



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2021 – 12:41 PM EST

PDB ID : 7L9E
Title : Crystal structure of apo-alpha glucosidase
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2021-01-03
Resolution : 2.29 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.25
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) : 2.25

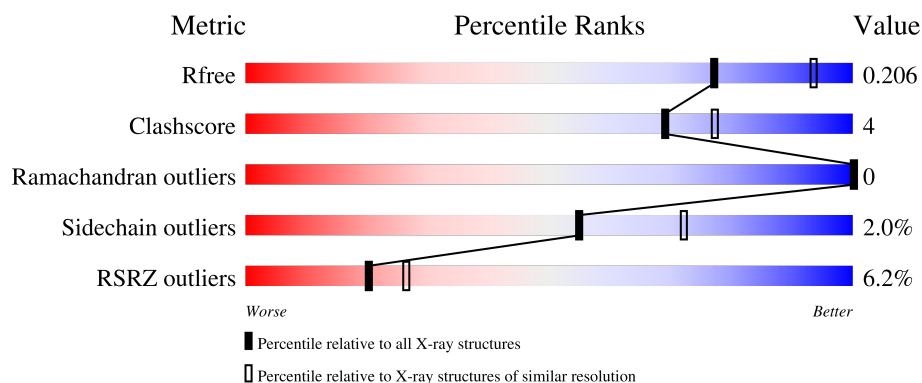
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	E	184	<div> <div>30%</div> <div>71% 8% 18%</div> </div>
1	G	184	<div> <div>68% 15% 17%</div> </div>
2	F	107	<div> <div>5%</div> <div>86% 12%</div> </div>
2	H	107	<div> <div>89% 11%</div> </div>
3	A	609	<div> <div>89% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	609	
4	B	134	
4	D	134	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PG4	A	1009	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15764 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 Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	150	Total	C	N	O	S	0	1	0
			1189	748	215	222	4			
1	G	153	Total	C	N	O	S	0	0	0
			1183	741	219	219	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	MET	-	initiating methionine	UNP Q8BHN3
E	3	GLY	-	expression tag	UNP Q8BHN3
E	4	ILE	-	expression tag	UNP Q8BHN3
E	5	LEU	-	expression tag	UNP Q8BHN3
E	6	PRO	-	expression tag	UNP Q8BHN3
E	7	SER	-	expression tag	UNP Q8BHN3
E	8	PRO	-	expression tag	UNP Q8BHN3
E	9	GLY	-	expression tag	UNP Q8BHN3
E	10	MET	-	expression tag	UNP Q8BHN3
E	11	PRO	-	expression tag	UNP Q8BHN3
E	12	ALA	-	expression tag	UNP Q8BHN3
E	13	LEU	-	expression tag	UNP Q8BHN3
E	14	LEU	-	expression tag	UNP Q8BHN3
E	15	SER	-	expression tag	UNP Q8BHN3
E	16	LEU	-	expression tag	UNP Q8BHN3
E	17	VAL	-	expression tag	UNP Q8BHN3
E	18	SER	-	expression tag	UNP Q8BHN3
E	19	LEU	-	expression tag	UNP Q8BHN3
E	20	LEU	-	expression tag	UNP Q8BHN3
E	21	SER	-	expression tag	UNP Q8BHN3
E	22	VAL	-	expression tag	UNP Q8BHN3
E	23	LEU	-	expression tag	UNP Q8BHN3
E	24	LEU	-	expression tag	UNP Q8BHN3
E	25	MET	-	expression tag	UNP Q8BHN3
E	26	GLY	-	expression tag	UNP Q8BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	27	CYS	-	expression tag	UNP Q8BHN3
E	28	VAL	-	expression tag	UNP Q8BHN3
E	29	ALA	-	expression tag	UNP Q8BHN3
E	30	GLU	-	expression tag	UNP Q8BHN3
E	31	THR	-	expression tag	UNP Q8BHN3
E	32	GLY	-	expression tag	UNP Q8BHN3
E	97	ASP	ASN	engineered mutation	UNP Q8BHN3
G	2	MET	-	initiating methionine	UNP Q8BHN3
G	3	GLY	-	expression tag	UNP Q8BHN3
G	4	ILE	-	expression tag	UNP Q8BHN3
G	5	LEU	-	expression tag	UNP Q8BHN3
G	6	PRO	-	expression tag	UNP Q8BHN3
G	7	SER	-	expression tag	UNP Q8BHN3
G	8	PRO	-	expression tag	UNP Q8BHN3
G	9	GLY	-	expression tag	UNP Q8BHN3
G	10	MET	-	expression tag	UNP Q8BHN3
G	11	PRO	-	expression tag	UNP Q8BHN3
G	12	ALA	-	expression tag	UNP Q8BHN3
G	13	LEU	-	expression tag	UNP Q8BHN3
G	14	LEU	-	expression tag	UNP Q8BHN3
G	15	SER	-	expression tag	UNP Q8BHN3
G	16	LEU	-	expression tag	UNP Q8BHN3
G	17	VAL	-	expression tag	UNP Q8BHN3
G	18	SER	-	expression tag	UNP Q8BHN3
G	19	LEU	-	expression tag	UNP Q8BHN3
G	20	LEU	-	expression tag	UNP Q8BHN3
G	21	SER	-	expression tag	UNP Q8BHN3
G	22	VAL	-	expression tag	UNP Q8BHN3
G	23	LEU	-	expression tag	UNP Q8BHN3
G	24	LEU	-	expression tag	UNP Q8BHN3
G	25	MET	-	expression tag	UNP Q8BHN3
G	26	GLY	-	expression tag	UNP Q8BHN3
G	27	CYS	-	expression tag	UNP Q8BHN3
G	28	VAL	-	expression tag	UNP Q8BHN3
G	29	ALA	-	expression tag	UNP Q8BHN3
G	30	GLU	-	expression tag	UNP Q8BHN3
G	31	THR	-	expression tag	UNP Q8BHN3
G	32	GLY	-	expression tag	UNP Q8BHN3
G	97	ASP	ASN	engineered mutation	UNP Q8BHN3

