



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:11 PM UTC

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:

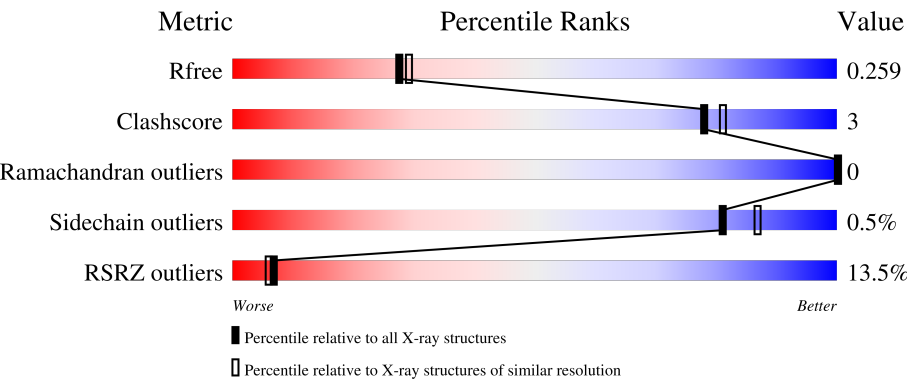
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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	9% 86% 6% 8%
1	B	798	5% 86% • 10%
1	C	798	22% 78% 10% 11%
1	D	798	6% 86% 6% 8%

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Mol	Chain	Length	Quality of chain
1	E	798	7% 84% 7% 9%
1	F	798	25% 80% 9% 11%

2 Entry composition [i](#)

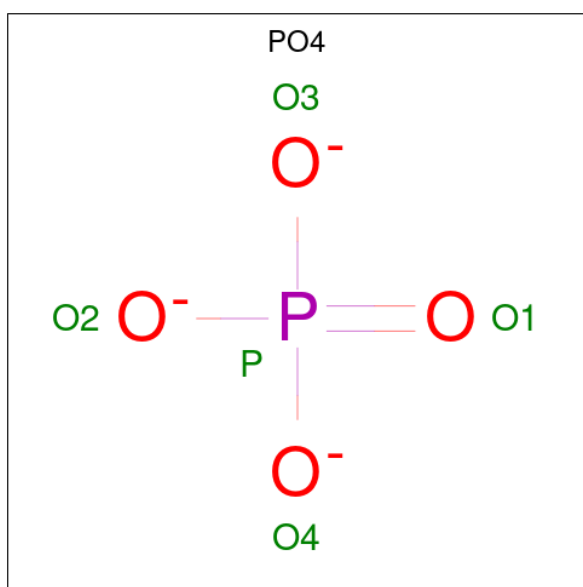
There are 4 unique types of molecules in this entry. The entry contains 36354 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	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: 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	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		

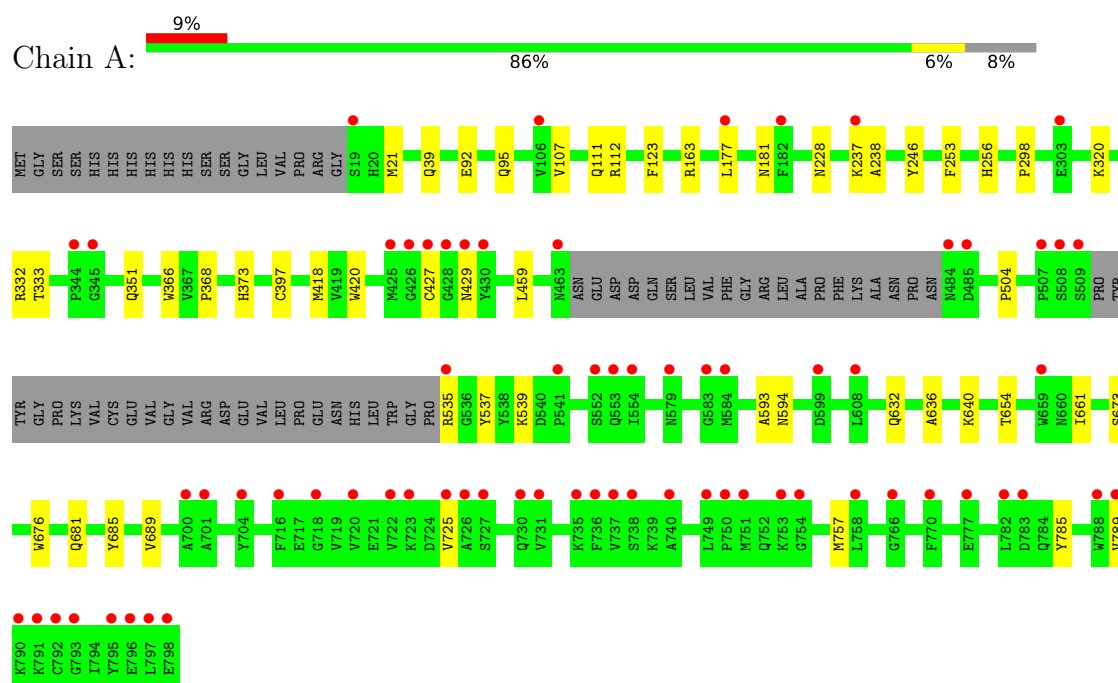
- Molecule 4 is water.

