



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:55 AM GMT

PDB ID : 3QF1
Title : Crystal structure of the complex of caprine lactoperoxidase with diethylenediamine at 2.6Å resolution
Authors : Pandey, N.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-01-21
Resolution : 2.60 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

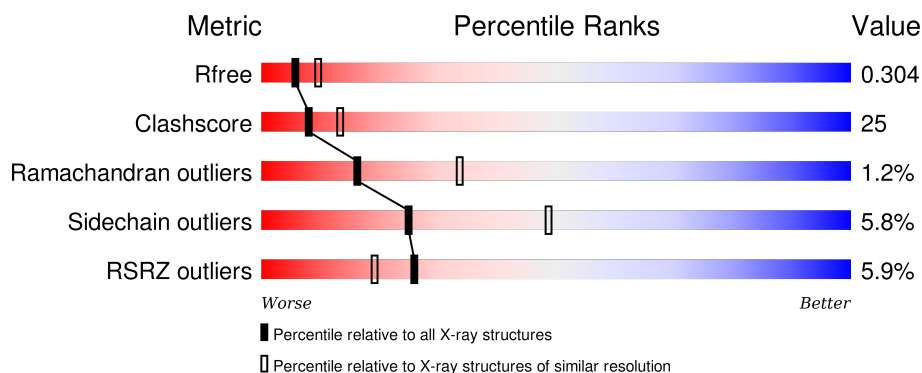
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>6%</div> <div>67%</div> <div>29%</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
6	IOD	A	620	-	-	X	-
7	PZE	A	6951	-	-	X	X
8	SCN	A	6788	-	-	-	X
9	GOL	A	597	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5060 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
			4757	3021	844	865	1	26			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

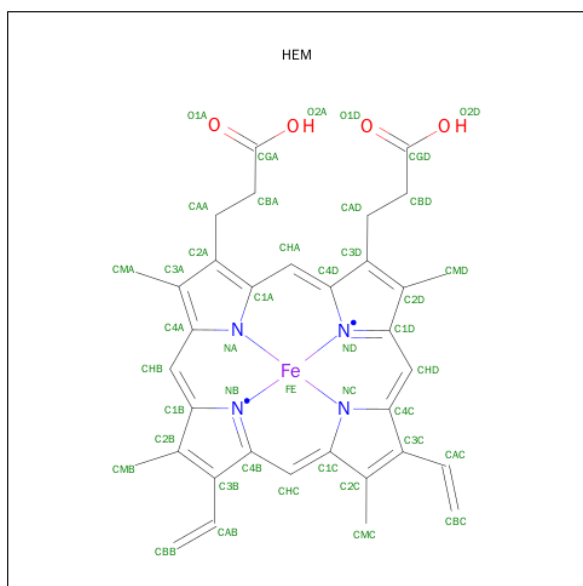
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

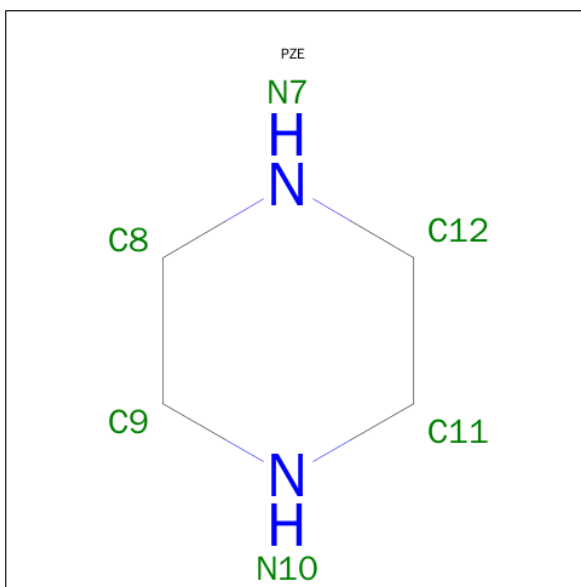


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

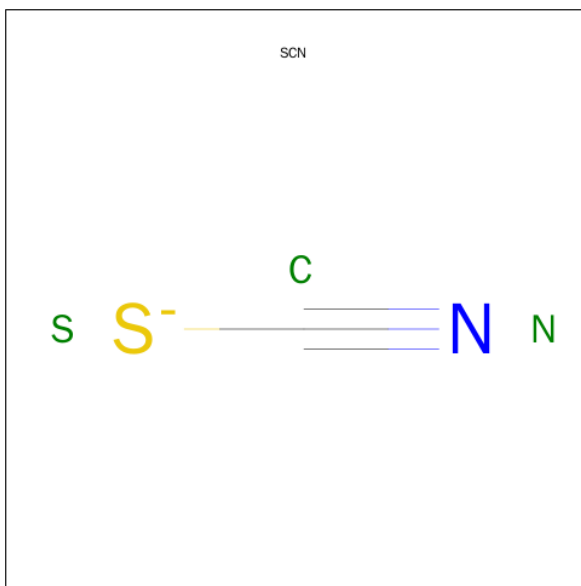
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	I	0	0
			10	10		

