



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2025 – 12:33 PM EST

PDB ID : 9NPL / pdb\_00009npl  
Title : Crystal structure of the inactive conformation of a glycoside hydrolase (CapGH2b - E553Q Mutant) from the GH2 family in the space group P1 at 2.25 Å  
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Deposited on : 2025-03-11  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

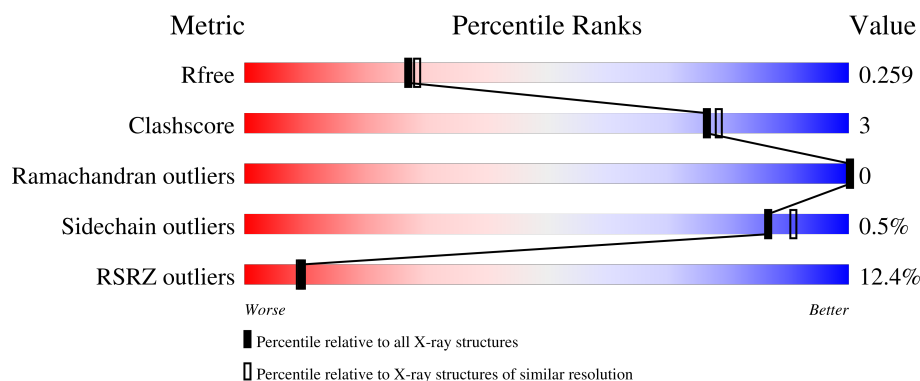
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	798	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>
1	B	798	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	798	<div> <div>21%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>11%</div> </div> </div>
1	D	798	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	798	<div><div></div><div>6%</div><div>84%</div><div>7%</div><div>9%</div></div>
1	F	798	<div><div></div><div>23%</div><div>80%</div><div>9%</div><div>11%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 36354 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 Glycoside hydrolase family 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5906	3773	1009	1094	30			
1	B	722	Total	C	N	O	S	0	0	0
			5806	3710	991	1076	29			
1	C	708	Total	C	N	O	S	0	0	0
			5698	3638	974	1057	29			
1	D	735	Total	C	N	O	S	0	0	0
			5909	3776	1011	1093	29			
1	E	726	Total	C	N	O	S	0	0	0
			5834	3726	996	1083	29			
1	F	708	Total	C	N	O	S	0	0	0
			5707	3651	975	1053	28			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0

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

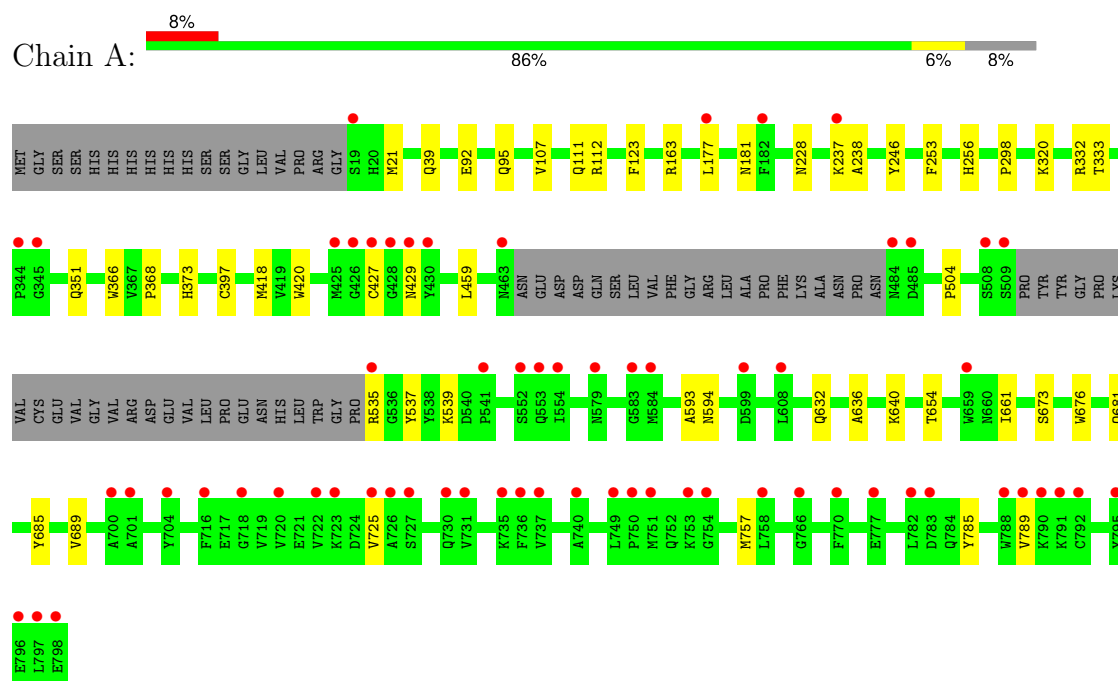
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total	O	0	0
			211	211		
4	B	272	Total	O	0	0
			272	272		
4	C	116	Total	O	0	0
			116	116		
4	D	224	Total	O	0	0
			224	224		
4	E	241	Total	O	0	0
			241	241		
4	F	92	Total	O	0	0
			92	92		

