



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 27, 2016 – 10:47 PM EST

PDB ID : 5K1E
Title : Crystal structure of an intermediate of lactoperoxidase with bound hypothiocynate at the substrate binding site on the distal heme side.
Authors : Singh, P.K.; Sirohi, H.V.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-05-18
Resolution : 2.07 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

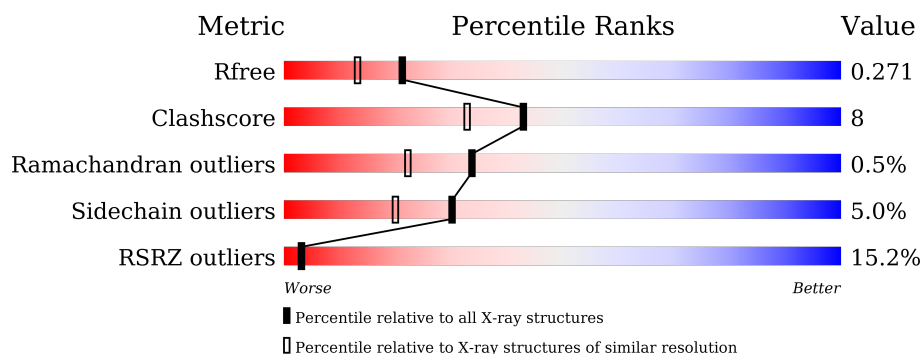
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	91344	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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. 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	<div> <div>15%</div> <div>84%</div> <div>15%</div> </div>

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
6	OSM	A	609	-	-	X	-
6	OSM	A	615	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	OSM	A	618	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5211 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
			4776	3039	848	861	1	27			

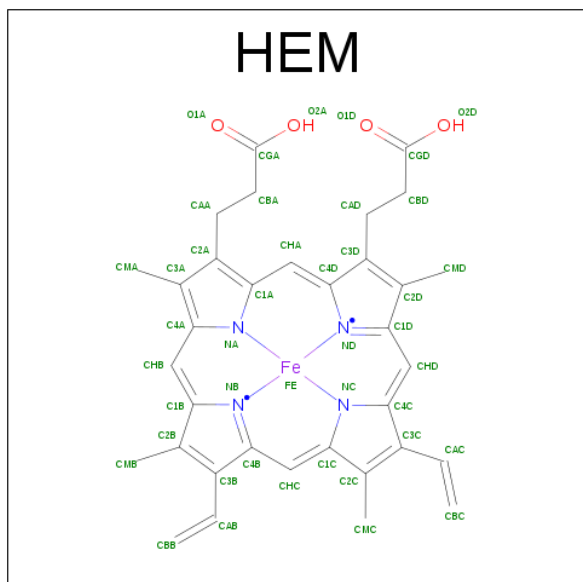
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	LYS	ASP	see sequence details	UNP P80025
A	547	MET	VAL	see sequence details	UNP P80025

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

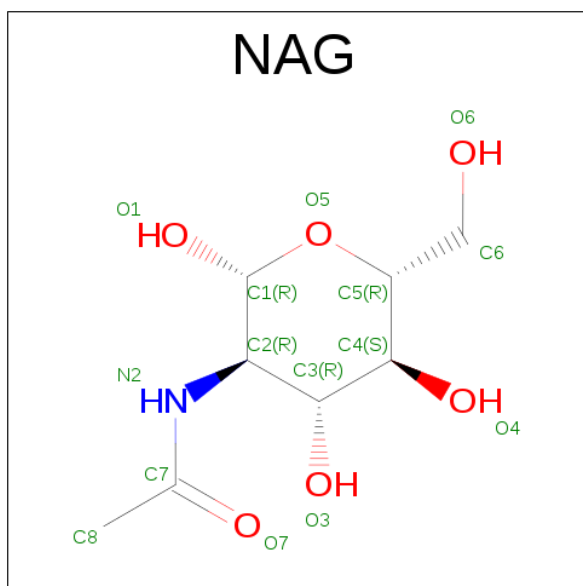
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