- Molecule 7 is PIPERAZINE (three-letter code: PZE) (formula: C₄H₁₀N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			6	4	2		

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



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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

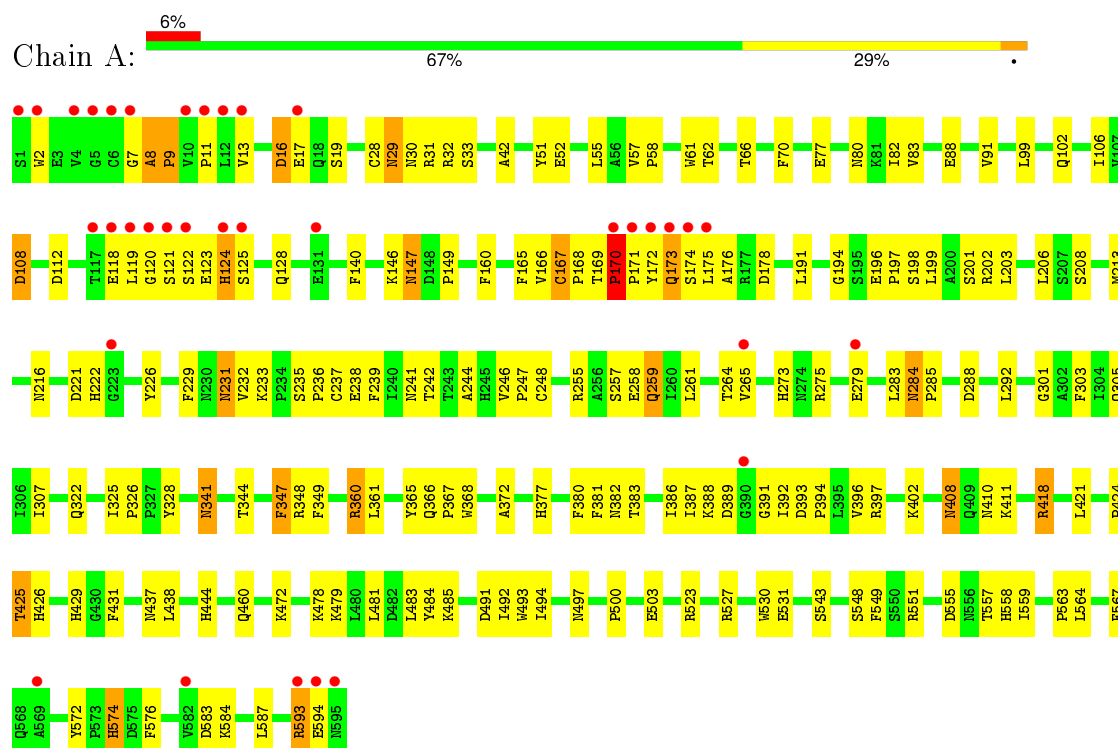
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	174	Total 174	O 174	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.15Å 80.18Å 76.73Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	44.15 – 2.60 44.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.15-2.60) 99.7 (44.15-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.256 0.233 , 0.304	Depositor DCC
R_{free} test set	1013 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.4	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	2 of 19804 reflections (0.010%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5060	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SCN, NAG, SEP, CA, EDO, PZE, 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	0/4875	0.85	2/6621 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	170	PRO	C-N-CD	-5.00	109.59	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4757	0	4645	233	0
2	A	28	0	26	0	0
3	A	28	0	25	2	0
4	A	1	0	0	0	0
5	A	43	0	30	4	0
6	A	10	0	0	9	0
7	A	6	0	10	6	0
8	A	3	0	0	0	0
9	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	4	0	6	0	0
11	A	174	0	0	5	0
All	All	5060	0	4750	238	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 25.