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		

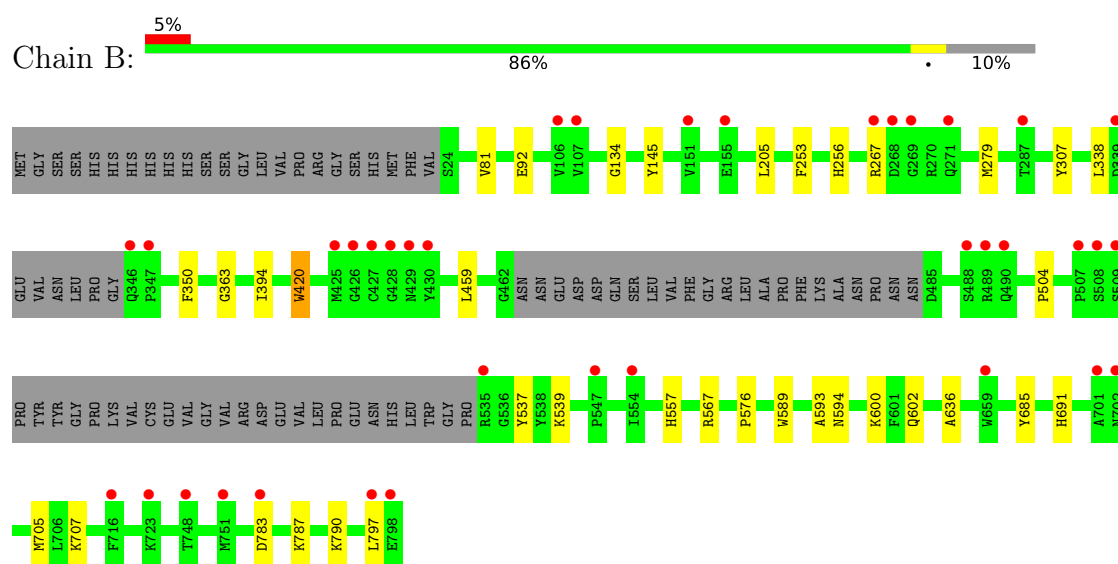
3 Residue-property plots [i](#)

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.

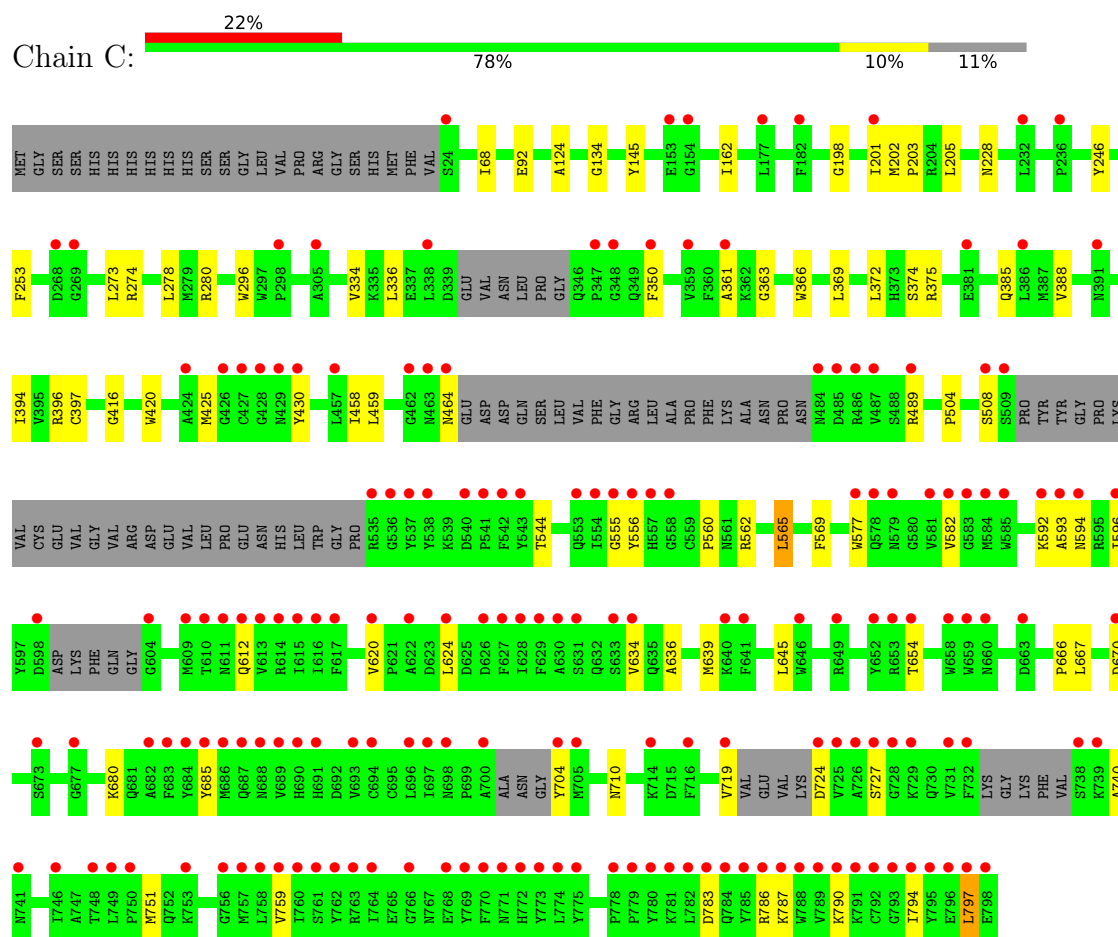
• Molecule 1: Glycoside hydrolase family 2



