



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:30 AM GMT

PDB ID : 2R5L
Title : Crystal structure of lactoperoxidase at 2.4Å resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Srinivasan, A.; Singh, T.P.
Deposited on : 2007-09-04
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

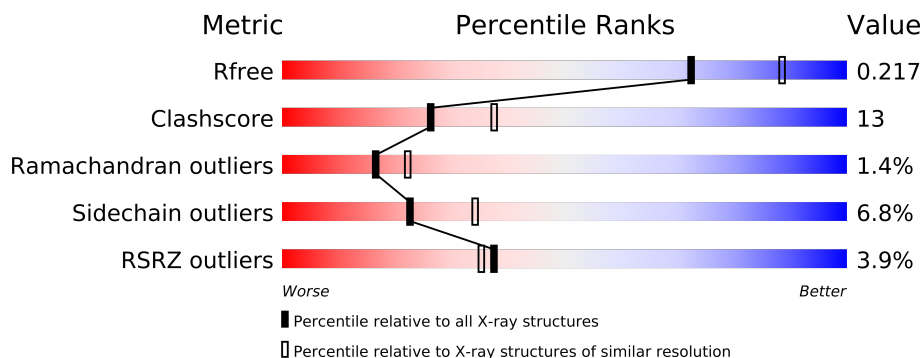
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	595	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	IOD	A	617	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5377 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			4757	3021	844	865	1	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

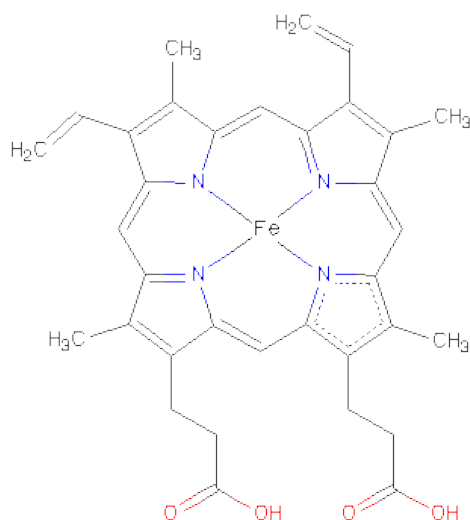
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	I	0	0
			10	10		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

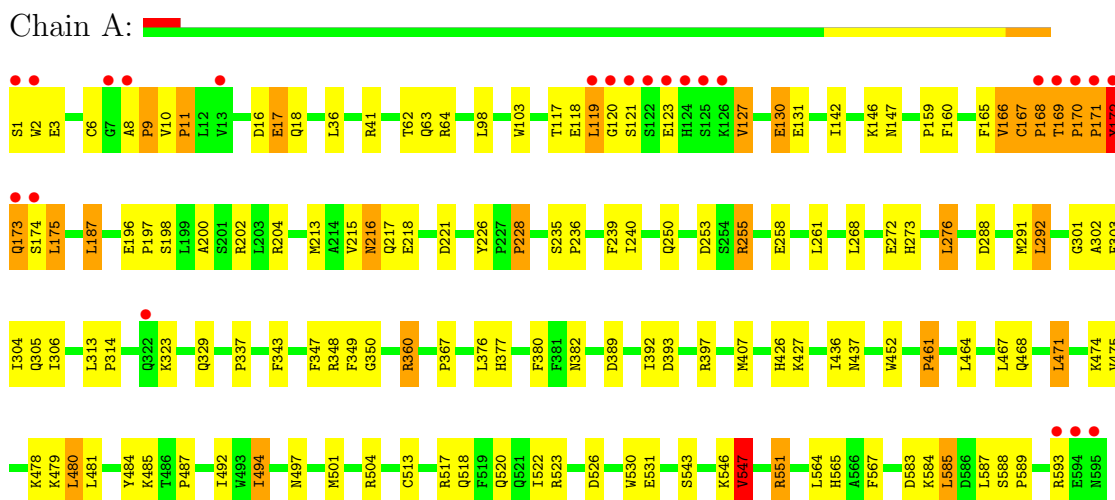
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	421	Total	O	0	0
			421	421		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	54.19Å 80.81Å 77.04Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 24.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.98-2.40) 97.8 (24.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.39Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.196 , 0.203 0.179 , 0.217	Depositor DCC
R_{free} test set	1274 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 24947 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5377	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, HEM, IOD, MAN

