



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:24 PM GMT

PDB ID : 4LJJ
Title : Crystal Structure of the Complex of goat Lactoperoxidase with Acrylonitrile at 1.98 Å Resolution
Authors : Kumar, M.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-07-05
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

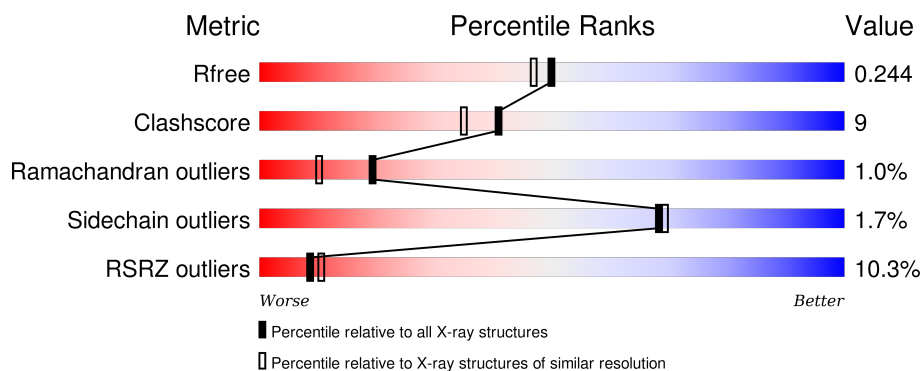
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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>10%</div> <div>83%</div> <div>15%</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
10	SCN	A	626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IOD	A	611	-	-	-	X
5	IOD	A	613	-	-	X	-
6	EDO	A	618	-	-	-	X
6	EDO	A	619	-	-	-	X
6	EDO	A	620	-	-	-	X
6	EDO	A	622	-	-	-	X
7	GOL	A	623	-	-	X	X
8	MPD	A	624	-	-	X	X

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 5248 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
			4758	3021	844	866	1	26			

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

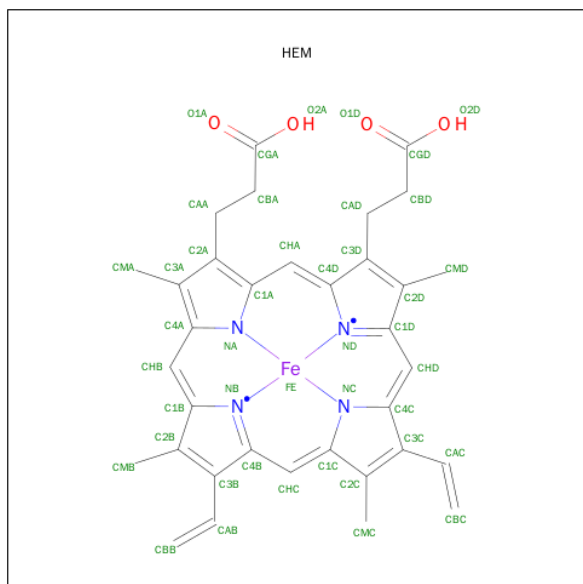


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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

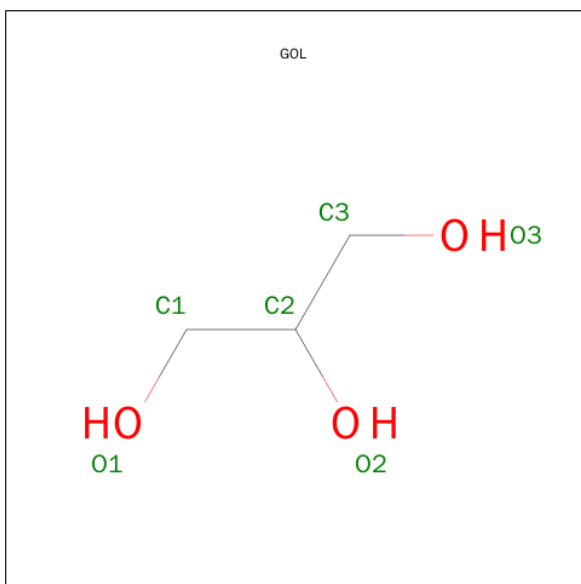
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	I	0	1
			13	13		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



