



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GJ1
Title : Crystal structure of Bovine lactoperoxidase at 2.3A resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Bhushan, A.; Singh, T.P.
Deposited on : 2006-03-30
Resolution : 2.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

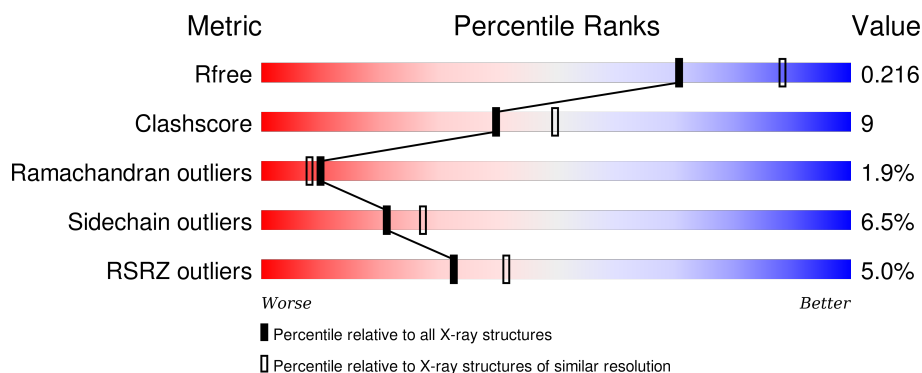
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	583	<div> <div>5%</div> <div>77%</div> <div>20%</div> <div>..</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
4	NO3	A	590	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NO3	A	591	-	X	-	X
8	OSM	A	702	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5198 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	583	Total	C	N	O	S	0	1	0
			4697	2991	835	846	25			

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

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

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

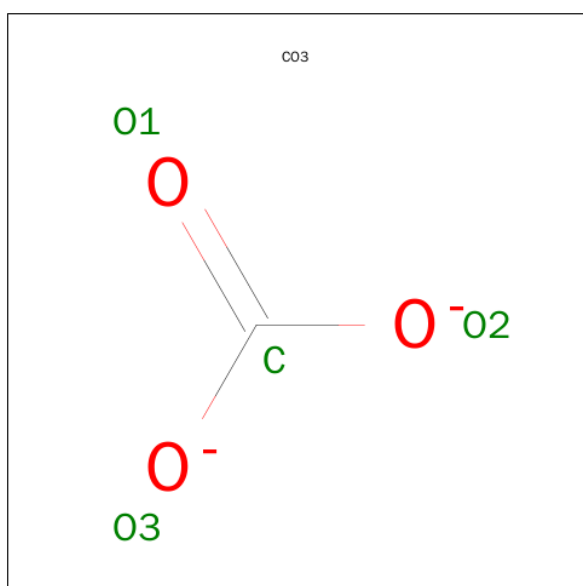
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).

