



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:04 PM UTC

PDB ID : 6F8Z / pdb_00006f8z
Title : Structure of the family GH92 alpha-mannosidase BT3130 from Bacteroides thetaiotaomicron
Authors : Thompson, A.J.; Spears, R.J.; Zhu, Y.; Suits, M.D.L.; Williams, S.J.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2017-12-13
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

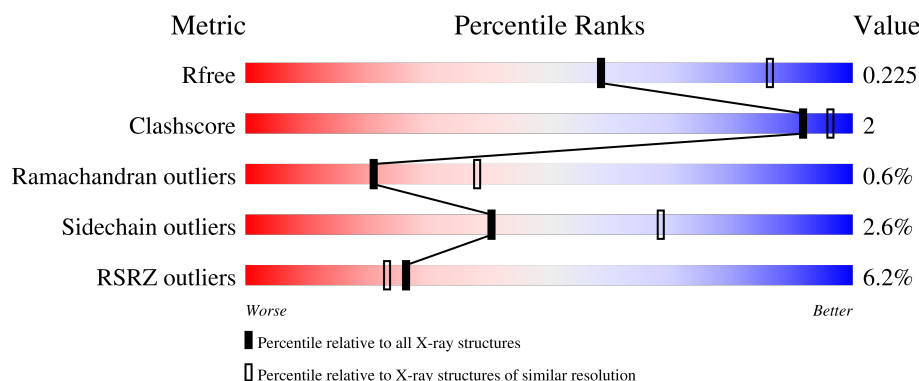
1 Overall quality at a glance

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	727	3% 92% 5% ..
1	B	727	3% 92% ..
1	C	727	12% 90% 6% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17983 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 Alpha-1,2-mannosidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	2	0
			5678	3610	963	1078	27			
1	B	703	Total	C	N	O	S	0	5	0
			5588	3565	939	1058	26			
1	C	700	Total	C	N	O	S	0	4	0
			5417	3438	918	1034	27			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP A0A174L250
A	18	GLY	-	expression tag	UNP A0A174L250
A	736	LEU	-	expression tag	UNP A0A174L250
A	737	GLU	-	expression tag	UNP A0A174L250
A	738	HIS	-	expression tag	UNP A0A174L250
A	739	HIS	-	expression tag	UNP A0A174L250
A	740	HIS	-	expression tag	UNP A0A174L250
A	741	HIS	-	expression tag	UNP A0A174L250
A	742	HIS	-	expression tag	UNP A0A174L250
A	743	HIS	-	expression tag	UNP A0A174L250
B	17	MET	-	initiating methionine	UNP A0A174L250
B	18	GLY	-	expression tag	UNP A0A174L250
B	736	LEU	-	expression tag	UNP A0A174L250
B	737	GLU	-	expression tag	UNP A0A174L250
B	738	HIS	-	expression tag	UNP A0A174L250
B	739	HIS	-	expression tag	UNP A0A174L250
B	740	HIS	-	expression tag	UNP A0A174L250
B	741	HIS	-	expression tag	UNP A0A174L250
B	742	HIS	-	expression tag	UNP A0A174L250
B	743	HIS	-	expression tag	UNP A0A174L250
C	17	MET	-	initiating methionine	UNP A0A174L250
C	18	GLY	-	expression tag	UNP A0A174L250
C	736	LEU	-	expression tag	UNP A0A174L250

