



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:31 AM UTC

PDB ID : 9NPE / pdb_00009npe
Title : Crystal structure of the inactive conformation of a glycoside hydrolase (CapGH2b) from the GH2 family in the space group P1 at 2.40 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 : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

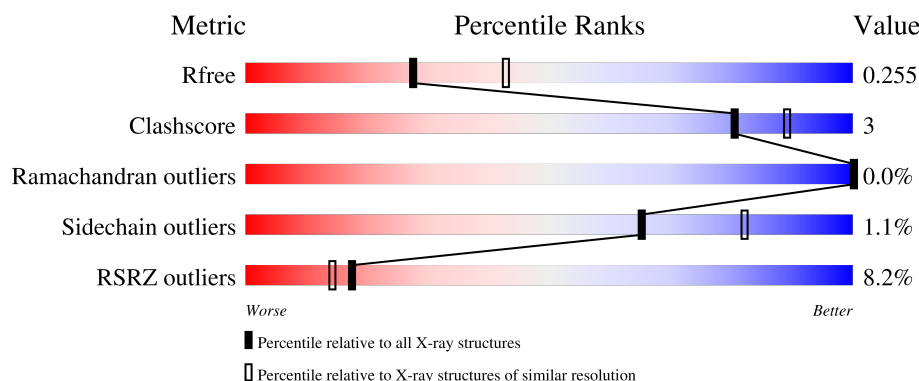
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	3% 84% 7% 8%
1	B	798	2% 85% 5% 9%
1	C	798	17% 79% 10% 10%
1	D	798	4% 87% 5% 8%
1	E	798	2% 85% 6% 9%

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Mol	Chain	Length	Quality of chain
1	F	798	15% 82% 9% 9%

2 Entry composition [i](#)

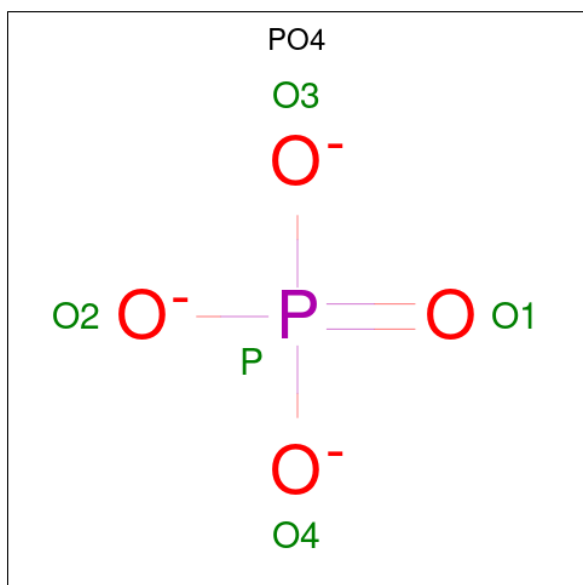
There are 4 unique types of molecules in this entry. The entry contains 37633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Se	0	0	0
			5914	3785	1009	1091	7	22			
1	B	726	Total	C	N	O	S	Se	0	0	0
			5843	3735	1000	1079	8	21			
1	C	715	Total	C	N	O	S	Se	0	0	0
			5762	3685	983	1066	7	21			
1	D	736	Total	C	N	O	S	Se	0	0	0
			5916	3783	1011	1092	8	22			
1	E	725	Total	C	N	O	S	Se	0	0	0
			5834	3732	998	1075	8	21			
1	F	724	Total	C	N	O	S	Se	0	0	0
			5826	3720	995	1083	7	21			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



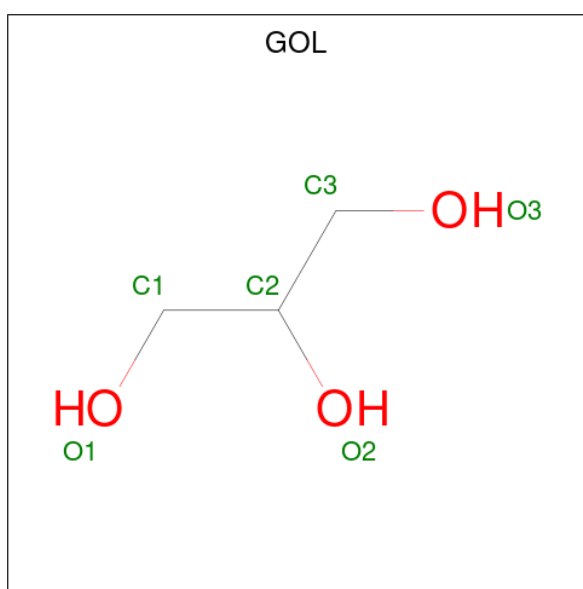
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	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
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	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	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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

