



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:55 AM UTC

PDB ID : 7FE3 / pdb_00007fe3
Title : Crystal structure of GH65 alpha-1,2-glucosidase from *Flavobacterium johnsoniae*
Authors : Nakamura, S.; Miyazaki, T.
Deposited on : 2021-07-19
Resolution : 1.54 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

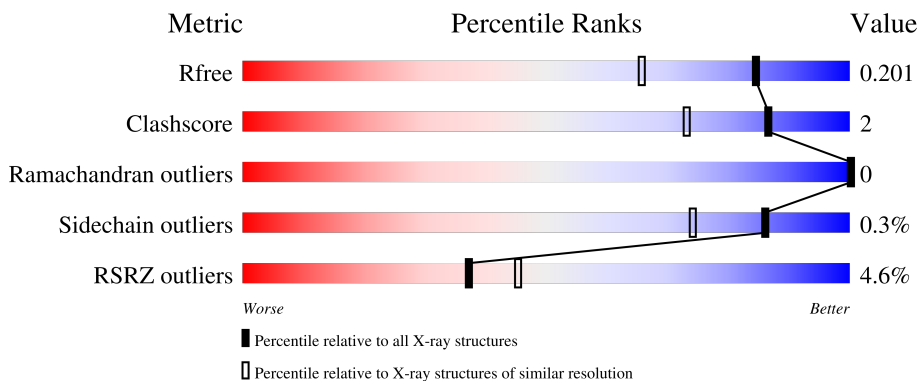
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	678	
1	B	678	
1	C	678	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17514 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 Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	659	5330	3392	898	1018	22	0	11	0
1	B	659	5305	3378	894	1011	22	0	8	0
1	C	659	5323	3390	896	1014	23	0	10	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP A5FBJ5
A	5	GLY	-	expression tag	UNP A5FBJ5
A	6	SER	-	expression tag	UNP A5FBJ5
A	7	SER	-	expression tag	UNP A5FBJ5
A	8	HIS	-	expression tag	UNP A5FBJ5
A	9	HIS	-	expression tag	UNP A5FBJ5
A	10	HIS	-	expression tag	UNP A5FBJ5
A	11	HIS	-	expression tag	UNP A5FBJ5
A	12	HIS	-	expression tag	UNP A5FBJ5
A	13	HIS	-	expression tag	UNP A5FBJ5
A	14	SER	-	expression tag	UNP A5FBJ5
A	15	SER	-	expression tag	UNP A5FBJ5
A	16	GLY	-	expression tag	UNP A5FBJ5
A	17	LEU	-	expression tag	UNP A5FBJ5
A	18	VAL	-	expression tag	UNP A5FBJ5
A	19	PRO	-	expression tag	UNP A5FBJ5
A	20	ARG	-	expression tag	UNP A5FBJ5
A	21	GLY	-	expression tag	UNP A5FBJ5
A	22	SER	-	expression tag	UNP A5FBJ5
A	23	HIS	-	expression tag	UNP A5FBJ5
B	4	MET	-	initiating methionine	UNP A5FBJ5
B	5	GLY	-	expression tag	UNP A5FBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
B	13	HIS	-	expression tag	UNP A5FBJ5
B	14	SER	-	expression tag	UNP A5FBJ5
B	15	SER	-	expression tag	UNP A5FBJ5
B	16	GLY	-	expression tag	UNP A5FBJ5
B	17	LEU	-	expression tag	UNP A5FBJ5
B	18	VAL	-	expression tag	UNP A5FBJ5
B	19	PRO	-	expression tag	UNP A5FBJ5
B	20	ARG	-	expression tag	UNP A5FBJ5
B	21	GLY	-	expression tag	UNP A5FBJ5
B	22	SER	-	expression tag	UNP A5FBJ5
B	23	HIS	-	expression tag	UNP A5FBJ5
C	4	MET	-	initiating methionine	UNP A5FBJ5
C	5	GLY	-	expression tag	UNP A5FBJ5
C	6	SER	-	expression tag	UNP A5FBJ5
C	7	SER	-	expression tag	UNP A5FBJ5
C	8	HIS	-	expression tag	UNP A5FBJ5
C	9	HIS	-	expression tag	UNP A5FBJ5
C	10	HIS	-	expression tag	UNP A5FBJ5
C	11	HIS	-	expression tag	UNP A5FBJ5
C	12	HIS	-	expression tag	UNP A5FBJ5
C	13	HIS	-	expression tag	UNP A5FBJ5
C	14	SER	-	expression tag	UNP A5FBJ5
C	15	SER	-	expression tag	UNP A5FBJ5
C	16	GLY	-	expression tag	UNP A5FBJ5
C	17	LEU	-	expression tag	UNP A5FBJ5
C	18	VAL	-	expression tag	UNP A5FBJ5
C	19	PRO	-	expression tag	UNP A5FBJ5
C	20	ARG	-	expression tag	UNP A5FBJ5
C	21	GLY	-	expression tag	UNP A5FBJ5
C	22	SER	-	expression tag	UNP A5FBJ5
C	23	HIS	-	expression tag	UNP A5FBJ5