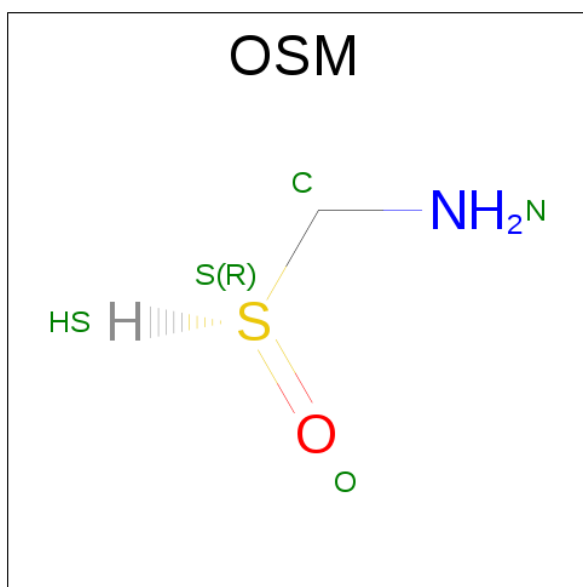


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			14	8	1	5		
4	A	1	Total	C	N	O		
			14	8	1	5		
4	A	1	Total	C	N	O		
			14	8	1	5		
4	A	1	Total	C	N	O		
			14	8	1	5		
4	A	1	Total	C	N	O		
			14	8	1	5		

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

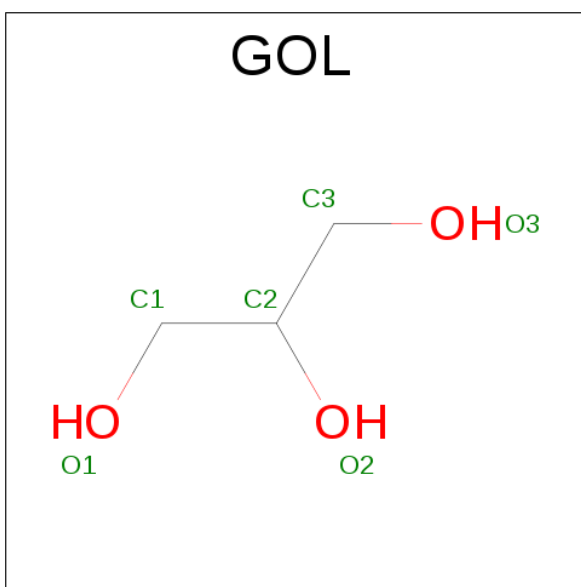
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total I		
			3 3	0	0

- Molecule 6 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



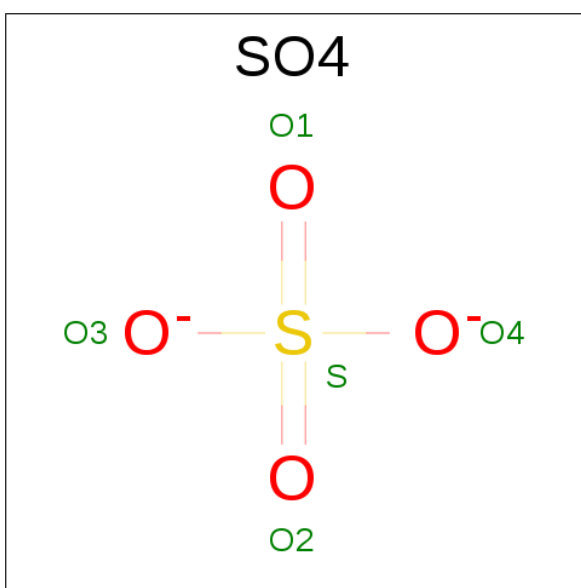
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		
6	A	1	Total	C	N	O	S	0	0
			4	1	1	1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