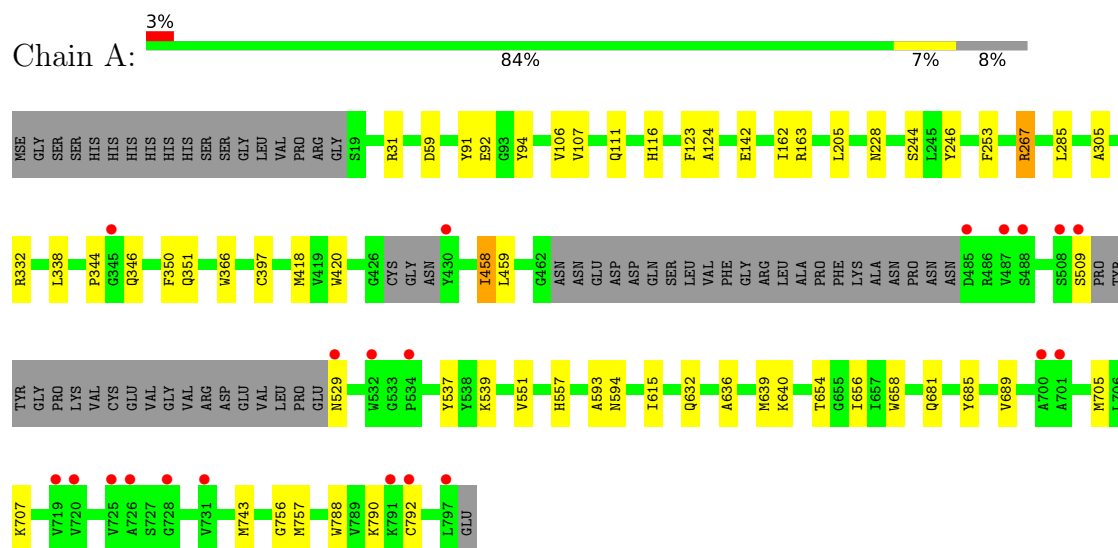
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	435	Total	O	0	0
			435	435		
4	B	407	Total	O	0	0
			407	407		
4	C	229	Total	O	0	0
			229	229		
4	D	419	Total	O	0	0
			419	419		
4	E	449	Total	O	0	0
			449	449		
4	F	265	Total	O	0	0
			265	265		

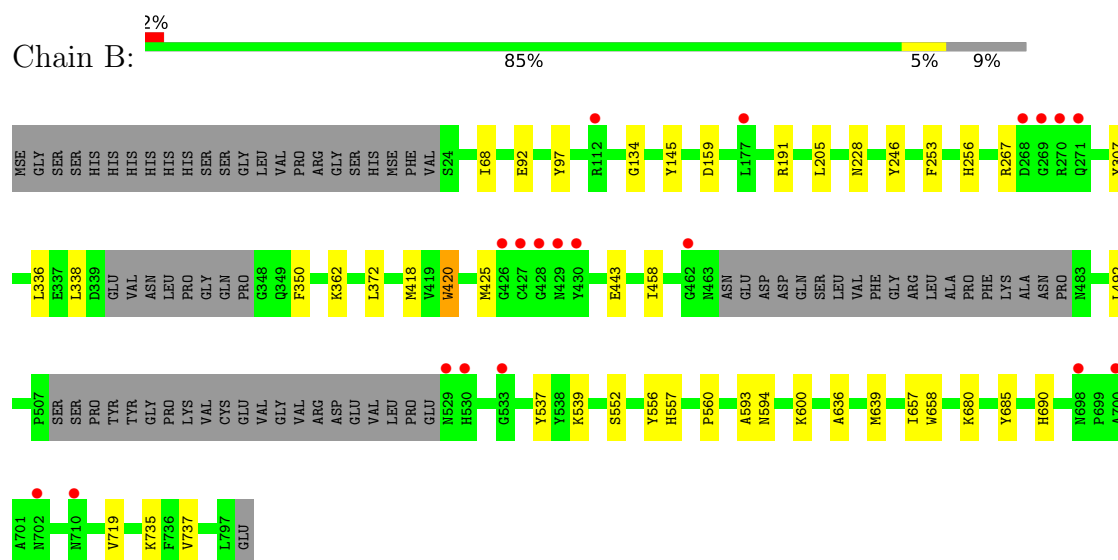
3 Residue-property plots [i](#)

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.

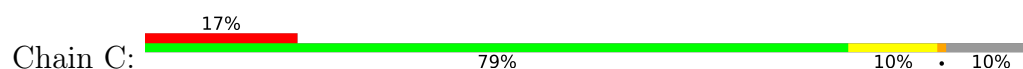
• Molecule 1: Glycoside hydrolase family 2