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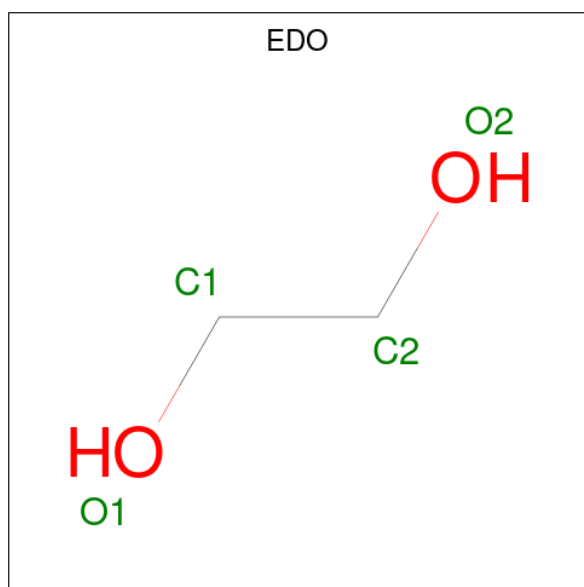
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Chain	Residue	Modelled	Actual	Comment	Reference
C	737	GLU	-	expression tag	UNP A0A174L250
C	738	HIS	-	expression tag	UNP A0A174L250
C	739	HIS	-	expression tag	UNP A0A174L250
C	740	HIS	-	expression tag	UNP A0A174L250
C	741	HIS	-	expression tag	UNP A0A174L250
C	742	HIS	-	expression tag	UNP A0A174L250
C	743	HIS	-	expression tag	UNP A0A174L250

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

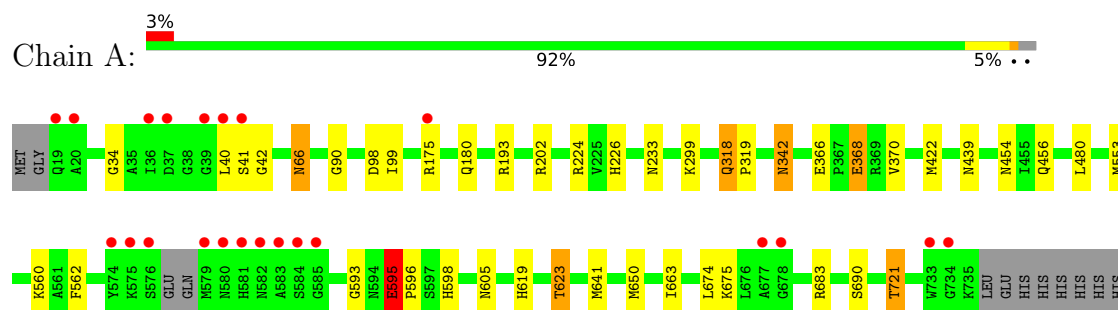
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	668	Total 668	O 668	0	0
4	B	417	Total 417	O 417	0	0
4	C	208	Total 208	O 208	0	0

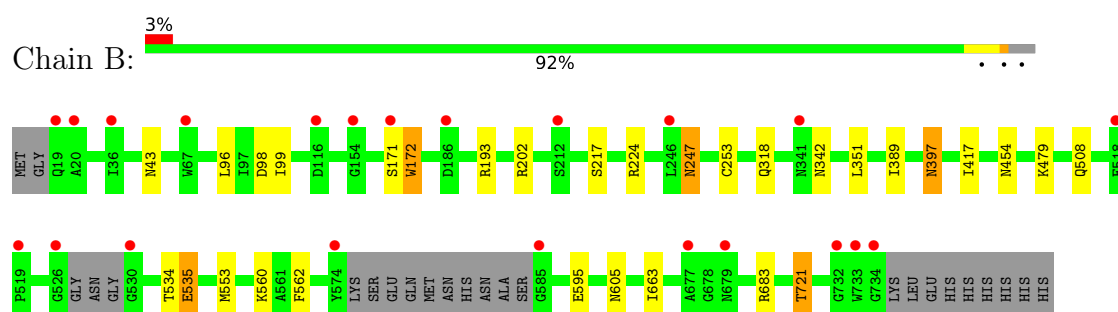
3 Residue-property plots [i](#)

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.

