



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 04:27 PM EDT

PDB ID : 3BIX
Title : Crystal structure of the extracellular esterase domain of Neuroligin-1
Authors : Arac, D.; Boucard, A.A.; Ozkan, E.; Strop, P.; Newell, E.; Sudhof, T.C.;
Brunger, A.T.
Deposited on : 2007-12-01
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

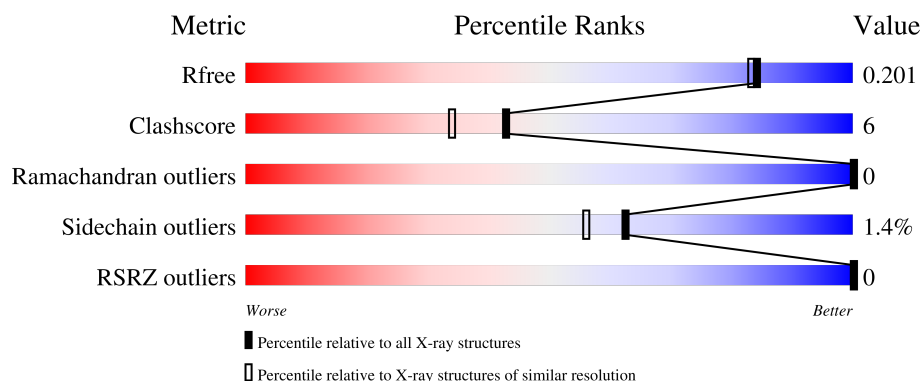
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




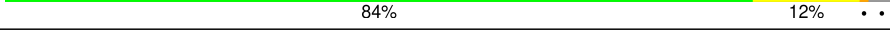
The reported resolution of this entry is 1.80 Å.

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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	574	
1	B	574	
1	C	574	
1	D	574	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19833 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 Neuroligin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	11	0
			4436	2858	738	823	17			
1	B	555	Total	C	N	O	S	0	8	0
			4422	2848	737	821	16			
1	C	555	Total	C	N	O	S	0	4	0
			4404	2830	736	822	16			
1	D	555	Total	C	N	O	S	0	11	0
			4436	2856	739	824	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ALA	-	expression tag	UNP Q62765
A	44	ASP	-	expression tag	UNP Q62765
A	45	PRO	-	expression tag	UNP Q62765
A	639	HIS	-	expression tag	UNP Q62765
A	640	HIS	-	expression tag	UNP Q62765
A	641	HIS	-	expression tag	UNP Q62765
A	642	HIS	-	expression tag	UNP Q62765
A	643	HIS	-	expression tag	UNP Q62765
A	644	HIS	-	expression tag	UNP Q62765
B	43	ALA	-	expression tag	UNP Q62765
B	44	ASP	-	expression tag	UNP Q62765
B	45	PRO	-	expression tag	UNP Q62765
B	639	HIS	-	expression tag	UNP Q62765
B	640	HIS	-	expression tag	UNP Q62765
B	641	HIS	-	expression tag	UNP Q62765
B	642	HIS	-	expression tag	UNP Q62765
B	643	HIS	-	expression tag	UNP Q62765
B	644	HIS	-	expression tag	UNP Q62765
C	43	ALA	-	expression tag	UNP Q62765
C	44	ASP	-	expression tag	UNP Q62765
C	45	PRO	-	expression tag	UNP Q62765

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	639	HIS	-	expression tag	UNP Q62765
C	640	HIS	-	expression tag	UNP Q62765
C	641	HIS	-	expression tag	UNP Q62765
C	642	HIS	-	expression tag	UNP Q62765
C	643	HIS	-	expression tag	UNP Q62765
C	644	HIS	-	expression tag	UNP Q62765
D	43	ALA	-	expression tag	UNP Q62765
D	44	ASP	-	expression tag	UNP Q62765
D	45	PRO	-	expression tag	UNP Q62765
D	639	HIS	-	expression tag	UNP Q62765
D	640	HIS	-	expression tag	UNP Q62765
D	641	HIS	-	expression tag	UNP Q62765
D	642	HIS	-	expression tag	UNP Q62765
D	643	HIS	-	expression tag	UNP Q62765
D	644	HIS	-	expression tag	UNP Q62765

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

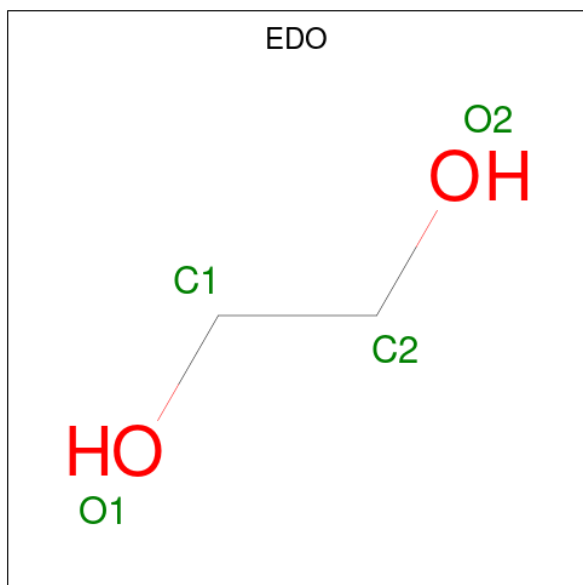
Continued from previous page...

