



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QL6
Title : Crystal structure of the complex of bovine lactoperoxidase with nimesulide at 1.7 Å resolution
Authors : Yamini, S.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-02-02
Resolution : 1.70 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

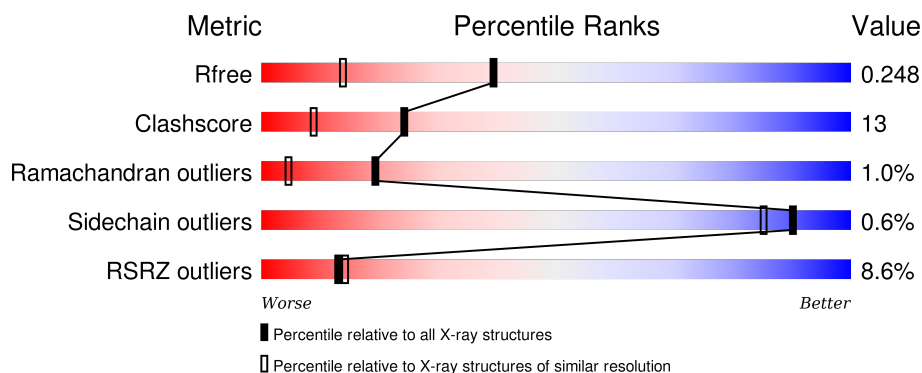
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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>9%</div> <div>81%</div> <div>16%</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
1	SEP	A	198	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEG	A	611	-	-	-	X
11	GOL	A	613	-	-	-	X
12	NIM	A	614	-	-	X	X
9	EDO	A	610	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 5489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

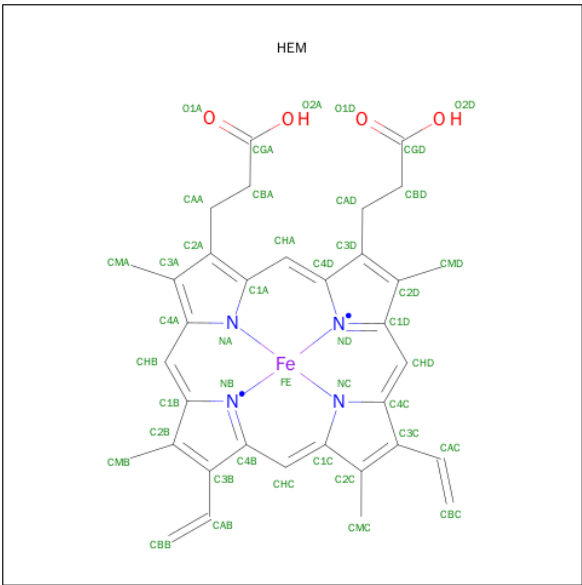
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

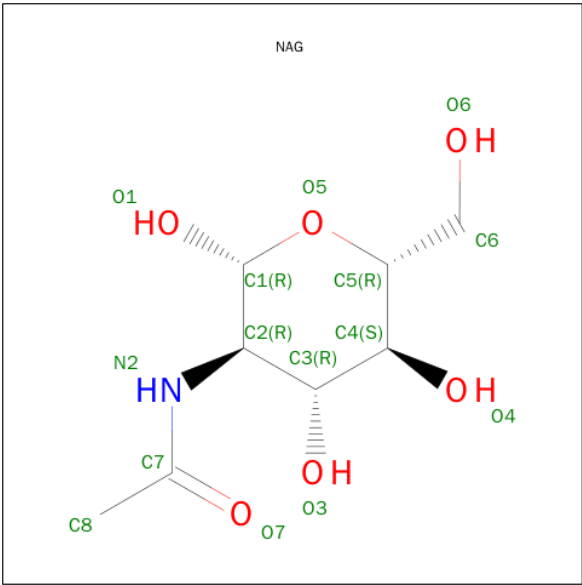
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

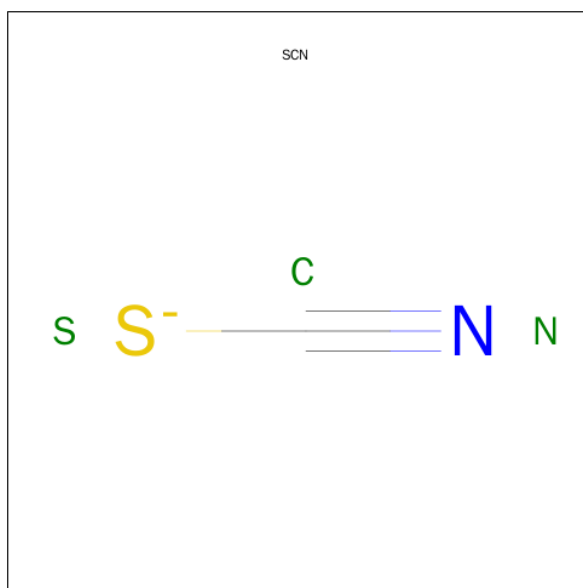
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

