



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 12:41 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
Authors : Martins, M.P.; Spadeto, J.P.M.; Miyamoto, R.Y.; Morais, M.A.B.; Murakami, M.T.
Deposited on : 2025-03-11
Resolution : 2.25 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	:	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

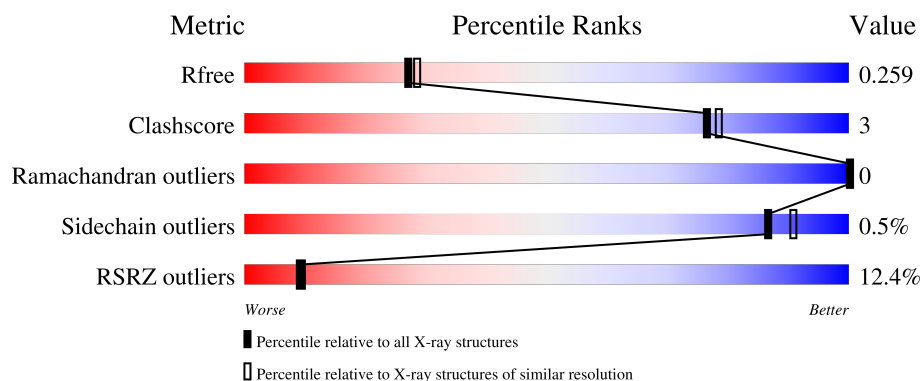
1 Overall quality at a glance

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 ≥ 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: O₄P).



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

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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	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: C₂H₆O₂).



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	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 C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 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		

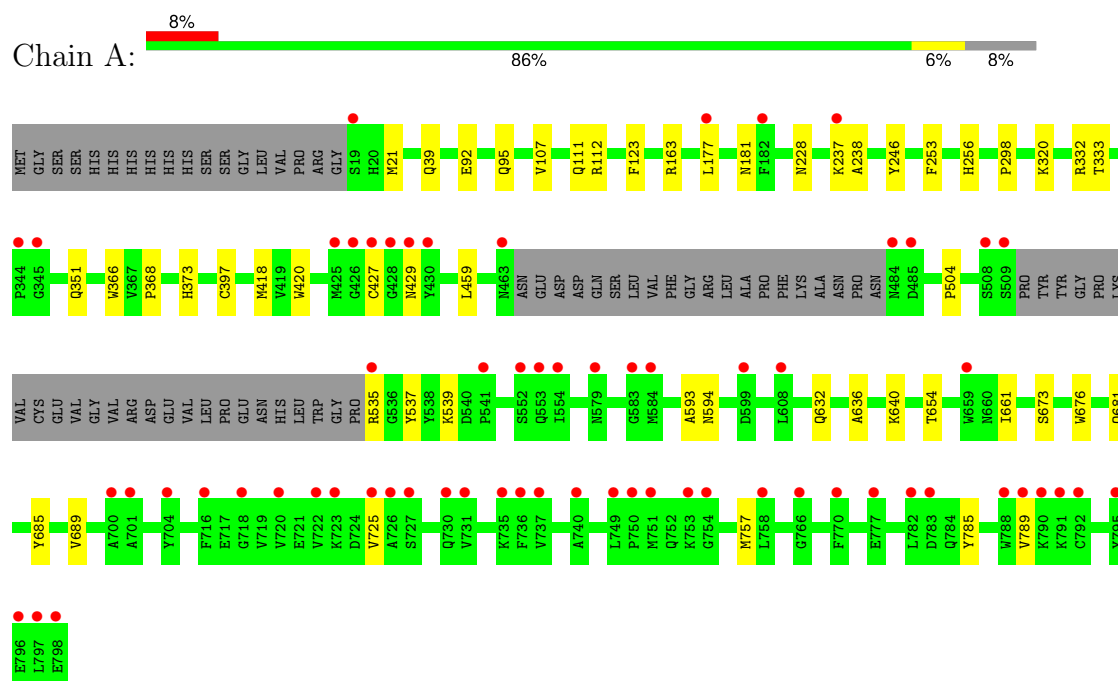
- Molecule 4 is water.

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		

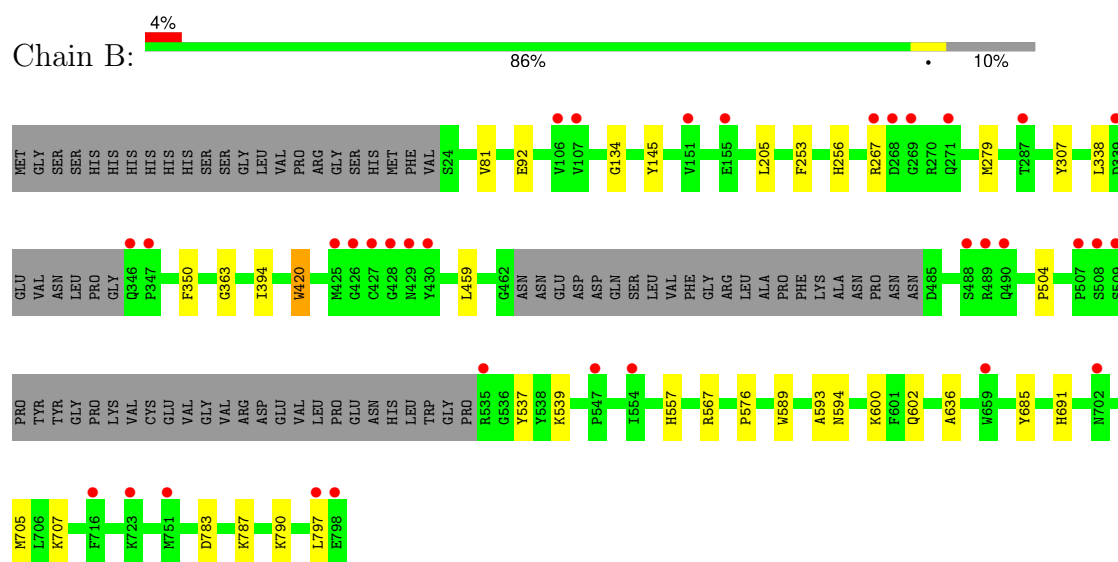
3 Residue-property plots [i](#)

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.

