



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:37 PM GMT

PDB ID : 4TWE
Title : Structure of ligand-free N-acetylated-alpha-linked-acidic-dipeptidase like protein (NAALADaseL)
Authors : Tykvart, J.; Barinka, C.; Lubkowski, J.; Sacha, P.; Konvalinka, J.
Deposited on : 2014-06-30
Resolution : 1.75 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

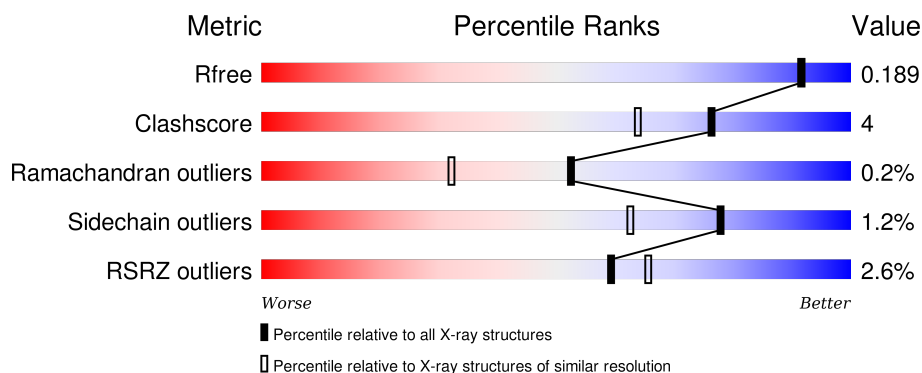
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	743	 2% 87% 8% 5%
1	B	743	 3% 88% 7% 5%

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
4	NAG	A	804	-	-	-	X
4	NAG	B	804	-	-	-	X
4	NAG	B	806	-	-	-	X
5	NAG	A	806	-	-	-	X
7	GOL	A	815	-	-	-	X
7	GOL	B	812	-	-	-	X
7	GOL	B	813	-	-	-	X
8	PEG	A	817	-	-	-	X
8	PEG	A	818	-	-	X	X
8	PEG	B	816	-	-	X	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13236 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 N-acetylated-alpha-linked acidic dipeptidase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	28	0
			5644	3572	966	1097	9			
1	B	706	Total	C	N	O	S	0	25	0
			5642	3573	967	1093	9			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9UQQ1
A	-1	LEU	-	expression tag	UNP Q9UQQ1
A	0	ASN	-	expression tag	UNP Q9UQQ1
A	1	ASP	-	expression tag	UNP Q9UQQ1
A	2	ILE	-	expression tag	UNP Q9UQQ1
A	3	PHE	-	expression tag	UNP Q9UQQ1
A	4	GLU	-	expression tag	UNP Q9UQQ1
A	5	ALA	-	expression tag	UNP Q9UQQ1
A	6	GLN	-	expression tag	UNP Q9UQQ1
A	7	LYS	-	expression tag	UNP Q9UQQ1
A	8	ILE	-	expression tag	UNP Q9UQQ1
A	9	GLU	-	expression tag	UNP Q9UQQ1
A	10	TRP	-	expression tag	UNP Q9UQQ1
A	11	HIS	-	expression tag	UNP Q9UQQ1
A	12	GLU	-	expression tag	UNP Q9UQQ1
A	13	GLY	-	expression tag	UNP Q9UQQ1
A	14	SER	-	expression tag	UNP Q9UQQ1
A	15	GLY	-	expression tag	UNP Q9UQQ1
A	16	SER	-	expression tag	UNP Q9UQQ1
A	17	GLY	-	expression tag	UNP Q9UQQ1
A	18	SER	-	expression tag	UNP Q9UQQ1
A	19	GLU	-	expression tag	UNP Q9UQQ1
A	20	ASN	-	expression tag	UNP Q9UQQ1
A	21	LEU	-	expression tag	UNP Q9UQQ1
A	22	TYR	-	expression tag	UNP Q9UQQ1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	PHE	-	expression tag	UNP Q9UQQ1
A	24	GLN	-	expression tag	UNP Q9UQQ1
A	25	GLY	-	expression tag	UNP Q9UQQ1
A	26	ARG	-	expression tag	UNP Q9UQQ1
A	27	SER	-	expression tag	UNP Q9UQQ1
B	-2	GLY	-	expression tag	UNP Q9UQQ1
B	-1	LEU	-	expression tag	UNP Q9UQQ1
B	0	ASN	-	expression tag	UNP Q9UQQ1
B	1	ASP	-	expression tag	UNP Q9UQQ1
B	2	ILE	-	expression tag	UNP Q9UQQ1
B	3	PHE	-	expression tag	UNP Q9UQQ1
B	4	GLU	-	expression tag	UNP Q9UQQ1
B	5	ALA	-	expression tag	UNP Q9UQQ1
B	6	GLN	-	expression tag	UNP Q9UQQ1
B	7	LYS	-	expression tag	UNP Q9UQQ1
B	8	ILE	-	expression tag	UNP Q9UQQ1
B	9	GLU	-	expression tag	UNP Q9UQQ1
B	10	TRP	-	expression tag	UNP Q9UQQ1
B	11	HIS	-	expression tag	UNP Q9UQQ1
B	12	GLU	-	expression tag	UNP Q9UQQ1
B	13	GLY	-	expression tag	UNP Q9UQQ1
B	14	SER	-	expression tag	UNP Q9UQQ1
B	15	GLY	-	expression tag	UNP Q9UQQ1
B	16	SER	-	expression tag	UNP Q9UQQ1
B	17	GLY	-	expression tag	UNP Q9UQQ1
B	18	SER	-	expression tag	UNP Q9UQQ1
B	19	GLU	-	expression tag	UNP Q9UQQ1
B	20	ASN	-	expression tag	UNP Q9UQQ1
B	21	LEU	-	expression tag	UNP Q9UQQ1
B	22	TYR	-	expression tag	UNP Q9UQQ1
B	23	PHE	-	expression tag	UNP Q9UQQ1
B	24	GLN	-	expression tag	UNP Q9UQQ1
B	25	GLY	-	expression tag	UNP Q9UQQ1
B	26	ARG	-	expression tag	UNP Q9UQQ1
B	27	SER	-	expression tag	UNP Q9UQQ1

