



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 11:13 PM EST

PDB ID : 6F9V
Title : Crystal structure of human Angiotensin-1 converting enzyme N-domain in complex with Sampatrilat.
Authors : Cozier, G.E.; Acharya, K.R.
Deposited on : 2017-12-15
Resolution : 1.69 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

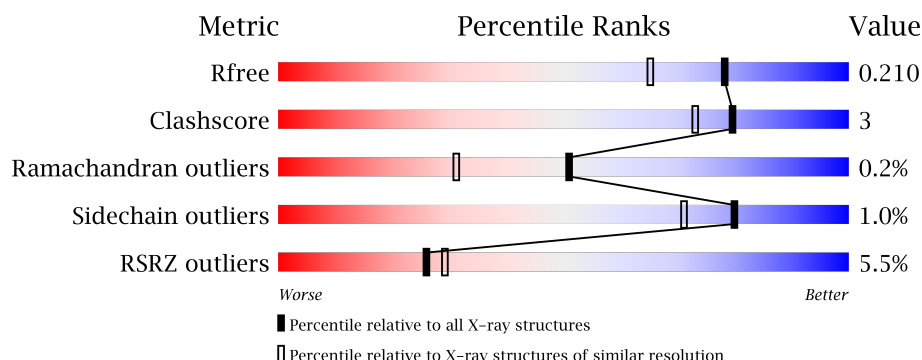
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	629	
1	B	629	

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	EDO	A	717	-	-	-	X
10	EDO	B	710	-	-	-	X
4	CL	A	703	-	-	-	X
4	CL	B	703	-	-	-	X
5	NAG	B	707	-	-	-	X
6	FUC	A	711	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 22601 atoms, of which 10587 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	97	0
			11127	3644	5432	981	1051	19			
1	B	604	Total	C	H	N	O	S	0	14	0
			9813	3216	4796	863	919	19			

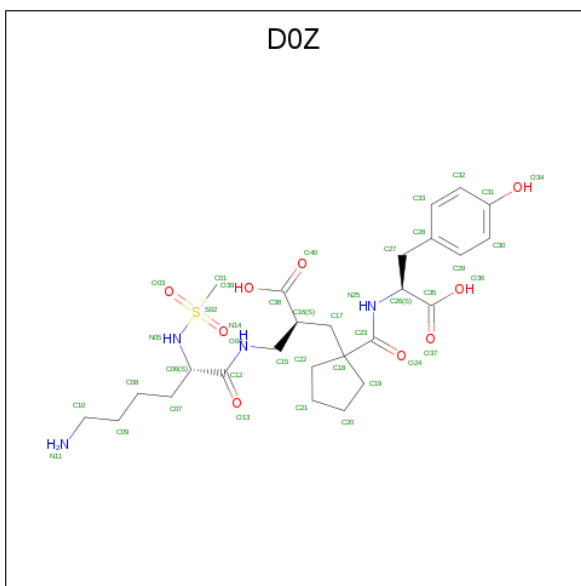
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	conflict	UNP P12821
A	25	GLN	ASN	conflict	UNP P12821
A	82	GLN	ASN	conflict	UNP P12821
A	117	GLN	ASN	conflict	UNP P12821
A	289	GLN	ASN	conflict	UNP P12821
A	545	ARG	GLN	conflict	UNP P12821
A	576	LEU	PRO	conflict	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	conflict	UNP P12821
B	25	GLN	ASN	conflict	UNP P12821
B	82	GLN	ASN	conflict	UNP P12821
B	117	GLN	ASN	conflict	UNP P12821
B	289	GLN	ASN	conflict	UNP P12821
B	545	ARG	GLN	conflict	UNP P12821
B	576	LEU	PRO	conflict	UNP P12821
B	629	LEU	-	expression tag	UNP P12821

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

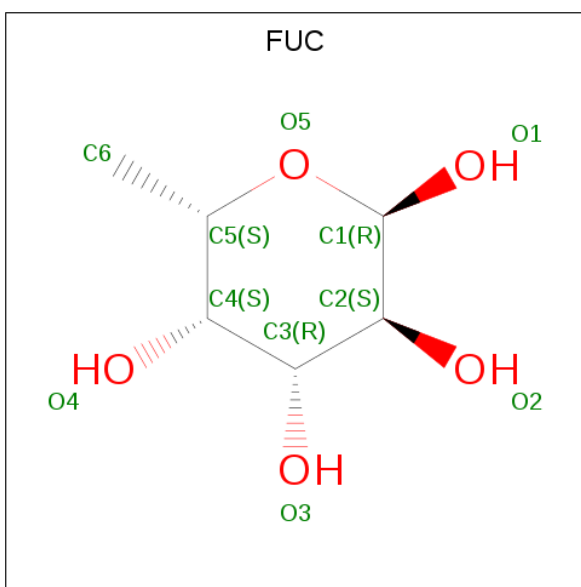
- Molecule 3 is Sampatrilat (three-letter code: D0Z) (formula: $C_{26}H_{40}N_4O_9S$).





