



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2024 – 10:48 AM JST

PDB ID : 7FE3  
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](mailto: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>.

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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	:	2.36.2
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)	:	2.36.2

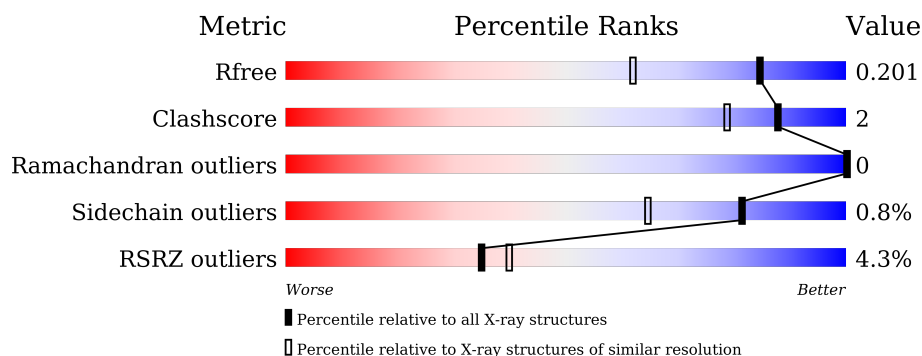
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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  $\geq 3$ , 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	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>5%</div> </div>
1	B	678	<div> <div>9%</div> <div>91%</div> <div>6%</div> <div>5%</div> </div>
1	C	678	<div> <div>0%</div> <div>92%</div> <div>5%</div> <div>5%</div> </div>

## 2 Entry composition

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
1	A	659	Total	C	N	O	S	0	11	0
			5330	3392	898	1018	22			
1	B	659	Total	C	N	O	S	0	8	0
			5305	3378	894	1011	22			
1	C	659	Total	C	N	O	S	0	10	0
			5323	3390	896	1014	23			

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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

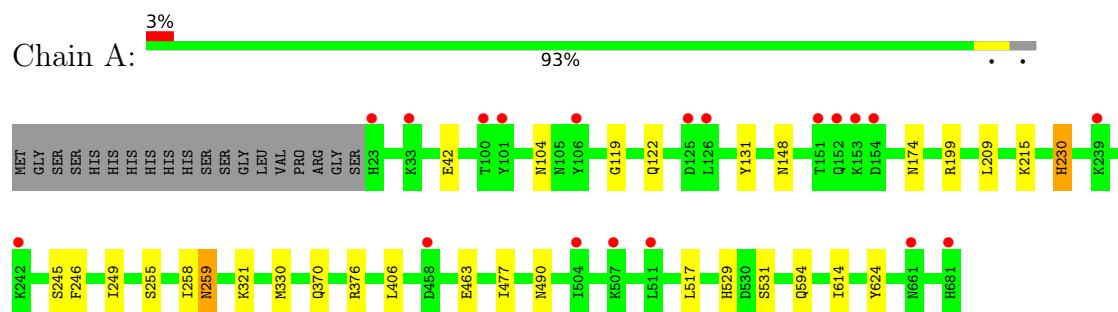
- Molecule 3 is water.

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

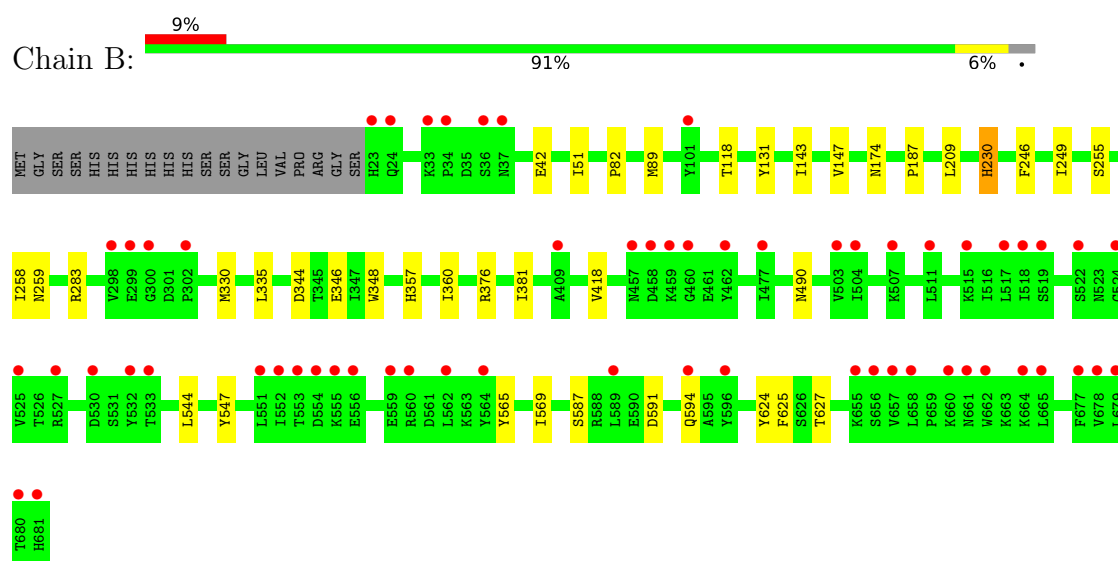
### 3 Residue-property plots [i](#)