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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

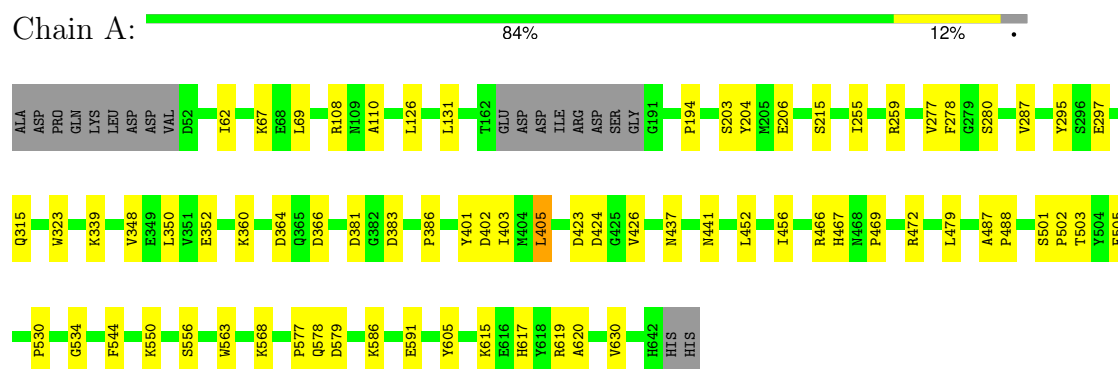
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	497	Total O 497 497	0	0
5	B	493	Total O 493 493	0	0
5	C	479	Total O 479 479	0	0
5	D	496	Total O 496 496	0	0

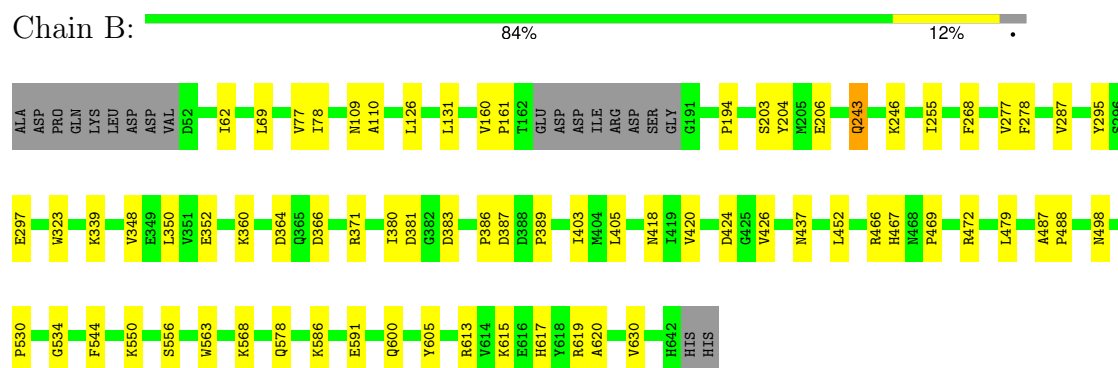
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

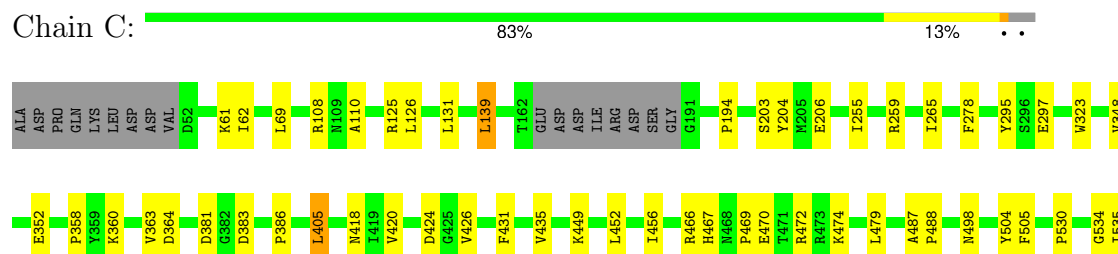
• Molecule 1: Neuroligin-1



• Molecule 1: Neuroligin-1

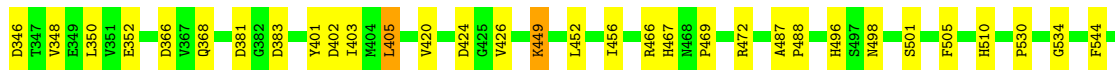
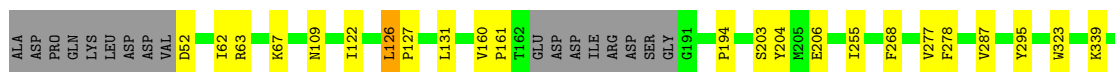
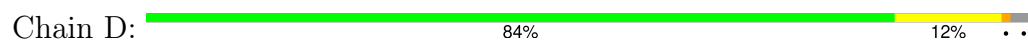