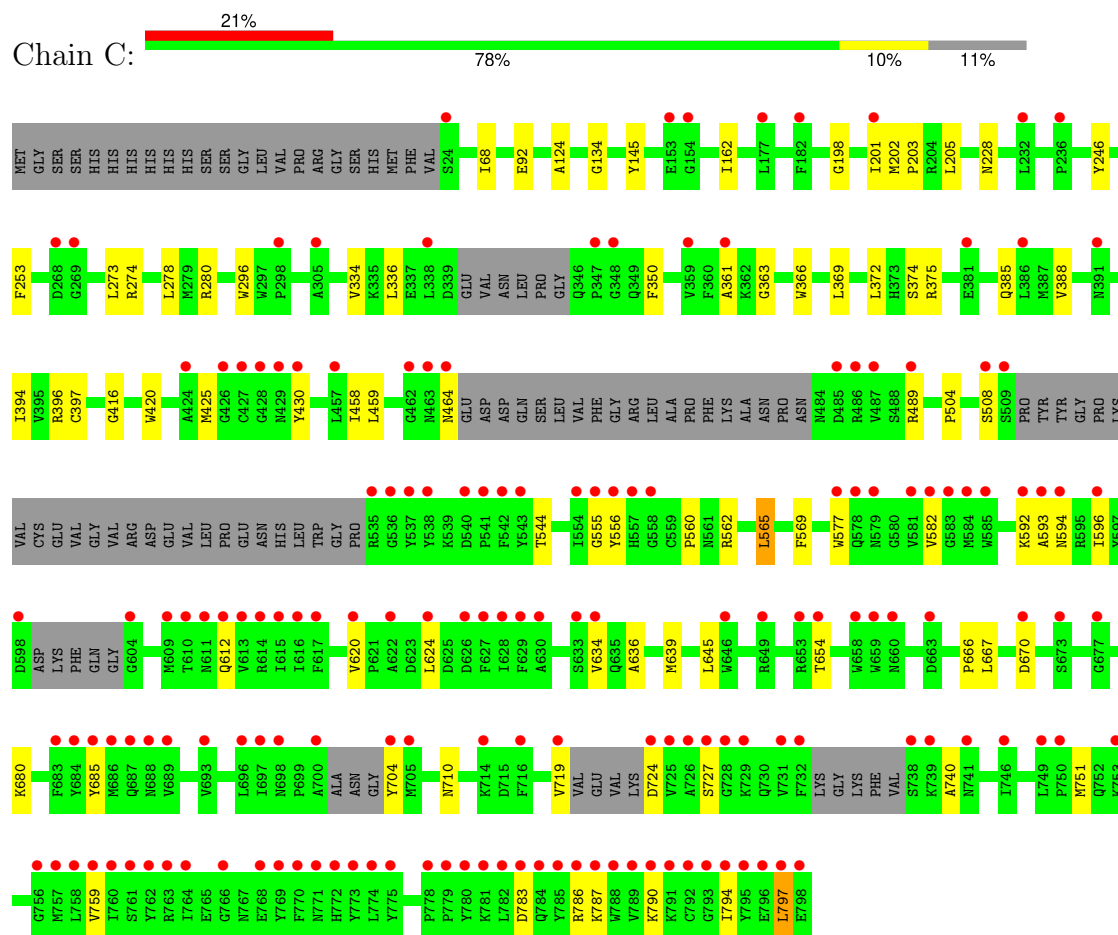
• Molecule 1: Glycoside hydrolase family 2



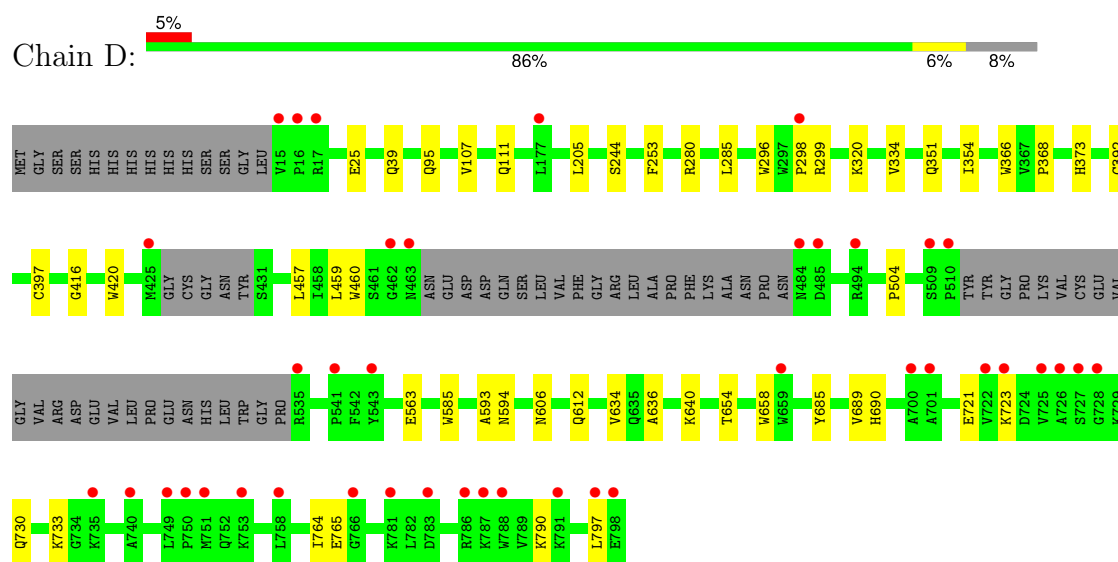
• Molecule 1: Glycoside hydrolase family 2



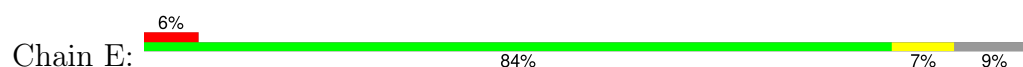
• Molecule 1: Glycoside hydrolase family 2