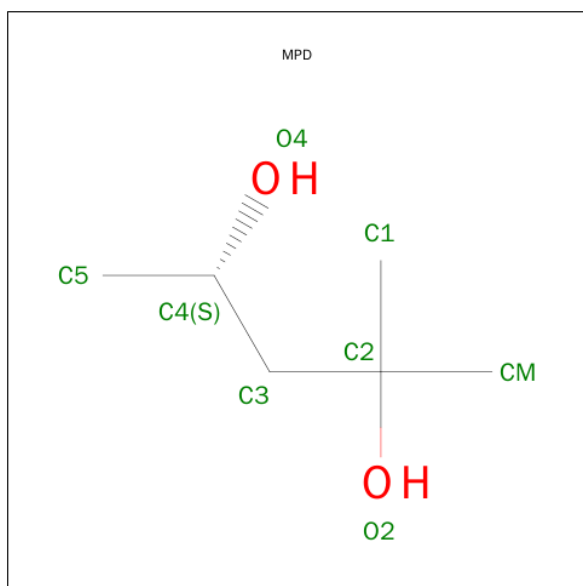
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



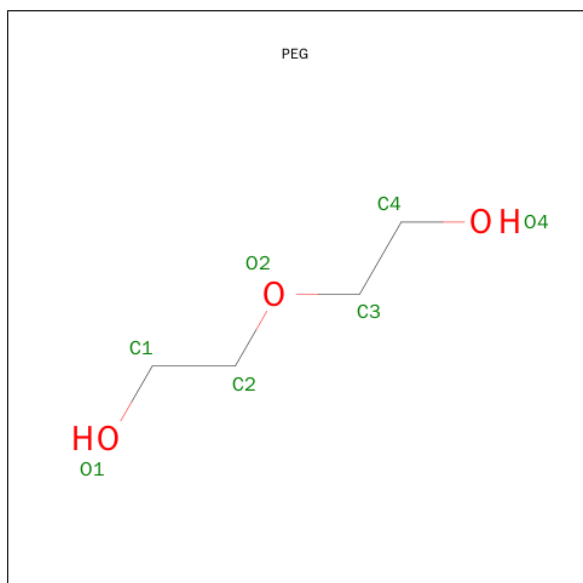
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



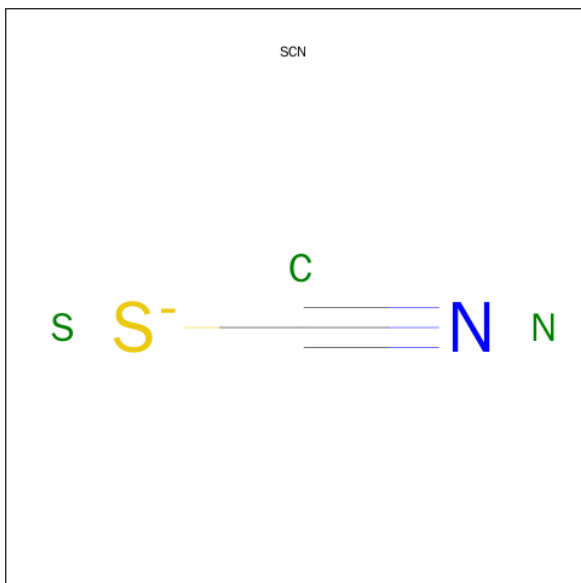
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 10 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

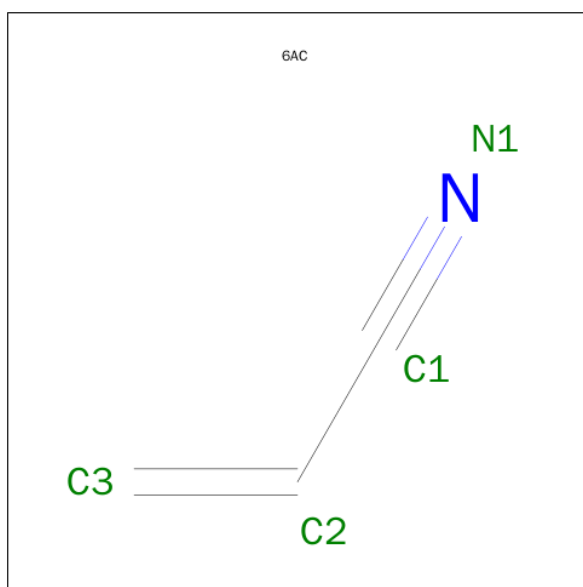


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 12 is PROP-2-ENENITRILE (three-letter code: 6AC) (formula: C₃H₃N).