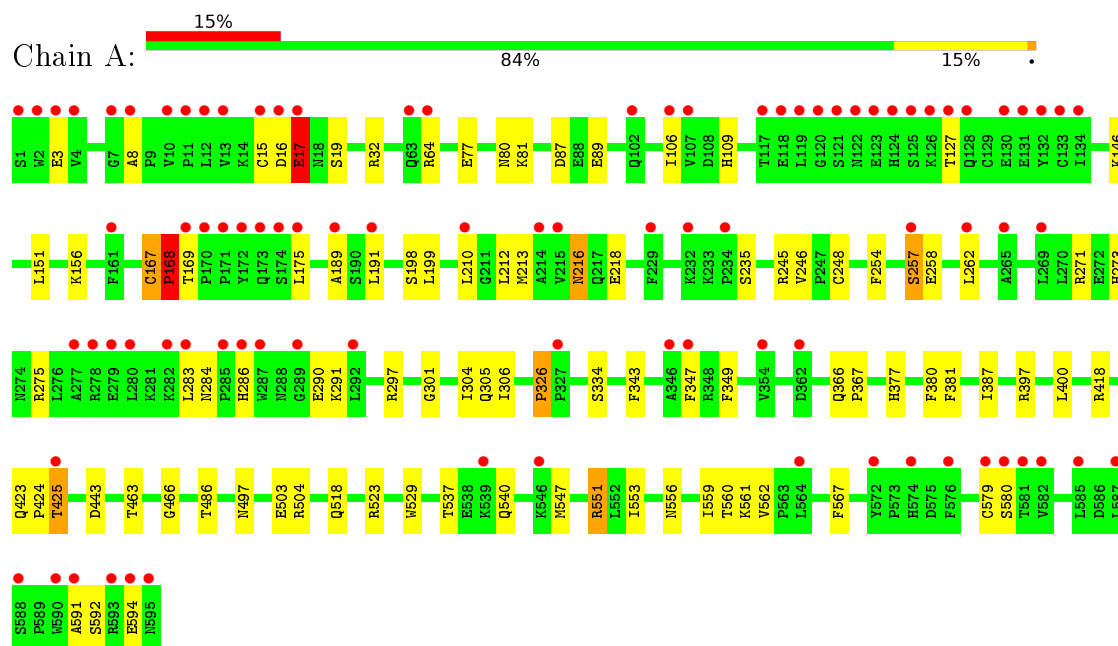
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	257	Total 257	O 257	0	0

3 Residue-property plots [i](#)

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	54.01Å 79.81Å 66.11Å 90.00° 93.01° 90.00°	Depositor
Resolution (Å)	34.17 – 2.07 34.15 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.4 (34.17-2.07) 94.5 (34.15-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.190 , 0.272 0.199 , 0.271	Depositor DCC
R_{free} test set	1001 reflections (3.20%)	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5211	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, SEP, CA, OSM, SO4, HEM, IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	1/4893 (0.0%)	0.85	6/6634 (0.1%)

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	503	GLU	CD-OE2	-6.12	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	CB-CA-C	-8.70	93.00	110.40
1	A	418	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	503	GLU	OE1-CD-OE2	-5.78	116.37	123.30
1	A	443	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	297	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	551	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	168	PRO	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	4776	0	4695	75	0
2	A	1	0	0	0	0
3	A	43	0	30	6	0
4	A	70	0	64	0	0
5	A	3	0	0	1	0
6	A	44	0	54	17	0
7	A	12	0	16	3	0
8	A	5	0	0	0	0
9	A	257	0	0	6	0
All	All	5211	0	4859	80	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 8.

