Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:58 PM GMT

PDB ID	:	4QJQ
Title	:	Crystal structure of goat lactoperoxidase in complex with octopamine at 2.1 Angstrom resolution
Authors	:	Singh, R.P.; Kushwaha, G.S.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2014-06-04
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

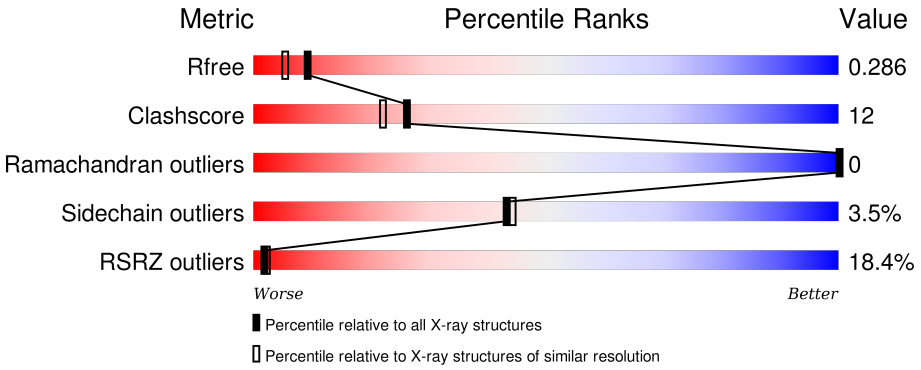
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	18% 83% 16%

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
5	IOD	A	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	OTR	A	614	-	-	X	-
8	PEG	A	615	-	-	-	X
9	EDO	A	624	-	-	-	X

2 Entry composition

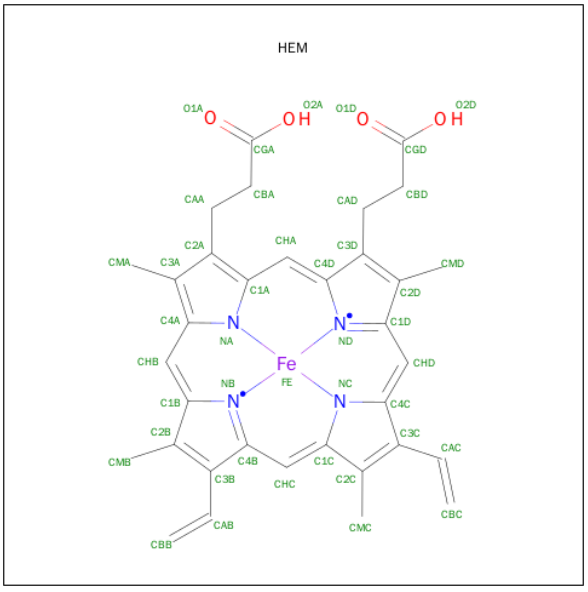
There are 10 unique types of molecules in this entry. The entry contains 5216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

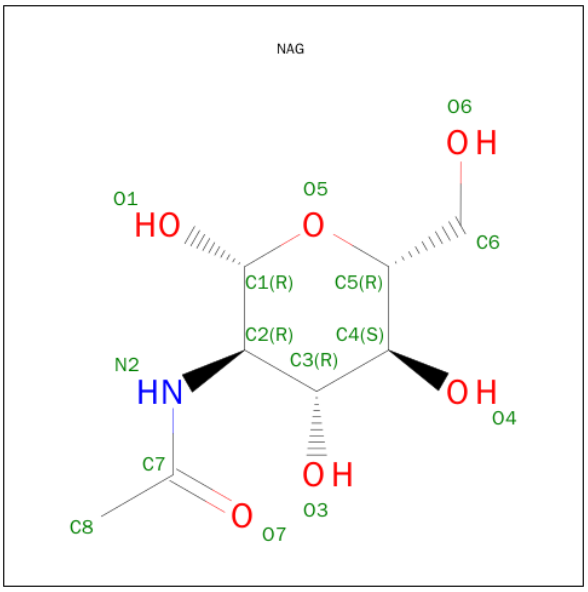
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4758	3021	844	866	1	26	0	0	0

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- 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 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0

