Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:51 PM GMT

PDB ID	:	4AQD
Title	:	Crystal structure of fully glycosylated human butyrylcholinesterase
Authors	:	Brazzolotto, X.; Wandhammer, M.; Ronco, C.; Trovaslet, M.; Jean, L.; Lockridge, O.; Renard, P.Y.; Nachon, F.
Deposited on	:	2012-04-16
Resolution	:	2.50 Å(reported)

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

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

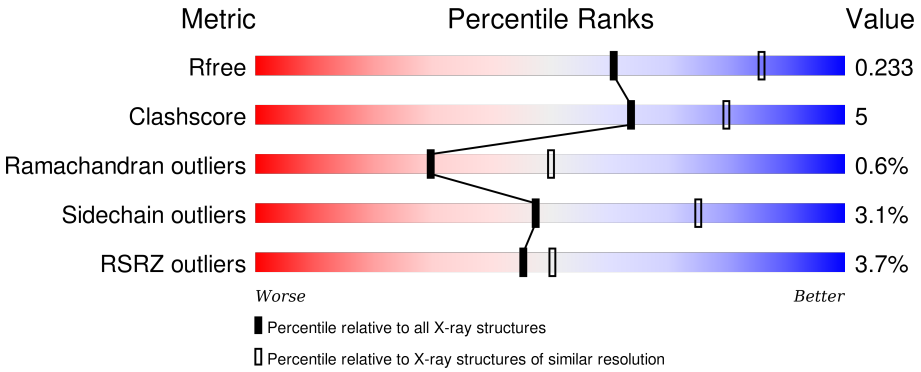
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	531	3% 87% 11%
1	B	531	4% 83% 14%

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	CL	B	1549	-	-	-	X
12	PEG	B	1530	-	-	-	X
12	PEG	B	1531	-	-	-	X
2	BAL	A	550	-	-	-	X
2	BAL	B	550	-	-	X	X
4	FUL	A	633	-	-	-	X
4	NAG	A	681	X	-	-	-
4	FUL	A	683	-	-	-	X
4	NAG	B	631	-	-	-	X
4	FUL	B	633	-	-	-	X
4	NAG	B	641	X	-	-	-
5	NAG	A	651	X	-	-	-
5	NAG	B	621	X	-	-	-
5	NAG	B	671	X	-	-	-
6	MAN	A	673	X	-	-	-
7	PG4	A	1531	-	-	-	X
8	EDO	A	1532	-	-	-	X
8	EDO	A	1536	-	-	-	X
8	EDO	A	1537	-	-	-	X
8	EDO	A	1538	-	-	-	X
8	EDO	A	1540	-	-	-	X
8	EDO	B	1532	-	-	-	X
8	EDO	B	1534	-	-	-	X
8	EDO	B	1539	-	-	-	X
8	EDO	B	1540	-	-	-	X
8	EDO	B	1541	-	-	-	X
9	UNX	A	1541	-	-	-	X
9	UNX	B	1542	-	-	-	X
9	UNX	B	1544	-	-	-	X

2 Entry composition

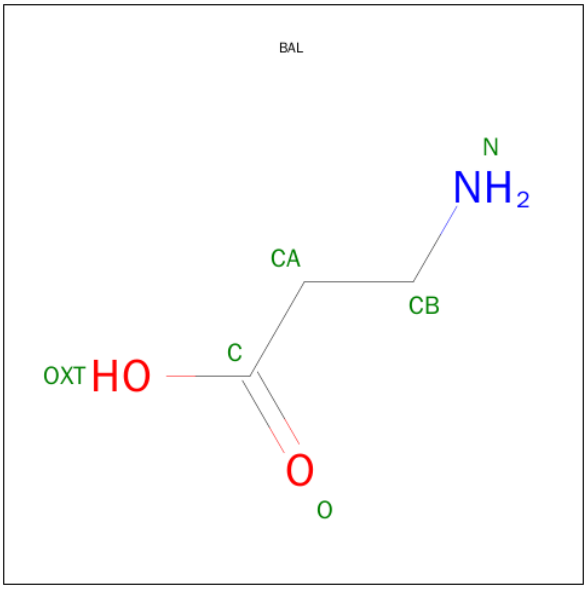
There are 13 unique types of molecules in this entry. The entry contains 9253 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BUTYRYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	12	3	0
			4222	2723	714	770	15			
1	B	526	Total	C	N	O	S	35	0	0
			4191	2704	705	767	15			

- Molecule 2 is BETA-ALANINE (three-letter code: BAL) (formula: $C_3H_7NO_2$).



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

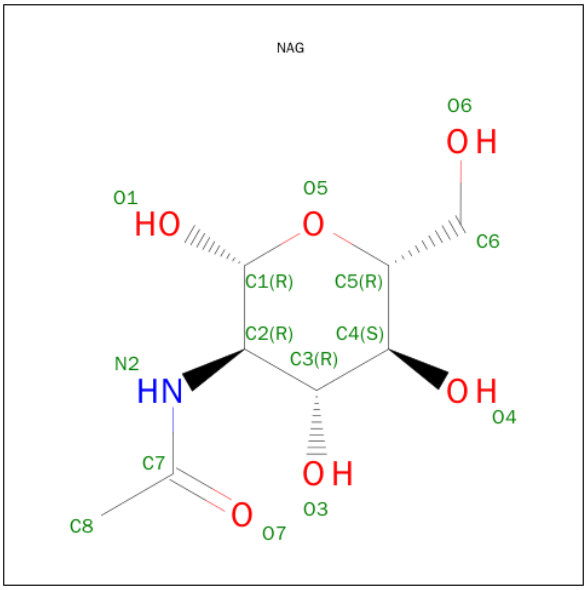
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total C N O 38 22 2 14	0	0
4	A	3	Total C N O 38 22 2 14	0	0
4	A	3	Total C N O 38 22 2 14	0	0
4	B	3	Total C N O 38 22 2 14	0	0
4	B	3	Total C N O 38 22 2 14	0	0
4	B	3	Total C N O 38 22 2 14	0	0