• Molecule 1: Neuroligin-1





- Molecule 1: Neuroligin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	173.74Å 173.74Å 108.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.88 – 1.80 45.88 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (45.88-1.80) 98.9 (45.88-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.75Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.185 , 0.205 0.181 , 0.201	Depositor DCC
R_{free} test set	16809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.470 for -h,-k,l 0.487 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19833	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, NI

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	0.32	0/4598	0.58	1/6280 (0.0%)
1	B	0.31	0/4575	0.58	0/6249
1	C	0.31	0/4545	0.58	0/6207
1	D	0.31	0/4598	0.58	1/6280 (0.0%)
All	All	0.31	0/18316	0.58	2/25016 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	402	ASP	N-CA-C	-5.08	97.29	111.00
1	A	402	ASP	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4436	0	4312	52	0
1	B	4422	0	4290	52	0
1	C	4404	0	4248	51	0
1	D	4436	0	4307	59	0
2	A	28	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	26	2	0
2	C	28	0	26	0	0
2	D	28	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	18	1	0
4	B	12	0	18	1	0
4	C	16	0	24	1	0
4	D	16	0	24	1	0
5	A	497	0	0	6	0
5	B	493	0	0	7	0
5	C	479	0	0	4	0
5	D	496	0	0	8	0
All	All	19833	0	17345	216	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 6.