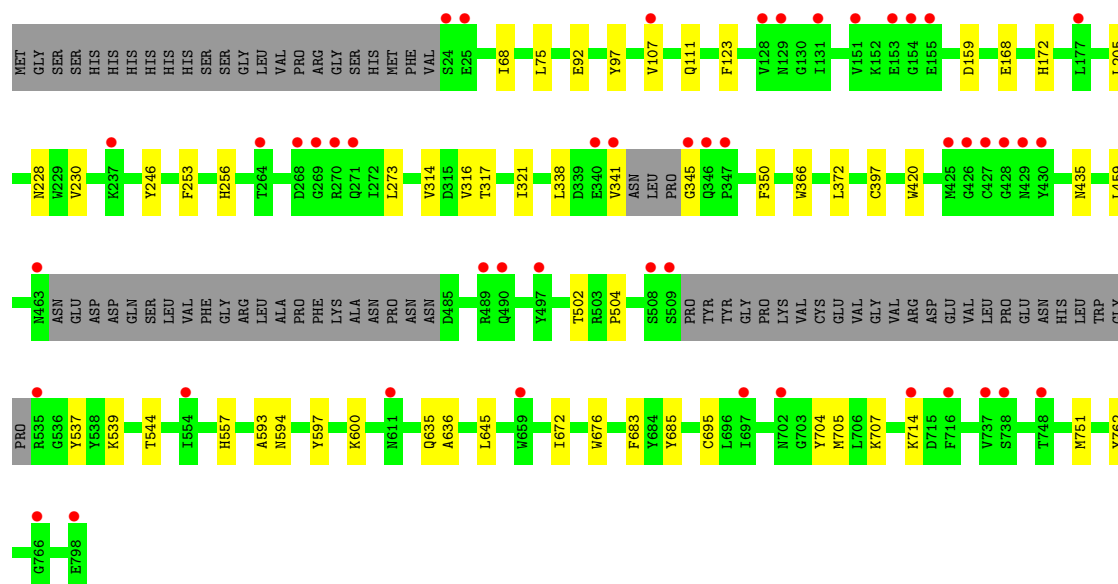


• Molecule 1: Glycoside hydrolase family 2

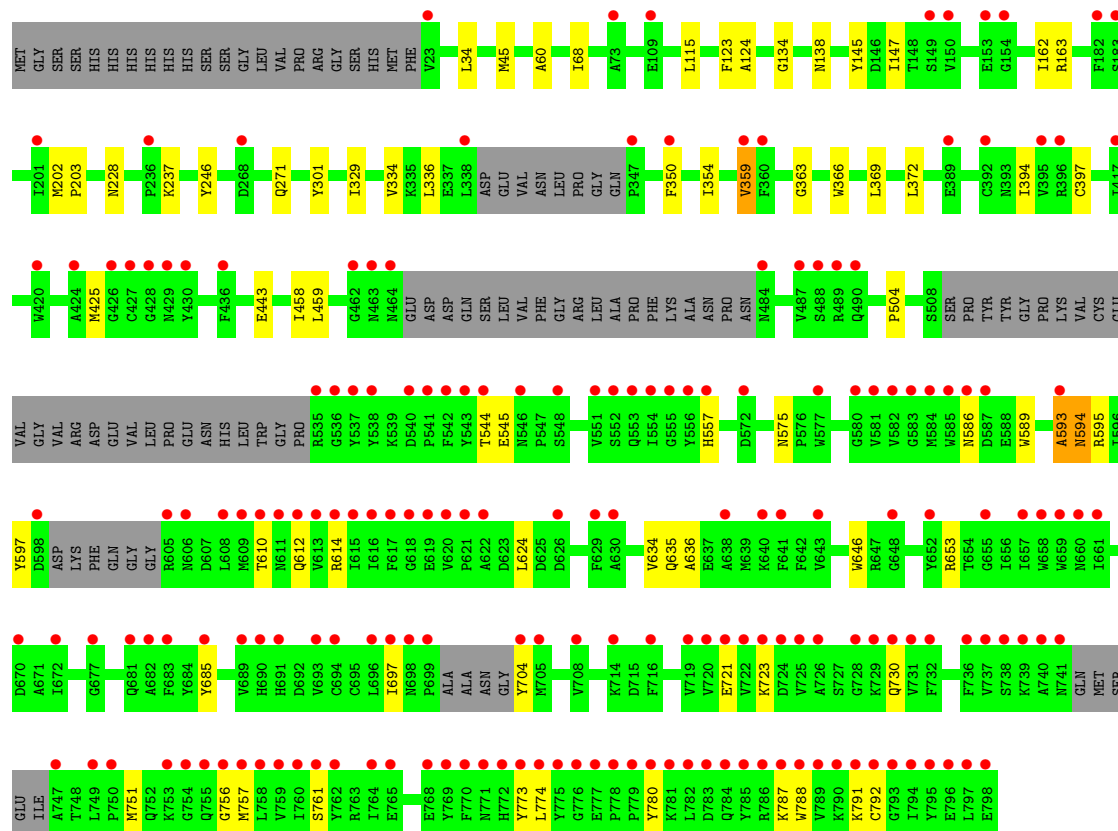
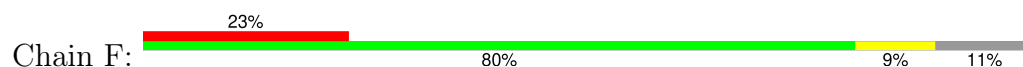


• Molecule 1: Glycoside hydrolase family 2





• Molecule 1: Glycoside hydrolase family 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	42.2	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.0	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	0.93	EDS
Total number of atoms	36354	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 17.19% 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: 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.