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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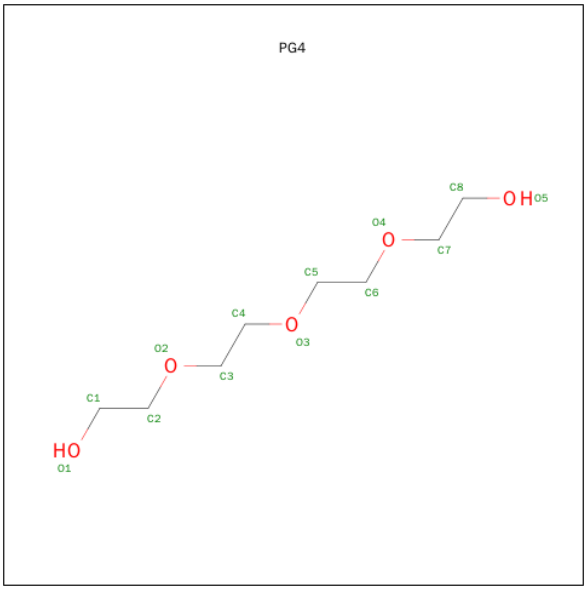
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

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

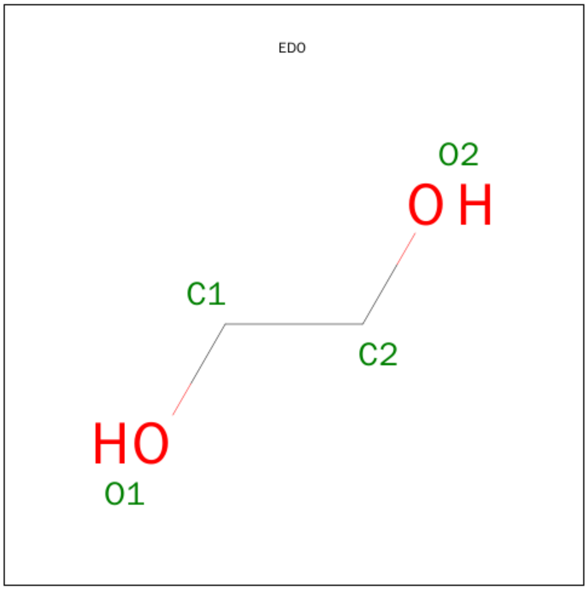
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total C N O 39 22 2 15	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

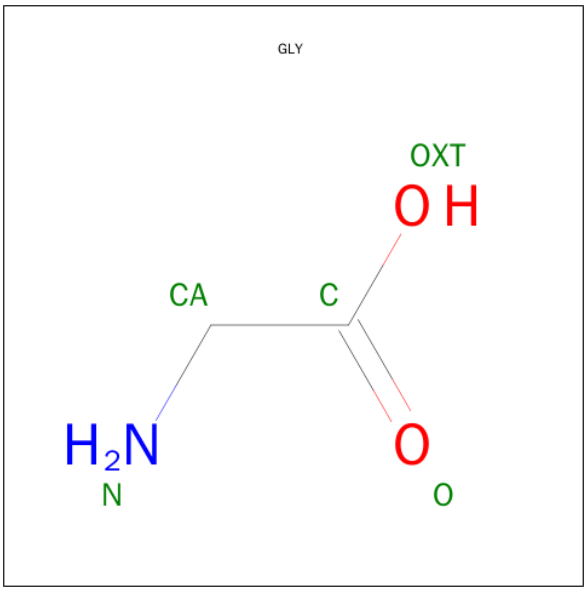
- Molecule 9 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	5	Total X 5 5	0	0
9	A	5	Total X 5 5	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

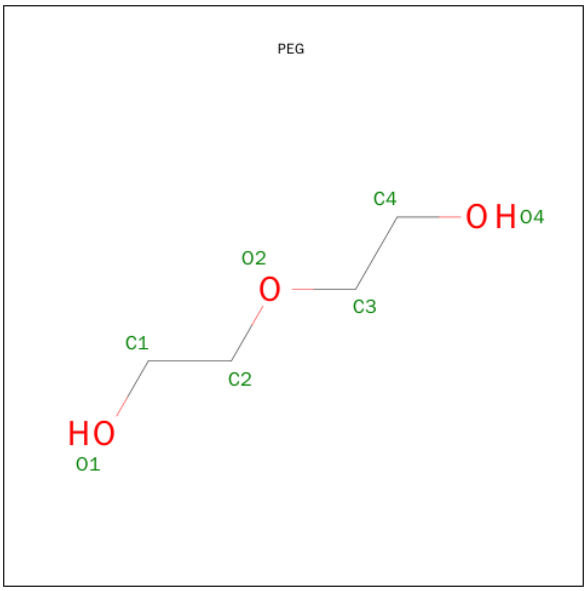
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	4	Total Cl 4 4	0	0
10	A	3	Total Cl 3 3	0	0

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 5 2 1 2	0	0
11	B	1	Total C N O 5 2 1 2	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 13 is water.