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	0.49	1/4875 (0.0%)	0.82	10/6621 (0.2%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	N-CA	6.27	1.57	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-CB-CG	-9.13	96.05	113.40
1	A	585	LEU	CA-CB-CG	6.88	131.13	115.30
1	A	461	PRO	CA-N-CD	-6.60	102.26	111.50
1	A	6	CYS	CA-CB-SG	5.94	124.69	114.00
1	A	228	PRO	CA-N-CD	-5.88	103.28	111.50
1	A	171	PRO	CA-N-CD	-5.80	103.38	111.50
1	A	547	VAL	CB-CA-C	-5.57	100.82	111.40
1	A	11	PRO	N-CA-C	5.48	126.35	112.10
1	A	172	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	587	LEU	CB-CG-CD1	-5.13	102.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4645	126	0
2	A	117	0	102	2	0
3	A	28	0	25	0	0
4	A	1	0	0	0	0
5	A	10	0	0	4	0
6	A	43	0	30	3	0
7	A	421	0	0	18	0
All	All	5377	0	4802	130	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:TRP:HB2	1:A:175:LEU:HD12	1.23	1.20
1:A:168:PRO:HG2	1:A:172:TYR:CE1	1.85	1.11
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.34	1.09
1:A:169:THR:CG2	1:A:170:PRO:HD3	1.89	1.02
1:A:2:TRP:HA	7:A:998:HOH:O	1.65	0.95
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.97	0.95
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.49	0.93
1:A:481:LEU:HD21	1:A:487:PRO:HD3	1.50	0.93
1:A:169:THR:HG22	1:A:170:PRO:CD	2.00	0.91
1:A:481:LEU:CD2	1:A:487:PRO:HD3	2.03	0.89
1:A:119:LEU:H	1:A:119:LEU:HD12	1.39	0.88
1:A:303:PHE:HD1	1:A:547:VAL:HG11	1.39	0.85
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.07	0.84
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.61	0.81
1:A:119:LEU:CD1	1:A:119:LEU:H	1.93	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.84	0.77
1:A:169:THR:CG2	1:A:170:PRO:CD	2.59	0.76
1:A:119:LEU:HD13	7:A:997:HOH:O	1.86	0.76
1:A:118:GLU:HG3	7:A:1000:HOH:O	1.86	0.76
1:A:119:LEU:HD21	1:A:169:THR:HG23	1.71	0.73
1:A:167:CYS:CB	1:A:168:PRO:CD	2.63	0.72
1:A:119:LEU:CD1	1:A:119:LEU:N	2.51	0.72
1:A:216:ASN:HD22	1:A:218:GLU:H	1.39	0.71
1:A:547:VAL:HG12	7:A:696:HOH:O	1.90	0.70
1:A:567:PHE:HB2	5:A:617:IOD:I	2.61	0.69
1:A:1:SER:HB2	7:A:995:HOH:O	1.93	0.68
1:A:253:ASP:OD2	1:A:255:ARG:HD3	1.95	0.67
1:A:169:THR:HG22	1:A:170:PRO:HD2	1.77	0.66
1:A:130:GLU:HG3	7:A:935:HOH:O	1.96	0.66
2:A:596:NAG:H61	2:A:597:NAG:C1	2.26	0.66
1:A:130:GLU:HG2	1:A:159:PRO:HG3	1.78	0.65
1:A:169:THR:H	1:A:170:PRO:HD2	1.61	0.64
