: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:275:ARG:HH11	1:A:555:ASP:HB2	1.72	0.53
1:A:281:LYS:C	1:A:283:LEU:N	2.67	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: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:OD1	1:A:122:ASN:O	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
1:A:407:MET:HE3	1:A:501:MET:HE3	1.94	0.49
1:A:286:HIS:N	1:A:286:HIS:ND1	2.39	0.49
1:A:230:ASN:C	1:A:230:ASN:OD1	2.54	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:361:LEU:CD1	1:A:401:ALA:HB3	2.42	0.49
1:A:241:ASN:CG	1:A:241:ASN:O	2.55	0.48
1:A:158:MET:HE1	1:A:432:ASP:HB2	1.94	0.48
1:A:551:ARG:NH1	1:A:582:VAL:O	2.46	0.48
1:A:78:VAL:HG13	1:A:82:ILE:HD12	1.95	0.48
1:A:167:CYS:C	1:A:168:PRO:O	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:32:ARG:HB3	7:A:801:HOH:O	2.12	0.47
1:A:281:LYS:HD3	1:A:292:LEU:HD11	1.97	0.47
1:A:551:ARG:HE	1:A:555:ASP:CG	2.23	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:332:ASN:CG	4:A:606:NAG:C1	2.89	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:94:GLN:O	1:A:569:ALA:CB	2.64	0.46
1:A:148:ASP:OD1	1:A:150:LYS:HB2	2.16	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: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:30:ASN:O	1:A:33:SER:C	2.53	0.45
1:A:57:LEU:HD22	1:A:61:TRP:CD1	2.52	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: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
1:A:62:THR:O	1:A:63:GLN:C	2.60	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:537:THR:O	1:A:538:GLU:C	2.60	0.44
1:A:32:ARG:HB2	7:A:801:HOH:O	2.15	0.44
1:A:56:ALA:HB2	1:A:177:ARG:CB	2.46	0.44
1:A:396:VAL:HA	1:A:399:LEU:HD12	2.01	0.43
1:A:298:LYS:NZ	1:A:535:VAL:O	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:HIS:CE1	5:A:607:BMM:C1	3.01	0.43
1:A:211:GLY:CA	7:A:757:HOH:O	2.66	0.43
1:A:95:ASN:HB3	1:A:96:ARG:HH12	1.83	0.42
3:A:602:HEM:HMC2	3:A:602:HEM:HBC2	2.00	0.42
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.98	0.42
1:A:227:LEU:CD1	1:A:251:ALA:HB2	2.49	0.42
1:A:446:MET:HA	1:A:446:MET:HE2	2.01	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:10:VAL:HG23	1:A:41:ARG:HH22	1.84	0.42
1:A:291:LYS:HE2	7:A:796:HOH:O	2.19	0.42
1:A:167:CYS:C	1:A:168:PRO:CD	2.82	0.42
1:A:94:GLN:O	1:A:569:ALA:HB3	2.20	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: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:407:MET:C	1:A:407:MET:SD	3.04	0.41
1:A:66:THR:HB	1:A:70:PHE:N	2.36	0.40
1:A:108:ASP:OD2	1:A:347:PHE:CD2	2.74	0.40
1:A:213:MET:HB3	1:A:270:LEU:HD11	2.02	0.40
1:A:95:ASN:HD21	4:A:603:NAG:C7	2.34	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:HD2	1:A:593:ARG:HA	1.85	0.40
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%)	6 7

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%)	481 (93%)	36 (7%)	14 22

All (36) 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	134	ILE
1	A	146	LYS
1	A	151	LEU
1	A	166	VAL

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Mol	Chain	Res	Type
1	A	168	PRO
1	A	174	SER
1	A	201	SER
1	A	240	ILE
1	A	241	ASN
1	A	257	SER
1	A	284	ASN
1	A	286	HIS
1	A	288	ASN
1	A	322	GLN
1	A	325	ILE
1	A	371	GLU
1	A	387	ILE
1	A	388	LYS
1	A	392	ILE
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	561	LYS
1	A	588	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	122	ASN
1	A	147	ASN
1	A	284	ASN
1	A	288	ASN
1	A	429	HIS
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN

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Mol	Chain	Res	Type
1	A	521	GLN
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	1.81	1 (12%)	7,12,14	2.08	2 (28%)