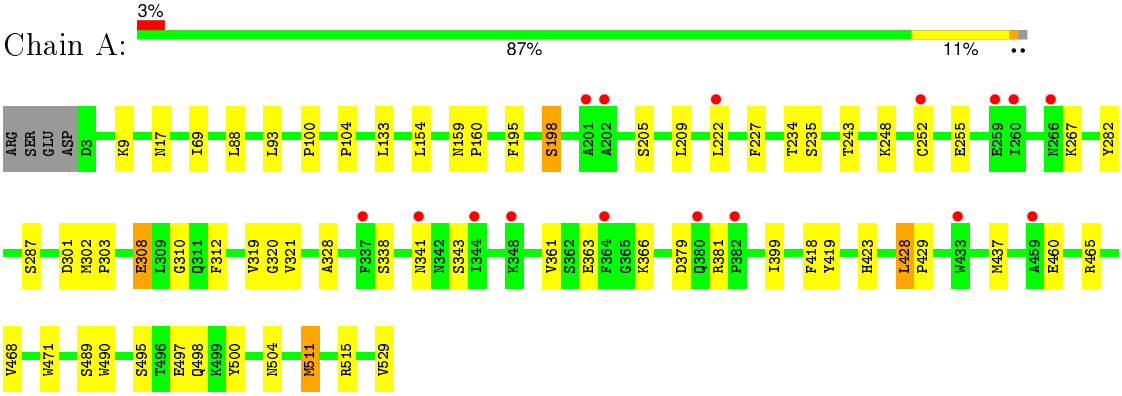
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	160	Total	O	0	0
			160	160		
13	B	118	Total	O	0	0
			118	118		

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.

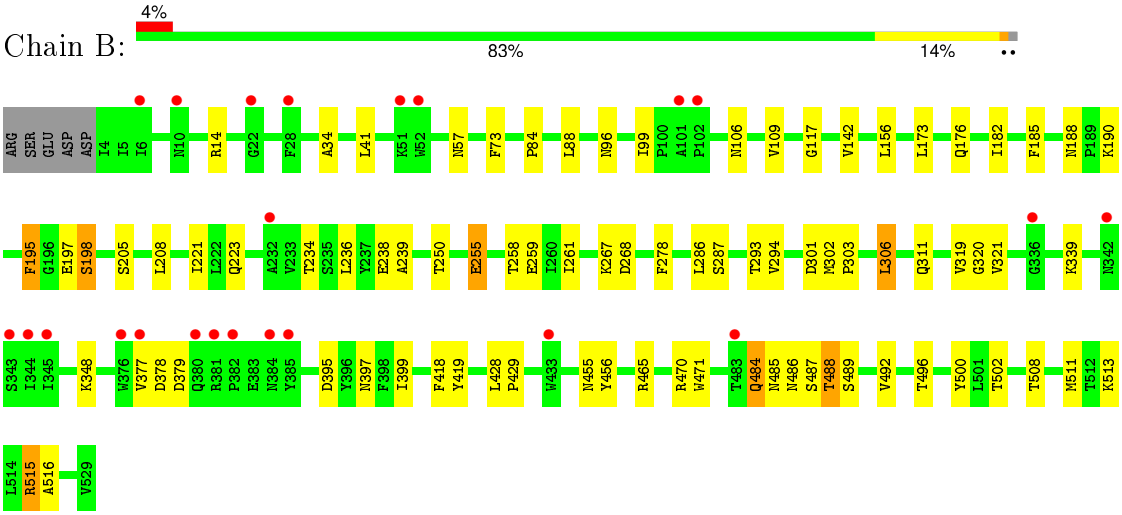
- Molecule 1: BUTYRYLCHOLINESTERASE

Chain A:



- Molecule 1: BUTYRYLCHOLINESTERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.75Å 79.26Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.50 46.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.04-2.50) 99.4 (46.17-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.232 0.164 , 0.233	Depositor DCC
R_{free} test set	1382 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 46097 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9253	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, UNX, EDO, PG4, BAL, PEG, FUL, 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	0.41	0/4351	0.57	0/5906
1	B	0.39	0/4310	0.54	0/5852
All	All	0.40	0/8661	0.56	0/11758

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
4	A	1	0
4	B	1	0
6	A	1	0
All	All	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	673	MAN	C1
4	A	681	NAG	C1
4	B	641	NAG	C1