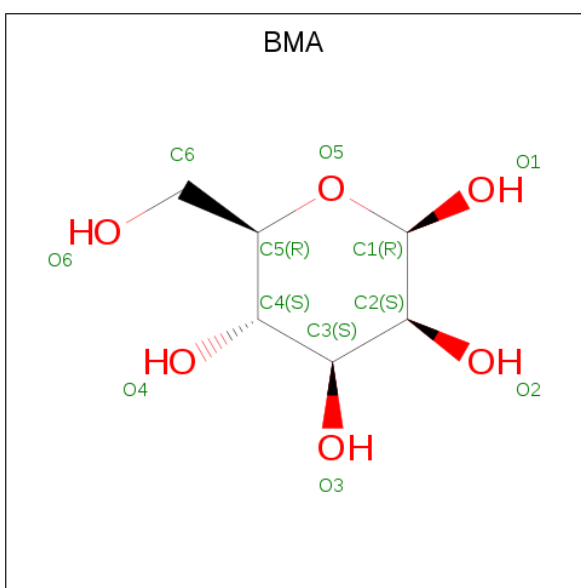
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
5	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 6 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			21	6	11	4		
6	A	1	Total	C	H	O	0	0
			20	6	10	4		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

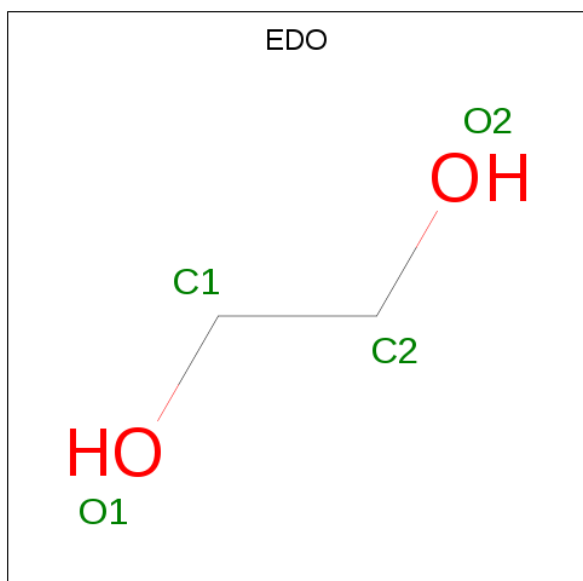


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

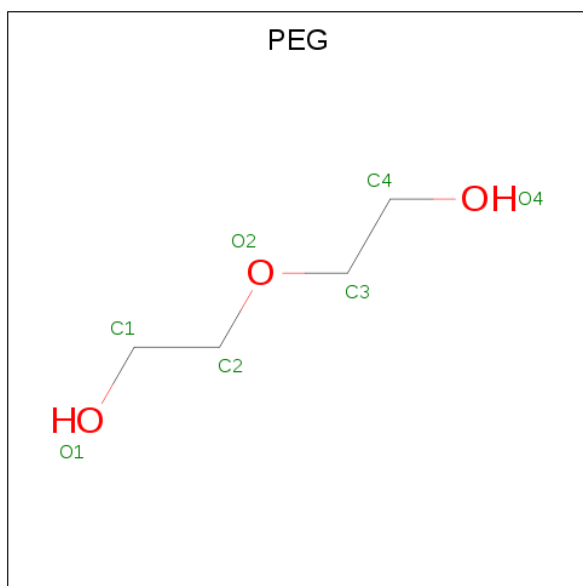
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	A	2	Total	Mg	0	0
			2	2		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



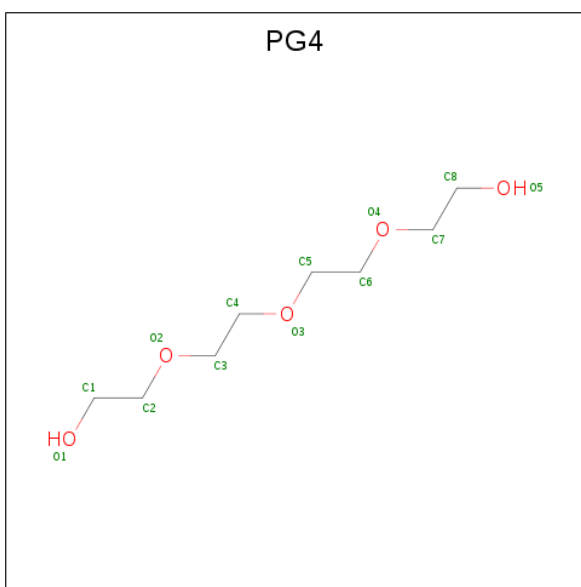
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	1
			9	2	5	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	A	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		
10	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