1:A:118:GLU:O	1:A:120:GLY:N	2.30	0.64
1:A:240:ILE:HD11	1:A:382:ASN:HA	1.79	0.64
1:A:172:TYR:HD2	1:A:173:GLN:H	1.45	0.63
1:A:127:VAL:HG13	1:A:131:GLU:HG3	1.80	0.63
1:A:168:PRO:CG	1:A:172:TYR:CE1	2.75	0.63
1:A:9:PRO:HG3	1:A:41:ARG:CZ	2.29	0.62
1:A:494:ILE:O	1:A:494:ILE:HD13	1.99	0.62
1:A:480:LEU:HD11	1:A:494:ILE:HD12	1.81	0.62
1:A:168:PRO:HG2	1:A:172:TYR:HE1	1.58	0.61
1:A:565:HIS:HB3	5:A:617:IOD:I	2.71	0.60
1:A:2:TRP:HB2	1:A:175:LEU:CD1	2.15	0.60
1:A:16:ASP:HB3	7:A:923:HOH:O	2.02	0.60
1:A:216:ASN:ND2	1:A:218:GLU:H	2.00	0.60
1:A:8:ALA:HB3	7:A:972:HOH:O	2.02	0.59
1:A:142:ILE:HD12	1:A:160:PHE:HB2	1.85	0.59
1:A:303:PHE:HD1	1:A:547:VAL:CG1	2.15	0.59
2:A:597:NAG:H3	2:A:598:MAN:O5	2.01	0.59
1:A:323:LYS:HE2	7:A:1012:HOH:O	2.02	0.59
1:A:103:TRP:HH2	1:A:304:ILE:HD13	1.67	0.59
1:A:481:LEU:HD21	1:A:487:PRO:CD	2.29	0.58
1:A:215:VAL:HA	1:A:228:PRO:HD3	1.84	0.58
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.86	0.58
1:A:63:GLN:HG2	7:A:913:HOH:O	2.02	0.58
1:A:169:THR:H	1:A:170:PRO:CD	2.18	0.57
1:A:120:GLY:HA3	1:A:123:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.86	0.57
1:A:146:LYS:O	1:A:147:ASN:HB2	2.05	0.56
1:A:215:VAL:CA	1:A:228:PRO:HD3	2.36	0.56
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.56
1:A:103:TRP:CH2	1:A:304:ILE:HD13	2.41	0.56
1:A:551:ARG:HD3	1:A:583:ASP:O	2.06	0.56
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.40	0.55
1:A:543:SER:HB3	1:A:585:LEU:HD12	1.88	0.55
1:A:303:PHE:CD1	1:A:547:VAL:HG11	2.31	0.55
1:A:17:GLU:N	7:A:923:HOH:O	2.40	0.55
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.42	0.54
1:A:588:SER:N	1:A:589:PRO:CD	2.70	0.54
1:A:215:VAL:C	1:A:228:PRO:HD3	2.28	0.54
1:A:288:ASP:O	1:A:292:LEU:HD22	2.08	0.53
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.89	0.53
1:A:62:THR:HG22	1:A:64:ARG:HG2	1.89	0.53
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.42	0.52
1:A:146:LYS:HE2	7:A:980:HOH:O	2.09	0.52
1:A:452:TRP:CD1	1:A:492:ILE:HD13	2.45	0.52
1:A:301:GLY:O	1:A:305:GLN:HG3	2.10	0.52
1:A:272:GLU:O	1:A:276:LEU:HD22	2.10	0.51
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.24	0.51
1:A:426:HIS:HB3	7:A:936:HOH:O	2.10	0.50
1:A:273:HIS:O	1:A:276:LEU:HB2	2.11	0.50
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.46	0.50
6:A:618:HEM:HBC2	6:A:618:HEM:HMC2	1.93	0.50