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	4222	0	4125	37	0
1	B	4191	0	4084	52	0
2	A	6	0	6	3	0
2	B	6	0	6	5	0
3	A	56	0	50	1	0
4	A	114	0	102	1	0
4	B	114	0	102	5	0
5	A	14	0	12	0	0
5	B	70	0	64	4	0
6	A	39	0	34	0	0
7	A	26	0	36	1	0
8	A	36	0	54	1	0
8	B	40	0	60	4	0
9	A	5	0	0	0	0
9	B	5	0	0	0	0
10	A	3	0	0	1	0
10	B	4	0	0	0	0
11	A	5	0	2	0	0
11	B	5	0	2	0	0
12	B	14	0	20	2	0
13	A	160	0	0	3	0
13	B	118	0	0	1	0
All	All	9253	0	8759	92	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 5.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:SER:OG	2:A:550:BAL:C	2.07	1.01
1:B:198:SER:OG	2:B:550:BAL:C	2.08	1.00
1:B:99:ILE:HD11	1:B:185:PHE:HB3	1.66	0.76
1:A:338:SER:HB3	1:A:341:ASN:HB2	1.69	0.74
4:B:631:NAG:H61	4:B:632:NAG:HN2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLU:OE1	13:A:2145:HOH:O	2.12	0.68
1:A:465[B]:ARG:NH2	13:A:2129:HOH:O	2.17	0.68
1:B:14:ARG:NH1	1:B:57:ASN:OD1	2.27	0.67
1:B:41:LEU:HB3	8:B:1539:EDO:H11	1.77	0.66
1:B:455:ASN:O	8:B:1534:EDO:O1	2.13	0.62
1:A:504:ASN:HB2	8:A:1536:EDO:H22	1.86	0.58
1:B:250:THR:HB	1:B:267:LYS:HE2	1.87	0.57
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.40	0.57
1:B:236:LEU:HD11	1:B:294:VAL:O	2.06	0.56
1:B:255:GLU:H	1:B:255:GLU:CD	2.09	0.56
1:B:259:GLU:HG3	4:B:641:NAG:H62	1.89	0.55
1:B:205:SER:HA	1:B:208:LEU:HD12	1.88	0.54
1:A:308:GLU:HA	7:A:1531:PG4:H82	1.89	0.54
1:A:361:VAL:O	1:A:366:LYS:NZ	2.34	0.54
1:A:319:VAL:O	1:A:418:PHE:HA	2.09	0.53
1:B:198:SER:HG	2:B:550:BAL:C	2.21	0.53
4:B:631:NAG:H61	4:B:632:NAG:N2	2.24	0.53
1:A:198:SER:CB	2:A:550:BAL:C	2.87	0.52
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.44	0.52
1:B:470:ARG:NH2	1:B:488:THR:HG22	2.25	0.51
1:B:428:LEU:HD12	1:B:429:PRO:HD2	1.90	0.51
1:B:429:PRO:HD3	12:B:1531:PEG:H31	1.91	0.51
1:B:195:PHE:HB3	1:B:221:ILE:HB	1.93	0.50
1:B:156:LEU:HD12	1:B:261:ILE:HD11	1.93	0.50
1:A:301:ASP:OD1	1:A:302:MET:N	2.43	0.50
1:A:100:PRO:HG2	1:A:104:PRO:HD3	1.94	0.50
1:B:428:LEU:HA	12:B:1531:PEG:H42	1.93	0.49
1:A:328:ALA:HB2	1:A:437:MET:HE3	1.94	0.49
1:B:513:LYS:HB3	1:B:516:ALA:HB2	1.94	0.49
1:B:198:SER:CB	2:B:550:BAL:C	2.91	0.48
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.94	0.48
1:A:495:SER:O	1:A:498:GLN:NE2	2.45	0.48
1:A:154:LEU:HD11	1:A:243:THR:HG23	1.96	0.48
1:A:287:SER:O	13:A:2089:HOH:O	2.20	0.48
1:B:377:VAL:HG23	1:B:378:ASP:H	1.80	0.47
1:A:133:LEU:HD23	1:A:468:VAL:HG13	1.97	0.47
1:A:248:LYS:HD3	4:A:633:FUL:H61	1.95	0.47
1:B:502:THR:O	1:B:508:THR:HB	2.15	0.47
1:B:197:GLU:HA	1:B:223:GLN:O	2.15	0.47
1:B:484:GLN:O	1:B:486:ASN:N	2.48	0.47
1:B:198:SER:HB3	2:B:550:BAL:OXT	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:THR:HG22	1:A:235:SER:O	2.15	0.46
1:B:455:ASN:HB3	13:B:2101:HOH:O	2.15	0.46
1:B:109:VAL:HG21	1:B:182:ILE:HG12	1.97	0.46
1:A:341:ASN:HB3	1:A:343:SER:H	1.80	0.45
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.98	0.45
1:A:198:SER:HG	2:A:550:BAL:C	2.25	0.45
1:B:320:GLY:HA3	1:B:419:TYR:CE2	2.52	0.45
1:B:487:SER:OG	1:B:488:THR:N	2.50	0.45
1:B:117:GLY:HA2	2:B:550:BAL:HA1	1.98	0.45
1:B:302:MET:HA	1:B:303:PRO:HD3	1.88	0.44
1:B:190:LYS:HZ1	5:B:621:NAG:H61	1.82	0.44
1:A:17:ASN:HD22	3:A:601:NAG:H83	1.83	0.44
1:B:234:THR:HG22	1:B:238:GLU:HB2	2.00	0.44
1:A:159:ASN:HA	1:A:160:PRO:HD3	1.89	0.44
1:B:190:LYS:HE2	5:B:621:NAG:H4	1.99	0.44
1:B:278:PHE:O	4:B:633:FUL:O4	2.33	0.43
4:B:661:NAG:H61	4:B:663:FUL:H2	1.83	0.43
1:A:69:ILE:HD11	1:A:88:LEU:HD11	2.01	0.43
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.54	0.43
1:B:301:ASP:HB3	1:B:306:LEU:HD13	2.00	0.43
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.88	0.43
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.75	0.43
1:A:321:VAL:HG11	1:A:399:ILE:HA	2.00	0.43
1:B:239:ALA:HB2	1:B:293:THR:HG21	2.00	0.43
1:A:227:PHE:CD1	1:A:303:PRO:HB2	2.54	0.42
1:B:395:ASP:OD2	1:B:515:ARG:NH1	2.52	0.42
1:A:209:LEU:HD23	1:A:312:PHE:HB3	2.00	0.42
1:A:489:SER:HA	10:A:1546:CL:CL	2.57	0.42
1:B:321:VAL:HG11	1:B:399:ILE:HA	2.00	0.42
1:A:419:TYR:HB3	1:A:490:TRP:CZ2	2.55	0.41
1:B:456:TYR:O	8:B:1534:EDO:H12	2.20	0.41
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.56	0.41
1:A:252:CYS:SG	1:A:267:LYS:HE3	2.61	0.41
1:B:84:PRO:HG2	1:B:88:LEU:HD21	2.01	0.41
1:B:500:TYR:CE1	1:B:511:MET:HB2	2.55	0.41
1:B:428:LEU:HA	1:B:429:PRO:HD3	1.87	0.41
1:B:106:ASN:HD22	5:B:621:NAG:C7	2.34	0.41
1:B:319:VAL:O	1:B:418:PHE:HA	2.20	0.41
1:B:397:ASN:HD21	8:B:1538:EDO:H21	1.86	0.41
1:B:188:ASN:ND2	5:B:621:NAG:H83	2.36	0.41
1:A:423:HIS:HE2	1:A:460:GLU:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HA	1:A:9:LYS:HD3	1.92	0.40
1:B:96:ASN:O	1:B:142:VAL:HA	2.21	0.40
1:B:73:PHE:CD1	1:B:339:LYS:HE3	2.56	0.40
1:B:488:THR:HG21	1:B:508:THR:OG1	2.20	0.40
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.83	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	528/531 (99%)	506 (96%)	20 (4%)	2 (0%)	39	61
1	B	524/531 (99%)	494 (94%)	26 (5%)	4 (1%)	24	41
All	All	1052/1062 (99%)	1000 (95%)	46 (4%)	6 (1%)	30	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	GLN
1	B	485	ASN
1	B	488	THR
1	B	489	SER
1	A	255	GLU
1	A	381	ARG