- Molecule 2 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	105	Total	C	N	O	S	0	0	0
			828	535	135	156	2			
2	H	107	Total	C	N	O	S	0	0	0
			835	538	138	157	2			

- Molecule 3 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	597	Total	C	N	O	S	0	6	0
			4858	3125	836	875	22			
3	C	597	Total	C	N	O	S	0	6	0
			4848	3120	834	872	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	967	SER	-	expression tag	UNP Q8BHN3
A	968	ALA	-	expression tag	UNP Q8BHN3
A	969	TRP	-	expression tag	UNP Q8BHN3
A	970	SER	-	expression tag	UNP Q8BHN3
A	971	HIS	-	expression tag	UNP Q8BHN3
A	972	PRO	-	expression tag	UNP Q8BHN3
A	973	GLN	-	expression tag	UNP Q8BHN3
A	974	PHE	-	expression tag	UNP Q8BHN3
A	975	GLU	-	expression tag	UNP Q8BHN3
A	976	LYS	-	expression tag	UNP Q8BHN3
A	977	LEU	-	expression tag	UNP Q8BHN3
A	978	GLU	-	expression tag	UNP Q8BHN3
C	967	SER	-	expression tag	UNP Q8BHN3
C	968	ALA	-	expression tag	UNP Q8BHN3
C	969	TRP	-	expression tag	UNP Q8BHN3
C	970	SER	-	expression tag	UNP Q8BHN3
C	971	HIS	-	expression tag	UNP Q8BHN3
C	972	PRO	-	expression tag	UNP Q8BHN3
C	973	GLN	-	expression tag	UNP Q8BHN3
C	974	PHE	-	expression tag	UNP Q8BHN3
C	975	GLU	-	expression tag	UNP Q8BHN3
C	976	LYS	-	expression tag	UNP Q8BHN3
C	977	LEU	-	expression tag	UNP Q8BHN3
C	978	GLU	-	expression tag	UNP Q8BHN3

