



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

PDB ID : 3TUW
Title : Crystal structure of lactoperoxidase complexed with pyrazinamide at 2.2Å resolution
Authors : Pandey, N.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-09-19
Resolution : 2.20 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

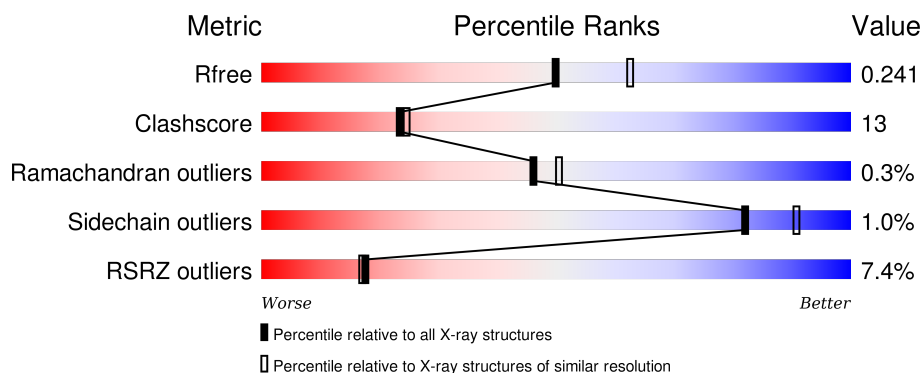
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>7%</div> <div>78%</div> <div>21%</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
10	PEG	A	603	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GOL	A	621	-	-	-	X
5	IOD	A	607	-	-	X	-
8	PZA	A	598	-	X	-	X

2 Entry composition [i](#)

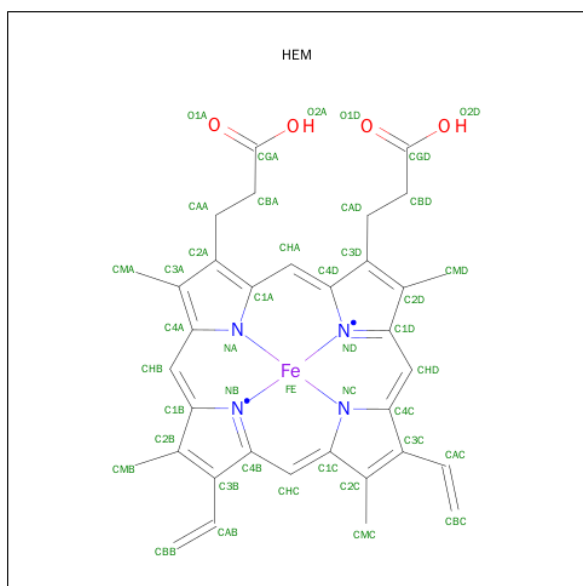
There are 13 unique types of molecules in this entry. The entry contains 5420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

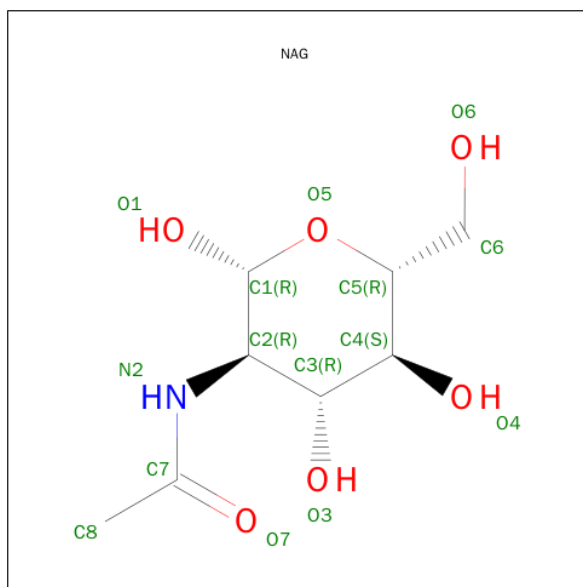
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

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



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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	I	0	0
			11	11		