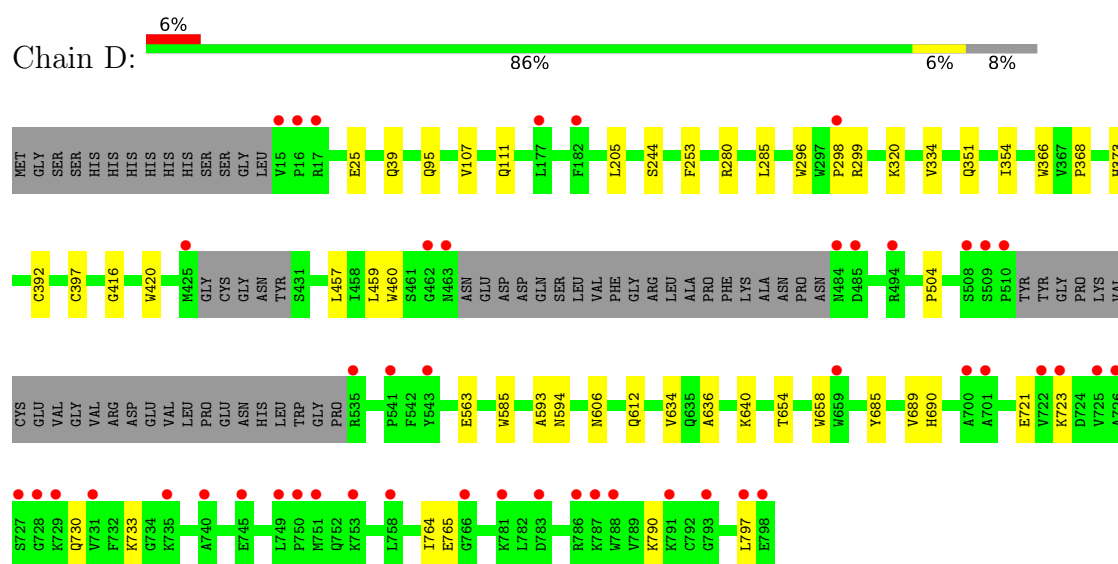
• Molecule 1: Glycoside hydrolase family 2



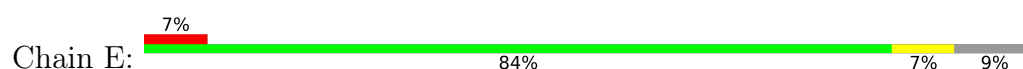
• Molecule 1: Glycoside hydrolase family 2

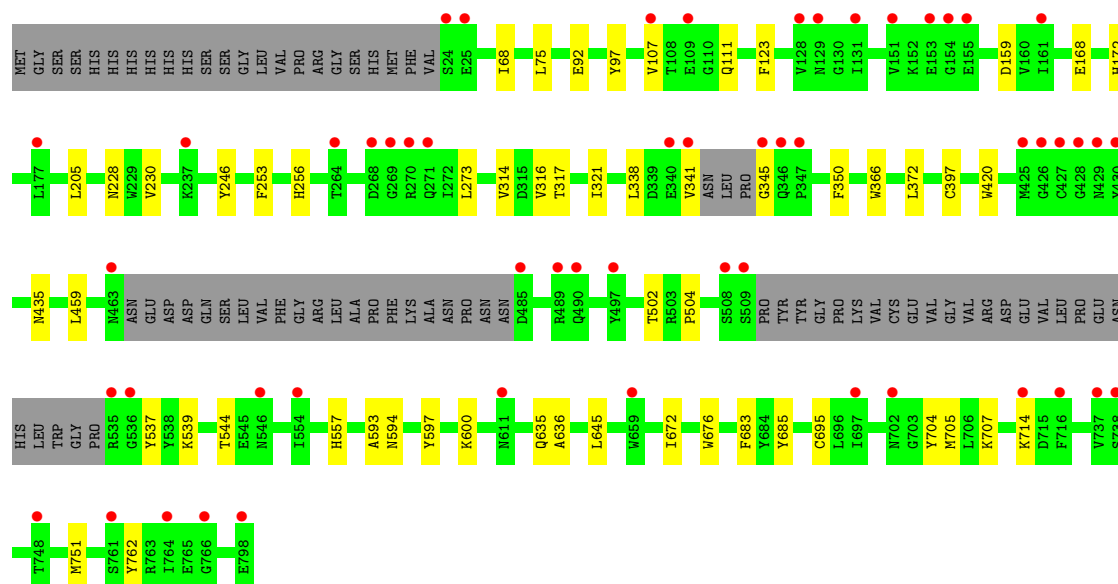


• Molecule 1: Glycoside hydrolase family 2

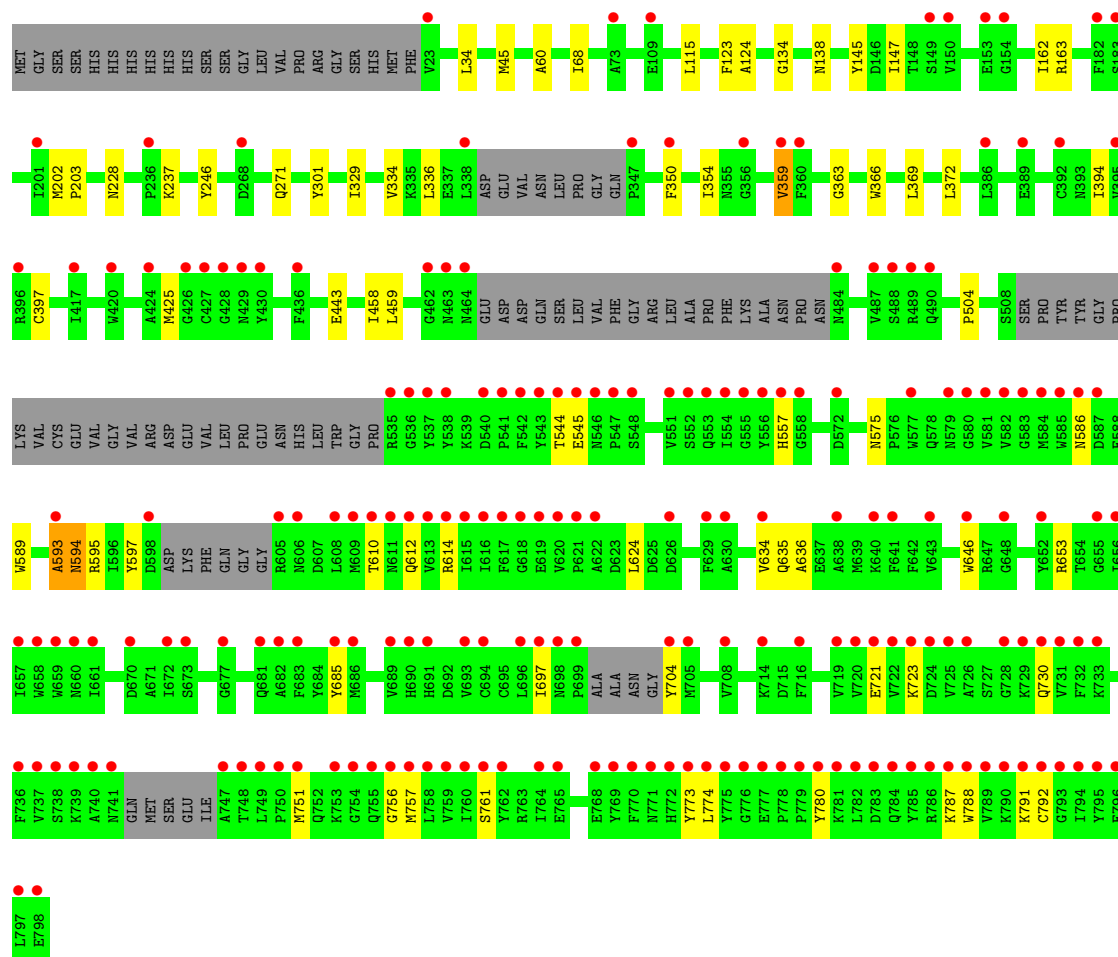
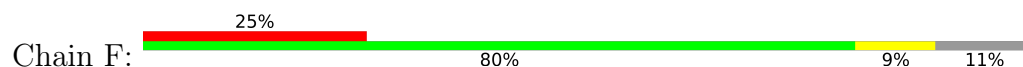


