



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:17 PM GMT

PDB ID : 3NYH
Title : Crystal structure of lactoperoxidase complexed simultaneously with thiocyanate ion, iodide ion, bromide ion, chloride ion through the substrate diffusion channel reveals a preferential queue of the inorganic substrates towards the distal heme cavity
Authors : Pandey, N.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2010-07-15
Resolution : 1.77 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>

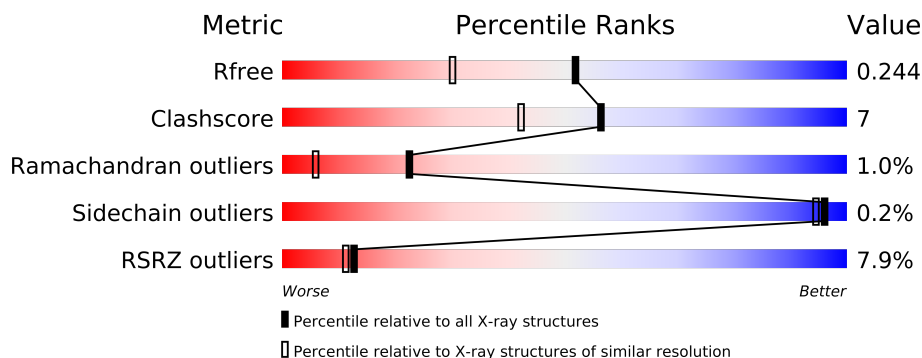
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.77 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	4987 (1.80-1.76)
Clashscore	79885	6152 (1.80-1.76)
Ramachandran outliers	78287	6074 (1.80-1.76)
Sidechain outliers	78261	6073 (1.80-1.76)
RSRZ outliers	66119	4990 (1.80-1.76)

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
10	GOL	A	615	-	X
10	GOL	A	617	-	X
12	MPD	A	626	-	X
15	SCN	A	629	X	-
4	NAG	A	596	-	X
4	NAG	A	604	-	X
7	IOD	A	616	-	X

2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 5734 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
			4774	3037	847	863	1	26			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	15	Total	I	0	0
			15	15		

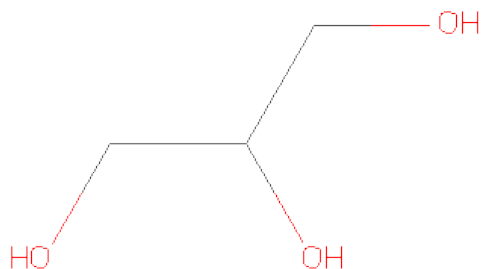
- Molecule 8 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Br	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

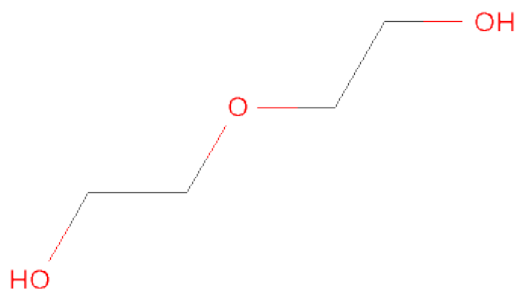
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



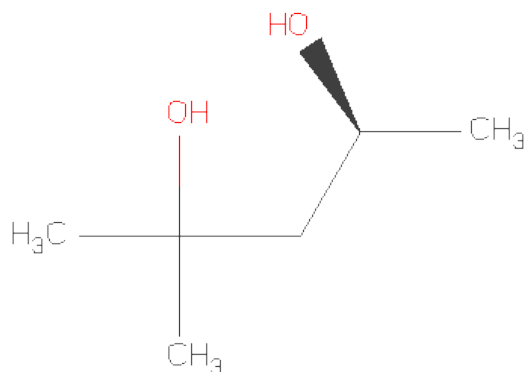
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



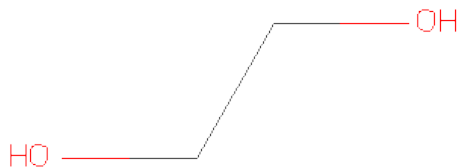
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

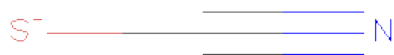


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Zn	0	0
			1	1		

- Molecule 15 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 16 is water.