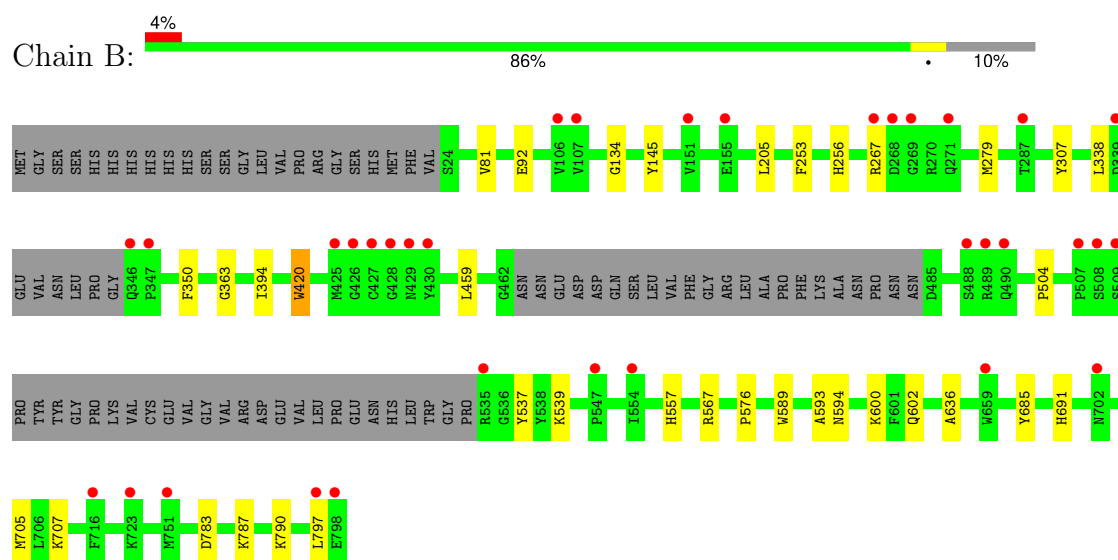
### 3 Residue-property plots [i](#)

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.