- Molecule 4 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	85	Total 603	C 356	N 101	O 136	S 10	0	0	0
4	D	84	Total 595	C 352	N 96	O 137	S 10	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression tag	UNP O08795
B	-9	GLY	-	expression tag	UNP O08795
B	-8	MET	-	expression tag	UNP O08795
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
B	0	SER	-	expression tag	UNP O08795
B	1	LEU	-	expression tag	UNP O08795
B	2	LEU	-	expression tag	UNP O08795
B	3	SER	-	expression tag	UNP O08795
B	4	VAL	-	expression tag	UNP O08795
B	5	LEU	-	expression tag	UNP O08795
B	6	LEU	-	expression tag	UNP O08795
B	7	MET	-	expression tag	UNP O08795
B	8	GLY	-	expression tag	UNP O08795
B	9	CYS	-	expression tag	UNP O08795
B	10	VAL	-	expression tag	UNP O08795
B	11	ALA	-	expression tag	UNP O08795
B	12	GLU	-	expression tag	UNP O08795
B	13	THR	-	expression tag	UNP O08795
B	14	GLY	-	expression tag	UNP O08795
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
D	-2	LEU	-	expression tag	UNP O08795
D	-1	VAL	-	expression tag	UNP O08795
D	0	SER	-	expression tag	UNP O08795
D	1	LEU	-	expression tag	UNP O08795
D	2	LEU	-	expression tag	UNP O08795
D	3	SER	-	expression tag	UNP O08795
D	4	VAL	-	expression tag	UNP O08795
D	5	LEU	-	expression tag	UNP O08795
D	6	LEU	-	expression tag	UNP O08795
D	7	MET	-	expression tag	UNP O08795
D	8	GLY	-	expression tag	UNP O08795
D	9	CYS	-	expression tag	UNP O08795
D	10	VAL	-	expression tag	UNP O08795
D	11	ALA	-	expression tag	UNP O08795
D	12	GLU	-	expression tag	UNP O08795
D	13	THR	-	expression tag	UNP O08795
D	14	GLY	-	expression tag	UNP O08795

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



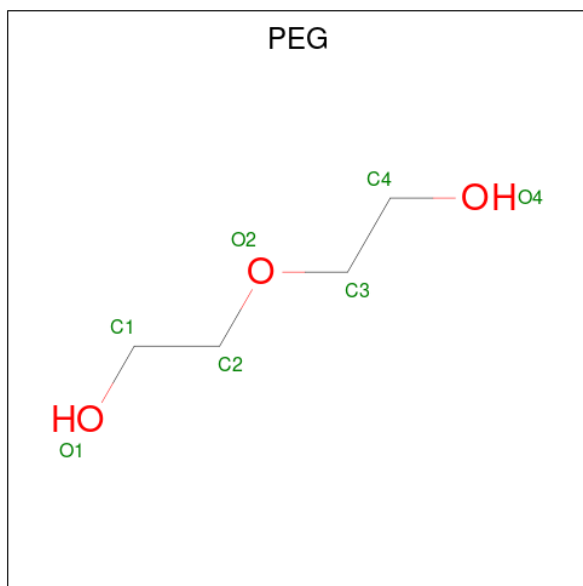
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



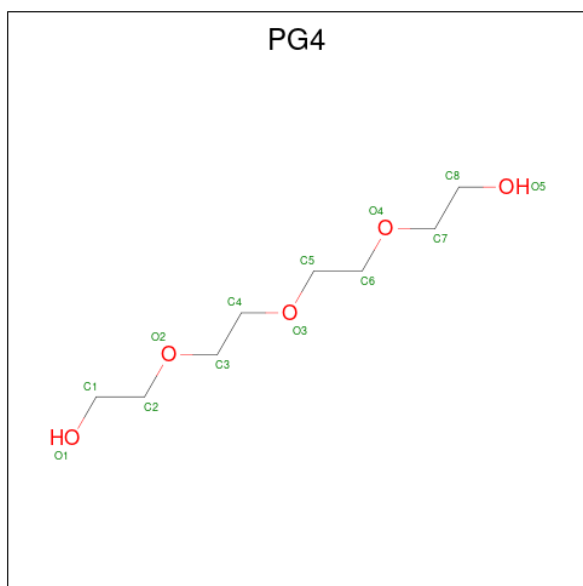
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

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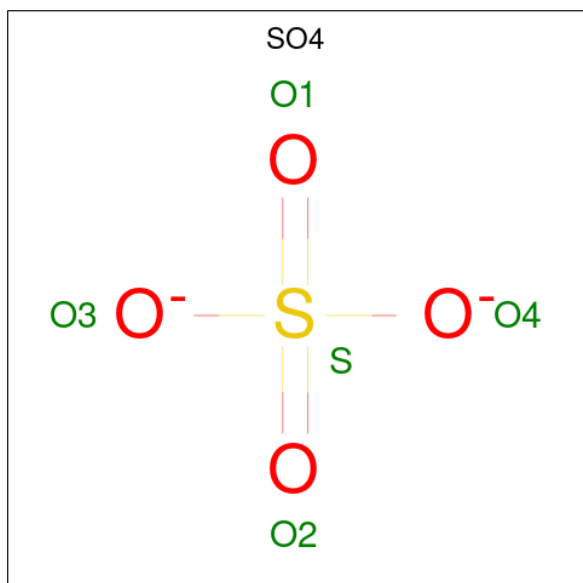
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Ca 2 2	0	0
9	D	2	Total Ca 2 2	0	0