• Molecule 1: Glycoside hydrolase family 2





• 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%)	81	87
1	C	613/689 (89%)	608 (99%)	5 (1%)	73	80
1	D	636/689 (92%)	634 (100%)	2 (0%)	86	90
1	E	626/689 (91%)	622 (99%)	4 (1%)	78	84
1	F	614/689 (89%)	611 (100%)	3 (0%)	81	87
All	All	3747/4134 (91%)	3730 (100%)	17 (0%)	81	87

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	B	809	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	EDO	A	810	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	D	810	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	C	804	-	3,3,3	0.25	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	808	-	4,4,4	1.63	1 (25%)	6,6,6	0.46	0
2	PO4	B	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	EDO	E	809	-	3,3,3	0.25	0	2,2,2	0.35	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	B	824	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	D	809	-	3,3,3	0.24	0	2,2,2	0.34	0
3	EDO	B	818	-	3,3,3	0.24	0	2,2,2	0.36	0
3	EDO	B	816	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	F	806	-	3,3,3	0.25	0	2,2,2	0.37	0
2	PO4	A	806	-	4,4,4	1.59	1 (25%)	6,6,6	0.48	0
3	EDO	B	813	-	3,3,3	0.26	0	2,2,2	0.31	0
3	EDO	D	811	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	B	805	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
3	EDO	B	820	-	3,3,3	0.26	0	2,2,2	0.29	0
3	EDO	F	805	-	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
2	PO4	B	806	-	4,4,4	1.61	1 (25%)	6,6,6	0.51	0
3	EDO	A	811	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	A	814	-	3,3,3	0.26	0	2,2,2	0.32	0
3	EDO	F	804	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	B	811	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	D	808	-	3,3,3	0.24	0	2,2,2	0.32	0
3	EDO	B	812	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	C	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.49	0
3	EDO	D	812	-	3,3,3	0.25	0	2,2,2	0.35	0
2	PO4	A	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
2	PO4	E	805	-	4,4,4	1.61	1 (25%)	6,6,6	0.50	0
2	PO4	E	804	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
2	PO4	B	801	-	4,4,4	1.58	1 (25%)	6,6,6	0.50	0
2	PO4	B	807	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	EDO	A	809	-	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
2	PO4	E	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.47	0
2	PO4	F	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.49	0
3	EDO	E	807	-	3,3,3	0.25	0	2,2,2	0.31	0
3	EDO	F	807	-	3,3,3	0.23	0	2,2,2	0.34	0
3	EDO	D	804	-	3,3,3	0.25	0	2,2,2	0.33	0
2	PO4	C	801	-	4,4,4	1.52	1 (25%)	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	E	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.49	0
3	EDO	D	807	-	3,3,3	0.23	0	2,2,2	0.31	0
3	EDO	D	805	-	3,3,3	0.24	0	2,2,2	0.33	0
3	EDO	B	821	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	A	813	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	B	804	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
2	PO4	F	803	-	4,4,4	1.63	1 (25%)	6,6,6	0.52	0
3	EDO	A	812	-	3,3,3	0.24	0	2,2,2	0.33	0
2	PO4	B	810	-	4,4,4	1.60	1 (25%)	6,6,6	0.49	0