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

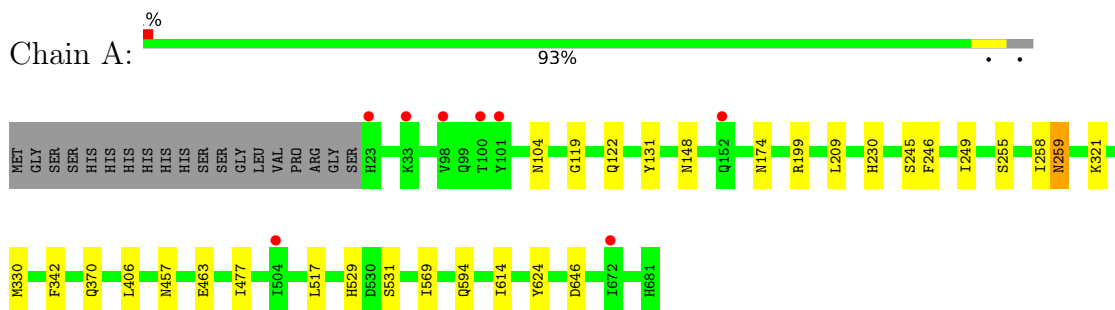
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	522	Total	O	0	0
			522	522		
3	B	393	Total	O	0	0
			393	393		
3	C	537	Total	O	0	0
			537	537		

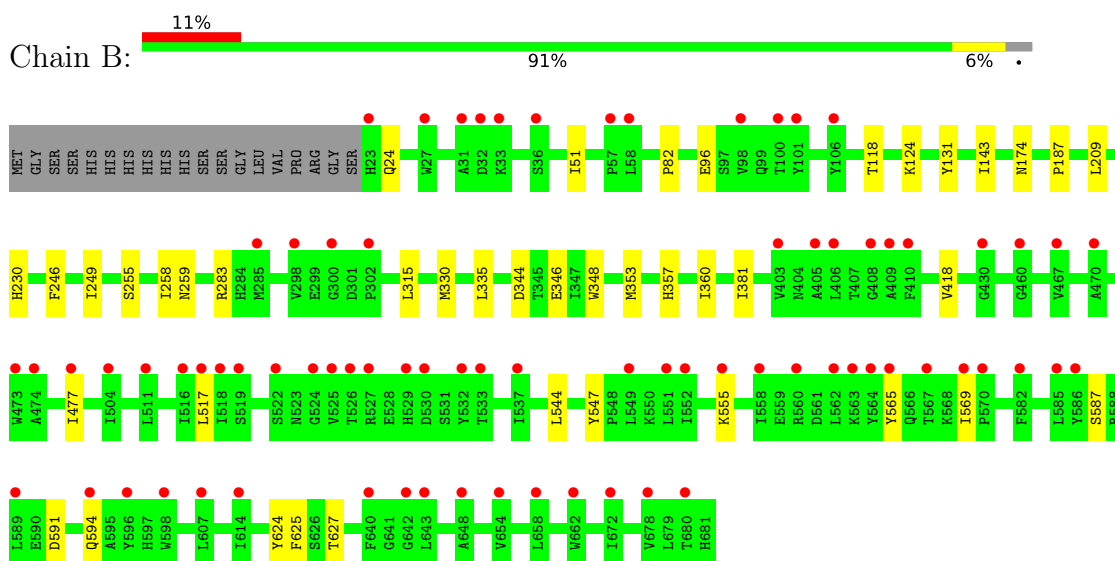
3 Residue-property plots [i](#)