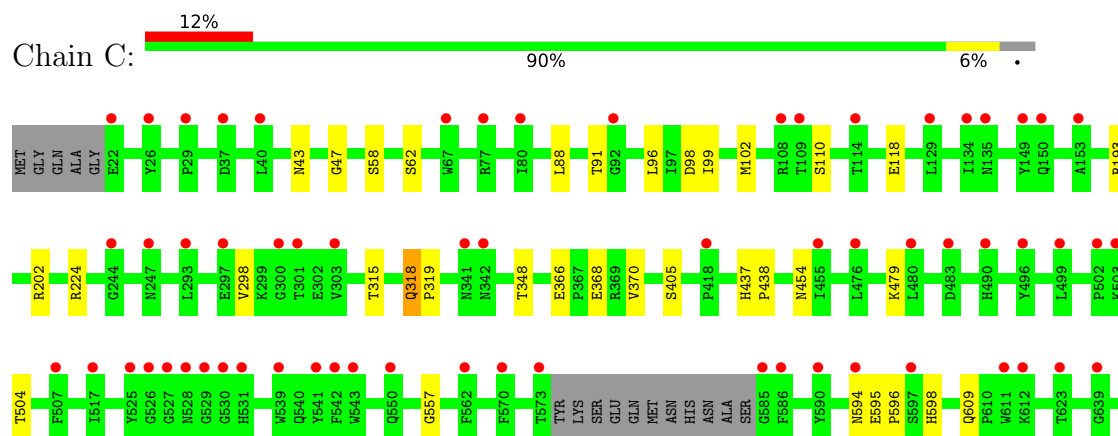
- Molecule 1: Alpha-1,2-mannosidase, putative

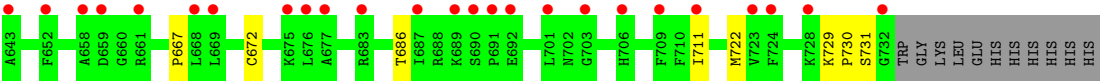


- Molecule 1: Alpha-1,2-mannosidase, putative



- Molecule 1: Alpha-1,2-mannosidase, putative





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	272.30Å 272.30Å 190.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.67 – 2.50 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.67-2.50) 99.9 (49.67-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.181 , 0.222 0.185 , 0.225	Depositor DCC
R_{free} test set	7011 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17983	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: CA, 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	0.67	1/5848 (0.0%)	0.82	2/7949 (0.0%)
1	B	0.65	0/5761	0.81	2/7834 (0.0%)
1	C	0.69	0/5589	0.85	5/7624 (0.1%)
All	All	0.67	1/17198 (0.0%)	0.83	9/23407 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	GLY	C-O	5.40	1.29	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	729	LYS	CA-C-N	6.16	127.54	119.84
1	C	729	LYS	C-N-CA	6.16	127.54	119.84
1	B	389	ILE	N-CA-C	-5.58	106.36	111.67
1	C	609	GLN	CA-C-N	5.31	125.63	119.47
1	C	609	GLN	C-N-CA	5.31	125.63	119.47
1	C	598	HIS	N-CA-C	5.29	117.80	111.71
1	A	598	HIS	N-CA-C	5.15	118.34	111.75
1	A	690	SER	N-CA-C	5.00	112.52	108.07
1	B	351	LEU	N-CA-C	5.00	116.73	111.28

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	5678	0	5300	25	0
1	B	5588	0	5201	10	0
1	C	5417	0	4861	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	4	0	6	1	0
4	A	668	0	0	4	3
4	B	417	0	0	4	0
4	C	208	0	0	2	0
All	All	17983	0	15368	51	3