All (80) 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:15:CYS:HB3	1:A:17:GLU:OE2	1.24	1.32
1:A:258:GLU:OE2	3:A:602:HEM:CMB	1.78	1.31
1:A:258:GLU:OE2	3:A:602:HEM:HMB1	1.13	1.26
1:A:257:SER:O	1:A:381:PHE:CD1	2.08	1.05
1:A:15:CYS:CB	1:A:17:GLU:OE2	2.05	1.04
1:A:258:GLU:HG3	6:A:609:OSM:HS	1.32	0.93
1:A:3:GLU:N	1:A:3:GLU:OE1	2.08	0.86
1:A:109:HIS:HE1	1:A:262:LEU:HD21	1.41	0.84
1:A:109:HIS:CE1	1:A:262:LEU:HD21	2.14	0.81
1:A:248:CYS:HB3	1:A:257:SER:OG	1.81	0.80
1:A:3:GLU:OE2	1:A:175:LEU:HD22	1.81	0.80
1:A:3:GLU:HB2	9:A:884:HOH:O	1.85	0.76
1:A:258:GLU:HG3	6:A:609:OSM:S	2.26	0.76
1:A:567:PHE:HB2	6:A:612:OSM:HS	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLY:HA3	6:A:615:OSM:H2	1.70	0.72
1:A:258:GLU:OE2	3:A:602:HEM:HMB2	1.84	0.71
1:A:257:SER:O	1:A:381:PHE:CE1	2.45	0.70
1:A:15:CYS:HB3	1:A:17:GLU:CD	2.10	0.67
1:A:109:HIS:HE1	1:A:262:LEU:CD2	2.08	0.67
3:A:602:HEM:HBC2	3:A:602:HEM:HMC1	1.77	0.66
1:A:216:ASN:HA	6:A:619:OSM:N	2.11	0.66
1:A:15:CYS:HB2	1:A:17:GLU:OE1	1.95	0.65
1:A:15:CYS:CB	1:A:17:GLU:CD	2.64	0.65
7:A:621:GOL:O1	9:A:701:HOH:O	2.15	0.64
1:A:258:GLU:CG	6:A:609:OSM:HS	2.07	0.63
1:A:109:HIS:ND1	9:A:704:HOH:O	2.30	0.63
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.61
3:A:602:HEM:HMB2	3:A:602:HEM:HBB2	1.84	0.59
1:A:109:HIS:CE1	1:A:262:LEU:CD2	2.86	0.56
1:A:17:GLU:OE2	1:A:17:GLU:N	2.38	0.56
1:A:16:ASP:HB2	1:A:19:SER:HB2	1.89	0.54
1:A:271:ARG:NH1	1:A:556:ASN:O	2.34	0.54
1:A:216:ASN:ND2	5:A:623:IOD:I	3.12	0.53
1:A:301:GLY:O	1:A:305:GLN:HG3	2.09	0.53
1:A:64:ARG:O	9:A:702:HOH:O	2.19	0.52
1:A:286:HIS:NE2	1:A:592:SER:O	2.43	0.51
1:A:466:GLY:CA	6:A:615:OSM:H2	2.41	0.50
1:A:199:LEU:HD22	1:A:254:PHE:CE1	2.47	0.49
1:A:397:ARG:HE	6:A:618:OSM:C	2.25	0.49
1:A:366:GLN:O	1:A:367:PRO:C	2.50	0.49
7:A:621:GOL:C1	9:A:701:HOH:O	2.60	0.49
1:A:198:SEP:C	7:A:621:GOL:HO2	2.24	0.49
1:A:8:ALA:HB3	1:A:168:PRO:HD2	1.95	0.48
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.49	0.47
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.48	0.47
1:A:397:ARG:HE	6:A:618:OSM:H1	1.79	0.47
1:A:16:ASP:CB	1:A:19:SER:HB2	2.44	0.47
1:A:561:LYS:HG2	6:A:618:OSM:O	2.15	0.47
1:A:15:CYS:HB2	1:A:17:GLU:CD	2.34	0.46
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.96	0.46
1:A:424:PRO:O	1:A:425:THR:HG22	2.16	0.46
1:A:537:THR:H	1:A:540:GLN:HE21	1.64	0.46
1:A:561:LYS:N	6:A:618:OSM:O	2.41	0.45
1:A:561:LYS:O	1:A:562:VAL:HG13	2.16	0.45
1:A:87:ASP:N	6:A:610:OSM:O	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:HB2	6:A:614:OSM:H2	1.98	0.45
1:A:400:LEU:HD11	1:A:553:ILE:HD13	1.98	0.44
1:A:397:ARG:NE	6:A:618:OSM:H1	2.33	0.44
1:A:306:ILE:HD12	1:A:547:MET:CE	2.47	0.44
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.99	0.44
1:A:17:GLU:OE2	1:A:17:GLU:CA	2.66	0.43
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.83	0.43
1:A:248:CYS:CB	1:A:257:SER:OG	2.59	0.43
1:A:466:GLY:HA3	6:A:615:OSM:C	2.44	0.43
3:A:602:HEM:CMB	3:A:602:HEM:HBB2	2.49	0.42
1:A:246:VAL:HG11	1:A:387:ILE:HD12	2.01	0.42
1:A:15:CYS:C	1:A:17:GLU:OE2	2.58	0.42
1:A:423:GLN:HA	1:A:423:GLN:HE21	1.85	0.42
1:A:425:THR:O	1:A:425:THR:HG23	2.19	0.42
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.55	0.41
1:A:283:LEU:O	1:A:284:ASN:ND2	2.53	0.41
1:A:156:LYS:HD3	9:A:951:HOH:O	2.21	0.41
1:A:290:GLU:O	1:A:291:LYS:C	2.59	0.41
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.55	0.41
1:A:559:ILE:O	1:A:579:CYS:SG	2.79	0.41
1:A:504:ARG:HA	6:A:613:OSM:H2	2.03	0.41
1:A:248:CYS:HB3	1:A:257:SER:CB	2.51	0.41
1:A:284:ASN:HD21	1:A:591:ALA:HA	1.86	0.41
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.51	0.40
1:A:463:THR:HG23	6:A:615:OSM: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%)	544 (92%)	45 (8%)	3 (0%)	34 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO
1	A	326	PRO
1	A	167	CYS