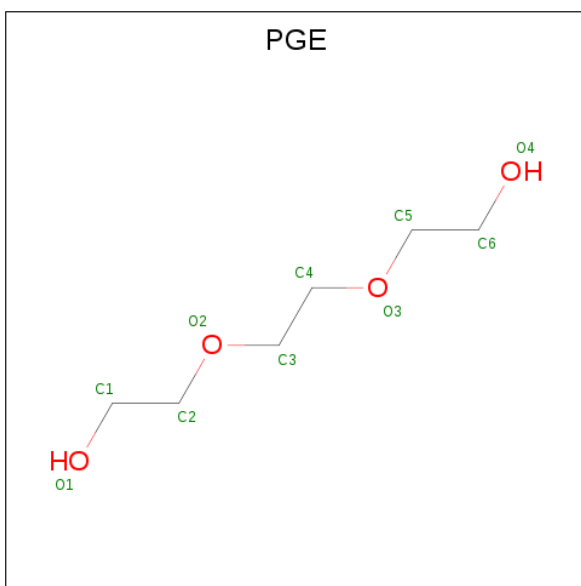
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	0	0
			17	4	10	3		
11	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			31	8	18	5		

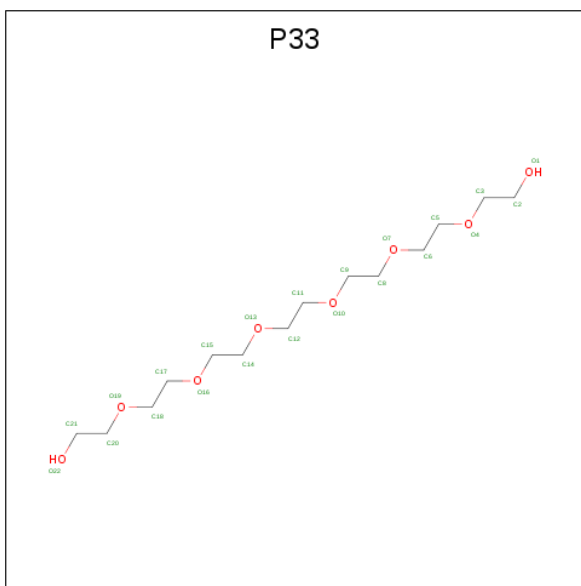
- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	H	O	0	0
			24	6	14	4		
13	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 14 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: P33)

(formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			52	14	30	8		

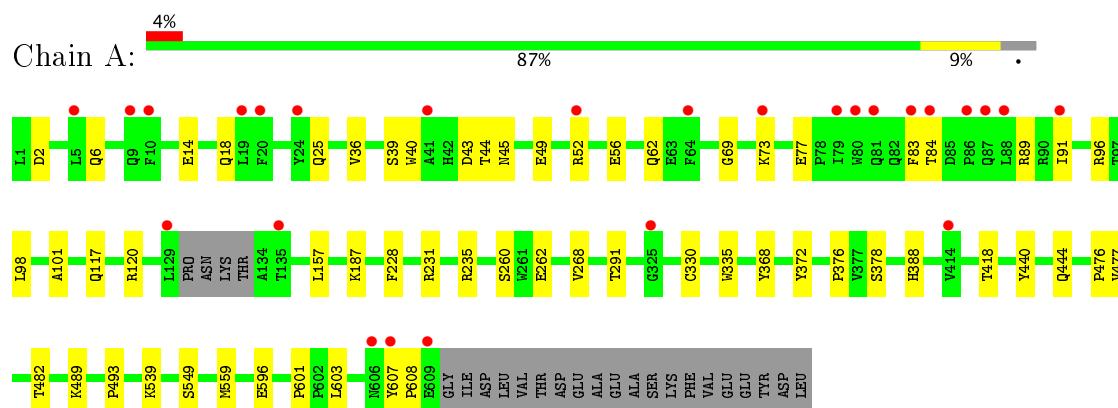
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	541	Total O 549 549	0	17
15	B	409	Total O 413 413	0	5