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.

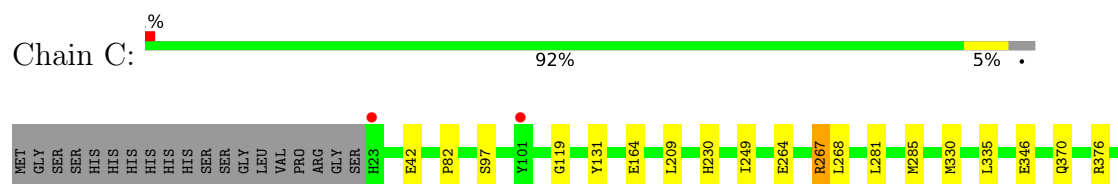
- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

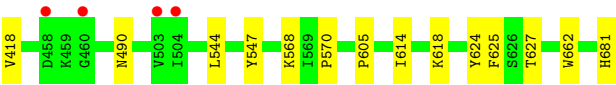


- Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65



- 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, $\alpha$ , $\beta$ , $\gamma$	122.83Å 193.97Å 111.73Å 90.00° 116.60° 90.00°	Depositor
Resolution (Å)	48.54 – 1.54 48.49 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.54-1.54) 99.3 (48.49-1.54)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.54Å)	Xtriage
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 (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17514	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.68	0/5459	0.78	1/7406 (0.0%)
1	B	0.68	0/5437	0.78	2/7376 (0.0%)
1	C	0.67	1/5455 (0.0%)	0.78	2/7400 (0.0%)
All	All	0.67	1/16351 (0.0%)	0.78	5/22182 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	GLU	CD-OE2	-5.40	1.19	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	267	ARG	CG-CD-NE	-5.54	100.16	111.80
1	C	376	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	376	ARG	NE-CZ-NH2	-5.25	117.68	120.30
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 ⓘ

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
1	B	5305	0	5190	23	0
1	C	5323	0	5207	18	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	62	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 (62) 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:381:ILE:HG22	1:C:268:LEU:HD21	1.91	0.52
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
1:B:89[B]:MET:HE1	1:B:147:VAL:HG21	1.98	0.46
1:C:370[A]:GLN:NE2	3:C:807:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:477:ILE:HD12	1:A:477:ILE:C	2.42	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

### 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	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

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%)	571 (99%)	5 (1%)	78	60
1	B	573/581 (99%)	569 (99%)	4 (1%)	84	68
1	C	575/581 (99%)	571 (99%)	4 (1%)	84	68
All	All	1724/1743 (99%)	1711 (99%)	13 (1%)	81	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	215	LYS
1	A	230	HIS
1	A	259	ASN
1	A	490	ASN