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

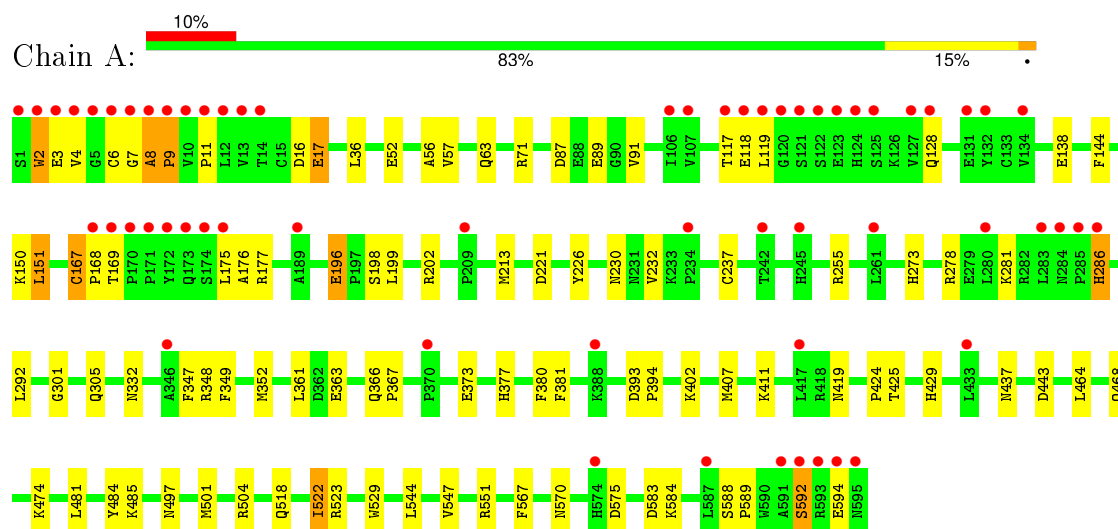
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	315	Total	O	0	1
			315	315		