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	-	3/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.81	1.62	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	4.55	118.54	106.67
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 oligosaccharides 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
3	HEM	A	602	1	50,50,50	1.78	9 (18%)	67,82,82	1.31	8 (11%)
4	NAG	A	603	-	14,14,15	0.60	0	17,19,21	1.80	1 (5%)
4	NAG	A	604	1	14,14,15	0.57	0	17,19,21	1.06	1 (5%)
4	NAG	A	605	-	14,14,15	0.48	0	17,19,21	1.61	2 (11%)
4	NAG	A	606	-	14,14,15	0.58	0	17,19,21	2.51	5 (29%)
5	BMM	A	607	-	0,1,1	-	-	-		

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	HEM	A	602	1	-	4/14/54/54	-
4	NAG	A	603	-	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	NAG	A	605	-	-	0/6/23/26	0/1/1/1
4	NAG	A	606	-	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3D-C2D	6.76	1.51	1.36
3	A	602	HEM	FE-NC	3.79	2.07	1.95
3	A	602	HEM	CAB-C3B	3.41	1.56	1.47
3	A	602	HEM	FE-ND	2.72	2.03	1.94
3	A	602	HEM	CAC-C3C	2.72	1.54	1.47
3	A	602	HEM	C3B-C2B	-2.52	1.32	1.37
3	A	602	HEM	FE-NB	2.42	2.02	1.94
3	A	602	HEM	FE-NA	2.32	2.02	1.95
3	A	602	HEM	CMA-C3A	2.27	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C1-O5-C5	6.71	121.17	112.19
4	A	606	NAG	C1-O5-C5	6.27	120.59	112.19
4	A	605	NAG	C1-O5-C5	5.90	120.10	112.19
3	A	602	HEM	C4D-ND-C1D	4.46	110.49	105.21
3	A	602	HEM	C3B-C2B-C1B	4.24	109.59	106.41
4	A	606	NAG	C4-C3-C2	4.23	117.22	111.02
4	A	606	NAG	C3-C4-C5	4.23	117.90	110.23
4	A	606	NAG	O5-C5-C6	3.29	114.06	107.66
3	A	602	HEM	CAD-C3D-C4D	3.15	130.19	124.70
3	A	602	HEM	CBA-CAA-C2A	-2.71	105.04	112.53
3	A	602	HEM	CHD-C1D-ND	2.62	127.24	124.42
3	A	602	HEM	CMD-C2D-C1D	2.58	129.06	125.03
4	A	604	NAG	O7-C7-N2	2.29	126.02	121.98
4	A	606	NAG	C2-N2-C7	2.23	125.89	122.90
3	A	602	HEM	C2B-C1B-NB	-2.10	107.42	109.84
3	A	602	HEM	O1A-CGA-CBA	-2.05	116.58	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	NAG	C6-C5-C4	-2.04	108.00	113.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