All (238) 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:202:ARG:NE	6:A:620:IOD:I	2.30	1.34
1:A:202:ARG:CZ	6:A:620:IOD:I	2.54	1.25
1:A:123:GLU:CG	1:A:125:SER:HB3	1.68	1.23
1:A:174:SER:HB2	1:A:175:LEU:HA	1.25	1.14
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.21	1.14
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.45	1.12
1:A:118:GLU:HG3	1:A:119:LEU:H	1.08	1.08
1:A:167:CYS:HB2	1:A:168:PRO:CD	1.85	1.07
1:A:167:CYS:CB	1:A:168:PRO:CD	2.34	1.05
1:A:169:THR:HB	1:A:170:PRO:HD3	1.39	1.04
1:A:593:ARG:H	1:A:593:ARG:HD3	1.21	1.04
1:A:123:GLU:HG3	1:A:125:SER:H	1.30	0.96
1:A:386:ILE:HG23	1:A:392:ILE:CD1	1.96	0.96
1:A:202:ARG:CD	6:A:620:IOD:I	2.85	0.95
1:A:386:ILE:CG2	1:A:392:ILE:HD11	1.96	0.95
1:A:118:GLU:CG	1:A:119:LEU:H	1.80	0.94
1:A:255:ARG:CD	7:A:6951:PZE:H9	1.97	0.94
1:A:52:GLU:HB3	1:A:57:VAL:HG12	1.48	0.93
1:A:123:GLU:HG3	1:A:125:SER:HB3	1.48	0.92
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.04	0.91
1:A:386:ILE:HG21	1:A:392:ILE:HD11	1.51	0.91
1:A:174:SER:CB	1:A:175:LEU:HA	2.01	0.90
1:A:301:GLY:O	1:A:305:GLN:HG3	1.71	0.90
1:A:174:SER:HB2	1:A:175:LEU:CA	2.00	0.90
1:A:118:GLU:HG3	1:A:119:LEU:N	1.86	0.90
1:A:8:ALA:N	1:A:9:PRO:HD3	1.88	0.89
1:A:393:ASP:HB3	1:A:559:ILE:HD11	1.58	0.86
1:A:386:ILE:HG23	1:A:392:ILE:HD13	1.57	0.85
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.12	0.84
1:A:106:ILE:HG13	1:A:265:VAL:HG11	1.59	0.83
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:CG2	1:A:392:ILE:CD1	2.55	0.81
1:A:231:ASN:N	1:A:231:ASN:HD22	1.78	0.80
1:A:593:ARG:N	1:A:593:ARG:HD3	1.96	0.80
1:A:255:ARG:HD2	7:A:6951:PZE:H9	1.62	0.79
1:A:173:GLN:N	1:A:173:GLN:NE2	2.30	0.79
1:A:82:ILE:HD11	1:A:479:LYS:HB3	1.64	0.79
1:A:169:THR:CB	1:A:170:PRO:HD3	2.07	0.79
1:A:175:LEU:O	1:A:175:LEU:HD12	1.82	0.79
1:A:9:PRO:O	1:A:11:PRO:HD3	1.83	0.79
1:A:123:GLU:CD	1:A:125:SER:HB3	2.04	0.78
1:A:82:ILE:HD11	1:A:479:LYS:CB	2.15	0.77
1:A:283:LEU:C	1:A:284:ASN:HD22	1.87	0.77
1:A:165:PHE:CE2	1:A:168:PRO:O	2.38	0.76
1:A:284:ASN:N	1:A:284:ASN:HD22	1.83	0.76
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.49	0.76
1:A:360:ARG:HH11	1:A:372:ALA:HA	1.50	0.76
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.02	0.75
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.69	0.75
1:A:123:GLU:CG	1:A:125:SER:CB	2.60	0.74
1:A:123:GLU:HG3	1:A:125:SER:N	2.01	0.74
1:A:123:GLU:HG3	1:A:125:SER:CB	2.16	0.74
5:A:618:HEM:HBC2	5:A:618:HEM:HMC1	1.70	0.73
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.71	0.73
1:A:172:TYR:C	1:A:173:GLN:NE2	2.43	0.72
1:A:255:ARG:HD3	7:A:6951:PZE:H9	1.70	0.72
1:A:7:GLY:O	1:A:8:ALA:HB3	1.87	0.72
1:A:168:PRO:CB	1:A:172:TYR:HB2	2.20	0.71
1:A:8:ALA:N	1:A:9:PRO:CD	2.52	0.71