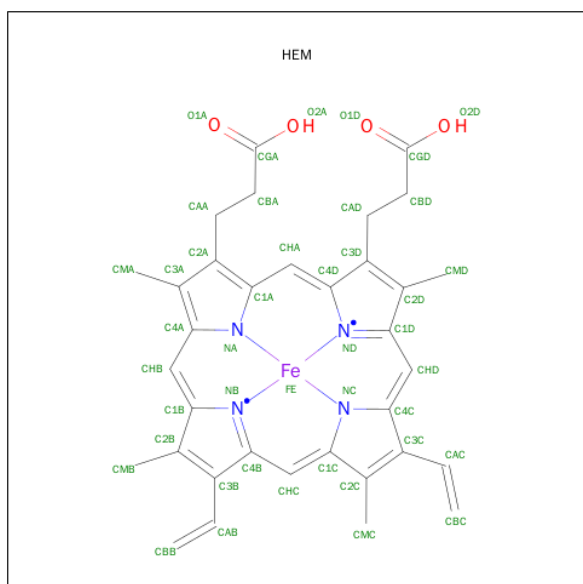


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

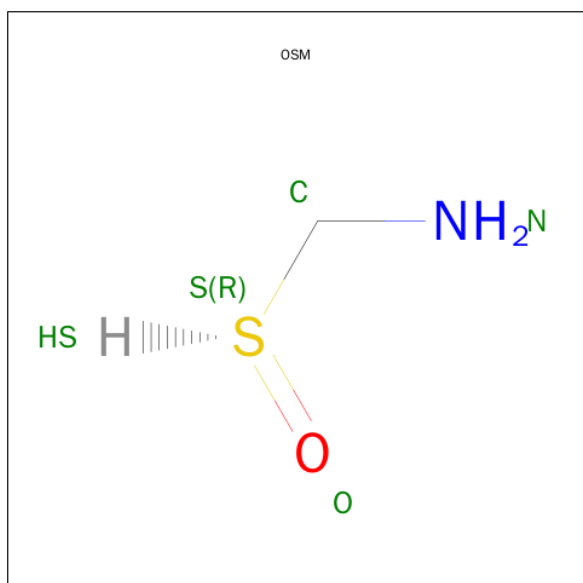
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).



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

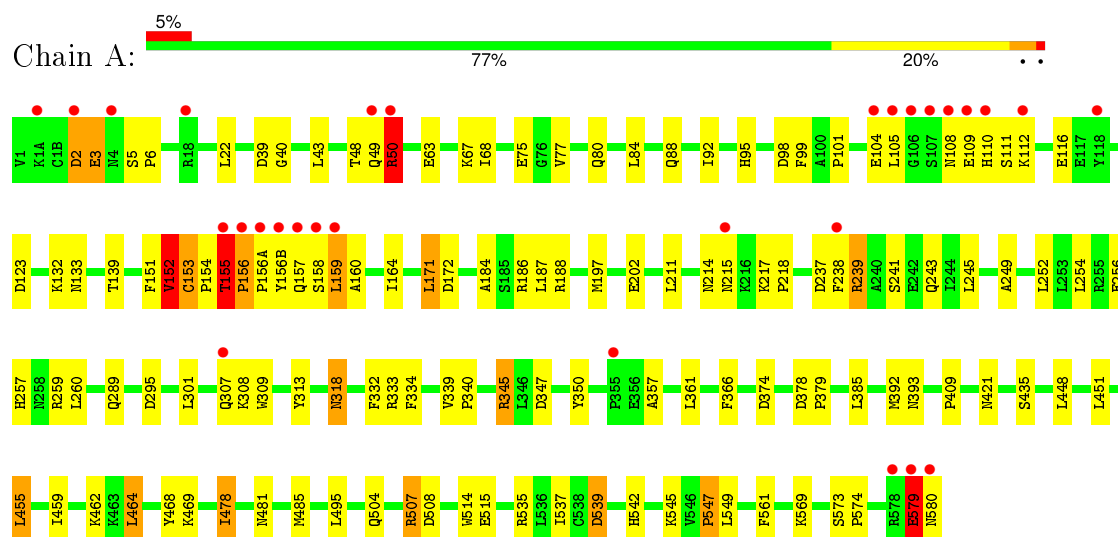
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	318	Total	O	0	0
			318	318		

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	54.63Å 80.67Å 77.68Å 90.00° 102.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 24.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 99.3 (24.46-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.174 , 0.219 0.172 , 0.216	Depositor DCC
R_{free} test set	931 reflections (3.31%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29120 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5198	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CO3, NAG, CA, OSM, HEM, NO3, 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	0.43	1/4822 (0.0%)	0.78	11/6538 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	PRO	C-N	5.13	1.45	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	547	PRO	C-N-CA	-5.72	107.40	121.70
1	A	374	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	295	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	172	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	152	VAL	N-CA-C	5.31	125.33	111.00
1	A	539	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	2	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	123	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	508	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	39	ASP	CB-CG-OD2	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4697	0	4619	80	0
2	A	84	0	75	0	0
3	A	39	0	34	3	0
4	A	8	0	0	0	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	A	43	0	30	2	0
8	A	4	0	5	2	0
9	A	318	0	0	11	0
All	All	5198	0	4763	85	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 9.

