Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2024 – 02:09 PM JST

PDB ID	:	8K2H
Title	:	Crystal structure of Group 2Oligosaccharide/Monosaccharide-releasing beta -N-acetylhexosaminidase NgaAt from Arabidopsis thaliana in complex with GalNAc-thiazoline
Authors	:	Sumida, T.; Fushinobu, S.
Deposited on	:	2023-07-12
Resolution	:	2.20 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:

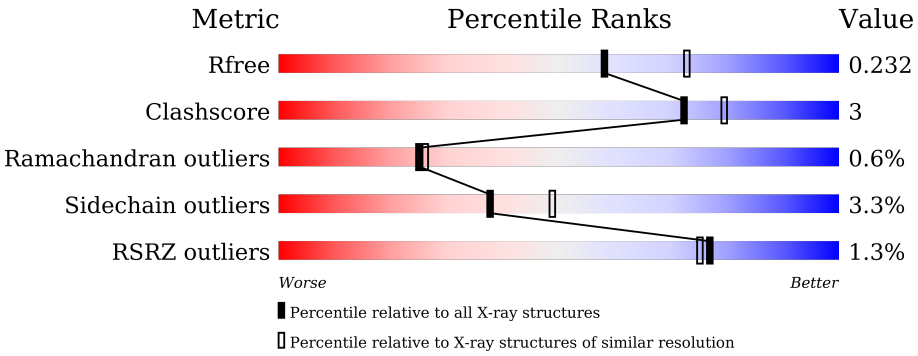
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

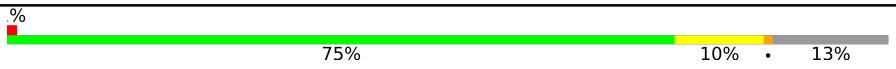
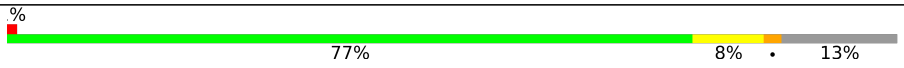
The reported resolution of this entry is 2.20 Å.

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	646	
1	B	646	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9285 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.

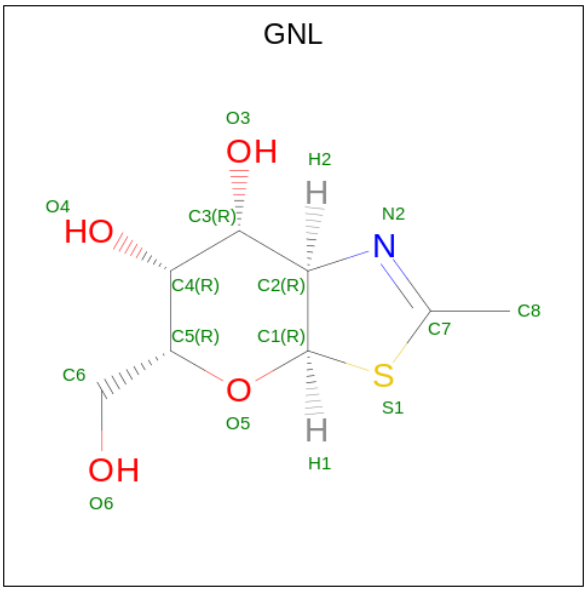
- Molecule 1 is a protein called Oligosaccharide/Monosaccharide-releasing beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	563	Total	C	N	O	S	0	1	0
			4493	2879	750	846	18			
1	A	560	Total	C	N	O	S	0	1	0
			4470	2867	747	838	18			

There are 6 discrepancies between the modelled and reference sequences:

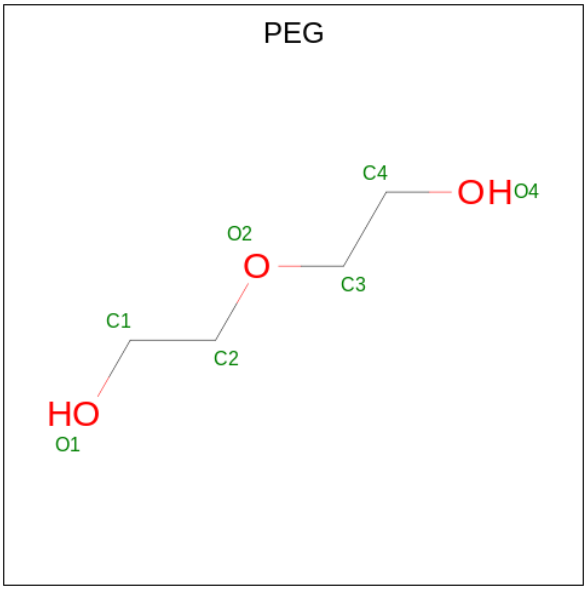
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q7Y231
B	-1	PRO	-	expression tag	UNP Q7Y231
B	0	GLY	-	expression tag	UNP Q7Y231
A	-2	GLY	-	expression tag	UNP Q7Y231
A	-1	PRO	-	expression tag	UNP Q7Y231
A	0	GLY	-	expression tag	UNP Q7Y231