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

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

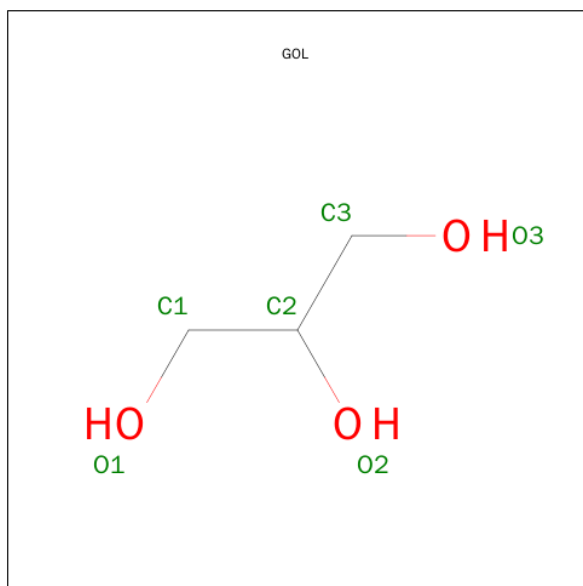
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		

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



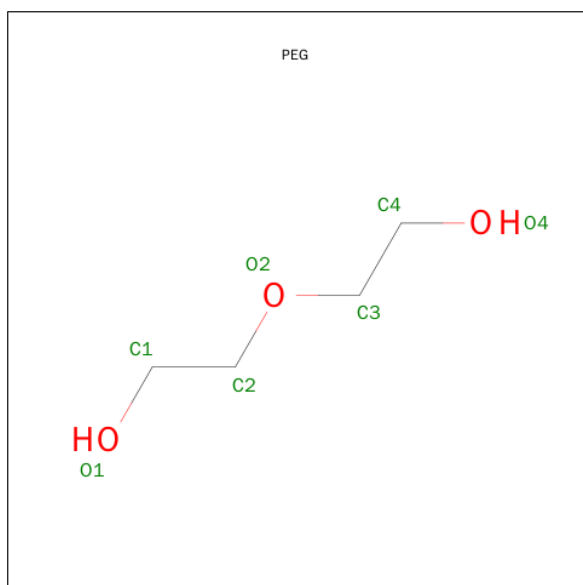
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			6	4	2		
8	B	1	Total	C	O	0	0
			7	4	3		

