



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 8K2I / pdb_00008k2i
Title : Crystal structure of Group 2 Oligosaccharide/Monosaccharide-releasing β -N-acetylhexosaminidase NgaAt from *Arabidopsis thaliana* in complex with GlcNAc-thiazoline
Authors : Sumida, T.; Fushinobu, S.
Deposited on : 2023-07-12
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

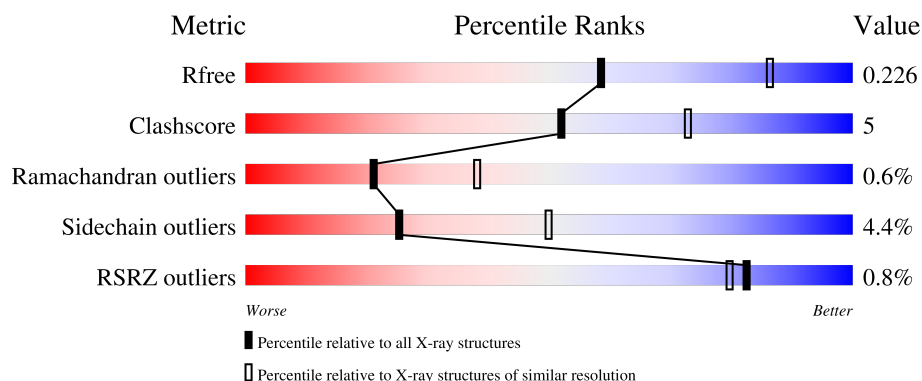
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	646	
1	B	646	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9217 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.

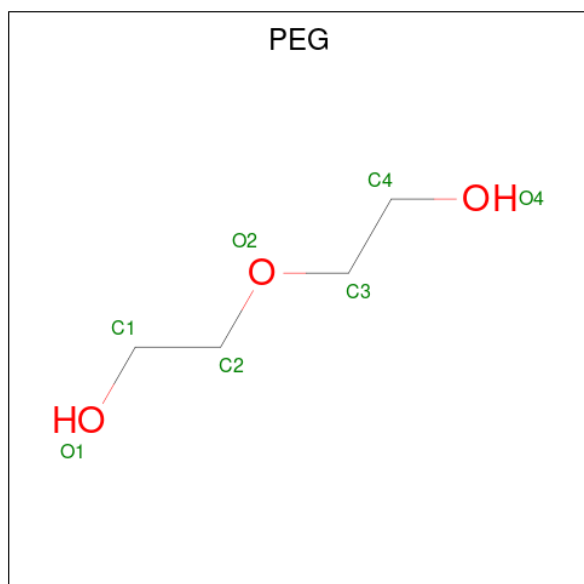
- Molecule 1 is a protein called Oligosaccharide/Monosaccharide-releasing beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	559	Total	C	N	O	S	0	1	0
			4463	2863	746	836	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:

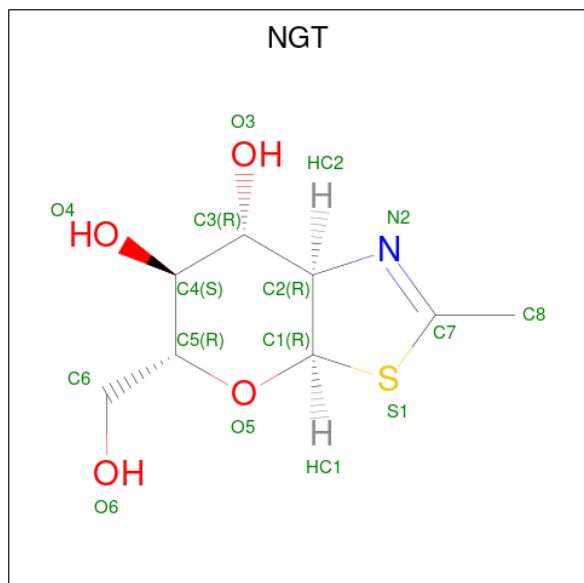
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q7Y231
B	-1	PRO	-	expression tag	UNP Q7Y231
B	0	GLY	-	expression tag	UNP Q7Y231
A	-2	GLY	-	expression tag	UNP Q7Y231
A	-1	PRO	-	expression tag	UNP Q7Y231
A	0	GLY	-	expression tag	UNP Q7Y231