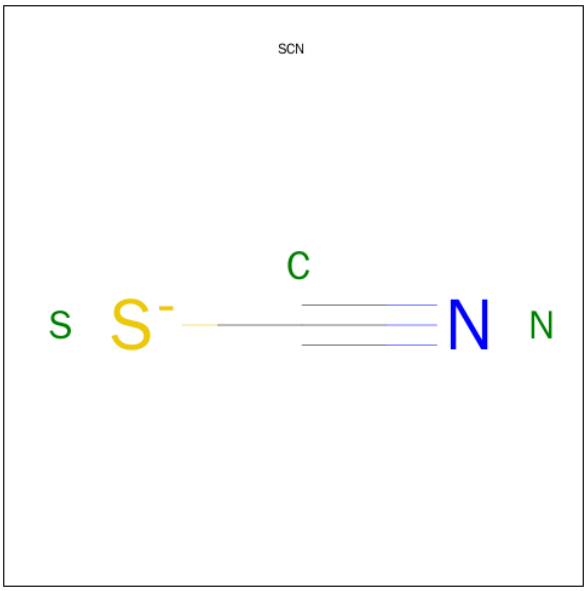
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

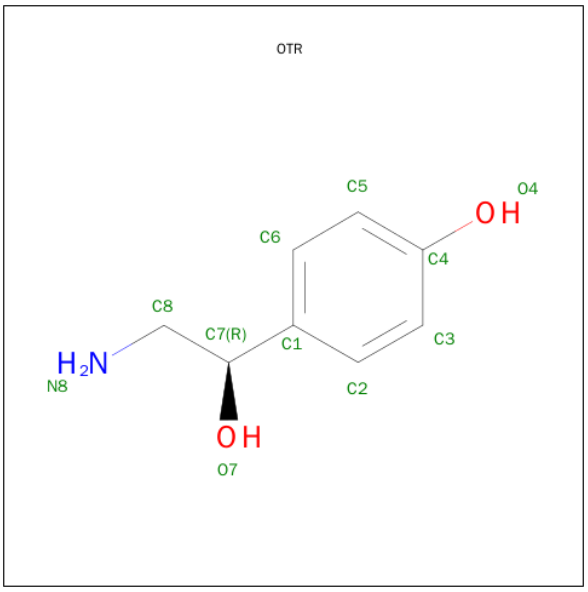
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	13	Total I 13 13	0	0

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



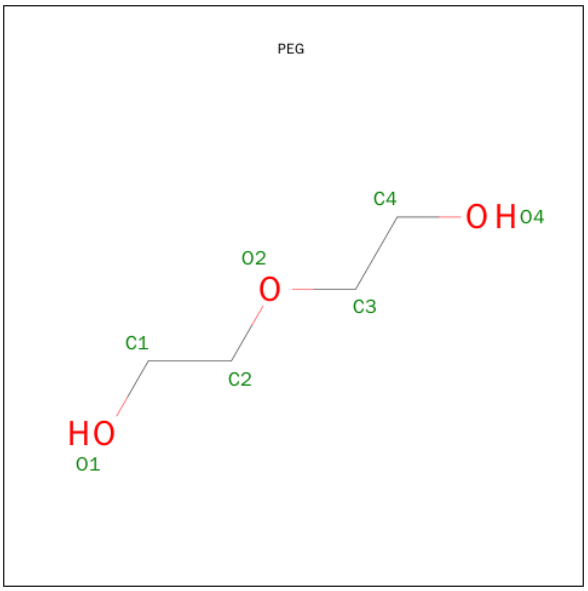
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	S		
6	A	1	3	1	1	1	0	0

- Molecule 7 is 4-(2R-AMINO-1-HYDROXYETHYL)PHENOL (three-letter code: OTR) (formula: $C_8H_{11}NO_2$).