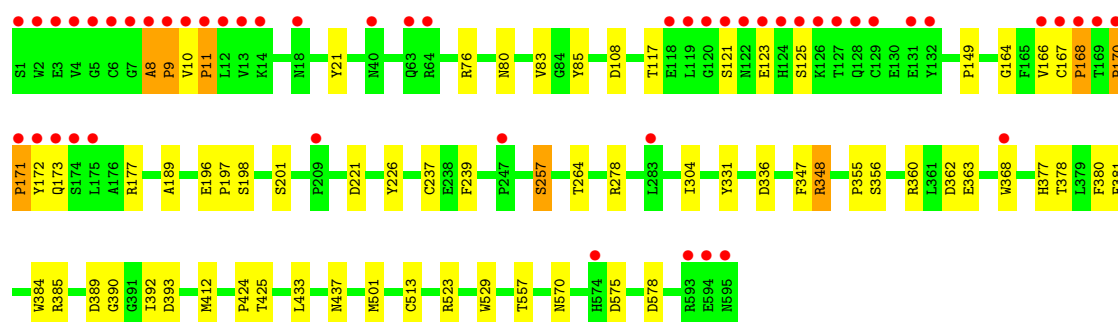
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	763	Total	O	0	0
			763	763		

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 ($\text{RSRZ} > 2$). 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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.23Å 79.84Å 77.55Å 90.00° 102.67° 90.00°	Depositor
Resolution (Å)	34.57 – 1.77 34.57 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.57-1.77) 98.3 (34.57-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.236 0.204 , 0.244	Depositor DCC
R_{free} test set	3107 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.3	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	7 of 61546 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5734	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: GOL, ZN, SCN, NAG, CL, CA, SEP, MPD, EDO, BR, PEG, 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	1.10	4/4891 (0.1%)	0.97	16/6634 (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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	TYR	CG-CD1	5.71	1.46	1.39
1	A	21	TYR	CD1-CE1	5.55	1.47	1.39
1	A	85	TYR	CE1-CZ	5.40	1.45	1.38
1	A	85	TYR	CE2-CZ	-5.36	1.31	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ALA	C-N-CD	-7.51	104.08	120.60
1	A	177	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	348	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	A	76	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	121	SER	N-CA-C	-6.37	93.79	111.00
1	A	173	GLN	N-CA-C	6.33	128.08	111.00
1	A	166	VAL	N-CA-C	6.28	127.96	111.00
1	A	76	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	578	ASP	CB-CG-OD1	5.33	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	MET	CG-SD-CE	-5.31	91.71	100.20
1	A	360	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	336	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	257	SER	O-C-N	-5.13	114.48	122.70
1	A	360	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	278	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	433	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	ARG	Mainchain
1	A	513	CYS	Mainchain