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 3 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (CCD ID: NGT) (formula: C₈H₁₃NO₄S).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	136	Total	O	0	0
			136	136		

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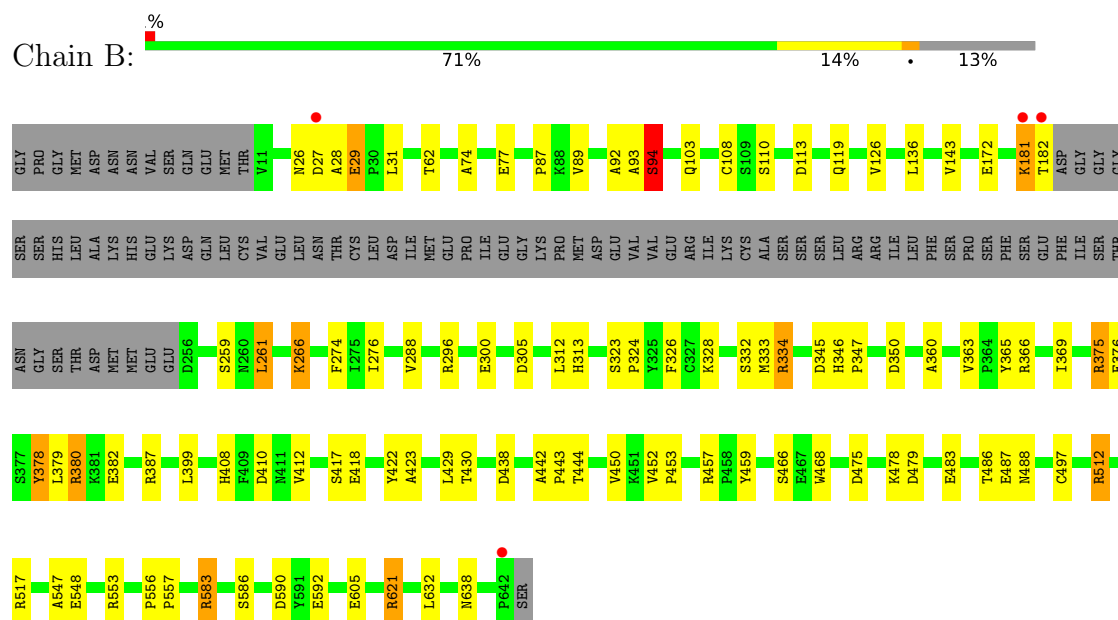
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total 105	O 105	0	0

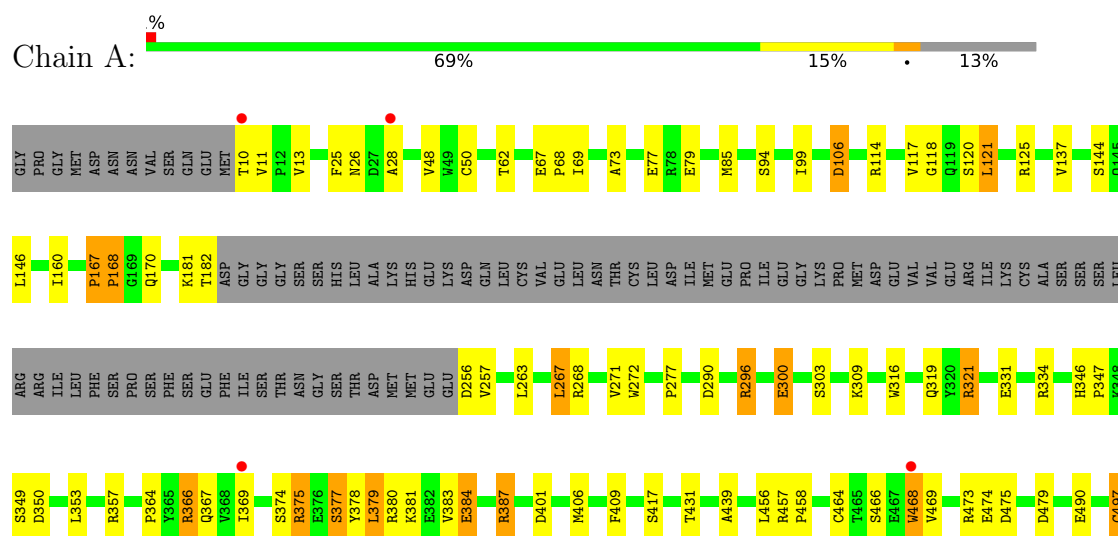
3 Residue-property plots [i](#)