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Mol	Chain	Res	Type
1	B	42	GLU
1	B	230	HIS
1	B	490	ASN
1	B	587	SER
1	C	42	GLU
1	C	97	SER
1	C	230	HIS
1	C	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	122	GLN
1	A	158	ASN
1	A	259	ASN
1	B	24	GLN
1	B	85	ASN
1	B	158	ASN
1	B	259	ASN
1	B	282	ASN
1	C	85	ASN
1	C	150	ASN
1	C	404	ASN
1	C	681	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	B	706	-	3,3,3	0.05	0	2,2,2	0.09	0
2	EDO	A	701	-	3,3,3	0.07	0	2,2,2	0.17	0
2	EDO	A	710	-	3,3,3	0.17	0	2,2,2	0.22	0
2	EDO	B	701	-	3,3,3	0.08	0	2,2,2	0.16	0
2	EDO	A	708	-	3,3,3	0.04	0	2,2,2	0.20	0
2	EDO	A	705	-	3,3,3	0.13	0	2,2,2	0.07	0
2	EDO	A	709	-	3,3,3	0.03	0	2,2,2	0.08	0
2	EDO	C	701	-	3,3,3	0.19	0	2,2,2	0.23	0
2	EDO	C	710	-	3,3,3	0.03	0	2,2,2	0.29	0
2	EDO	C	706	-	3,3,3	0.16	0	2,2,2	0.05	0
2	EDO	B	704	-	3,3,3	0.26	0	2,2,2	0.16	0
2	EDO	A	706	-	3,3,3	0.21	0	2,2,2	0.40	0
2	EDO	C	703	-	3,3,3	0.28	0	2,2,2	0.59	0
2	EDO	C	705	-	3,3,3	0.08	0	2,2,2	0.44	0
2	EDO	C	709	-	3,3,3	0.07	0	2,2,2	0.04	0
2	EDO	C	708	-	3,3,3	0.22	0	2,2,2	0.14	0
2	EDO	C	702	-	3,3,3	0.26	0	2,2,2	0.08	0
2	EDO	C	704	-	3,3,3	0.08	0	2,2,2	0.17	0
2	EDO	A	703	-	3,3,3	0.10	0	2,2,2	0.48	0
2	EDO	A	702	-	3,3,3	0.32	0	2,2,2	0.12	0
2	EDO	B	702	-	3,3,3	0.04	0	2,2,2	0.11	0
2	EDO	B	705	-	3,3,3	0.09	0	2,2,2	0.23	0
2	EDO	C	707	-	3,3,3	0.24	0	2,2,2	0.37	0
2	EDO	A	707	-	3,3,3	0.24	0	2,2,2	0.21	0
2	EDO	A	704	-	3,3,3	0.16	0	2,2,2	0.25	0
2	EDO	B	703	-	3,3,3	0.13	0	2,2,2	0.25	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	EDO	B	706	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	A	710	-	-	0/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	708	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	A	709	-	-	0/1/1/1	-
2	EDO	C	701	-	-	0/1/1/1	-
2	EDO	C	710	-	-	0/1/1/1	-
2	EDO	C	706	-	-	0/1/1/1	-
2	EDO	B	704	-	-	0/1/1/1	-
2	EDO	A	706	-	-	1/1/1/1	-
2	EDO	C	703	-	-	0/1/1/1	-
2	EDO	C	705	-	-	0/1/1/1	-
2	EDO	C	709	-	-	0/1/1/1	-
2	EDO	C	708	-	-	1/1/1/1	-
2	EDO	C	702	-	-	0/1/1/1	-
2	EDO	C	704	-	-	0/1/1/1	-
2	EDO	A	703	-	-	1/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-
2	EDO	C	707	-	-	0/1/1/1	-
2	EDO	A	707	-	-	1/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-