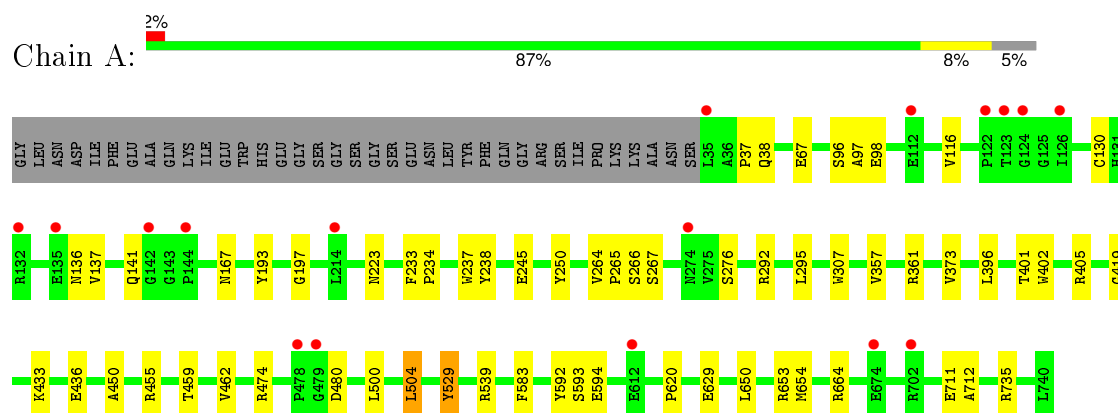
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	824	Total	O	0	4
			827	827		
9	B	803	Total	O	0	5
			806	806		

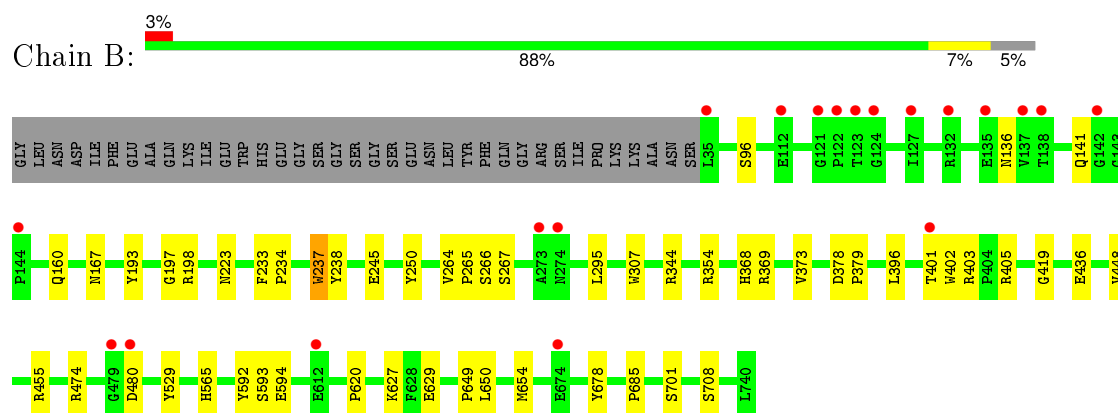
3 Residue-property plots [i](#)

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: N-acetylated-alpha-linked acidic dipeptidase-like protein



- Molecule 1: N-acetylated-alpha-linked acidic dipeptidase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.51Å 174.84Å 208.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.14 – 1.75 29.14 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.14-1.75) 98.4 (29.14-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.188 0.167 , 0.189	Depositor DCC
R_{free} test set	1757 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	7 of 176202 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.40 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9720e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, BMA, NAG, CA, PEG

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	0.94	2/5812 (0.0%)	0.87	8/7924 (0.1%)
1	B	0.94	2/5793 (0.0%)	0.88	5/7898 (0.1%)
All	All	0.94	4/11605 (0.0%)	0.88	13/15822 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	SER	CB-OG	5.54	1.49	1.42
1	A	130	CYS	CB-SG	5.51	1.91	1.82
1	A	529	TYR	CD1-CE1	5.19	1.47	1.39
1	B	708	SER	C-O	5.12	1.33	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	B	405	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	405	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	B	405	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	504	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	A	405	ARG	CG-CD-NE	-5.80	99.61	111.80
1	A	653	ARG	NE-CZ-NH2	-5.44	117.58	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	369	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	403	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	361	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	583	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	B	405	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267[B]	SER	Peptide