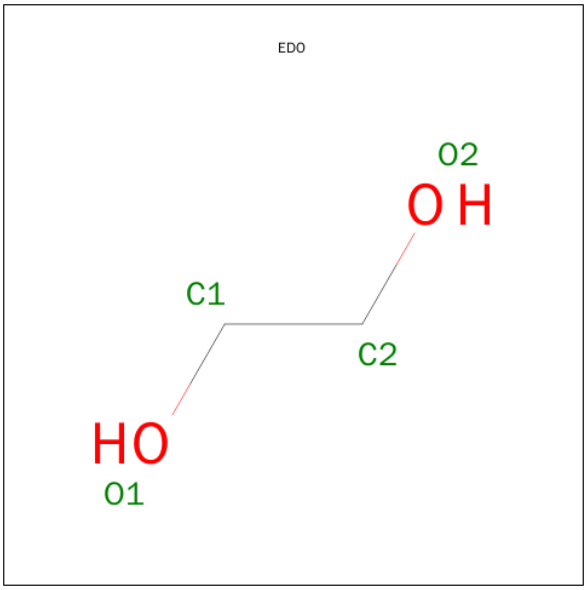
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	11	8	1	2	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is water.

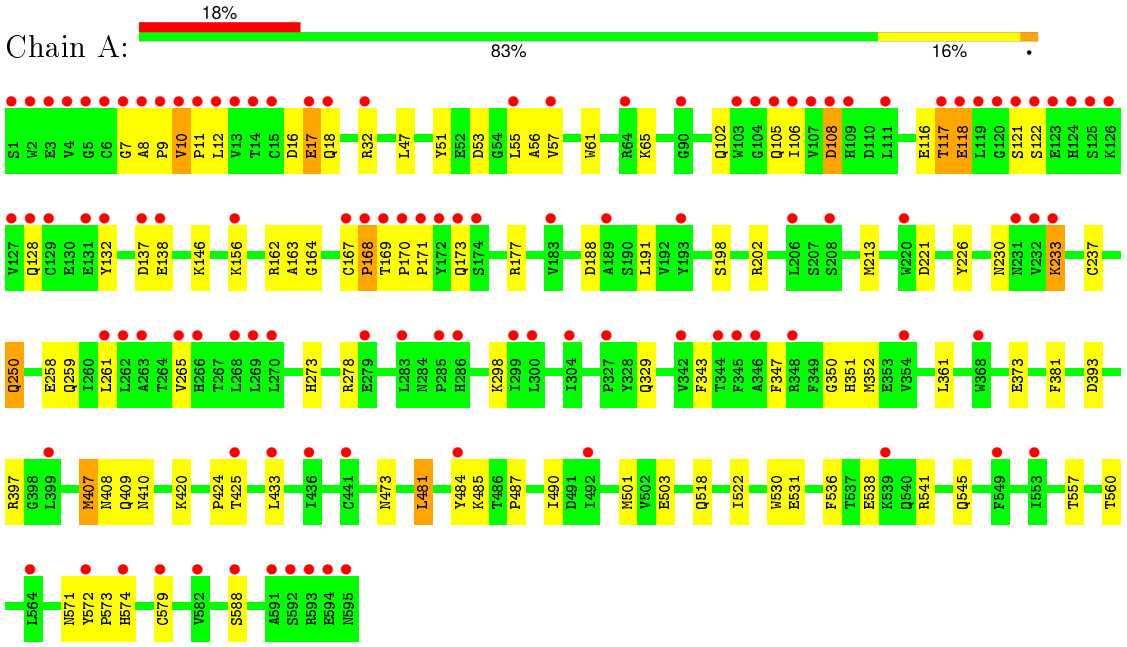
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	309	Total O 309 309	0	0

3 Residue-property plots (i)

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

- Molecule 1: Lactoperoxidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.95Å 80.36Å 75.39Å 90.00° 102.81° 90.00°	Depositor
Resolution (Å)	73.51 – 2.10 33.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (73.51-2.10) 99.2 (33.86-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.204 , 0.278 0.220 , 0.286	Depositor DCC
R_{free} test set	1834 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.922	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 36652 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SCN, NAG, SEP, CA, EDO, PEG, HEM, OTR, 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	0.63	1/4876 (0.0%)	0.77	3/6621 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	N-CD	5.03	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	188	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	10	VAL	C-N-CD	-5.03	109.54	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	4758	0	4644	111	0
2	A	43	0	30	14	0
3	A	56	0	52	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	13	0	0	2	0
6	A	3	0	0	0	0
7	A	11	0	10	9	0
8	A	14	0	20	1	0
9	A	8	0	12	2	0
10	A	309	0	0	19	0
All	All	5216	0	4768	119	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 12.