3	EDO	E	806	-	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
3	EDO	B	817	-	3,3,3	0.24	0	2,2,2	0.32	0
3	EDO	B	822	-	3,3,3	0.25	0	2,2,2	0.32	0
3	EDO	D	806	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	C	807	-	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	F	801	-	4,4,4	1.50	1 (25%)	6,6,6	0.58	0
3	EDO	B	815	-	3,3,3	0.25	0	2,2,2	0.35	0
3	EDO	B	823	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	A	801	-	4,4,4	1.60	1 (25%)	6,6,6	0.47	0
3	EDO	E	808	-	3,3,3	0.25	0	2,2,2	0.32	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
3	EDO	C	806	-	3,3,3	0.26	0	2,2,2	0.33	0
2	PO4	A	807	-	4,4,4	0.74	0	6,6,6	0.48	0
2	PO4	A	805	-	4,4,4	1.65	1 (25%)	6,6,6	0.48	0
3	EDO	A	808	-	3,3,3	0.25	0	2,2,2	0.34	0
2	PO4	A	803	-	4,4,4	1.64	1 (25%)	6,6,6	0.49	0
2	PO4	D	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	EDO	B	814	-	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	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.48	0
3	EDO	A	815	-	3,3,3	0.25	0	2,2,2	0.33	0
3	EDO	E	810	-	3,3,3	0.24	0	2,2,2	0.32	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	E	808	-	-	0/1/1/1	-
3	EDO	A	808	-	-	0/1/1/1	-
3	EDO	F	804	-	-	0/1/1/1	-
3	EDO	A	810	-	-	1/1/1/1	-
3	EDO	D	810	-	-	0/1/1/1	-
3	EDO	A	813	-	-	0/1/1/1	-
3	EDO	B	811	-	-	0/1/1/1	-
3	EDO	D	808	-	-	1/1/1/1	-
3	EDO	B	812	-	-	0/1/1/1	-
3	EDO	E	810	-	-	0/1/1/1	-
3	EDO	C	804	-	-	0/1/1/1	-
3	EDO	D	812	-	-	0/1/1/1	-
3	EDO	A	812	-	-	0/1/1/1	-
3	EDO	E	809	-	-	0/1/1/1	-
3	EDO	F	808	-	-	0/1/1/1	-
3	EDO	B	824	-	-	1/1/1/1	-
3	EDO	B	814	-	-	1/1/1/1	-
3	EDO	D	809	-	-	0/1/1/1	-
3	EDO	B	818	-	-	0/1/1/1	-
3	EDO	E	806	-	-	0/1/1/1	-
3	EDO	B	816	-	-	0/1/1/1	-
3	EDO	D	813	-	-	0/1/1/1	-
3	EDO	A	809	-	-	0/1/1/1	-
3	EDO	F	806	-	-	1/1/1/1	-
3	EDO	B	817	-	-	1/1/1/1	-
3	EDO	B	813	-	-	1/1/1/1	-
3	EDO	B	822	-	-	0/1/1/1	-
3	EDO	D	811	-	-	0/1/1/1	-
3	EDO	D	806	-	-	0/1/1/1	-
3	EDO	B	819	-	-	1/1/1/1	-
3	EDO	E	807	-	-	0/1/1/1	-
3	EDO	B	820	-	-	0/1/1/1	-
3	EDO	F	807	-	-	0/1/1/1	-
3	EDO	D	804	-	-	0/1/1/1	-
3	EDO	C	807	-	-	1/1/1/1	-
3	EDO	C	805	-	-	0/1/1/1	-
3	EDO	B	823	-	-	0/1/1/1	-
3	EDO	B	815	-	-	0/1/1/1	-
3	EDO	F	805	-	-	0/1/1/1	-
3	EDO	A	811	-	-	0/1/1/1	-
3	EDO	A	814	-	-	0/1/1/1	-
3	EDO	D	805	-	-	0/1/1/1	-
3	EDO	A	815	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	821	-	-	0/1/1/1	-
3	EDO	C	803	-	-	1/1/1/1	-
3	EDO	D	807	-	-	0/1/1/1	-
3	EDO	C	806	-	-	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	A	810	EDO	1	0
3	B	824	EDO	1	0
3	F	806	EDO	1	0
3	A	814	EDO	1	0
3	F	804	EDO	1	0
3	B	811	EDO	1	0
3	D	808	EDO	1	0
3	B	812	EDO	1	0
3	E	807	EDO	1	0
3	D	805	EDO	1	0
3	C	805	EDO	2	0
3	E	808	EDO	1	0
3	B	819	EDO	1	0
3	C	806	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%)	0.52	70 (9%)	14 13	27, 43, 73, 86	0
1	B	722/798 (90%)	0.49	37 (5%)	33 32	28, 41, 61, 76	0
1	C	708/798 (88%)	1.26	176 (24%)	2 1	35, 53, 93, 114	0
1	D	735/798 (92%)	0.42	47 (6%)	25 24	27, 42, 72, 84	0
1	E	726/798 (90%)	0.59	54 (7%)	20 19	28, 42, 65, 89	0
1	F	708/798 (88%)	1.40	200 (28%)	1 1	34, 58, 101, 114	0
All	All	4334/4788 (90%)	0.78	584 (13%)	7 6	27, 45, 84, 114	0