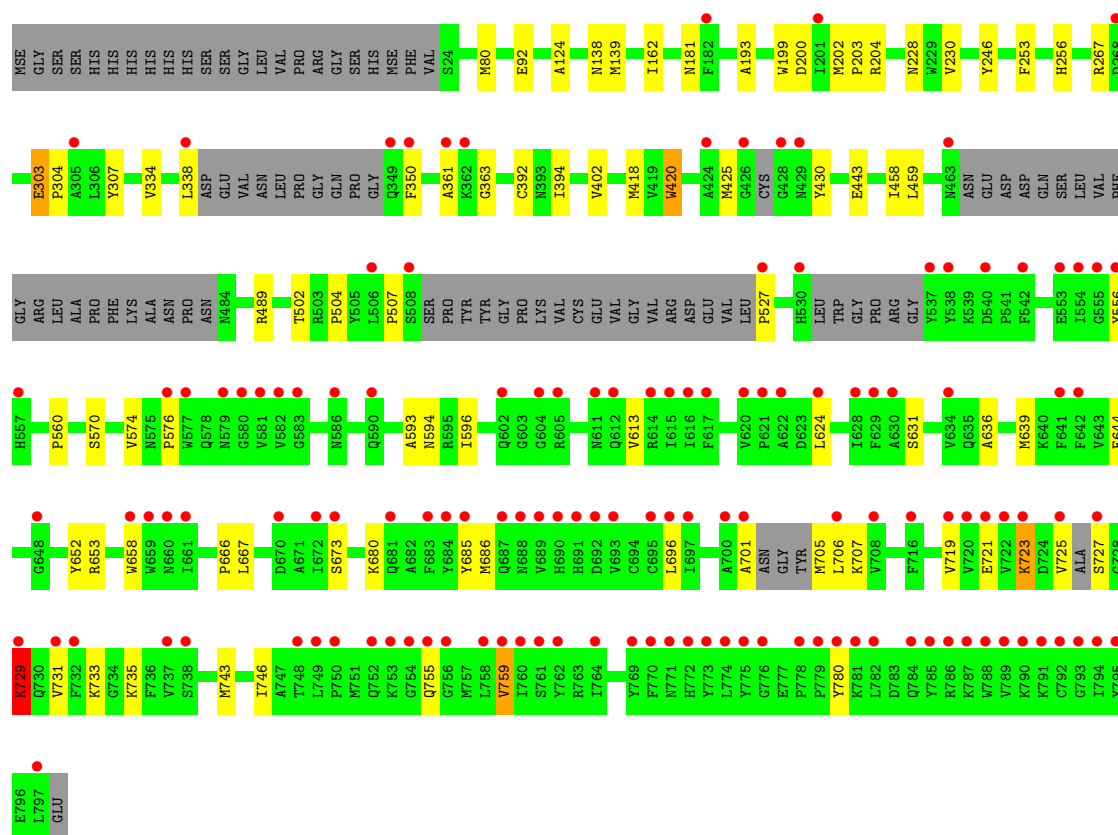


• Molecule 1: Glycoside hydrolase family 2

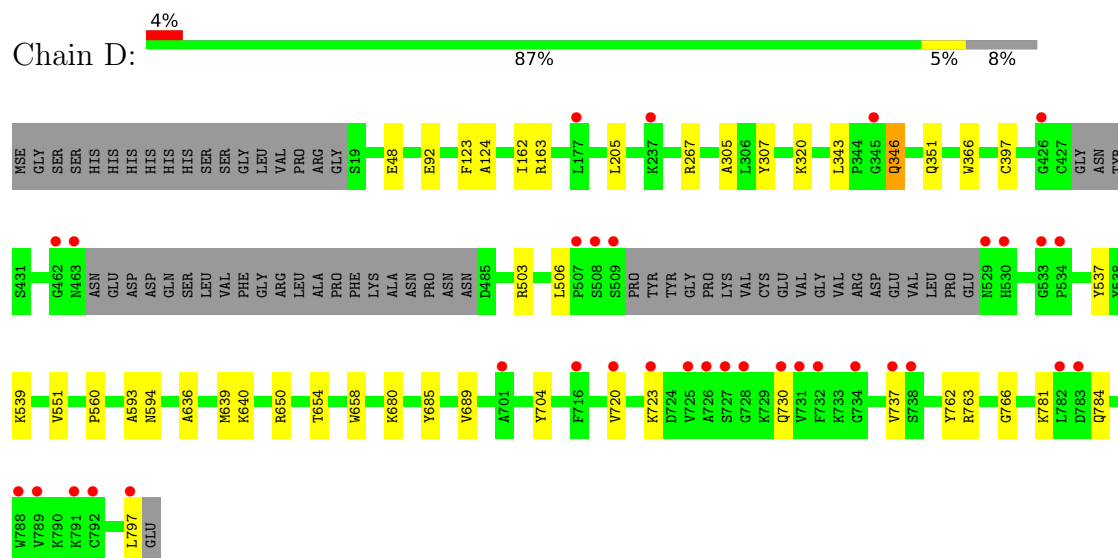


• Molecule 1: Glycoside hydrolase family 2

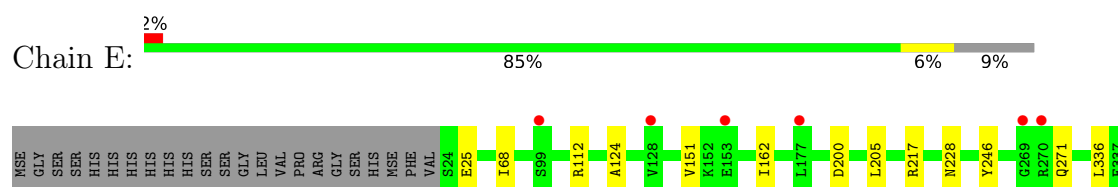


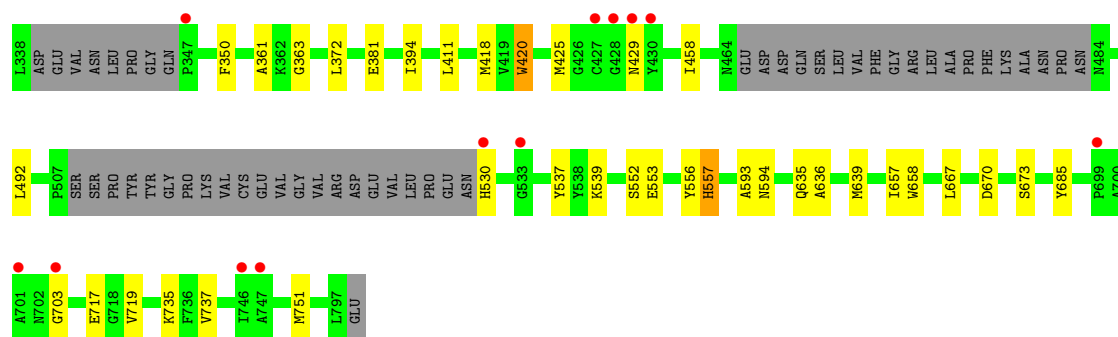


- Molecule 1: Glycoside hydrolase family 2

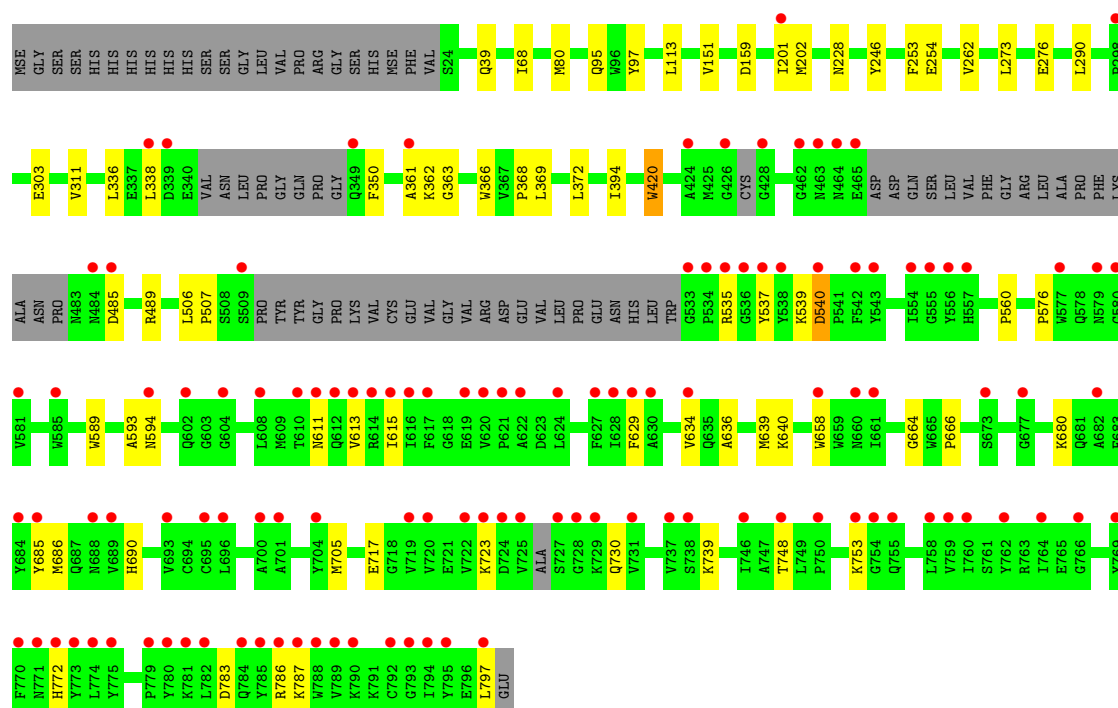
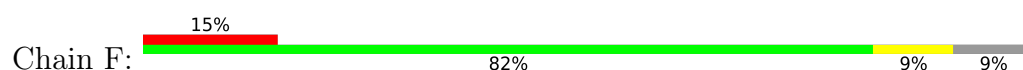


- Molecule 1: Glycoside hydrolase family 2





● 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	122.52Å 124.14Å 133.60Å 89.30° 117.29° 103.48°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.40) 99.6 (20.00-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.41Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.222 , 0.255 0.222 , 0.255	Depositor DCC
R_{free} test set	13180 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	37633	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.25% 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: PO4, GOL

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	0.15	0/6048	0.34	0/8175
1	B	0.12	0/5974	0.34	0/8075
1	C	0.15	0/5887	0.33	0/7951
1	D	0.12	0/6049	0.32	0/8176
1	E	0.13	0/5966	0.34	0/8064
1	F	0.12	0/5952	0.32	0/8040
All	All	0.13	0/35876	0.33	0/48481