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



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.28Å 133.83Å 150.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.71 – 2.50 47.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.71-2.50) 100.0 (47.71-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.157 , 0.230 0.165 , 0.226	Depositor DCC
R_{free} test set	2489 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9217	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NGT, CL

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	0.93	0/4604	1.44	28/6288 (0.4%)
1	B	0.96	2/4597 (0.0%)	1.44	30/6278 (0.5%)
All	All	0.94	2/9201 (0.0%)	1.44	58/12566 (0.5%)

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	15
1	B	0	9
All	All	0	24

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	350	ASP	CG-OD1	6.03	1.36	1.25
1	B	94	SER	CA-CB	-5.18	1.46	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	THR	CA-CB-OG1	-10.23	94.26	109.60
1	B	488	ASN	CB-CA-C	-8.28	97.69	111.02
1	B	89	VAL	CA-C-O	-7.21	114.21	121.49
1	A	502	ASP	CB-CA-C	7.07	120.68	109.52
1	A	300	GLU	CB-CG-CD	6.97	124.44	112.60
1	B	62	THR	CA-CB-OG1	-6.90	99.25	109.60
1	A	77	GLU	CB-CG-CD	6.86	124.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ASP	CA-CB-CG	-6.72	105.88	112.60
1	A	25	PHE	CA-CB-CG	6.67	120.47	113.80
1	A	106	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	256	ASP	CB-CA-C	6.51	122.47	110.10
1	A	256	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	300	GLU	CB-CA-C	6.22	119.17	109.84
1	B	363	VAL	CA-C-O	6.16	125.53	119.62
1	A	526	GLU	CB-CG-CD	6.12	123.01	112.60
1	B	266	LYS	CB-CA-C	6.05	120.33	110.22
1	B	410	ASP	CB-CA-C	-5.97	101.50	110.88
1	B	590	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	350	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	479	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	87	PRO	CB-CA-C	-5.87	103.89	111.46
1	B	638	ASN	N-CA-CB	5.80	119.28	110.28
1	B	457	ARG	O-C-N	-5.73	116.68	121.38
1	A	384	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	623	THR	CA-CB-OG1	-5.72	101.02	109.60
1	B	77	GLU	CB-CG-CD	5.67	122.25	112.60
1	A	633	ARG	CA-C-N	5.67	126.39	120.03
1	A	633	ARG	C-N-CA	5.67	126.39	120.03
1	A	479	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	79	GLU	CB-CG-CD	5.64	122.18	112.60
1	A	167	PRO	N-CA-C	5.61	117.55	110.70
1	B	438	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	313	HIS	CA-CB-CG	-5.49	108.31	113.80
1	A	331	GLU	CB-CG-CD	5.46	121.89	112.60
1	A	475	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	290	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	62	THR	CB-CA-C	5.41	116.50	108.87
1	B	305	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	272	TRP	CA-C-N	5.31	127.82	120.29
1	A	272	TRP	C-N-CA	5.31	127.82	120.29
1	B	345	ASP	CA-CB-CG	-5.30	107.30	112.60
1	B	324	PRO	CB-CA-C	-5.29	104.30	111.12