All (216) 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:D:126:LEU:HD23	1:D:126:LEU:H	1.28	0.95
1:D:126:LEU:H	1:D:126:LEU:CD2	1.96	0.78
1:B:62[B]:ILE:HD11	1:B:110:ALA:HB2	1.66	0.76
1:A:62[A]:ILE:HD11	1:A:110:ALA:HB2	1.68	0.75
1:C:613:ARG:NE	1:C:615:LYS:HE2	2.03	0.74
1:B:613:ARG:NE	1:B:615:LYS:HE2	2.05	0.70
1:D:449:LYS:HD3	1:D:449:LYS:H	1.57	0.69
1:B:371:ARG:HH21	1:B:437[B]:ASN:ND2	1.91	0.69
1:A:381:ASP:OD2	1:A:383:ASP:HB3	1.95	0.67
1:A:403[B]:ILE:HD13	1:A:502:PRO:O	1.95	0.66
1:B:380[A]:ILE:HD11	1:B:389:PRO:HD3	1.77	0.66
1:A:62[A]:ILE:HD12	1:A:108:ARG:O	1.96	0.66
1:C:62[A]:ILE:HD11	1:C:110:ALA:HB2	1.78	0.65
1:C:62[A]:ILE:HD12	1:C:108:ARG:O	1.96	0.65
1:B:348:VAL:O	1:B:352:GLU:HG3	1.97	0.64
1:D:126:LEU:HD23	1:D:126:LEU:N	2.09	0.63
1:B:77[A]:VAL:HG13	1:B:160:VAL:O	1.98	0.63
1:A:403[B]:ILE:HD13	1:A:403[B]:ILE:H	1.63	0.63
1:B:466:ARG:HG2	5:B:1005:HOH:O	1.98	0.63
1:B:126:LEU:HD12	1:B:126:LEU:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PRO:HG2	1:B:568:LYS:HG2	1.81	0.62
1:A:360:LYS:HE3	1:A:364:ASP:OD2	2.00	0.62
1:A:550:LYS:HB3	1:A:586:LYS:HG2	1.81	0.62
1:C:126:LEU:HD12	1:C:126:LEU:O	2.00	0.61
1:D:550:LYS:HB3	1:D:586:LYS:HG2	1.82	0.61
1:A:126:LEU:HB2	1:A:131:LEU:HD11	1.81	0.61
1:D:62[B]:ILE:HD11	1:D:268:PHE:CZ	2.35	0.61
1:A:194:PRO:HG2	1:A:568:LYS:HG2	1.83	0.61
1:B:371:ARG:HH21	1:B:437[B]:ASN:HD21	1.49	0.61
1:C:617:HIS:HB3	1:C:620:ALA:HB2	1.83	0.61
1:C:126:LEU:HB2	1:C:131:LEU:HD11	1.82	0.61
1:B:617:HIS:HB3	1:B:620:ALA:HB2	1.84	0.60
1:C:194:PRO:HG2	1:C:568:LYS:HG2	1.82	0.60
1:A:403[B]:ILE:HD11	1:A:503:THR:OG1	2.01	0.60
1:A:617:HIS:HB3	1:A:620:ALA:HB2	1.84	0.60
1:C:619:ARG:HA	4:C:13:EDO:H21	1.83	0.60
1:D:469:PRO:HG3	5:D:1087:HOH:O	2.02	0.59
1:D:617:HIS:HB3	1:D:620:ALA:HB2	1.84	0.59
1:A:348:VAL:O	1:A:352:GLU:HG3	2.02	0.59
1:C:348:VAL:O	1:C:352:GLU:HG3	2.03	0.59
1:B:550:LYS:HB3	1:B:586:LYS:HG2	1.84	0.59
1:D:381:ASP:OD2	1:D:383:ASP:HB3	2.03	0.59
1:A:126:LEU:HD12	1:A:126:LEU:O	2.02	0.58
1:D:613:ARG:HD3	1:D:615:LYS:HE2	1.84	0.58
1:D:348:VAL:O	1:D:352:GLU:HG3	2.03	0.58
1:C:487:ALA:HB3	1:C:488:PRO:HD3	1.86	0.58
1:A:405:LEU:N	1:A:405:LEU:HD23	2.19	0.57
1:D:194:PRO:HG2	1:D:568:LYS:HG2	1.85	0.57
1:D:449:LYS:HD3	1:D:449:LYS:N	2.19	0.57
1:A:403[B]:ILE:HD12	1:A:501:SER:HB3	1.86	0.57
1:D:449:LYS:H	1:D:449:LYS:CD	2.18	0.57
1:D:401:TYR:O	1:D:403[A]:ILE:HD12	2.05	0.57
1:C:466:ARG:HG2	5:C:865:HOH:O	2.05	0.56
1:C:255:ILE:HD13	1:C:295:TYR:HB3	1.86	0.56
1:A:401:TYR:O	1:A:403[A]:ILE:HD12	2.05	0.56
1:C:259:ARG:HH12	1:C:297:GLU:CD	2.09	0.56
1:D:405:LEU:HD13	1:D:505:PHE:CD2	2.41	0.56
1:B:578:GLN:O	1:B:591:GLU:HG2	2.06	0.56
1:A:277[B]:VAL:HG12	1:A:287:VAL:HG22	1.88	0.56
1:D:466:ARG:HG2	5:D:878:HOH:O	2.05	0.56
1:A:487:ALA:HB3	1:A:488:PRO:HD3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ILE:HD13	1:B:295:TYR:HB3	1.88	0.56
1:A:67:LYS:HE3	5:A:1032:HOH:O	2.06	0.55
1:B:243:GLN:HE21	1:B:246:LYS:NZ	2.05	0.55
1:B:469:PRO:HG3	5:B:1091:HOH:O	2.06	0.55
1:B:487:ALA:HB3	1:B:488:PRO:HD3	1.89	0.55
1:A:578:GLN:O	1:A:591:GLU:HG2	2.06	0.55
1:A:259:ARG:HH12	1:A:297:GLU:CD	2.09	0.55
1:C:405:LEU:N	1:C:405:LEU:HD23	2.21	0.55
1:D:510:HIS:CD2	1:D:555[A]:LEU:HD23	2.42	0.55
1:C:381:ASP:OD2	1:C:383:ASP:HB3	2.06	0.55
1:C:449:LYS:HB2	1:C:449:LYS:NZ	2.22	0.55
1:A:466:ARG:HG2	5:A:873:HOH:O	2.06	0.55
2:A:1:NAG:H83	5:A:812:HOH:O	2.06	0.54
1:B:277[A]:VAL:HG12	1:B:287:VAL:HG22	1.89	0.54
1:B:405:LEU:N	1:B:405:LEU:HD23	2.23	0.54