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	4774	0	4687	57	0
2	A	43	0	30	3	0
3	A	1	0	0	0	0
4	A	28	0	26	0	0
5	A	28	0	25	0	0
6	A	39	0	34	2	0
7	A	15	0	0	3	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	18	0	24	5	0
11	A	7	0	10	2	0
12	A	8	0	13	6	0
13	A	4	0	4	2	0
14	A	1	0	0	0	0
15	A	3	0	0	0	0
16	A	763	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5734	0	4853	64	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 7.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:603:MAN:O6	16:A:1096:HOH:O	1.94	0.86
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.63	0.81
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.10	0.81
1:A:197:PRO:HB3	12:A:626:MPD:H12	1.63	0.80
12:A:626:MPD:H11	12:A:626:MPD:H53	1.63	0.79
1:A:201:SER:HB2	12:A:626:MPD:H51	1.64	0.78
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.64	0.77
1:A:356:SER:N	7:A:616:IOD:I	2.86	0.76
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.16	0.76
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.70	0.74
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.72	0.70
12:A:626:MPD:C5	12:A:626:MPD:H11	2.31	0.60
1:A:363:GLU:H	13:A:627:EDO:H21	1.65	0.60
1:A:377:HIS:CD2	10:A:617:GOL:H2	2.38	0.58
1:A:8:ALA:N	1:A:9:PRO:CD	2.66	0.58
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.02	0.57
1:A:198:SEP:H	1:A:198:SEP:P	2.29	0.55
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.42	0.55
1:A:168:PRO:HG2	1:A:172:TYR:HB2	1.85	0.55
1:A:8:ALA:H	1:A:9:PRO:CD	2.19	0.54
1:A:377:HIS:HD2	10:A:617:GOL:H2	1.73	0.54
1:A:196:GLU:HB3	1:A:198:SEP:O2P	2.08	0.53
1:A:197:PRO:HD2	1:A:198:SEP:O3P	2.09	0.52
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.38	0.52
1:A:257:SER:O	1:A:381:PHE:HA	2.09	0.52
1:A:368:TRP:CH2	1:A:389:ASP:O	2.63	0.52
1:A:393:ASP:OD1	1:A:557:THR:HB	2.10	0.52
1:A:355:PRO:HA	7:A:616:IOD:I	2.80	0.51
12:A:626:MPD:C5	12:A:626:MPD:C1	2.89	0.51
1:A:9:PRO:C	1:A:11:PRO:HD3	2.30	0.51
1:A:425:THR:O	1:A:425:THR:HG22	2.11	0.50
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.59	0.50
1:A:570:ASN:HD22	1:A:575:ASP:HB3	1.76	0.50
1:A:264:THR:HG23	1:A:392:ILE:HB	1.93	0.49
1:A:424:PRO:O	1:A:425:THR:HB	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:PRO:O	1:A:11:PRO:HD3	2.12	0.49
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.95	0.48
1:A:197:PRO:O	12:A:626:MPD:H52	2.13	0.48
1:A:378:THR:HG22	10:A:617:GOL:H12	1.97	0.47
1:A:8:ALA:H	1:A:9:PRO:HD2	1.79	0.47
1:A:149:PRO:HB2	11:A:625:PEG:H41	1.97	0.47
1:A:10:VAL:HG21	16:A:1333:HOH:O	2.15	0.46
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.46	0.46
1:A:239:PHE:N	10:A:613:GOL:H31	2.31	0.46
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.98	0.46
1:A:237:CYS:HA	1:A:381:PHE:O	2.16	0.45
2:A:605:HEM:HMC2	2:A:605:HEM:HBC2	1.99	0.45
1:A:378:THR:HA	10:A:617:GOL:H12	2.00	0.44
1:A:108:ASP:C	1:A:108:ASP:OD1	2.55	0.44
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.53	0.44
1:A:123:GLU:HG3	1:A:125:SER:H	1.83	0.44
1:A:384:TRP:CZ2	6:A:601:NAG:H2	2.52	0.43
1:A:355:PRO:CA	7:A:616:IOD:I	3.37	0.43
1:A:424:PRO:O	1:A:425:THR:CB	2.66	0.43
1:A:80:ASN:OD1	11:A:625:PEG:H22	2.18	0.43
1:A:363:GLU:HB2	13:A:627:EDO:H22	2.00	0.43
1:A:362:ASP:HA	1:A:368:TRP:HD1	1.84	0.43
2:A:605:HEM:HBB2	2:A:605:HEM:HMB2	2.00	0.42
1:A:167:CYS:CB	1:A:168:PRO:CD	2.88	0.42
2:A:605:HEM:HBB2	2:A:605:HEM:CMB	2.49	0.42
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.45	0.42
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.54	0.41
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.31	0.41
1:A:83:VAL:O	1:A:412:MET:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	555 (94%)	31 (5%)	6 (1%)	22 6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	11	PRO
1	A	170	PRO
1	A	171	PRO
1	A	168	PRO
1	A	390	GLY