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	A	706	EDO	O1-C1-C2-O2
2	C	708	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	708	EDO	1	0
2	A	706	EDO	3	0
2	C	707	EDO	3	0
2	A	707	EDO	2	0
2	B	703	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	659/678 (97%)	-0.09	19 (2%) 51 58	18, 26, 44, 67	0
1	B	659/678 (97%)	0.37	60 (9%) 9 10	17, 32, 62, 75	0
1	C	659/678 (97%)	-0.17	6 (0%) 84 86	19, 27, 40, 53	0
All	All	1977/2034 (97%)	0.04	85 (4%) 35 40	17, 28, 51, 75	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	8.0
1	B	517	LEU	7.3
1	B	680	THR	5.8
1	A	504	ILE	4.5
1	B	679	LEU	4.3
1	B	657	VAL	4.3
1	B	662	TRP	4.3
1	C	504	ILE	4.2
1	B	458	ASP	4.1
1	B	527	ARG	3.9
1	B	460	GLY	3.8
1	A	100	THR	3.8
1	A	23	HIS	3.8
1	B	660	LYS	3.7
1	A	152	GLN	3.7
1	B	459	LYS	3.6
1	B	298	VAL	3.6
1	B	101	TYR	3.6
1	B	589	LEU	3.5
1	B	661	ASN	3.5
1	B	518	ILE	3.5
1	B	658	LEU	3.5
1	B	300	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	665	LEU	3.4
1	B	533	THR	3.4
1	B	511	LEU	3.3
1	A	239	LYS	3.3
1	A	33	LYS	3.2
1	B	23	HIS	3.2
1	B	552	ILE	3.2
1	B	524	GLY	3.1
1	C	101	TYR	3.1
1	B	681	HIS	3.1
1	B	519	SER	3.0
1	A	125	ASP	3.0
1	B	553	THR	3.0
1	B	677	PHE	2.9
1	B	477	ILE	2.9
1	A	242	LYS	2.9
1	B	504	ILE	2.9
1	B	555	LYS	2.9
1	B	678	VAL	2.9
1	B	24	GLN	2.8
1	C	503	VAL	2.8
1	A	151	THR	2.8
1	B	564	TYR	2.8
1	B	554	ASP	2.8
1	B	33	LYS	2.8
1	B	655	LYS	2.8
1	B	556	GLU	2.8
1	A	661	ASN	2.7
1	B	302	PRO	2.7
1	B	522	SER	2.6
1	B	596	TYR	2.6
1	C	23	HIS	2.6
1	B	525	VAL	2.6
1	A	153	LYS	2.5
1	B	462	TYR	2.5
1	B	532	TYR	2.5
1	B	37	ASN	2.5
1	A	126	LEU	2.5
1	B	457	ASN	2.4
1	A	681	HIS	2.4
1	B	36	SER	2.4
1	B	559	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	530	ASP	2.4
1	C	458	ASP	2.3
1	B	34	PRO	2.3
1	B	562	LEU	2.2
1	A	106	TYR	2.2
1	B	503	VAL	2.2
1	B	664	LYS	2.2
1	B	299	GLU	2.2
1	B	560	ARG	2.2
1	A	507	LYS	2.1
1	B	515	LYS	2.1
1	C	460	GLY	2.1
1	B	594	GLN	2.1
1	B	551	LEU	2.1
1	B	656	SER	2.1
1	B	409	ALA	2.1
1	A	458	ASP	2.1
1	A	511	LEU	2.1
1	B	507	LYS	2.0
1	A	154	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	EDO	A	705	4/4	0.83	0.13	35,35,37,37	0
2	EDO	B	705	4/4	0.85	0.22	46,50,51,54	0
2	EDO	C	709	4/4	0.86	0.17	30,35,36,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	C	707	4/4	0.89	0.10	26,28,30,30	0
2	EDO	B	701	4/4	0.89	0.17	28,29,32,33	0
2	EDO	C	710	4/4	0.89	0.20	40,45,46,47	0
2	EDO	A	707	4/4	0.90	0.33	37,46,47,49	0
2	EDO	C	708	4/4	0.91	0.26	35,41,42,50	0
2	EDO	B	706	4/4	0.91	0.10	37,39,40,42	0
2	EDO	A	709	4/4	0.91	0.12	34,35,38,38	0
2	EDO	A	710	4/4	0.92	0.07	32,32,34,36	0
2	EDO	A	706	4/4	0.92	0.15	27,30,32,33	0
2	EDO	B	703	4/4	0.92	0.07	30,30,31,32	0
2	EDO	C	703	4/4	0.93	0.12	24,25,29,29	0
2	EDO	B	704	4/4	0.94	0.12	28,30,31,31	0
2	EDO	A	704	4/4	0.95	0.08	26,30,33,34	0
2	EDO	A	708	4/4	0.95	0.16	37,38,38,38	0
2	EDO	C	705	4/4	0.95	0.06	28,32,34,36	0
2	EDO	C	706	4/4	0.95	0.08	31,32,33,35	0
2	EDO	C	704	4/4	0.96	0.07	33,34,35,35	0
2	EDO	C	702	4/4	0.97	0.07	23,23,23,24	0
2	EDO	A	703	4/4	0.97	0.11	22,22,26,27	0
2	EDO	B	702	4/4	0.97	0.08	29,29,30,30	0
2	EDO	A	701	4/4	0.98	0.06	21,21,21,22	0
2	EDO	A	702	4/4	0.98	0.09	21,21,22,23	0
2	EDO	C	701	4/4	0.98	0.13	22,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.