1:B:381:ASP:OD2	1:B:383:ASP:HB3	2.08	0.54
1:D:277[A]:VAL:HG12	1:D:287:VAL:HG22	1.90	0.54
1:B:613:ARG:HD2	5:B:1073:HOH:O	2.06	0.54
1:D:487:ALA:HB3	1:D:488:PRO:HD3	1.90	0.54
1:C:126:LEU:HB2	1:C:131:LEU:CD1	2.38	0.54
1:B:619:ARG:HA	4:B:6:EDO:H11	1.90	0.53
1:D:510:HIS:CD2	1:D:555[B]:LEU:HD22	2.43	0.53
1:A:255[B]:ILE:HD13	1:A:295:TYR:HB3	1.91	0.52
1:C:601:LYS:NZ	1:C:601:LYS:HB3	2.23	0.52
1:D:403[B]:ILE:HD13	1:D:496:HIS:CG	2.44	0.52
1:A:126:LEU:HB2	1:A:131:LEU:CD1	2.40	0.52
1:D:203:SER:O	1:D:204:TYR:HB2	2.10	0.51
1:B:62[A]:ILE:HD11	1:B:268:PHE:CZ	2.46	0.51
1:B:530:PRO:HG3	1:B:544:PHE:CE1	2.44	0.51
1:D:255:ILE:HD13	1:D:295:TYR:HB3	1.93	0.51
1:B:613:ARG:HE	1:B:615:LYS:HE2	1.73	0.51
1:D:621:ASN:HB2	4:D:645:EDO:H11	1.93	0.51
1:D:126:LEU:HB2	1:D:131:LEU:CD2	2.41	0.51
1:D:496:HIS:HB3	1:D:501[A]:SER:OG	2.11	0.51
1:B:203:SER:O	1:B:204:TYR:HB2	2.11	0.51
1:D:452:LEU:HD21	1:D:630:VAL:HG13	1.92	0.51
1:D:530:PRO:HG3	1:D:544:PHE:CE1	2.45	0.51
1:C:358:PRO:HG2	1:D:498[B]:ASN:OD1	2.10	0.50
1:D:405:LEU:HD13	1:D:505:PHE:HD2	1.76	0.50
1:C:530:PRO:HG3	1:C:544:PHE:CE1	2.46	0.50
1:A:69:LEU:HD21	1:A:215:SER:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:SER:O	1:C:204:TYR:HB2	2.11	0.50
1:B:466:ARG:NH1	1:B:467:HIS:NE2	2.60	0.49
1:A:619:ARG:HA	4:A:4:EDO:H11	1.94	0.49
1:B:77[A]:VAL:HG12	1:B:78:ILE:N	2.27	0.49
1:A:530:PRO:HG3	1:A:544:PHE:CE1	2.47	0.48
1:A:203:SER:O	1:A:204:TYR:HB2	2.13	0.48
1:A:426:VAL:O	1:A:472:ARG:HD2	2.14	0.48
2:B:2:NAG:H81	5:B:813:HOH:O	2.14	0.48
1:B:498[A]:ASN:HD21	1:B:600:GLN:NE2	2.12	0.48
1:B:360:LYS:HD2	1:B:364:ASP:OD2	2.13	0.47
1:B:498[A]:ASN:OD1	1:B:600:GLN:NE2	2.48	0.47
1:C:426:VAL:O	1:C:472:ARG:HD2	2.15	0.47
1:D:126:LEU:HD21	5:D:753:HOH:O	2.14	0.47
1:B:109:ASN:ND2	2:B:2:NAG:C7	2.78	0.47
1:C:386:PRO:HD3	5:C:784:HOH:O	2.15	0.46
1:C:550:LYS:HB3	1:C:586:LYS:HG3	1.97	0.46
1:A:405:LEU:HD23	1:A:405:LEU:H	1.79	0.46
1:C:605:TYR:CZ	1:C:615:LYS:HB2	2.51	0.46
1:D:62[B]:ILE:HD11	1:D:268:PHE:HZ	1.78	0.46
1:D:339:LYS:HE3	1:D:366:ASP:O	2.16	0.46
1:C:550:LYS:HB2	1:C:586:LYS:HE2	1.97	0.46
1:B:339:LYS:HE3	1:B:366:ASP:O	2.16	0.46
1:B:371:ARG:NH2	1:B:437[B]:ASN:ND2	2.61	0.46
1:C:504:TYR:CZ	1:C:597:ARG:HG2	2.51	0.46
1:A:452:LEU:HD21	1:A:630:VAL:HG13	1.98	0.46
1:C:255:ILE:HD13	1:C:295:TYR:CB	2.46	0.46
1:C:360:LYS:HE3	1:C:364:ASP:OD2	2.15	0.46
1:B:452:LEU:HD21	1:B:630:VAL:HG13	1.99	0.45
1:C:588:ASN:O	1:C:591:GLU:HG3	2.16	0.45
1:D:52:ASP:N	5:D:1004:HOH:O	2.50	0.45
1:D:126:LEU:HA	1:D:127:PRO:HD3	1.79	0.45
1:B:126:LEU:HB2	1:B:131:LEU:CD2	2.47	0.45
1:A:479:LEU:C	1:A:479:LEU:HD23	2.38	0.45
1:A:577:PRO:HG2	1:A:579:ASP:OD2	2.16	0.45
1:B:488:PRO:HG3	5:B:953:HOH:O	2.17	0.45
1:C:452:LEU:HD21	1:C:630:VAL:HG13	1.99	0.45
1:A:403[A]:ILE:CD1	1:A:501:SER:HB3	2.46	0.44
1:B:426:VAL:O	1:B:472:ARG:HD2	2.16	0.44
1:C:534:GLY:HA2	1:C:556:SER:OG	2.17	0.44
2:D:4:NAG:H81	5:D:827:HOH:O	2.17	0.44
1:A:437[A]:ASN:OD1	1:A:441:ASN:ND2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:VAL:CG1	1:B:424:ASP:HA	2.47	0.44
1:B:255:ILE:HD13	1:B:295:TYR:CB	2.47	0.44
1:D:452:LEU:O	1:D:456:ILE:HG12	2.18	0.44
1:D:588:ASN:O	1:D:591:GLU:HG3	2.18	0.44
1:B:403:ILE:HG22	1:B:405:LEU:HD22	2.00	0.44
1:D:62[B]:ILE:HD11	1:D:268:PHE:CE1	2.52	0.44
1:A:280:SER:HA	1:A:315:GLN:O	2.18	0.44
1:D:420:VAL:CG1	1:D:424:ASP:HA	2.48	0.43
1:D:467:HIS:O	1:D:469:PRO:HD3	2.18	0.43
1:A:605:TYR:CZ	1:A:615:LYS:HB2	2.53	0.43
1:B:467:HIS:O	1:B:469:PRO:HD3	2.19	0.43
1:C:452:LEU:O	1:C:456:ILE:HG12	2.18	0.43