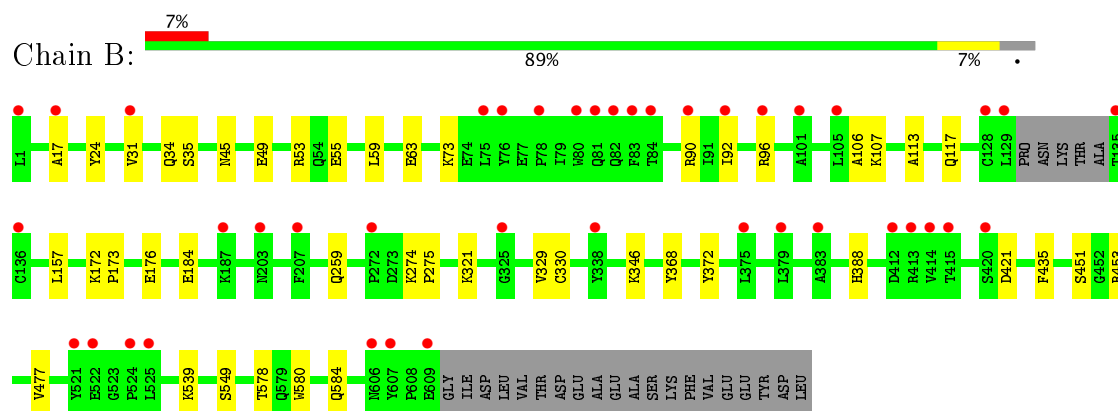
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Angiotensin-converting enzyme



• Molecule 1: Angiotensin-converting enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.22Å 77.22Å 83.11Å 88.36° 64.20° 75.29°	Depositor
Resolution (Å)	21.97 – 1.69 74.35 – 1.69	Depositor EDS
% Data completeness (in resolution range)	97.1 (21.97-1.69) 94.0 (74.35-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.183 , 0.212 0.182 , 0.210	Depositor DCC
R_{free} test set	2503 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22601	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, PGE, NAG, CL, ZN, D0Z, PG4, BMA, FUC, EDO, P33, PEG, MAN

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	0.57	0/5873	0.67	0/7993
1	B	0.51	0/5200	0.61	0/7080
All	All	0.54	0/11073	0.64	0/15073

There are no bond length outliers.

There are no bond angle outliers.

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	5695	5432	5412	42	0
1	B	5017	4796	4759	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	40	38	0	1	0
3	B	40	38	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	70	64	60	1	0
5	B	42	42	39	1	0
6	A	20	21	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	11	9	9	0	0
8	A	11	10	10	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
10	A	12	17	18	3	0
10	B	16	24	24	1	0
11	A	7	10	10	0	0
11	B	7	10	10	0	0
12	A	13	18	18	5	0
13	B	20	28	28	0	0
14	B	22	30	30	0	0
15	A	549	0	0	10	0
15	B	413	0	0	6	0
All	All	12014	10587	10447	69	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 3.