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 (51) 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:C:711:ILE:HG21	1:C:722:MET:HE1	1.59	0.84
1:A:439:ASN:HD22	1:A:456:GLN:HE22	1.41	0.67
1:A:619:HIS:O	1:A:623:THR:HB	1.95	0.67
1:A:422:MET:HE2	1:A:480:LEU:HD21	1.82	0.60
1:C:98:ASP:OD2	1:C:202:ARG:NH2	2.36	0.57
1:B:534:THR:O	1:B:535:GLU:C	2.50	0.54
1:A:202:ARG:HD3	4:A:1096:HOH:O	2.08	0.53
1:A:66:ASN:HD22	3:A:802:EDO:H12	1.74	0.52
1:C:202:ARG:HD3	4:C:1037:HOH:O	2.11	0.51
1:C:102:MET:HE2	1:C:110:SER:HA	1.93	0.51
1:A:342:ASN:HD22	1:A:342:ASN:N	2.09	0.49
1:B:98:ASP:OD2	1:B:202:ARG:NH2	2.46	0.49
1:A:342:ASN:ND2	1:A:342:ASN:H	2.11	0.49
1:C:98:ASP:CG	1:C:202:ARG:HH22	2.20	0.49
1:B:202:ARG:HD3	4:B:1110:HOH:O	2.12	0.49
1:A:180:GLN:HE21	1:A:233:ASN:HD21	1.61	0.48
1:A:342:ASN:HD22	1:A:342:ASN:H	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:OD2	1:A:202:ARG:NH2	2.47	0.47
1:C:298:VAL:HG12	1:C:672:CYS:CB	2.44	0.47
1:C:224:ARG:NH2	4:C:1001:HOH:O	2.47	0.47
1:A:650:MET:SD	1:A:674:LEU:HD11	2.54	0.47
4:A:1154:HOH:O	1:B:721:THR:HG21	2.15	0.47
1:A:721:THR:HG22	4:A:1462:HOH:O	2.15	0.46
1:A:721:THR:HG21	4:B:1105:HOH:O	2.15	0.46
1:B:171[A]:SER:O	1:B:172:TRP:CG	2.69	0.46
1:C:437:HIS:HB2	1:C:438:PRO:CD	2.46	0.46
1:C:47:GLY:HA3	1:C:58:SER:HB2	1.99	0.45
1:A:224:ARG:NH2	4:A:907:HOH:O	2.50	0.45
1:A:318:GLN:HA	1:A:319:PRO:C	2.41	0.45
1:C:88:LEU:HD13	1:C:91:THR:HG21	1.99	0.44
1:B:397:ASN:C	1:B:397:ASN:HD22	2.25	0.44
1:A:34:GLY:O	1:A:41:SER:HB2	2.17	0.44
1:B:553:MET:HG2	1:B:562:PHE:CG	2.53	0.43
1:A:439:ASN:ND2	1:A:456:GLN:HE22	2.13	0.43
1:C:366:GLU:O	1:C:370:VAL:HG23	2.17	0.43
1:A:366:GLU:O	1:A:370:VAL:HG23	2.19	0.43
1:C:595:GLU:N	1:C:596:PRO:CD	2.82	0.43
1:C:318:GLN:HA	1:C:319:PRO:C	2.44	0.43
1:B:224:ARG:NH2	4:B:1004:HOH:O	2.51	0.43
1:C:298:VAL:HG12	1:C:672:CYS:HB2	2.01	0.42
1:A:224:ARG:HE	1:A:226:HIS:CE1	2.37	0.42
1:A:368:GLU:H	1:A:368:GLU:CD	2.28	0.42
1:C:667:PRO:HB2	1:C:686:THR:HG21	2.01	0.42
1:C:298:VAL:HG12	1:C:672:CYS:HB3	2.02	0.42
1:B:508:GLN:NE2	4:B:1010:HOH:O	2.53	0.41
1:A:42:GLY:O	1:A:90:GLY:HA2	2.20	0.41
1:A:595:GLU:N	1:A:596:PRO:CD	2.83	0.41
1:B:605:ASN:HD22	1:B:663:ILE:CG2	2.34	0.41
1:A:605:ASN:HD22	1:A:663:ILE:CG2	2.33	0.40
1:A:553:MET:HG2	1:A:562:PHE:CG	2.56	0.40
1:A:98:ASP:CG	1:A:202:ARG:HH22	2.29	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:962:HOH:O	4:A:962:HOH:O[10_664]	1.88	0.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1081:HOH:O	4:A:1081:HOH:O[10_664]	1.96	0.24
4:A:1410:HOH:O	4:A:1410:HOH:O[10_664]	2.05	0.15

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	713/727 (98%)	688 (96%)	23 (3%)	2 (0%)	36	55
1	B	702/727 (97%)	672 (96%)	26 (4%)	4 (1%)	21	38
1	C	700/727 (96%)	662 (95%)	32 (5%)	6 (1%)	14	27
All	All	2115/2181 (97%)	2022 (96%)	81 (4%)	12 (1%)	21	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	TRP
1	B	247	ASN
1	B	535	GLU
1	C	731	SER
1	C	348	THR
1	C	118	GLU
1	A	99	ILE
1	B	99	ILE
1	C	99	ILE
1	C	730	PRO
1	A	595	GLU
1	C	557	GLY