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.

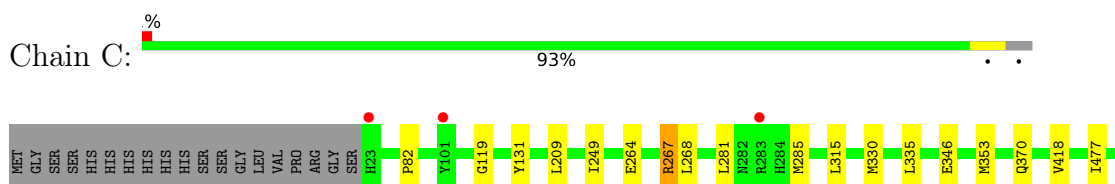
- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.83Å 193.97Å 111.73Å 90.00° 116.60° 90.00°	Depositor
Resolution (Å)	48.54 – 1.54 48.54 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.54-1.54) 99.3 (48.54-1.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.54Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.171 , 0.192 0.181 , 0.201	Depositor DCC
R_{free} test set	16770 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17514	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

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	0.96	0/5459	1.13	5/7406 (0.1%)
1	B	0.97	0/5437	1.20	1/7376 (0.0%)
1	C	0.96	0/5455	1.12	1/7400 (0.0%)
All	All	0.97	0/16351	1.15	7/22182 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	ASN	CA-C-N	5.75	128.26	120.38
1	A	457	ASN	C-N-CA	5.75	128.26	120.38
1	A	569	ILE	CA-C-O	5.42	122.16	119.12
1	C	267	ARG	CG-CD-NE	-5.38	100.16	112.00
1	A	342	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	646	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	187	PRO	N-CD-CG	-5.03	95.65	103.20

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	5330	0	5206	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5305	0	5190	25	0
1	C	5323	0	5207	20	0
2	A	40	0	60	6	0
2	B	24	0	36	1	0
2	C	40	0	60	3	0
3	A	522	0	0	4	0
3	B	393	0	0	0	0
3	C	537	0	0	1	0
All	All	17514	0	15759	66	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 2.