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	455/456 (100%)	444 (98%)	11 (2%)	57 82
1	B	451/456 (99%)	434 (96%)	17 (4%)	40 67
All	All	906/912 (99%)	878 (97%)	28 (3%)	47 75

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	PHE
1	A	198	SER
1	A	282	TYR
1	A	308	GLU
1	A	363	GLU
1	A	379	ASP
1	A	428	LEU
1	A	471	TRP
1	A	511	MET
1	A	515	ARG
1	A	529	VAL
1	B	176	GLN
1	B	195	PHE
1	B	198	SER
1	B	255	GLU
1	B	258	THR
1	B	268	ASP
1	B	286	LEU
1	B	287	SER
1	B	306	LEU
1	B	311	GLN
1	B	348	LYS
1	B	379	ASP
1	B	465	ARG
1	B	471	TRP
1	B	492	VAL
1	B	496	THR
1	B	515	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

25 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	601	1,3	14,14,15	0.65	0	15,19,21	1.02	1 (6%)
3	NAG	A	602	3	14,14,15	0.46	0	15,19,21	1.21	2 (13%)
4	NAG	A	611	1,4	14,14,15	0.53	0	15,19,21	1.45	2 (13%)
4	NAG	A	612	4	14,14,15	0.48	0	15,19,21	1.48	1 (6%)
4	FUL	A	613	4	10,10,11	0.66	0	14,14,16	1.11	2 (14%)
3	NAG	A	621	1,3	14,14,15	0.59	0	15,19,21	1.14	2 (13%)
3	NAG	A	622	3	14,14,15	0.62	0	15,19,21	1.12	2 (13%)
4	NAG	A	631	1,4	14,14,15	0.49	0	15,19,21	1.28	1 (6%)
4	NAG	A	632	4	14,14,15	0.49	0	15,19,21	1.30	2 (13%)
4	FUL	A	633	4	10,10,11	0.58	0	14,14,16	1.42	3 (21%)
6	NAG	A	671	1,6	14,14,15	0.42	0	15,19,21	1.18	1 (6%)
6	NAG	A	672	6	14,14,15	0.63	0	15,19,21	1.16	1 (6%)
6	MAN	A	673	6	11,11,12	0.59	0	14,15,17	1.27	2 (14%)
4	NAG	A	681	1,4	14,14,15	0.68	0	15,19,21	1.13	1 (6%)
4	NAG	A	682	4	14,14,15	0.54	0	15,19,21	0.73	0
4	FUL	A	683	4	10,10,11	0.58	0	14,14,16	0.90	0
4	NAG	B	631	1,4	14,14,15	0.38	0	15,19,21	1.74	2 (13%)
4	NAG	B	632	4	14,14,15	0.44	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FUL	B	633	4	10,10,11	0.61	0	14,14,16	1.70	2 (14%)
4	NAG	B	641	1,4	14,14,15	0.48	0	15,19,21	1.16	1 (6%)
4	NAG	B	642	4	14,14,15	0.46	0	15,19,21	0.94	1 (6%)
4	FUL	B	643	4	10,10,11	0.56	0	14,14,16	0.86	0
4	NAG	B	661	1,4	14,14,15	0.51	0	15,19,21	1.51	2 (13%)
4	NAG	B	662	4	14,14,15	0.56	0	15,19,21	1.28	1 (6%)
4	FUL	B	663	4	10,10,11	0.59	0	14,14,16	1.04	1 (7%)