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.17	0.71
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.20	0.71
1:A:248:CYS:HB3	1:A:257:SER:OG	1.90	0.71
1:A:255:ARG:HB3	7:A:6951:PZE:H11	1.72	0.70
1:A:29:ASN:HD21	1:A:527:ARG:H	1.38	0.70
1:A:124:HIS:O	1:A:128:GLN:HB2	1.92	0.70
1:A:120:GLY:HA2	1:A:123:GLU:HB2	1.71	0.69
1:A:172:TYR:C	1:A:173:GLN:HE21	1.94	0.69
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.93	0.68
1:A:438:LEU:CD2	1:A:494:ILE:HD11	2.24	0.68
1:A:367:PRO:HG3	9:A:597:GOL:C1	2.23	0.68
1:A:367:PRO:HG3	9:A:597:GOL:H12	1.76	0.68
1:A:120:GLY:HA2	1:A:123:GLU:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:C	1:A:203:LEU:H	1.98	0.67
1:A:391:GLY:O	1:A:394:PRO:HD2	1.95	0.66
6:A:609:IOD:I	11:A:691:HOH:O	2.83	0.66
1:A:175:LEU:HD12	1:A:175:LEU:C	2.17	0.65
1:A:118:GLU:O	1:A:119:LEU:HB3	1.94	0.65
1:A:381:PHE:CE2	1:A:424:PRO:HD3	2.32	0.64
1:A:106:ILE:HD11	1:A:265:VAL:HG12	1.79	0.64
1:A:7:GLY:C	1:A:9:PRO:HD3	2.17	0.64
1:A:82:ILE:HD13	1:A:479:LYS:HD3	1.80	0.62
1:A:388:LYS:HE3	3:A:602:NAG:O6	1.99	0.62
1:A:551:ARG:HD3	1:A:583:ASP:O	1.99	0.62
1:A:106:ILE:CG1	1:A:265:VAL:HG11	2.29	0.62
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.35	0.62
1:A:83:VAL:HG12	1:A:418:ARG:HD2	1.79	0.62
1:A:194:GLY:HA3	1:A:199:LEU:HD23	1.82	0.61
1:A:393:ASP:HB3	1:A:559:ILE:CD1	2.29	0.61
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.36	0.61
1:A:118:GLU:OE2	1:A:118:GLU:HA	2.00	0.61
1:A:368:TRP:CE3	1:A:368:TRP:O	2.53	0.61
1:A:484:TYR:O	1:A:485:LYS:HB2	1.99	0.61
1:A:16:ASP:O	1:A:17:GLU:HB2	2.01	0.60
1:A:275:ARG:HE	1:A:555:ASP:HB3	1.66	0.60
1:A:572:TYR:HE2	11:A:785:HOH:O	1.83	0.60
1:A:118:GLU:CG	1:A:119:LEU:N	2.50	0.60
1:A:16:ASP:OD2	1:A:19:SER:HB2	2.01	0.60
1:A:284:ASN:N	1:A:285:PRO:HD3	2.16	0.60
1:A:438:LEU:HD22	1:A:494:ILE:HD11	1.83	0.60
1:A:258:GLU:HG3	7:A:6951:PZE:C12	2.31	0.60
1:A:424:PRO:O	1:A:425:THR:HB	2.00	0.60
1:A:88:GLU:O	1:A:91:VAL:HG22	2.01	0.60
1:A:7:GLY:O	1:A:8:ALA:CB	2.50	0.60
1:A:438:LEU:HD21	1:A:494:ILE:HG13	1.84	0.59
1:A:106:ILE:CD1	1:A:265:VAL:CG1	2.80	0.59
1:A:408:ASN:HD22	1:A:410:ASN:H	1.50	0.59
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.31	0.59
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.83	0.59
1:A:173:GLN:N	1:A:173:GLN:HE21	1.99	0.59
1:A:326:PRO:O	1:A:523:ARG:NH2	2.33	0.59
1:A:231:ASN:N	1:A:231:ASN:ND2	2.50	0.59
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.38	0.59
1:A:425:THR:HG22	1:A:426:HIS:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ARG:H	1:A:593:ARG:CD	2.05	0.58
1:A:168:PRO:HB2	1:A:172:TYR:HB2	1.86	0.58
1:A:201:SER:OG	1:A:206:LEU:HD11	2.02	0.58
1:A:574:HIS:C	1:A:574:HIS:ND1	2.58	0.58
1:A:202:ARG:HD2	6:A:620:IOD:I	2.73	0.58