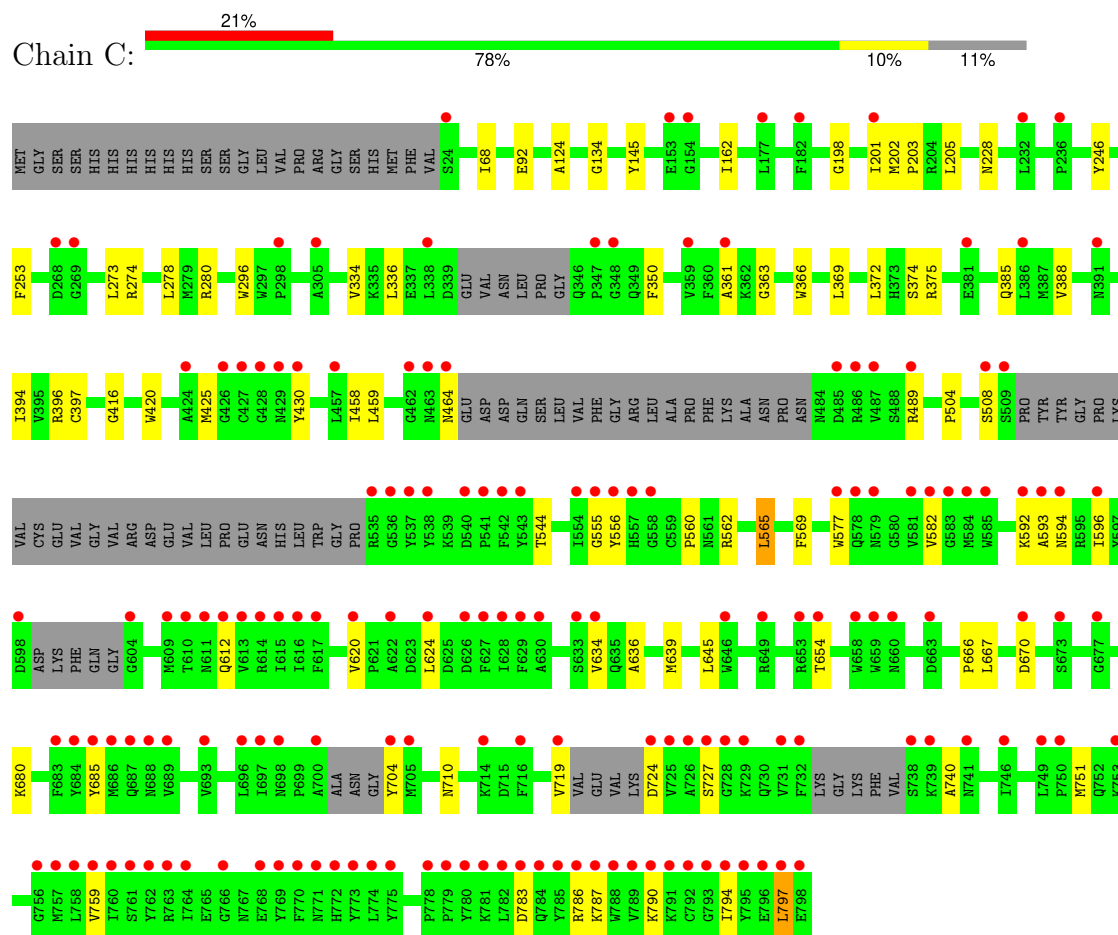
#### • Molecule 1: Glycoside hydrolase family 2



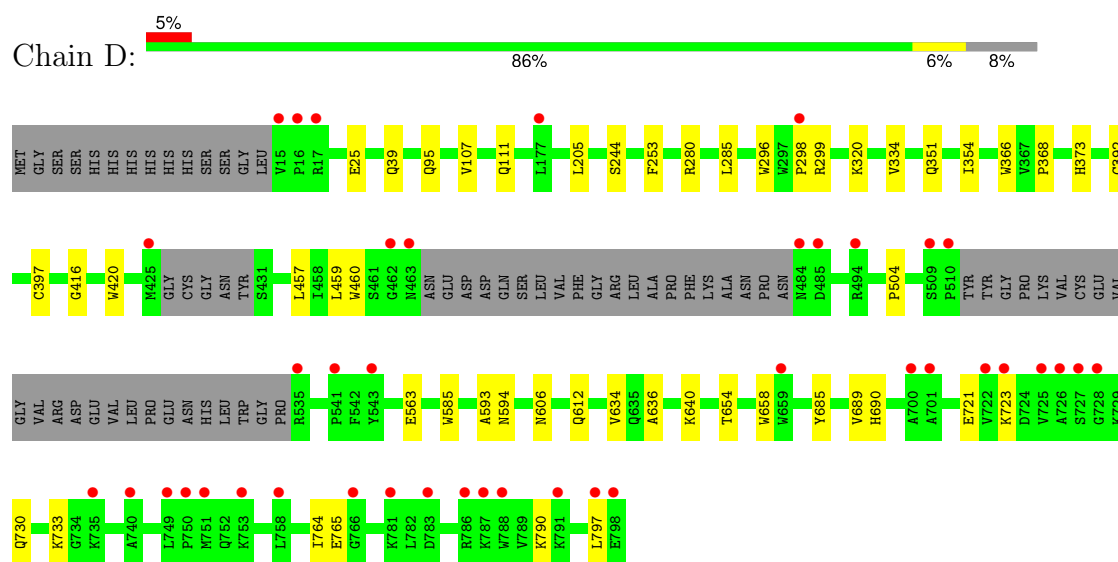
#### • Molecule 1: Glycoside hydrolase family 2



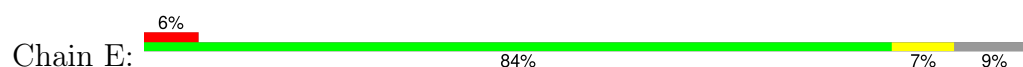
• Molecule 1: Glycoside hydrolase family 2