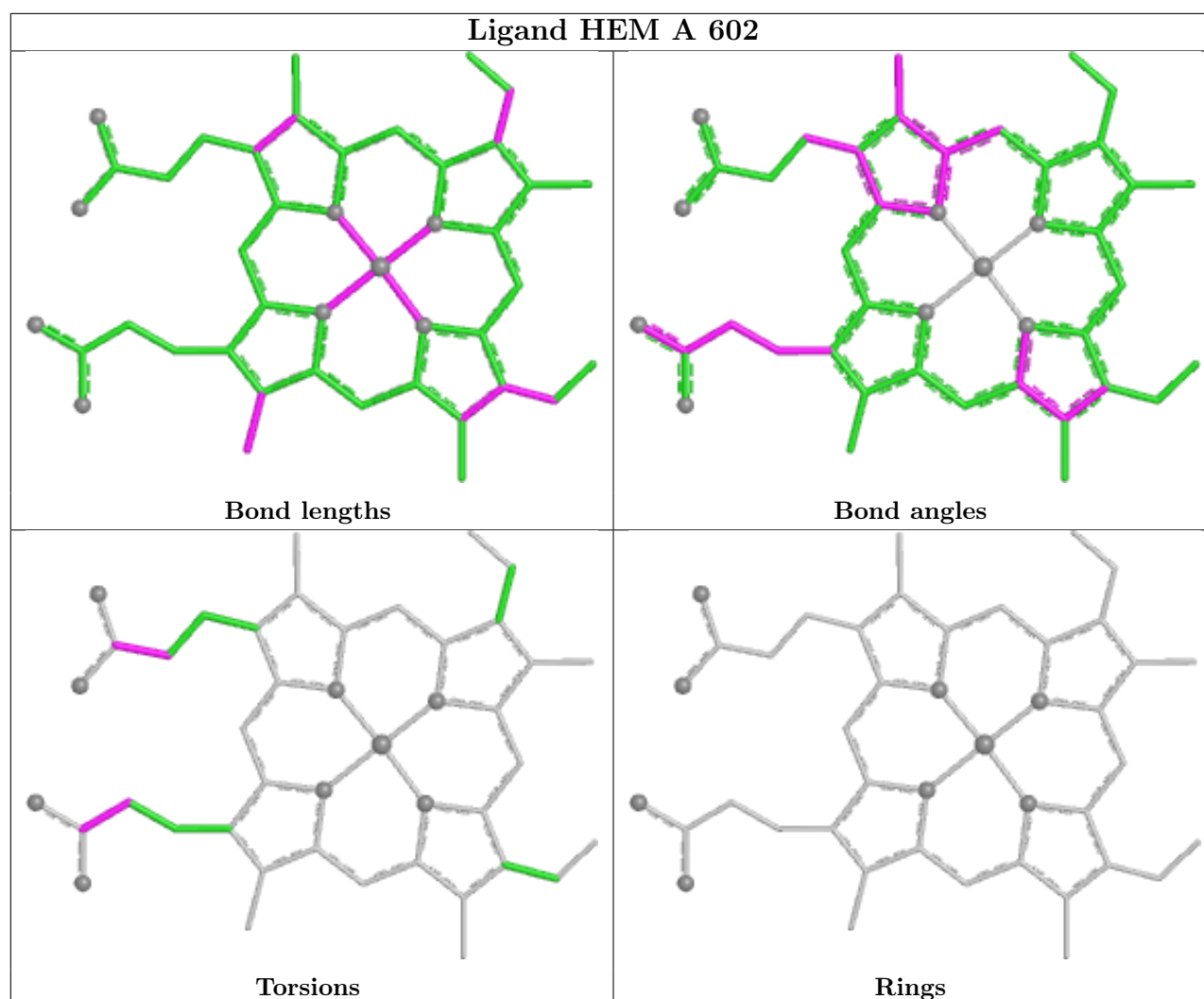
Mol	Chain	Res	Type	Atoms
4	A	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
3	A	602	HEM	CAA-CBA-CGA-O1A
3	A	602	HEM	CAA-CBA-CGA-O2A
3	A	602	HEM	CAD-CBD-CGD-O2D
3	A	602	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

5 monomers are involved in 29 short contacts:

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

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



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, 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	594/595 (99%)	0.52	62 (10%) 11 9	14, 35, 72, 103	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	6.9
1	A	2	TRP	6.4
1	A	120	GLY	5.7
1	A	10	VAL	5.3
1	A	175	LEU	4.7
1	A	7	GLY	4.1
1	A	170	PRO	4.0
1	A	174	SER	3.9
1	A	13	VAL	3.9
1	A	8	ALA	3.8
1	A	9	PRO	3.6
1	A	211	GLY	3.5
1	A	289	GLY	3.4
1	A	172	TYR	3.3
1	A	4	VAL	3.3
1	A	121	SER	3.2
1	A	223	GLY	3.2
1	A	332	ASN	3.2
1	A	591	ALA	3.1
1	A	561	LYS	3.1
1	A	210	LEU	3.0
1	A	118	GLU	2.9
1	A	119	LEU	2.9
1	A	173	GLN	2.9
1	A	1	SER	2.8
1	A	168	PRO	2.8
1	A	171	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	284	ASN	2.8
1	A	56	ALA	2.7
1	A	167	CYS	2.7
1	A	161	PHE	2.7
1	A	11	PRO	2.7
1	A	214	ALA	2.7
1	A	287	TRP	2.6
1	A	136	GLY	2.5
1	A	206	LEU	2.5
1	A	572	TYR	2.5
1	A	280	LEU	2.5
1	A	124	HIS	2.5
1	A	169	THR	2.5
1	A	283	LEU	2.5
1	A	33	SER	2.5
1	A	547	VAL	2.4
1	A	220	TRP	2.3
1	A	562	VAL	2.2
1	A	3	GLU	2.2
1	A	122	ASN	2.2
1	A	277	ALA	2.2
1	A	595	ASN	2.2
1	A	593	ARG	2.2
1	A	208	SER	2.2
1	A	592	SER	2.2
1	A	132	TYR	2.1
1	A	129	CYS	2.1
1	A	209	PRO	2.1
1	A	18	ASN	2.1
1	A	115	PRO	2.1
1	A	241	ASN	2.1
1	A	425	THR	2.1
1	A	474	LYS	2.1
1	A	578	ASP	2.1
1	A	95	ASN	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.76	0.16	41,43,53,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