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%)	516 (100%)	1 (0%)	96 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	347	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
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	6.10	3 (33%)	10,12,14	1.44	2 (20%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	O-C	17.67	1.23	1.11
1	A	198	SEP	P-O1P	3.04	1.61	1.51
1	A	198	SEP	CA-C	2.51	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	P-OG-CB	-2.83	110.00	118.19
1	A	198	SEP	C-CA-N	-2.54	111.30	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

5 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$
5	NAG	A	599	1,5	12,14,15	0.73	0	15,19,21	1.24	3 (20%)
5	NAG	A	600	5	12,14,15	0.82	0	15,19,21	1.99	3 (20%)
6	NAG	A	601	1,6	12,14,15	0.82	0	15,19,21	1.03	0
6	NAG	A	602	6	12,14,15	0.48	0	15,19,21	1.95	5 (33%)
6	MAN	A	603	6	10,11,12	0.65	0	11,15,17	1.59	1 (9%)

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
5	NAG	A	599	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
6	NAG	A	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	602	6	-	0/6/23/26	0/1/1/1
6	MAN	A	603	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	NAG	O5-C5-C4	5.03	117.04	110.65
6	A	603	MAN	O5-C5-C6	4.84	112.06	106.98
5	A	600	NAG	O5-C5-C6	3.86	111.03	106.98
5	A	600	NAG	C3-C2-N2	-3.69	106.14	111.76
6	A	602	NAG	C3-C2-N2	2.83	116.07	111.76
5	A	600	NAG	O5-C5-C4	-2.76	107.15	110.65
5	A	599	NAG	O4-C4-C5	2.68	116.35	109.28
6	A	602	NAG	O3-C3-C2	2.62	114.59	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	NAG	C4-C3-C2	-2.11	106.16	111.32
5	A	599	NAG	C3-C2-N2	-2.06	108.62	111.76
6	A	602	NAG	O5-C5-C6	2.05	109.14	106.98
5	A	599	NAG	O5-C5-C6	-2.02	104.86	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 29 ligands modelled in this entry, 19 are monoatomic - leaving 10 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	596	1	12,14,15	0.65	0	15,19,21	1.23	1 (6%)
4	NAG	A	604	1	12,14,15	0.72	1 (8%)	15,19,21	1.05	2 (13%)
2	HEM	A	605	1,16	49,50,50	2.98	19 (38%)	46,82,82	2.36	13 (28%)
10	GOL	A	613	-	5,5,5	0.55	0	5,5,5	0.34	0
10	GOL	A	615	-	5,5,5	0.94	0	5,5,5	0.41	0
10	GOL	A	617	-	5,5,5	1.03	0	5,5,5	0.48	0
11	PEG	A	625	-	6,6,6	0.92	0	5,5,5	1.32	1 (20%)
12	MPD	A	626	-	7,7,7	2.65	1 (14%)	10,10,10	1.78	1 (10%)
13	EDO	A	627	-	3,3,3	1.46	0	2,2,2	0.81	0
15	SCN	A	629	-	2,2,2	1.85	1 (50%)	1,1,1	3.47	1 (100%)