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%)	491 (95%)	26 (5%)	30	20

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	32	ARG
1	A	89	GLU
1	A	127	THR
1	A	146	LYS
1	A	151	LEU
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	210	LEU
1	A	212	LEU
1	A	216	ASN
1	A	218	GLU
1	A	235	SER
1	A	245	ARG
1	A	257	SER
1	A	275	ARG
1	A	326	PRO
1	A	334	SER
1	A	347	PHE
1	A	425	THR
1	A	486	THR

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Mol	Chain	Res	Type
1	A	551	ARG
1	A	560	THR
1	A	580	SER
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	284	ASN
1	A	329	GLN
1	A	423	GLN
1	A	497	ASN
1	A	521	GLN
1	A	565	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	7,9,10	1.32	1 (14%)	8,12,14	4.70	5 (62%)

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	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	2.45	1.66	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	-2.93	99.71	107.08
1	A	198	SEP	O2P-P-OG	-2.19	100.32	106.72
1	A	198	SEP	O2P-P-O1P	2.65	119.29	110.63
1	A	198	SEP	O3P-P-OG	3.98	118.34	106.72
1	A	198	SEP	OG-CB-CA	11.69	118.44	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	1,9	24,50,50	1.61	2 (8%)	16,82,82	1.74	3 (18%)
4	NAG	A	603	1	14,14,15	0.55	0	15,19,21	1.71	2 (13%)
4	NAG	A	604	1,4	14,14,15	0.52	0	15,19,21	1.56	3 (20%)
4	NAG	A	605	4	14,14,15	0.31	0	15,19,21	1.60	3 (20%)
4	NAG	A	606	1	14,14,15	0.77	0	15,19,21	1.48	1 (6%)
4	NAG	A	607	1	14,14,15	0.74	0	15,19,21	1.45	2 (13%)
6	OSM	A	609	-	1,3,3	0.48	0	0,2,2	0.00	-
6	OSM	A	610	-	1,3,3	0.49	0	0,2,2	0.00	-
6	OSM	A	611	-	1,3,3	0.58	0	0,2,2	0.00	-
6	OSM	A	612	-	1,3,3	0.58	0	0,2,2	0.00	-
6	OSM	A	613	-	1,3,3	0.33	0	0,2,2	0.00	-
6	OSM	A	614	-	1,3,3	0.45	0	0,2,2	0.00	-
6	OSM	A	615	-	1,3,3	0.00	0	0,2,2	0.00	-
6	OSM	A	616	-	1,3,3	0.62	0	0,2,2	0.00	-
6	OSM	A	617	-	1,3,3	0.56	0	0,2,2	0.00	-
6	OSM	A	618	-	1,3,3	0.28	0	0,2,2	0.00	-
6	OSM	A	619	-	1,3,3	0.10	0	0,2,2	0.00	-
7	GOL	A	620	-	5,5,5	0.25	0	5,5,5	0.26	0
7	GOL	A	621	-	5,5,5	0.75	0	5,5,5	0.40	0
8	SO4	A	624	-	4,4,4	0.94	0	6,6,6	3.42	2 (33%)