- Molecule 2 is (3aR,5R,6R,7R,7aR)-5-(hydroxymethyl)-2-methyl-5,6,7,7a-tetrahydro-3aH-pyrano[3,2-d][1,3]thiazole-6,7-diol (three-letter code: GNL) (formula: $C_8H_{13}NO_4S$).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

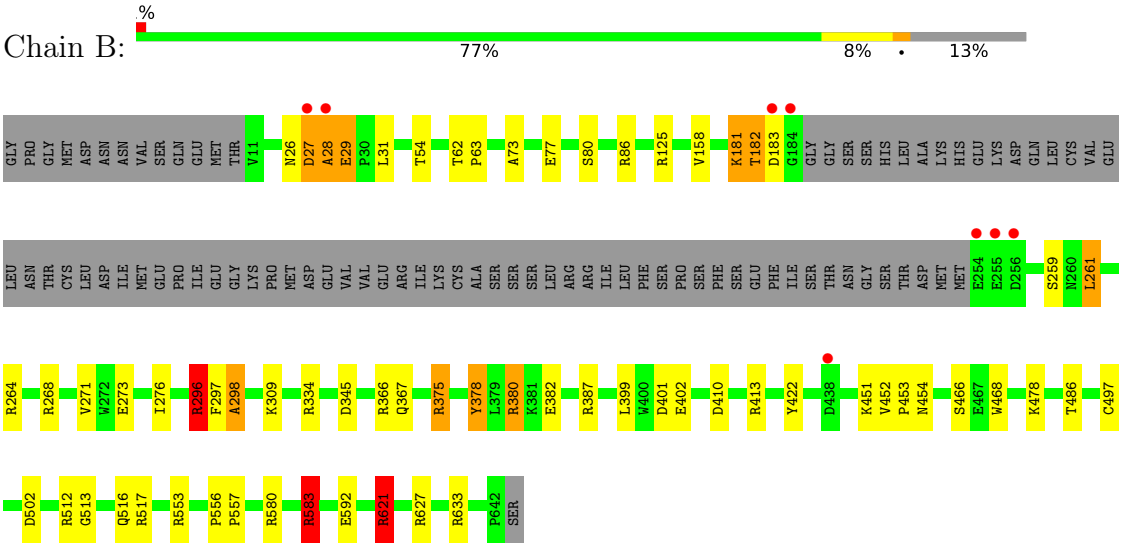
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	154	Total O 154 154	0	0
5	A	125	Total O 125 125	0	0

3 Residue-property plots (i)

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.

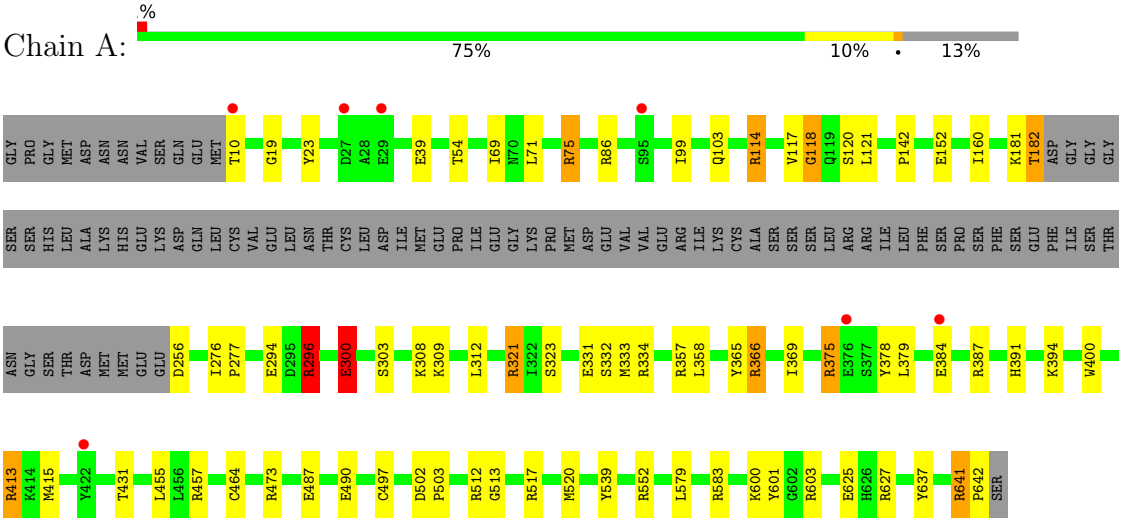
• Molecule 1: Oligosaccharide/Monosaccharide-releasing beta-N-acetylhexosaminidase