All (69) 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:B:321:LYS:O	15:B:801:HOH:O	1.98	0.80
1:A:77[B]:GLU:OE1	1:A:96[B]:ARG:NE	2.21	0.74
1:A:40[B]:TRP:CE2	1:A:44:THR:HG21	2.25	0.72
1:A:84[B]:THR:OG1	15:A:1032[B]:HOH:O	2.10	0.69
1:B:106:ALA:O	15:B:803:HOH:O	2.13	0.67
1:A:549:SER:OG	15:A:801:HOH:O	2.14	0.65
1:B:55:GLU:OE2	15:B:804:HOH:O	2.14	0.65
1:A:39[B]:SER:O	1:A:43[B]:ASP:N	2.29	0.60
1:A:98[B]:LEU:HB3	1:A:101:ALA:HB3	1.86	0.58
1:A:83[B]:PHE:O	1:A:89[B]:ARG:NH1	2.37	0.57
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.85	0.56
1:A:73[B]:LYS:NZ	15:A:805:HOH:O	2.29	0.56
1:B:329:VAL:O	1:B:346:LYS:HE2	2.05	0.55
1:A:601:PRO:O	15:A:802:HOH:O	2.18	0.55
1:A:62[B]:GLN:HG3	15:A:1144:HOH:O	2.06	0.54
1:A:91[B]:ILE:HG12	1:A:378:SER:HB2	1.91	0.53
1:B:578:THR:HG23	10:B:710:EDO:H11	1.90	0.53
1:A:418:THR:HG23	10:A:716[A]:EDO:C2	2.39	0.53
1:B:90:ARG:NH1	1:B:549:SER:O	2.37	0.53
1:A:539:LYS:HE3	1:A:559:MET:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14[B]:GLU:HB3	15:A:931[B]:HOH:O	2.10	0.52
1:B:580:TRP:O	1:B:584:GLN:HG2	2.10	0.51
1:B:73:LYS:HG3	1:B:96:ARG:HG3	1.92	0.51
1:A:40[B]:TRP:O	1:A:44:THR:N	2.28	0.50
1:B:31:VAL:O	1:B:34:GLN:HG3	2.12	0.50
1:B:49:GLU:HG3	1:B:53:ARG:CZ	2.42	0.49
1:A:73[A]:LYS:HG3	1:A:77[A]:GLU:HB2	1.94	0.49
1:A:2:ASP:O	1:A:6[B]:GLN:HG3	2.12	0.48
1:A:117:GLN:HG2	1:A:120[B]:ARG:HH22	1.79	0.47
1:A:52:ARG:NH1	1:A:56:GLU:OE2	2.47	0.47
1:B:24:TYR:OH	15:B:805:HOH:O	2.18	0.47
1:A:444[B]:GLN:NE2	15:A:816:HOH:O	2.39	0.47
1:B:59:LEU:O	1:B:63:GLU:HG3	2.15	0.47
3:B:702:D0Z:C38	3:B:702:D0Z:C22	2.94	0.46
1:B:539:LYS:HG3	15:B:1139:HOH:O	2.16	0.46
1:A:268:VAL:O	12:A:720:PG4:H42	2.14	0.46
1:B:172:LYS:O	1:B:176[A]:GLU:HG3	2.16	0.46
1:B:451:SER:OG	1:B:453:ARG:HG2	2.15	0.46
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.46	0.46
1:A:235:ARG:HH22	12:A:720:PG4:H32	1.81	0.45
1:A:418:THR:HG23	10:A:716[A]:EDO:H21	1.98	0.45
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.99	0.45
1:A:596:GLU:OE2	5:B:707:NAG:O7	2.34	0.44
1:A:330:CYS:O	15:A:803:HOH:O	2.21	0.44
1:A:489:LYS:O	1:A:493:PRO:HD2	2.18	0.44
1:B:107:LYS:NZ	1:B:184[A]:GLU:OE1	2.47	0.44
3:A:702:D0Z:C22	3:A:702:D0Z:C38	2.95	0.44
1:B:172:LYS:HB3	1:B:173:PRO:HD3	1.99	0.43
1:A:49:GLU:OE1	1:A:52:ARG:NH2	2.44	0.43
1:A:69[B]:GLY:HA3	1:A:98[B]:LEU:HD11	2.00	0.43
1:B:17:ALA:HB1	1:B:92:ILE:HD11	2.01	0.43
6:A:711:FUC:H62	15:A:1086:HOH:O	2.18	0.43
1:A:482:THR:HG21	5:A:712:NAG:O7	2.19	0.43
1:A:260[B]:SER:HB3	1:A:262[B]:GLU:OE1	2.18	0.42
1:A:418:THR:HG23	10:A:716[A]:EDO:H22	2.02	0.42
1:A:607:TYR:CG	1:A:608:PRO:HA	2.53	0.42
1:A:187:LYS:NZ	15:A:836:HOH:O	2.51	0.42
1:A:157:LEU:HD13	1:A:476:PRO:HB2	2.02	0.41
1:A:440:TYR:O	1:A:444[B]:GLN:HG2	2.21	0.41
1:B:184[B]:GLU:OE2	15:B:806:HOH:O	2.21	0.41
1:A:477:VAL:HG12	1:A:603:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:O	1:B:117:GLN:HG3	2.20	0.41
1:A:18[B]:GLN:OE1	1:A:18[B]:GLN:HA	2.19	0.41
1:A:231:ARG:HG3	12:A:720:PG4:H71	2.03	0.41
12:A:720:PG4:H51	12:A:720:PG4:H72	1.83	0.41
1:A:25[A]:GLN:OE1	1:A:376:PRO:CB	2.69	0.40
1:B:259:GLN:O	1:B:435:PHE:HA	2.21	0.40
1:A:36[B]:VAL:HG13	1:A:335:TRP:HE3	1.85	0.40
1:A:228:PHE:CZ	12:A:720:PG4:H52	2.56	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	698/629 (111%)	685 (98%)	12 (2%)	1 (0%)	55	34
1	B	614/629 (98%)	600 (98%)	13 (2%)	1 (0%)	51	31
All	All	1312/1258 (104%)	1285 (98%)	25 (2%)	2 (0%)	51	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN