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	590/618 (96%)	574 (97%)	16 (3%)	39	67
1	B	578/618 (94%)	562 (97%)	16 (3%)	38	66
1	C	537/618 (87%)	525 (98%)	12 (2%)	45	73
All	All	1705/1854 (92%)	1661 (97%)	44 (3%)	40	68

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

Mol	Chain	Res	Type
1	A	40	LEU
1	A	66	ASN
1	A	175	ARG
1	A	193	ARG
1	A	299	LYS
1	A	318	GLN
1	A	342	ASN
1	A	368	GLU
1	A	454	ASN
1	A	560	LYS
1	A	595	GLU
1	A	623	THR
1	A	641	MET
1	A	675	LYS
1	A	683	ARG
1	A	721	THR
1	B	43	ASN
1	B	96	LEU
1	B	193	ARG
1	B	217	SER
1	B	247	ASN
1	B	253	CYS
1	B	318	GLN
1	B	342	ASN
1	B	397	ASN
1	B	417	ILE

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Mol	Chain	Res	Type
1	B	454	ASN
1	B	479	LYS
1	B	560	LYS
1	B	595	GLU
1	B	683	ARG
1	B	721	THR
1	C	43	ASN
1	C	62	SER
1	C	96	LEU
1	C	193	ARG
1	C	315	THR
1	C	318	GLN
1	C	368	GLU
1	C	405	SER
1	C	454	ASN
1	C	479	LYS
1	C	504	THR
1	C	594	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	126	GLN
1	A	135	ASN
1	A	147	HIS
1	A	150	GLN
1	A	180	GLN
1	A	187	HIS
1	A	226	HIS
1	A	267	GLN
1	A	292	GLN
1	A	318	GLN
1	A	342	ASN
1	A	403	ASN
1	A	439	ASN
1	A	454	ASN
1	A	466	GLN
1	A	487	GLN
1	A	490	HIS
1	A	498	ASN
1	A	508	GLN