1:D:255:ILE:HD13	1:D:295:TYR:CB	2.48	0.43
1:C:420:VAL:CG1	1:C:424:ASP:HA	2.48	0.43
1:C:449:LYS:HB2	1:C:449:LYS:HZ3	1.82	0.43
1:D:67:LYS:HE3	5:D:1058:HOH:O	2.16	0.43
1:A:452:LEU:O	1:A:456[A]:ILE:HG12	2.19	0.43
1:B:605:TYR:CZ	1:B:615:LYS:HB2	2.54	0.43
1:C:139:LEU:HD12	1:C:139:LEU:HA	1.88	0.43
1:D:605:TYR:CZ	1:D:615:LYS:HB2	2.53	0.43
1:A:255[B]:ILE:HD13	1:A:295:TYR:CB	2.48	0.43
1:A:339:LYS:HE3	1:A:366:ASP:O	2.19	0.43
1:A:386:PRO:HD3	5:A:787:HOH:O	2.19	0.43
1:C:467:HIS:O	1:C:469:PRO:HD3	2.18	0.43
1:D:350:LEU:C	1:D:350:LEU:HD23	2.38	0.43
1:B:534:GLY:HA2	1:B:556:SER:OG	2.18	0.42
1:D:109:ASN:ND2	2:D:4:NAG:C7	2.82	0.42
1:B:350:LEU:C	1:B:350:LEU:HD23	2.40	0.42
1:B:62[A]:ILE:HD11	1:B:268:PHE:CE1	2.55	0.42
1:B:479:LEU:HD23	1:B:479:LEU:C	2.40	0.42
1:C:259:ARG:HH11	1:C:259:ARG:HG2	1.83	0.42
1:C:498[A]:ASN:HD21	1:C:600:GLN:NE2	2.17	0.42
1:C:69:LEU:HD12	1:C:69:LEU:N	2.34	0.42
1:C:535:ILE:N	1:C:536:PRO:CD	2.82	0.42
1:C:578:GLN:O	1:C:591:GLU:HA	2.20	0.42
1:D:160:VAL:HA	1:D:161:PRO:HD3	1.92	0.42
1:A:467:HIS:O	1:A:469:PRO:HD3	2.18	0.42
1:A:488:PRO:HG3	5:A:935:HOH:O	2.19	0.42
1:A:405:LEU:N	1:A:405:LEU:CD2	2.82	0.42
1:B:386:PRO:HG3	5:B:799:HOH:O	2.20	0.42
1:D:578:GLN:O	1:D:591:GLU:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:HD12	1:D:405:LEU:H	1.84	0.41
1:B:160:VAL:HA	1:B:161:PRO:HD3	1.92	0.41
1:C:431:PHE:O	1:C:435:VAL:HG23	2.21	0.41
1:D:426:VAL:O	1:D:472:ARG:HD2	2.20	0.41
1:C:470:GLU:O	1:C:474:LYS:HG3	2.19	0.41
1:D:52:ASP:OD1	1:D:63:ARG:NH1	2.54	0.41
1:A:423:ASP:O	1:A:424:ASP:HB2	2.20	0.41
1:D:122:ILE:HD12	1:D:122:ILE:C	2.40	0.41
1:D:488:PRO:HG3	5:D:1111:HOH:O	2.20	0.41
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.41
1:D:534:GLY:HA2	1:D:556:SER:OG	2.20	0.41
1:D:576:VAL:HA	1:D:577:PRO:HD3	1.93	0.41
1:A:259:ARG:NH1	5:A:1116:HOH:O	2.52	0.41
1:A:405:LEU:O	1:A:505:PHE:HA	2.21	0.41
1:A:534:GLY:HA2	1:A:556:SER:OG	2.20	0.41
1:A:578:GLN:O	1:A:591:GLU:HA	2.21	0.41
1:B:426:VAL:HA	5:B:853:HOH:O	2.20	0.41
1:C:61:LYS:NZ	5:C:939:HOH:O	2.54	0.41
1:C:265:ILE:HD12	1:C:265:ILE:HA	1.95	0.41
1:C:405:LEU:O	1:C:505:PHE:HA	2.20	0.41
1:C:125:ARG:NH1	1:C:363:VAL:O	2.54	0.41
1:C:479:LEU:HD23	1:C:479:LEU:C	2.41	0.41
1:D:346:ASP:OD2	1:D:348:VAL:HB	2.21	0.41
1:C:537:MET:HE2	1:C:583:ILE:HG13	2.02	0.40
1:D:126:LEU:HB2	1:D:131:LEU:HD21	2.02	0.40
1:D:368:GLN:NE2	5:D:929:HOH:O	2.54	0.40
1:D:405:LEU:O	1:D:505:PHE:HA	2.22	0.40
1:C:488:PRO:HG3	5:C:944:HOH:O	2.20	0.40
1:B:69:LEU:N	1:B:69:LEU:HD12	2.37	0.40
1:B:380[A]:ILE:HD12	1:B:387:ASP:O	2.21	0.40
1:A:360:LYS:HA	1:A:360:LYS:HD2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	562/574 (98%)	538 (96%)	24 (4%)	0	100	100
1	B	559/574 (97%)	537 (96%)	22 (4%)	0	100	100
1	C	555/574 (97%)	533 (96%)	22 (4%)	0	100	100
1	D	562/574 (98%)	538 (96%)	24 (4%)	0	100	100
All	All	2238/2296 (98%)	2146 (96%)	92 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/494 (99%)	483 (99%)	5 (1%)	73	68
1	B	485/494 (98%)	478 (99%)	7 (1%)	62	56
1	C	481/494 (97%)	473 (98%)	8 (2%)	56	47
1	D	488/494 (99%)	481 (99%)	7 (1%)	62	56
All	All	1942/1976 (98%)	1915 (99%)	27 (1%)	62	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	GLU
1	A	278	PHE
1	A	323	TRP
1	A	405	LEU
1	A	563	TRP
1	B	206	GLU
1	B	243	GLN
1	B	278	PHE
1	B	297	GLU
1	B	323	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	418	ASN
1	B	563	TRP
1	C	139	LEU
1	C	206	GLU
1	C	278	PHE
1	C	323	TRP
1	C	405	LEU
1	C	418	ASN
1	C	563	TRP