5:A:618:HEM:HBC2	5:A:618:HEM:CMC	2.35	0.57
1:A:393:ASP:N	1:A:394:PRO:CD	2.68	0.57
1:A:438:LEU:CD2	1:A:494:ILE:CD1	2.83	0.57
1:A:368:TRP:HE3	1:A:368:TRP:O	1.88	0.56
1:A:91:VAL:CG1	1:A:411:LYS:HD3	2.35	0.56
1:A:202:ARG:NH2	6:A:620:IOD:I	3.06	0.56
1:A:264:THR:HG23	1:A:392:ILE:CG2	2.36	0.56
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.88	0.56
1:A:438:LEU:HD22	1:A:494:ILE:CD1	2.36	0.56
1:A:259:GLN:HE21	1:A:261:LEU:HB2	1.71	0.56
1:A:283:LEU:C	1:A:284:ASN:ND2	2.58	0.55
1:A:118:GLU:O	1:A:119:LEU:CB	2.54	0.55
1:A:106:ILE:CD1	1:A:265:VAL:HG12	2.36	0.55
1:A:196:GLU:CB	1:A:198:SEP:O2P	2.54	0.55
1:A:99:LEU:HG	1:A:567:PHE:HE1	1.72	0.55
1:A:341:ASN:ND2	1:A:444:HIS:ND1	2.43	0.55
1:A:259:GLN:HG2	1:A:261:LEU:H	1.71	0.55
1:A:102:GLN:HE22	1:A:259:GLN:HE22	1.52	0.54
1:A:82:ILE:HD11	1:A:479:LYS:HB2	1.89	0.54
1:A:201:SER:C	1:A:203:LEU:N	2.60	0.54
1:A:2:TRP:CZ3	1:A:174:SER:OG	2.55	0.54
1:A:191:LEU:H	1:A:191:LEU:HD23	1.72	0.54
1:A:222:HIS:HB2	1:A:558:HIS:HE1	1.73	0.53
1:A:140:PHE:O	1:A:160:PHE:HB3	2.09	0.53
1:A:264:THR:HG23	1:A:392:ILE:HG23	1.90	0.52
1:A:174:SER:CB	1:A:175:LEU:CA	2.70	0.52
1:A:361:LEU:HB3	1:A:365:TYR:HA	1.90	0.52
3:A:602:NAG:H62	3:A:603:NAG:N2	2.24	0.52
1:A:16:ASP:OD1	1:A:16:ASP:C	2.49	0.51
1:A:408:ASN:ND2	1:A:410:ASN:H	2.08	0.51
1:A:438:LEU:HD21	1:A:494:ILE:CG1	2.41	0.50
1:A:194:GLY:CA	1:A:199:LEU:HD23	2.41	0.50
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.46	0.50
1:A:77:GLU:OE2	1:A:483:LEU:HD21	2.11	0.50
1:A:288:ASP:O	1:A:292:LEU:HG	2.11	0.50
1:A:52:GLU:OE1	1:A:62:THR:OG1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CD1	1:A:175:LEU:C	2.80	0.50
1:A:557:THR:OG1	1:A:559:ILE:HG12	2.11	0.50
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.08	0.50
1:A:106:ILE:CD1	1:A:265:VAL:HG11	2.41	0.49
1:A:257:SER:O	1:A:381:PHE:HA	2.12	0.49
1:A:392:ILE:HG22	1:A:396:VAL:HG23	1.94	0.49
1:A:30:ASN:HB3	1:A:33:SER:O	2.13	0.49
1:A:559:ILE:HD13	1:A:559:ILE:N	2.26	0.49
1:A:165:PHE:HE2	1:A:168:PRO:O	1.94	0.49
1:A:175:LEU:O	1:A:176:ALA:C	2.50	0.49
1:A:284:ASN:N	1:A:284:ASN:ND2	2.54	0.48
1:A:258:GLU:HG3	7:A:6951:PZE:H12A	1.95	0.48
1:A:146:LYS:O	1:A:147:ASN:HB2	2.13	0.48
1:A:366:GLN:O	1:A:367:PRO:C	2.51	0.48
1:A:491:ASP:HA	11:A:765:HOH:O	2.12	0.48
1:A:13:VAL:O	1:A:13:VAL:HG23	2.13	0.48
1:A:123:GLU:CD	1:A:125:SER:CB	2.78	0.47
1:A:123:GLU:HG3	1:A:125:SER:CA	2.43	0.47
1:A:438:LEU:HD21	1:A:494:ILE:CD1	2.44	0.47
1:A:275:ARG:NE	1:A:555:ASP:HB3	2.28	0.47
1:A:393:ASP:O	1:A:397:ARG:HG3	2.14	0.47
1:A:106:ILE:HD11	1:A:265:VAL:CG1	2.41	0.47
1:A:425:THR:HG23	1:A:425:THR:O	2.14	0.47
1:A:233:LYS:HE2	1:A:238:GLU:OE2	2.14	0.47
1:A:112:ASP:OD2	5:A:618:HEM:O1D	2.33	0.47