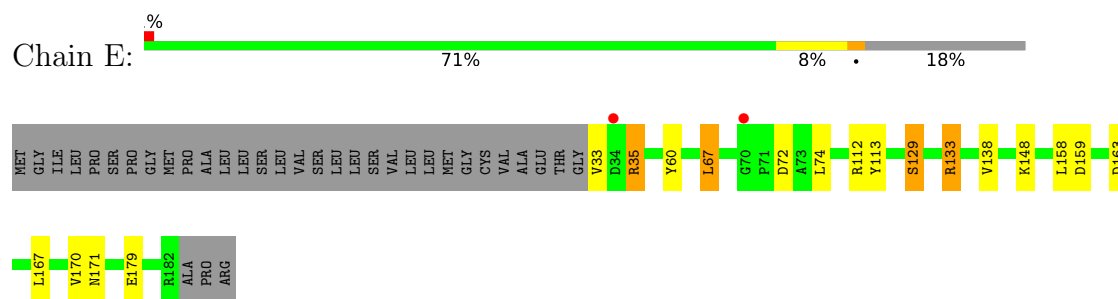
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	61	Total O 61 61	0	0
10	F	45	Total O 45 45	0	0
10	A	249	Total O 249 249	0	0
10	B	25	Total O 25 25	0	0
10	G	24	Total O 24 24	0	0
10	H	31	Total O 31 31	0	0
10	C	223	Total O 223 223	0	0
10	D	22	Total O 22 22	0	0

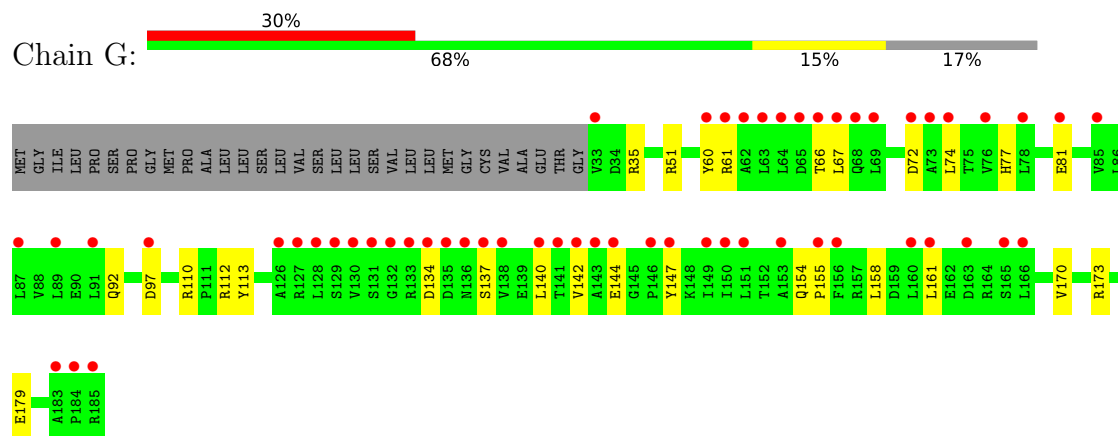
3 Residue-property plots

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.

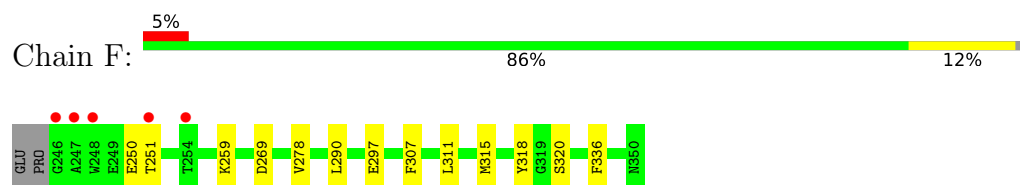
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



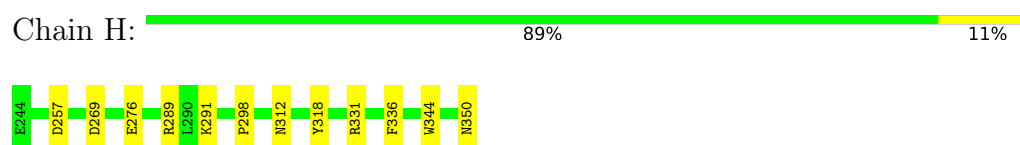
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