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

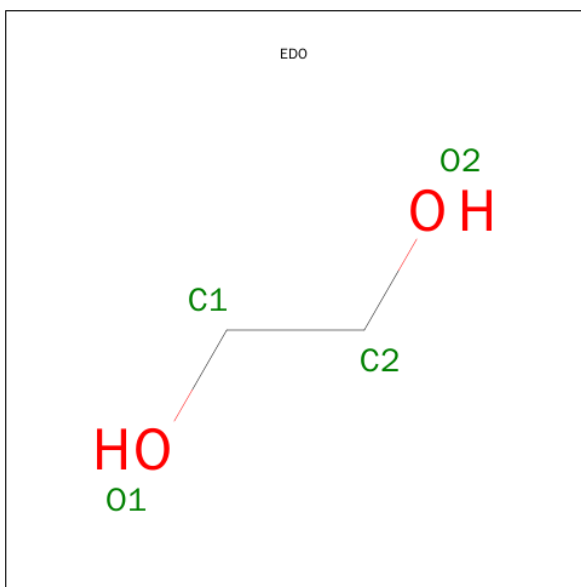
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total	I	0	0
			14	14		

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



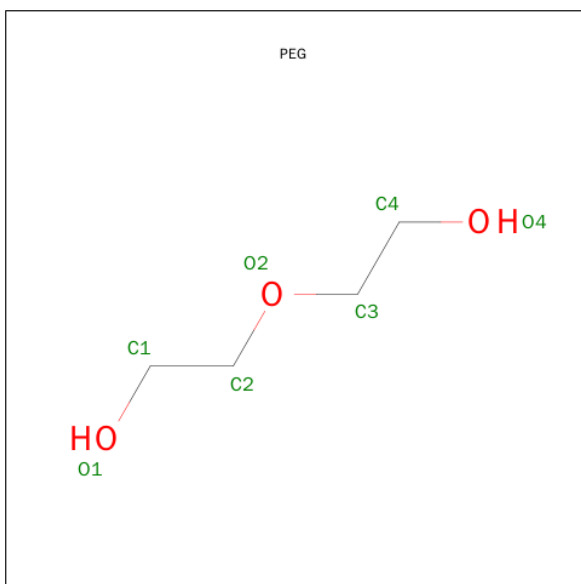
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



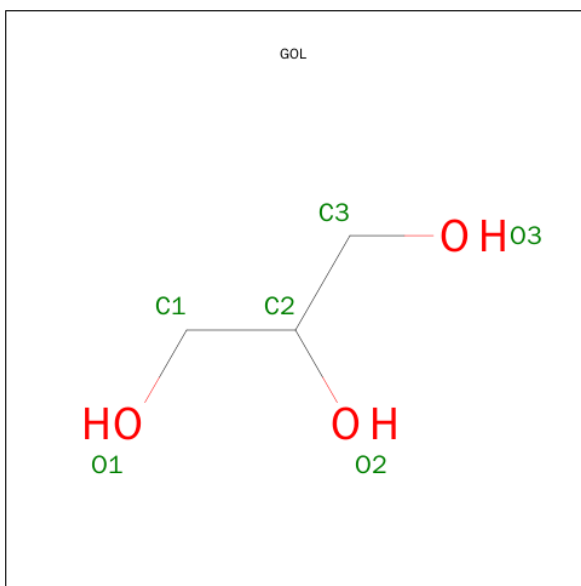
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