3 Residue-property plots [i](#)

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

- Molecule 1: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.05Å 80.34Å 76.12Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	74.22 – 1.98 35.33 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.0 (74.22-1.98) 98.1 (35.33-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.242 0.193 , 0.244	Depositor DCC
R_{free} test set	2189 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 43538 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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, MPD, SCN, NAG, SEP, 6AC, CA, EDO, PEG, 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	0.90	1/4876 (0.0%)	0.86	5/6621 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	TRP	CD2-CE2	5.20	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	LEU	CA-CB-CG	5.27	127.41	115.30
1	A	278	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	443	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	255	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	504	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	4758	0	4642	74	0
2	A	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	0	0
4	A	43	0	30	1	0
5	A	13	0	0	5	0
6	A	20	0	28	5	0
7	A	6	0	6	4	0
8	A	8	0	14	11	0
9	A	7	0	10	0	0
10	A	3	0	0	1	0
11	A	1	0	0	0	0
12	A	4	0	3	0	0
13	A	315	0	0	3	0
All	All	5248	0	4797	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (84) 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)
8:A:624:MPD:C5	8:A:624:MPD:H12	1.39	1.32
8:A:624:MPD:C1	8:A:624:MPD:H53	1.60	1.31
1:A:202:ARG:HD3	8:A:624:MPD:H11	1.33	1.03
8:A:624:MPD:H52	8:A:624:MPD:H12	1.52	0.90
5:A:614:IOD:I	13:A:718:HOH:O	2.59	0.90
8:A:624:MPD:C1	8:A:624:MPD:C5	2.21	0.89
1:A:117:THR:HG21	1:A:138:GLU:OE1	1.75	0.86
1:A:2:TRP:CD1	1:A:175:LEU:HD13	2.16	0.81
1:A:202:ARG:HD3	8:A:624:MPD:C1	2.12	0.79
5:A:613:IOD:I	13:A:981:HOH:O	2.70	0.78
8:A:624:MPD:H53	8:A:624:MPD:H12	0.76	0.76
1:A:150:LYS:HG3	7:A:623:GOL:H12	1.74	0.67
1:A:551:ARG:HD3	1:A:583:ASP:O	1.93	0.67
1:A:419:ASN:HD21	7:A:623:GOL:H32	1.60	0.67
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.77	0.66
1:A:63:GLN:O	1:A:71:ARG:NH1	2.33	0.61
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.36	0.60
1:A:429:HIS:CE1	6:A:618:EDO:H22	2.36	0.60
1:A:196:GLU:HB3	1:A:198:SEP:O3P	2.02	0.60
1:A:424:PRO:O	1:A:425:THR:HB	2.01	0.59
1:A:36:LEU:HD23	6:A:619:EDO:H12	1.85	0.59
1:A:407:MET:HB3	1:A:501:MET:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.85	0.58
1:A:2:TRP:HB2	1:A:175:LEU:HD22	1.86	0.57
1:A:373:GLU:HG2	5:A:615:IOD:I	2.75	0.56
1:A:592:SER:OG	1:A:594:GLU:OE2	2.23	0.56
8:A:624:MPD:C1	8:A:624:MPD:H52	2.21	0.56
1:A:237:CYS:HA	1:A:381:PHE:O	2.06	0.55
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.04	0.54
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.55	0.54
1:A:144:PHE:HB2	1:A:151:LEU:HD13	1.90	0.53
1:A:407:MET:HB3	1:A:501:MET:HE3	1.91	0.53
1:A:464:LEU:HA	1:A:481:LEU:HD12	1.91	0.53
1:A:52:GLU:CG	1:A:57:VAL:HG12	2.38	0.53
1:A:419:ASN:ND2	7:A:623:GOL:H32	2.24	0.52
1:A:175:LEU:HD12	1:A:176:ALA:H	1.75	0.52
1:A:119:LEU:CD2	1:A:169:THR:HG22	2.40	0.52
1:A:419:ASN:ND2	7:A:623:GOL:H11	2.25	0.52
1:A:551:ARG:CD	1:A:583:ASP:O	2.58	0.51
8:A:624:MPD:H52	8:A:624:MPD:O2	2.09	0.51
1:A:118:GLU:OE2	1:A:118:GLU:HA	2.10	0.51
1:A:361:LEU:HD21	6:A:622:EDO:H21	1.93	0.50
1:A:8:ALA:N	1:A:9:PRO:CD	2.74	0.50
1:A:7:GLY:O	1:A:8:ALA:HB3	2.12	0.49
1:A:230:ASN:ND2	10:A:626:SCN:S	2.77	0.49
1:A:567:PHE:HB2	5:A:613:IOD:I	2.83	0.49
4:A:606:HEM:HBC2	4:A:606:HEM:HMC2	1.95	0.48
1:A:567:PHE:HD2	5:A:613:IOD:I	2.67	0.48
1:A:119:LEU:HD21	1:A:169:THR:HG22	1.95	0.47
1:A:518:GLN:O	1:A:522:ILE:HG23	2.14	0.47
1:A:522:ILE:HG13	1:A:523:ARG:N	2.29	0.47
1:A:301:GLY:O	1:A:305:GLN:HG3	2.15	0.46
1:A:361:LEU:CD2	6:A:622:EDO:H21	2.46	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.96	0.46
1:A:202:ARG:CD	8:A:624:MPD:H11	2.25	0.45
1:A:570:ASN:HD22	1:A:575:ASP:HB3	1.81	0.45
1:A:407:MET:HE3	1:A:407:MET:C	2.36	0.45
1:A:230:ASN:OD1	1:A:232:VAL:HG22	2.16	0.45
1:A:281:LYS:HD3	1:A:292:LEU:HD11	1.98	0.45
1:A:402:LYS:NZ	6:A:622:EDO:H12	2.32	0.44
1:A:352:MET:CB	1:A:407:MET:HG2	2.47	0.44
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	1:A:57:VAL:HG12	2.00	0.43
1:A:167:CYS:CB	1:A:168:PRO:CD	2.97	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.54	0.43
1:A:352:MET:HB3	1:A:407:MET:HG2	2.01	0.42
1:A:393:ASP:HB2	1:A:394:PRO:HD3	2.01	0.42
1:A:332:ASN:OD1	1:A:332:ASN:C	2.57	0.42
1:A:9:PRO:O	1:A:11:PRO:HD3	2.20	0.42
1:A:484:TYR:O	1:A:485:LYS:HB2	2.19	0.42
1:A:366:GLN:O	1:A:367:PRO:C	2.58	0.41
1:A:196:GLU:CB	1:A:198:SEP:O3P	2.68	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.85	0.41
1:A:286:HIS:N	1:A:286:HIS:ND1	2.64	0.41
1:A:199:LEU:HD12	8:A:624:MPD:H13	2.01	0.41
1:A:6:CYS:SG	1:A:7:GLY:N	2.94	0.41
1:A:551:ARG:HB3	13:A:895:HOH:O	2.21	0.41
1:A:87:ASP:OD1	1:A:89:GLU:HB2	2.20	0.41
1:A:230:ASN:ND2	1:A:232:VAL:HG22	2.36	0.41
1:A:544:LEU:O	1:A:547:VAL:HG22	2.20	0.41
1:A:2:TRP:HD1	1:A:175:LEU:HD13	1.78	0.41
1:A:16:ASP:O	1:A:17:GLU:CB	2.69	0.41
1:A:91:VAL:HG12	1:A:411:LYS:HD2	2.03	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%)	559 (94%)	27 (5%)	6 (1%)	19 10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	A	17	GLU
1	A	3	GLU
1	A	9	PRO
1	A	56	ALA