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	596	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	HEM	A	605	1,16	-	0/14/114/114	0/0/8/8
10	GOL	A	613	-	-	0/4/4/4	0/0/0/0
10	GOL	A	615	-	-	0/4/4/4	0/0/0/0
10	GOL	A	617	-	-	0/4/4/4	0/0/0/0
11	PEG	A	625	-	-	0/4/4/4	0/0/0/0
12	MPD	A	626	-	-	0/5/5/5	0/0/0/0
13	EDO	A	627	-	-	0/1/1/1	0/0/0/0
15	SCN	A	629	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C2B-C1B	10.24	1.47	1.44
2	A	605	HEM	C4A-C3A	7.47	1.49	1.40
12	A	626	MPD	O2-C2	-6.94	1.24	1.44
2	A	605	HEM	C2D-C1D	-6.47	1.42	1.44
2	A	605	HEM	C3C-C2C	-5.77	1.33	1.43
2	A	605	HEM	C3B-C2B	-5.23	1.34	1.43
2	A	605	HEM	C3B-CAB	4.53	1.54	1.40
2	A	605	HEM	C3C-CAC	4.50	1.54	1.40
2	A	605	HEM	C3D-C4D	-3.66	1.43	1.44
2	A	605	HEM	CMC-C2C	3.61	1.58	1.47
2	A	605	HEM	CAD-CBD	3.24	1.61	1.52
2	A	605	HEM	FE-NA	3.09	2.05	1.92
2	A	605	HEM	CMB-C2B	3.01	1.56	1.47
2	A	605	HEM	CMD-C2D	2.82	1.56	1.47
2	A	605	HEM	CBD-CGD	2.78	1.57	1.50
2	A	605	HEM	C1B-NB	-2.53	1.34	1.39
2	A	605	HEM	C3D-C2D	2.53	1.48	1.43
15	A	629	SCN	C-S	2.29	1.78	1.63
2	A	605	HEM	CHB-C1B	2.13	1.38	1.35
2	A	605	HEM	CHA-C4D	2.09	1.38	1.35
2	A	605	HEM	FE-ND	2.06	2.05	1.97
4	A	604	NAG	O5-C5	-2.01	1.41	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C3B-C4B-NB	-7.45	108.67	114.00
2	A	605	HEM	CHD-C1D-ND	5.67	129.30	124.58
2	A	605	HEM	CAD-C3D-C4D	5.31	134.08	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C4D-ND-C1D	4.82	110.10	105.16
2	A	605	HEM	CBD-CAD-C3D	-4.41	104.74	114.37
2	A	605	HEM	C2D-C1D-ND	-4.25	107.91	112.93
12	A	626	MPD	O2-C2-C1	-4.03	92.74	107.98
15	A	629	SCN	S-C-N	-3.47	153.99	176.18
2	A	605	HEM	CHC-C4B-NB	3.09	127.15	124.58
2	A	605	HEM	CHD-C4C-NC	-2.98	122.14	124.73
4	A	596	NAG	O5-C5-C4	2.95	114.39	110.65
2	A	605	HEM	CHC-C1C-NC	2.64	127.03	124.73
2	A	605	HEM	CMB-C2B-C3B	2.45	131.93	126.16
4	A	604	NAG	C3-C2-N2	-2.31	108.24	111.76
2	A	605	HEM	O1D-CGD-CBD	-2.17	115.55	123.03
2	A	605	HEM	C1B-NB-C4B	2.15	107.36	105.16
11	A	625	PEG	O4-C4-C3	2.12	125.53	111.80
2	A	605	HEM	C2A-C1A-CHA	-2.12	121.99	126.00
4	A	604	NAG	O5-C5-C4	-2.05	108.06	110.65