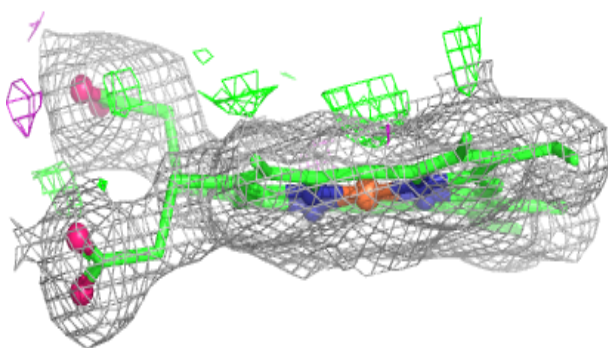
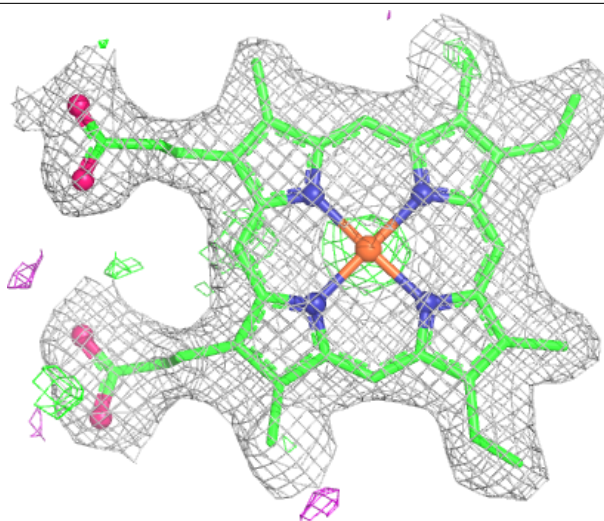
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	603	14/15	0.59	0.15	51,57,59,60	0
4	NAG	A	606	14/15	0.62	0.14	46,52,58,59	0
4	NAG	A	604	14/15	0.77	0.12	51,59,61,62	0
4	NAG	A	605	14/15	0.86	0.10	47,49,53,54	0
6	IOD	A	620	1/1	0.91	0.16	98,98,98,98	0
6	IOD	A	611	1/1	0.94	0.06	57,57,57,57	0
6	IOD	A	616	1/1	0.95	0.16	91,91,91,91	0
6	IOD	A	615	1/1	0.96	0.11	101,101,101,101	0
6	IOD	A	609	1/1	0.96	0.05	53,53,53,53	0
6	IOD	A	613	1/1	0.96	0.06	59,59,59,59	0
6	IOD	A	612	1/1	0.97	0.07	62,62,62,62	0
3	HEM	A	602	43/43	0.97	0.06	11,18,22,24	0
6	IOD	A	617	1/1	0.97	0.11	96,96,96,96	0
6	IOD	A	614	1/1	0.97	0.12	69,69,69,69	0
5	BMM	A	607	2/2	0.98	0.12	26,26,26,31	0
6	IOD	A	618	1/1	0.98	0.23	95,95,95,95	0
6	IOD	A	619	1/1	0.98	0.19	97,97,97,97	0
6	IOD	A	610	1/1	0.98	0.07	50,50,50,50	0
2	CA	A	601	1/1	0.99	0.01	26,26,26,26	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 [i](#)

There are no such residues in this entry.