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5914	0	5738	31	0
1	B	5843	0	5664	25	0
1	C	5762	0	5591	47	0
1	D	5916	0	5740	23	0
1	E	5834	0	5662	24	0
1	F	5826	0	5643	39	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	0	0
2	C	30	0	0	0	0
2	D	20	0	0	0	0
2	E	30	0	0	0	0
2	F	15	0	0	0	0
3	A	24	0	32	0	0
3	B	42	0	56	1	0
3	C	36	0	48	0	0
3	D	30	0	40	1	0
3	E	30	0	40	1	0
3	F	42	0	56	0	0
4	A	435	0	0	0	0
4	B	407	0	0	0	0
4	C	229	0	0	0	0
4	D	419	0	0	0	0
4	E	449	0	0	0	0
4	F	265	0	0	1	0
All	All	37633	0	34310	183	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 (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ALA:N	1:C:594:ASN:HA	2.14	0.63
1:F:593:ALA:N	1:F:594:ASN:HA	2.15	0.61
1:D:593:ALA:N	1:D:594:ASN:HA	2.16	0.60
1:A:593:ALA:N	1:A:594:ASN:HA	2.17	0.59
1:F:228:ASN:HB3	1:F:246:TYR:HB2	1.84	0.59
1:E:381:GLU:HG2	1:E:411:LEU:HD11	1.84	0.58
1:C:721:GLU:HG3	1:C:733:LYS:HD2	1.86	0.57
1:F:273:LEU:HD13	1:F:290:LEU:HD23	1.87	0.57
1:F:201:ILE:HD12	1:F:202:MSE:HG2	1.86	0.57
1:D:723:LYS:HG2	1:D:730:GLN:HA	1.87	0.56
1:B:552:SER:HA	1:B:657:ILE:HB	1.88	0.56
1:F:537:TYR:CZ	1:F:539:LYS:HB2	2.42	0.55
1:F:361:ALA:HB1	1:F:394:ILE:HG21	1.89	0.55
1:C:723:LYS:HA	1:C:731:VAL:HG23	1.88	0.55
1:B:253:PHE:CZ	1:C:92:GLU:HB2	2.42	0.54
1:C:80:MSE:HB3	1:C:666:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:639:MSE:HE1	1:C:658:TRP:HB2	1.89	0.54
1:E:593:ALA:N	1:E:594:ASN:HA	2.22	0.54
1:B:593:ALA:N	1:B:594:ASN:HA	2.22	0.54
1:A:705:MSE:HG2	1:A:707:LYS:HE2	1.88	0.54
1:C:425:MSE:HG3	1:C:430:TYR:CE1	2.43	0.53
1:C:723:LYS:HG3	1:C:759:VAL:HG13	1.90	0.53
1:B:97:TYR:HE1	1:B:159:ASP:HB3	1.73	0.53
1:C:303:GLU:HG2	1:C:304:PRO:HD2	1.90	0.53
1:A:640:LYS:HG3	1:A:689:VAL:HG11	1.91	0.53
1:A:537:TYR:CE2	1:A:539:LYS:HB2	2.44	0.52
1:E:639:MSE:HE1	1:E:658:TRP:HB2	1.89	0.52
1:F:639:MSE:HE3	1:F:686:MSE:HE2	1.91	0.52
1:D:720:VAL:HG23	1:D:762:TYR:HB3	1.90	0.52
1:E:719:VAL:HG12	1:E:735:LYS:HG2	1.92	0.52
1:B:639:MSE:HE1	1:B:658:TRP:HB2	1.90	0.52
1:F:489:ARG:NH1	1:F:507:PRO:HB2	2.25	0.52
1:A:418:MSE:HB3	1:A:458:ILE:HG12	1.93	0.51
1:A:253:PHE:CZ	1:B:92:GLU:HB2	2.46	0.51
1:C:636:ALA:HB1	1:C:685:TYR:CG	2.45	0.51
1:F:336:LEU:HD11	1:F:350:PHE:CD1	2.46	0.51
1:F:613:VAL:HA	1:F:634:VAL:HG21	1.93	0.51
1:D:92:GLU:HB2	1:F:253:PHE:CZ	2.46	0.51
1:E:425:MSE:HE1	1:E:492:LEU:HD11	1.93	0.51
1:B:191:ARG:HD3	1:B:443:GLU:OE1	2.10	0.51
1:A:639:MSE:HE1	1:A:658:TRP:HB2	1.93	0.50
1:B:719:VAL:HG22	1:B:735:LYS:HG2	1.94	0.50
1:F:636:ALA:HB1	1:F:685:TYR:CG	2.46	0.50
1:F:783:ASP:O	1:F:787:LYS:HG3	2.12	0.50
1:B:636:ALA:HB1	1:B:685:TYR:CG	2.47	0.49
1:F:797:LEU:H	1:F:797:LEU:HD23	1.76	0.49
1:A:92:GLU:HB2	1:C:253:PHE:CZ	2.48	0.49
1:A:123:PHE:HB3	1:A:163:ARG:NH2	2.28	0.49
1:C:644:GLU:HG2	1:C:696:LEU:HD22	1.93	0.49
1:C:652:TYR:HD2	1:C:653:ARG:HE	1.59	0.49
1:A:537:TYR:HB2	1:A:615:ILE:HG21	1.95	0.49
1:C:639:MSE:HE3	1:C:686:MSE:HE2	1.95	0.49
1:F:560:PRO:HA	1:F:680:LYS:HE2	1.94	0.49
1:E:530:HIS:N	1:E:553:GLU:HB2	2.28	0.48
1:C:729:LYS:HE2	1:C:729:LYS:HB2	1.55	0.48
1:D:781:LYS:HB3	1:D:784:GLN:HG3	1.95	0.48
1:A:107:VAL:HG13	1:A:111:GLN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:MSE:HE1	1:A:792:CYS:HB2	1.96	0.48