Chain B:



• Molecule 1: Oligosaccharide/Monosaccharide-releasing beta-N-acetylhexosaminidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.85Å 134.04Å 149.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.07 – 2.20 48.02 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.07-2.20) 100.0 (48.02-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.169 , 0.229 0.177 , 0.232	Depositor DCC
R_{free} test set	3690 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9285	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNL, CL, 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	0.73	4/4604 (0.1%)	1.11	17/6288 (0.3%)
1	B	0.76	4/4627 (0.1%)	1.13	20/6318 (0.3%)
All	All	0.75	8/9231 (0.1%)	1.12	37/12606 (0.3%)

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	12
1	B	0	9
All	All	0	21

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CD-OE1	6.59	1.32	1.25
1	B	296	ARG	CD-NE	-6.06	1.36	1.46
1	B	273	GLU	CD-OE1	5.90	1.32	1.25
1	A	300	GLU	CD-OE2	5.86	1.32	1.25
1	A	152	GLU	CD-OE2	5.80	1.32	1.25
1	B	77	GLU	CD-OE2	5.61	1.31	1.25
1	B	402	GLU	CD-OE1	-5.43	1.19	1.25
1	A	294	GLU	CD-OE1	5.03	1.31	1.25

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	ARG	NE-CZ-NH2	-19.05	110.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	ARG	NE-CZ-NH2	-12.61	113.99	120.30
1	A	296	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	A	86	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	B	413	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	296	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	517	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	357	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	B	86	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	297	PHE	C-N-CA	-6.70	104.96	121.70
1	A	75	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	39	GLU	CB-CA-C	-6.65	97.10	110.40
1	B	583	ARG	CD-NE-CZ	6.62	132.87	123.60
1	A	357	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	86	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	268	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	580	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	B	633	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	603	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	256	ASP	CB-CA-C	6.02	122.43	110.40
1	B	583	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	268	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	321	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	297	PHE	CB-CA-C	5.59	121.58	110.40
1	A	366	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	114	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	297	PHE	O-C-N	-5.49	113.92	122.70
1	B	410	ASP	CB-CA-C	-5.39	99.61	110.40
1	B	334	ARG	CB-CA-C	-5.39	99.62	110.40
1	A	520	MET	CG-SD-CE	5.37	108.80	100.20
1	B	125	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	86	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	486	THR	CA-CB-OG1	-5.29	97.90	109.00
1	B	298	ALA	CB-CA-C	5.17	117.86	110.10
1	A	603	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	264	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	387	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	118	GLY	Peptide
1	A	296	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	512	ARG	Sidechain
1	A	517	ARG	Sidechain
1	A	552	ARG	Sidechain
1	A	627	ARG	Sidechain
1	A	641	ARG	Sidechain
1	B	182	THR	Peptide
1	B	296	ARG	Sidechain
1	B	298	ALA	Mainchain
1	B	380	ARG	Sidechain
1	B	512	ARG	Sidechain
1	B	553	ARG	Sidechain
1	B	583	ARG	Sidechain
1	B	621	ARG	Sidechain
1	B	627	ARG	Sidechain