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	5644	0	5470	45	0
1	B	5642	0	5461	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	42	0	39	0	0
4	B	56	0	52	1	0
5	A	56	0	50	1	0
5	B	56	0	50	0	0
6	A	39	0	34	0	0
7	A	18	0	24	0	0
7	B	24	0	32	3	0
8	A	13	0	17	11	0
8	B	7	0	10	4	0
9	A	827	0	0	17	0
9	B	806	0	0	9	0
All	All	13236	0	11239	87	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 4.

All (87) 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:250[A]:TYR:HD2	9:B:1341:HOH:O	1.29	1.13
1:B:436[A]:GLU:OE2	9:B:1598:HOH:O	1.78	0.98
1:A:539[B]:ARG:NH1	9:A:1548:HOH:O	1.96	0.97
1:A:250[A]:TYR:HD2	9:A:1437:HOH:O	1.49	0.94
1:B:250[A]:TYR:CD2	9:B:1341:HOH:O	2.10	0.92
1:A:250[A]:TYR:CD2	9:A:1437:HOH:O	2.23	0.88
1:B:197:GLY:HA2	8:B:816:PEG:H11	1.58	0.86
1:A:436[A]:GLU:OE2	9:A:1611:HOH:O	1.99	0.81
1:B:198:ARG:HG3	8:B:816:PEG:H12	1.68	0.74
8:A:818:PEG:H41	9:A:1514:HOH:O	1.90	0.72
1:B:265[A]:PRO:HA	9:B:1256:HOH:O	1.89	0.72
1:A:37:PRO:HA	8:A:818:PEG:H31	1.72	0.72
1:A:620:PRO:HG2	1:B:266[A]:SER:HB2	1.73	0.70
1:B:448[B]:VAL:HG21	1:B:565:HIS:CE1	2.26	0.70
1:A:38:GLN:H	8:A:818:PEG:C2	2.09	0.66
9:A:1013:HOH:O	1:B:654[B]:MET:HG2	1.98	0.64
1:B:197:GLY:CA	8:B:816:PEG:H11	2.29	0.61
1:A:474:ARG:NH2	1:A:480[A]:ASP:O	2.34	0.61
1:A:233:PHE:CD1	1:A:234:PRO:HA	2.37	0.59
1:A:197:GLY:HA2	8:A:817:PEG:H22	1.83	0.58
1:B:396[A]:LEU:HG	1:B:402[A]:TRP:HB3	1.86	0.57
1:A:37:PRO:CA	8:A:818:PEG:H31	2.35	0.56
1:B:354[B]:ARG:HG2	1:B:354[B]:ARG:HH11	1.70	0.56
1:A:433:LYS:HE2	7:B:813:GOL:H2	1.87	0.55
1:B:198:ARG:H	8:B:816:PEG:C1	2.19	0.55
1:A:654[B]:MET:HG2	9:B:1043:HOH:O	2.08	0.53
1:B:233:PHE:CD1	1:B:234:PRO:HA	2.44	0.53
1:A:265[B]:PRO:HA	9:A:1198:HOH:O	2.07	0.53
1:A:396:LEU:HG	1:A:402[A]:TRP:HB3	1.91	0.52
1:A:116:VAL:HG23	9:A:1413:HOH:O	2.10	0.51
1:A:396:LEU:CD1	1:A:401[A]:THR:HB	2.41	0.51
1:A:136:ASN:HA	1:A:141:GLN:HB2	1.92	0.51
1:B:474:ARG:NH2	1:B:480[A]:ASP:O	2.44	0.50
1:B:448[B]:VAL:CG2	1:B:565:HIS:CE1	2.93	0.50
1:B:354[B]:ARG:CG	1:B:354[B]:ARG:HH11	2.25	0.50
1:A:37:PRO:HA	8:A:818:PEG:C3	2.40	0.49
1:A:38:GLN:H	8:A:818:PEG:H21	1.76	0.49
1:B:594:GLU:HG3	9:B:1094:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:SER:HB3	1:B:629:GLU:HG2	1.94	0.49
1:B:237:TRP:CE3	7:B:814:GOL:H31	2.48	0.48
1:A:459:THR:O	1:A:462:VAL:HG22	2.13	0.48