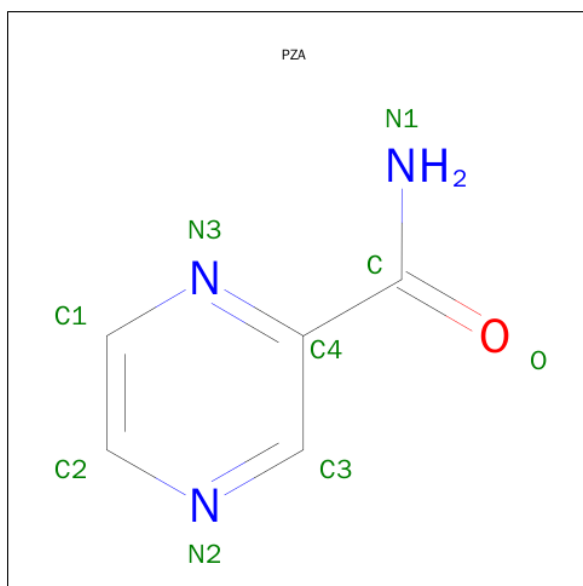
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

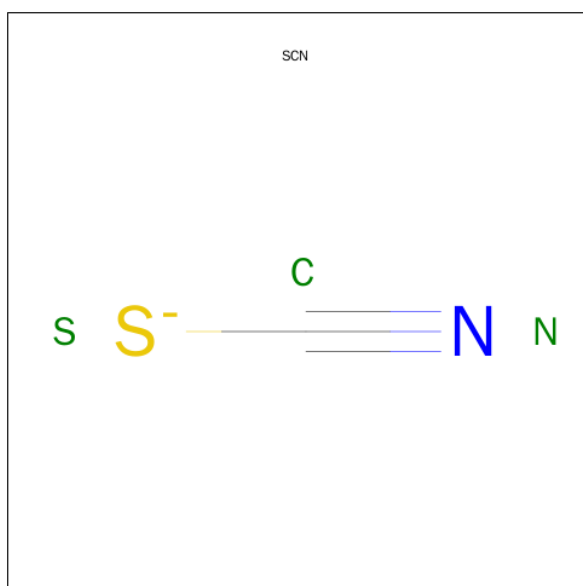
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is PYRAZINE-2-CARBOXAMIDE (three-letter code: PZA) (formula: C₅H₅N₃O).



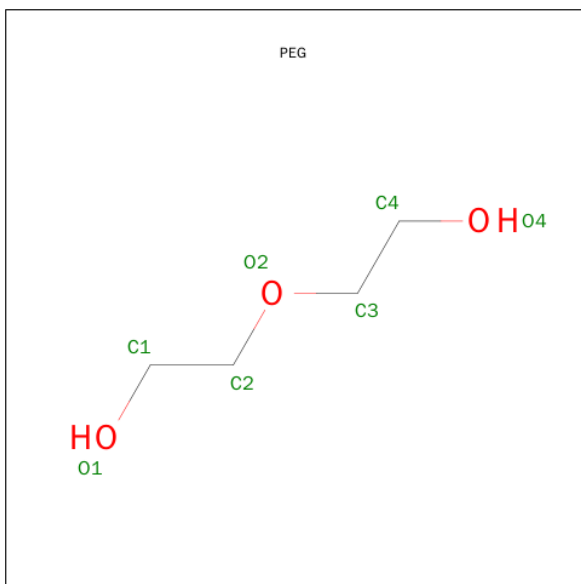
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 9 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



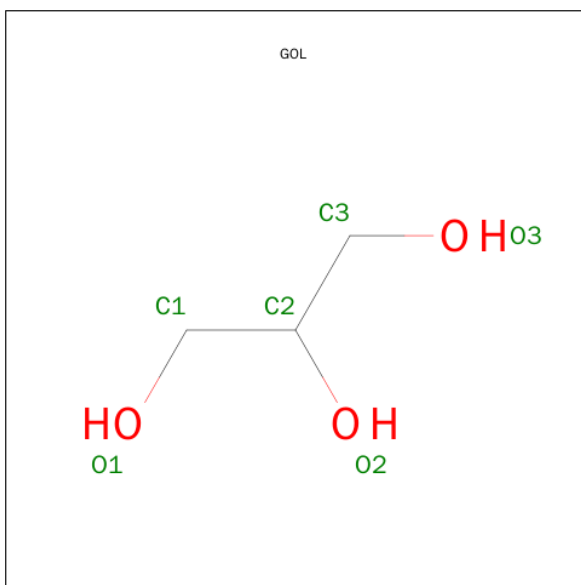
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	S	0	0
			3	1	1	1		