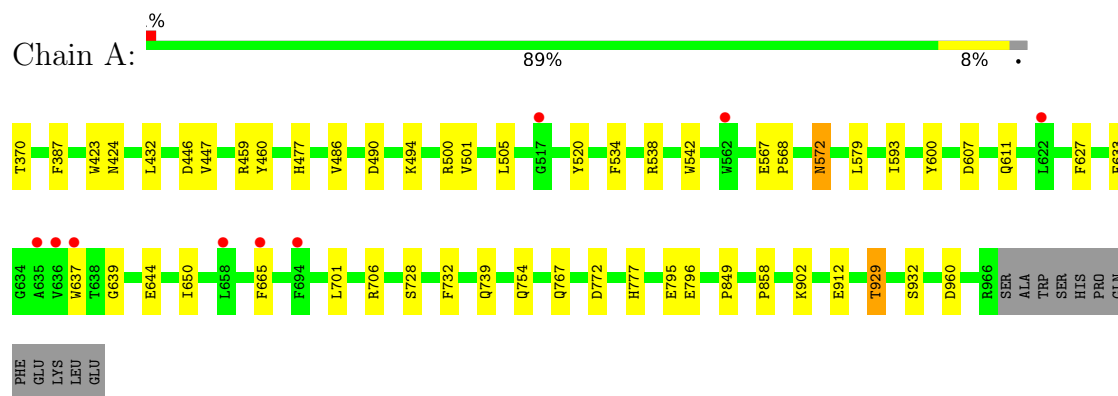
- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2



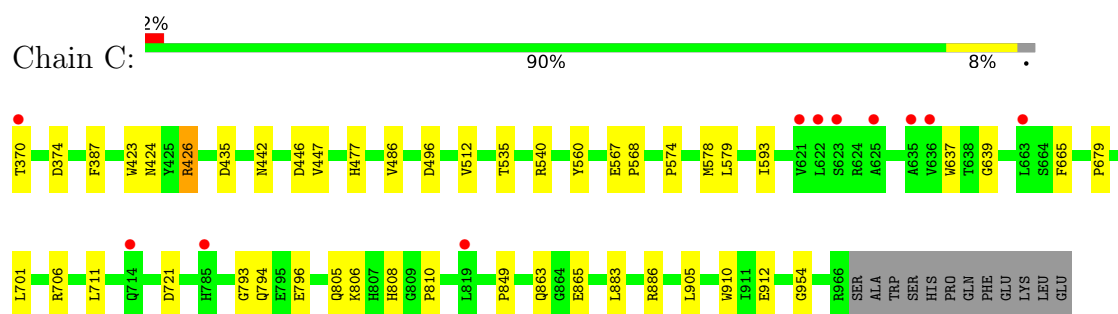
- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2



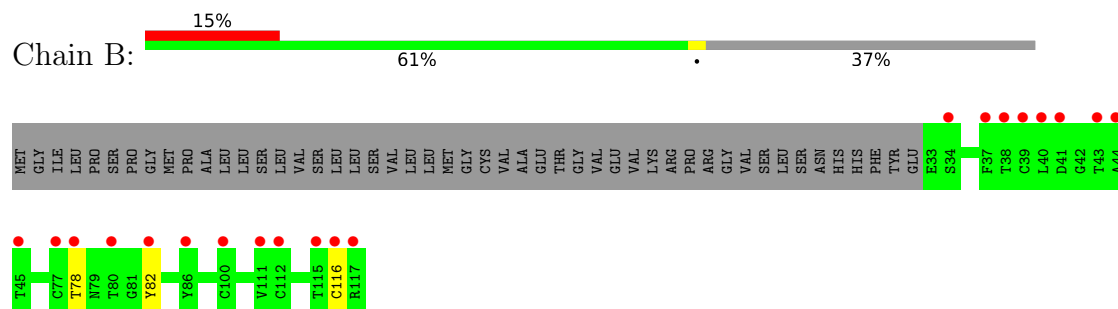
● Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3