All (85) 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:92:ILE:HD11	1:A:249:ALA:HB1	1.52	0.90
1:A:153:CYS:CB	1:A:154:PRO:HD3	2.00	0.90
1:A:547:PRO:HD3	1:A:561:PHE:CE2	2.07	0.89
1:A:153:CYS:HB2	1:A:154:PRO:HD3	1.60	0.84
1:A:155:THR:H	1:A:156:PRO:HD2	1.45	0.82
1:A:459:ILE:H	1:A:459:ILE:HD12	1.46	0.81
1:A:153:CYS:HB2	1:A:154:PRO:CD	2.12	0.79
1:A:109:GLU:HB3	1:A:112:LYS:HE2	1.63	0.79
1:A:153:CYS:CB	1:A:154:PRO:CD	2.64	0.75
1:A:2:ASP:HB3	9:A:999:HOH:O	1.88	0.74
1:A:48:THR:HG22	1:A:50:ARG:HG3	1.72	0.71
1:A:237:ASP:OD2	1:A:239:ARG:HD3	1.90	0.71
1:A:547:PRO:HD3	1:A:561:PHE:CD2	2.25	0.70
1:A:92:ILE:HD11	1:A:249:ALA:CB	2.24	0.67
7:A:605:HEM:HMC2	7:A:605:HEM:HBC2	1.77	0.66
1:A:153:CYS:HB3	1:A:154:PRO:HD3	1.78	0.65
1:A:109:GLU:HG3	1:A:111:SER:H	1.62	0.65
1:A:68:ILE:HG21	1:A:478:ILE:HD11	1.79	0.64
3:A:587:MAN:H61	9:A:785:HOH:O	1.96	0.64
1:A:545:LYS:HG3	9:A:856:HOH:O	1.99	0.62
1:A:345:ARG:NH1	1:A:357:ALA:HA	2.17	0.59
1:A:333:ARG:HH11	1:A:421:ASN:ND2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:HIS:NE2	8:A:702:OSM:S	2.73	0.59
1:A:211:LEU:HD23	1:A:254:LEU:HD22	1.84	0.59
1:A:345:ARG:HH12	1:A:357:ALA:HA	1.68	0.59
1:A:155:THR:H	1:A:156:PRO:CD	2.08	0.59
1:A:154:PRO:HG2	1:A:156(B):TYR:CD1	2.38	0.58
1:A:459:ILE:HD12	1:A:459:ILE:N	2.18	0.58
1:A:569:LYS:HD3	9:A:928:HOH:O	2.03	0.56
1:A:514:TRP:CE2	1:A:515:GLU:HG3	2.40	0.56
1:A:75:GLU:HG3	9:A:863:HOH:O	2.06	0.56
1:A:256:GLU:OE1	1:A:259:ARG:HD3	2.06	0.56
1:A:197:MET:HG2	1:A:257:HIS:CD2	2.41	0.55
1:A:392:MET:HB3	1:A:485:MET:CE	2.37	0.54
1:A:573:SER:N	1:A:574:PRO:CD	2.71	0.54
1:A:318:ASN:HD22	1:A:318:ASN:C	2.12	0.53
1:A:155:THR:N	1:A:156:PRO:HD2	2.21	0.53
1:A:68:ILE:HD12	1:A:464:LEU:HD13	1.90	0.53
1:A:385:LEU:HD11	1:A:537:ILE:HD13	1.91	0.53
1:A:152:VAL:O	1:A:153:CYS:C	2.46	0.52
1:A:308:LYS:HE3	1:A:309:TRP:CZ2	2.44	0.51
1:A:459:ILE:H	1:A:459:ILE:CD1	2.20	0.51
1:A:151:PHE:O	1:A:164:ILE:HD11	2.09	0.51
1:A:535:ARG:HD3	1:A:569:LYS:HA	1.92	0.51
1:A:49:GLN:O	1:A:50:ARG:HB3	2.11	0.50
1:A:366:PHE:CZ	1:A:409:PRO:HG3	2.47	0.50