All (66) 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:209:LEU:HD11	1:B:249:ILE:CD1	2.01	0.90
1:C:614:ILE:HD11	2:C:707:EDO:H21	1.59	0.83
1:A:209:LEU:HD11	1:A:249:ILE:CD1	2.09	0.82
1:B:209:LEU:HD11	1:B:249:ILE:HD11	1.61	0.82
1:A:209:LEU:HD11	1:A:249:ILE:HD11	1.62	0.81
1:A:614:ILE:HD11	2:A:706:EDO:H12	1.70	0.74
1:B:209:LEU:HD11	1:B:249:ILE:HD12	1.71	0.71
1:C:614:ILE:CD1	2:C:707:EDO:H21	2.27	0.65
1:A:209:LEU:HD11	1:A:249:ILE:HD12	1.83	0.58
1:B:330:MET:HA	1:B:624:TYR:O	2.07	0.55
1:A:614:ILE:CD1	2:A:706:EDO:H12	2.37	0.54
1:A:330:MET:HA	1:A:624:TYR:O	2.09	0.53
1:C:281:LEU:O	1:C:285[A]:MET:HG2	2.09	0.52
1:B:96:GLU:OE1	1:B:124:LYS:NZ	2.41	0.52
1:B:381:ILE:HG22	1:C:268:LEU:HD21	1.91	0.52
1:C:315:LEU:HD23	1:C:353:MET:HE3	1.93	0.50
1:B:82:PRO:HD3	1:B:335:LEU:HD21	1.94	0.50
1:B:544:LEU:HA	1:B:547:TYR:O	2.12	0.50
1:B:259:ASN:ND2	1:B:259:ASN:H	2.09	0.50
1:C:614:ILE:CG1	2:C:707:EDO:H21	2.43	0.49
1:A:259:ASN:ND2	1:A:259:ASN:H	2.10	0.49
1:C:330:MET:HA	1:C:624:TYR:O	2.13	0.49
1:B:591:ASP:OD2	1:B:594:GLN:HG3	2.14	0.47
1:C:346:GLU:HG2	1:C:418:VAL:HA	1.97	0.47
1:C:662:TRP:O	1:C:681:HIS:CE1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370[A]:GLN:NE2	3:C:807:HOH:O	2.47	0.46
1:B:381:ILE:CG2	1:C:268:LEU:HD21	2.46	0.46
1:A:406:LEU:HA	2:A:707:EDO:H21	1.98	0.46
1:A:477:ILE:HD12	1:A:477:ILE:C	2.42	0.45
1:C:625:PHE:CZ	1:C:627:THR:HB	2.52	0.45
1:A:246:PHE:HA	2:A:708:EDO:H22	1.99	0.45
1:A:594:GLN:NE2	3:A:803:HOH:O	2.41	0.45
1:B:315:LEU:HD23	1:B:353:MET:HE3	1.98	0.45
1:C:209:LEU:HD11	1:C:249:ILE:CD1	2.46	0.45
1:B:565:TYR:O	1:B:569:ILE:HD12	2.17	0.45
1:C:82:PRO:HG3	1:C:335[B]:LEU:HD11	1.99	0.45
1:C:264:GLU:OE1	1:C:267:ARG:NH2	2.49	0.45
1:A:199:ARG:HG2	3:A:828:HOH:O	2.16	0.45