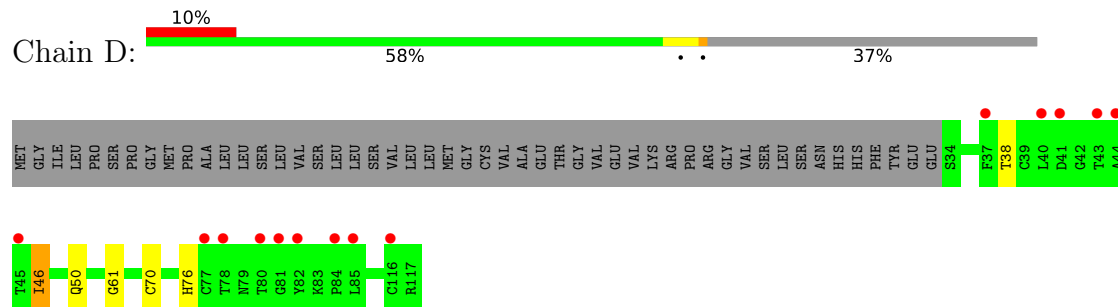
● Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3



● Molecule 4: Glucosidase 2 subunit beta



● Molecule 4: Glucosidase 2 subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.97Å 102.97Å 240.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.33 – 2.29 49.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.33-2.29) 96.3 (49.87-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.206 0.180 , 0.206	Depositor DCC
R_{free} test set	2019 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l 0.035 for h,-h-k,-l 0.020 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15764	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, PG4, CA, PEG, SO4

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	E	0.25	0/1211	0.49	0/1643
1	G	0.24	0/1203	0.52	2/1636 (0.1%)
2	F	0.25	0/856	0.48	0/1171
2	H	0.25	0/863	0.47	0/1181
3	A	0.26	0/5039	0.46	0/6865
3	C	0.26	0/5029	0.46	0/6852
4	B	0.26	0/614	0.51	0/840
4	D	0.26	0/606	0.51	0/831
All	All	0.25	0/15421	0.47	2/21019 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	35	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	G	97	ASP	CB-CG-OD2	5.24	123.02	118.30

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	E	1189	0	1215	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1183	0	1172	17	1
2	F	828	0	765	11	0
2	H	835	0	777	11	0
3	A	4858	0	4624	37	0
3	C	4848	0	4615	26	0
4	B	603	0	493	1	0
4	D	595	0	482	3	0
5	A	36	0	52	10	0
5	B	4	0	6	0	0
5	C	32	0	48	3	0
5	E	12	0	18	0	0
5	F	4	0	6	1	0
5	G	4	0	6	1	0
6	A	21	0	30	1	0
7	A	13	0	18	0	0
8	A	10	0	0	1	0
8	C	5	0	0	0	0
9	B	2	0	0	0	0
9	D	2	0	0	0	0
10	A	249	0	0	6	0
10	B	25	0	0	0	0
10	C	223	0	0	7	0
10	D	22	0	0	1	0
10	E	61	0	0	5	0
10	F	45	0	0	1	0
10	G	24	0	0	6	0
10	H	31	0	0	1	0
All	All	15764	0	14327	110	1

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 4.

The worst 5 of 110 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)
5:A:1006:EDO:O1	10:A:1101:HOH:O	1.92	0.87
3:A:796:GLU:OE1	10:A:1102:HOH:O	1.93	0.86
3:C:721:ASP:OD1	10:C:1101:HOH:O	1.98	0.82
1:G:110:ARG:NH2	10:G:304:HOH:O	2.16	0.79
1:E:60:TYR:OH	10:E:301:HOH:O	2.02	0.78

All (1) 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)
1:E:72:ASP:OD1	1:G:110:ARG:NH1[3_565]	2.18	0.02

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	E	149/184 (81%)	143 (96%)	6 (4%)	0	100	100
1	G	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
2	F	103/107 (96%)	97 (94%)	6 (6%)	0	100	100
2	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	A	601/609 (99%)	590 (98%)	11 (2%)	0	100	100
3	C	601/609 (99%)	589 (98%)	12 (2%)	0	100	100
4	B	83/134 (62%)	82 (99%)	1 (1%)	0	100	100
4	D	82/134 (61%)	79 (96%)	3 (4%)	0	100	100
All	All	1875/2068 (91%)	1826 (97%)	49 (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	E	134/163 (82%)	128 (96%)	6 (4%)	27	39
1	G	126/163 (77%)	123 (98%)	3 (2%)	49	66
2	F	87/92 (95%)	86 (99%)	1 (1%)	73	86
2	H	88/92 (96%)	88 (100%)	0	100	100
3	A	521/529 (98%)	511 (98%)	10 (2%)	57	73
3	C	519/529 (98%)	509 (98%)	10 (2%)	57	73
4	B	67/116 (58%)	66 (98%)	1 (2%)	65	79
4	D	67/116 (58%)	65 (97%)	2 (3%)	41	57
All	All	1609/1800 (89%)	1576 (98%)	33 (2%)	55	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	806	LYS
3	C	808	HIS
4	D	46	ILE
3	A	637	TRP
3	A	572	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	572	ASN
3	C	563	ASN
3	C	808	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