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	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
4	NAG	A	611	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	612	4	-	0/6/23/26	0/1/1/1
4	FUL	A	613	4	-	0/0/17/20	0/1/1/1
3	NAG	A	621	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	622	3	-	0/6/23/26	0/1/1/1
4	NAG	A	631	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	632	4	-	0/6/23/26	0/1/1/1
4	FUL	A	633	4	-	0/0/17/20	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	672	6	-	0/6/23/26	0/1/1/1
6	MAN	A	673	6	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	A	681	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	682	4	-	0/6/23/26	0/1/1/1
4	FUL	A	683	4	-	0/0/17/20	0/1/1/1
4	NAG	B	631	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	632	4	-	0/6/23/26	0/1/1/1
4	FUL	B	633	4	-	0/0/17/20	0/1/1/1
4	NAG	B	641	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	B	642	4	-	0/6/23/26	0/1/1/1
4	FUL	B	643	4	-	0/0/17/20	0/1/1/1
4	NAG	B	661	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	662	4	-	0/6/23/26	0/1/1/1
4	FUL	B	663	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	631	NAG	O4-C4-C3	-3.52	102.41	110.34
6	A	673	MAN	C1-C2-C3	-3.12	105.86	109.54
3	A	622	NAG	C1-O5-C5	-2.92	108.55	112.25
3	A	602	NAG	C4-C3-C2	-2.46	107.41	111.23
3	A	621	NAG	O4-C4-C3	-2.45	104.81	110.34
4	A	633	FUL	O5-C1-C2	-2.44	106.89	110.86
6	A	673	MAN	O5-C1-C2	-2.40	106.96	110.86
4	A	633	FUL	C1-C2-C3	-2.33	106.78	109.54
4	B	661	NAG	C6-C5-C4	-2.15	107.70	113.02
4	A	613	FUL	O5-C1-C2	-2.06	107.51	110.86
4	B	642	NAG	C4-C3-C2	-2.02	108.09	111.23
4	B	632	NAG	C1-O5-C5	2.02	114.81	112.25
4	A	632	NAG	O5-C5-C6	2.10	111.89	107.35
3	A	622	NAG	C4-C3-C2	2.23	114.70	111.23
4	B	633	FUL	C1-C2-C3	2.36	112.33	109.54
4	A	613	FUL	O5-C5-C6	2.37	110.05	106.13
4	B	663	FUL	O5-C5-C6	2.44	110.17	106.13
4	A	633	FUL	O2-C2-C1	2.53	114.28	109.21
3	A	602	NAG	C1-O5-C5	2.56	115.50	112.25
3	A	621	NAG	C4-C3-C2	2.71	115.44	111.23
3	A	601	NAG	C4-C3-C2	2.77	115.53	111.23
6	A	671	NAG	C1-O5-C5	2.81	115.81	112.25
4	A	611	NAG	C1-O5-C5	2.92	115.95	112.25
4	A	611	NAG	O4-C4-C3	3.02	117.13	110.34
6	A	672	NAG	C4-C3-C2	3.04	115.96	111.23
4	A	681	NAG	C4-C3-C2	3.47	116.62	111.23
4	B	641	NAG	C1-O5-C5	3.63	116.86	112.25
4	B	662	NAG	C2-N2-C7	3.75	127.86	123.04
4	A	631	NAG	C1-O5-C5	4.00	117.32	112.25
4	A	632	NAG	C1-O5-C5	4.11	117.46	112.25
4	B	661	NAG	C1-O5-C5	4.34	117.75	112.25
4	B	633	FUL	C1-O5-C5	4.41	119.19	112.38
4	A	612	NAG	C1-O5-C5	4.51	117.98	112.25
4	B	631	NAG	C1-O5-C5	4.87	118.43	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	673	MAN	C1
4	A	681	NAG	C1
4	B	641	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAG	1	0
4	A	633	FUL	1	0
4	B	631	NAG	2	0
4	B	632	NAG	2	0
4	B	633	FUL	1	0
4	B	641	NAG	1	0
4	B	661	NAG	1	0
4	B	663	FUL	1	0