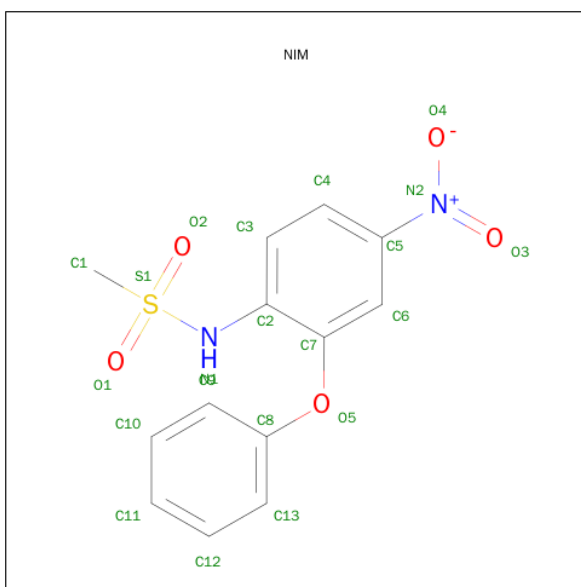
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 12 is 4-NITRO-2-PHENOXYMETHANESULFONANILIDE (three-letter code: NIM) (formula: $C_{13}H_{12}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	S	0	0
			21	13	2	5	1		

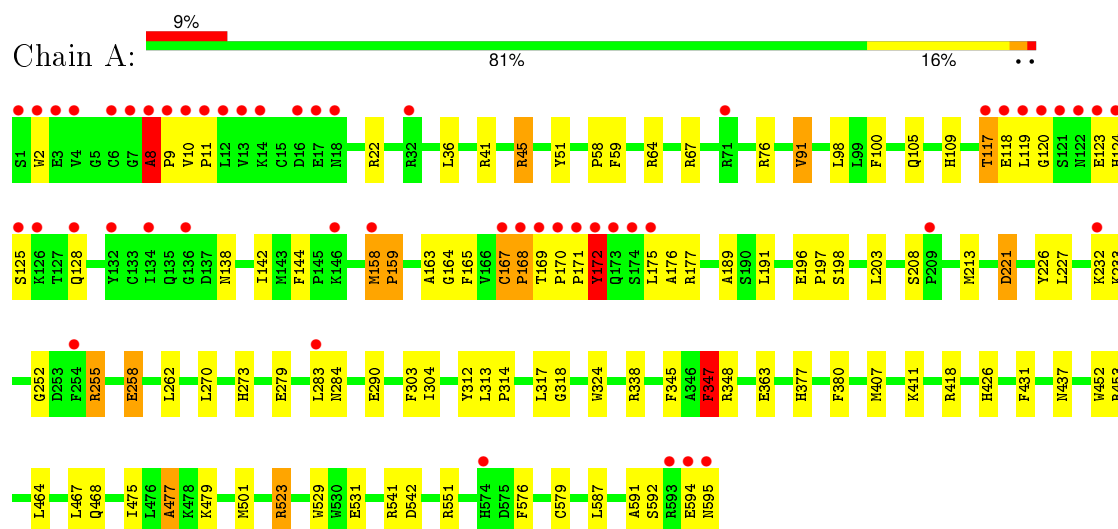
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	535	Total	O	0	0
			535	535		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.92Å 79.50Å 77.72Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	26.71 – 1.70 26.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (26.71-1.70) 94.9 (26.71-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.246 0.216 , 0.248	Depositor DCC
R_{free} test set	3384 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 67233 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5489	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: GOL, ZN, SCN, NAG, NIM, CA, SEP, EDO, HEM, PEG, 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	1.23	13/4891 (0.3%)	1.15	26/6634 (0.4%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TYR	CE2-CZ	-7.74	1.28	1.38
1	A	347	PHE	C-N	6.98	1.50	1.34
1	A	477	ALA	C-N	6.67	1.49	1.34
1	A	576	PHE	CE1-CZ	5.89	1.48	1.37
1	A	100	PHE	CE1-CZ	5.73	1.48	1.37
1	A	163	ALA	CA-CB	5.72	1.64	1.52
1	A	312	TYR	CG-CD1	5.65	1.46	1.39
1	A	91	VAL	CB-CG1	-5.61	1.41	1.52
1	A	324	TRP	CG-CD1	-5.21	1.29	1.36
1	A	452	TRP	CZ3-CH2	5.17	1.48	1.40
1	A	312	TYR	CE2-CZ	5.17	1.45	1.38
1	A	303	PHE	CE2-CZ	5.17	1.47	1.37
1	A	258	GLU	CD-OE1	-5.02	1.20	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ALA	CB-CA-C	-8.21	97.79	110.10
1	A	541	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	542	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	67	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	541	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	418	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	76	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	45	ARG	NE-CZ-NH2	-7.07	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	HIS	N-CA-C	-6.57	93.27	111.00
1	A	551	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	22	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	117	THR	CB-CA-C	-6.23	94.79	111.60
1	A	347	PHE	O-C-N	6.14	132.53	122.70
1	A	255	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	191	LEU	CB-CG-CD1	-6.04	100.73	111.00
1	A	453	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	418	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	345	PHE	CB-CG-CD2	-5.88	116.68	120.80
1	A	98	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	A	22	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	159	PRO	CB-CA-C	-5.38	98.55	112.00
1	A	312	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	A	221	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	467	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	523	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	158	MET	C-N-CD	-5.01	109.58	120.60