1:A:214:ASN:OD1	1:A:215:ASN:N	2.45	0.50
3:A:586:NAG:H62	3:A:587:MAN:H2	1.94	0.49
1:A:451:LEU:HG	1:A:455:LEU:HD22	1.93	0.49
1:A:171:LEU:HD13	1:A:289:GLN:HA	1.94	0.49
1:A:48:THR:HG22	1:A:50:ARG:CG	2.40	0.48
1:A:393:ASN:HB2	9:A:872:HOH:O	2.12	0.48
1:A:159:LEU:HD22	1:A:160:ALA:H	1.79	0.48
1:A:159:LEU:CD2	1:A:160:ALA:H	2.29	0.46
1:A:49:GLN:O	1:A:50:ARG:CB	2.63	0.45
1:A:217:LYS:HA	1:A:218:PRO:C	2.36	0.45
1:A:313:TYR:HD1	1:A:507:ARG:HD3	1.80	0.45
1:A:184:ALA:O	1:A:188:ARG:HG3	2.16	0.45
3:A:586:NAG:C6	3:A:587:MAN:H2	2.47	0.45
1:A:392:MET:HB3	1:A:485:MET:HE3	1.98	0.45
1:A:40:GLY:HA2	9:A:885:HOH:O	2.17	0.44
1:A:88:GLN:OE1	1:A:243:GLN:NE2	2.51	0.44
1:A:241:SER:O	1:A:366:PHE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASP:O	1:A:350:TYR:N	2.44	0.44
1:A:259:ARG:NH2	9:A:879:HOH:O	2.44	0.44
7:A:605:HEM:NA	8:A:702:OSM:S	2.91	0.43
1:A:5:SER:HA	1:A:6:PRO:HD3	1.81	0.43
1:A:238[B]:PHE:HD2	1:A:238[B]:PHE:O	2.01	0.43
1:A:259:ARG:HD2	1:A:539:ASP:HB3	2.00	0.42
1:A:104:GLU:HB3	1:A:105:LEU:H	1.53	0.42
1:A:542:HIS:ND1	9:A:710:HOH:O	2.37	0.42
1:A:307:GLN:HG3	9:A:886:HOH:O	2.19	0.42
1:A:378:ASP:HB2	1:A:379:PRO:HD3	2.00	0.42
1:A:99:PHE:O	1:A:101:PRO:HD3	2.19	0.42
1:A:151:PHE:CD1	1:A:151:PHE:N	2.86	0.42
1:A:334:PHE:HA	1:A:481:ASN:HD21	1.83	0.42
1:A:313:TYR:CD1	1:A:507:ARG:HD3	2.53	0.42
1:A:579:GLU:HB2	1:A:580:ASN:H	1.11	0.41
1:A:339:VAL:HA	1:A:340:PRO:HD3	1.90	0.41
1:A:132:LYS:O	1:A:133:ASN:HB2	2.20	0.41
1:A:22:LEU:HA	1:A:22:LEU:HD12	1.94	0.41
1:A:462:LYS:HE2	1:A:462:LYS:HB2	1.85	0.40
1:A:80:GLN:NE2	9:A:971:HOH:O	2.32	0.40
1:A:468:TYR:O	1:A:469:LYS:HB2	2.21	0.40
1:A:63:GLU:OE2	1:A:67:LYS:NZ	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	582/583 (100%)	555 (95%)	16 (3%)	11 (2%)	10 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	153	CYS
1	A	152	VAL
1	A	158	SER
1	A	155	THR
1	A	157	GLN
1	A	579	GLU
1	A	3	GLU
1	A	108	ASN
1	A	156	PRO
1	A	156(A)	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	510/509 (100%)	477 (94%)	33 (6%)	21	27