1:A:396:LEU:HD12	1:A:401[A]:THR:HB	1.96	0.48
1:A:500:LEU:CD2	5:A:812:NAG:H82	2.44	0.48
1:B:167:ASN:HB2	1:B:307:TRP:CD2	2.49	0.48
1:B:264:VAL:HB	1:B:265[B]:PRO:HD2	1.96	0.47
1:A:264:VAL:O	1:A:265[B]:PRO:C	2.52	0.47
1:B:136:ASN:HA	1:B:141:GLN:HB2	1.97	0.47
1:A:711[B]:GLU:HG3	1:A:712:ALA:N	2.30	0.47
1:A:96[A]:SER:HB3	9:A:1599:HOH:O	2.15	0.47
1:B:167:ASN:HB2	1:B:307:TRP:CE3	2.50	0.46
1:A:67:GLU:HG2	9:A:1634:HOH:O	2.16	0.46
1:A:97:ALA:O	1:A:98:GLU:HG2	2.16	0.45
1:B:264:VAL:O	1:B:265[A]:PRO:C	2.53	0.45
1:B:396[A]:LEU:HD12	1:B:401[A]:THR:HB	1.98	0.45
1:A:654[B]:MET:HE1	9:A:1513:HOH:O	2.16	0.45
1:B:264:VAL:HB	1:B:265[B]:PRO:CD	2.47	0.45
1:A:594:GLU:HG3	9:A:1278:HOH:O	2.17	0.45
1:B:701[B]:SER:OG	9:B:1696:HOH:O	2.21	0.44
1:A:419:GLY:HA3	9:A:1437:HOH:O	2.17	0.44
1:B:223:ASN:HA	1:B:238:TYR:CD1	2.52	0.44
1:A:37:PRO:HB3	8:A:818:PEG:H31	1.98	0.44
1:A:735:ARG:HD2	9:A:1571:HOH:O	2.17	0.44
1:A:37:PRO:CB	8:A:818:PEG:H31	2.48	0.44
1:A:593:SER:HB3	1:A:629:GLU:HG2	1.99	0.44
1:A:654[B]:MET:CE	9:A:1513:HOH:O	2.65	0.44
1:B:265[B]:PRO:O	1:B:266[B]:SER:HB2	2.18	0.44
1:B:627:LYS:NZ	9:B:1312:HOH:O	2.32	0.43
1:A:266[B]:SER:CB	1:B:620:PRO:HG2	2.48	0.43
1:A:620:PRO:HG2	1:B:266[A]:SER:CB	2.44	0.43
8:A:818:PEG:C4	9:A:1514:HOH:O	2.59	0.43
1:A:223:ASN:HA	1:A:238:TYR:CD1	2.53	0.43
1:B:419:GLY:HA3	9:B:1341:HOH:O	2.18	0.43
1:B:378:ASP:HA	1:B:379:PRO:HA	1.92	0.42
1:A:292[A]:ARG:NH2	9:A:907:HOH:O	2.52	0.42
1:A:357:VAL:HG11	8:A:818:PEG:H42	2.01	0.42
1:A:167:ASN:HB2	1:A:307:TRP:CD2	2.55	0.42
1:A:193:TYR:CE2	1:A:245:GLU:HB3	2.56	0.41
1:B:650:LEU:O	1:B:654[A]:MET:HG3	2.20	0.41
1:B:368:HIS:CE1	1:B:379:PRO:HB3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:O	1:A:137:VAL:HG12	2.21	0.41
1:B:678:TYR:CD1	1:B:685:PRO:HD3	2.56	0.41
1:B:193:TYR:CE2	1:B:245:GLU:HB3	2.55	0.41
1:B:344:ARG:CZ	7:B:812:GOL:H31	2.50	0.41
1:B:480[A]:ASP:CG	1:B:480[A]:ASP:O	2.56	0.41
1:B:354[B]:ARG:NH1	1:B:354[B]:ARG:CG	2.84	0.40
1:A:650:LEU:O	1:A:654[A]:MET:HG3	2.21	0.40
1:B:160:GLN:HB3	4:B:806:NAG:H82	2.04	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	732/743 (98%)	714 (98%)	16 (2%)	2 (0%)	46	25
1	B	729/743 (98%)	706 (97%)	22 (3%)	1 (0%)	56	36
All	All	1461/1486 (98%)	1420 (97%)	38 (3%)	3 (0%)	52	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	A	450	ALA
1	B	373	VAL