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	4774	0	4686	119	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	43	0	30	4	0
5	A	42	0	39	1	0
6	A	28	0	25	0	0
7	A	14	0	0	0	0
8	A	3	0	0	0	0
9	A	8	0	12	2	0
10	A	7	0	10	1	0
11	A	12	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	21	0	12	12	0
13	A	535	0	0	0	0
All	All	5489	0	4828	127	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 13.

All (127) 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:171:PRO:CA	1:A:172:TYR:HB2	1.42	1.47
1:A:171:PRO:HA	1:A:172:TYR:CB	1.36	1.35
12:A:614:NIM:H6	12:A:614:NIM:H9	1.16	1.12
12:A:614:NIM:H6	12:A:614:NIM:C9	1.78	1.10
12:A:614:NIM:H9	12:A:614:NIM:C6	1.79	1.08
1:A:118:GLU:C	1:A:119:LEU:HD12	1.78	1.03
1:A:258:GLU:HB2	12:A:614:NIM:H3	1.36	1.02
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.42	1.01
1:A:165:PHE:CZ	1:A:169:THR:O	2.20	0.94
1:A:197:PRO:HG2	1:A:198:SEP:O3P	1.65	0.94
1:A:8:ALA:HB3	1:A:9:PRO:CD	1.97	0.94
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.49	0.92
1:A:283:LEU:HD11	1:A:591:ALA:HB2	1.52	0.91
1:A:165:PHE:HZ	1:A:169:THR:O	1.52	0.91
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.01	0.91
1:A:258:GLU:CB	12:A:614:NIM:H3	2.02	0.90
1:A:120:GLY:HA3	1:A:123:GLU:OE2	1.73	0.89
1:A:118:GLU:O	1:A:119:LEU:HD12	1.72	0.89
1:A:167:CYS:CB	1:A:168:PRO:CD	2.53	0.86
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.55	0.86
1:A:171:PRO:CA	1:A:172:TYR:CB	2.18	0.86
1:A:283:LEU:HD21	1:A:591:ALA:N	1.96	0.80
1:A:10:VAL:HG23	1:A:41:ARG:HH22	1.47	0.79
1:A:169:THR:HB	1:A:170:PRO:HD3	1.63	0.79
1:A:120:GLY:CA	1:A:123:GLU:OE2	2.36	0.74
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.88	0.73
1:A:119:LEU:HD13	1:A:138:ASN:ND2	2.06	0.70
1:A:2:TRP:HZ2	1:A:175:LEU:HD21	1.57	0.70
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.21	0.69
1:A:283:LEU:HD11	1:A:591:ALA:CB	2.22	0.69
4:A:605:HEM:O1D	12:A:614:NIM:H10	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.40	0.68
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.91	0.68
1:A:197:PRO:CG	1:A:198:SEP:O3P	2.41	0.66
1:A:172:TYR:CE2	1:A:177:ARG:HA	2.31	0.65
1:A:10:VAL:HG23	1:A:41:ARG:NH2	2.13	0.64
1:A:119:LEU:N	1:A:119:LEU:HD12	2.12	0.64
1:A:8:ALA:CB	1:A:9:PRO:CD	2.73	0.64
1:A:123:GLU:HG2	1:A:124:HIS:N	2.12	0.64
1:A:165:PHE:CE1	1:A:168:PRO:O	2.52	0.63
1:A:172:TYR:HE2	1:A:177:ARG:CB	2.13	0.62
1:A:125:SER:HA	1:A:128:GLN:HB3	1.82	0.61
1:A:123:GLU:HG2	1:A:124:HIS:H	1.65	0.61
1:A:142:ILE:HB	1:A:158:MET:HG3	1.83	0.61
1:A:142:ILE:HB	1:A:158:MET:CG	2.31	0.60
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.84	0.60
1:A:169:THR:N	1:A:170:PRO:HD2	2.17	0.59
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.83	0.59
1:A:158:MET:HG3	1:A:158:MET:O	2.05	0.57
1:A:258:GLU:HG3	12:A:614:NIM:C3	2.35	0.56
1:A:283:LEU:HD21	1:A:591:ALA:CA	2.34	0.56
1:A:531:GLU:O	1:A:531:GLU:HG2	2.05	0.56
12:A:614:NIM:C6	12:A:614:NIM:C9	2.46	0.56
1:A:363:GLU:HB2	11:A:613:GOL:H12	1.87	0.56
4:A:605:HEM:HBB2	4:A:605:HEM:CMB	2.36	0.55
1:A:159:PRO:HG2	1:A:431:PHE:CE2	2.41	0.55
1:A:258:GLU:CG	12:A:614:NIM:H3	2.37	0.55
1:A:169:THR:N	1:A:170:PRO:CD	2.70	0.54