All (119) 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:53:ASP:CG	1:A:55:LEU:HB2	1.45	1.37
1:A:258:GLU:OE2	2:A:601:HEM:HMB3	1.45	1.15
1:A:108:ASP:OD2	2:A:601:HEM:HMD1	1.46	1.15
1:A:484:TYR:CE1	1:A:490:ILE:HA	1.91	1.05
1:A:108:ASP:OD2	2:A:601:HEM:CMD	2.06	1.02
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.40	1.02
1:A:53:ASP:OD1	1:A:55:LEU:HB2	1.63	0.99
1:A:53:ASP:CG	1:A:55:LEU:CB	2.31	0.98
1:A:51:TYR:CG	1:A:55:LEU:O	2.22	0.91
1:A:138:GLU:O	1:A:162:ARG:HG3	1.74	0.88
1:A:53:ASP:OD2	1:A:55:LEU:CB	2.22	0.87
1:A:258:GLU:HG3	7:A:614:OTR:C3	2.05	0.85
1:A:53:ASP:OD2	1:A:55:LEU:HB2	1.75	0.83
1:A:258:GLU:OE2	2:A:601:HEM:CMB	2.29	0.80
1:A:10:VAL:HB	1:A:11:PRO:HA	1.64	0.80
1:A:51:TYR:CB	1:A:55:LEU:O	2.30	0.80
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.11	0.79
1:A:53:ASP:OD1	1:A:55:LEU:CB	2.29	0.78
5:A:621:IOD:I	10:A:993:HOH:O	2.70	0.77
1:A:258:GLU:HG3	7:A:614:OTR:C2	2.14	0.77
1:A:156:LYS:NZ	10:A:981:HOH:O	2.17	0.77
1:A:572:TYR:CG	1:A:573:PRO:HA	2.20	0.76
1:A:258:GLU:HG3	7:A:614:OTR:H3	1.67	0.76
1:A:572:TYR:CD2	1:A:573:PRO:HA	2.20	0.74
1:A:258:GLU:CG	7:A:614:OTR:H3	2.18	0.74
1:A:53:ASP:OD2	1:A:55:LEU:HB3	1.93	0.69
2:A:601:HEM:CHA	10:A:937:HOH:O	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:HA3	2:A:601:HEM:CAC	2.23	0.68
1:A:51:TYR:CD2	1:A:55:LEU:O	2.46	0.68
1:A:137:ASP:CB	10:A:925:HOH:O	2.40	0.68
1:A:137:ASP:HB2	10:A:925:HOH:O	1.94	0.68
1:A:278:ARG:NH1	10:A:827:HOH:O	2.26	0.67
1:A:484:TYR:CZ	1:A:490:ILE:HA	2.30	0.67
1:A:132:TYR:HE2	10:A:736:HOH:O	1.78	0.66
1:A:230:ASN:HB2	1:A:250:GLN:HG2	1.78	0.65
1:A:381:PHE:HZ	7:A:614:OTR:H81	1.60	0.64
1:A:481:LEU:O	1:A:485:LYS:HA	1.97	0.64
1:A:484:TYR:CD2	1:A:490:ILE:HG12	2.33	0.64
1:A:106:ILE:HG13	1:A:265:VAL:HG11	1.81	0.63
1:A:230:ASN:HB2	1:A:250:GLN:CG	2.30	0.62
1:A:102:GLN:HG3	1:A:265:VAL:HG21	1.82	0.61
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.35	0.61
1:A:261:LEU:O	1:A:265:VAL:HG23	2.02	0.60
1:A:407:MET:SD	1:A:408:ASN:N	2.75	0.59
1:A:409:GLN:OE1	1:A:473:ASN:ND2	2.34	0.58
1:A:105:GLN:HG3	2:A:601:HEM:C1C	2.40	0.57
1:A:381:PHE:CZ	7:A:614:OTR:H81	2.40	0.56
1:A:7:GLY:N	1:A:167:CYS:SG	2.77	0.56
1:A:420:LYS:NZ	10:A:912:HOH:O	2.38	0.56
1:A:137:ASP:HB3	10:A:925:HOH:O	2.04	0.56
1:A:258:GLU:CB	7:A:614:OTR:H3	2.35	0.56
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.40	0.56
2:A:601:HEM:HMB1	2:A:601:HEM:CBB	2.26	0.55
1:A:258:GLU:HG3	7:A:614:OTR:H2	1.88	0.55
1:A:424:PRO:O	1:A:425:THR:OG1	2.13	0.55
1:A:53:ASP:OD1	1:A:55:LEU:CA	2.55	0.55
1:A:572:TYR:CG	1:A:573:PRO:CA	2.89	0.55
1:A:173:GLN:NE2	10:A:983:HOH:O	2.40	0.54
1:A:8:ALA:HB2	1:A:167:CYS:HB2	1.90	0.54
1:A:169:THR:HB	1:A:170:PRO:HD2	1.89	0.53
1:A:588:SER:HB2	10:A:940:HOH:O	2.10	0.53