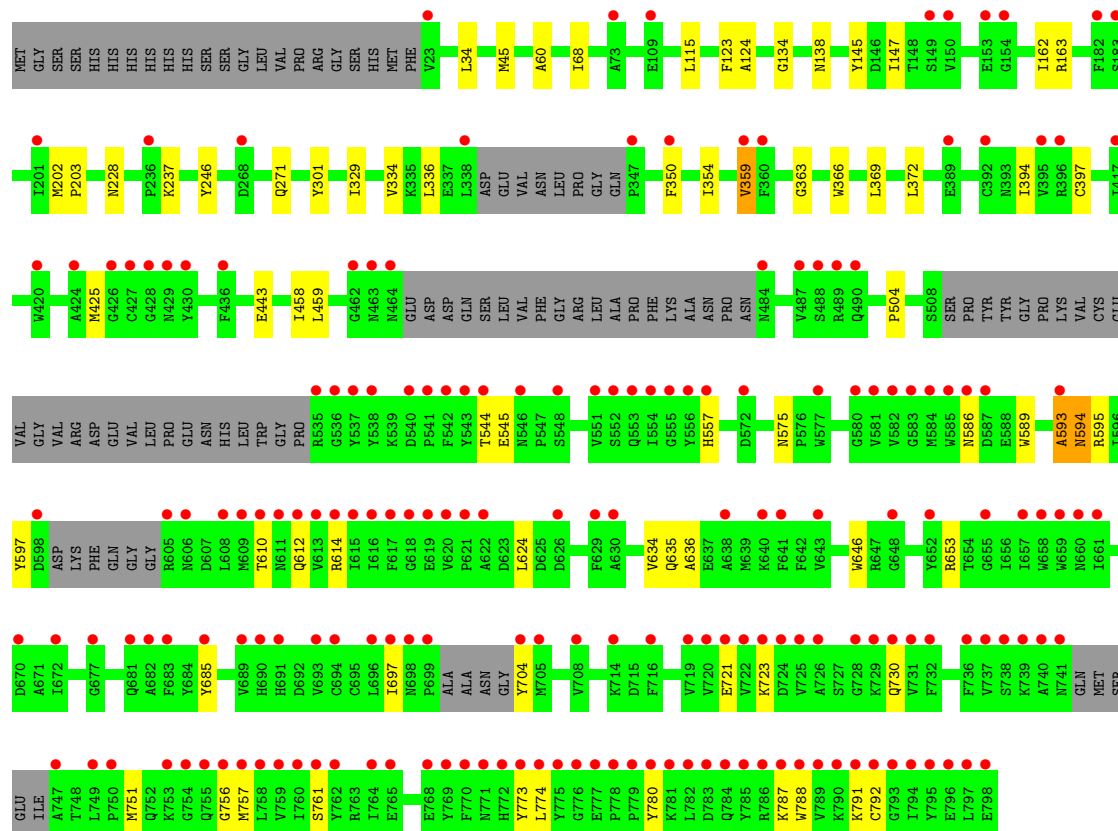


• Molecule 1: Glycoside hydrolase family 2



• Molecule 1: Glycoside hydrolase family 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.98Å 124.41Å 133.48Å 89.21° 117.47° 103.29°	Depositor
Resolution (Å)	47.41 – 2.25 47.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.41-2.25) 96.8 (47.41-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.230 , 0.260 0.230 , 0.259	Depositor DCC
$R_{free}$ test set	15611 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	36354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.19% 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, PO4

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	0.13	0/6059	0.33	0/8225
1	B	0.10	0/5955	0.31	0/8080
1	C	0.16	0/5841	0.32	0/7925
1	D	0.12	0/6062	0.32	0/8228
1	E	0.12	0/5983	0.31	0/8118
1	F	0.13	0/5852	0.32	0/7939
All	All	0.13	0/35752	0.32	0/48515

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	535	ARG	Sidechain
1	F	593	ALA	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5906	0	5729	29	0
1	B	5806	0	5635	23	0
1	C	5698	0	5514	47	0
1	D	5909	0	5741	29	0
1	E	5834	0	5659	30	0
1	F	5707	0	5545	41	0
2	A	35	0	0	0	0
2	B	50	0	0	0	0
2	C	10	0	0	0	0
2	D	15	0	0	0	0
2	E	25	0	0	0	0
2	F	15	0	0	0	0
3	A	32	0	48	2	0
3	B	56	0	84	4	0
3	C	20	0	30	3	0
3	D	40	0	60	2	0
3	E	20	0	30	2	0
3	F	20	0	30	2	0
4	A	211	0	0	0	0
4	B	272	0	0	0	0
4	C	116	0	0	0	0
4	D	224	0	0	0	0
4	E	241	0	0	1	0
4	F	92	0	0	0	0
All	All	36354	0	34105	192	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 3.