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.87	0.54
1:A:347:PHE:HD1	1:A:347:PHE:O	1.90	0.54
1:A:119:LEU:HD11	1:A:169:THR:CG2	2.38	0.54
1:A:347:PHE:O	1:A:347:PHE:CD1	2.60	0.54
1:A:8:ALA:CB	1:A:9:PRO:HD3	2.32	0.53
1:A:468:GLN:HG2	1:A:477:ALA:HB3	1.90	0.52
1:A:109:HIS:CE1	1:A:262:LEU:HD21	2.44	0.52
1:A:159:PRO:HG2	1:A:431:PHE:HE2	1.75	0.52
4:A:605:HEM:HBB2	4:A:605:HEM:HMB2	1.92	0.51
1:A:284:ASN:HD21	1:A:592:SER:H	1.58	0.51
1:A:171:PRO:CA	1:A:172:TYR:HB3	2.31	0.51
1:A:123:GLU:CG	1:A:124:HIS:H	2.23	0.51
1:A:171:PRO:CB	1:A:172:TYR:CB	2.87	0.51
1:A:258:GLU:HG3	12:A:614:NIM:H3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.46	0.50
1:A:91:VAL:HG12	1:A:411:LYS:HD3	1.94	0.50
1:A:172:TYR:CE2	1:A:177:ARG:HB2	2.46	0.50
1:A:109:HIS:HE1	1:A:262:LEU:CD2	2.25	0.50
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.47	0.50
1:A:125:SER:HA	1:A:128:GLN:CB	2.41	0.49
1:A:171:PRO:CB	1:A:172:TYR:HB3	2.42	0.49
1:A:594:GLU:O	1:A:595:ASN:HB2	2.13	0.48
1:A:172:TYR:CZ	1:A:177:ARG:HA	2.48	0.48
1:A:172:TYR:HE2	1:A:177:ARG:HG3	1.78	0.48
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.48	0.48
1:A:169:THR:HB	1:A:170:PRO:CD	2.39	0.48
1:A:175:LEU:HG	1:A:176:ALA:N	2.28	0.48
1:A:119:LEU:CD1	1:A:119:LEU:N	2.76	0.48
1:A:119:LEU:HD13	1:A:138:ASN:HD22	1.78	0.48
1:A:123:GLU:CG	1:A:124:HIS:N	2.76	0.48
1:A:36:LEU:HD11	11:A:612:GOL:H2	1.96	0.47
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.79	0.47
1:A:317:LEU:O	1:A:318:GLY:C	2.52	0.47
1:A:172:TYR:CE2	1:A:177:ARG:CB	2.95	0.47
1:A:144:PHE:HE2	1:A:158:MET:CE	2.28	0.47
1:A:313:LEU:N	1:A:314:PRO:CD	2.77	0.47
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.97	0.47
1:A:36:LEU:HD23	9:A:610:EDO:H12	1.97	0.47
1:A:232:LYS:HG2	1:A:233:LYS:N	2.30	0.46
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.96	0.46
1:A:197:PRO:HD2	1:A:198:SEP:O3P	2.15	0.46
1:A:109:HIS:HE1	1:A:262:LEU:HD21	1.81	0.46
1:A:91:VAL:CG1	1:A:411:LYS:HD3	2.46	0.46
1:A:208:SER:HB3	5:A:599:NAG:H62	1.98	0.46
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.98	0.46
1:A:58:PRO:O	1:A:59:PHE:C	2.54	0.46
1:A:255:ARG:HG2	12:A:614:NIM:C1	2.46	0.45
1:A:197:PRO:CD	1:A:198:SEP:O3P	2.64	0.45
1:A:125:SER:HA	1:A:128:GLN:HE21	1.81	0.45
1:A:279:GLU:OE2	1:A:587:LEU:HD12	2.17	0.45
1:A:119:LEU:CD1	1:A:138:ASN:ND2	2.78	0.45
1:A:109:HIS:CE1	1:A:262:LEU:CD2	3.00	0.45
1:A:105:GLN:HG2	1:A:109:HIS:NE2	2.32	0.44
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.53	0.44
1:A:172:TYR:HE2	1:A:177:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASN:ND2	1:A:592:SER:H	2.16	0.44
1:A:45:ARG:HB2	10:A:611:PEG:H21	2.00	0.44
1:A:119:LEU:CD1	1:A:138:ASN:HD21	2.31	0.43
1:A:464:LEU:O	1:A:468:GLN:HG3	2.18	0.43
1:A:172:TYR:HE2	1:A:177:ARG:HB2	1.78	0.43
1:A:175:LEU:HG	1:A:176:ALA:H	1.84	0.43
1:A:142:ILE:HB	1:A:158:MET:HG2	2.00	0.43
4:A:605:HEM:O1D	12:A:614:NIM:C10	2.63	0.42
1:A:594:GLU:O	1:A:595:ASN:CB	2.67	0.42
1:A:338:ARG:HD3	9:A:610:EDO:H11	2.01	0.41
1:A:475:ILE:CG2	1:A:479:LYS:HE3	2.50	0.41
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.20	0.41
1:A:407:MET:HB3	1:A:501:MET:HE3	2.01	0.41
1:A:172:TYR:CE2	1:A:177:ARG:CA	3.02	0.41