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%)	0.63	50 (8%)	11 10	12, 25, 70, 114	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	19.8
1	A	2	TRP	19.4
1	A	12	LEU	14.7
1	A	119	LEU	13.8
1	A	7	GLY	13.7
1	A	4	VAL	12.3
1	A	171	PRO	12.0
1	A	124	HIS	11.8
1	A	10	VAL	11.5
1	A	172	TYR	10.9
1	A	8	ALA	10.5
1	A	122	ASN	9.7
1	A	121	SER	8.7
1	A	128	GLN	8.6
1	A	120	GLY	8.5
1	A	595	ASN	7.8
1	A	173	GLN	7.5
1	A	14	LYS	7.2
1	A	594	GLU	7.0
1	A	125	SER	6.3
1	A	1	SER	6.2
1	A	6	CYS	6.1
1	A	593	ARG	5.9
1	A	127	THR	5.6
1	A	3	GLU	5.5
1	A	5	GLY	5.4
1	A	123	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	170	PRO	4.9
1	A	174	SER	4.9
1	A	11	PRO	4.6
1	A	129	CYS	4.0
1	A	118	GLU	3.9
1	A	126	LYS	3.8
1	A	283	LEU	3.8
1	A	9	PRO	3.4
1	A	169	THR	3.3
1	A	64	ARG	2.9
1	A	132	TYR	2.8
1	A	209	PRO	2.4
1	A	166	VAL	2.4
1	A	167	CYS	2.3
1	A	168	PRO	2.3
1	A	40	ASN	2.3
1	A	18	ASN	2.2
1	A	247	PRO	2.2
1	A	63	GLN	2.2
1	A	574	HIS	2.2
1	A	175	LEU	2.1
1	A	368	TRP	2.1
1	A	131	GLU	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. 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	0.32	9.80	21,38,44,48	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
6	NAG	A	602	14/15	0.28	5.24	52,58,64,68	0
6	NAG	A	601	14/15	0.20	1.83	25,33,42,44	0
5	NAG	A	599	14/15	0.11	0.59	30,39,42,49	0
5	NAG	A	600	14/15	0.38	-	56,60,61,62	0
6	MAN	A	603	11/12	0.42	-	72,75,77,78	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(Å ²)	Q<0.9
10	GOL	A	617	6/6	0.28	37.39	18,22,26,28	0
12	MPD	A	626	8/8	0.34	12.88	22,36,39,42	0
10	GOL	A	615	6/6	0.31	8.44	24,26,27,28	0
4	NAG	A	604	14/15	0.31	7.87	30,34,39,39	0
7	IOD	A	616	1/1	0.17	4.39	54,54,54,54	1
4	NAG	A	596	14/15	0.29	2.53	48,53,56,56	0
15	SCN	A	629	3/3	0.16	0.74	34,34,35,37	0
10	GOL	A	613	6/6	0.35	0.40	19,26,27,27	0
11	PEG	A	625	7/7	0.22	0.30	12,25,34,35	0
2	HEM	A	605	43/43	0.12	-0.12	12,14,18,20	0
7	IOD	A	623	1/1	0.08	-0.33	34,34,34,34	1
7	IOD	A	622	1/1	0.09	-0.37	43,43,43,43	0
3	CA	A	606	1/1	0.09	-0.43	15,15,15,15	0
13	EDO	A	627	4/4	0.09	-0.48	18,19,20,23	0
7	IOD	A	614	1/1	0.05	-1.55	32,32,32,32	1
7	IOD	A	609	1/1	0.04	-1.86	41,41,41,41	1
7	IOD	A	620	1/1	0.06	-2.09	38,38,38,38	1
7	IOD	A	624	1/1	0.05	-2.22	39,39,39,39	1
7	IOD	A	612	1/1	0.04	-2.33	32,32,32,32	0
7	IOD	A	610	1/1	0.04	-2.75	42,42,42,42	0
9	CL	A	598	1/1	0.07	-2.99	26,26,26,26	0
7	IOD	A	607	1/1	0.02	-3.24	19,19,19,19	0
7	IOD	A	608	1/1	0.03	-3.79	31,31,31,31	0
7	IOD	A	618	1/1	0.05	-3.84	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	IOD	A	621	1/1	0.03	-4.88	38,38,38,38	1
8	BR	A	597	1/1	0.03	-4.99	28,28,28,28	0
7	IOD	A	611	1/1	0.04	-6.87	25,25,25,25	0
7	IOD	A	619	1/1	0.04	-10.83	42,42,42,42	0
14	ZN	A	628	1/1	0.03	-12.16	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.