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.49	0.47
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.50	0.46
1:A:82:ILE:CD1	1:A:479:LYS:HD3	2.45	0.46
1:A:551:ARG:CD	1:A:583:ASP:O	2.63	0.46
1:A:202:ARG:NH1	6:A:620:IOD:I	3.16	0.46
1:A:438:LEU:HD21	1:A:494:ILE:HD11	1.97	0.45
1:A:58:PRO:HG2	1:A:61:TRP:HB2	1.99	0.45
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.81	0.45
1:A:460:GLN:NE2	11:A:738:HOH:O	2.50	0.45
1:A:66:THR:HB	1:A:70:PHE:N	2.32	0.45
1:A:408:ASN:C	1:A:408:ASN:HD22	2.19	0.44
1:A:237:CYS:HA	1:A:381:PHE:O	2.18	0.44
1:A:472:LYS:HD2	1:A:500:PRO:HG2	1.99	0.44
1:A:548:SER:OG	1:A:551:ARG:HB2	2.18	0.44
1:A:349:PHE:CD1	1:A:349:PHE:C	2.90	0.44
1:A:258:GLU:O	1:A:380:PHE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:CYS:HA	1:A:383:THR:HG21	2.00	0.44
1:A:303:PHE:O	1:A:307:ILE:HG12	2.17	0.44
1:A:52:GLU:OE1	1:A:62:THR:CB	2.65	0.44
1:A:392:ILE:O	1:A:393:ASP:C	2.56	0.44
1:A:9:PRO:O	1:A:11:PRO:CD	2.62	0.43
1:A:236:PRO:HB3	6:A:619:IOD:I	2.88	0.43
1:A:393:ASP:N	1:A:394:PRO:HD3	2.33	0.43
1:A:402:LYS:HA	1:A:402:LYS:HD3	1.70	0.43
1:A:108:ASP:HB2	1:A:347:PHE:CD2	2.54	0.43
1:A:424:PRO:O	1:A:425:THR:CB	2.65	0.43
1:A:325:ILE:HG22	1:A:523:ARG:NH2	2.33	0.43
1:A:28:CYS:O	1:A:527:ARG:NH2	2.47	0.43
1:A:377:HIS:O	1:A:429:HIS:CD2	2.72	0.43
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.98	0.42
1:A:559:ILE:HG23	6:A:611:IOD:I	2.90	0.42
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.77	0.42
1:A:344:THR:O	1:A:348:ARG:HG3	2.18	0.42
1:A:196:GLU:OE2	1:A:198:SEP:O2P	2.37	0.42
1:A:120:GLY:HA2	1:A:123:GLU:HB3	1.98	0.42
1:A:31:ARG:HH11	1:A:31:ARG:HD3	1.70	0.42
1:A:408:ASN:HB3	1:A:411:LYS:HB2	2.02	0.42
1:A:492:ILE:O	1:A:493:TRP:C	2.58	0.42
1:A:279:GLU:OE2	1:A:279:GLU:HA	2.19	0.42
1:A:368:TRP:CH2	1:A:389:ASP:O	2.73	0.42
1:A:124:HIS:O	1:A:128:GLN:N	2.52	0.42
1:A:421:LEU:HB3	1:A:431:PHE:HB2	2.01	0.42
1:A:241:ASN:O	1:A:242:THR:C	2.59	0.42
1:A:99:LEU:HD21	1:A:549:PHE:CD2	2.54	0.41
1:A:51:TYR:CD2	1:A:55:LEU:O	2.73	0.41
1:A:232:VAL:HG21	11:A:749:HOH:O	2.20	0.41
1:A:173:GLN:HB2	1:A:174:SER:HA	2.03	0.41
1:A:283:LEU:C	1:A:285:PRO:HD3	2.40	0.41
1:A:80:ASN:HA	1:A:418:ARG:NH2	2.36	0.41
1:A:198:SEP:O	1:A:202:ARG:HB2	2.21	0.41
1:A:174:SER:HB2	1:A:175:LEU:C	2.41	0.41
1:A:201:SER:O	1:A:203:LEU:N	2.53	0.41
1:A:80:ASN:OD1	1:A:418:ARG:NH2	2.54	0.41
1:A:241:ASN:ND2	1:A:244:ALA:HB2	2.35	0.41
1:A:283:LEU:HB3	1:A:284:ASN:ND2	2.36	0.40
5:A:618:HEM:HMC1	5:A:618:HEM:CBC	2.46	0.40
1:A:236:PRO:HA	1:A:239:PHE:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:OD2	1:A:108:ASP:C	2.60	0.40
1:A:123:GLU:OE2	1:A:125:SER:HB2	2.21	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	592/595 (100%)	551 (93%)	34 (6%)	7 (1%)	16	33