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%)	560 (95%)	26 (4%)	6 (1%)	19 4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	172	TYR
1	A	579	CYS
1	A	8	ALA
1	A	168	PRO

5.3.2 Protein sidechains [i](#)

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%)	514 (99%)	3 (1%)	90	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	172	TYR
1	A	347	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	147	ASN
1	A	173	GLN
1	A	231	ASN
1	A	284	ASN
1	A	364	ASN
1	A	437	ASN
1	A	497	ASN
1	A	570	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	198	1	8,9,10	1.88	1 (12%)	8,12,14	3.79	4 (50%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O2P	3.37	1.66	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	-6.18	88.78	106.56
1	A	198	SEP	OG-P-O1P	-2.75	100.15	107.14
1	A	198	SEP	O3P-P-O1P	4.56	125.26	110.58
1	A	198	SEP	O3P-P-OG	6.68	125.80	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	5	0

5.5 Carbohydrates ⓘ

2 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	$\# Z > 2$
6	NAG	A	601	1,6	14,14,15	1.13	1 (7%)	15,19,21	1.52	3 (20%)
6	NAG	A	602	6	14,14,15	0.75	0	15,19,21	2.16	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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	NAG	C4-C5	2.22	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	NAG	O4-C4-C3	-2.44	104.85	110.34
6	A	601	NAG	O5-C5-C6	-2.13	102.75	107.35
6	A	602	NAG	O5-C5-C6	2.01	111.70	107.35
6	A	601	NAG	C6-C5-C4	3.36	121.30	113.02
6	A	602	NAG	C1-O5-C5	6.85	120.94	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 16 are monoatomic - leaving 11 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$
5	NAG	A	596	1	14,14,15	0.59	0	15,19,21	1.81	6 (40%)
5	NAG	A	599	1	14,14,15	0.90	1 (7%)	15,19,21	1.30	1 (6%)
5	NAG	A	604	1	14,14,15	0.85	0	15,19,21	1.31	2 (13%)
4	HEM	A	605	1,12	30,50,50	3.37	12 (40%)	24,82,82	2.88	12 (50%)
9	EDO	A	609	-	3,3,3	0.49	0	2,2,2	0.93	0
9	EDO	A	610	-	3,3,3	0.59	0	2,2,2	0.55	0
10	PEG	A	611	-	6,6,6	0.33	0	5,5,5	1.08	0
11	GOL	A	612	-	5,5,5	0.51	0	5,5,5	0.94	0
11	GOL	A	613	-	5,5,5	2.02	2 (40%)	5,5,5	1.31	1 (20%)
12	NIM	A	614	4	20,22,22	2.08	4 (20%)	29,31,31	3.68	8 (27%)
8	SCN	A	615	-	2,2,2	1.67	1 (50%)	1,1,1	0.37	0