1:B:344:ASP:O	1:B:348:TRP:HB2	2.17	0.44
1:B:346:GLU:HG2	1:B:418:VAL:HA	1.99	0.44
1:A:119:GLY:HA3	1:A:131:TYR:CZ	2.53	0.44
1:B:255:SER:HA	1:B:258:ILE:O	2.18	0.44
1:A:104:ASN:ND2	1:A:122:GLN:HB3	2.33	0.43
1:A:463:GLU:HG2	1:A:517:LEU:HD12	2.00	0.43
1:B:118:THR:HA	1:B:131:TYR:O	2.19	0.43
1:B:477:ILE:C	1:B:477:ILE:HD12	2.44	0.43
1:C:119:GLY:HA3	1:C:131:TYR:CZ	2.54	0.42
1:A:370[B]:GLN:NE2	3:A:814:HOH:O	2.52	0.42
1:A:406:LEU:HD23	2:A:707:EDO:H21	2.02	0.42
1:A:174:ASN:HB3	1:A:230:HIS:CG	2.55	0.42
1:B:259:ASN:H	1:B:259:ASN:HD22	1.68	0.42
1:A:148:ASN:OD1	1:A:245:SER:HB2	2.20	0.42
1:B:283[B]:ARG:HD2	1:B:283[B]:ARG:HA	1.94	0.41
1:C:477:ILE:HD12	1:C:477:ILE:C	2.45	0.41
1:A:529:HIS:CE1	1:A:531:SER:HB2	2.55	0.41
1:A:321:LYS:HE3	3:A:1263:HOH:O	2.21	0.41
1:A:614:ILE:CG1	2:A:706:EDO:H12	2.50	0.41
1:B:174:ASN:HB3	1:B:230:HIS:CG	2.56	0.41
1:C:544:LEU:HA	1:C:547:TYR:O	2.21	0.41
1:B:625:PHE:CZ	1:B:627:THR:HB	2.55	0.41
1:A:255:SER:HA	1:A:258:ILE:O	2.21	0.40
1:B:246:PHE:HA	2:B:703:EDO:H22	2.02	0.40
1:B:357:HIS:HB2	1:B:360:ILE:HD12	2.03	0.40
1:C:605:PRO:HB2	1:C:618:LYS:HG2	2.03	0.40
1:C:568:LYS:O	1:C:570:PRO:HD3	2.21	0.40
1:B:51:ILE:HD11	1:B:143:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	668/678 (98%)	647 (97%)	21 (3%)	0	100	100
1	B	665/678 (98%)	641 (96%)	24 (4%)	0	100	100
1	C	667/678 (98%)	648 (97%)	19 (3%)	0	100	100
All	All	2000/2034 (98%)	1936 (97%)	64 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	576/581 (99%)	575 (100%)	1 (0%)	87	77
1	B	573/581 (99%)	569 (99%)	4 (1%)	76	55
1	C	575/581 (99%)	575 (100%)	0	100	100
All	All	1724/1743 (99%)	1719 (100%)	5 (0%)	86	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	ASN
1	B	24	GLN