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



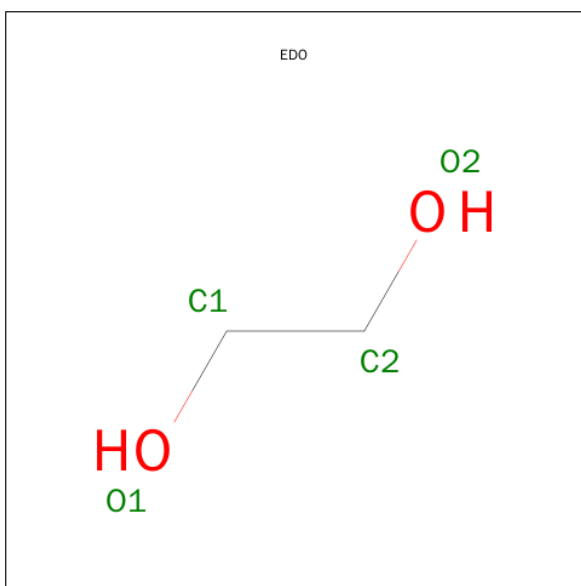
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		

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



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

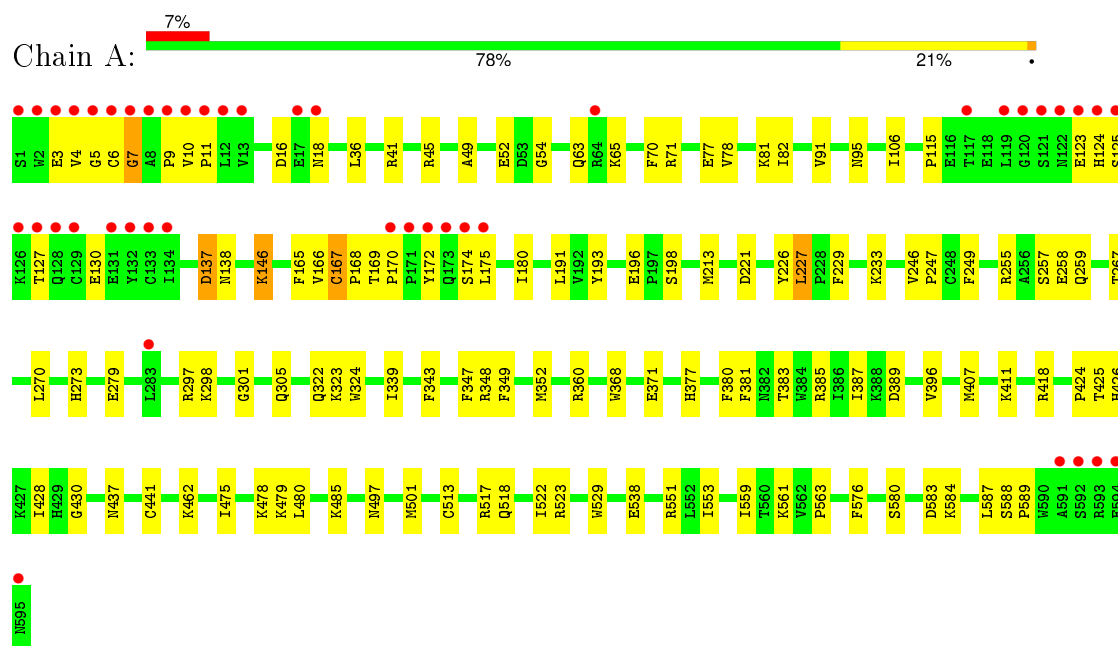
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	474	Total	O	0	0
			474	474		

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 79.72Å 77.00Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	43.96 – 2.20 43.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.96-2.20) 98.5 (43.96-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.12 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.216 0.195 , 0.241	Depositor DCC
R_{free} test set	1604 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.925	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 32019 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5420	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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, ZN, SCN, NAG, SEP, CA, EDO, PEG, HEM, IOD, PZA

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	0.54	0/4891	0.77	1/6634 (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	227	LEU	CA-CB-CG	5.75	128.52	115.30