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	516/516 (100%)	507 (98%)	9 (2%)	68	69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	128	GLN
1	A	177	ARG
1	A	196	GLU
1	A	286	HIS
1	A	347	PHE
1	A	363	GLU
1	A	522	ILE
1	A	592	SER

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	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN
1	A	595	ASN

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	2.89	3 (37%)	8,12,14	4.05	6 (75%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/6/8/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	-6.16	1.30	1.51
1	A	198	SEP	P-O2P	-3.83	1.41	1.54
1	A	198	SEP	OG-CB	2.76	1.56	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	-7.76	84.21	106.56
1	A	198	SEP	O3P-P-O1P	-3.76	98.46	110.58
1	A	198	SEP	O2P-P-OG	2.71	114.36	106.56
1	A	198	SEP	O2P-P-O1P	3.09	120.53	110.58
1	A	198	SEP	OG-CB-CA	4.11	111.78	108.27
1	A	198	SEP	OG-P-O1P	4.64	118.96	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	2	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	603	1,3	14,14,15	0.70	0	15,19,21	1.10	1 (6%)
3	NAG	A	604	3	14,14,15	0.67	0	15,19,21	2.47	3 (20%)

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	603	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	604	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	NAG	C4-C3-C2	-4.97	103.50	111.23
3	A	603	NAG	O4-C4-C3	-2.30	105.16	110.34
3	A	604	NAG	C3-C4-C5	2.25	114.12	110.20
3	A	604	NAG	C1-O5-C5	7.17	121.35	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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	NAG	A	601	1	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
2	NAG	A	602	1	14,14,15	0.51	0	15,19,21	0.98	1 (6%)
2	NAG	A	605	1	14,14,15	0.52	0	15,19,21	1.39	3 (20%)
4	HEM	A	606	1,13	30,50,50	2.29	14 (46%)	24,82,82	2.80	10 (41%)
6	EDO	A	618	-	3,3,3	1.24	0	2,2,2	1.46	1 (50%)
6	EDO	A	619	-	3,3,3	0.61	0	2,2,2	0.13	0
6	EDO	A	620	-	3,3,3	0.88	0	2,2,2	0.64	0
6	EDO	A	621	-	3,3,3	0.26	0	2,2,2	0.20	0
6	EDO	A	622	-	3,3,3	1.03	0	2,2,2	1.06	0
7	GOL	A	623	-	5,5,5	2.25	2 (40%)	5,5,5	3.99	2 (40%)
8	MPD	A	624	-	6,7,7	1.36	1 (16%)	7,10,10	0.98	0
9	PEG	A	625	-	6,6,6	0.51	0	5,5,5	0.55	0
10	SCN	A	626	-	2,2,2	1.29	0	1,1,1	0.61	0
12	6AC	A	629[A]	-	2,3,3	7.01	2 (100%)	1,2,2	0.27	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	NAG	A	601	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	605	1	-	0/6/23/26	0/1/1/1
4	HEM	A	606	1,13	-	0/10/54/54	0/0/8/8
6	EDO	A	618	-	-	0/1/1/1	0/0/0/0
6	EDO	A	619	-	-	0/1/1/1	0/0/0/0
6	EDO	A	620	-	-	0/1/1/1	0/0/0/0
6	EDO	A	621	-	-	0/1/1/1	0/0/0/0
6	EDO	A	622	-	-	0/1/1/1	0/0/0/0
7	GOL	A	623	-	-	0/4/4/4	0/0/0/0
8	MPD	A	624	-	-	0/5/5/5	0/0/0/0
9	PEG	A	625	-	-	0/4/4/4	0/0/0/0
10	SCN	A	626	-	-	0/0/0/0	0/0/0/0
12	6AC	A	629[A]	-	-	0/0/1/1	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	629[A]	6AC	C2-C1	-9.66	1.25	1.42