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	4470	0	4363	33	0
1	B	4493	0	4375	28	0
2	A	14	0	13	0	0
2	B	14	0	13	1	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
4	A	1	0	0	0	0
5	A	125	0	0	1	0
5	B	154	0	0	1	0
All	All	9285	0	8784	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (61) 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:69:ILE:HD12	1:A:69:ILE:N	2.01	0.76
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.51	0.73
1:B:466:SER:OG	1:B:468[A]:TRP:CD1	2.48	0.66
1:A:457:ARG:NH1	1:A:490:GLU:OE1	2.30	0.64
1:A:375:ARG:HG2	1:A:375:ARG:HH11	1.63	0.63
1:A:300:GLU:H	1:A:300:GLU:CD	2.01	0.62
1:A:181:LYS:O	1:A:182:THR:C	2.36	0.62
1:A:413:ARG:NH1	1:A:455:LEU:O	2.32	0.60
1:B:28:ALA:O	1:B:29:GLU:HB3	2.01	0.59
1:A:600:LYS:HB3	1:A:601:TYR:CD2	2.38	0.58
1:A:641:ARG:N	1:A:642:PRO:HD2	2.21	0.56
1:B:452:VAL:N	1:B:453:PRO:CD	2.68	0.56
1:B:27:ASP:O	1:B:29:GLU:N	2.38	0.56
1:A:117:VAL:O	1:A:118:GLY:C	2.41	0.55
1:B:621:ARG:HB2	1:B:621:ARG:NH1	2.22	0.54
1:A:69:ILE:N	1:A:69:ILE:CD1	2.69	0.54
1:B:375:ARG:HG3	1:B:375:ARG:NH1	2.22	0.53
1:B:375:ARG:NH1	1:B:375:ARG:CG	2.72	0.53
1:B:375:ARG:HH11	1:B:375:ARG:CG	2.21	0.51
1:B:62:THR:HG22	1:B:63:PRO:HD2	1.94	0.50
1:A:332:SER:O	1:A:400:TRP:CH2	2.65	0.50
1:A:121:LEU:HD12	1:A:160:ILE:HG12	1.93	0.49
1:B:73:ALA:O	1:B:271:VAL:HA	2.11	0.49
1:A:365:TYR:CZ	1:A:415:MET:HG2	2.48	0.49
1:A:296:ARG:HD2	5:A:879:HOH:O	2.13	0.48
1:B:583:ARG:HD2	5:B:867:HOH:O	2.13	0.47
1:A:375:ARG:HH11	1:A:375:ARG:CG	2.26	0.47
1:A:391:HIS:HB2	1:A:394:LYS:HE2	1.97	0.47
1:A:276:ILE:O	1:A:277:PRO:C	2.52	0.47
1:A:637:TYR:CE1	1:A:641:ARG:HD2	2.50	0.47
1:A:300:GLU:HG2	1:A:303:SER:HB3	1.96	0.47
1:A:312:LEU:C	1:A:312:LEU:HD23	2.34	0.47
1:B:367:GLN:HG3	1:B:378:TYR:CG	2.50	0.47
1:A:54:THR:O	1:A:513:GLY:HA3	2.15	0.47
1:B:276:ILE:HG23	1:B:592:GLU:HG3	1.96	0.46
1:A:375:ARG:CZ	1:A:375:ARG:HB3	2.46	0.46
1:A:332:SER:O	1:A:400:TRP:CZ3	2.69	0.46
1:B:54:THR:O	1:B:513:GLY:HA3	2.15	0.45
1:A:579:LEU:O	1:A:583:ARG:HD3	2.16	0.45
1:B:366:ARG:HH11	1:B:366:ARG:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:HB3	1:A:358:LEU:HD12	1.99	0.45
1:B:401:ASP:OD1	2:B:701:GNL:N2	2.51	0.44
1:A:366:ARG:HB3	1:A:375:ARG:HD2	2.00	0.44
1:A:431:THR:HA	1:A:464:CYS:O	2.18	0.44
1:B:181:LYS:HA	1:B:181:LYS:HD2	1.54	0.43
1:B:380:ARG:HG3	1:B:422:TYR:CD1	2.53	0.43
1:B:366:ARG:HB2	1:B:366:ARG:NH1	2.33	0.43
1:B:451:LYS:HD3	1:B:454:ASN:HD22	1.83	0.43
1:B:309:LYS:HD3	1:B:309:LYS:HA	1.91	0.43
1:A:366:ARG:CB	1:A:375:ARG:HD2	2.49	0.42
1:A:69:ILE:HG22	1:A:71:LEU:HG	2.00	0.42
1:A:309:LYS:HD3	1:A:309:LYS:HA	1.78	0.42
1:A:375:ARG:CG	1:A:375:ARG:NH1	2.82	0.41
1:B:28:ALA:O	1:B:29:GLU:CB	2.68	0.41
1:B:516:GLN:OE1	1:B:583:ARG:HG2	2.20	0.41
1:B:556:PRO:HA	1:B:557:PRO:HD3	2.00	0.41
1:B:378:TYR:CZ	1:B:382:GLU:HG3	2.56	0.41
1:B:80:SER:HA	1:B:158:VAL:O	2.21	0.40
1:A:19:GLY:HA3	1:A:23:TYR:CD2	2.57	0.40
1:A:103:GLN:HA	1:A:142:PRO:O	2.21	0.40
1:B:259:SER:OG	1:B:261:LEU:HB2	2.21	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	557/646 (86%)	543 (98%)	12 (2%)	2 (0%)	34	37
1	B	560/646 (87%)	544 (97%)	11 (2%)	5 (1%)	17	16
All	All	1117/1292 (86%)	1087 (97%)	23 (2%)	7 (1%)	25	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ALA
1	B	26	ASN
1	B	183	ASP
1	B	29	GLU
1	A	497	CYS
1	B	497	CYS
1	A	333	MET