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	4774	0	4687	120	1
2	A	43	0	30	7	0
3	A	42	0	39	2	0
4	A	28	0	25	0	0
5	A	11	0	0	4	0
6	A	1	0	0	0	0
7	A	1	0	0	0	1
8	A	9	0	5	2	0
9	A	3	0	0	0	0
10	A	14	0	18	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	12	0	16	4	0
12	A	8	0	10	1	0
13	A	474	0	0	18	0
All	All	5420	0	4830	130	1

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 (130) 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:167:CYS:HB2	1:A:168:PRO:CD	1.81	1.10
1:A:167:CYS:CB	1:A:168:PRO:HD3	1.83	1.08
2:A:605:HEM:HMC2	2:A:605:HEM:HBC2	1.39	1.04
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.40	1.04
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.60	1.02
2:A:605:HEM:HBB2	2:A:605:HEM:HMB1	1.40	0.98
1:A:167:CYS:CB	1:A:168:PRO:CD	2.36	0.94
1:A:255:ARG:HA	8:A:598:PZA:N2	1.82	0.94
1:A:462:LYS:HD2	13:A:974:HOH:O	1.68	0.93
1:A:168:PRO:HB2	1:A:170:PRO:O	1.73	0.89
1:A:169:THR:HG23	13:A:780:HOH:O	1.75	0.86
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.58	0.84
1:A:54:GLY:HA2	13:A:936:HOH:O	1.79	0.82
2:A:605:HEM:HBC2	2:A:605:HEM:CMC	2.09	0.82
2:A:605:HEM:HBB2	2:A:605:HEM:CMB	2.10	0.81
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.63	0.79
1:A:95:ASN:HD22	11:A:621:GOL:H12	1.49	0.77
1:A:63:GLN:HG2	1:A:71:ARG:HH12	1.49	0.77
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.69	0.74
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.70	0.73
1:A:426:HIS:HE1	13:A:1057:HOH:O	1.73	0.71
1:A:424:PRO:O	1:A:425:THR:HB	1.89	0.70
1:A:517:ARG:HD3	13:A:1128:HOH:O	1.91	0.69
1:A:233:LYS:HD3	13:A:927:HOH:O	1.92	0.69
1:A:339:ILE:HD13	1:A:522:ILE:HD11	1.76	0.68
1:A:70:PHE:CG	1:A:485:LYS:HB2	2.29	0.68
1:A:9:PRO:CD	1:A:167:CYS:HA	2.23	0.67
1:A:425:THR:O	1:A:425:THR:HG22	1.96	0.66
1:A:428:ILE:O	1:A:428:ILE:HD12	1.95	0.66
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HD3	1:A:167:CYS:HA	1.77	0.66
1:A:279:GLU:HG2	1:A:587:LEU:HD12	1.78	0.65
5:A:612:IOD:I	13:A:1072:HOH:O	2.83	0.65
3:A:596:NAG:O7	11:A:621:GOL:H11	1.97	0.64
1:A:63:GLN:CG	1:A:71:ARG:HH12	2.11	0.64
1:A:352:MET:HB3	1:A:407:MET:HG2	1.82	0.61
2:A:605:HEM:HMC2	2:A:605:HEM:CBC	2.24	0.61
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.61
1:A:9:PRO:HG3	1:A:167:CYS:O	2.00	0.61
2:A:605:HEM:CBB	2:A:605:HEM:HMB1	2.25	0.61
1:A:166:VAL:O	1:A:168:PRO:HD2	2.01	0.60
1:A:124:HIS:HB2	1:A:127:THR:HB	1.83	0.60
1:A:175:LEU:HD12	13:A:1106:HOH:O	2.02	0.59
1:A:387:ILE:HG21	12:A:623:EDO:H12	1.84	0.59
1:A:580:SER:HA	11:A:622:GOL:O2	2.02	0.59
1:A:428:ILE:HD13	1:A:430:GLY:CA	2.33	0.58
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.39	0.58
1:A:518:GLN:O	1:A:522:ILE:HG12	2.05	0.57
1:A:65:LYS:NZ	13:A:981:HOH:O	2.36	0.57
1:A:165:PHE:CZ	1:A:169:THR:O	2.57	0.56
1:A:323:LYS:HD3	1:A:324:TRP:CE2	2.41	0.56
1:A:559:ILE:HG23	5:A:607:IOD:I	2.76	0.55
1:A:169:THR:N	1:A:170:PRO:HD2	2.20	0.55
1:A:169:THR:H	1:A:170:PRO:HD2	1.72	0.55
1:A:52:GLU:HG2	13:A:981:HOH:O	2.07	0.55
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.03	0.55
1:A:18:ASN:ND2	13:A:1008:HOH:O	2.41	0.54
1:A:428:ILE:HD13	1:A:430:GLY:N	2.23	0.54
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.90	0.53
5:A:614:IOD:I	13:A:1014:HOH:O	2.89	0.53
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.36	0.53
1:A:259:GLN:HG2	2:A:605:HEM:CBB	2.39	0.53