7	A	623	GOL	O2-C2	-4.24	1.30	1.43
4	A	606	HEM	C3B-C4B	-4.07	1.48	1.51
4	A	606	HEM	C2D-C3D	-3.82	1.43	1.54
4	A	606	HEM	CAD-C3D	-3.23	1.47	1.54
4	A	606	HEM	C3B-CAB	-2.70	1.46	1.51
8	A	624	MPD	O2-C2	-2.60	1.37	1.44
4	A	606	HEM	C2C-C1C	-2.13	1.48	1.52
7	A	623	GOL	O3-C3	2.05	1.51	1.42
4	A	606	HEM	FE-NC	2.17	2.04	1.95
12	A	629[A]	6AC	C1-N1	2.23	1.20	1.14
4	A	606	HEM	CHD-C1D	2.24	1.45	1.38
4	A	606	HEM	CHC-C4B	2.31	1.45	1.38
4	A	606	HEM	C4A-CHB	2.54	1.46	1.39
4	A	606	HEM	FE-NB	2.82	2.12	1.97
4	A	606	HEM	C2A-C3A	2.90	1.46	1.37
4	A	606	HEM	CHD-C4C	3.93	1.45	1.36
4	A	606	HEM	C1C-NC	3.97	1.40	1.36
4	A	606	HEM	CHC-C1C	3.98	1.45	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	623	GOL	O2-C2-C1	-7.39	74.75	108.65
4	A	606	HEM	CBD-CAD-C3D	-3.74	102.67	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	HEM	C3B-C4B-CHC	-2.62	119.47	123.16
2	A	605	NAG	O3-C3-C4	-2.54	104.61	110.34
2	A	605	NAG	C2-N2-C7	-2.20	120.22	123.04
2	A	602	NAG	C1-O5-C5	-2.08	109.61	112.25
6	A	618	EDO	O1-C1-C2	-2.01	98.10	112.54
4	A	606	HEM	CAA-C2A-C1A	2.23	129.43	127.01
2	A	601	NAG	C1-O5-C5	2.34	115.21	112.25
4	A	606	HEM	CMD-C2D-C3D	2.93	127.29	114.35
2	A	605	NAG	O5-C5-C6	3.01	113.86	107.35
4	A	606	HEM	C1D-CHD-C4C	3.35	131.42	125.82
7	A	623	GOL	C3-C2-C1	3.95	126.60	111.12
4	A	606	HEM	C2C-C1C-NC	4.31	117.48	110.21
4	A	606	HEM	CMB-C2B-C3B	4.62	128.06	116.53
4	A	606	HEM	CAD-C3D-C4D	4.78	129.34	112.47
4	A	606	HEM	CAD-C3D-C2D	5.25	128.30	113.22
4	A	606	HEM	CMC-C2C-C3C	6.03	131.59	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	HEM	1	0
6	A	618	EDO	1	0
6	A	619	EDO	1	0
6	A	622	EDO	3	0
7	A	623	GOL	4	0
8	A	624	MPD	11	0
10	A	626	SCN	1	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%)	0.67	61 (10%) 9 10	16, 32, 94, 174	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	GLY	23.0
1	A	172	TYR	17.3
1	A	1	SER	16.2
1	A	119	LEU	13.2
1	A	122	SER	13.2
1	A	173	GLN	12.5
1	A	121	SER	11.0
1	A	12	LEU	9.8
1	A	2	TRP	9.6
1	A	4	VAL	8.9
1	A	595	ASN	8.4
1	A	120	GLY	8.4
1	A	174	SER	8.3
1	A	9	PRO	7.8
1	A	6	CYS	6.8
1	A	5	GLY	6.5
1	A	169	THR	6.4
1	A	13	VAL	5.8
1	A	171	PRO	5.6
1	A	132	TYR	5.5
1	A	593	ARG	5.3
1	A	11	PRO	5.3
1	A	594	GLU	5.1
1	A	125	SER	4.9
1	A	170	PRO	4.7
1	A	124	HIS	4.7
1	A	283	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	4.4
1	A	10	VAL	4.2
1	A	127	VAL	3.9
1	A	128	GLN	3.9
1	A	118	GLU	3.8
1	A	168	PRO	3.7
1	A	123	GLU	3.6
1	A	209	PRO	3.3
1	A	285	PRO	3.3
1	A	245	HIS	3.3
1	A	8	ALA	2.8
1	A	592	SER	2.6
1	A	433	LEU	2.6
1	A	234	PRO	2.6
1	A	574	HIS	2.5
1	A	591	ALA	2.5
1	A	587	LEU	2.5
1	A	286	HIS	2.4
1	A	280	LEU	2.4
1	A	107	VAL	2.3
1	A	14	THR	2.3
1	A	284	ASN	2.3
1	A	346	ALA	2.3
1	A	131	GLU	2.2
1	A	175	LEU	2.2
1	A	242	THR	2.2
1	A	388	LYS	2.1
1	A	261	LEU	2.1
1	A	370	PRO	2.1
1	A	189	ALA	2.1
1	A	106	ILE	2.1
1	A	417	LEU	2.0
1	A	117	THR	2.0
1	A	134	VAL	2.0