All (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
1:B:81:VAL:HG21	3:B:811:EDO:H22	1.84	0.59
1:A:593:ALA:N	1:A:594:ASN:HA	2.16	0.59
1:B:600:LYS:HG3	1:D:320:LYS:HB2	1.85	0.58
1:F:612:GLN:HB3	1:F:634:VAL:HG11	1.85	0.58
1:C:205:LEU:HD23	3:C:806:EDO:H12	1.84	0.58
1:C:201:ILE:HD12	1:C:202:MET:HG2	1.86	0.57
1:B:253:PHE:CZ	1:C:92:GLU:HB2	2.40	0.57
1:D:593:ALA:N	1:D:594:ASN:HA	2.20	0.56
1:E:341:VAL:HB	1:E:345:GLY:HA2	1.88	0.56
1:F:237:LYS:H	1:F:237:LYS:HD2	1.71	0.56
1:F:459:LEU:HD23	1:F:504:PRO:HG2	1.89	0.55
1:A:459:LEU:HD23	1:A:504:PRO:HG2	1.87	0.55
1:F:787:LYS:HE2	1:F:791:LYS:HD2	1.89	0.55
1:E:593:ALA:N	1:E:594:ASN:HA	2.21	0.54
1:C:592:LYS:HG3	1:C:667:LEU:HA	1.89	0.54
1:C:787:LYS:HA	1:C:790:LYS:HE3	1.89	0.54
1:C:459:LEU:HD23	1:C:504:PRO:HG2	1.90	0.54
1:B:459:LEU:HD23	1:B:504:PRO:HG2	1.90	0.54
1:B:593:ALA:N	1:B:594:ASN:HA	2.23	0.54
1:C:612:GLN:HB3	1:C:634:VAL:HG11	1.89	0.53
1:A:636:ALA:HB1	1:A:685:TYR:CG	2.43	0.53
1:C:228:ASN:HB3	1:C:246:TYR:HB2	1.91	0.53
1:C:350:PHE:O	1:C:654:THR:HG21	2.10	0.52
1:D:636:ALA:HB1	1:D:685:TYR:CG	2.45	0.52
1:F:202:MET:HE3	1:F:203:PRO:HD2	1.91	0.52
1:D:368:PRO:HB3	1:D:373:HIS:HE1	1.74	0.52
1:F:586:ASN:HD21	1:F:589:TRP:CD1	2.28	0.52
1:F:636:ALA:HB1	1:F:685:TYR:CG	2.45	0.52
1:C:556:TYR:H	1:C:639:MET:HE2	1.75	0.51
1:A:92:GLU:HB2	1:C:253:PHE:CZ	2.46	0.51
1:D:790:LYS:HD2	1:D:797:LEU:HD11	1.92	0.51
1:B:267:ARG:HD3	1:B:307:TYR:CE2	2.46	0.50
1:D:253:PHE:CZ	1:E:92:GLU:HB2	2.47	0.50
1:D:368:PRO:HB3	1:D:373:HIS:CE1	2.47	0.50
1:E:636:ALA:HB1	1:E:685:TYR:CG	2.47	0.50
1:D:107:VAL:HG13	1:D:111:GLN:HB2	1.93	0.50
1:F:593:ALA:N	1:F:594:ASN:HA	2.27	0.49
1:A:228:ASN:HB3	1:A:246:TYR:HB2	1.95	0.49
1:A:537:TYR:CE2	1:A:539:LYS:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:MET:HA	1:B:279:MET:HE2	1.94	0.49
1:C:636:ALA:HB1	1:C:685:TYR:CG	2.48	0.49
1:C:366:TRP:HB3	1:C:397:CYS:HA	1.94	0.49
1:B:567:ARG:HG3	3:B:812:EDO:H12	1.95	0.49
1:C:278:LEU:HD23	1:C:280:ARG:NH1	2.28	0.49
1:B:636:ALA:HB1	1:B:685:TYR:CG	2.48	0.49
1:E:316:VAL:HG23	1:E:317:THR:HG23	1.94	0.48
1:C:385:GLN:HA	1:C:388:VAL:HG12	1.96	0.48
1:F:366:TRP:HB3	1:F:397:CYS:HA	1.96	0.48
1:A:177:LEU:HB3	1:A:429:ASN:HB3	1.95	0.48
1:C:783:ASP:O	1:C:787:LYS:HG2	2.13	0.48
1:B:537:TYR:CE2	1:B:539:LYS:HB2	2.49	0.48
1:E:544:THR:HA	1:E:645:LEU:HD21	1.95	0.48
1:C:724:ASP:HB3	1:C:727:SER:OG	2.13	0.47
1:E:253:PHE:HA	1:E:256:HIS:ND1	2.29	0.47
1:F:756:GLY:HA2	1:F:788:TRP:CE2	2.49	0.47
1:F:595:ARG:HG2	1:F:597:TYR:O	2.14	0.47
1:E:107:VAL:HG13	1:E:111:GLN:HB2	1.96	0.47
1:D:640:LYS:HG3	1:D:689:VAL:HG11	1.95	0.47
1:A:640:LYS:HG3	1:A:689:VAL:HG11	1.97	0.47
1:F:723:LYS:HB3	1:F:730:GLN:HA	1.96	0.47
1:D:612:GLN:HB3	1:D:634:VAL:HG11	1.96	0.47
1:A:253:PHE:CZ	1:B:92:GLU:HB2	2.50	0.47
1:B:602:GLN:HG3	3:B:824:EDO:H22	1.96	0.47
1:C:704:TYR:CE2	1:C:751:MET:HA	2.50	0.47
1:F:721:GLU:HG3	1:F:761:SER:HB2	1.97	0.47
1:D:764:ILE:HG22	1:D:765:GLU:HG3	1.97	0.46
1:C:296:TRP:CZ2	1:C:416:GLY:HA2	2.49	0.46
1:C:786:ARG:HG3	1:C:797:LEU:HD21	1.97	0.46
1:A:320:LYS:HB2	1:E:600:LYS:HG3	1.98	0.46
1:B:363:GLY:HA3	1:B:394:ILE:O	2.15	0.46
1:F:329:ILE:HB	3:F:806:EDO:H11	1.96	0.46
1:F:646:TRP:CD1	1:F:653:ARG:HB3	2.51	0.46
1:A:181:ASN:HB3	1:A:427:CYS:O	2.16	0.46
1:D:366:TRP:HB3	1:D:397:CYS:HA	1.98	0.46
1:E:338:LEU:HD13	1:E:350:PHE:HB3	1.96	0.46
1:F:45:MET:SD	1:F:163:ARG:HD3	2.55	0.46
1:A:112:ARG:HG3	3:A:814:EDO:H12	1.98	0.46
1:B:420:TRP:C	1:B:420:TRP:CD1	2.94	0.46
1:A:298:PRO:HB3	1:A:418:MET:HG3	1.98	0.46
1:D:563:GLU:HG2	3:D:808:EDO:H21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:TRP:CZ2	1:D:416:GLY:HA2	2.51	0.46
1:E:230:VAL:HG13	1:E:502:THR:HG21	1.98	0.45
1:F:334:VAL:HG21	1:F:458:ILE:HB	1.98	0.45
1:B:253:PHE:HA	1:B:256:HIS:ND1	2.32	0.45
1:D:299:ARG:HD3	1:D:392:CYS:O	2.16	0.45
1:C:334:VAL:HG21	1:C:458:ILE:HB	1.97	0.45
1:F:610:THR:O	1:F:614:ARG:HG3	2.17	0.45
1:A:253:PHE:HA	1:A:256:HIS:ND1	2.32	0.45
1:A:332:ARG:HG2	1:A:333:THR:N	2.31	0.45
1:F:575:ASN:HA	1:F:624:LEU:HD12	1.99	0.45
1:C:425:MET:HG3	1:C:430:TYR:CE1	2.52	0.45
1:F:363:GLY:HA3	1:F:394:ILE:O	2.17	0.45
1:A:366:TRP:HB3	1:A:397:CYS:HA	1.99	0.45
1:D:593:ALA:HB3	1:D:594:ASN:C	2.42	0.45
1:A:351:GLN:HB2	1:A:654:THR:HG21	1.97	0.44
1:B:338:LEU:HD13	1:B:350:PHE:HB3	1.98	0.44