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	1,9	-	0/6/54/54	0/0/8/8
4	NAG	A	603	1	-	0/6/23/26	0/1/1/1
4	NAG	A	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	605	4	-	0/6/23/26	0/1/1/1
4	NAG	A	606	1	-	0/6/23/26	0/1/1/1
4	NAG	A	607	1	-	0/6/23/26	0/1/1/1
6	OSM	A	609	-	-	0/0/1/1	0/0/0/0
6	OSM	A	610	-	-	0/0/1/1	0/0/0/0
6	OSM	A	611	-	-	0/0/1/1	0/0/0/0
6	OSM	A	612	-	-	0/0/1/1	0/0/0/0
6	OSM	A	613	-	-	0/0/1/1	0/0/0/0
6	OSM	A	614	-	-	0/0/1/1	0/0/0/0
6	OSM	A	615	-	-	0/0/1/1	0/0/0/0
6	OSM	A	616	-	-	0/0/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OSM	A	617	-	-	0/0/1/1	0/0/0/0
6	OSM	A	618	-	-	0/0/1/1	0/0/0/0
6	OSM	A	619	-	-	0/0/1/1	0/0/0/0
7	GOL	A	620	-	-	0/4/4/4	0/0/0/0
7	GOL	A	621	-	-	0/4/4/4	0/0/0/0
8	SO4	A	624	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C4C-NC	-5.70	1.29	1.36
3	A	602	HEM	C4D-ND	-2.63	1.33	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	CBA-CAA-C2A	-4.33	104.88	112.49
3	A	602	HEM	CBD-CAD-C3D	-3.45	106.42	112.47
4	A	605	NAG	C3-C4-C5	2.00	113.80	110.23
3	A	602	HEM	CMC-C2C-C3C	2.07	129.15	125.09
4	A	604	NAG	O7-C7-N2	2.19	126.31	121.84
4	A	607	NAG	O5-C5-C4	2.32	113.98	110.13
4	A	604	NAG	O5-C5-C4	2.32	113.98	110.13
4	A	605	NAG	O5-C5-C4	2.60	114.44	110.13
4	A	603	NAG	O5-C5-C4	2.95	115.02	110.13
4	A	606	NAG	C4-C3-C2	3.22	116.34	111.34
4	A	604	NAG	C1-O5-C5	3.39	117.12	112.14
8	A	624	SO4	O4-S-O3	3.91	124.84	109.09
4	A	605	NAG	C1-O5-C5	4.14	118.23	112.14
4	A	603	NAG	C1-O5-C5	4.21	118.33	112.14
4	A	607	NAG	C1-O5-C5	4.34	118.52	112.14
8	A	624	SO4	O2-S-O1	7.03	133.08	109.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HEM	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	OSM	3	0
6	A	610	OSM	1	0
6	A	612	OSM	1	0
6	A	613	OSM	1	0
6	A	614	OSM	1	0
6	A	615	OSM	4	0
6	A	618	OSM	5	0
6	A	619	OSM	1	0
7	A	621	GOL	3	0