1:A:216:ASN:HD22	1:A:217:GLN:N	2.10	0.49
1:A:165:PHE:HZ	1:A:170:PRO:O	1.94	0.49
1:A:481:LEU:HD22	1:A:487:PRO:HD3	1.89	0.49
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.77	0.49
1:A:197:PRO:O	1:A:198:SEP:C	2.59	0.49
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.94	0.49
1:A:393:ASP:O	1:A:397:ARG:HG3	2.13	0.48
1:A:593:ARG:HA	1:A:593:ARG:HD3	1.71	0.48
1:A:302:ALA:O	1:A:306:ILE:HG13	2.14	0.48
1:A:494:ILE:C	1:A:494:ILE:HD13	2.34	0.48
1:A:475:VAL:HG12	1:A:479:LYS:HE3	1.95	0.47
1:A:585:LEU:HA	7:A:669:HOH:O	2.14	0.47
1:A:175:LEU:HD11	7:A:995:HOH:O	2.15	0.47
1:A:407:MET:HB3	1:A:501:MET:CE	2.45	0.47
1:A:160:PHE:HD2	1:A:436:ILE:CD1	2.28	0.47
1:A:171:PRO:O	1:A:172:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:513:CYS:O	1:A:517:ARG:HG2	2.15	0.47
1:A:119:LEU:HD12	1:A:119:LEU:N	2.09	0.46
1:A:392:ILE:C	1:A:392:ILE:HD12	2.37	0.45
1:A:169:THR:N	1:A:170:PRO:HD2	2.31	0.45
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.52	0.45
1:A:258:GLU:HG3	5:A:608:IOD:I	2.87	0.44
1:A:584:LYS:HB3	7:A:761:HOH:O	2.16	0.44
1:A:202:ARG:HD2	1:A:250:GLN:HE22	1.82	0.44
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.53	0.44
1:A:119:LEU:HD13	1:A:119:LEU:N	2.33	0.43
1:A:216:ASN:ND2	5:A:610:IOD:I	3.22	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.53	0.43
1:A:174:SER:OG	1:A:175:LEU:N	2.52	0.42
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.69	0.42
1:A:522:ILE:HD12	1:A:522:ILE:C	2.39	0.42
1:A:142:ILE:HD11	1:A:160:PHE:CD2	2.55	0.42
1:A:522:ILE:O	1:A:526:ASP:HB2	2.19	0.42
1:A:350:GLY:HA3	6:A:618:HEM:CBC	2.50	0.42
1:A:484:TYR:O	1:A:485:LYS:HB2	2.19	0.42
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.67	0.41
1:A:118:GLU:C	1:A:120:GLY:H	2.24	0.41
1:A:8:ALA:N	1:A:9:PRO:HD3	2.35	0.41
1:A:63:GLN:HB2	7:A:987:HOH:O	2.20	0.41
1:A:36:LEU:HG	1:A:337:PRO:HD2	2.03	0.41
1:A:313:LEU:N	1:A:314:PRO:CD	2.83	0.41
1:A:142:ILE:CD1	1:A:160:PHE:HB2	2.49	0.41
1:A:166:VAL:HG22	1:A:166:VAL:H	1.68	0.40
1:A:142:ILE:HD11	1:A:436:ILE:HD13	2.03	0.40
1:A:235:SER:HA	1:A:236:PRO:HD3	1.93	0.40
1:A:200:ALA:O	1:A:204:ARG:HG3	2.21	0.40
6:A:618:HEM:HAA1	7:A:685:HOH:O	2.22	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%)	553 (93%)	31 (5%)	8 (1%)	16	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	172	TYR
1	A	166	VAL
1	A	17	GLU
1	A	9	PRO