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	612/616 (99%)	605 (99%)	7 (1%)	80	66
1	B	609/616 (99%)	602 (99%)	7 (1%)	80	66
All	All	1221/1232 (99%)	1207 (99%)	14 (1%)	78	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	TRP
1	A	276	SER
1	A	295	LEU
1	A	455	ARG
1	A	504	LEU
1	A	529	TYR
1	A	592	TYR
1	B	96	SER
1	B	237	TRP
1	B	295	LEU
1	B	455	ARG
1	B	529	TYR
1	B	592	TYR
1	B	649	PRO

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](#)

11 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	$\# Z > 2$
5	NAG	A	806	1,5	14,14,15	0.55	0	15,19,21	1.21	1 (6%)
5	NAG	A	807	5	14,14,15	0.70	0	15,19,21	1.68	3 (20%)
6	NAG	A	809	1,6	14,14,15	0.63	0	15,19,21	1.20	1 (6%)
6	NAG	A	810	6	14,14,15	0.50	0	15,19,21	0.84	0
6	BMA	A	811	6	11,11,12	0.73	0	14,15,17	1.17	1 (7%)
5	NAG	A	812	1,5	14,14,15	0.82	0	15,19,21	1.42	3 (20%)
5	NAG	A	813	5	14,14,15	0.85	0	15,19,21	1.70	3 (20%)
5	NAG	B	808	1,5	14,14,15	0.59	0	15,19,21	0.81	0
5	NAG	B	809	5	14,14,15	0.58	0	15,19,21	1.10	1 (6%)
5	NAG	B	810	1,5	14,14,15	0.93	0	15,19,21	1.55	3 (20%)
5	NAG	B	811	5	14,14,15	0.97	1 (7%)	15,19,21	1.43	2 (13%)

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
5	NAG	A	806	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	807	5	-	0/6/23/26	0/1/1/1
6	NAG	A	809	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	810	6	-	0/6/23/26	0/1/1/1
6	BMA	A	811	6	-	0/2/19/22	0/1/1/1
5	NAG	A	812	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	813	5	-	0/6/23/26	0/1/1/1
5	NAG	B	808	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	809	5	-	0/6/23/26	0/1/1/1
5	NAG	B	810	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	811	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	811	NAG	O5-C1	-2.48	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	811	NAG	O4-C4-C3	-3.81	101.75	110.34
6	A	809	NAG	O7-C7-C8	-3.09	116.40	122.06
5	A	813	NAG	O4-C4-C3	-2.90	103.81	110.34
5	A	807	NAG	C3-C2-N2	-2.54	104.49	110.56
5	A	807	NAG	C3-C4-C5	-2.28	106.22	110.20
5	B	810	NAG	C6-C5-C4	-2.23	107.51	113.02
5	B	810	NAG	O6-C6-C5	-2.19	104.11	111.33
5	A	812	NAG	O7-C7-C8	-2.15	118.11	122.06
5	B	809	NAG	C1-O5-C5	2.08	114.89	112.25
5	A	812	NAG	O7-C7-N2	2.20	126.35	121.86
5	A	806	NAG	C1-O5-C5	2.50	115.43	112.25
5	B	811	NAG	C3-C4-C5	2.87	115.20	110.20
6	A	811	BMA	C1-C2-C3	2.96	113.04	109.54
5	A	812	NAG	C1-O5-C5	2.98	116.03	112.25
5	A	813	NAG	C1-O5-C5	3.34	116.48	112.25
5	A	807	NAG	C2-N2-C7	3.48	127.51	123.04
5	B	810	NAG	C1-O5-C5	3.73	116.98	112.25
5	A	813	NAG	C3-C4-C5	3.92	117.03	110.20