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	596	1	-	0/6/23/26	0/1/1/1
5	NAG	A	599	1	-	0/6/23/26	0/1/1/1
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
4	HEM	A	605	1,12	-	0/10/54/54	0/0/8/8
9	EDO	A	609	-	-	0/1/1/1	0/0/0/0
9	EDO	A	610	-	-	0/1/1/1	0/0/0/0
10	PEG	A	611	-	-	0/4/4/4	0/0/0/0
11	GOL	A	612	-	-	0/4/4/4	0/0/0/0
11	GOL	A	613	-	-	0/4/4/4	0/0/0/0
12	NIM	A	614	4	-	0/13/13/13	0/2/2/2
8	SCN	A	615	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	C3B-C4B	-12.03	1.41	1.51
12	A	614	NIM	S1-N1	-7.66	1.52	1.63
4	A	605	HEM	C3D-C4D	-7.40	1.42	1.51
4	A	605	HEM	C2C-C1C	-5.50	1.42	1.52
11	A	613	GOL	O2-C2	-3.33	1.33	1.43
12	A	614	NIM	C1-S1	-3.04	1.66	1.75
4	A	605	HEM	C2B-C1B	-2.87	1.42	1.51
4	A	605	HEM	C2D-C3D	-2.52	1.47	1.54
11	A	613	GOL	C1-C2	-2.29	1.43	1.52
4	A	605	HEM	C2D-C1D	-2.11	1.44	1.51
5	A	599	NAG	O5-C1	-2.05	1.40	1.43
4	A	605	HEM	CBC-CAC	2.12	1.41	1.29
4	A	605	HEM	FE-NB	2.14	2.08	1.97
8	A	615	SCN	C-S	2.25	1.78	1.63
12	A	614	NIM	O2-S1	2.34	1.48	1.43
12	A	614	NIM	O1-S1	2.37	1.48	1.43
4	A	605	HEM	FE-NC	2.59	2.06	1.95
4	A	605	HEM	CMC-C2C	3.85	1.62	1.53
4	A	605	HEM	C1C-NC	4.32	1.41	1.36
4	A	605	HEM	C4C-NC	4.52	1.41	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	614	NIM	C4-C5-N2	-9.30	111.99	119.48
12	A	614	NIM	C3-C2-N1	-7.24	105.36	120.94
12	A	614	NIM	O2-S1-O1	-6.39	109.49	118.77
4	A	605	HEM	CAA-C2A-C1A	-4.48	122.14	127.01
4	A	605	HEM	C3B-CAB-CBB	-4.00	118.31	124.46
4	A	605	HEM	C1D-CHD-C4C	-3.78	119.50	125.82
4	A	605	HEM	CMA-C3A-C4A	-3.37	122.78	128.36
12	A	614	NIM	O3-N2-C5	-3.37	112.83	118.89
4	A	605	HEM	C2C-C1C-NC	-3.25	104.73	110.21
5	A	604	NAG	C2-N2-C7	-3.11	119.05	123.04
4	A	605	HEM	CBD-CAD-C3D	-3.04	104.72	113.55
4	A	605	HEM	C4B-CHC-C1C	-2.78	121.17	125.82
5	A	599	NAG	C1-O5-C5	-2.52	109.05	112.25
5	A	596	NAG	O5-C5-C6	-2.31	102.34	107.35
5	A	596	NAG	C4-C3-C2	-2.15	107.89	111.23
11	A	613	GOL	O2-C2-C1	-2.12	98.93	108.65
5	A	596	NAG	O6-C6-C5	-2.08	104.45	111.33
5	A	604	NAG	O6-C6-C5	-2.07	104.50	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
12	A	614	NIM	C1-S1-N1	2.10	109.48	106.83
4	A	605	HEM	C2D-C3D-C4D	2.25	105.32	101.50
5	A	596	NAG	C3-C2-N2	2.27	116.00	110.56
5	A	596	NAG	O4-C4-C5	2.29	115.30	109.24
5	A	596	NAG	C6-C5-C4	3.24	121.00	113.02
4	A	605	HEM	CAD-C3D-C2D	3.66	123.73	113.22
4	A	605	HEM	CMB-C2B-C3B	4.38	127.47	116.53
4	A	605	HEM	CMC-C2C-C3C	5.06	129.15	116.53
4	A	605	HEM	CAD-C3D-C4D	5.09	130.42	112.47
12	A	614	NIM	C2-N1-S1	5.86	141.36	124.05
12	A	614	NIM	C7-C2-N1	6.48	132.82	118.50
12	A	614	NIM	C6-C5-N2	10.56	128.06	118.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	599	NAG	1	0
4	A	605	HEM	4	0
9	A	610	EDO	2	0
10	A	611	PEG	1	0
11	A	612	GOL	1	0
11	A	613	GOL	1	0
12	A	614	NIM	12	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%)	0.54	51 (8%) 13 14	8, 21, 63, 99	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	16.3
1	A	2	TRP	15.8
1	A	119	LEU	15.3
1	A	13	VAL	13.3
1	A	4	VAL	13.0
1	A	173	GLN	11.5
1	A	121	SER	10.7
1	A	593	ARG	10.4
1	A	595	ASN	9.9
1	A	125	SER	9.7
1	A	122	ASN	9.7
1	A	172	TYR	8.9
1	A	12	LEU	8.8
1	A	7	GLY	8.6
1	A	124	HIS	8.4
1	A	10	VAL	7.9
1	A	6	CYS	7.2
1	A	169	THR	7.0
1	A	170	PRO	6.9
1	A	123	GLU	6.7
1	A	118	GLU	6.5
1	A	9	PRO	5.6
1	A	8	ALA	5.5
1	A	168	PRO	5.4
1	A	158	MET	5.3
1	A	11	PRO	5.1
1	A	120	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	4.7
1	A	14	LYS	4.6
1	A	175	LEU	4.4
1	A	174	SER	4.4
1	A	594	GLU	4.3
1	A	3	GLU	3.9
1	A	283	LEU	3.8
1	A	126	LYS	3.6
1	A	232	LYS	3.4
1	A	128	GLN	3.3
1	A	132	TYR	3.3
1	A	18	ASN	3.2
1	A	16	ASP	3.2
1	A	167	CYS	3.2
1	A	254	PHE	2.8
1	A	17	GLU	2.8
1	A	146	LYS	2.5
1	A	32	ARG	2.5
1	A	574	HIS	2.4
1	A	117	THR	2.3
1	A	209	PRO	2.2
1	A	134	ILE	2.1
1	A	136	GLY	2.1
1	A	71	ARG	2.1