1:C:202:MSE:HE3	1:C:203:PRO:HD2	1.96	0.48
1:C:363:GLY:HA3	1:C:394:ILE:O	2.13	0.48
1:C:719:VAL:HG12	1:C:735:LYS:HG2	1.95	0.48
1:A:338:LEU:HD23	1:A:350:PHE:HB3	1.96	0.47
1:F:705:MSE:HE1	1:F:748:THR:HG22	1.96	0.47
1:A:31:ARG:HD2	1:A:59:ASP:HB3	1.97	0.47
1:F:362:LYS:HD2	1:F:690:HIS:CD2	2.50	0.47
1:A:228:ASN:HB3	1:A:246:TYR:HB2	1.97	0.47
1:C:203:PRO:HD3	1:C:667:LEU:HD11	1.96	0.47
1:D:343:LEU:HB3	1:D:346:GLN:HB3	1.95	0.47
1:F:262:VAL:HG22	1:F:276:GLU:HG2	1.96	0.47
1:F:537:TYR:HB2	1:F:615:ILE:HG21	1.96	0.47
1:C:560:PRO:HA	1:C:680:LYS:HE2	1.96	0.47
1:E:228:ASN:HB3	1:E:246:TYR:HB2	1.97	0.47
1:F:363:GLY:HA3	1:F:394:ILE:O	2.15	0.47
1:B:600:LYS:HG3	1:D:320:LYS:HB2	1.97	0.46
1:E:418:MSE:HB3	1:E:458:ILE:HG12	1.97	0.46
1:B:134:GLY:HA3	1:B:145:TYR:CE1	2.50	0.46
1:A:529:ASN:HA	1:A:551:VAL:HA	1.97	0.46
1:E:420:TRP:C	1:E:420:TRP:CD1	2.93	0.46
1:F:68:ILE:HG13	1:F:372:LEU:HD13	1.97	0.46
1:A:636:ALA:HB1	1:A:685:TYR:CG	2.51	0.46
1:C:701:ALA:HB2	1:C:705:MSE:N	2.31	0.46
1:F:639:MSE:HE1	1:F:658:TRP:HB2	1.97	0.46
1:C:338:LEU:HD23	1:C:350:PHE:HB3	1.97	0.46
1:D:537:TYR:CE2	1:D:539:LYS:HB2	2.51	0.46
1:E:363:GLY:HA3	1:E:394:ILE:O	2.16	0.46
1:D:636:ALA:HB1	1:D:685:TYR:CG	2.50	0.46
1:A:366:TRP:HB3	1:A:397:CYS:HA	1.98	0.46
1:B:420:TRP:C	1:B:420:TRP:CD1	2.94	0.46
1:A:267:ARG:HH12	1:A:305:ALA:HB1	1.81	0.45
1:B:362:LYS:HD2	1:B:690:HIS:CD2	2.51	0.45
1:C:230:VAL:HG13	1:C:502:THR:HG21	1.97	0.45
1:E:717:GLU:HG2	1:E:737:VAL:HG22	1.98	0.45
1:A:707:LYS:HD3	1:A:743:MSE:SE	2.66	0.45
1:C:755:GLN:HB2	1:C:780:TYR:CE2	2.52	0.45
1:D:650:ARG:NH2	3:D:806:GOL:H11	2.31	0.45
1:A:244:SER:HB3	1:A:285:LEU:HD11	1.98	0.45
1:B:425:MSE:HE1	1:B:492:LEU:HD11	1.98	0.45
1:C:267:ARG:HD2	1:C:307:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:MSE:HE1	1:D:658:TRP:HB2	1.98	0.45
1:E:636:ALA:HB1	1:E:685:TYR:CG	2.52	0.45
1:D:366:TRP:HB3	1:D:397:CYS:HA	1.99	0.45
1:F:39:GLN:HB2	1:F:95:GLN:HG3	1.99	0.45
1:B:362:LYS:HE3	1:B:690:HIS:O	2.17	0.45
1:E:557:HIS:O	1:E:635:GLN:HB2	2.17	0.45
1:F:537:TYR:O	1:F:540:ASP:HB2	2.17	0.45
1:D:560:PRO:HA	1:D:680:LYS:HE2	1.99	0.45
1:C:489:ARG:NH1	1:C:507:PRO:HB2	2.32	0.44
1:E:594:ASN:HB2	1:E:667:LEU:HD22	1.99	0.44
1:F:113:LEU:HD23	1:F:151:VAL:HG11	1.99	0.44
1:A:551:VAL:HG23	1:A:656:ILE:HA	1.99	0.44
1:C:418:MSE:HB3	1:C:458:ILE:HD13	2.00	0.44
1:F:254:GLU:HG2	4:F:1030:HOH:O	2.18	0.44
1:D:267:ARG:HD3	1:D:307:TYR:CE2	2.53	0.44
1:E:124:ALA:HB2	1:E:162:ILE:HG12	1.99	0.44
1:C:489:ARG:CZ	1:C:507:PRO:HB2	2.48	0.43
1:B:338:LEU:HD23	1:B:350:PHE:HB3	1.99	0.43
1:B:228:ASN:HB3	1:B:246:TYR:HB2	1.99	0.43
1:D:267:ARG:HH12	1:D:305:ALA:HB1	1.83	0.43
1:C:228:ASN:HB3	1:C:246:TYR:HB2	1.99	0.43
1:F:420:TRP:C	1:F:420:TRP:CD1	2.96	0.43
1:C:361:ALA:HB1	1:C:394:ILE:HG21	2.01	0.43
1:F:611:ASN:O	1:F:615:ILE:HG12	2.17	0.43
1:D:763:ARG:NH1	1:D:766:GLY:HA2	2.33	0.43
1:F:338:LEU:HD23	1:F:350:PHE:HB3	1.99	0.43
1:B:253:PHE:HA	1:B:256:HIS:ND1	2.34	0.43
1:F:80:MSE:HB3	1:F:666:PRO:HG2	2.01	0.43
1:A:756:GLY:HA2	1:A:788:TRP:CZ2	2.54	0.42
1:E:537:TYR:CE2	1:E:539:LYS:HB2	2.53	0.42
1:F:739:LYS:HD3	1:F:739:LYS:HA	1.81	0.42
1:C:363:GLY:HA2	1:C:392:CYS:SG	2.59	0.42