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	A	170	PRO
1	A	171	PRO
1	A	147	ASN
1	A	9	PRO
1	A	149	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	516/516 (100%)	486 (94%)	30 (6%)	25	49

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	29	ASN
1	A	32	ARG
1	A	108	ASP
1	A	121	SER
1	A	122	SER
1	A	124	HIS
1	A	173	GLN
1	A	208	SER
1	A	216	ASN
1	A	231	ASN
1	A	235	SER
1	A	259	GLN
1	A	284	ASN
1	A	322	GLN
1	A	341	ASN
1	A	347	PHE
1	A	360	ARG
1	A	382	ASN
1	A	408	ASN
1	A	418	ARG
1	A	425	THR
1	A	481	LEU
1	A	503	GLU
1	A	543	SER
1	A	564	LEU
1	A	574	HIS
1	A	587	LEU
1	A	593	ARG
1	A	594	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	68	ASN
1	A	102	GLN

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	173	GLN
1	A	216	ASN
1	A	222	HIS
1	A	231	ASN
1	A	250	GLN
1	A	284	ASN
1	A	294	GLN
1	A	341	ASN
1	A	364	ASN
1	A	366	GLN
1	A	382	ASN
1	A	403	ASN
1	A	408	ASN
1	A	429	HIS
1	A	497	ASN
1	A	558	HIS