1:A:10:VAL:CB	1:A:11:PRO:HA	2.36	0.52
1:A:393:ASP:OD1	1:A:557:THR:HB	2.09	0.52
1:A:259:GLN:HG2	2:A:601:HEM:CBB	2.40	0.51
1:A:233:LYS:HG3	1:A:233:LYS:O	2.08	0.51
1:A:116:GLU:HA	1:A:163:ALA:HA	1.92	0.51
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.93	0.51
1:A:298:LYS:HE2	1:A:536:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:O	1:A:397:ARG:NE	2.41	0.51
1:A:481:LEU:O	1:A:485:LYS:N	2.43	0.50
1:A:10:VAL:HB	1:A:11:PRO:CA	2.36	0.50
1:A:108:ASP:OD2	2:A:601:HEM:HMD2	2.06	0.50
1:A:484:TYR:CD1	1:A:490:ILE:HA	2.41	0.50
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.94	0.50
1:A:481:LEU:O	1:A:485:LYS:CA	2.59	0.49
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.46	0.49
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.42	0.49
1:A:237:CYS:HA	1:A:381:PHE:O	2.13	0.48
1:A:560:THR:HA	1:A:579:CYS:SG	2.52	0.48
1:A:57:VAL:HG13	1:A:61:TRP:CG	2.48	0.48
1:A:118:GLU:O	1:A:121:SER:HB2	2.14	0.48
1:A:16:ASP:OD1	1:A:16:ASP:C	2.52	0.48
1:A:198:SEP:P	1:A:198:SEP:H	2.36	0.48
1:A:536:PHE:O	1:A:541:ARG:NH1	2.48	0.47
1:A:588:SER:CB	10:A:940:HOH:O	2.63	0.47
1:A:329:GLN:HG2	10:A:941:HOH:O	2.14	0.47
1:A:167:CYS:O	1:A:169:THR:HG23	2.14	0.47
1:A:47:LEU:HA	8:A:616:PEG:H21	1.97	0.46
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.50	0.46
1:A:17:GLU:HG3	1:A:18:GLN:N	2.31	0.45
1:A:51:TYR:HB3	1:A:55:LEU:O	2.14	0.45
1:A:574:HIS:HB2	10:A:903:HOH:O	2.16	0.45
1:A:530:TRP:CZ2	1:A:531:GLU:HG3	2.51	0.45
1:A:56:ALA:HB1	1:A:177:ARG:HD3	2.00	0.44
1:A:433:LEU:HD13	2:A:601:HEM:HMA1	1.99	0.44
1:A:481:LEU:HD21	1:A:487:PRO:HD3	2.00	0.44
9:A:625:EDO:H11	10:A:988:HOH:O	2.17	0.44
1:A:571:ASN:N	1:A:571:ASN:HD22	2.15	0.44
1:A:424:PRO:HG2	7:A:614:OTR:H82	1.99	0.43
1:A:572:TYR:CE1	1:A:573:PRO:HB3	2.52	0.43
1:A:51:TYR:CD1	1:A:57:VAL:O	2.72	0.43
9:A:625:EDO:C1	10:A:988:HOH:O	2.65	0.43
1:A:171:PRO:HG2	1:A:173:GLN:HB2	2.00	0.43
1:A:484:TYR:O	1:A:485:LYS:HB2	2.18	0.43
1:A:53:ASP:OD1	1:A:55:LEU:N	2.53	0.42
1:A:51:TYR:HD1	1:A:57:VAL:O	2.02	0.42
1:A:373:GLU:HB2	5:A:622:IOD:I	2.90	0.42
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.41
1:A:9:PRO:CB	1:A:11:PRO:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:O	1:A:168:PRO:C	2.57	0.41
1:A:407:MET:HB3	1:A:501:MET:CE	2.50	0.41
1:A:572:TYR:C	1:A:572:TYR:CD1	2.93	0.41
1:A:137:ASP:HB3	1:A:138:GLU:H	1.66	0.41
1:A:117:THR:CG2	10:A:853:HOH:O	2.68	0.41
1:A:202:ARG:HD3	10:A:933:HOH:O	2.20	0.41
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.56	0.40
1:A:522:ILE:HD12	1:A:522:ILE:C	2.42	0.40
1:A:484:TYR:CE2	1:A:490:ILE:HG12	2.57	0.40
1:A:122:SER:HB2	10:A:797:HOH:O	2.22	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%)	564 (95%)	28 (5%)	0	100 100