1:A:352:MET:CB	1:A:407:MET:HG2	2.40	0.52
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.91	0.52
1:A:551:ARG:HD3	1:A:583:ASP:O	2.10	0.52
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.56	0.52
1:A:301:GLY:O	1:A:305:GLN:HG3	2.10	0.52
1:A:428:ILE:HD13	1:A:430:GLY:HA3	1.90	0.52
1:A:407:MET:HB3	1:A:501:MET:HE3	1.91	0.52
1:A:322:GLN:HG2	13:A:687:HOH:O	2.10	0.51
1:A:36:LEU:HD11	10:A:619:PEG:H32	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LYS:NZ	13:A:746:HOH:O	2.44	0.50
1:A:428:ILE:C	1:A:428:ILE:HD12	2.32	0.50
1:A:115:PRO:HG2	13:A:1037:HOH:O	2.12	0.50
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.47	0.49
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.94	0.49
1:A:6:CYS:SG	1:A:7:GLY:N	2.86	0.49
1:A:385:ARG:O	1:A:389:ASP:HB3	2.12	0.49
1:A:424:PRO:O	1:A:425:THR:CB	2.59	0.49
1:A:428:ILE:CD1	1:A:430:GLY:N	2.77	0.48
1:A:257:SER:O	1:A:381:PHE:HA	2.14	0.48
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.78	0.48
1:A:517:ARG:CD	13:A:1128:HOH:O	2.57	0.48
1:A:227:LEU:CD2	1:A:270:LEU:HD22	2.41	0.48
1:A:584:LYS:HE3	11:A:622:GOL:H11	1.97	0.47
3:A:596:NAG:H4	13:A:1056:HOH:O	2.15	0.47
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.49	0.47
1:A:324:TRP:CZ2	1:A:513:CYS:HB2	2.50	0.47
1:A:360:ARG:NH2	1:A:371:GLU:O	2.43	0.47
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.95	0.47
1:A:123:GLU:HG3	1:A:125:SER:H	1.80	0.47
1:A:169:THR:HB	1:A:170:PRO:CD	2.45	0.46
1:A:425:THR:CG2	1:A:425:THR:O	2.61	0.46
1:A:227:LEU:HD21	1:A:267:THR:HA	1.97	0.46
1:A:428:ILE:CD1	1:A:430:GLY:H	2.28	0.46
1:A:258:GLU:HB2	8:A:598:PZA:H4	1.98	0.46
1:A:428:ILE:HD12	1:A:430:GLY:H	1.79	0.46
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.44	0.46
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.46	0.46
1:A:561:LYS:HD2	5:A:607:IOD:I	2.86	0.45
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.47	0.45
1:A:418:ARG:HH22	10:A:603:PEG:C4	2.29	0.45
1:A:36:LEU:CD1	10:A:619:PEG:H32	2.47	0.45
1:A:16:ASP:C	1:A:16:ASP:OD1	2.54	0.44
1:A:478:LYS:HE3	1:A:478:LYS:HB2	1.71	0.44
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.83	0.44
1:A:249:PHE:CE1	1:A:383:THR:HG23	2.53	0.44
1:A:249:PHE:CZ	1:A:383:THR:HG23	2.52	0.43
1:A:407:MET:HB3	1:A:501:MET:CE	2.48	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:193:TYR:OH	1:A:297:ARG:HA	2.19	0.42
1:A:124:HIS:HB2	1:A:127:THR:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CD2	1:A:485:LYS:HB2	2.54	0.42
1:A:246:VAL:HG11	1:A:387:ILE:HD12	2.01	0.42
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.54	0.42
1:A:10:VAL:HA	1:A:11:PRO:HD3	1.88	0.42
1:A:172:TYR:CE2	1:A:174:SER:HB3	2.55	0.41
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.50	0.41
1:A:137:ASP:HB3	1:A:138:ASN:H	1.64	0.41
1:A:91:VAL:CG1	1:A:411:LYS:HD3	2.50	0.41
1:A:172:TYR:CE2	1:A:174:SER:N	2.86	0.41
1:A:298:LYS:HG3	13:A:1061:HOH:O	2.20	0.41
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.51	0.41
1:A:172:TYR:HE2	1:A:174:SER:HB3	1.86	0.41
1:A:462:LYS:HA	1:A:462:LYS:HD3	1.81	0.41
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.03	0.41
1:A:106:ILE:HG23	1:A:191:LEU:HD11	2.02	0.41
1:A:4:VAL:HG13	1:A:5:GLY:N	2.36	0.41
1:A:368:TRP:CE3	1:A:368:TRP:O	2.75	0.40
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLU:OE1	7:A:618:ZN:ZN[2_545]	1.35	0.85