1:E:123:PHE:CD2	1:E:168:GLU:HG3	2.51	0.44
1:D:459:LEU:HD23	1:D:504:PRO:HG2	1.99	0.44
1:B:790:LYS:HB2	1:B:797:LEU:HD11	1.98	0.44
1:C:489:ARG:HH22	1:C:508:SER:HB3	1.82	0.44
1:D:457:LEU:HD21	1:D:460:TRP:CZ2	2.53	0.44
1:C:555:GLY:HA3	1:C:670:ASP:OD2	2.17	0.44
1:E:672:ILE:HD12	1:E:683:PHE:HA	2.00	0.44
1:A:632:GLN:HB3	1:A:681:GLN:HB2	2.00	0.44
1:F:271:GLN:HB2	3:F:804:EDO:H22	2.00	0.44
1:C:134:GLY:HA3	1:C:145:TYR:CE1	2.53	0.44
1:D:244:SER:HB3	1:D:285:LEU:HD11	1.99	0.44
1:E:714:LYS:HE2	4:E:1003:HOH:O	2.18	0.43
1:B:134:GLY:HA3	1:B:145:TYR:CE1	2.52	0.43
1:C:710:ASN:ND2	1:C:740:ALA:HA	2.34	0.43
1:E:366:TRP:HB3	1:E:397:CYS:HA	2.00	0.43
1:D:658:TRP:HE1	1:D:690:HIS:CE1	2.37	0.43
1:C:396:ARG:HG3	1:C:420:TRP:CG	2.53	0.43
1:F:124:ALA:HB2	1:F:162:ILE:HG12	2.00	0.43
1:F:774:LEU:HD21	1:F:780:TYR:CZ	2.53	0.43
1:F:757:MET:HE3	1:F:757:MET:HB2	1.97	0.43
1:C:366:TRP:CZ2	1:C:369:LEU:HD21	2.54	0.43
1:C:577:TRP:CE2	1:C:582:VAL:HG13	2.54	0.43
1:D:723:LYS:HG2	1:D:730:GLN:HA	2.00	0.43
1:E:636:ALA:HB1	1:E:685:TYR:CD2	2.53	0.43
1:F:336:LEU:HD11	1:F:350:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:HB3	1:A:163:ARG:NH2	2.34	0.42
1:F:544:THR:HG23	1:F:545:GLU:HG3	2.01	0.42
1:F:138:ASN:HD21	1:F:443:GLU:HB2	1.84	0.42
1:A:107:VAL:HG13	1:A:111:GLN:HB2	2.01	0.42
1:B:691:HIS:ND1	3:B:819:EDO:H12	2.34	0.42
1:E:537:TYR:CE2	1:E:539:LYS:HB2	2.55	0.42
1:C:375:ARG:HG2	3:C:805:EDO:H22	2.00	0.42
1:F:557:HIS:O	1:F:635:GLN:HB2	2.20	0.42
1:F:301:TYR:CE1	1:F:359:VAL:HG23	2.54	0.42
1:A:21:MET:HE2	1:A:21:MET:HA	2.02	0.42
1:A:39:GLN:HB2	1:A:95:GLN:HG3	2.02	0.42
1:A:676:TRP:HB3	3:A:810:EDO:H21	2.02	0.42
1:C:363:GLY:HA3	1:C:394:ILE:O	2.20	0.42
1:F:228:ASN:HB3	1:F:246:TYR:HB2	2.02	0.42
1:B:705:MET:HG3	1:B:707:LYS:HG3	2.00	0.42
1:C:560:PRO:HA	1:C:680:LYS:HE2	2.02	0.42
1:D:298:PRO:HD3	1:D:354:ILE:HG21	2.02	0.42
1:E:68:ILE:HG13	1:E:372:LEU:HD13	2.00	0.42
1:E:228:ASN:HB3	1:E:246:TYR:HB2	2.02	0.42
1:E:314:VAL:HG22	1:E:321:ILE:HG12	2.02	0.42
1:F:336:LEU:HD12	1:F:336:LEU:HA	1.91	0.42
1:A:725:VAL:HG21	1:A:757:MET:HE2	2.01	0.42
1:C:202:MET:HE3	1:C:203:PRO:HD2	2.02	0.42
1:D:280:ARG:HD3	1:E:597:TYR:CG	2.54	0.42
1:F:68:ILE:HG13	1:F:372:LEU:HD13	2.01	0.42
1:C:562:ARG:CZ	1:C:624:LEU:HD22	2.50	0.41
1:E:97:TYR:HE1	1:E:159:ASP:HB3	1.84	0.41
1:F:354:ILE:HG12	1:F:359:VAL:HG11	2.02	0.41
1:F:115:LEU:HB2	1:F:147:ILE:HD13	2.01	0.41
1:F:366:TRP:HZ2	1:F:369:LEU:HD11	1.85	0.41
1:F:697:ILE:HB	1:F:773:TYR:CD2	2.55	0.41
1:A:661:ILE:O	1:A:673:SER:HB3	2.20	0.41
1:B:576:PRO:HB3	1:B:589:TRP:CE2	2.54	0.41
1:F:134:GLY:HA3	1:F:145:TYR:CE1	2.55	0.41
1:E:172:HIS:ND1	3:E:808:EDO:H12	2.35	0.41
1:F:123:PHE:HB3	1:F:163:ARG:NH2	2.36	0.41
1:D:585:TRP:CE2	1:D:606:ASN:HB3	2.55	0.41
1:C:198:GLY:HA3	1:C:596:ILE:HD12	2.03	0.41
1:D:420:TRP:CD1	1:D:420:TRP:C	2.98	0.41
1:A:237:LYS:HG3	1:A:238:ALA:N	2.34	0.41
1:B:636:ALA:HB1	1:B:685:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LEU:HD22	1:C:274:ARG:H	1.86	0.41
1:C:420:TRP:C	1:C:420:TRP:CD1	2.98	0.41
1:D:39:GLN:HB2	1:D:95:GLN:HG3	2.02	0.41
1:D:351:GLN:HB2	1:D:654:THR:HG21	2.03	0.41
1:E:704:TYR:CE2	1:E:751:MET:HA	2.55	0.41
1:A:785:TYR:O	1:A:789:VAL:HG23	2.20	0.41
1:C:374:SER:OG	3:C:805:EDO:H21	2.20	0.41
1:E:420:TRP:C	1:E:420:TRP:CD1	2.99	0.41
1:E:557:HIS:O	1:E:635:GLN:HB2	2.20	0.41
1:A:368:PRO:HB3	1:A:373:HIS:HE1	1.86	0.40
1:A:420:TRP:CD1	1:A:420:TRP:C	2.99	0.40
1:C:124:ALA:HB2	1:C:162:ILE:HG12	2.03	0.40
1:E:695:CYS:HB2	1:E:762:TYR:CD1	2.56	0.40
1:B:783:ASP:O	1:B:787:LYS:HG3	2.21	0.40
1:C:592:LYS:HE3	1:C:666:PRO:O	2.21	0.40
1:C:759:VAL:HG13	1:C:794:ILE:HD11	2.03	0.40
1:F:34:LEU:HB2	1:F:60:ALA:HB2	2.03	0.40
1:C:361:ALA:HB1	1:C:394:ILE:HG21	2.04	0.40
1:F:704:TYR:CE2	1:F:751:MET:HA	2.56	0.40
1:C:68:ILE:HG13	1:C:372:LEU:HD13	2.03	0.40
1:C:336:LEU:HD11	1:C:350:PHE:CD1	2.57	0.40
1:C:544:THR:HA	1:C:645:LEU:HD21	2.03	0.40
1:C:565:LEU:HD12	1:C:569:PHE:HE2	1.86	0.40
1:E:705:MET:HG3	1:E:707:LYS:HG3	2.03	0.40
1:F:788:TRP:O	1:F:792:CYS:HB2	2.21	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	729/798 (91%)	706 (97%)	23 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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
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