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	516/516 (100%)	481 (93%)	35 (7%)	22	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	18	GLN
1	A	98	LEU
1	A	117	THR
1	A	121	SER
1	A	127	VAL
1	A	130	GLU
1	A	172	TYR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	216	ASN
1	A	255	ARG
1	A	261	LEU
1	A	268	LEU

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	291	MET
1	A	292	LEU
1	A	329	GLN
1	A	347	PHE
1	A	360	ARG
1	A	367	PRO
1	A	376	LEU
1	A	461	PRO
1	A	464	LEU
1	A	471	LEU
1	A	480	LEU
1	A	494	ILE
1	A	504	ARG
1	A	520	GLN
1	A	523	ARG
1	A	546	LYS
1	A	547	VAL
1	A	551	ARG
1	A	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	217	GLN
1	A	222	HIS
1	A	329	GLN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	521	GLN
1	A	545	GLN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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	9,9,10	6.61	2 (22%)	10,12,14	2.89	6 (60%)

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	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	18.98	1.24	1.11
1	A	198	SEP	CA-C	4.91	1.57	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	C-CA-N	-5.32	108.51	113.83
1	A	198	SEP	O2P-P-O1P	-3.79	98.04	110.44
1	A	198	SEP	O3P-P-OG	3.12	115.26	106.65
1	A	198	SEP	P-OG-CB	3.04	126.97	118.19
1	A	198	SEP	O3P-P-O1P	-2.69	101.65	110.44
1	A	198	SEP	O2P-P-OG	2.65	113.96	106.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

11 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	596	1,2	12,14,15	0.66	0	15,19,21	0.73	0
2	NAG	A	597	2	12,14,15	0.69	0	15,19,21	0.83	0
2	MAN	A	598	2	10,11,12	0.51	0	11,15,17	0.65	0
2	NAG	A	599	1,2	12,14,15	0.54	0	15,19,21	0.86	0
2	NAG	A	600	2	12,14,15	0.48	0	15,19,21	0.96	1 (6%)
2	MAN	A	601	2	10,11,12	0.55	0	11,15,17	0.58	0
2	NAG	A	602	1,2	12,14,15	0.48	0	15,19,21	0.82	0
2	NAG	A	603	2	12,14,15	0.60	0	15,19,21	1.13	2 (13%)
2	MAN	A	604	2	10,11,12	0.45	0	11,15,17	0.41	0
3	NAG	A	605	1,3	12,14,15	0.80	0	15,19,21	1.27	2 (13%)
3	NAG	A	606	3	12,14,15	0.48	0	15,19,21	0.89	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	MAN	A	598	2	-	0/2/19/22	0/1/1/1
2	NAG	A	599	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	2	-	0/6/23/26	0/1/1/1
2	MAN	A	601	2	-	0/2/19/22	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	2	-	0/6/23/26	0/1/1/1
2	MAN	A	604	2	-	0/2/19/22	0/1/1/1
3	NAG	A	605	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	606	3	-	0/6/23/26	1/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	NAG	C4-C3-C2	2.98	118.62	111.32
3	A	606	NAG	C3-C2-N2	-2.63	107.76	111.76
2	A	600	NAG	C3-C2-N2	-2.49	107.97	111.76
3	A	605	NAG	C3-C2-N2	-2.44	108.05	111.76
2	A	603	NAG	O5-C5-C4	2.15	113.38	110.65
2	A	603	NAG	C2-N2-C7	-2.14	119.50	123.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	606	NAG	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 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	$\# Z > 2$
6	HEM	A	618	1,7	49,50,50	2.55	16 (32%)	46,82,82	1.87	8 (17%)