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	597/541 (110%)	593 (99%)	4 (1%)	87	81
1	B	533/541 (98%)	527 (99%)	6 (1%)	78	68
All	All	1130/1082 (104%)	1120 (99%)	10 (1%)	80	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	THR
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	35	SER
1	B	330	CYS
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	D0Z	A	702	2	34,41,41	2.42	10 (29%)	39,57,57	2.32	11 (28%)
5	NAG	A	705	1	14,14,15	0.26	0	15,19,21	0.62	0
6	FUC	A	706	5	9,10,11	0.86	0	13,14,16	1.01	0
7	BMA	A	707	8,5	11,11,12	0.75	0	13,15,17	0.86	0
8	MAN	A	708	7	11,11,12	1.64	2 (18%)	13,15,17	1.59	3 (23%)
5	NAG	A	709	1,5,6	14,14,15	0.72	1 (7%)	15,19,21	0.58	0
5	NAG	A	710	5,7	14,14,15	0.70	1 (7%)	15,19,21	0.76	0
6	FUC	A	711	5	9,10,11	1.08	1 (11%)	13,14,16	0.77	0
5	NAG	A	712	1,5,6	14,14,15	0.63	0	15,19,21	0.72	0
5	NAG	A	713	5	14,14,15	0.56	0	15,19,21	0.40	0
10	EDO	A	716[A]	-	3,3,3	0.46	0	2,2,2	0.65	0
10	EDO	A	717	-	3,3,3	0.34	0	2,2,2	0.34	0
10	EDO	A	718	-	3,3,3	0.50	0	2,2,2	0.24	0
11	PEG	A	719	-	6,6,6	0.53	0	5,5,5	0.37	0
12	PG4	A	720	-	12,12,12	0.55	0	11,11,11	0.71	0
3	D0Z	B	702	2	34,41,41	2.42	10 (29%)	39,57,57	2.69	10 (25%)
5	NAG	B	705	1	14,14,15	0.48	0	15,19,21	0.42	0
5	NAG	B	706	1	14,14,15	0.61	0	15,19,21	0.65	0
5	NAG	B	707	1	14,14,15	0.52	0	15,19,21	0.65	0
10	EDO	B	709	-	3,3,3	0.54	0	2,2,2	0.23	0
10	EDO	B	710	-	3,3,3	0.54	0	2,2,2	0.11	0
10	EDO	B	711	-	3,3,3	0.52	0	2,2,2	0.26	0
10	EDO	B	712	-	3,3,3	0.46	0	2,2,2	0.32	0
13	PGE	B	713	-	9,9,9	0.27	0	8,8,8	0.48	0
13	PGE	B	714	-	9,9,9	0.31	0	8,8,8	0.43	0
11	PEG	B	715	-	6,6,6	0.47	0	5,5,5	0.28	0
14	P33	B	716	-	21,21,21	0.59	0	20,20,20	0.61	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	D0Z	A	702	2	-	0/38/55/55	0/2/2/2
5	NAG	A	705	1	-	0/6/23/26	0/1/1/1
6	FUC	A	706	5	-	0/0/17/20	0/1/1/1
7	BMA	A	707	8,5	-	0/2/19/22	0/1/1/1
8	MAN	A	708	7	-	0/2/19/22	0/1/1/1
5	NAG	A	709	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	710	5,7	-	0/6/23/26	0/1/1/1
6	FUC	A	711	5	-	0/0/17/20	0/1/1/1
5	NAG	A	712	1,5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	713	5	-	0/6/23/26	0/1/1/1
10	EDO	A	716[A]	-	-	0/1/1/1	0/0/0/0
10	EDO	A	717	-	-	0/1/1/1	0/0/0/0
10	EDO	A	718	-	-	0/1/1/1	0/0/0/0
11	PEG	A	719	-	-	0/4/4/4	0/0/0/0
12	PG4	A	720	-	-	0/10/10/10	0/0/0/0
3	D0Z	B	702	2	-	0/38/55/55	0/2/2/2
5	NAG	B	705	1	-	0/6/23/26	0/1/1/1
5	NAG	B	706	1	-	0/6/23/26	0/1/1/1
5	NAG	B	707	1	-	0/6/23/26	0/1/1/1
10	EDO	B	709	-	-	0/1/1/1	0/0/0/0
10	EDO	B	710	-	-	0/1/1/1	0/0/0/0
10	EDO	B	711	-	-	0/1/1/1	0/0/0/0
10	EDO	B	712	-	-	0/1/1/1	0/0/0/0
13	PGE	B	713	-	-	0/7/7/7	0/0/0/0
13	PGE	B	714	-	-	0/7/7/7	0/0/0/0
11	PEG	B	715	-	-	0/4/4/4	0/0/0/0
14	P33	B	716	-	-	0/19/19/19	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	D0Z	C22-C18	-6.18	1.40	1.54