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(\AA^2)	Q<0.9
1	SEP	A	198	10/11	0.97	0.14	-	16,36,42,52	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(\AA^2)	Q<0.9
3	NAG	A	603	14/15	0.81	0.17	0.41	49,52,55,56	0
3	NAG	A	604	14/15	0.66	0.27	-	61,66,67,71	14

6.4 Ligands

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(\AA^2)	Q<0.9
6	EDO	A	618	4/4	0.93	0.32	7.58	17,19,24,36	0
6	EDO	A	620	4/4	0.68	0.21	5.98	38,41,43,45	0
6	EDO	A	619	4/4	0.84	0.21	4.34	35,48,51,57	0
8	MPD	A	624	8/8	0.82	0.27	3.91	21,38,45,50	0
5	IOD	A	611	1/1	0.98	0.14	3.14	31,31,31,31	1
10	SCN	A	626	3/3	0.79	0.16	2.97	35,35,39,47	3
7	GOL	A	623	6/6	0.93	0.14	2.86	24,26,34,36	0
6	EDO	A	622	4/4	0.90	0.15	2.32	28,33,39,40	0
2	NAG	A	602	14/15	0.71	0.19	1.77	57,63,65,68	0
4	HEM	A	606	43/43	0.97	0.18	0.92	16,20,24,27	0
6	EDO	A	621	4/4	0.85	0.21	0.46	33,35,41,49	0
9	PEG	A	625	7/7	0.81	0.30	0.16	39,57,76,77	7
5	IOD	A	608	1/1	0.98	0.10	-0.56	35,35,35,35	1
5	IOD	A	612	1/1	0.97	0.06	-0.92	55,55,55,55	1
5	IOD	A	615	1/1	0.97	0.09	-0.96	49,49,49,49	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CA	A	627	1/1	0.99	0.10	-1.62	24,24,24,24	0
5	IOD	A	630	1/1	1.00	0.05	-2.45	28,28,28,28	0
5	IOD	A	616	1/1	0.98	0.03	-2.50	53,53,53,53	1
5	IOD	A	607	1/1	0.97	0.04	-2.78	49,49,49,49	1
12	6AC	A	629[A]	4/4	0.99	0.19	-	17,17,19,19	4
2	NAG	A	601	14/15	0.66	0.35	-	57,61,63,63	0
5	IOD	A	628[B]	1/1	0.99	0.11	-	25,25,25,25	1
5	IOD	A	617	1/1	0.89	0.24	-	65,65,65,65	1
5	IOD	A	613	1/1	0.93	0.14	-	62,62,62,62	1
5	IOD	A	609	1/1	0.99	0.05	-	38,38,38,38	1
5	IOD	A	614	1/1	0.94	0.13	-	56,56,56,56	1
2	NAG	A	605	14/15	0.46	0.35	-	59,63,67,68	14
5	IOD	A	610	1/1	0.88	0.11	-	57,57,57,57	1

6.5 Other polymers ⓘ

There are no such residues in this entry.