1:C:725:VAL:C	1:C:727:SER:HB2	2.44	0.42
1:A:124:ALA:HB2	1:A:162:ILE:HG12	2.01	0.42
1:A:420:TRP:CD2	1:A:459:LEU:HD23	2.55	0.42
1:C:576:PRO:HD3	1:C:624:LEU:HD13	2.00	0.42
1:E:68:ILE:HG13	1:E:372:LEU:HD13	2.01	0.42
1:C:707:LYS:HD3	1:C:743:MSE:SE	2.70	0.42
1:E:703:GLY:HA2	1:E:751:MSE:HE2	2.01	0.42
1:A:116:HIS:HE1	1:A:142:GLU:HG2	1.85	0.42
1:E:25:GLU:HG3	1:E:217:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:506:LEU:HD23	1:F:506:LEU:HA	1.86	0.42
1:C:204:ARG:HB2	1:C:596:ILE:HG23	2.01	0.42
1:D:123:PHE:HB3	1:D:163:ARG:NH2	2.35	0.42
1:E:200:ASP:OD2	3:E:807:GOL:H2	2.20	0.42
1:F:640:LYS:HE2	1:F:772:HIS:CE1	2.54	0.42
1:C:139:MSE:CE	1:C:193:ALA:H	2.33	0.42
1:A:344:PRO:HD2	1:E:271:GLN:HB3	2.02	0.42
1:E:336:LEU:HD11	1:E:350:PHE:CD1	2.55	0.42
1:C:124:ALA:HB2	1:C:162:ILE:HG12	2.01	0.41
1:F:97:TYR:HE1	1:F:159:ASP:HB3	1.85	0.41
1:A:91:TYR:HA	1:A:94:TYR:CD1	2.54	0.41
1:C:253:PHE:HA	1:C:256:HIS:ND1	2.35	0.41
1:E:552:SER:HA	1:E:657:ILE:HB	2.01	0.41
1:F:723:LYS:HG3	1:F:730:GLN:HA	2.01	0.41
1:C:138:ASN:HD21	1:C:443:GLU:HB2	1.84	0.41
1:C:570:SER:O	1:C:574:VAL:HG23	2.19	0.41
1:D:124:ALA:HB2	1:D:162:ILE:HG12	2.01	0.41
1:A:351:GLN:HB2	1:A:654:THR:HG21	2.01	0.41
1:C:139:MSE:HE3	1:C:402:VAL:HG12	2.01	0.41
1:C:459:LEU:HD12	1:C:504:PRO:O	2.21	0.41
1:C:706:LEU:HG	1:C:746:ILE:HD12	2.02	0.41
1:B:737:VAL:H	3:B:811:GOL:H12	1.86	0.41
1:C:181:ASN:HA	1:C:527:PRO:HG3	2.01	0.41
1:D:351:GLN:HB2	1:D:654:THR:HG21	2.03	0.41
1:D:640:LYS:HG3	1:D:689:VAL:HG11	2.01	0.41
1:B:418:MSE:HB3	1:B:458:ILE:HD13	2.03	0.41
1:B:537:TYR:CE2	1:B:539:LYS:HB2	2.56	0.41
1:A:790:LYS:HB2	1:A:790:LYS:HE3	1.81	0.41
1:C:613:VAL:HG22	1:C:631:SER:HA	2.02	0.41
1:C:199:TRP:HD1	1:C:200:ASP:OD1	2.03	0.41
1:D:48:GLU:H	1:D:48:GLU:CD	2.29	0.41
1:D:797:LEU:H	1:D:797:LEU:HD22	1.86	0.41
1:B:336:LEU:HD11	1:B:350:PHE:CD1	2.56	0.41
1:B:560:PRO:HA	1:B:680:LYS:HE2	2.03	0.41
1:C:420:TRP:CD1	1:C:420:TRP:C	2.99	0.41
1:F:629:PHE:CE2	1:F:786:ARG:HG3	2.56	0.41
1:D:506:LEU:HD12	1:D:506:LEU:HA	1.96	0.40
1:F:366:TRP:CZ2	1:F:369:LEU:HD21	2.56	0.40
1:A:632:GLN:HB3	1:A:681:GLN:HB2	2.04	0.40
1:B:68:ILE:HG13	1:B:372:LEU:HD13	2.02	0.40
1:B:267:ARG:HD2	1:B:307:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:ALA:HB1	1:E:394:ILE:HG21	2.03	0.40
1:F:368:PRO:O	1:F:664:GLY:HA3	2.21	0.40
1:F:576:PRO:HB3	1:F:589:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	727/798 (91%)	702 (97%)	25 (3%)	0	100	100
1	B	718/798 (90%)	694 (97%)	24 (3%)	0	100	100
1	C	699/798 (88%)	676 (97%)	22 (3%)	1 (0%)	48	64
1	D	728/798 (91%)	708 (97%)	20 (3%)	0	100	100
1	E	717/798 (90%)	686 (96%)	31 (4%)	0	100	100
1	F	712/798 (89%)	684 (96%)	28 (4%)	0	100	100
All	All	4301/4788 (90%)	4150 (96%)	150 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	729	LYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	635/666 (95%)	627 (99%)	8 (1%)	61	80
1	B	626/666 (94%)	622 (99%)	4 (1%)	78	89
1	C	620/666 (93%)	612 (99%)	8 (1%)	61	80
1	D	636/666 (96%)	630 (99%)	6 (1%)	70	85
1	E	625/666 (94%)	616 (99%)	9 (1%)	59	79
1	F	626/666 (94%)	618 (99%)	8 (1%)	61	80
All	All	3768/3996 (94%)	3725 (99%)	43 (1%)	65	82