1	C	601	LYS
1	D	126	LEU
1	D	206	GLU
1	D	278	PHE
1	D	323	TRP
1	D	405	LEU
1	D	449	LYS
1	D	563	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	ASN
1	A	418	ASN
1	A	441	ASN
1	A	498	ASN
1	A	621	ASN
1	B	243	GLN
1	B	400	ASN
1	B	418	ASN
1	B	441	ASN
1	B	600	GLN
1	C	418	ASN
1	C	441	ASN
1	C	621	ASN
1	D	400	ASN
1	D	418	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	EDO	A	646	-	3,3,3	0.41	0	2,2,2	0.39	0
4	EDO	B	6	-	3,3,3	0.39	0	2,2,2	0.34	0
2	NAG	B	2	1	14,14,15	0.65	0	17,19,21	0.53	0
2	NAG	C	3	1	14,14,15	0.53	0	17,19,21	0.67	1 (5%)
4	EDO	B	11	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	D	14	-	3,3,3	0.41	0	2,2,2	0.40	0
4	EDO	C	15	-	3,3,3	0.41	0	2,2,2	0.40	0
2	NAG	A	1	1	14,14,15	0.51	0	17,19,21	0.66	1 (5%)
2	NAG	D	4	1	14,14,15	0.64	0	17,19,21	0.55	0
4	EDO	A	645	-	3,3,3	0.42	0	2,2,2	0.37	0
2	NAG	D	5	1	14,14,15	0.55	0	17,19,21	0.63	0
2	NAG	C	6	1	14,14,15	0.55	0	17,19,21	0.62	0
4	EDO	D	9	-	3,3,3	0.39	0	2,2,2	0.42	0
4	EDO	C	13	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EDO	C	2	-	3,3,3	0.41	0	2,2,2	0.37	0
2	NAG	A	8	1	14,14,15	0.56	0	17,19,21	0.63	0
4	EDO	D	12	-	3,3,3	0.50	0	2,2,2	0.30	0
4	EDO	D	645	-	3,3,3	0.39	0	2,2,2	0.37	0
4	EDO	A	4	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	B	645	-	3,3,3	0.38	0	2,2,2	0.40	0
2	NAG	B	7	1	14,14,15	0.56	0	17,19,21	0.63	0
4	EDO	C	10	-	3,3,3	0.40	0	2,2,2	0.39	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	EDO	A	646	-	-	0/1/1/1	-
4	EDO	B	6	-	-	0/1/1/1	-
2	NAG	B	2	1	-	4/6/23/26	0/1/1/1
2	NAG	C	3	1	-	4/6/23/26	0/1/1/1
4	EDO	B	11	-	-	0/1/1/1	-
4	EDO	D	14	-	-	0/1/1/1	-
4	EDO	C	15	-	-	0/1/1/1	-
2	NAG	A	1	1	-	3/6/23/26	0/1/1/1
2	NAG	D	4	1	-	4/6/23/26	0/1/1/1
4	EDO	A	645	-	-	0/1/1/1	-
2	NAG	D	5	1	-	4/6/23/26	0/1/1/1
2	NAG	C	6	1	-	4/6/23/26	0/1/1/1
4	EDO	D	9	-	-	0/1/1/1	-
4	EDO	C	13	-	-	0/1/1/1	-
4	EDO	C	2	-	-	0/1/1/1	-
2	NAG	A	8	1	-	4/6/23/26	0/1/1/1
4	EDO	D	12	-	-	1/1/1/1	-
4	EDO	D	645	-	-	0/1/1/1	-
4	EDO	A	4	-	-	0/1/1/1	-
4	EDO	B	645	-	-	0/1/1/1	-
2	NAG	B	7	1	-	4/6/23/26	0/1/1/1
4	EDO	C	10	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	NAG	C2-N2-C7	-2.10	120.08	122.90
2	A	1	NAG	C2-N2-C7	-2.04	120.16	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAG	C1-C2-N2-C7
2	A	1	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	8	NAG	C8-C7-N2-C2
2	A	8	NAG	O7-C7-N2-C2
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	7	NAG	C8-C7-N2-C2
2	B	7	NAG	O7-C7-N2-C2
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	C	6	NAG	C8-C7-N2-C2
2	C	6	NAG	O7-C7-N2-C2
2	D	4	NAG	C8-C7-N2-C2
2	D	4	NAG	O7-C7-N2-C2
2	D	5	NAG	C8-C7-N2-C2
2	D	5	NAG	O7-C7-N2-C2
2	A	1	NAG	C8-C7-N2-C2
2	D	5	NAG	O5-C5-C6-O6
2	A	8	NAG	O5-C5-C6-O6
2	B	7	NAG	O5-C5-C6-O6
2	A	8	NAG	C4-C5-C6-O6
2	D	5	NAG	C4-C5-C6-O6
2	B	7	NAG	C4-C5-C6-O6
2	C	6	NAG	O5-C5-C6-O6
2	C	6	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	D	4	NAG	C3-C2-N2-C7
2	C	3	NAG	C1-C2-N2-C7
4	D	12	EDO	O1-C1-C2-O2
2	D	4	NAG	C1-C2-N2-C7
2	C	3	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	6	EDO	1	0
2	B	2	NAG	2	0
2	A	1	NAG	1	0
2	D	4	NAG	2	0
4	C	13	EDO	1	0
4	D	645	EDO	1	0
4	A	4	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	555/574 (96%)	-1.42	0 100 100	9, 21, 39, 46	11 (1%)
1	B	555/574 (96%)	-1.42	0 100 100	9, 22, 40, 45	8 (1%)
1	C	555/574 (96%)	-1.43	0 100 100	13, 22, 39, 47	4 (0%)
1	D	555/574 (96%)	-1.42	0 100 100	9, 21, 39, 46	11 (1%)
All	All	2220/2296 (96%)	-1.42	0 100 100	9, 22, 39, 47	34 (1%)