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	43	LEU
1	A	50	ARG
1	A	77	VAL
1	A	84	LEU
1	A	110	HIS
1	A	116	GLU
1	A	139	THR
1	A	155	THR
1	A	159	LEU
1	A	171	LEU
1	A	186	ARG
1	A	187	LEU
1	A	202	GLU
1	A	239	ARG
1	A	245	LEU

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Mol	Chain	Res	Type
1	A	252	LEU
1	A	260	LEU
1	A	301	LEU
1	A	318	ASN
1	A	332	PHE
1	A	345	ARG
1	A	361	LEU
1	A	435	SER
1	A	448	LEU
1	A	455	LEU
1	A	464	LEU
1	A	478	ILE
1	A	495	LEU
1	A	504	GLN
1	A	507	ARG
1	A	549	LEU
1	A	579	GLU

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	26	ASN
1	A	108	ASN
1	A	133	ASN
1	A	318	ASN
1	A	349	ASN
1	A	408	GLN
1	A	421	ASN
1	A	452	GLN
1	A	481	ASN
1	A	504	GLN
1	A	529	GLN
1	A	555	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

9 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	581	1,2	14,14,15	0.56	0	15,19,21	0.83	1 (6%)
2	NAG	A	582	2	14,14,15	0.70	1 (7%)	15,19,21	1.27	2 (13%)
2	NAG	A	583	1,2	14,14,15	0.59	0	15,19,21	0.72	0
2	NAG	A	584	2	14,14,15	0.68	0	15,19,21	1.32	2 (13%)
3	NAG	A	585	1,3	14,14,15	0.65	0	15,19,21	0.95	0
3	NAG	A	586	3	14,14,15	0.55	0	15,19,21	1.33	1 (6%)
3	MAN	A	587	3	11,11,12	0.48	0	14,15,17	1.13	1 (7%)
2	NAG	A	588	1,2	14,14,15	0.62	0	15,19,21	1.43	1 (6%)
2	NAG	A	589	2	14,14,15	0.57	0	15,19,21	1.25	2 (13%)

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	581	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	582	2	-	0/6/23/26	0/1/1/1
2	NAG	A	583	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	584	2	-	0/6/23/26	0/1/1/1
3	NAG	A	585	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	586	3	-	0/6/23/26	0/1/1/1
3	MAN	A	587	3	-	0/2/19/22	1/1/1/1
2	NAG	A	588	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	589	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	582	NAG	O5-C1	-2.08	1.40	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	582	NAG	C1-O5-C5	-3.00	108.44	112.25
2	A	581	NAG	C2-N2-C7	-2.07	120.38	123.04
2	A	589	NAG	C3-C4-C5	2.17	113.98	110.20
2	A	584	NAG	C3-C4-C5	2.29	114.19	110.20
2	A	582	NAG	C4-C3-C2	2.53	115.16	111.23
2	A	584	NAG	C4-C3-C2	2.93	115.78	111.23
3	A	587	MAN	C1-O5-C5	2.95	116.00	112.25
2	A	589	NAG	C4-C3-C2	3.16	116.15	111.23
2	A	588	NAG	C4-C3-C2	4.07	117.55	111.23
3	A	586	NAG	C1-O5-C5	4.43	117.87	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	587	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	586	NAG	2	0
3	A	587	MAN	3	0

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	NO3	A	590	-	3,3,3	3.25	3 (100%)	3,3,3	0.16	0
4	NO3	A	591	-	3,3,3	2.91	3 (100%)	3,3,3	0.08	0
7	HEM	A	605	1,8	30,50,50	2.35	7 (23%)	24,82,82	2.40	10 (41%)
5	CO3	A	688	-	0,3,3	0.00	-	0,3,3	0.00	-
8	OSM	A	702	7	1,3,3	0.52	0	0,2,2	0.00	-