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%)	572 (97%)	18 (3%)	2 (0%)	46 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	7	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	512 (99%)	5 (1%)	82	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	137	ASP
1	A	146	LYS
1	A	347	PHE
1	A	441	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	GLN
1	A	364	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN
1	A	574	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	1.02	0	8,12,14	1.47	2 (25%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O-C-CA	-2.05	120.15	125.49
1	A	198	SEP	OG-CB-CA	2.47	110.38	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates ⓘ

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$
4	NAG	A	601	1,4	14,14,15	2.16	4 (28%)	15,19,21	1.97	5 (33%)
4	NAG	A	602	4	14,14,15	1.04	2 (14%)	15,19,21	2.31	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
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	O4-C4	-5.86	1.28	1.43
4	A	601	NAG	O5-C5	-3.75	1.35	1.43
4	A	601	NAG	C4-C5	-2.69	1.47	1.53
4	A	602	NAG	C1-C2	-2.17	1.49	1.52
4	A	601	NAG	C3-C2	-2.14	1.47	1.52
4	A	602	NAG	C3-C2	-2.07	1.47	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	NAG	C4-C3-C2	-5.94	101.99	111.23
4	A	601	NAG	O4-C4-C5	-3.75	99.31	109.24
4	A	601	NAG	C1-O5-C5	-3.35	108.00	112.25
4	A	601	NAG	O4-C4-C3	-2.44	104.83	110.34
4	A	602	NAG	C2-N2-C7	-2.28	120.11	123.04
4	A	601	NAG	C4-C3-C2	-2.16	107.87	111.23
4	A	602	NAG	C3-C2-N2	2.53	116.63	110.56
4	A	602	NAG	C3-C4-C5	3.17	115.73	110.20
4	A	601	NAG	C3-C4-C5	3.69	116.64	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	NAG	C1-O5-C5	4.25	117.64	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 [i](#)