All (584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLY	7.1
1	C	427	CYS	6.2
1	E	429	ASN	6.0
1	F	538	TYR	5.4
1	D	510	PRO	5.3
1	E	427	CYS	5.3
1	C	726	ALA	5.3
1	B	427	CYS	5.2
1	C	535	ARG	5.2
1	E	463	ASN	5.1
1	F	462	GLY	5.1
1	C	700	ALA	5.1
1	F	779	PRO	5.0
1	F	427	CYS	5.0
1	F	347	PRO	4.9
1	F	797	LEU	4.9
1	C	463	ASN	4.9
1	D	798	GLU	4.9
1	F	769	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	578	GLN	4.8
1	E	341	VAL	4.8
1	F	338	LEU	4.8
1	A	798	GLU	4.8
1	C	464	ASN	4.8
1	F	536	GLY	4.8
1	C	792	CYS	4.8
1	C	659	TRP	4.8
1	C	797	LEU	4.7
1	E	426	GLY	4.6
1	C	426	GLY	4.6
1	F	581	VAL	4.6
1	F	615	ILE	4.6
1	F	616	ILE	4.6
1	F	789	VAL	4.5
1	D	797	LEU	4.5
1	A	427	CYS	4.5
1	A	554	ILE	4.4
1	F	764	ILE	4.4
1	F	774	LEU	4.4
1	F	617	PHE	4.4
1	F	429	ASN	4.4
1	C	788	TRP	4.4
1	C	770	PHE	4.4
1	F	463	ASN	4.3
1	F	464	ASN	4.3
1	C	536	GLY	4.3
1	A	430	TYR	4.3
1	C	719	VAL	4.2
1	F	780	TYR	4.2
1	C	614	ARG	4.2
1	F	698	ASN	4.2
1	B	798	GLU	4.2
1	F	693	VAL	4.2
1	F	759	VAL	4.2
1	C	764	ILE	4.1
1	F	760	ILE	4.1
1	C	795	TYR	4.1
1	F	785	TYR	4.1
1	D	15	VAL	4.1
1	F	726	ALA	4.1
1	C	537	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	604	GLY	4.1
1	A	429	ASN	4.1
1	C	542	PHE	4.0
1	F	542	PHE	4.0
1	C	554	ILE	4.0
1	A	725	VAL	4.0
1	F	487	VAL	4.0
1	C	462	GLY	4.0
1	F	614	ARG	4.0
1	F	685	TYR	4.0
1	F	699	PRO	4.0
1	C	731	VAL	4.0
1	C	615	ILE	4.0
1	C	738	SER	4.0
1	E	535	ARG	3.9
1	F	757	MET	3.9
1	F	754	GLY	3.9
1	F	753	LYS	3.9
1	B	509	SER	3.9
1	C	775	TYR	3.9
1	F	541	PRO	3.9
1	F	554	ILE	3.9
1	F	621	PRO	3.9
1	C	789	VAL	3.9
1	D	16	PRO	3.8
1	C	538	TYR	3.8
1	F	620	VAL	3.8
1	B	428	GLY	3.8
1	F	758	LEU	3.8
1	C	347	PRO	3.8
1	C	620	VAL	3.8
1	F	154	GLY	3.8
1	C	617	PHE	3.8
1	F	540	ASP	3.8
1	F	747	ALA	3.8
1	C	760	ILE	3.8
1	F	535	ARG	3.8
1	C	555	GLY	3.8
1	C	581	VAL	3.8
1	E	425	MET	3.7
1	C	509	SER	3.7
1	C	794	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	774	LEU	3.7
1	A	791	LYS	3.7
1	B	430	TYR	3.7
1	F	153	GLU	3.7
1	F	682	ALA	3.7
1	D	727	SER	3.7
1	F	793	GLY	3.7
1	F	23	VAL	3.7
1	A	463	ASN	3.7
1	E	430	TYR	3.7
1	C	154	GLY	3.7
1	E	177	LEU	3.7
1	C	732	PHE	3.6
1	F	629	PHE	3.6
1	F	630	ALA	3.6
1	E	798	GLU	3.6
1	C	759	VAL	3.6
1	D	725	VAL	3.6
1	E	490	GLN	3.6
1	F	489	ARG	3.6
1	A	426	GLY	3.6
1	F	788	TRP	3.6
1	C	798	GLU	3.6
1	B	429	ASN	3.6
1	C	660	ASN	3.6
1	F	737	VAL	3.6
1	F	794	ILE	3.5
1	C	543	TYR	3.5
1	F	537	TYR	3.5
1	F	690	HIS	3.5
1	C	630	ALA	3.5
1	F	659	TRP	3.5
1	C	616	ILE	3.5
1	F	755	GLN	3.5
1	A	726	ALA	3.4
1	F	792	CYS	3.4
1	C	685	TYR	3.4
1	C	779	PRO	3.4
1	C	725	VAL	3.4
1	E	345	GLY	3.4
1	C	430	TYR	3.4
1	C	785	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	795	TYR	3.4
1	E	264	THR	3.4
1	C	761	SER	3.4
1	C	793	GLY	3.4
1	C	724	ASP	3.4
1	F	723	LYS	3.4
1	F	798	GLU	3.4
1	F	426	GLY	3.4
1	A	797	LEU	3.3
1	F	584	MET	3.3
1	C	182	PHE	3.3
1	C	780	TYR	3.3
1	C	773	TYR	3.3
1	F	772	HIS	3.3
1	B	508	SER	3.3
1	F	722	VAL	3.3
1	E	428	GLY	3.3
1	F	389	GLU	3.3
1	F	787	LYS	3.3
1	A	788	TRP	3.3
1	E	509	SER	3.3
1	C	670	ASP	3.3
1	F	670	ASP	3.3
1	F	741	ASN	3.3
1	F	749	LEU	3.3
1	F	605	ARG	3.3
1	C	796	GLU	3.3
1	F	730	GLN	3.3
1	F	430	TYR	3.3
1	F	704	TYR	3.3
1	D	700	ALA	3.2
1	F	782	LEU	3.2
1	E	346	GLN	3.2
1	C	769	TYR	3.2
1	A	731	VAL	3.2
1	D	723	LYS	3.2
1	F	796	GLU	3.2
1	A	792	CYS	3.2
1	F	762	TYR	3.2
1	C	540	ASP	3.2
1	F	236	PRO	3.2
1	C	784	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	736	PHE	3.2
1	F	731	VAL	3.1
1	C	556	TYR	3.1
1	A	730	GLN	3.1
1	C	696	LEU	3.1
1	F	587	ASP	3.1
1	F	648	GLY	3.1
1	F	756	GLY	3.1
1	C	746	ILE	3.1