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	205	LEU
1	B	420	TRP
1	B	557	HIS
1	C	464	ASN
1	C	565	LEU
1	C	620	VAL
1	C	719	VAL
1	C	797	LEU

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Mol	Chain	Res	Type
1	D	205	LEU
1	D	334	VAL
1	E	75	LEU
1	E	205	LEU
1	E	273	LEU
1	E	435	ASN
1	F	359	VAL
1	F	425	MET
1	F	594	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	484	ASN
1	A	579	ASN
1	A	606	ASN
1	A	742	GLN
1	A	752	GLN
1	A	772	HIS
1	B	228	ASN
1	B	429	ASN
1	B	553	GLN
1	B	575	ASN
1	B	635	GLN
1	B	702	ASN
1	C	26	GLN
1	C	111	GLN
1	C	349	GLN
1	C	351	GLN
1	C	365	ASN
1	C	385	GLN
1	C	590	GLN
1	C	606	ASN
1	C	691	HIS
1	C	752	GLN
1	D	228	ASN
1	D	351	GLN
1	D	611	ASN
1	D	681	GLN
1	D	772	HIS
1	E	26	GLN

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Mol	Chain	Res	Type
1	E	228	ASN
1	E	349	GLN
1	E	549	GLN
1	E	575	ASN
1	E	635	GLN
1	F	365	ASN
1	F	553	GLN
1	F	594	ASN
1	F	741	ASN
1	F	752	GLN

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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. '2' 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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
2	A	804	PO4	P-O1	2.80	1.57	1.50
2	E	802	PO4	P-O1	2.80	1.57	1.50
2	E	805	PO4	P-O1	2.79	1.57	1.50
2	B	809	PO4	P-O1	2.78	1.57	1.50
2	B	801	PO4	P-O1	2.77	1.57	1.50
2	E	803	PO4	P-O1	2.77	1.57	1.50
2	A	801	PO4	P-O1	2.76	1.57	1.50
2	B	810	PO4	P-O1	2.76	1.57	1.50
2	B	803	PO4	P-O1	2.76	1.57	1.50
2	B	806	PO4	P-O1	2.76	1.57	1.50
2	B	802	PO4	P-O1	2.75	1.57	1.50
2	F	802	PO4	P-O1	2.75	1.57	1.50
2	B	805	PO4	P-O1	2.74	1.57	1.50
2	A	806	PO4	P-O1	2.74	1.57	1.50
2	B	807	PO4	P-O1	2.74	1.57	1.50
2	D	801	PO4	P-O1	2.74	1.57	1.50
2	E	801	PO4	P-O1	2.74	1.57	1.50
2	B	804	PO4	P-O1	2.73	1.57	1.50
2	D	802	PO4	P-O1	2.73	1.57	1.50
2	D	803	PO4	P-O1	2.73	1.57	1.50
2	E	804	PO4	P-O1	2.72	1.56	1.50
2	A	802	PO4	P-O1	2.72	1.56	1.50
2	C	801	PO4	P-O1	2.63	1.56	1.50
2	F	801	PO4	P-O1	2.56	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (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
3	A	810	EDO	O1-C1-C2-O2
3	D	808	EDO	O1-C1-C2-O2
3	B	814	EDO	O1-C1-C2-O2
3	F	806	EDO	O1-C1-C2-O2
3	C	803	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

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	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