The worst 5 of 192 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:D:721:GLU:HB3	1:D:733:LYS:HD3	1.80	0.63
1:E:459:LEU:HD23	1:E:504:PRO:HG2	1.82	0.61
1:E:676:TRP:HB3	3:E:807:EDO:H21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ALA:N	1:C:594:ASN:HA	2.16	0.61
1:D:25:GLU:HB2	3:D:805:EDO:H21	1.84	0.60

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	729/798 (91%)	706 (97%)	23 (3%)	0	100	100
1	B	714/798 (90%)	689 (96%)	25 (4%)	0	100	100
1	C	692/798 (87%)	668 (96%)	24 (4%)	0	100	100
1	D	727/798 (91%)	706 (97%)	21 (3%)	0	100	100
1	E	718/798 (90%)	696 (97%)	22 (3%)	0	100	100
1	F	694/798 (87%)	672 (97%)	22 (3%)	0	100	100
All	All	4274/4788 (89%)	4137 (97%)	137 (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	635/689 (92%)	635 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	623/689 (90%)	620 (100%)	3 (0%)	86	91
1	C	613/689 (89%)	608 (99%)	5 (1%)	79	86
1	D	636/689 (92%)	634 (100%)	2 (0%)	91	94
1	E	626/689 (91%)	622 (99%)	4 (1%)	84	89
1	F	614/689 (89%)	611 (100%)	3 (0%)	86	91
All	All	3747/4134 (91%)	3730 (100%)	17 (0%)	86	91

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	359	VAL
1	F	594	ASN
1	C	797	LEU
1	D	205	LEU
1	D	334	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	26	GLN
1	F	553	GLN
1	E	228	ASN
1	E	575	ASN
1	F	741	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