1	A	559	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	475	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	312	LEU	CA-C-N	5.26	127.59	120.65
1	B	312	LEU	C-N-CA	5.26	127.59	120.65
1	B	376	GLU	CB-CG-CD	5.23	121.49	112.60
1	B	332	SER	CA-C-N	5.23	131.47	123.47
1	B	332	SER	C-N-CA	5.23	131.47	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	GLU	CB-CG-CD	5.19	121.43	112.60
1	A	582	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	517	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	B	583	ARG	N-CA-CB	5.16	118.24	110.30
1	A	257	VAL	CB-CA-C	-5.15	104.81	111.20
1	A	137	VAL	N-CA-C	5.13	113.52	107.77
1	B	444	THR	CA-CB-OG1	5.12	117.28	109.60
1	B	586	SER	N-CA-C	-5.12	105.78	111.36
1	A	502	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	THR	Peptide
1	A	114	ARG	Sidechain
1	A	28	ALA	Peptide
1	A	296	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	334	ARG	Sidechain
1	A	357	ARG	Sidechain
1	A	380	ARG	Sidechain
1	A	387	ARG	Sidechain
1	A	473	ARG	Sidechain
1	A	512	ARG	Sidechain
1	A	517	ARG	Sidechain
1	A	522	ARG	Sidechain
1	A	627	ARG	Sidechain
1	A	641	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	333	MET	Peptide
1	B	334	ARG	Sidechain
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	94	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	4470	0	4363	46	0
1	B	4463	0	4356	44	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
3	A	14	0	13	2	0
3	B	14	0	13	0	0
4	A	1	0	0	1	0
5	A	105	0	0	0	0
5	B	136	0	0	0	0
All	All	9217	0	8765	90	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 (90) 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:466:SER:HG	1:B:468[A]:TRP:CD1	1.91	0.89
1:B:378:TYR:CE2	1:B:382:GLU:HG3	2.16	0.80
1:B:375:ARG:HG3	1:B:375:ARG:HH11	1.48	0.78
1:B:466:SER:OG	1:B:468[A]:TRP:CD1	2.38	0.76
1:A:466:SER:HG	1:A:468[A]:TRP:CD1	2.09	0.71
1:A:387:ARG:HG3	1:A:387:ARG:HH11	1.57	0.68
1:B:103:GLN:HG3	1:B:143:VAL:HG22	1.79	0.64
1:A:26:ASN:O	1:A:26:ASN:OD1	2.16	0.63
1:A:377:SER:O	1:A:381:LYS:HG3	1.99	0.63
1:B:346:HIS:ND1	1:B:347:PRO:HD2	2.15	0.61
1:B:369:ILE:O	1:B:369:ILE:HD12	2.00	0.61
1:A:316:TRP:O	1:A:319:GLN:HG2	2.02	0.60
1:A:69:ILE:HD12	1:A:69:ILE:N	2.17	0.59
1:B:366:ARG:HH11	1:B:366:ARG:CB	2.14	0.59
1:A:379:LEU:O	1:A:383:VAL:HG23	2.03	0.59
1:A:26:ASN:O	1:A:26:ASN:CG	2.46	0.59
1:B:375:ARG:HH11	1:B:375:ARG:CG	2.17	0.58
1:B:380:ARG:HG3	1:B:422:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ALA:O	1:A:271:VAL:HA	2.06	0.55
1:B:365:TYR:OH	1:B:418:GLU:OE1	2.26	0.54
1:A:532:LEU:C	1:A:532:LEU:HD23	2.33	0.53
1:A:117:VAL:O	1:A:118:GLY:C	2.47	0.53
1:A:50:CYS:SG	1:A:69:ILE:HD11	2.48	0.53
1:A:181:LYS:O	1:A:182:THR:C	2.53	0.52
1:A:406:MET:HE2	1:A:439:ALA:HB3	1.90	0.52
1:A:409:PHE:HD1	1:A:456:LEU:HD21	1.75	0.52
1:A:641:ARG:HD2	4:A:703:CL:CL	2.47	0.52
1:B:181:LYS:HD2	1:B:182:THR:N	2.25	0.52
1:B:288:VAL:O	1:B:326:PHE:HA	2.11	0.51
1:B:452:VAL:N	1:B:453:PRO:CD	2.74	0.51