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	490/566 (87%)	473 (96%)	17 (4%)	36	46
1	B	492/566 (87%)	477 (97%)	15 (3%)	41	53
All	All	982/1132 (87%)	950 (97%)	32 (3%)	38	49

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	ASP
1	B	31	LEU
1	B	181	LYS
1	B	182	THR
1	B	261	LEU
1	B	296	ARG
1	B	345	ASP
1	B	375	ARG
1	B	378	TYR
1	B	387	ARG
1	B	399	LEU
1	B	478	LYS
1	B	502	ASP
1	B	583	ARG
1	B	621	ARG
1	A	75	ARG

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	120	SER
1	A	182	THR
1	A	300	GLU
1	A	308	LYS
1	A	369	ILE
1	A	375	ARG
1	A	378	TYR
1	A	379	LEU
1	A	384	GLU
1	A	473	ARG
1	A	487	GLU
1	A	502	ASP
1	A	503	PRO
1	A	539	TYR
1	A	625	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	ASN
1	A	504	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GNL	B	701	-	13,15,15	2.38	3 (23%)	12,22,22	1.46	2 (16%)
3	PEG	A	702	-	6,6,6	0.43	0	5,5,5	0.24	0
2	GNL	A	701	-	13,15,15	1.17	1 (7%)	12,22,22	0.94	1 (8%)
3	PEG	B	702	-	6,6,6	0.27	0	5,5,5	0.24	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNL	B	701	-	-	0/2/30/30	0/2/2/2
3	PEG	A	702	-	-	4/4/4/4	-
2	GNL	A	701	-	-	0/2/30/30	0/2/2/2
3	PEG	B	702	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GNL	C7-S1	7.53	1.83	1.77
2	A	701	GNL	C7-S1	-3.43	1.74	1.77
2	B	701	GNL	C7-N2	2.83	1.29	1.27
2	B	701	GNL	O5-C1	-2.10	1.39	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	GNL	O3-C3-C2	3.93	118.12	109.14
2	B	701	GNL	C1-O5-C5	2.27	116.77	112.58
2	A	701	GNL	O3-C3-C2	2.11	113.96	109.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	PEG	O2-C3-C4-O4
3	A	702	PEG	O1-C1-C2-O2
3	A	702	PEG	O2-C3-C4-O4
3	A	702	PEG	C1-C2-O2-C3
3	B	702	PEG	C1-C2-O2-C3
3	A	702	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	GNL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	560/646 (86%)	-0.34	7 (1%)	77	75	28, 45, 82, 131	0
1	B	563/646 (87%)	-0.38	8 (1%)	75	73	26, 39, 72, 141	0
All	All	1123/1292 (86%)	-0.36	15 (1%)	77	75	26, 42, 77, 141	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	GLY	9.5
1	B	183	ASP	7.7
1	B	254	GLU	7.0
1	B	255	GLU	4.2
1	B	27	ASP	4.2
1	A	27	ASP	4.0
1	B	28	ALA	3.8
1	A	422	TYR	3.7
1	A	376	GLU	3.6
1	B	256	ASP	3.5
1	A	29	GLU	2.5
1	A	10	THR	2.2
1	B	438	ASP	2.1
1	A	384	GLU	2.1
1	A	95	SER	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

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. 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	B-factors(Å^2)	Q<0.9
3	PEG	B	702	7/7	0.92	0.09	49,56,59,61	0
3	PEG	A	702	7/7	0.94	0.12	54,65,66,72	0
4	CL	A	703	1/1	0.95	0.07	65,65,65,65	0
2	GNL	A	701	14/14	0.97	0.09	29,34,37,38	0
2	GNL	B	701	14/14	0.98	0.09	29,32,35,35	0

6.5 Other polymers

There are no such residues in this entry.