77 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	PO4	E	804	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
3	EDO	B	811	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	B	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
2	PO4	A	803	-	4,4,4	1.64	1 (25%)	6,6,6	0.49	0
2	PO4	B	806	-	4,4,4	1.61	1 (25%)	6,6,6	0.51	0
3	EDO	B	822	-	3,3,3	0.25	0	2,2,2	0.32	0
2	PO4	A	801	-	4,4,4	1.60	1 (25%)	6,6,6	0.47	0
3	EDO	B	814	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	B	805	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
3	EDO	A	809	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	D	811	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	D	810	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	A	810	-	3,3,3	0.25	0	2,2,2	0.32	0
2	PO4	A	804	-	4,4,4	1.62	1 (25%)	6,6,6	0.50	0
3	EDO	C	807	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	D	805	-	3,3,3	0.24	0	2,2,2	0.33	0
2	PO4	A	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
3	EDO	D	809	-	3,3,3	0.24	0	2,2,2	0.34	0
3	EDO	A	811	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	F	805	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	C	805	-	3,3,3	0.25	0	2,2,2	0.29	0
2	PO4	E	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.47	0
2	PO4	A	806	-	4,4,4	1.59	1 (25%)	6,6,6	0.48	0
3	EDO	D	804	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	D	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	EDO	F	807	-	3,3,3	0.23	0	2,2,2	0.34	0
3	EDO	B	815	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	B	824	-	3,3,3	0.24	0	2,2,2	0.33	0
2	PO4	B	808	-	4,4,4	1.63	1 (25%)	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	E	805	-	4,4,4	1.61	1 (25%)	6,6,6	0.50	0
3	EDO	A	814	-	3,3,3	0.26	0	2,2,2	0.32	0
3	EDO	B	813	-	3,3,3	0.26	0	2,2,2	0.31	0
2	PO4	A	805	-	4,4,4	1.65	1 (25%)	6,6,6	0.48	0
3	EDO	F	806	-	3,3,3	0.25	0	2,2,2	0.37	0
3	EDO	E	810	-	3,3,3	0.24	0	2,2,2	0.32	0
2	PO4	D	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.52	0
3	EDO	F	808	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	A	815	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	F	803	-	4,4,4	1.63	1 (25%)	6,6,6	0.52	0
2	PO4	B	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.48	0
3	EDO	E	807	-	3,3,3	0.25	0	2,2,2	0.31	0
2	PO4	B	801	-	4,4,4	1.58	1 (25%)	6,6,6	0.50	0
3	EDO	B	818	-	3,3,3	0.24	0	2,2,2	0.36	0
2	PO4	B	807	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
2	PO4	C	801	-	4,4,4	1.52	1 (25%)	6,6,6	0.57	0
2	PO4	E	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	EDO	D	806	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	B	817	-	3,3,3	0.24	0	2,2,2	0.32	0
3	EDO	D	808	-	3,3,3	0.24	0	2,2,2	0.32	0
3	EDO	B	821	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	B	816	-	3,3,3	0.24	0	2,2,2	0.33	0
2	PO4	F	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.49	0
3	EDO	D	812	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	C	806	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	D	807	-	3,3,3	0.23	0	2,2,2	0.31	0
3	EDO	B	823	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	A	807	-	4,4,4	0.74	0	6,6,6	0.48	0
2	PO4	C	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
3	EDO	B	812	-	3,3,3	0.25	0	2,2,2	0.34	0
3	EDO	B	820	-	3,3,3	0.26	0	2,2,2	0.29	0
3	EDO	A	813	-	3,3,3	0.25	0	2,2,2	0.34	0
3	EDO	E	809	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	E	806	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	D	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.48	0
2	PO4	B	809	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	EDO	E	808	-	3,3,3	0.25	0	2,2,2	0.32	0
2	PO4	F	801	-	4,4,4	1.50	1 (25%)	6,6,6	0.58	0
2	PO4	B	810	-	4,4,4	1.60	1 (25%)	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	F	804	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	E	801	-	4,4,4	1.56	1 (25%)	6,6,6	0.47	0
3	EDO	C	804	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	A	808	-	3,3,3	0.25	0	2,2,2	0.34	0
3	EDO	D	813	-	3,3,3	0.26	0	2,2,2	0.30	0
2	PO4	B	804	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	EDO	A	812	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	B	819	-	3,3,3	0.24	0	2,2,2	0.34	0
3	EDO	C	803	-	3,3,3	0.25	0	2,2,2	0.33	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	D	804	-	-	0/1/1/1	-
3	EDO	D	806	-	-	0/1/1/1	-
3	EDO	B	811	-	-	0/1/1/1	-
3	EDO	F	807	-	-	0/1/1/1	-
3	EDO	B	815	-	-	0/1/1/1	-
3	EDO	B	824	-	-	1/1/1/1	-
3	EDO	F	804	-	-	0/1/1/1	-
3	EDO	B	822	-	-	0/1/1/1	-
3	EDO	B	817	-	-	1/1/1/1	-
3	EDO	C	804	-	-	0/1/1/1	-
3	EDO	A	814	-	-	0/1/1/1	-
3	EDO	B	813	-	-	1/1/1/1	-
3	EDO	F	806	-	-	1/1/1/1	-
3	EDO	B	814	-	-	1/1/1/1	-
3	EDO	E	810	-	-	0/1/1/1	-
3	EDO	D	808	-	-	1/1/1/1	-
3	EDO	A	809	-	-	0/1/1/1	-
3	EDO	B	821	-	-	0/1/1/1	-
3	EDO	D	811	-	-	0/1/1/1	-
3	EDO	B	816	-	-	0/1/1/1	-
3	EDO	D	810	-	-	0/1/1/1	-
3	EDO	A	808	-	-	0/1/1/1	-
3	EDO	A	810	-	-	1/1/1/1	-
3	EDO	F	808	-	-	0/1/1/1	-
3	EDO	D	812	-	-	0/1/1/1	-
3	EDO	C	807	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	813	-	-	0/1/1/1	-
3	EDO	D	805	-	-	0/1/1/1	-
3	EDO	C	806	-	-	0/1/1/1	-
3	EDO	D	809	-	-	0/1/1/1	-
3	EDO	A	811	-	-	0/1/1/1	-
3	EDO	A	812	-	-	0/1/1/1	-
3	EDO	B	823	-	-	0/1/1/1	-
3	EDO	D	807	-	-	0/1/1/1	-
3	EDO	A	815	-	-	0/1/1/1	-
3	EDO	F	805	-	-	0/1/1/1	-
3	EDO	E	807	-	-	0/1/1/1	-
3	EDO	B	819	-	-	1/1/1/1	-
3	EDO	B	812	-	-	0/1/1/1	-
3	EDO	C	805	-	-	0/1/1/1	-
3	EDO	B	820	-	-	0/1/1/1	-
3	EDO	B	818	-	-	0/1/1/1	-
3	EDO	A	813	-	-	0/1/1/1	-
3	EDO	E	809	-	-	0/1/1/1	-
3	EDO	C	803	-	-	1/1/1/1	-
3	EDO	E	806	-	-	0/1/1/1	-
3	EDO	E	808	-	-	0/1/1/1	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	805	PO4	P-O1	2.81	1.57	1.50
2	B	808	PO4	P-O1	2.81	1.57	1.50
2	A	803	PO4	P-O1	2.81	1.57	1.50
2	F	803	PO4	P-O1	2.80	1.57	1.50
2	C	802	PO4	P-O1	2.80	1.57	1.50