Of 25 ligands modelled in this entry, 13 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	596	1	14,14,15	1.12	2 (14%)	15,19,21	1.21	1 (6%)
8	PZA	A	598	-	9,9,9	1.55	1 (11%)	11,11,11	2.28	6 (54%)
3	NAG	A	599	1	14,14,15	1.08	2 (14%)	15,19,21	0.91	0
10	PEG	A	603	-	6,6,6	2.04	1 (16%)	5,5,5	1.32	1 (20%)
3	NAG	A	604	1	14,14,15	1.04	2 (14%)	15,19,21	1.09	1 (6%)
2	HEM	A	605	1,13	30,50,50	2.30	10 (33%)	24,82,82	2.34	10 (41%)
10	PEG	A	619	-	6,6,6	2.03	1 (16%)	5,5,5	1.14	1 (20%)
9	SCN	A	620	-	2,2,2	2.58	1 (50%)	1,1,1	0.16	0
11	GOL	A	621	-	5,5,5	0.76	0	5,5,5	0.66	0
11	GOL	A	622	-	5,5,5	0.41	0	5,5,5	0.31	0
12	EDO	A	623	-	3,3,3	3.15	1 (33%)	2,2,2	1.37	0
12	EDO	A	624	-	3,3,3	2.60	1 (33%)	2,2,2	1.29	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
3	NAG	A	596	1	-	0/6/23/26	0/1/1/1
8	PZA	A	598	-	-	4/4/4/4	0/1/1/1
3	NAG	A	599	1	-	0/6/23/26	0/1/1/1
10	PEG	A	603	-	-	0/4/4/4	0/0/0/0
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
2	HEM	A	605	1,13	-	0/10/54/54	0/0/8/8
10	PEG	A	619	-	-	0/4/4/4	0/0/0/0
9	SCN	A	620	-	-	0/0/0/0	0/0/0/0
11	GOL	A	621	-	-	0/4/4/4	0/0/0/0
11	GOL	A	622	-	-	0/4/4/4	0/0/0/0
12	EDO	A	623	-	-	0/1/1/1	0/0/0/0
12	EDO	A	624	-	-	0/1/1/1	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEM	C3B-C4B	-7.54	1.45	1.51
2	A	605	HEM	C3D-C4D	-5.42	1.44	1.51
12	A	623	EDO	O2-C2	-5.20	1.14	1.42
10	A	603	PEG	O4-C4	-4.70	1.16	1.42
10	A	619	PEG	O4-C4	-4.61	1.17	1.42
12	A	624	EDO	O2-C2	-4.47	1.17	1.42
2	A	605	HEM	C2C-C1C	-4.25	1.44	1.52
3	A	599	NAG	O5-C5	-2.58	1.37	1.43
3	A	604	NAG	O5-C5	-2.47	1.38	1.43
3	A	596	NAG	O5-C1	-2.45	1.39	1.43
3	A	596	NAG	O5-C5	-2.40	1.38	1.43
3	A	604	NAG	O5-C1	-2.34	1.39	1.43
2	A	605	HEM	C2B-C1B	-2.15	1.44	1.51
3	A	599	NAG	O5-C1	-2.12	1.40	1.43
2	A	605	HEM	C2D-C1D	-2.00	1.45	1.51
2	A	605	HEM	FE-NB	2.04	2.08	1.97
2	A	605	HEM	FE-ND	2.09	2.08	1.97
2	A	605	HEM	C1C-NC	2.38	1.38	1.36
2	A	605	HEM	FE-NC	2.63	2.06	1.95
2	A	605	HEM	C3B-CAB	2.69	1.56	1.51
9	A	620	SCN	C-S	3.57	1.86	1.63
8	A	598	PZA	O-C	4.21	1.33	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C3B-CAB-CBB	-3.25	119.47	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	605	HEM	C3C-CAC-CBC	-3.00	119.85	124.46
3	A	596	NAG	C4-C3-C2	-2.93	106.67	111.23
8	A	598	PZA	C4-C3-N2	-2.63	119.33	122.11
3	A	604	NAG	C2-N2-C7	-2.59	119.71	123.04
2	A	605	HEM	C3B-C4B-NB	-2.28	107.27	111.63
8	A	598	PZA	C1-C2-N2	-2.22	118.94	121.94
8	A	598	PZA	C2-C1-N3	-2.09	119.66	122.25
10	A	619	PEG	O4-C4-C3	2.33	126.44	112.03
2	A	605	HEM	C2D-C3D-C4D	2.38	105.53	101.50
2	A	605	HEM	C3B-C4B-CHC	2.39	126.53	123.16
8	A	598	PZA	C2-N2-C3	2.61	121.65	116.84
10	A	603	PEG	O4-C4-C3	2.66	128.43	112.03
8	A	598	PZA	C1-N3-C4	3.03	120.99	116.92
2	A	605	HEM	CMD-C2D-C3D	3.05	127.86	114.35
2	A	605	HEM	CMC-C2C-C3C	3.45	125.15	116.53
2	A	605	HEM	CMB-C2B-C3B	3.76	125.91	116.53
8	A	598	PZA	C4-C-N1	3.94	120.07	116.21
2	A	605	HEM	CAD-C3D-C4D	4.46	128.21	112.47
2	A	605	HEM	CAD-C3D-C2D	4.54	126.26	113.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	598	PZA	O-C-C4-N3
8	A	598	PZA	N3-C4-C-N1
8	A	598	PZA	O-C-C4-C3
8	A	598	PZA	C3-C4-C-N1