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%)	0.87	90 (15%) 3 3	23, 47, 106, 168	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	18.9
1	A	172	TYR	14.3
1	A	173	GLN	13.5
1	A	121	SER	12.7
1	A	120	GLY	12.7
1	A	119	LEU	10.2
1	A	122	ASN	8.8
1	A	257	SER	8.7
1	A	1	SER	7.7
1	A	7	GLY	7.1
1	A	10	VAL	7.0
1	A	594	GLU	7.0
1	A	593	ARG	6.4
1	A	126	LYS	6.3
1	A	132	TYR	6.0
1	A	171	PRO	5.7
1	A	582	VAL	5.7
1	A	174	SER	5.7
1	A	127	THR	5.6
1	A	595	ASN	5.4
1	A	124	HIS	5.3
1	A	131	GLU	5.1
1	A	283	LEU	5.1
1	A	4	VAL	5.1
1	A	282	LYS	4.9
1	A	17	GLU	4.7
1	A	214	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	4.5
1	A	170	PRO	4.3
1	A	12	LEU	4.0
1	A	16	ASP	3.7
1	A	169	THR	3.6
1	A	210	LEU	3.6
1	A	576	PHE	3.4
1	A	581	THR	3.4
1	A	63	GLN	3.4
1	A	123	GLU	3.4
1	A	286	HIS	3.3
1	A	161	PHE	3.3
1	A	280	LEU	3.2
1	A	327	PRO	3.2
1	A	262	LEU	3.2
1	A	265	ALA	3.2
1	A	13	VAL	3.1
1	A	591	ALA	3.1
1	A	277	ALA	3.1
1	A	3	GLU	3.1
1	A	574	HIS	3.1
1	A	11	PRO	3.1
1	A	287	TRP	3.0
1	A	64	ARG	3.0
1	A	539	LYS	2.9
1	A	425	THR	2.9
1	A	107	VAL	2.8
1	A	125	SER	2.8
1	A	572	TYR	2.8
1	A	587	LEU	2.8
1	A	579	CYS	2.8
1	A	585	LEU	2.8
1	A	232	LYS	2.8
1	A	354	VAL	2.7
1	A	546	LYS	2.7
1	A	128	GLN	2.7
1	A	117	THR	2.6
1	A	15	CYS	2.6
1	A	118	GLU	2.6
1	A	175	LEU	2.5
1	A	189	ALA	2.5
1	A	588	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	191	LEU	2.5
1	A	590	TRP	2.5
1	A	215	VAL	2.4
1	A	278	ARG	2.4
1	A	134	ILE	2.4
1	A	130	GLU	2.4
1	A	133	CYS	2.4
1	A	102	GLN	2.4
1	A	229	PHE	2.3
1	A	106	ILE	2.3
1	A	347	PHE	2.2
1	A	362	ASP	2.2
1	A	285	PRO	2.2
1	A	580	SER	2.1
1	A	289	GLY	2.1
1	A	269	LEU	2.1
1	A	564	LEU	2.1
1	A	234	PRO	2.1
1	A	292	LEU	2.1
1	A	346	ALA	2.0
1	A	279	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.91	0.14	-	43,50,63,69	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	HEM	A	602	43/43	0.97	0.20	0.51	23,27,33,34	0
4	NAG	A	606	14/15	0.88	0.17	0.47	58,61,68,69	0
6	OSM	A	617	4/4	0.98	0.12	0.19	33,43,46,47	0
6	OSM	A	611	4/4	0.96	0.13	0.16	38,43,45,52	0
6	OSM	A	612	4/4	0.96	0.16	0.12	52,53,53,53	0
8	SO4	A	624	5/5	0.96	0.16	0.07	26,33,50,55	0
7	GOL	A	620	6/6	0.94	0.14	-0.06	48,50,54,58	0
7	GOL	A	621	6/6	0.92	0.12	-0.31	31,32,36,38	0
6	OSM	A	614	4/4	0.99	0.12	-0.38	26,28,42,46	0
6	OSM	A	610	4/4	0.99	0.10	-0.54	36,43,46,48	0
4	NAG	A	604	14/15	0.78	0.19	-0.55	52,70,82,83	0
6	OSM	A	613	4/4	0.97	0.10	-0.67	49,51,52,55	0
6	OSM	A	615	4/4	0.98	0.08	-0.84	24,25,30,33	0
5	IOD	A	608	1/1	1.00	0.08	-1.24	29,29,29,29	0
6	OSM	A	616	4/4	0.96	0.09	-1.46	40,44,45,52	0
6	OSM	A	618	4/4	0.91	0.11	-1.58	57,57,63,64	0
2	CA	A	601	1/1	0.98	0.10	-1.85	33,33,33,33	0
6	OSM	A	619	4/4	0.99	0.10	-2.04	26,26,26,29	4
5	IOD	A	623	1/1	0.99	0.08	-2.52	48,48,48,48	1
5	IOD	A	622	1/1	0.97	0.04	-2.55	64,64,64,64	1
4	NAG	A	605	14/15	0.76	0.24	-	77,88,93,110	0
6	OSM	A	609	4/4	0.98	0.16	-	44,51,53,54	0
4	NAG	A	607	14/15	0.68	0.27	-	64,72,88,92	0
4	NAG	A	603	14/15	0.76	0.31	-	68,73,79,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.