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	8,9,10	0.93	0	8,12,14	1.46	1 (12%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	2.16	112.65	107.14

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 [i](#)

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	$\# Z > 2$
3	NAG	A	602	1,3	14,14,15	0.44	0	15,19,21	1.04	0
3	NAG	A	603	3	14,14,15	0.74	0	15,19,21	2.12	5 (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	NAG	A	602	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C4-C3-C2	-3.88	105.20	111.23
3	A	603	NAG	C3-C4-C5	2.07	113.81	110.20
3	A	603	NAG	C3-C2-N2	2.55	116.67	110.56
3	A	603	NAG	O3-C3-C2	2.84	114.73	109.11
3	A	603	NAG	C1-O5-C5	4.92	118.49	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAG	2	0
3	A	603	NAG	1	0

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 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	$\# Z > 2$
9	GOL	A	597	-	5,5,5	0.35	0	5,5,5	0.24	0
10	EDO	A	598	-	3,3,3	0.28	0	2,2,2	0.79	0
2	NAG	A	599	1	14,14,15	0.38	0	15,19,21	0.99	1 (6%)
2	NAG	A	605	1	14,14,15	0.73	0	15,19,21	2.34	4 (26%)
5	HEM	A	618	1,11	30,50,50	2.68	8 (26%)	24,82,82	2.27	6 (25%)
8	SCN	A	6788	-	2,2,2	1.99	1 (50%)	1,1,1	0.20	0
7	PZE	A	6951	-	6,6,6	0.45	0	6,6,6	1.94	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
9	GOL	A	597	-	-	0/4/4/4	0/0/0/0
10	EDO	A	598	-	-	0/1/1/1	0/0/0/0
2	NAG	A	599	1	-	0/6/23/26	0/1/1/1
2	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	HEM	A	618	1,11	-	0/10/54/54	0/0/8/8
8	SCN	A	6788	-	-	0/0/0/0	0/0/0/0
7	PZE	A	6951	-	-	0/0/6/6	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	618	HEM	C3B-C4B	-10.66	1.42	1.51
5	A	618	HEM	C3D-C4D	-5.85	1.44	1.51
5	A	618	HEM	C2C-C1C	-4.15	1.44	1.52
5	A	618	HEM	C2A-C3A	-2.41	1.30	1.37
5	A	618	HEM	C2B-C1B	-2.39	1.44	1.51
5	A	618	HEM	C2D-C1D	-2.35	1.44	1.51
5	A	618	HEM	CMC-C2C	2.15	1.58	1.53
8	A	6788	SCN	C-S	2.75	1.81	1.63
5	A	618	HEM	C3B-CAB	2.84	1.56	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	618	HEM	CBA-CAA-C2A	-5.26	103.09	112.53
5	A	618	HEM	CBD-CAD-C3D	-2.20	107.16	113.55
2	A	599	NAG	C4-C3-C2	2.08	114.46	111.23
2	A	605	NAG	O7-C7-N2	2.62	127.21	121.86
7	A	6951	PZE	C11-N10-C9	2.89	119.92	110.33
7	A	6951	PZE	C12-N7-C8	2.93	120.06	110.33
5	A	618	HEM	CMB-C2B-C3B	3.65	125.64	116.53
5	A	618	HEM	CMC-C2C-C3C	3.67	125.70	116.53
2	A	605	NAG	C4-C3-C2	3.72	117.01	111.23
5	A	618	HEM	CAD-C3D-C2D	4.61	126.47	113.22
2	A	605	NAG	C3-C4-C5	4.73	118.44	110.20
5	A	618	HEM	CAD-C3D-C4D	5.08	130.38	112.47
2	A	605	NAG	C2-N2-C7	5.60	130.23	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	597	GOL	2	0
5	A	618	HEM	4	0
7	A	6951	PZE	6	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%)	0.24	35 (5%) 26 19	22, 42, 79, 99	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	10.2
1	A	595	ASN	9.0
1	A	12	LEU	6.4
1	A	390	GLY	5.7
1	A	594	GLU	5.7
1	A	7	GLY	5.5
1	A	173	GLN	5.2
1	A	4	VAL	5.2
1	A	2	TRP	5.1
1	A	175	LEU	5.1
1	A	13	VAL	5.0
1	A	171	PRO	4.9
1	A	124	HIS	4.6
1	A	121	SER	4.5
1	A	11	PRO	3.9
1	A	1	SER	3.7
1	A	6	CYS	3.7
1	A	172	TYR	3.6
1	A	120	GLY	3.4
1	A	10	VAL	2.9
1	A	118	GLU	2.9
1	A	125	SER	2.8
1	A	5	GLY	2.7
1	A	117	THR	2.6
1	A	119	LEU	2.5
1	A	569	ALA	2.5
1	A	593	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	582	VAL	2.3
1	A	265	VAL	2.3
1	A	279	GLU	2.3
1	A	131	GLU	2.2
1	A	122	SER	2.2
1	A	223	GLY	2.1
1	A	17	GLU	2.1
1	A	170	PRO	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	0.86	0.30	-	45,48,49,51	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
3	NAG	A	602	14/15	0.88	0.15	-0.54	60,61,63,63	0
3	NAG	A	603	14/15	0.73	0.31	-	79,80,81,81	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.

less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	PZE	A	6951	6/6	0.83	0.54	12.01	35,35,36,36	6
9	GOL	A	597	6/6	0.73	0.26	4.24	45,50,51,52	0
8	SCN	A	6788	3/3	0.74	0.33	4.16	47,47,48,50	0
2	NAG	A	599	14/15	0.87	0.21	0.18	68,71,72,73	0
5	HEM	A	618	43/43	0.97	0.16	-0.97	17,22,29,32	0
6	IOD	A	616	1/1	0.98	0.06	-1.20	83,83,83,83	0
4	CA	A	607	1/1	0.97	0.09	-1.59	36,36,36,36	0
6	IOD	A	611	1/1	0.98	0.04	-3.45	78,78,78,78	0
6	IOD	A	615	1/1	0.97	0.08	-3.63	54,54,54,54	0
6	IOD	A	612	1/1	0.99	0.04	-3.83	58,58,58,58	0
6	IOD	A	609	1/1	1.00	0.04	-4.60	46,46,46,46	0
6	IOD	A	610	1/1	0.96	0.05	-4.74	82,82,82,82	0
6	IOD	A	619	1/1	0.98	0.04	-8.19	73,73,73,73	0
6	IOD	A	620	1/1	0.98	0.10	-	47,47,47,47	1
10	EDO	A	598	4/4	0.94	0.17	-	44,44,45,46	0
6	IOD	A	1618	1/1	0.98	0.04	-	80,80,80,80	0
6	IOD	A	617	1/1	0.98	0.08	-	64,64,64,64	1
2	NAG	A	605	14/15	0.67	0.30	-	77,78,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.