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	819	EDO	O1-C1-C2-O2
3	B	817	EDO	O1-C1-C2-O2
3	B	824	EDO	O1-C1-C2-O2
3	B	813	EDO	O1-C1-C2-O2
3	C	807	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	811	EDO	1	0
3	A	810	EDO	1	0
3	D	805	EDO	1	0
3	C	805	EDO	2	0
3	B	824	EDO	1	0
3	A	814	EDO	1	0
3	F	806	EDO	1	0
3	E	807	EDO	1	0
3	D	808	EDO	1	0
3	C	806	EDO	1	0
3	B	812	EDO	1	0
3	E	808	EDO	1	0
3	F	804	EDO	1	0
3	B	819	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	735/798 (92%)	0.42	65 (8%)	17 17	27, 43, 73, 86	0
1	B	722/798 (90%)	0.39	34 (4%)	37 37	28, 41, 61, 76	0
1	C	708/798 (88%)	1.16	164 (23%)	2 3	35, 53, 93, 114	0
1	D	735/798 (92%)	0.32	41 (5%)	31 31	27, 42, 72, 84	0
1	E	726/798 (90%)	0.49	47 (6%)	26 25	28, 42, 65, 89	0
1	F	708/798 (88%)	1.31	186 (26%)	2 2	34, 58, 101, 114	0
All	All	4334/4788 (90%)	0.68	537 (12%)	9 9	27, 45, 84, 114	0

The worst 5 of 537 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLY	6.9
1	C	427	CYS	6.1
1	E	429	ASN	6.0
1	F	538	TYR	5.3
1	D	510	PRO	5.2