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Mol	Chain	Res	Type
1	A	528	ASN
1	A	531	HIS
1	A	550	GLN
1	A	580	ASN
1	A	605	ASN
1	A	619	HIS
1	A	697	GLN
1	B	43	ASN
1	B	44	ASN
1	B	147	HIS
1	B	292	GLN
1	B	318	GLN
1	B	342	ASN
1	B	391	GLN
1	B	397	ASN
1	B	403	ASN
1	B	454	ASN
1	B	466	GLN
1	B	487	GLN
1	B	594	ASN
1	B	605	ASN
1	B	713	HIS
1	C	28	ASN
1	C	43	ASN
1	C	115	HIS
1	C	147	HIS
1	C	238	HIS
1	C	275	HIS
1	C	292	GLN
1	C	318	GLN
1	C	437	HIS
1	C	456	GLN
1	C	458	GLN
1	C	531	HIS
1	C	594	ASN
1	C	605	ASN
1	C	622	ASN
1	C	635	ASN
1	C	697	GLN
1	C	713	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
3	EDO	A	802	-	3,3,3	0.55	0	2,2,2	0.46	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
3	EDO	A	802	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	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, 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	715/727 (98%)	-0.38	22 (3%)	51	47	21, 34, 59, 128	2 (0%)
1	B	703/727 (96%)	0.06	22 (3%)	51	47	23, 46, 75, 107	5 (0%)
1	C	700/727 (96%)	1.00	88 (12%)	8	6	31, 70, 99, 138	4 (0%)
All	All	2118/2181 (97%)	0.22	132 (6%)	26	23	21, 47, 90, 138	11 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	732	GLY	7.2
1	A	581	HIS	7.1
1	A	576	SER	7.1
1	B	67[A]	TRP	6.9
1	B	585	GLY	6.1
1	A	583	ALA	5.7
1	A	19	GLN	5.4
1	A	579	MET	5.2
1	A	584	SER	5.1
1	A	582	ASN	5.0
1	C	585	GLY	5.0
1	B	19	GLN	5.0
1	C	341	ASN	4.3
1	A	580	ASN	4.2
1	C	22	GLU	4.1
1	C	342	ASN	4.0
1	C	528	ASN	4.0
1	B	574	TYR	4.0
1	C	247	ASN	3.8
1	C	527	GLY	3.8
1	C	573	THR	3.8
1	B	677	ALA	3.7
1	A	40	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	659	ASP	3.7
1	A	734	GLY	3.6
1	C	483	ASP	3.6
1	C	669	LEU	3.5
1	B	734	GLY	3.5
1	C	701	LEU	3.4
1	C	80	ILE	3.4
1	B	171[A]	SER	3.4
1	B	186	ASP	3.3
1	B	20	ALA	3.3
1	A	41	SER	3.3
1	C	539	TRP	3.3
1	C	114	THR	3.3
1	C	691	PRO	3.3
1	C	109	THR	3.3
1	C	67	TRP	3.1
1	B	679	ASN	3.1
1	A	574	TYR	3.1
1	A	585	GLY	3.1
1	A	677	ALA	3.1
1	C	134	ILE	3.1
1	C	499	LEU	3.0
1	A	37	ASP	3.0
1	C	724	PHE	3.0
1	C	594	ASN	3.0
1	C	529	GLY	3.0
1	C	153	ALA	2.9
1	C	525	TYR	2.9
1	C	723	VAL	2.9
1	C	26	TYR	2.8
1	A	575	LYS	2.8
1	B	732	GLY	2.8
1	B	341	ASN	2.8
1	C	703	GLY	2.7
1	C	244	GLY	2.7
1	C	507	PHE	2.7
1	C	597	SER	2.7
1	B	530	GLY	2.7
1	C	108	ARG	2.7
1	C	303	VAL	2.7
1	C	455	ILE	2.6
1	C	692	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	733	TRP	2.6
1	B	526	GLY	2.6
1	B	518	GLU	2.6
1	C	297	GLU	2.6
1	C	480	LEU	2.6
1	C	677	ALA	2.6
1	C	490	HIS	2.6
1	C	531	HIS	2.6
1	C	37	ASP	2.5
1	C	711	ILE	2.5
1	C	550	GLN	2.5
1	A	733	TRP	2.5
1	C	675	LYS	2.5
1	C	135	ASN	2.4
1	B	246	LEU	2.4
1	B	116	ASP	2.4
1	C	502	PRO	2.3
1	A	36	ILE	2.3
1	C	586	PHE	2.3
1	C	612	LYS	2.3
1	C	689	LYS	2.3
1	C	77[A]	ARG	2.3
1	C	639	GLY	2.3
1	C	683	ARG	2.3
1	C	150	GLN	2.3
1	C	149	TYR	2.3
1	C	301	THR	2.3
1	C	661	ARG	2.3
1	C	517	ILE	2.3
1	C	476	LEU	2.3
1	B	519	PRO	2.3
1	C	643	ALA	2.2
1	C	658	ALA	2.2
1	C	293	LEU	2.2
1	C	503	LYS	2.2
1	C	652	PHE	2.2
1	C	496	TYR	2.2
1	C	687	ILE	2.2
1	C	690	SER	2.2
1	C	542	PHE	2.2
1	C	611	TRP	2.2
1	C	530	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	541	TYR	2.2
1	C	676	LEU	2.2
1	C	562	PHE	2.2
1	C	92	GLY	2.1
1	C	668	LEU	2.1
1	C	570	PHE	2.1
1	C	709	PHE	2.1
1	C	129	LEU	2.1
1	B	36	ILE	2.1
1	C	418	PRO	2.1
1	C	300	GLY	2.1
1	B	212	SER	2.1
1	C	29	PRO	2.1
1	C	40	LEU	2.1
1	A	39	GLY	2.1
1	A	175	ARG	2.1
1	C	623	THR	2.1
1	C	728	LYS	2.1
1	C	590	TYR	2.1
1	C	706	HIS	2.1
1	A	20	ALA	2.0
1	A	678	GLY	2.0
1	B	154	GLY	2.0
1	C	526	GLY	2.0
1	C	543	TRP	2.0

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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
3	EDO	A	802	4/4	0.91	0.14	44,44,47,48	0
2	CA	A	801	1/1	0.93	0.11	58,58,58,58	0
2	CA	C	900	1/1	0.99	0.09	81,81,81,81	0
2	CA	B	900	1/1	0.99	0.09	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.