1	F	577	TRP	3.1
1	D	462	GLY	3.1
1	F	655	GLY	3.1
1	C	787	LYS	3.1
1	F	543	TYR	3.1
1	B	346	GLN	3.1
1	C	756	GLY	3.1
1	C	766	GLY	3.1
1	F	428	GLY	3.1
1	A	535	ARG	3.1
1	C	359	VAL	3.1
1	F	720	VAL	3.1
1	F	781	LYS	3.1
1	B	425	MET	3.1
1	F	201	ILE	3.0
1	C	758	LEU	3.0
1	F	582	VAL	3.0
1	A	751	MET	3.0
1	B	702	ASN	3.0
1	C	579	ASN	3.0
1	B	797	LEU	3.0
1	C	782	LEU	3.0
1	F	725	VAL	3.0
1	C	610	THR	3.0
1	F	556	TYR	3.0
1	A	484	ASN	3.0
1	F	583	GLY	3.0
1	C	646	TRP	3.0
1	C	622	ALA	2.9
1	D	177	LEU	2.9
1	A	553	GLN	2.9
1	F	786	ARG	2.9
1	F	697	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	773	TYR	2.9
1	F	580	GLY	2.9
1	F	611	ASN	2.9
1	F	771	ASN	2.9
1	F	182	PHE	2.9
1	F	350	PHE	2.9
1	A	722	VAL	2.9
1	F	689	VAL	2.9
1	A	727	SER	2.9
1	C	704	TYR	2.9
1	A	750	PRO	2.9
1	B	723	LYS	2.9
1	F	770	PHE	2.9
1	A	659	TRP	2.9
1	B	107	VAL	2.9
1	C	201	ILE	2.9
1	B	268	ASP	2.9
1	E	508	SER	2.9
1	E	702	ASN	2.9
1	C	763	ARG	2.9
1	F	424	ALA	2.9
1	E	25	GLU	2.9
1	F	610	THR	2.9
1	A	508	SER	2.8
1	C	781	LYS	2.8
1	F	714	LYS	2.8
1	B	489	ARG	2.8
1	F	652	TYR	2.8
1	F	775	TYR	2.8
1	C	612	GLN	2.8
1	C	429	ASN	2.8
1	A	177	LEU	2.8
1	A	740	ALA	2.8
1	F	619	GLU	2.8
1	C	577	TRP	2.8
1	F	585	TRP	2.8
1	C	673	SER	2.8
1	D	543	TYR	2.8
1	C	361	ALA	2.8
1	A	723	LYS	2.8
1	B	151	VAL	2.8
1	D	722	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	131	ILE	2.8
1	C	611	ASN	2.8
1	C	663	ASP	2.8
1	F	268	ASP	2.8
1	A	718	GLY	2.8
1	C	558	GLY	2.8
1	F	618	GLY	2.8
1	C	624	LEU	2.8
1	C	749	LEU	2.8
1	F	593	ALA	2.8
1	E	489	ARG	2.8
1	A	720	VAL	2.8
1	C	582	VAL	2.8
1	F	613	VAL	2.8
1	F	691	HIS	2.7
1	C	428	GLY	2.7
1	E	340	GLU	2.7
1	C	729	LYS	2.7
1	A	701	ALA	2.7
1	C	683	PHE	2.7
1	F	359	VAL	2.7
1	C	598	ASP	2.7
1	E	697	ILE	2.7
1	A	754	GLY	2.7
1	A	552	SER	2.7
1	D	541	PRO	2.7
1	C	757	MET	2.7
1	C	177	LEU	2.7
1	D	726	ALA	2.7
1	D	740	ALA	2.7
1	A	182	PHE	2.7
1	F	724	ASP	2.7
1	C	596	ILE	2.7
1	D	509	SER	2.7
1	C	338	LEU	2.7
1	C	557	HIS	2.7
1	A	579	ASN	2.7
1	B	287	THR	2.7
1	D	753	LYS	2.7
1	F	791	LYS	2.7
1	F	776	GLY	2.7
1	A	509	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	727	SER	2.7
1	F	420	TRP	2.7
1	C	772	HIS	2.6
1	F	790	LYS	2.6
1	C	634	VAL	2.6
1	C	771	ASN	2.6
1	F	643	VAL	2.6
1	E	554	ILE	2.6
1	C	508	SER	2.6
1	F	761	SER	2.6
1	F	739	LYS	2.6
1	F	768	GLU	2.6
1	C	489	ARG	2.6
1	C	762	TYR	2.6
1	F	484	ASN	2.6
1	E	270	ARG	2.6
1	A	19	SER	2.6
1	C	633	SER	2.6
1	F	557	HIS	2.6
1	A	782	LEU	2.6
1	A	790	LYS	2.6
1	D	788	TRP	2.6
1	F	73	ALA	2.6
1	F	732	PHE	2.6
1	C	583	GLY	2.6
1	C	609	MET	2.6
1	C	613	VAL	2.6
1	C	693	VAL	2.6
1	C	24	SER	2.6
1	F	183	SER	2.6
1	F	661	ILE	2.6
1	F	608	LEU	2.6
1	A	783	ASP	2.6
1	C	594	ASN	2.6
1	C	688	ASN	2.6
1	B	751	MET	2.6
1	C	689	VAL	2.6
1	C	778	PRO	2.6
1	E	716	PHE	2.6
1	F	641	PHE	2.6
1	F	395	VAL	2.6
1	F	778	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	787	LYS	2.6
1	B	271	GLN	2.5
1	F	612	GLN	2.5
1	F	622	ALA	2.5
1	F	740	ALA	2.5
1	E	268	ASP	2.5
1	F	544	THR	2.5
1	F	750	PRO	2.5
1	C	487	VAL	2.5
1	E	237	LYS	2.5
1	F	548	SER	2.5
1	F	677	GLY	2.5
1	F	658	TRP	2.5
1	A	777	GLU	2.5
1	F	721	GLU	2.5
1	F	777	GLU	2.5
1	F	696	LEU	2.5
1	A	584	MET	2.5
1	B	339	ASP	2.5
1	C	153	GLU	2.5
1	F	488	SER	2.5
1	C	786	ARG	2.5
1	D	749	LEU	2.5
1	D	791	LYS	2.5
1	C	741	ASN	2.5
1	F	546	ASN	2.5
1	F	598	ASP	2.5
1	C	424	ALA	2.5
1	E	347	PRO	2.5
1	A	789	VAL	2.4
1	C	716	PHE	2.4
1	B	554	ILE	2.4
1	F	657	ILE	2.4
1	C	658	TRP	2.4
1	E	497	TYR	2.4
1	A	753	LYS	2.4
1	C	753	LYS	2.4
1	F	626	ASP	2.4
1	F	638	ALA	2.4
1	C	677	GLY	2.4
1	E	269	GLY	2.4
1	F	392	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	VAL	2.4