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
5	A	812	NAG	1	0

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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
4	NAG	A	804	1	14,14,15	0.51	0	15,19,21	1.17	1 (6%)
4	NAG	A	805	1	14,14,15	0.61	0	15,19,21	2.06	2 (13%)
4	NAG	A	808	1	14,14,15	0.62	0	15,19,21	1.59	2 (13%)
7	GOL	A	814	-	5,5,5	0.57	0	5,5,5	0.99	0
7	GOL	A	815	-	5,5,5	0.40	0	5,5,5	0.35	0
7	GOL	A	816	-	5,5,5	0.21	0	5,5,5	0.77	0
8	PEG	A	817	-	6,6,6	0.60	0	5,5,5	0.58	0
8	PEG	A	818	-	5,5,6	0.60	0	4,4,5	0.83	0
4	NAG	B	804	1	14,14,15	0.43	0	15,19,21	1.23	1 (6%)
4	NAG	B	805	1	14,14,15	0.66	0	15,19,21	1.92	2 (13%)
4	NAG	B	806	1	14,14,15	0.57	0	15,19,21	1.11	0
4	NAG	B	807	1	14,14,15	0.66	0	15,19,21	1.56	3 (20%)
7	GOL	B	812	-	5,5,5	0.33	0	5,5,5	0.39	0
7	GOL	B	813	-	5,5,5	0.35	0	5,5,5	0.33	0
7	GOL	B	814	-	5,5,5	0.29	0	5,5,5	0.90	0
7	GOL	B	815	-	5,5,5	0.30	0	5,5,5	0.76	0
8	PEG	B	816	-	6,6,6	0.63	0	5,5,5	0.49	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
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
4	NAG	A	805	1	-	0/6/23/26	0/1/1/1
4	NAG	A	808	1	-	0/6/23/26	0/1/1/1
7	GOL	A	814	-	-	0/4/4/4	0/0/0/0
7	GOL	A	815	-	-	0/4/4/4	0/0/0/0
7	GOL	A	816	-	-	0/4/4/4	0/0/0/0
8	PEG	A	817	-	-	0/4/4/4	0/0/0/0
8	PEG	A	818	-	-	0/3/3/4	0/0/0/0
4	NAG	B	804	1	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1	-	0/6/23/26	0/1/1/1
4	NAG	B	806	1	-	0/6/23/26	0/1/1/1
4	NAG	B	807	1	-	0/6/23/26	0/1/1/1
7	GOL	B	812	-	-	0/4/4/4	0/0/0/0
7	GOL	B	813	-	-	0/4/4/4	0/0/0/0
7	GOL	B	814	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	815	-	-	0/4/4/4	0/0/0/0
8	PEG	B	816	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	805	NAG	C2-N2-C7	-4.03	117.86	123.04
4	A	808	NAG	C2-N2-C7	-3.39	118.68	123.04
4	B	807	NAG	C3-C4-C5	-3.37	104.32	110.20
4	A	805	NAG	C2-N2-C7	-2.84	119.39	123.04
4	B	807	NAG	C2-N2-C7	-2.65	119.63	123.04
4	B	804	NAG	C1-O5-C5	2.01	114.79	112.25
4	A	804	NAG	C1-O5-C5	2.44	115.35	112.25
4	B	807	NAG	C1-O5-C5	2.60	115.55	112.25
4	A	808	NAG	C1-O5-C5	2.87	115.89	112.25
4	B	805	NAG	C1-O5-C5	5.33	119.02	112.25
4	A	805	NAG	C1-O5-C5	6.64	120.67	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	817	PEG	1	0
8	A	818	PEG	10	0
4	B	806	NAG	1	0
7	B	812	GOL	1	0
7	B	813	GOL	1	0
7	B	814	GOL	1	0
8	B	816	PEG	4	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	706/743 (95%)	-0.12	17 (2%) 62 69	15, 23, 39, 59	0
1	B	706/743 (95%)	-0.11	20 (2%) 56 62	14, 23, 40, 59	0
All	All	1412/1486 (95%)	-0.12	37 (2%) 59 65	14, 23, 39, 59	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	THR	9.1
1	A	35	LEU	6.6
1	B	124	GLY	6.6
1	B	35	LEU	6.4
1	A	123	THR	6.0
1	A	126	ILE	4.7
1	A	124	GLY	4.0
1	B	132	ARG	3.7
1	A	144	PRO	3.6
1	B	144	PRO	3.6
1	A	132	ARG	3.4
1	B	612	GLU	3.4
1	A	142	GLY	3.3
1	A	612	GLU	3.2
1	B	122	PRO	2.9
1	A	135	GLU	2.8
1	B	137	VAL	2.7
1	B	274	ASN	2.7
1	A	702	ARG	2.7
1	B	127	ILE	2.7
1	A	122	PRO	2.6
1	A	274	ASN	2.6
1	A	479[A]	GLY	2.6
1	B	479[A]	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	121	GLY	2.5
1	B	142	GLY	2.5
1	A	112	GLU	2.4
1	A	674[A]	GLU	2.4
1	B	135[A]	GLU	2.4
1	B	674	GLU	2.3
1	A	214	LEU	2.3
1	B	112	GLU	2.3
1	B	138	THR	2.2
1	B	273	ALA	2.2
1	A	478	PRO	2.2
1	B	480[A]	ASP	2.1
1	B	401[A]	THR	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](#)