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	596	NAG	2	0
8	A	598	PZA	2	0
10	A	603	PEG	1	0
2	A	605	HEM	7	0
10	A	619	PEG	2	0
11	A	621	GOL	2	0
11	A	622	GOL	2	0
12	A	623	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	0.22	44 (7%) 17 17	15, 31, 71, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	15.7
1	A	172	TYR	11.9
1	A	121	SER	8.9
1	A	171	PRO	8.5
1	A	7	GLY	8.1
1	A	4	VAL	7.6
1	A	119	LEU	7.0
1	A	173	GLN	7.0
1	A	8	ALA	6.4
1	A	122	ASN	6.4
1	A	12	LEU	6.2
1	A	6	CYS	6.2
1	A	124	HIS	6.0
1	A	593	ARG	5.7
1	A	595	ASN	5.5
1	A	283	LEU	5.4
1	A	120	GLY	5.3
1	A	1	SER	5.2
1	A	174	SER	4.8
1	A	170	PRO	4.6
1	A	594	GLU	4.0
1	A	132	TYR	3.9
1	A	18	ASN	3.8
1	A	128	GLN	3.8
1	A	3	GLU	3.5
1	A	125	SER	3.5
1	A	10	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	123	GLU	3.5
1	A	133	CYS	3.2
1	A	13	VAL	3.0
1	A	592	SER	2.8
1	A	126	LYS	2.7
1	A	5	GLY	2.6
1	A	591	ALA	2.5
1	A	11	PRO	2.4
1	A	175	LEU	2.4
1	A	127	THR	2.4
1	A	64	ARG	2.4
1	A	117	THR	2.3
1	A	17	GLU	2.3
1	A	134	ILE	2.3
1	A	129	CYS	2.2
1	A	9	PRO	2.2
1	A	131	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.91	0.19	-	34,44,45,45	0

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	A	601	14/15	0.91	0.14	-0.14	43,47,54,55	0
4	NAG	A	602	14/15	0.77	0.23	-	59,66,73,73	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
11	GOL	A	621	6/6	0.89	0.28	12.98	38,41,47,51	0
10	PEG	A	603	7/7	0.77	0.23	8.21	29,33,38,42	0
8	PZA	A	598	9/9	0.77	0.43	7.19	37,38,40,40	9
11	GOL	A	622	6/6	0.77	0.19	1.33	61,64,66,68	0
2	HEM	A	605	43/43	0.94	0.20	1.21	14,18,22,24	0
9	SCN	A	620	3/3	0.91	0.17	0.69	43,43,45,46	0
10	PEG	A	619	7/7	0.88	0.12	0.37	48,50,52,53	0
12	EDO	A	623	4/4	0.93	0.16	-0.20	32,34,36,39	0
3	NAG	A	599	14/15	0.89	0.11	-0.79	41,51,53,54	0
6	CA	A	606	1/1	0.99	0.07	-2.00	19,19,19,19	0
5	IOD	A	607	1/1	0.96	0.05	-2.45	53,53,53,53	0
5	IOD	A	609	1/1	0.99	0.03	-2.48	58,58,58,58	0
5	IOD	A	610	1/1	0.98	0.04	-3.10	58,58,58,58	0
5	IOD	A	615	1/1	1.00	0.04	-3.22	27,27,27,27	0
5	IOD	A	616	1/1	0.99	0.05	-3.64	36,36,36,36	0
5	IOD	A	608	1/1	0.99	0.03	-	40,40,40,40	0
3	NAG	A	604	14/15	0.76	0.24	-	49,59,63,64	0
5	IOD	A	617	1/1	0.98	0.04	-	58,58,58,58	0
5	IOD	A	614	1/1	0.94	0.05	-	58,58,58,58	1
7	ZN	A	618	1/1	0.96	0.06	-	45,45,45,45	0
5	IOD	A	612	1/1	0.95	0.05	-	53,53,53,53	1
5	IOD	A	611	1/1	0.98	0.07	-	71,71,71,71	0
3	NAG	A	596	14/15	0.76	0.27	-	53,67,77,86	0
5	IOD	A	613	1/1	0.95	0.04	-	74,74,74,74	1
12	EDO	A	624	4/4	0.88	0.18	-	28,32,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.