1:A:263:LEU:HD23	1:A:263:LEU:C	2.35	0.50
1:A:457:ARG:NH1	1:A:490:GLU:OE2	2.44	0.50
1:B:378:TYR:C	1:B:378:TYR:CD1	2.88	0.50
1:A:167:PRO:O	1:A:168:PRO:O	2.30	0.50
1:B:126:VAL:HG22	1:B:136:LEU:HD23	1.93	0.49
1:A:167:PRO:C	1:A:168:PRO:O	2.54	0.49
1:A:366:ARG:HB3	1:A:375:ARG:HD2	1.95	0.49
1:B:366:ARG:NH1	1:B:366:ARG:HB2	2.28	0.48
1:A:566:GLY:HA2	1:A:576:VAL:HG23	1.96	0.47
1:B:369:ILE:HD12	1:B:369:ILE:C	2.39	0.47
1:A:641:ARG:N	1:A:642:PRO:CD	2.77	0.47
1:B:92:ALA:O	1:B:94:SER:N	2.47	0.47
1:A:613:THR:O	1:A:628:PRO:HB3	2.14	0.47
1:B:172:GLU:OE1	1:B:266:LYS:NZ	2.40	0.47
1:B:378:TYR:CD1	1:B:379:LEU:N	2.83	0.47
1:A:121:LEU:HD12	1:A:160:ILE:HG12	1.96	0.46
1:B:387:ARG:HD2	1:B:423:ALA:HB2	1.97	0.46
1:A:296:ARG:NH2	1:A:547:ALA:O	2.45	0.46
1:A:48:VAL:HG22	1:A:85:MET:HG2	1.98	0.46
1:A:364:PRO:HG2	1:A:378:TYR:OH	2.16	0.46
1:A:401:ASP:OD1	3:A:702:NGT:N2	2.49	0.46
1:B:417:SER:HB3	1:B:459:TYR:CE1	2.52	0.45
1:A:497:CYS:HB3	3:A:702:NGT:S1	2.56	0.45
1:B:28:ALA:O	1:B:29:GLU:HB3	2.16	0.45
1:B:429:LEU:HD23	1:B:430:THR:N	2.31	0.45
1:A:431:THR:HA	1:A:464:CYS:O	2.17	0.44
1:B:366:ARG:HH11	1:B:366:ARG:HB3	1.79	0.44
1:A:387:ARG:HG3	1:A:387:ARG:NH1	2.31	0.44
1:A:505:PRO:O	1:A:506:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ALA:O	1:B:93:ALA:C	2.60	0.44
1:B:442:ALA:HB1	1:B:443:PRO:CD	2.48	0.44
1:A:349:SER:O	1:A:353:LEU:HG	2.18	0.43
1:B:259:SER:OG	1:B:261:LEU:HB2	2.17	0.43
1:A:504:HIS:HD2	1:A:522:ARG:HH12	1.67	0.43
1:A:267:LEU:HD12	1:A:267:LEU:N	2.34	0.43
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.73	0.42
1:A:346:HIS:ND1	1:A:347:PRO:HD2	2.34	0.42
1:B:126:VAL:HG22	1:B:136:LEU:CD2	2.48	0.42
1:A:167:PRO:O	1:A:168:PRO:C	2.59	0.42
1:A:106:ASP:OD1	1:A:117:VAL:HG23	2.20	0.42
1:B:108:CYS:HA	1:B:113:ASP:O	2.19	0.42
1:B:547:ALA:O	1:B:548:GLU:C	2.61	0.42
1:B:74:ALA:HB1	1:B:274:PHE:O	2.20	0.42
1:B:452:VAL:N	1:B:453:PRO:HD2	2.33	0.42
1:B:366:ARG:CB	1:B:366:ARG:NH1	2.83	0.42
1:B:408:HIS:O	1:B:412:VAL:HG23	2.20	0.41
1:B:450:VAL:O	1:B:483:GLU:HG3	2.19	0.41
1:B:632:LEU:C	1:B:632:LEU:HD23	2.45	0.41
1:B:556:PRO:O	1:B:557:PRO:C	2.61	0.41
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.51	0.41
1:A:267:LEU:C	1:A:268:ARG:HG3	2.41	0.41
1:B:92:ALA:C	1:B:94:SER:H	2.29	0.41
1:B:276:ILE:HG23	1:B:592:GLU:HG3	2.03	0.41
1:B:323:SER:HB3	1:B:360:ALA:O	2.20	0.41
1:B:375:ARG:CG	1:B:375:ARG:NH1	2.77	0.40
1:B:181:LYS:HD2	1:B:182:THR:H	1.84	0.40
1:A:125:ARG:HD3	1:A:146:LEU:CD1	2.51	0.40
1:A:125:ARG:HD3	1:A:146:LEU:HD12	2.02	0.40
1:A:277:PRO:O	1:A:321:ARG:NH2	2.52	0.40
1:A:584:LEU:HD12	1:A:584:LEU:C	2.47	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	557/646 (86%)	536 (96%)	18 (3%)	3 (0%)	24	43
1	B	556/646 (86%)	533 (96%)	19 (3%)	4 (1%)	18	34
All	All	1113/1292 (86%)	1069 (96%)	37 (3%)	7 (1%)	21	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO
1	B	26	ASN
1	B	29	GLU
1	A	497	CYS
1	B	334	ARG
1	B	497	CYS
1	A	303	SER