There are no Ramachandran outliers to report.

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%)	498 (96%)	18 (4%)	43 44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	GLU
1	A	32	ARG
1	A	65	LYS
1	A	117	THR
1	A	118	GLU
1	A	128	GLN
1	A	146	LYS
1	A	233	LYS
1	A	250	GLN
1	A	347	PHE
1	A	352	MET
1	A	407	MET
1	A	410	ASN
1	A	481	LEU
1	A	503	GLU
1	A	538	GLU
1	A	545	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	147	ASN
1	A	250	GLN
1	A	423	GLN
1	A	545	GLN
1	A	571	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	0.69	0	8,12,14	1.52	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(^{o})	Ideal(^{o})
1	A	198	SEP	O-C-CA	-2.66	118.56	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 14 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	$\#\|Z\| > 2$
2	HEM	A	601	10	30,50,50	2.27	7 (23%)	24,82,82	2.47	11 (45%)
3	NAG	A	602	1	14,14,15	0.80	1 (7%)	15,19,21	1.25	1 (6%)
3	NAG	A	603	1	14,14,15	0.63	0	15,19,21	1.47	2 (13%)
3	NAG	A	604	1	14,14,15	0.58	0	15,19,21	1.47	1 (6%)
3	NAG	A	605	1	14,14,15	0.57	0	15,19,21	1.16	1 (6%)
6	SCN	A	613	-	2,2,2	1.20	0	1,1,1	2.20	1 (100%)
7	OTR	A	614	-	11,11,11	2.40	5 (45%)	13,14,14	1.90	2 (15%)
8	PEG	A	615	-	6,6,6	0.49	0	5,5,5	0.34	0
8	PEG	A	616	-	6,6,6	0.52	0	5,5,5	0.76	0
9	EDO	A	624	-	3,3,3	0.53	0	2,2,2	0.22	0
9	EDO	A	625	-	3,3,3	0.43	0	2,2,2	1.25	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
2	HEM	A	601	10	-	0/10/54/54	0/0/8/8
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	603	1	-	0/6/23/26	0/1/1/1
3	NAG	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	SCN	A	613	-	-	0/0/0/0	0/0/0/0
7	OTR	A	614	-	-	0/6/6/6	0/1/1/1
8	PEG	A	615	-	-	0/4/4/4	0/0/0/0
8	PEG	A	616	-	-	0/4/4/4	0/0/0/0
9	EDO	A	624	-	-	0/1/1/1	0/0/0/0
9	EDO	A	625	-	-	0/1/1/1	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C2D-C3D	-6.48	1.35	1.54
2	A	601	HEM	C2C-C1C	-6.20	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	614	OTR	C1-C7	-4.97	1.44	1.52
2	A	601	HEM	C3B-C4B	-3.65	1.48	1.51
2	A	601	HEM	C3D-C4D	-3.42	1.47	1.51
7	A	614	OTR	C3-C4	-3.28	1.32	1.38
2	A	601	HEM	C2B-C1B	-2.85	1.42	1.51
7	A	614	OTR	C2-C1	-2.69	1.34	1.39
7	A	614	OTR	O4-C4	-2.66	1.30	1.37
7	A	614	OTR	C5-C4	-2.52	1.33	1.38
3	A	602	NAG	O5-C1	-2.36	1.39	1.43
2	A	601	HEM	FE-NB	2.50	2.10	1.97
2	A	601	HEM	FE-NC	3.26	2.08	1.95