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 10 are unknown and 7 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
7	PG4	A	1530	-	12,12,12	0.66	0	11,11,11	1.48	0
7	PG4	A	1531	-	12,12,12	0.68	0	11,11,11	1.45	0
8	EDO	A	1532	-	3,3,3	0.51	0	2,2,2	0.47	0
8	EDO	A	1533	-	3,3,3	0.53	0	2,2,2	0.30	0
8	EDO	A	1534	-	3,3,3	0.54	0	2,2,2	0.36	0
8	EDO	A	1535	-	3,3,3	0.51	0	2,2,2	0.28	0
8	EDO	A	1536	-	3,3,3	0.47	0	2,2,2	0.52	0
8	EDO	A	1537	-	3,3,3	0.53	0	2,2,2	0.38	0
8	EDO	A	1538	-	3,3,3	0.49	0	2,2,2	0.35	0
8	EDO	A	1539	-	3,3,3	0.51	0	2,2,2	0.24	0
8	EDO	A	1540	-	3,3,3	0.58	0	2,2,2	0.14	0
11	GLY	A	1643	-	1,4,4	0.54	0	0,4,4	0.00	-
2	BAL	A	550	-	1,5,5	0.12	0	0,5,5	0.00	-
5	NAG	A	651	1	14,14,15	0.55	0	15,19,21	0.52	0
12	PEG	B	1530	-	6,6,6	0.60	0	5,5,5	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PEG	B	1531	-	6,6,6	0.69	0	5,5,5	1.21	0
8	EDO	B	1532	-	3,3,3	0.52	0	2,2,2	0.38	0
8	EDO	B	1533	-	3,3,3	0.50	0	2,2,2	0.34	0
8	EDO	B	1534	-	3,3,3	0.46	0	2,2,2	0.67	0
8	EDO	B	1535	-	3,3,3	0.53	0	2,2,2	0.27	0
8	EDO	B	1536	-	3,3,3	0.47	0	2,2,2	0.49	0
8	EDO	B	1537	-	3,3,3	0.46	0	2,2,2	0.64	0
8	EDO	B	1538	-	3,3,3	0.48	0	2,2,2	0.36	0
8	EDO	B	1539	-	3,3,3	0.46	0	2,2,2	0.40	0
8	EDO	B	1540	-	3,3,3	0.50	0	2,2,2	0.40	0
8	EDO	B	1541	-	3,3,3	0.44	0	2,2,2	0.54	0
11	GLY	B	1642	-	1,4,4	0.55	0	0,4,4	0.00	-
2	BAL	B	550	-	1,5,5	0.09	0	0,5,5	0.00	-
5	NAG	B	601	1	14,14,15	0.62	0	15,19,21	1.19	2 (13%)
5	NAG	B	611	1	14,14,15	0.43	0	15,19,21	0.87	1 (6%)
5	NAG	B	621	1	14,14,15	0.57	0	15,19,21	1.57	2 (13%)
5	NAG	B	651	1	14,14,15	0.52	0	15,19,21	1.39	1 (6%)
5	NAG	B	671	1	14,14,15	0.56	0	15,19,21	0.82	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
7	PG4	A	1530	-	-	0/10/10/10	0/0/0/0
7	PG4	A	1531	-	-	0/10/10/10	0/0/0/0
8	EDO	A	1532	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1533	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1534	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1535	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1536	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1537	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1538	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1539	-	-	0/1/1/1	0/0/0/0
8	EDO	A	1540	-	-	0/1/1/1	0/0/0/0
11	GLY	A	1643	-	-	0/0/2/2	0/0/0/0
2	BAL	A	550	-	-	0/1/3/3	0/0/0/0
5	NAG	A	651	1	1/1/5/7	1/6/23/26	0/1/1/1
12	PEG	B	1530	-	-	0/4/4/4	0/0/0/0
12	PEG	B	1531	-	-	0/4/4/4	0/0/0/0
8	EDO	B	1532	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	1533	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1534	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1535	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1536	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1537	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1538	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1539	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1540	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1541	-	-	0/1/1/1	0/0/0/0
11	GLY	B	1642	-	-	0/0/2/2	0/0/0/0
2	BAL	B	550	-	-	0/1/3/3	0/0/0/0
5	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	611	1	-	0/6/23/26	0/1/1/1
5	NAG	B	621	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	651	1	-	0/6/23/26	0/1/1/1
5	NAG	B	671	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	NAG	C4-C3-C2	2.26	114.74	111.23
5	B	611	NAG	C1-O5-C5	2.72	115.70	112.25
5	B	601	NAG	C1-O5-C5	3.10	116.19	112.25
5	B	621	NAG	C1-O5-C5	3.53	116.73	112.25
5	B	621	NAG	C2-N2-C7	3.64	127.72	123.04
5	B	651	NAG	C1-O5-C5	4.58	118.06	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	651	NAG	C1
5	B	671	NAG	C1
5	B	621	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	651	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1531	PG4	1	0
8	A	1536	EDO	1	0
2	A	550	BAL	3	0
12	B	1531	PEG	2	0
8	B	1534	EDO	2	0
8	B	1538	EDO	1	0
8	B	1539	EDO	1	0
2	B	550	BAL	5	0
5	B	621	NAG	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	527/531 (99%)	-0.05	16 (3%)	54	59	26, 44, 72, 117	4 (0%)
1	B	526/531 (99%)	0.08	23 (4%)	38	43	27, 52, 88, 119	12 (2%)
All	All	1053/1062 (99%)	0.01	39 (3%)	45	50	26, 48, 81, 119	16 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	344	ILE	4.4
1	B	380	GLN	4.1
1	A	380	GLN	4.0
1	B	382	PRO	3.3
1	B	384	ASN	3.2
1	B	52	TRP	3.0
1	B	336	GLY	3.0
1	A	344	ILE	2.9
1	B	343	SER	2.8