3	A	702	D0Z	C22-C18	-5.16	1.43	1.54
3	A	702	D0Z	C19-C20	-3.55	1.40	1.52
3	B	702	D0Z	O13-C12	-3.42	1.16	1.23
3	B	702	D0Z	C19-C20	-3.07	1.41	1.52
5	A	710	NAG	O5-C1	-2.39	1.39	1.43
6	A	711	FUC	O5-C1	-2.31	1.39	1.43
3	A	702	D0Z	O13-C12	-2.21	1.19	1.23
5	A	709	NAG	O5-C1	-2.10	1.40	1.43
3	A	702	D0Z	O04-S02	2.29	1.47	1.43
3	A	702	D0Z	O34-C31	2.31	1.42	1.37
3	B	702	D0Z	O34-C31	2.40	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	D0Z	O04-S02	2.59	1.48	1.43
3	A	702	D0Z	C22-C21	2.60	1.61	1.52
3	B	702	D0Z	C22-C21	2.75	1.61	1.52
3	B	702	D0Z	S02-N05	3.45	1.69	1.62
8	A	708	MAN	C1-C2	3.53	1.60	1.52
3	B	702	D0Z	C23-N25	3.78	1.41	1.34
8	A	708	MAN	C2-C3	3.87	1.57	1.52
3	A	702	D0Z	S02-N05	4.75	1.72	1.62
3	B	702	D0Z	C12-N14	5.12	1.44	1.33
3	A	702	D0Z	C23-N25	5.15	1.44	1.34
3	A	702	D0Z	C12-N14	6.05	1.45	1.33
3	A	702	D0Z	C19-C18	6.36	1.68	1.54
3	B	702	D0Z	C19-C18	7.18	1.70	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	D0Z	O03-S02-O04	-12.80	99.40	118.78
3	A	702	D0Z	O03-S02-O04	-9.23	104.81	118.78
3	B	702	D0Z	C16-C15-N14	-4.74	106.41	112.29
3	A	702	D0Z	C16-C15-N14	-3.37	108.11	112.29
3	B	702	D0Z	C12-C06-N05	-2.66	103.83	110.93
3	A	702	D0Z	C07-C06-N05	-2.51	105.53	110.27
3	A	702	D0Z	C08-C07-C06	-2.45	106.21	114.01
3	B	702	D0Z	O13-C12-N14	-2.43	118.38	123.07
3	B	702	D0Z	C32-C33-C28	-2.41	117.70	121.02
3	A	702	D0Z	O24-C23-N25	-2.27	118.03	122.72
3	A	702	D0Z	C30-C29-C28	-2.26	117.90	121.02
8	A	708	MAN	O2-C2-C3	-2.17	105.91	110.17
3	B	702	D0Z	C20-C19-C18	2.12	107.51	104.95
8	A	708	MAN	O5-C1-C2	2.22	114.26	110.79
3	B	702	D0Z	C33-C28-C29	2.34	121.87	118.16
3	B	702	D0Z	C21-C22-C18	2.61	108.10	104.95
3	A	702	D0Z	C33-C28-C29	2.75	122.52	118.16
3	A	702	D0Z	O24-C23-C18	2.79	126.06	121.85
3	A	702	D0Z	O03-S02-C01	2.87	113.26	108.35
8	A	708	MAN	C1-C2-C3	3.34	113.89	109.65
3	B	702	D0Z	O03-S02-N05	3.79	113.15	107.26
3	B	702	D0Z	O04-S02-C01	3.87	114.97	108.35
3	A	702	D0Z	C22-C18-C19	4.19	107.15	102.33
3	A	702	D0Z	O04-S02-C01	4.83	116.61	108.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	D0Z	1	0
6	A	711	FUC	1	0
5	A	712	NAG	1	0
10	A	716[A]	EDO	3	0
12	A	720	PG4	5	0
3	B	702	D0Z	1	0
5	B	707	NAG	1	0
10	B	710	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	605/629 (96%)	0.48	26 (4%)	36 41	20, 28, 48, 90	0
1	B	604/629 (96%)	0.64	41 (6%)	18 21	20, 37, 65, 86	0
All	All	1209/1258 (96%)	0.56	67 (5%)	26 29	20, 32, 59, 90	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	7.8
1	B	1	LEU	5.4
1	B	414	VAL	5.4
1	B	413	ARG	5.3
1	B	129	LEU	4.2
1	B	415	THR	4.1
1	A	607	TYR	4.1
1	B	135	THR	4.1
1	B	325	GLY	4.1
1	A	80[A]	TRP	3.9
1	B	105	LEU	3.8
1	B	90	ARG	3.8
1	B	84	THR	3.8
1	B	82	GLN	3.7
1	B	78	PRO	3.7
1	A	609	GLU	3.5
1	B	81	GLN	3.5