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	614	OTR	O7-C7-C1	-4.49	101.14	111.20
2	A	601	HEM	C3B-CAB-CBB	-2.90	120.01	124.46
2	A	601	HEM	C4B-CHC-C1C	-2.89	120.99	125.82
2	A	601	HEM	C3C-CAC-CBC	-2.87	120.05	124.46
7	A	614	OTR	C3-C2-C1	-2.82	118.30	121.20
3	A	603	NAG	O6-C6-C5	-2.64	102.61	111.33
2	A	601	HEM	C1D-CHD-C4C	-2.54	121.57	125.82
3	A	604	NAG	O7-C7-C8	-2.52	117.43	122.06
2	A	601	HEM	C3B-C4B-NB	-2.32	107.19	111.63
6	A	613	SCN	S-C-N	-2.20	161.10	175.94
3	A	602	NAG	C1-O5-C5	2.28	115.14	112.25
3	A	605	NAG	C1-O5-C5	2.34	115.22	112.25
2	A	601	HEM	CMD-C2D-C3D	2.82	126.82	114.35
2	A	601	HEM	C2D-C3D-C4D	2.85	106.34	101.50
3	A	603	NAG	C1-O5-C5	3.92	117.22	112.25
2	A	601	HEM	CMB-C2B-C3B	3.94	126.38	116.53
2	A	601	HEM	CMC-C2C-C3C	3.95	126.39	116.53
2	A	601	HEM	CAD-C3D-C4D	4.08	126.86	112.47
2	A	601	HEM	CAD-C3D-C2D	4.73	126.80	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	14	0
7	A	614	OTR	9	0
8	A	616	PEG	1	0
9	A	625	EDO	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	1.20	109 (18%) 2 2	37, 58, 118, 207	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	22.2
1	A	171	PRO	18.6
1	A	119	LEU	16.5
1	A	3	GLU	15.7
1	A	1	SER	14.6
1	A	55	LEU	13.4
1	A	13	VAL	13.2
1	A	168	PRO	12.5
1	A	121	SER	11.7
1	A	172	TYR	11.6
1	A	6	CYS	11.4
1	A	124	HIS	11.4
1	A	120	GLY	10.4
1	A	10	VAL	10.2
1	A	169	THR	10.1
1	A	170	PRO	8.9
1	A	122	SER	8.4
1	A	594	GLU	8.2
1	A	173	GLN	7.9
1	A	595	ASN	7.5
1	A	118	GLU	7.2
1	A	5	GLY	7.1
1	A	4	VAL	6.8
1	A	125	SER	6.3
1	A	593	ARG	6.3
1	A	127	VAL	5.9
1	A	129	CYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	5.7
1	A	592	SER	5.3
1	A	425	THR	5.2
1	A	572	TYR	5.1
1	A	132	TYR	5.0
1	A	126	LYS	4.8
1	A	107	VAL	4.6
1	A	269	LEU	4.5
1	A	9	PRO	4.3
1	A	106	ILE	4.3
1	A	7	GLY	4.2
1	A	300	LEU	4.2
1	A	231	ASN	4.2
1	A	574	HIS	3.9
1	A	17	GLU	3.9
1	A	111	LEU	3.8
1	A	484	TYR	3.8
1	A	174	SER	3.8
1	A	123	GLU	3.8
1	A	8	ALA	3.7
1	A	128	GLN	3.7
1	A	167	CYS	3.6
1	A	262	LEU	3.5
1	A	591	ALA	3.4
1	A	283	LEU	3.4
1	A	441	CYS	3.3
1	A	399	LEU	3.3
1	A	345	PHE	3.3
1	A	588	SER	3.3
1	A	11	PRO	3.3
1	A	279	GLU	3.2
1	A	18	GLN	3.2
1	A	348	ARG	3.2
1	A	208	SER	3.2
1	A	15	CYS	3.2
1	A	268	LEU	3.2
1	A	346	ALA	3.1
1	A	232	VAL	3.1
1	A	206	LEU	3.1