1	B	716	PHE	2.4
1	F	150	VAL	2.4
1	F	729	LYS	2.4
1	F	705	MET	2.4
1	C	684	TYR	2.4
1	D	485	ASP	2.4
1	E	153	GLU	2.4
1	A	428	GLY	2.4
1	C	593	ALA	2.4
1	C	728	GLY	2.4
1	F	738	SER	2.4
1	E	737	VAL	2.4
1	F	719	VAL	2.4
1	A	795	TYR	2.4
1	A	796	GLU	2.4
1	C	750	PRO	2.4
1	F	555	GLY	2.4
1	C	584	MET	2.4
1	F	784	GLN	2.4
1	C	585	TRP	2.4
1	C	783	ASP	2.3
1	D	298	PRO	2.3
1	A	237	LYS	2.3
1	E	714	LYS	2.3
1	B	488	SER	2.3
1	A	425	MET	2.3
1	C	686	MET	2.3
1	F	708	VAL	2.3
1	C	649	ARG	2.3
1	D	494	ARG	2.3
1	A	485	ASP	2.3
1	F	660	ASN	2.3
1	F	640	LYS	2.3
1	B	267	ARG	2.3
1	C	628	ILE	2.3
1	C	697	ILE	2.3
1	F	417	ILE	2.3
1	F	672	ILE	2.3
1	A	716	PHE	2.3
1	A	737	VAL	2.3
1	B	155	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	490	GLN	2.3
1	C	381	GLU	2.3
1	C	768	GLU	2.3
1	C	386	LEU	2.3
1	D	463	ASN	2.3
1	D	735	LYS	2.3
1	D	781	LYS	2.3
1	E	611	ASN	2.3
1	A	541	PRO	2.3
1	B	507	PRO	2.3
1	A	345	GLY	2.3
1	B	269	GLY	2.3
1	D	728	GLY	2.3
1	D	701	ALA	2.3
1	C	654	THR	2.3
1	D	17	ARG	2.3
1	E	24	SER	2.3
1	C	687	GLN	2.3
1	F	109	GLU	2.3
1	F	683	PHE	2.3
1	F	716	PHE	2.3
1	C	232	LEU	2.3
1	C	391	ASN	2.3
1	B	347	PRO	2.3
1	A	583	GLY	2.3
1	F	728	GLY	2.3
1	C	629	PHE	2.2
1	E	151	VAL	2.3
1	F	436	PHE	2.2
1	C	698	ASN	2.2
1	E	129	ASN	2.2
1	B	547	PRO	2.2
1	C	486	ARG	2.2
1	C	705	MET	2.2
1	D	751	MET	2.2
1	D	766	GLY	2.2
1	C	305	ALA	2.2
1	F	765	GLU	2.2
1	B	659	TRP	2.2
1	C	592	LYS	2.2
1	D	758	LEU	2.2
1	A	770	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	627	PHE	2.2
1	C	485	ASP	2.2
1	D	484	ASN	2.2
1	C	298	PRO	2.2
1	E	766	GLY	2.2
1	A	700	ALA	2.2
1	E	738	SER	2.2
1	F	552	SER	2.2
1	D	659	TRP	2.2
1	E	659	TRP	2.2
1	A	758	LEU	2.2
1	F	551	VAL	2.2
1	B	535	ARG	2.2
1	D	783	ASP	2.2
1	F	572	ASP	2.2
1	F	783	ASP	2.2
1	C	236	PRO	2.2
1	D	750	PRO	2.2
1	A	766	GLY	2.2
1	E	154	GLY	2.2
1	E	107	VAL	2.2
1	E	128	VAL	2.2
1	F	360	PHE	2.2
1	F	606	ASN	2.2
1	A	344	PRO	2.2
1	A	735	LYS	2.2
1	E	155	GLU	2.2
1	F	553	GLN	2.2
1	F	681	GLN	2.2
1	A	704	TYR	2.1
1	D	535	ARG	2.1
1	A	749	LEU	2.1
1	C	457	LEU	2.1
1	D	425	MET	2.1
1	F	646	TRP	2.1
1	A	736	PHE	2.1
1	C	541	PRO	2.1
1	E	271	GLN	2.1
1	F	490	GLN	2.1
1	C	269	GLY	2.1
1	C	348	GLY	2.1
1	B	701	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	682	ALA	2.1
1	E	748	THR	2.1
1	F	149	SER	2.1
1	A	608	LEU	2.1
1	F	609	MET	2.1
1	C	790	LYS	2.1
1	C	626	ASP	2.1
1	C	641	PHE	2.1
1	F	558	GLY	2.1
1	C	653	ARG	2.1
1	F	396	ARG	2.1
1	F	694	CYS	2.1
1	C	714	LYS	2.1
1	F	386	LEU	2.1
1	A	599	ASP	2.1
1	C	268	ASP	2.1
1	F	586	ASN	2.1
1	F	656	ILE	2.1
1	C	691	HIS	2.1
1	D	182	PHE	2.1
1	D	793	GLY	2.1
1	D	786	ARG	2.1
1	E	761	SER	2.1
1	F	673	SER	2.1
1	C	739	LYS	2.1
1	B	783	ASP	2.1
1	E	485	ASP	2.1
1	C	652	TYR	2.1
1	D	731	VAL	2.1
1	F	634	VAL	2.1
1	E	536	GLY	2.1
1	F	356	GLY	2.1
1	C	791	LYS	2.0
1	C	748	THR	2.0
1	F	748	THR	2.0
1	F	751	MET	2.0
1	A	303	GLU	2.0
1	E	109	GLU	2.0
1	F	545	GLU	2.0
1	C	553	GLN	2.0
1	C	484	ASN	2.0
1	E	546	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	579	ASN	2.0
1	E	764	ILE	2.0
1	A	507	PRO	2.0
1	A	106	VAL	2.0
1	A	793	GLY	2.0
1	C	350	PHE	2.0
1	D	745	GLU	2.0
1	F	686	MET	2.0
1	A	738	SER	2.0
1	B	748	THR	2.0
1	C	631	SER	2.0
1	D	508	SER	2.0
1	C	690	HIS	2.0
1	C	694	CYS	2.0
1	E	161	ILE	2.0
1	F	547	PRO	2.0
1	C	640	LYS	2.0
1	D	729	LYS	2.0
1	F	733	LYS	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($\text{\AA}^2$)	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

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

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