There are no RSRZ outliers to report.

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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	0.95	0.07	48,53,55,56	0
2	NAG	B	2	14/15	0.96	0.06	49,54,56,56	0
2	NAG	C	3	14/15	0.96	0.07	48,53,54,55	0
2	NAG	C	6	14/15	0.96	0.08	54,57,59,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	5	14/15	0.96	0.09	55,59,60,61	0
4	EDO	B	6	4/4	0.96	0.13	38,40,41,41	0
4	EDO	D	645	4/4	0.96	0.13	38,39,39,41	0
2	NAG	A	8	14/15	0.97	0.09	56,60,61,62	0
4	EDO	A	4	4/4	0.97	0.11	37,39,40,40	0
2	NAG	B	7	14/15	0.97	0.08	54,58,59,60	0
2	NAG	D	4	14/15	0.97	0.07	49,54,57,57	0
4	EDO	C	13	4/4	0.98	0.09	39,41,41,41	0
4	EDO	D	12	4/4	0.98	0.07	39,39,39,40	0
4	EDO	B	11	4/4	0.99	0.06	34,36,38,40	0
4	EDO	C	2	4/4	0.99	0.04	31,31,31,32	0
4	EDO	A	646	4/4	0.99	0.04	24,26,28,29	0
4	EDO	C	15	4/4	0.99	0.05	39,39,41,43	0
4	EDO	A	645	4/4	0.99	0.05	30,30,31,31	0
4	EDO	D	9	4/4	0.99	0.03	24,25,27,29	0
4	EDO	B	645	4/4	0.99	0.03	24,25,27,29	0
4	EDO	D	14	4/4	0.99	0.06	40,42,43,45	0
3	NI	B	1	1/1	1.00	0.02	28,28,28,28	0
3	NI	A	2	1/1	1.00	0.01	28,28,28,28	0
4	EDO	C	10	4/4	1.00	0.04	25,27,29,30	0

6.5 Other polymers

There are no such residues in this entry.