1	A	64	ARG	3.1
1	A	564	LEU	3.0
1	A	261	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	3.0
1	A	344	THR	2.9
1	A	492	ILE	2.9
1	A	104	GLY	2.8
1	A	265	VAL	2.8
1	A	233	LYS	2.7
1	A	117	THR	2.7
1	A	304	ILE	2.7
1	A	105	GLN	2.7
1	A	109	HIS	2.6
1	A	220	TRP	2.6
1	A	137	ASP	2.6
1	A	156	LYS	2.5
1	A	183	VAL	2.5
1	A	286	HIS	2.5
1	A	90	GLY	2.5
1	A	193	TYR	2.5
1	A	436	ILE	2.4
1	A	266	HIS	2.4
1	A	103	TRP	2.4
1	A	131	GLU	2.4
1	A	549	PHE	2.3
1	A	342	VAL	2.3
1	A	263	ALA	2.3
1	A	138	GLU	2.3
1	A	368	TRP	2.2
1	A	327	PRO	2.2
1	A	579	CYS	2.2
1	A	433	LEU	2.2
1	A	14	THR	2.1
1	A	57	VAL	2.1
1	A	354	VAL	2.1
1	A	539	LYS	2.1
1	A	299	ILE	2.1
1	A	270	LEU	2.1
1	A	582	VAL	2.1
1	A	553	ILE	2.0
1	A	285	PRO	2.0
1	A	32	ARG	2.0
1	A	108	ASP	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, 95^{th} 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	0.71	0.27	-	51,57,69,79	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
9	EDO	A	624	4/4	0.88	0.31	4.84	54,55,57,58	0
5	IOD	A	622	1/1	0.86	0.15	4.46	123,123,123,123	0
8	PEG	A	615	7/7	0.87	0.18	3.43	63,69,73,76	0
7	OTR	A	614	11/11	0.89	0.31	1.88	28,52,63,68	0
8	PEG	A	616	7/7	0.87	0.20	1.12	67,71,77,79	0
2	HEM	A	601	43/43	0.90	0.25	0.74	31,37,47,52	0
3	NAG	A	602	14/15	0.89	0.16	0.63	50,59,72,77	0
3	NAG	A	605	14/15	0.94	0.17	0.18	56,62,72,74	0
6	SCN	A	613	3/3	0.71	0.14	-0.12	62,62,83,93	0
5	IOD	A	617	1/1	0.92	0.11	-0.37	105,105,105,105	0
5	IOD	A	619	1/1	0.93	0.15	-0.43	148,148,148,148	0
5	IOD	A	607	1/1	0.99	0.12	-0.51	49,49,49,49	0
4	CA	A	606	1/1	0.97	0.13	-1.46	45,45,45,45	0
5	IOD	A	611	1/1	0.99	0.03	-1.60	88,88,88,88	0
5	IOD	A	609	1/1	0.96	0.04	-2.45	79,79,79,79	0
5	IOD	A	620	1/1	0.97	0.05	-2.74	83,83,83,83	0
5	IOD	A	608	1/1	0.97	0.06	-3.46	71,71,71,71	0
5	IOD	A	618	1/1	0.84	0.09	-	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	IOD	A	621	1/1	0.85	0.10	-	134,134,134,134	0
5	IOD	A	623	1/1	0.76	0.10	-	119,119,119,119	0
5	IOD	A	612	1/1	0.93	0.06	-	113,113,113,113	0
5	IOD	A	610	1/1	0.99	0.03	-	82,82,82,82	0
3	NAG	A	604	14/15	0.88	0.23	-	71,86,93,98	0
3	NAG	A	603	14/15	0.83	0.34	-	76,85,92,93	0
9	EDO	A	625	4/4	0.98	0.21	-	40,40,43,52	0

6.5 Other polymers

There are no such residues in this entry.