All (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
1	C	535	ARG	5.2
1	E	427	CYS	5.2
1	B	427	CYS	5.1
1	C	726	ALA	5.1
1	E	463	ASN	5.1
1	D	798	GLU	5.0
1	F	462	GLY	4.9
1	F	779	PRO	4.9
1	C	700	ALA	4.9
1	F	427	CYS	4.9
1	C	463	ASN	4.9
1	A	798	GLU	4.8
1	F	347	PRO	4.8
1	C	578	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
1	F	797	LEU	4.8
1	C	464	ASN	4.7
1	F	338	LEU	4.7
1	F	769	TYR	4.7
1	E	341	VAL	4.7
1	C	792	CYS	4.7
1	F	536	GLY	4.7
1	C	797	LEU	4.6
1	C	659	TRP	4.6
1	E	426	GLY	4.5
1	C	426	GLY	4.5
1	F	615	ILE	4.5
1	F	581	VAL	4.4
1	F	616	ILE	4.4
1	F	789	VAL	4.4
1	A	427	CYS	4.4
1	D	797	LEU	4.4
1	A	554	ILE	4.3
1	F	764	ILE	4.3
1	F	429	ASN	4.3
1	F	774	LEU	4.3
1	F	463	ASN	4.3
1	F	464	ASN	4.3
1	F	617	PHE	4.3
1	C	770	PHE	4.2
1	B	798	GLU	4.2
1	C	614	ARG	4.2
1	C	788	TRP	4.2
1	C	536	GLY	4.2
1	F	698	ASN	4.1
1	A	430	TYR	4.1
1	C	719	VAL	4.1
1	F	780	TYR	4.1
1	C	764	ILE	4.0
1	F	760	ILE	4.0
1	F	693	VAL	4.0
1	F	759	VAL	4.0
1	F	614	ARG	4.0
1	A	429	ASN	4.0
1	C	795	TYR	4.0
1	F	785	TYR	4.0
1	D	15	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	726	ALA	4.0
1	C	604	GLY	3.9
1	E	535	ARG	3.9
1	F	753	LYS	3.9
1	C	554	ILE	3.9
1	C	537	TYR	3.9
1	C	542	PHE	3.9
1	F	542	PHE	3.9
1	F	699	PRO	3.9
1	A	725	VAL	3.9
1	F	487	VAL	3.9
1	C	462	GLY	3.9
1	C	738	SER	3.9
1	F	685	TYR	3.9
1	F	757	MET	3.8
1	C	615	ILE	3.8
1	C	731	VAL	3.8
1	B	509	SER	3.8
1	F	754	GLY	3.8
1	F	541	PRO	3.8
1	F	621	PRO	3.8
1	F	554	ILE	3.8
1	C	775	TYR	3.7
1	F	535	ARG	3.7
1	D	16	PRO	3.7
1	A	791	LYS	3.7
1	F	153	GLU	3.7
1	F	540	ASP	3.7
1	C	789	VAL	3.7
1	C	347	PRO	3.7
1	F	758	LEU	3.7
1	B	428	GLY	3.7
1	F	620	VAL	3.7
1	C	538	TYR	3.7
1	F	154	GLY	3.7
1	C	620	VAL	3.7
1	C	509	SER	3.7
1	E	425	MET	3.7
1	C	617	PHE	3.7
1	C	760	ILE	3.7
1	D	727	SER	3.6
1	E	798	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	747	ALA	3.6
1	A	463	ASN	3.6
1	C	555	GLY	3.6
1	C	794	ILE	3.6
1	C	581	VAL	3.6
1	C	774	LEU	3.6
1	C	798	GLU	3.6
1	F	489	ARG	3.6
1	F	682	ALA	3.6
1	B	430	TYR	3.6
1	F	793	GLY	3.6
1	F	23	VAL	3.6
1	E	177	LEU	3.6
1	C	154	GLY	3.5
1	E	430	TYR	3.5
1	E	490	GLN	3.5
1	C	732	PHE	3.5
1	F	629	PHE	3.5
1	F	630	ALA	3.5
1	B	429	ASN	3.5
1	C	660	ASN	3.5
1	C	759	VAL	3.5
1	D	725	VAL	3.5
1	A	426	GLY	3.5
1	F	794	ILE	3.4
1	F	737	VAL	3.4
1	F	690	HIS	3.4
1	F	788	TRP	3.4
1	F	755	GLN	3.4
1	F	723	LYS	3.4
1	C	543	TYR	3.4
1	F	537	TYR	3.4
1	F	798	GLU	3.4
1	C	616	ILE	3.3
1	F	792	CYS	3.3
1	C	630	ALA	3.3
1	C	724	ASP	3.3
1	C	779	PRO	3.3
1	C	761	SER	3.3
1	A	726	ALA	3.3
1	E	264	THR	3.3
1	F	659	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	389	GLU	3.3
1	F	787	LYS	3.3
1	C	725	VAL	3.3
1	C	685	TYR	3.3
1	E	345	GLY	3.3
1	C	796	GLU	3.3
1	F	584	MET	3.3
1	C	430	TYR	3.3
1	C	785	TYR	3.3
1	C	793	GLY	3.3
1	F	795	TYR	3.3
1	F	605	ARG	3.2
1	B	508	SER	3.2
1	A	797	LEU	3.2
1	F	426	GLY	3.2
1	C	670	ASP	3.2
1	F	670	ASP	3.2
1	F	772	HIS	3.2
1	D	723	LYS	3.2
1	F	796	GLU	3.2
1	C	182	PHE	3.2
1	E	509	SER	3.2
1	F	741	ASN	3.2
1	C	780	TYR	3.2
1	F	730	GLN	3.2
1	E	428	GLY	3.2
1	F	722	VAL	3.2
1	E	346	GLN	3.2
1	C	773	TYR	3.2
1	F	749	LEU	3.2
1	C	540	ASP	3.1
1	F	782	LEU	3.1
1	C	784	GLN	3.1
1	A	788	TRP	3.1
1	D	700	ALA	3.1
1	F	430	TYR	3.1
1	F	704	TYR	3.1
1	A	792	CYS	3.1
1	A	731	VAL	3.1
1	C	769	TYR	3.1
1	F	236	PRO	3.1
1	C	787	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	730	GLN	3.1
1	F	587	ASP	3.1
1	F	762	TYR	3.1
1	F	781	LYS	3.1
1	F	736	PHE	3.0
1	A	535	ARG	3.0
1	C	696	LEU	3.0
1	F	731	VAL	3.0
1	B	346	GLN	3.0
1	C	556	TYR	3.0
1	C	746	ILE	3.0
1	F	648	GLY	3.0
1	F	756	GLY	3.0
1	D	462	GLY	3.0
1	F	655	GLY	3.0
1	B	425	MET	3.0
1	C	756	GLY	2.9
1	C	766	GLY	2.9
1	F	201	ILE	2.9
1	F	428	GLY	2.9
1	F	543	TYR	2.9
1	F	577	TRP	2.9
1	C	359	VAL	2.9
1	F	720	VAL	2.9
1	A	751	MET	2.9
1	C	758	LEU	2.9
1	B	702	ASN	2.9
1	C	579	ASN	2.9
1	F	786	ARG	2.9
1	F	582	VAL	2.9
1	B	723	LYS	2.9
1	A	484	ASN	2.9
1	A	553	GLN	2.9
1	C	610	THR	2.9
1	B	797	LEU	2.9
1	C	782	LEU	2.9
1	F	611	ASN	2.9
1	F	771	ASN	2.9
1	F	725	VAL	2.8
1	E	25	GLU	2.8
1	C	781	LYS	2.8
1	F	714	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	763	ARG	2.8
1	F	583	GLY	2.8
1	D	177	LEU	2.8
1	F	697	ILE	2.8
1	A	727	SER	2.8
1	F	556	TYR	2.8
1	B	268	ASP	2.8
1	C	622	ALA	2.8
1	B	489	ARG	2.8
1	F	580	GLY	2.8
1	E	702	ASN	2.8
1	E	508	SER	2.8
1	F	773	TYR	2.8
1	A	750	PRO	2.8
1	F	182	PHE	2.8
1	F	350	PHE	2.8
1	F	619	GLU	2.8
1	A	722	VAL	2.8
1	C	646	TRP	2.8
1	F	689	VAL	2.8
1	C	612	GLN	2.8
1	C	201	ILE	2.8
1	A	508	SER	2.8
1	A	723	LYS	2.8
1	C	704	TYR	2.8
1	F	770	PHE	2.8
1	B	107	VAL	2.8
1	F	610	THR	2.8
1	C	429	ASN	2.8
1	F	424	ALA	2.7
1	A	659	TRP	2.7
1	C	729	LYS	2.7
1	C	673	SER	2.7
1	E	340	GLU	2.7
1	E	489	ARG	2.7
1	C	663	ASP	2.7
1	F	268	ASP	2.7
1	F	652	TYR	2.7
1	F	775	TYR	2.7
1	A	177	LEU	2.7
1	C	611	ASN	2.7
1	A	740	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	131	ILE	2.7