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	NO3	A	590	-	-	0/0/0/0	0/0/0/0
4	NO3	A	591	-	-	0/0/0/0	0/0/0/0
7	HEM	A	605	1,8	-	0/10/54/54	0/0/8/8
5	CO3	A	688	-	-	0/0/0/0	0/0/0/0
8	OSM	A	702	7	-	0/0/1/1	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	605	HEM	C3B-C4B	-9.13	1.43	1.51
7	A	605	HEM	C3D-C4D	-4.22	1.46	1.51
7	A	605	HEM	C2C-C1C	-3.91	1.45	1.52
7	A	605	HEM	C2D-C1D	-2.12	1.44	1.51
7	A	605	HEM	C2B-C1B	-2.05	1.45	1.51
7	A	605	HEM	CAA-C2A	2.19	1.55	1.52
4	A	591	NO3	O2-N	2.70	1.39	1.25
4	A	591	NO3	O3-N	2.73	1.39	1.25
4	A	590	NO3	O2-N	2.80	1.39	1.25
4	A	590	NO3	O3-N	2.89	1.40	1.25
4	A	591	NO3	O1-N	3.27	1.37	1.24
7	A	605	HEM	FE-NC	3.34	2.09	1.95
4	A	590	NO3	O1-N	3.93	1.40	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	605	HEM	CBA-CAA-C2A	-3.34	106.53	112.53
7	A	605	HEM	C3B-CAB-CBB	-3.09	119.72	124.46
7	A	605	HEM	CMA-C3A-C4A	-2.24	124.66	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	605	HEM	CAA-C2A-C1A	-2.04	124.79	127.01
7	A	605	HEM	C2D-C3D-C4D	2.11	105.07	101.50
7	A	605	HEM	CMD-C2D-C3D	3.23	128.64	114.35
7	A	605	HEM	CMB-C2B-C3B	3.72	125.83	116.53
7	A	605	HEM	CAD-C3D-C4D	4.25	127.44	112.47
7	A	605	HEM	CMC-C2C-C3C	4.59	127.98	116.53
7	A	605	HEM	CAD-C3D-C2D	4.96	127.48	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	605	HEM	2	0
8	A	702	OSM	2	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	583/583 (100%)	-0.13	29 (4%) 32 41	11, 24, 48, 71	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	SER	10.2
1	A	107	SER	9.6
1	A	157	GLN	8.3
1	A	156(B)	TYR	7.9
1	A	580	ASN	7.8
1	A	156	PRO	7.1
1	A	108	ASN	6.8
1	A	579	GLU	6.4
1	A	578	ARG	5.5
1	A	156(A)	PRO	5.4
1	A	105	LEU	5.1
1	A	159	LEU	4.7
1	A	106	GLY	3.9
1	A	110	HIS	3.8
1	A	155	THR	3.5
1	A	112	LYS	3.1
1	A	49	GLN	2.8
1	A	2	ASP	2.7
1	A	118	TYR	2.7
1	A	18	ARG	2.6
1	A	4	ASN	2.6
1	A	215	ASN	2.6
1	A	109	GLU	2.4
1	A	238[A]	PHE	2.4
1	A	307	GLN	2.2
1	A	355	PRO	2.1
1	A	1(A)	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	2.1
1	A	50	ARG	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [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
2	NAG	A	581	14/15	0.83	0.24	1.79	45,52,55,61	0
2	NAG	A	583	14/15	0.94	0.13	0.31	34,42,46,51	0
3	NAG	A	585	14/15	0.92	0.12	-0.07	43,46,49,54	0
3	NAG	A	586	14/15	0.78	0.34	-	59,64,65,67	0
2	NAG	A	588	14/15	0.77	0.23	-	51,58,60,65	0
3	MAN	A	587	11/12	0.77	0.40	-	69,70,70,71	0
2	NAG	A	584	14/15	0.74	0.32	-	55,57,60,61	0
2	NAG	A	589	14/15	0.66	0.46	-	68,71,72,72	0
2	NAG	A	582	14/15	0.74	0.54	-	65,69,71,71	0

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
8	OSM	A	702	4/4	0.80	0.20	9.48	45,45,45,46	0
4	NO3	A	591	4/4	0.96	0.16	2.88	16,17,18,18	0
4	NO3	A	590	4/4	0.91	0.17	1.11	51,51,52,52	0
6	CA	A	701	1/1	0.99	0.06	-1.70	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	HEM	A	605	43/43	0.99	0.08	-1.77	10,13,16,17	0
5	CO3	A	688	4/4	0.90	0.15	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.