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Mol	Chain	Res	Type
1	B	517	LEU
1	B	555	LYS
1	B	587	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	85	ASN
1	A	104	ASN
1	A	105	ASN
1	A	108	GLN
1	A	150	ASN
1	A	171	ASN
1	A	178	ASN
1	A	183	HIS
1	A	185	ASN
1	A	206	ASN
1	A	259	ASN
1	A	539	GLN
1	A	571	GLN
1	A	608	ASN
1	B	85	ASN
1	B	108	GLN
1	B	171	ASN
1	B	183	HIS
1	B	259	ASN
1	B	282	ASN
1	B	480	ASN
1	B	539	GLN
1	B	571	GLN
1	B	608	ASN
1	C	85	ASN
1	C	108	GLN
1	C	150	ASN
1	C	178	ASN
1	C	185	ASN
1	C	206	ASN
1	C	539	GLN
1	C	571	GLN
1	C	608	ASN
1	C	681	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](#)

26 ligands 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	$\# Z > 2$
2	EDO	A	704	-	3,3,3	0.16	0	2,2,2	0.18	0
2	EDO	A	702	-	3,3,3	0.32	0	2,2,2	0.08	0
2	EDO	A	709	-	3,3,3	0.03	0	2,2,2	0.01	0
2	EDO	C	709	-	3,3,3	0.07	0	2,2,2	0.09	0
2	EDO	C	708	-	3,3,3	0.22	0	2,2,2	0.11	0
2	EDO	B	705	-	3,3,3	0.08	0	2,2,2	0.16	0
2	EDO	A	705	-	3,3,3	0.13	0	2,2,2	0.04	0
2	EDO	A	707	-	3,3,3	0.24	0	2,2,2	0.23	0
2	EDO	B	706	-	3,3,3	0.05	0	2,2,2	0.04	0
2	EDO	C	710	-	3,3,3	0.03	0	2,2,2	0.21	0
2	EDO	A	703	-	3,3,3	0.09	0	2,2,2	0.39	0
2	EDO	C	703	-	3,3,3	0.28	0	2,2,2	0.50	0
2	EDO	A	708	-	3,3,3	0.04	0	2,2,2	0.13	0
2	EDO	C	704	-	3,3,3	0.08	0	2,2,2	0.12	0
2	EDO	C	702	-	3,3,3	0.26	0	2,2,2	0.12	0
2	EDO	C	706	-	3,3,3	0.16	0	2,2,2	0.07	0
2	EDO	A	710	-	3,3,3	0.17	0	2,2,2	0.15	0
2	EDO	C	701	-	3,3,3	0.19	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	701	-	3,3,3	0.08	0	2,2,2	0.12	0
2	EDO	A	701	-	3,3,3	0.07	0	2,2,2	0.12	0
2	EDO	B	704	-	3,3,3	0.26	0	2,2,2	0.12	0
2	EDO	B	703	-	3,3,3	0.13	0	2,2,2	0.19	0
2	EDO	C	707	-	3,3,3	0.23	0	2,2,2	0.31	0
2	EDO	B	702	-	3,3,3	0.04	0	2,2,2	0.05	0
2	EDO	C	705	-	3,3,3	0.08	0	2,2,2	0.35	0
2	EDO	A	706	-	3,3,3	0.20	0	2,2,2	0.32	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-
2	EDO	A	709	-	-	0/1/1/1	-
2	EDO	C	709	-	-	0/1/1/1	-
2	EDO	C	708	-	-	1/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	A	707	-	-	1/1/1/1	-
2	EDO	B	706	-	-	0/1/1/1	-
2	EDO	C	710	-	-	0/1/1/1	-
2	EDO	A	703	-	-	1/1/1/1	-
2	EDO	C	703	-	-	0/1/1/1	-
2	EDO	A	708	-	-	0/1/1/1	-
2	EDO	C	704	-	-	0/1/1/1	-
2	EDO	C	702	-	-	0/1/1/1	-
2	EDO	C	706	-	-	0/1/1/1	-
2	EDO	A	710	-	-	0/1/1/1	-
2	EDO	C	701	-	-	0/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	B	704	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	C	707	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	C	705	-	-	0/1/1/1	-
2	EDO	A	706	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	703	EDO	O1-C1-C2-O2
2	C	708	EDO	O1-C1-C2-O2
2	A	706	EDO	O1-C1-C2-O2
2	A	707	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	707	EDO	2	0
2	A	708	EDO	1	0
2	B	703	EDO	1	0
2	C	707	EDO	3	0
2	A	706	EDO	3	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, 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	659/678 (97%)	0.15	8 (1%) 76 82	10, 26, 44, 67	11 (1%)
1	B	659/678 (97%)	0.73	77 (11%) 9 12	11, 31, 62, 75	8 (1%)