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	$\# Z > 2$
5	EDO	C	1004	-	3,3,3	0.46	0	2,2,2	0.40	0
5	EDO	C	1001	-	3,3,3	0.51	0	2,2,2	0.30	0
5	EDO	G	201	-	3,3,3	0.41	0	2,2,2	0.41	0
5	EDO	A	1006	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	A	1001	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	A	1003	3	3,3,3	0.48	0	2,2,2	0.33	0
7	PG4	A	1009	-	12,12,12	0.53	0	11,11,11	0.20	0
5	EDO	C	1003	-	3,3,3	0.46	0	2,2,2	0.41	0
5	EDO	C	1006	-	3,3,3	0.42	0	2,2,2	0.49	0
6	PEG	A	1004	-	6,6,6	0.50	0	5,5,5	0.33	0
5	EDO	E	201	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	1007	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	F	401	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	A	1008	-	3,3,3	0.53	0	2,2,2	0.18	0
8	SO4	C	1009	-	4,4,4	0.13	0	6,6,6	0.11	0
5	EDO	C	1002	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	C	1005	-	3,3,3	0.48	0	2,2,2	0.32	0
8	SO4	A	1014	-	4,4,4	0.13	0	6,6,6	0.12	0
5	EDO	A	1010	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	B	603	-	3,3,3	0.44	0	2,2,2	0.47	0
5	EDO	A	1013	-	3,3,3	0.56	0	2,2,2	0.27	0
5	EDO	A	1011	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	C	1008	-	3,3,3	0.58	0	2,2,2	0.25	0
5	EDO	E	202	-	3,3,3	0.42	0	2,2,2	0.42	0
5	EDO	A	1012	3	3,3,3	0.46	0	2,2,2	0.44	0
6	PEG	A	1005	-	6,6,6	0.48	0	5,5,5	0.49	0
6	PEG	A	1002	-	6,6,6	0.48	0	5,5,5	0.26	0
5	EDO	C	1007	-	3,3,3	0.43	0	2,2,2	0.45	0
8	SO4	A	1015	-	4,4,4	0.13	0	6,6,6	0.11	0
5	EDO	E	203	-	3,3,3	0.40	0	2,2,2	0.44	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
5	EDO	C	1004	-	-	0/1/1/1	-
5	EDO	C	1001	-	-	1/1/1/1	-
5	EDO	G	201	-	-	1/1/1/1	-
5	EDO	A	1006	-	-	1/1/1/1	-
5	EDO	A	1001	-	-	1/1/1/1	-
5	EDO	A	1003	3	-	1/1/1/1	-
7	PG4	A	1009	-	-	5/10/10/10	-
5	EDO	C	1003	-	-	1/1/1/1	-
5	EDO	C	1006	-	-	1/1/1/1	-
6	PEG	A	1004	-	-	1/4/4/4	-
5	EDO	E	201	-	-	1/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	F	401	-	-	1/1/1/1	-
5	EDO	A	1008	-	-	0/1/1/1	-
5	EDO	C	1002	-	-	1/1/1/1	-
5	EDO	C	1005	-	-	0/1/1/1	-
5	EDO	A	1010	-	-	0/1/1/1	-
5	EDO	B	603	-	-	0/1/1/1	-
5	EDO	A	1013	-	-	0/1/1/1	-
5	EDO	A	1011	-	-	1/1/1/1	-
5	EDO	C	1008	-	-	0/1/1/1	-
5	EDO	E	202	-	-	0/1/1/1	-
5	EDO	A	1012	3	-	1/1/1/1	-
6	PEG	A	1005	-	-	3/4/4/4	-
6	PEG	A	1002	-	-	3/4/4/4	-
5	EDO	C	1007	-	-	0/1/1/1	-
5	EDO	E	203	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1004	PEG	O2-C3-C4-O4
5	E	201	EDO	O1-C1-C2-O2
5	A	1001	EDO	O1-C1-C2-O2