1	C	598	ASP	2.7
1	B	151	VAL	2.7
1	D	722	VAL	2.7
1	F	691	HIS	2.7
1	C	361	ALA	2.7
1	D	543	TYR	2.7
1	D	753	LYS	2.7
1	F	791	LYS	2.7
1	A	718	GLY	2.6
1	C	558	GLY	2.6
1	F	618	GLY	2.6
1	C	624	LEU	2.6
1	C	749	LEU	2.6
1	C	577	TRP	2.6
1	F	585	TRP	2.6
1	A	552	SER	2.6
1	F	724	ASP	2.6
1	F	790	LYS	2.6
1	A	720	VAL	2.6
1	C	582	VAL	2.6
1	F	613	VAL	2.6
1	F	593	ALA	2.6
1	C	428	GLY	2.6
1	C	757	MET	2.6
1	E	697	ILE	2.6
1	D	509	SER	2.6
1	D	541	PRO	2.6
1	F	739	LYS	2.6
1	C	683	PHE	2.6
1	F	359	VAL	2.6
1	A	701	ALA	2.6
1	A	754	GLY	2.6
1	F	768	GLU	2.6
1	C	177	LEU	2.6
1	A	579	ASN	2.6
1	C	596	ILE	2.6
1	A	509	SER	2.6
1	C	727	SER	2.6
1	A	790	LYS	2.6
1	C	557	HIS	2.6
1	C	489	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	270	ARG	2.6
1	A	182	PHE	2.6
1	D	726	ALA	2.6
1	D	740	ALA	2.6
1	B	287	THR	2.6
1	C	338	LEU	2.6
1	C	771	ASN	2.6
1	C	508	SER	2.6
1	C	772	HIS	2.6
1	F	761	SER	2.6
1	F	776	GLY	2.5
1	F	484	ASN	2.5
1	D	787	LYS	2.5
1	E	554	ILE	2.5
1	A	19	SER	2.5
1	C	633	SER	2.5
1	C	634	VAL	2.5
1	F	643	VAL	2.5
1	E	237	LYS	2.5
1	F	557	HIS	2.5
1	C	24	SER	2.5
1	F	183	SER	2.5
1	A	783	ASP	2.5
1	C	609	MET	2.5
1	F	420	TRP	2.5
1	A	782	LEU	2.5
1	C	594	ASN	2.5
1	C	688	ASN	2.5
1	B	271	GLN	2.5
1	F	612	GLN	2.5
1	C	762	TYR	2.5
1	F	661	ILE	2.5
1	E	268	ASP	2.5
1	A	777	GLU	2.5
1	B	751	MET	2.5
1	F	721	GLU	2.5
1	F	777	GLU	2.5
1	C	583	GLY	2.5
1	C	613	VAL	2.5
1	C	693	VAL	2.5
1	F	73	ALA	2.5
1	F	732	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	608	LEU	2.5
1	C	778	PRO	2.5
1	F	778	PRO	2.5
1	F	548	SER	2.4
1	C	153	GLU	2.4
1	D	791	LYS	2.4
1	D	788	TRP	2.4
1	C	689	VAL	2.4
1	E	716	PHE	2.4
1	F	395	VAL	2.4
1	F	641	PHE	2.4
1	C	786	ARG	2.4
1	F	544	THR	2.4
1	F	750	PRO	2.4
1	B	339	ASP	2.4
1	A	753	LYS	2.4
1	C	753	LYS	2.4
1	F	622	ALA	2.4
1	F	740	ALA	2.4
1	C	487	VAL	2.4
1	A	584	MET	2.4
1	F	488	SER	2.4
1	F	598	ASP	2.4
1	F	729	LYS	2.4
1	F	677	GLY	2.4
1	F	696	LEU	2.4
1	C	741	ASN	2.4
1	F	546	ASN	2.4
1	E	153	GLU	2.4
1	F	626	ASP	2.4
1	D	749	LEU	2.4
1	F	658	TRP	2.3
1	A	796	GLU	2.3
1	E	347	PRO	2.3
1	B	554	ILE	2.3
1	D	485	ASP	2.3
1	F	657	ILE	2.3
1	C	424	ALA	2.3
1	A	789	VAL	2.3
1	F	392	CYS	2.3
1	F	705	MET	2.3
1	A	237	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	716	PHE	2.3
1	E	714	LYS	2.3
1	F	738	SER	2.3
1	C	677	GLY	2.3
1	E	269	GLY	2.3
1	E	497	TYR	2.3
1	F	638	ALA	2.3
1	F	640	LYS	2.3
1	B	106	VAL	2.3
1	F	150	VAL	2.3
1	B	716	PHE	2.3
1	C	658	TRP	2.3
1	C	649	ARG	2.3
1	D	494	ARG	2.3
1	C	783	ASP	2.3
1	F	784	GLN	2.3
1	A	428	GLY	2.3
1	C	728	GLY	2.3
1	C	684	TYR	2.3
1	C	584	MET	2.3
1	D	735	LYS	2.3
1	D	781	LYS	2.3
1	B	155	GLU	2.3
1	C	381	GLU	2.3
1	C	768	GLU	2.3
1	C	593	ALA	2.3
1	C	750	PRO	2.3
1	E	737	VAL	2.3
1	F	719	VAL	2.3
1	B	267	ARG	2.3
1	A	485	ASP	2.3
1	B	488	SER	2.3
1	F	555	GLY	2.3
1	A	425	MET	2.2
1	A	795	TYR	2.2
1	C	686	MET	2.2
1	F	109	GLU	2.2
1	F	660	ASN	2.2
1	D	298	PRO	2.2
1	D	17	ARG	2.2
1	B	490	GLN	2.2
1	D	463	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	611	ASN	2.2
1	F	708	VAL	2.2
1	C	687	GLN	2.2
1	C	592	LYS	2.2
1	E	24	SER	2.2
1	C	628	ILE	2.2
1	C	697	ILE	2.2
1	F	417	ILE	2.2
1	F	672	ILE	2.2
1	C	585	TRP	2.2
1	F	765	GLU	2.2
1	C	386	LEU	2.2
1	C	391	ASN	2.2
1	C	486	ARG	2.2
1	A	541	PRO	2.2
1	B	507	PRO	2.2
1	C	654	THR	2.2
1	A	737	VAL	2.2
1	A	716	PHE	2.2
1	A	345	GLY	2.2
1	B	269	GLY	2.2
1	D	728	GLY	2.2
1	C	232	LEU	2.2
1	C	698	ASN	2.2
1	E	129	ASN	2.2
1	B	347	PRO	2.2
1	D	701	ALA	2.2
1	F	683	PHE	2.2
1	F	716	PHE	2.2
1	C	485	ASP	2.2
1	C	705	MET	2.2
1	D	751	MET	2.2
1	A	583	GLY	2.1
1	F	728	GLY	2.1
1	B	535	ARG	2.1
1	D	484	ASN	2.1
1	B	547	PRO	2.1
1	A	735	LYS	2.1
1	E	151	VAL	2.1
1	C	629	PHE	2.1
1	F	436	PHE	2.1
1	D	783	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	155	GLU	2.1
1	F	572	ASP	2.1
1	F	783	ASP	2.1
1	D	766	GLY	2.1
1	E	738	SER	2.1
1	F	552	SER	2.1
1	D	758	LEU	2.1
1	C	298	PRO	2.1
1	C	305	ALA	2.1
1	A	770	PHE	2.1
1	C	627	PHE	2.1
1	D	535	ARG	2.1
1	E	766	GLY	2.1
1	A	758	LEU	2.1
1	C	236	PRO	2.1
1	C	790	LYS	2.1
1	D	750	PRO	2.1
1	F	553	GLN	2.1
1	F	606	ASN	2.1
1	F	681	GLN	2.1
1	B	659	TRP	2.1
1	A	700	ALA	2.1
1	F	551	VAL	2.1
1	A	766	GLY	2.1
1	E	154	GLY	2.1
1	C	714	LYS	2.1
1	E	271	GLN	2.1
1	F	490	GLN	2.1
1	A	344	PRO	2.1
1	D	659	TRP	2.1
1	E	659	TRP	2.1
1	D	425	MET	2.1
1	C	653	ARG	2.0
1	F	396	ARG	2.0
1	E	107	VAL	2.0
1	E	128	VAL	2.0
1	F	360	PHE	2.0
1	C	626	ASP	2.0
1	F	149	SER	2.0
1	C	739	LYS	2.0
1	A	749	LEU	2.0
1	C	457	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	541	PRO	2.0
1	F	609	MET	2.0
1	D	786	ARG	2.0
1	E	748	THR	2.0
1	A	704	TYR	2.0
1	A	599	ASP	2.0
1	A	736	PHE	2.0
1	C	268	ASP	2.0
1	C	269	GLY	2.0
1	C	348	GLY	2.0
1	C	791	LYS	2.0
1	A	608	LEU	2.0
1	F	586	ASN	2.0
1	F	694	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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.