### 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

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	PO4	B	803	5/5	0.29	0.22	80,83,89,100	0
2	PO4	E	805	5/5	0.31	0.20	81,82,90,90	0
2	PO4	A	801	5/5	0.36	0.20	84,89,94,100	0
2	PO4	A	806	5/5	0.36	0.19	86,95,103,103	0
2	PO4	B	809	5/5	0.41	0.20	65,76,79,87	0
2	PO4	B	805	5/5	0.46	0.14	85,89,94,96	0
2	PO4	B	808	5/5	0.52	0.19	59,68,73,82	0
2	PO4	D	802	5/5	0.54	0.31	45,45,48,49	5
2	PO4	B	804	5/5	0.54	0.17	64,75,83,86	0
2	PO4	B	810	5/5	0.55	0.16	73,73,86,89	0
2	PO4	F	803	5/5	0.56	0.19	63,65,76,78	0
2	PO4	A	805	5/5	0.58	0.25	55,59,73,77	0
2	PO4	A	804	5/5	0.60	0.14	74,75,85,92	0
2	PO4	E	803	5/5	0.60	0.16	61,67,76,81	0
2	PO4	F	802	5/5	0.61	0.16	81,89,96,100	0
2	PO4	B	806	5/5	0.63	0.20	64,67,71,76	0
2	PO4	E	802	5/5	0.63	0.16	74,78,83,93	0
2	PO4	A	807	5/5	0.65	0.16	74,74,82,83	0
3	EDO	F	808	4/4	0.66	0.24	85,85,87,87	0
3	EDO	F	805	4/4	0.67	0.20	70,70,72,72	0
3	EDO	A	809	4/4	0.68	0.24	69,71,75,76	0
2	PO4	C	802	5/5	0.69	0.19	57,61,66,71	0
2	PO4	B	807	5/5	0.70	0.24	47,48,50,55	5
3	EDO	D	810	4/4	0.70	0.20	54,56,58,59	0
3	EDO	E	808	4/4	0.71	0.21	44,47,50,51	0
3	EDO	C	804	4/4	0.72	0.23	44,46,50,50	0
2	PO4	E	804	5/5	0.73	0.23	47,49,51,57	5
3	EDO	D	809	4/4	0.74	0.23	72,74,74,75	0
3	EDO	C	805	4/4	0.75	0.22	47,50,55,57	0
3	EDO	B	815	4/4	0.75	0.18	56,62,62,65	0
2	PO4	A	803	5/5	0.75	0.16	60,64,67,77	0
3	EDO	B	824	4/4	0.76	0.19	46,47,49,51	0
2	PO4	B	802	5/5	0.76	0.18	36,45,55,57	5
3	EDO	D	811	4/4	0.78	0.21	45,53,56,60	0
3	EDO	B	818	4/4	0.78	0.18	58,58,60,65	0
3	EDO	E	806	4/4	0.79	0.20	48,50,53,56	0
3	EDO	E	809	4/4	0.79	0.16	58,60,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	823	4/4	0.80	0.18	61,62,62,63	0
3	EDO	B	811	4/4	0.80	0.23	54,54,54,54	0
3	EDO	F	807	4/4	0.80	0.18	48,51,52,53	0
3	EDO	B	812	4/4	0.80	0.22	49,53,54,56	0
3	EDO	C	803	4/4	0.81	0.17	49,52,52,53	0
2	PO4	D	803	5/5	0.83	0.23	38,41,43,44	5
3	EDO	C	807	4/4	0.83	0.18	50,55,56,58	0
3	EDO	D	807	4/4	0.83	0.18	41,43,44,47	0
3	EDO	A	814	4/4	0.84	0.16	52,53,54,54	0
3	EDO	F	806	4/4	0.84	0.22	48,48,50,51	0
3	EDO	D	813	4/4	0.85	0.18	42,44,47,49	0
3	EDO	A	815	4/4	0.85	0.17	50,50,51,55	0
3	EDO	D	805	4/4	0.85	0.21	52,52,54,57	0
3	EDO	A	810	4/4	0.85	0.19	47,48,55,56	0
3	EDO	B	822	4/4	0.86	0.21	47,48,48,49	0
3	EDO	B	821	4/4	0.87	0.21	50,51,52,57	0
3	EDO	B	820	4/4	0.88	0.15	48,51,52,54	0
3	EDO	E	807	4/4	0.88	0.15	43,45,48,51	0
3	EDO	A	813	4/4	0.88	0.15	45,52,52,54	0
3	EDO	B	819	4/4	0.88	0.15	39,43,43,51	0
3	EDO	C	806	4/4	0.89	0.16	44,47,47,48	0
3	EDO	B	816	4/4	0.89	0.15	47,57,57,60	0
3	EDO	B	813	4/4	0.90	0.14	42,43,44,44	0
3	EDO	D	806	4/4	0.90	0.18	42,48,49,50	0
3	EDO	A	812	4/4	0.90	0.13	49,52,53,54	0
2	PO4	C	801	5/5	0.90	0.12	51,51,52,56	0
3	EDO	B	817	4/4	0.90	0.19	35,40,43,45	0
3	EDO	A	811	4/4	0.91	0.12	54,56,58,59	0
3	EDO	D	808	4/4	0.91	0.15	46,47,49,54	0
2	PO4	E	801	5/5	0.92	0.14	50,51,54,55	0
2	PO4	D	801	5/5	0.92	0.17	44,48,59,65	0
3	EDO	D	804	4/4	0.92	0.13	35,36,40,41	0
3	EDO	F	804	4/4	0.92	0.11	59,60,60,63	0
3	EDO	E	810	4/4	0.93	0.13	36,37,40,42	0
2	PO4	F	801	5/5	0.93	0.11	50,52,54,59	0
3	EDO	D	812	4/4	0.94	0.10	40,41,46,47	0
3	EDO	B	814	4/4	0.94	0.20	38,40,42,44	0
2	PO4	A	802	5/5	0.94	0.15	44,49,54,55	0
2	PO4	B	801	5/5	0.94	0.14	49,49,56,57	0
3	EDO	A	808	4/4	0.95	0.09	40,41,44,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.