5	A	1003	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	C	1001	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	201	EDO	1	0
5	A	1006	EDO	3	0
5	A	1001	EDO	1	0
5	A	1003	EDO	1	0
5	C	1006	EDO	1	0
5	A	1007	EDO	1	0
5	F	401	EDO	1	0
5	A	1008	EDO	2	0
5	A	1010	EDO	1	0
5	A	1011	EDO	1	0
6	A	1005	PEG	1	0
5	C	1007	EDO	2	0
8	A	1015	SO4	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	E	150/184 (81%)	-0.16	2 (1%) 77 81	37, 51, 75, 106	0
1	G	153/184 (83%)	1.37	56 (36%) 0 0	45, 75, 98, 113	0
2	F	105/107 (98%)	0.01	5 (4%) 30 37	33, 41, 76, 97	0
2	H	107/107 (100%)	0.15	0 100 100	37, 54, 74, 104	0
3	A	597/609 (98%)	-0.15	9 (1%) 73 79	30, 40, 59, 80	0
3	C	597/609 (98%)	-0.04	11 (1%) 68 74	31, 43, 63, 102	0
4	B	85/134 (63%)	0.72	20 (23%) 0 1	38, 58, 106, 144	0
4	D	84/134 (62%)	0.67	14 (16%) 1 2	36, 59, 105, 119	0
All	All	1878/2068 (90%)	0.11	117 (6%) 20 26	30, 46, 83, 144	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	81	GLY	8.4
4	D	82	TYR	7.0
4	D	80	THR	6.8
4	B	82	TYR	6.7
2	F	247	ALA	5.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	EDO	C	1001	4/4	0.77	0.32	59,62,63,68	0
7	PG4	A	1009	13/13	0.77	0.41	56,72,85,88	0
5	EDO	C	1007	4/4	0.81	0.36	57,63,63,64	0
6	PEG	A	1004	7/7	0.82	0.27	43,62,71,74	0
5	EDO	C	1002	4/4	0.82	0.21	54,55,64,65	0
6	PEG	A	1005	7/7	0.83	0.16	50,66,76,80	0
5	EDO	A	1010	4/4	0.84	0.19	57,59,63,68	0
6	PEG	A	1002	7/7	0.86	0.14	58,63,71,76	0
5	EDO	A	1006	4/4	0.86	0.19	47,55,58,67	0
5	EDO	G	201	4/4	0.87	0.22	62,65,67,71	0
5	EDO	A	1008	4/4	0.88	0.19	50,60,65,73	0
5	EDO	A	1012	4/4	0.88	0.40	52,52,62,72	0
5	EDO	C	1006	4/4	0.89	0.24	54,56,58,71	0
5	EDO	B	603	4/4	0.90	0.27	59,60,60,61	0
8	SO4	A	1014	5/5	0.91	0.15	79,80,83,109	0
5	EDO	C	1005	4/4	0.92	0.10	51,55,57,60	0
5	EDO	E	202	4/4	0.92	0.16	49,55,62,62	0
8	SO4	A	1015	5/5	0.92	0.25	78,90,99,100	0
5	EDO	A	1001	4/4	0.93	0.09	51,51,58,58	0
5	EDO	A	1003	4/4	0.93	0.32	61,69,74,85	0
5	EDO	E	201	4/4	0.93	0.09	57,57,62,71	0
5	EDO	A	1007	4/4	0.93	0.10	54,56,63,65	0
5	EDO	C	1004	4/4	0.94	0.15	49,50,52,70	0
5	EDO	F	401	4/4	0.94	0.19	49,52,57,63	0
5	EDO	A	1011	4/4	0.95	0.28	50,54,55,64	0
5	EDO	C	1003	4/4	0.96	0.19	53,54,60,64	0
5	EDO	C	1008	4/4	0.96	0.34	38,48,53,58	0
5	EDO	E	203	4/4	0.97	0.18	41,42,53,67	0
5	EDO	A	1013	4/4	0.97	0.38	44,46,47,54	0
8	SO4	C	1009	5/5	0.97	0.30	64,66,85,99	0
9	CA	D	601	1/1	0.98	0.04	48,48,48,48	0
9	CA	B	602	1/1	0.99	0.06	41,41,41,41	0
9	CA	B	601	1/1	0.99	0.06	49,49,49,49	0
9	CA	D	602	1/1	0.99	0.08	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.