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
6	HEM	A	618	1,7	-	0/14/114/114	0/0/8/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	618	HEM	C3D-C4D	6.63	1.46	1.44
6	A	618	HEM	C4A-C3A	5.85	1.47	1.40
6	A	618	HEM	C2B-C1B	5.64	1.46	1.44
6	A	618	HEM	C3C-C2C	-5.53	1.34	1.43
6	A	618	HEM	C3B-C2B	-5.26	1.34	1.43
6	A	618	HEM	C3C-CAC	4.90	1.55	1.40
6	A	618	HEM	C3B-CAB	4.68	1.55	1.40
6	A	618	HEM	C3D-C2D	4.39	1.51	1.43
6	A	618	HEM	FE-NC	3.65	2.11	1.97
6	A	618	HEM	FE-NA	2.96	2.05	1.92
6	A	618	HEM	CMC-C2C	2.50	1.55	1.47
6	A	618	HEM	CMB-C2B	2.50	1.55	1.47
6	A	618	HEM	CAA-C2A	2.39	1.56	1.52
6	A	618	HEM	FE-ND	2.34	2.06	1.97
6	A	618	HEM	CMD-C2D	2.17	1.54	1.47
6	A	618	HEM	C2D-C1D	-2.13	1.44	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	618	HEM	C3B-C4B-NB	-8.10	108.20	114.00
6	A	618	HEM	C4D-ND-C1D	4.58	109.85	105.16
6	A	618	HEM	CHC-C4B-NB	3.48	127.48	124.58
6	A	618	HEM	CHD-C1D-ND	3.38	127.40	124.58
6	A	618	HEM	CAD-C3D-C4D	2.59	129.18	124.53
6	A	618	HEM	C2D-C1D-ND	-2.58	109.88	112.93
6	A	618	HEM	C1B-NB-C4B	2.21	107.43	105.16
6	A	618	HEM	CBD-CAD-C3D	-2.20	109.57	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	595/595 (100%)	-0.16	24 (4%)	36 34	8, 22, 59, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	10.8
1	A	174	SER	9.1
1	A	2	TRP	8.1
1	A	173	GLN	7.9
1	A	1	SER	7.6
1	A	121	SER	6.9
1	A	119	LEU	6.8
1	A	595	ASN	6.8
1	A	122	SER	6.6
1	A	120	GLY	5.1
1	A	172	TYR	4.2
1	A	593	ARG	4.2
1	A	171	PRO	4.2
1	A	594	GLU	4.1
1	A	124	HIS	3.9
1	A	169	THR	3.4
1	A	13	VAL	3.1
1	A	8	ALA	2.9
1	A	170	PRO	2.8
1	A	126	LYS	2.7
1	A	322	GLN	2.3
1	A	168	PRO	2.3
1	A	125	SER	2.2
1	A	123	GLU	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.20	1.44	2,22,24,28	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	605	14/15	0.23	11.10	52,56,59,64	0
2	NAG	A	597	14/15	0.36	4.65	63,68,69,72	0
2	NAG	A	603	14/15	0.30	3.78	56,58,62,67	0
2	NAG	A	600	14/15	0.31	3.58	59,63,65,68	0
2	NAG	A	596	14/15	0.17	0.40	43,46,51,57	0
2	NAG	A	602	14/15	0.13	-0.03	36,41,44,50	0
2	NAG	A	599	14/15	0.12	-0.10	41,44,48,54	0
2	MAN	A	604	11/12	0.42	-	70,73,74,74	0
3	NAG	A	606	14/15	0.45	-	68,71,73,73	0
2	MAN	A	598	11/12	0.39	-	74,76,76,77	0
2	MAN	A	601	11/12	0.45	-	71,73,73,74	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	IOD	A	617	1/1	0.24	4.51	77,77,77,77	0
5	IOD	A	613	1/1	0.17	0.63	66,66,66,66	0
5	IOD	A	609	1/1	0.08	-1.18	21,21,21,21	0
5	IOD	A	612	1/1	0.06	-1.34	68,68,68,68	0
4	CA	A	607	1/1	0.08	-1.46	16,16,16,16	0
6	HEM	A	618	43/43	0.08	-1.52	8,13,19,20	0
5	IOD	A	614	1/1	0.04	-1.55	65,65,65,65	0
5	IOD	A	610	1/1	0.06	-2.05	64,64,64,64	0
5	IOD	A	616	1/1	0.03	-2.36	52,52,52,52	0
5	IOD	A	615	1/1	0.06	-2.53	65,65,65,65	0
5	IOD	A	611	1/1	0.06	-3.45	66,66,66,66	0
5	IOD	A	608	1/1	0.06	-4.13	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.