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
5	NAG	A	806	14/15	0.95	0.14	3.31	34,38,50,50	0
5	NAG	A	812	14/15	0.93	0.11	1.42	22,26,38,41	0
5	NAG	B	810	14/15	0.95	0.13	1.12	22,27,36,40	0
6	NAG	A	809	14/15	0.97	0.07	-0.27	23,27,30,32	0
5	NAG	B	808	14/15	0.98	0.07	-0.32	22,25,29,32	0
6	BMA	A	811	11/12	0.79	0.31	-	60,64,67,67	0
6	NAG	A	810	14/15	0.93	0.16	-	34,38,45,48	0
5	NAG	B	811	14/15	0.75	0.31	-	45,53,55,56	0
5	NAG	A	807	14/15	0.66	0.49	-	60,64,69,70	0
5	NAG	B	809	14/15	0.95	0.17	-	33,39,44,44	0
5	NAG	A	813	14/15	0.73	0.33	-	50,58,60,62	0

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(Å ²)	Q<0.9
8	PEG	B	816	7/7	0.89	0.23	8.88	38,41,44,46	0
8	PEG	A	817	7/7	0.84	0.27	7.12	38,39,47,49	0
8	PEG	A	818	6/7	0.85	0.22	6.60	36,40,43,45	0
7	GOL	A	815	6/6	0.90	0.17	4.81	38,47,48,48	0
7	GOL	B	813	6/6	0.81	0.21	3.71	64,66,67,68	0
7	GOL	B	812	6/6	0.88	0.17	3.63	45,49,49,49	0
4	NAG	B	806	14/15	0.89	0.14	2.95	34,39,44,49	0
4	NAG	B	804	14/15	0.90	0.29	2.82	54,60,63,66	0
4	NAG	A	804	14/15	0.91	0.28	2.09	54,58,61,63	0
7	GOL	B	814	6/6	0.89	0.14	1.42	40,42,46,49	0
7	GOL	A	814	6/6	0.74	0.26	1.34	46,48,50,53	0
7	GOL	B	815	6/6	0.84	0.19	1.08	45,53,53,54	0
7	GOL	A	816	6/6	0.89	0.14	0.89	39,47,48,48	0
2	ZN	B	802	1/1	1.00	0.07	-1.54	20,20,20,20	0
3	CA	A	803	1/1	1.00	0.04	-1.58	17,17,17,17	0
2	ZN	A	802	1/1	0.99	0.05	-1.99	19,19,19,19	0
3	CA	B	803	1/1	1.00	0.03	-2.31	18,18,18,18	0
2	ZN	B	801	1/1	1.00	0.05	-2.48	20,20,20,20	0
2	ZN	A	801	1/1	1.00	0.02	-7.64	19,19,19,19	0
4	NAG	A	805	14/15	0.93	0.14	-	32,39,46,49	0
4	NAG	B	807	14/15	0.92	0.20	-	35,39,47,49	0
4	NAG	B	805	14/15	0.93	0.12	-	38,45,49,52	0
4	NAG	A	808	14/15	0.89	0.15	-	34,41,48,49	0

6.5 Other polymers

There are no such residues in this entry.