1	C	659/678 (97%)	0.10	6 (0%) 81 86	10, 27, 40, 53	10 (1%)
All	All	1977/2034 (97%)	0.33	91 (4%) 37 45	10, 27, 51, 75	29 (1%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	5.2
1	A	101	TYR	5.1
1	C	672	ILE	4.3
1	B	101	TYR	4.3
1	B	517	LEU	4.0
1	B	564	TYR	3.8
1	B	98	VAL	3.6
1	B	562	LEU	3.6
1	B	558	ILE	3.6
1	B	477	ILE	3.5
1	B	532	TYR	3.4
1	B	473	TRP	3.4
1	B	408	GLY	3.3
1	B	537	ILE	3.3
1	B	467	VAL	3.3
1	B	569	ILE	3.3
1	B	406	LEU	3.2
1	B	525	VAL	3.2
1	B	672	ILE	3.1
1	B	524	GLY	3.1
1	A	672	ILE	3.1
1	B	298	VAL	3.0
1	B	518	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	285	MET	2.9
1	B	405	ALA	2.8
1	C	503	VAL	2.8
1	B	533	THR	2.8
1	B	565	TYR	2.8
1	B	662	TRP	2.7
1	B	585	LEU	2.6
1	B	598	TRP	2.6
1	A	504	ILE	2.6
1	A	23	HIS	2.6
1	B	589	LEU	2.6
1	A	152	GLN	2.6
1	B	516	ILE	2.6
1	A	100	THR	2.6
1	B	410	PHE	2.6
1	B	403	VAL	2.6
1	C	101	TYR	2.5
1	B	100	THR	2.5
1	B	300	GLY	2.5
1	B	460	GLY	2.4
1	B	552	ILE	2.4
1	B	529	HIS	2.4
1	B	57	PRO	2.4
1	B	614	ILE	2.4
1	B	551	LEU	2.4
1	B	563	LYS	2.4
1	B	648	ALA	2.4
1	B	33	LYS	2.4
1	B	526	THR	2.4
1	B	567	THR	2.4
1	B	658	LEU	2.4
1	C	283[A]	ARG	2.4
1	B	586	TYR	2.4
1	B	474	ALA	2.3
1	B	654	VAL	2.3
1	B	23	HIS	2.3
1	B	582	PHE	2.3
1	C	23	HIS	2.3
1	A	98	VAL	2.3
1	B	555	LYS	2.3
1	B	302	PRO	2.2
1	B	511	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	504	ILE	2.2
1	B	106	TYR	2.2
1	B	560	ARG	2.2
1	B	31	ALA	2.2
1	B	470	ALA	2.2
1	B	522	SER	2.2
1	B	527	ARG	2.2
1	B	607	LEU	2.1
1	B	519	SER	2.1
1	B	594	GLN	2.1
1	B	642	GLY	2.1
1	C	504	ILE	2.1
1	A	33	LYS	2.1
1	B	430	GLY	2.1
1	B	640	PHE	2.1
1	B	678	VAL	2.1
1	B	530	ASP	2.1
1	B	570	PRO	2.1
1	B	32	ASP	2.1
1	B	58	LEU	2.0
1	B	596	TYR	2.0
1	B	680	THR	2.0
1	B	27	TRP	2.0
1	B	549	LEU	2.0
1	B	643	LEU	2.0
1	B	36	SER	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(\AA^2)	Q<0.9
2	EDO	B	705	4/4	0.86	0.13	46,50,51,54	0
2	EDO	A	707	4/4	0.87	0.17	37,46,47,49	0
2	EDO	C	709	4/4	0.87	0.14	30,35,36,39	0
2	EDO	C	710	4/4	0.87	0.14	40,45,46,47	0
2	EDO	B	706	4/4	0.88	0.11	37,39,40,42	0
2	EDO	C	708	4/4	0.89	0.16	35,41,42,50	0
2	EDO	A	705	4/4	0.89	0.11	35,35,37,37	0
2	EDO	A	709	4/4	0.89	0.13	34,35,38,38	0
2	EDO	C	707	4/4	0.91	0.12	26,28,30,30	0
2	EDO	A	706	4/4	0.92	0.15	27,30,32,33	0
2	EDO	A	710	4/4	0.92	0.09	32,32,34,36	0
2	EDO	B	701	4/4	0.92	0.13	28,29,32,33	0
2	EDO	B	703	4/4	0.92	0.10	30,30,31,32	0
2	EDO	A	708	4/4	0.92	0.10	37,38,38,38	0
2	EDO	B	704	4/4	0.93	0.11	28,30,31,31	0
2	EDO	A	704	4/4	0.94	0.10	26,30,33,34	0
2	EDO	C	703	4/4	0.94	0.10	24,25,29,29	0
2	EDO	C	704	4/4	0.94	0.08	33,34,35,35	0
2	EDO	C	706	4/4	0.94	0.09	31,32,33,35	0
2	EDO	C	705	4/4	0.95	0.08	28,32,34,36	0
2	EDO	B	702	4/4	0.95	0.07	29,29,30,30	0
2	EDO	A	703	4/4	0.96	0.08	22,22,26,27	0
2	EDO	C	702	4/4	0.97	0.06	23,23,23,24	0
2	EDO	A	702	4/4	0.97	0.06	21,21,22,23	0
2	EDO	C	701	4/4	0.97	0.06	22,24,24,24	0
2	EDO	A	701	4/4	0.98	0.05	21,21,21,22	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.