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	0.84	0.25	-	16,25,38,40	0

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
6	NAG	A	601	14/15	0.94	0.10	-0.21	20,27,38,38	0
6	NAG	A	602	14/15	0.67	0.26	-	43,52,57,59	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
12	NIM	A	614	21/21	0.59	0.52	9.92	4,27,34,39	21
9	EDO	A	610	4/4	0.76	0.23	7.69	22,30,32,33	0
11	GOL	A	613	6/6	0.81	0.28	5.33	21,26,36,42	0
10	PEG	A	611	7/7	0.88	0.19	3.71	24,28,32,34	0
7	IOD	A	720	1/1	0.97	0.08	1.51	37,37,37,37	1
7	IOD	A	719	1/1	0.98	0.13	0.88	21,21,21,21	1
11	GOL	A	612	6/6	0.68	0.15	0.68	38,41,43,44	0
5	NAG	A	599	14/15	0.83	0.13	0.39	28,35,40,44	0
8	SCN	A	615	3/3	0.95	0.10	0.09	33,33,34,35	0
4	HEM	A	605	43/43	0.98	0.08	-0.42	4,11,15,17	0
7	IOD	A	715	1/1	0.97	0.04	-0.92	40,40,40,40	1
7	IOD	A	721	1/1	0.84	0.07	-1.00	106,106,106,106	0
2	CA	A	606	1/1	1.00	0.06	-1.29	12,12,12,12	0
7	IOD	A	713	1/1	0.99	0.07	-1.40	43,43,43,43	1
7	IOD	A	711	1/1	0.97	0.04	-1.44	31,31,31,31	0
7	IOD	A	718	1/1	0.99	0.04	-1.61	35,35,35,35	1
7	IOD	A	708	1/1	0.99	0.03	-1.95	27,27,27,27	0
7	IOD	A	710	1/1	0.99	0.04	-2.51	24,24,24,24	0
7	IOD	A	707	1/1	1.00	0.02	-5.02	17,17,17,17	0
7	IOD	A	712	1/1	0.98	0.07	-	36,36,36,36	1
7	IOD	A	714	1/1	0.88	0.06	-	46,46,46,46	1
5	NAG	A	604	14/15	0.77	0.24	-	32,39,42,45	0
3	ZN	A	617	1/1	0.98	0.02	-	28,28,28,28	0
5	NAG	A	596	14/15	0.73	0.26	-	41,45,48,48	0
9	EDO	A	609	4/4	0.89	0.15	-	28,31,31,35	0
7	IOD	A	722	1/1	0.99	0.14	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	IOD	A	709	1/1	0.96	0.11	-	57,57,57,57	1

6.5 Other polymers [i](#)

There are no such residues in this entry.