1	A	9[A]	GLN	3.5
1	B	420	SER	3.4
1	A	73[A]	LYS	3.1
1	B	412	ASP	3.1
1	A	79[A]	ILE	3.1
1	B	609	GLU	3.1
1	B	136	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	606	ASN	3.0
1	B	375	LEU	3.0
1	B	80	TRP	2.9
1	B	524	PRO	2.9
1	B	75	LEU	2.7
1	A	91[A]	ILE	2.7
1	B	101	ALA	2.7
1	A	83[A]	PHE	2.7
1	B	31	VAL	2.7
1	A	84[A]	THR	2.7
1	A	606	ASN	2.6
1	A	5[A]	LEU	2.6
1	B	17	ALA	2.6
1	B	522	GLU	2.6
1	B	83	PHE	2.6
1	A	19[A]	LEU	2.6
1	B	76	TYR	2.5
1	B	92	ILE	2.5
1	B	128	CYS	2.4
1	A	64[A]	PHE	2.4
1	A	129	LEU	2.4
1	A	10[A]	PHE	2.3
1	B	607	TYR	2.3
1	B	272	PRO	2.3
1	B	521	TYR	2.3
1	A	414	VAL	2.3
1	A	41[A]	ALA	2.3
1	B	96	ARG	2.2
1	A	88[A]	LEU	2.2
1	B	187	LYS	2.2
1	B	525	LEU	2.2
1	A	81[A]	GLN	2.2
1	A	86[A]	PRO	2.2
1	A	135	THR	2.2
1	A	87[A]	GLN	2.2
1	A	24[A]	TYR	2.1
1	A	52	ARG	2.1
1	B	338	TYR	2.1
1	B	207	PHE	2.1
1	B	383	ALA	2.1
1	B	379	LEU	2.1
1	A	20[A]	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	203	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
10	EDO	A	717	4/4	0.95	0.24	11.09	29,34,45,45	10
4	CL	B	703	1/1	0.98	0.18	6.04	30,30,30,30	0
4	CL	A	703	1/1	1.00	0.17	5.72	22,22,22,22	0
6	FUC	A	711	10/11	0.86	0.14	4.08	51,61,79,84	0
5	NAG	B	707	14/15	0.65	0.15	3.68	46,58,71,76	0
10	EDO	B	710	4/4	0.87	0.24	2.84	30,46,50,56	10
9	MG	B	708	1/1	0.99	0.14	2.00	24,24,24,24	0
5	NAG	A	705	14/15	0.80	0.19	1.54	49,63,75,77	0
10	EDO	B	709	4/4	0.75	0.13	1.36	54,65,68,70	0
5	NAG	B	705	14/15	0.75	0.21	1.06	52,70,80,84	28
12	PG4	A	720	13/13	0.83	0.13	0.97	27,51,64,70	31
3	D0Z	B	702	40/40	0.96	0.11	0.83	18,27,42,46	0
14	P33	B	716	22/22	0.83	0.13	0.66	37,55,69,74	0
13	PGE	B	713	10/10	0.85	0.13	0.48	36,45,53,53	24
10	EDO	A	716[A]	4/4	0.88	0.17	0.15	30,38,48,58	9
5	NAG	A	712	14/15	0.91	0.11	0.14	34,47,58,65	0
13	PGE	B	714	10/10	0.93	0.10	0.09	38,47,65,66	0
3	D0Z	A	702	40/40	0.96	0.11	-0.01	19,28,41,48	0
9	MG	A	715	1/1	0.94	0.12	-0.27	35,35,35,35	0
5	NAG	A	709	14/15	0.95	0.11	-0.38	32,42,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	FUC	A	706	10/11	0.86	0.14	-0.68	34,44,55,64	21
11	PEG	B	715	7/7	0.80	0.13	-0.69	45,62,71,82	0
10	EDO	B	712	4/4	0.84	0.14	-0.78	54,65,77,82	0
11	PEG	A	719	7/7	0.89	0.13	-0.94	39,47,57,57	17
9	MG	A	714	1/1	0.97	0.08	-1.62	33,33,33,33	0
10	EDO	A	718	4/4	0.86	0.09	-2.27	48,57,67,73	0
5	NAG	A	713	14/15	0.72	0.21	-	53,76,96,100	0
10	EDO	B	711	4/4	0.92	0.07	-	47,57,62,72	0
5	NAG	A	710	14/15	0.91	0.13	-	38,54,67,69	0
2	ZN	A	701	1/1	1.00	0.14	-	21,21,21,21	0
5	NAG	B	706	14/15	0.82	0.33	-	52,76,92,99	0
2	ZN	B	701	1/1	1.00	0.15	-	22,22,22,22	0
8	MAN	A	708	11/12	0.54	0.23	-	85,106,127,132	0
7	BMA	A	707	11/12	0.61	0.19	-	63,73,88,92	0
4	CL	B	704	1/1	0.96	0.18	-	35,35,35,35	0
4	CL	A	704	1/1	0.99	0.15	-	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.