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	205	LEU
1	A	267	ARG
1	A	332	ARG
1	A	346	GLN
1	A	458	ILE
1	A	509	SER
1	A	557	HIS
1	B	205	LEU
1	B	420	TRP
1	B	556	TYR
1	B	557	HIS
1	C	303	GLU
1	C	334	VAL
1	C	420	TRP
1	C	556	TYR
1	C	673	SER
1	C	723	LYS
1	C	729	LYS
1	C	759	VAL
1	D	205	LEU
1	D	346	GLN
1	D	503	ARG
1	D	551	VAL
1	D	704	TYR
1	D	737	VAL
1	E	112	ARG
1	E	151	VAL
1	E	205	LEU
1	E	420	TRP

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Mol	Chain	Res	Type
1	E	429	ASN
1	E	556	TYR
1	E	557	HIS
1	E	670	ASP
1	E	673	SER
1	F	303	GLU
1	F	311	VAL
1	F	420	TRP
1	F	485	ASP
1	F	535	ARG
1	F	540	ASP
1	F	717	GLU
1	F	753	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	228	ASN
1	A	752	GLN
1	B	26	GLN
1	B	379	HIS
1	B	730	GLN
1	B	767	ASN
1	C	463	ASN
1	C	529	ASN
1	C	594	ASN
1	C	635	GLN
1	C	688	ASN
1	C	711	ASN
1	D	172	HIS
1	D	271	GLN
1	D	557	HIS
1	D	575	ASN
1	D	702	ASN
1	E	228	ASN
1	E	464	ASN
1	E	575	ASN
1	E	687	GLN
1	E	784	GLN
1	F	228	ASN
1	F	385	GLN