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	490/566 (87%)	461 (94%)	29 (6%)	18	37
1	B	489/566 (86%)	474 (97%)	15 (3%)	35	62
All	All	979/1132 (86%)	935 (96%)	44 (4%)	25	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	ASP
1	B	31	LEU
1	B	110	SER
1	B	119	GLN
1	B	181	LYS
1	B	261	LEU

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Mol	Chain	Res	Type
1	B	300	GLU
1	B	328	LYS
1	B	375	ARG
1	B	378	TYR
1	B	399	LEU
1	B	478	LYS
1	B	512	ARG
1	B	605	GLU
1	B	621	ARG
1	A	11	VAL
1	A	13	VAL
1	A	94	SER
1	A	99	ILE
1	A	120	SER
1	A	121	LEU
1	A	144	SER
1	A	170	GLN
1	A	267	LEU
1	A	300	GLU
1	A	366	ARG
1	A	367	GLN
1	A	369	ILE
1	A	374	SER
1	A	375	ARG
1	A	377	SER
1	A	379	LEU
1	A	384	GLU
1	A	417	SER
1	A	458	PRO
1	A	468[A]	TRP
1	A	468[B]	TRP
1	A	469	VAL
1	A	474	GLU
1	A	532	LEU
1	A	584	LEU
1	A	600	LYS
1	A	625	GLU
1	A	641	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	GLN
1	B	103	GLN
1	A	70	ASN
1	A	119	GLN
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 oligosaccharides 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	PEG	A	701	-	6,6,6	0.36	0	5,5,5	0.37	0
3	NGT	A	702	-	13,15,15	1.10	1 (7%)	14,22,22	0.98	1 (7%)
2	PEG	B	701	-	6,6,6	0.34	0	5,5,5	0.30	0
3	NGT	B	702	-	13,15,15	1.68	1 (7%)	14,22,22	1.33	4 (28%)

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	PEG	A	701	-	-	2/4/4/4	-
3	NGT	A	702	-	-	0/2/30/30	0/2/2/2
2	PEG	B	701	-	-	2/4/4/4	-
3	NGT	B	702	-	-	0/2/30/30	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NGT	C7-S1	-5.79	1.72	1.77
3	A	702	NGT	C7-S1	-2.96	1.74	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NGT	O3-C3-C2	2.95	115.63	109.16
3	B	702	NGT	C3-C4-C5	-2.19	106.27	110.23
3	B	702	NGT	O3-C3-C4	-2.07	105.50	110.38
3	B	702	NGT	C1-O5-C5	2.01	116.17	112.56
3	A	702	NGT	C1-O5-C5	2.01	116.17	112.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	PEG	O2-C3-C4-O4
2	A	701	PEG	O1-C1-C2-O2
2	B	701	PEG	C1-C2-O2-C3
2	A	701	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NGT	2	0

5.7 Other polymers [i](#)

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 [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	560/646 (86%)	-0.43	5 (0%)	81 78	32, 57, 94, 151	1 (0%)
1	B	559/646 (86%)	-0.59	4 (0%)	84 81	23, 49, 83, 157	1 (0%)
All	All	1119/1292 (86%)	-0.51	9 (0%)	82 80	23, 53, 89, 157	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	642	PRO	4.0
1	A	10	THR	3.2
1	A	468[A]	TRP	3.2
1	B	642	PRO	3.0
1	A	369	ILE	2.7
1	A	28	ALA	2.4
1	B	182	THR	2.3
1	B	181	LYS	2.1
1	B	27	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	PEG	B	701	7/7	0.93	0.10	59,66,74,80	0
2	PEG	A	701	7/7	0.93	0.11	58,73,80,81	0
4	CL	A	703	1/1	0.95	0.08	82,82,82,82	0
3	NGT	A	702	14/14	0.99	0.04	41,45,51,51	0
3	NGT	B	702	14/14	0.99	0.04	37,41,47,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.