1	A	348	LYS	2.8
1	B	342	ASN	2.8
1	B	102	PRO	2.6
1	B	381	ARG	2.6
1	A	201	ALA	2.5
1	B	385	TYR	2.5
1	B	28	PHE	2.4
1	A	337	PHE	2.4
1	A	259	GLU	2.4
1	B	433	TRP	2.4
1	A	364	PHE	2.3
1	A	222	LEU	2.3
1	B	22	GLY	2.3
1	A	266	ASN	2.2
1	A	252	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	6	ILE	2.2
1	B	232	ALA	2.2
1	B	10	ASN	2.2
1	B	345	ILE	2.2
1	B	483	THR	2.2
1	B	101	ALA	2.1
1	A	459	ALA	2.1
1	B	51	LYS	2.1
1	B	376	TRP	2.1
1	A	202	ALA	2.1
1	B	377	VAL	2.1
1	A	433	TRP	2.1
1	A	382	PRO	2.1
1	A	341	ASN	2.0
1	A	260	ILE	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	FUL	A	633	10/11	0.83	0.47	9.81	125,130,131,132	0
4	FUL	A	683	10/11	0.88	0.20	6.27	90,100,106,108	0
4	FUL	B	633	10/11	0.78	0.29	4.07	96,106,109,112	0
4	NAG	B	631	14/15	0.90	0.28	3.68	71,91,107,111	0
6	NAG	A	672	14/15	0.93	0.14	0.58	66,81,91,108	0
6	NAG	A	671	14/15	0.95	0.12	-0.15	43,57,71,71	0
4	NAG	A	611	14/15	0.92	0.15	-0.34	67,78,96,103	0
6	MAN	A	673	11/12	0.74	0.29	-	118,125,131,137	0
4	NAG	A	631	14/15	0.74	0.27	-	97,111,128,137	0
4	NAG	A	682	14/15	0.73	0.41	-	104,116,121,121	0
4	NAG	A	681	14/15	0.80	0.26	-	92,101,109,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	661	14/15	0.86	0.19	-	67,78,101,111	0
4	NAG	A	632	14/15	0.74	0.67	-	145,148,151,153	0
4	FUL	B	663	10/11	0.69	0.37	-	124,127,131,132	0
3	NAG	A	621	14/15	0.90	0.18	-	42,64,70,92	0
4	FUL	A	613	10/11	0.88	0.22	-	96,98,100,101	0
3	NAG	A	602	14/15	0.80	0.37	-	91,100,108,111	0
3	NAG	A	601	14/15	0.92	0.24	-	51,65,83,91	0
4	NAG	B	641	14/15	0.94	0.21	-	72,89,102,108	0
4	NAG	B	632	14/15	0.90	0.34	-	90,105,112,113	0
4	NAG	B	662	14/15	0.77	0.38	-	88,106,120,121	0
4	NAG	A	612	14/15	0.82	0.27	-	90,105,113,116	0
3	NAG	A	622	14/15	0.74	0.40	-	93,108,123,124	0
4	FUL	B	643	10/11	0.84	0.41	-	119,124,127,127	0
4	NAG	B	642	14/15	0.83	0.40	-	110,115,126,126	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	EDO	B	1539	4/4	0.95	0.44	14.11	57,59,61,61	0
9	UNX	B	1544	1/1	0.98	0.57	9.37	67,67,67,67	0
9	UNX	B	1542	1/1	0.99	0.63	9.16	59,59,59,59	0
8	EDO	B	1541	4/4	0.90	0.25	9.14	74,75,76,78	0
8	EDO	A	1537	4/4	0.91	0.32	9.12	51,52,58,64	0
12	PEG	B	1530	7/7	0.81	0.42	8.07	66,86,98,100	0
9	UNX	A	1541	1/1	0.99	0.53	7.82	58,58,58,58	0
8	EDO	A	1538	4/4	0.97	0.25	7.55	61,65,67,68	0
12	PEG	B	1531	7/7	0.86	0.31	6.90	70,73,88,89	0
8	EDO	A	1536	4/4	0.87	0.32	6.59	74,76,77,82	0
8	EDO	A	1532	4/4	0.90	0.31	5.38	64,66,68,76	0
7	PG4	A	1531	13/13	0.90	0.29	4.96	59,80,87,92	0
8	EDO	A	1540	4/4	0.86	0.20	3.92	64,65,72,73	0
10	CL	B	1549	1/1	0.74	0.22	3.78	95,95,95,95	0
2	BAL	B	550	6/6	0.89	0.33	3.09	49,55,68,79	0
8	EDO	B	1534	4/4	0.85	0.30	2.72	55,65,69,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	EDO	B	1540	4/4	0.92	0.30	2.67	67,74,81,81	0
2	BAL	A	550	6/6	0.94	0.28	2.57	50,56,70,84	0
8	EDO	B	1532	4/4	0.91	0.19	2.44	62,64,69,79	0
11	GLY	B	1642	5/5	0.89	0.16	1.98	57,60,68,70	0
8	EDO	B	1538	4/4	0.90	0.22	1.76	64,65,67,69	0
8	EDO	A	1533	4/4	0.80	0.25	1.12	68,74,75,78	0
8	EDO	B	1535	4/4	0.92	0.16	0.82	68,75,76,77	0
10	CL	A	1546	1/1	0.92	0.16	0.71	73,73,73,73	0
8	EDO	B	1537	4/4	0.90	0.15	0.40	69,73,76,77	0
5	NAG	B	651	14/15	0.92	0.26	-0.31	56,71,80,87	0
5	NAG	A	651	14/15	0.91	0.25	-0.39	58,78,87,91	0
10	CL	B	1550	1/1	0.90	0.16	-0.56	82,82,82,82	0
8	EDO	B	1533	4/4	0.96	0.12	-1.06	65,73,74,76	0
8	EDO	A	1534	4/4	0.87	0.12	-1.13	66,71,75,76	0
11	GLY	A	1643	5/5	0.96	0.11	-1.28	42,48,53,58	0
5	NAG	B	671	14/15	0.74	0.19	-	92,103,111,112	0
8	EDO	A	1539	4/4	0.94	0.49	-	77,82,84,85	0
9	UNX	A	1544	1/1	0.97	0.56	-	53,53,53,53	0
9	UNX	B	1548	1/1	0.81	0.08	-	68,68,68,68	0
10	CL	B	1546	1/1	0.84	0.49	-	102,102,102,102	0
10	CL	A	1547	1/1	0.66	0.23	-	99,99,99,99	0
9	UNX	B	1545	1/1	0.97	0.63	-	53,53,53,53	0
9	UNX	A	1543	1/1	0.82	1.29	-	83,83,83,83	0
5	NAG	B	621	14/15	0.89	0.28	-	75,88,96,97	0
9	UNX	A	1548	1/1	0.41	0.20	-	71,71,71,71	0
8	EDO	A	1535	4/4	0.76	0.19	-	84,85,88,88	0
5	NAG	B	611	14/15	0.77	0.19	-	102,109,114,116	0
9	UNX	A	1542	1/1	0.98	0.46	-	54,54,54,54	0
8	EDO	B	1536	4/4	0.88	0.48	-	64,65,73,74	0
10	CL	B	1547	1/1	0.90	0.12	-	96,96,96,96	0
5	NAG	B	601	14/15	0.66	0.33	-	94,104,119,120	0
10	CL	A	1545	1/1	0.86	0.08	-	90,90,90,90	0
9	UNX	B	1543	1/1	0.96	0.62	-	43,43,43,43	0
7	PG4	A	1530	13/13	0.84	0.32	-	76,82,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.