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Mol	Chain	Res	Type
1	F	549	GLN
1	F	557	HIS
1	F	681	GLN
1	F	784	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.50	0
2	PO4	D	801	-	4,4,4	1.60	1 (25%)	6,6,6	0.53	0
2	PO4	A	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.51	0
3	GOL	B	807	-	5,5,5	0.37	0	5,5,5	0.51	0
2	PO4	C	804	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	GOL	B	809	-	5,5,5	0.30	0	5,5,5	0.37	0
3	GOL	D	806	-	5,5,5	0.35	0	5,5,5	0.39	0
2	PO4	D	804	-	4,4,4	1.58	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	E	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.47	0
3	GOL	C	810	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	F	810	-	5,5,5	0.34	0	5,5,5	0.42	0
2	PO4	C	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
2	PO4	C	806	-	4,4,4	1.58	1 (25%)	6,6,6	0.47	0
3	GOL	A	805	-	5,5,5	0.35	0	5,5,5	0.45	0
3	GOL	B	810	-	5,5,5	0.35	0	5,5,5	0.36	0
2	PO4	B	801	-	4,4,4	1.61	1 (25%)	6,6,6	0.46	0
3	GOL	B	806	-	5,5,5	0.34	0	5,5,5	0.39	0
3	GOL	B	805	-	5,5,5	0.33	0	5,5,5	0.37	0
2	PO4	F	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.48	0
3	GOL	B	808	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	F	804	-	5,5,5	0.36	0	5,5,5	0.48	0
2	PO4	E	805	-	4,4,4	1.61	1 (25%)	6,6,6	0.51	0
3	GOL	B	811	-	5,5,5	0.35	0	5,5,5	0.41	0
3	GOL	E	808	-	5,5,5	0.32	0	5,5,5	0.49	0
2	PO4	A	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.44	0
3	GOL	F	805	-	5,5,5	0.31	0	5,5,5	0.37	0
3	GOL	F	809	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	E	810	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	F	806	-	5,5,5	0.33	0	5,5,5	0.38	0
2	PO4	A	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
3	GOL	F	808	-	5,5,5	0.32	0	5,5,5	0.35	0
2	PO4	E	806	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
2	PO4	E	804	-	4,4,4	1.61	1 (25%)	6,6,6	0.47	0
3	GOL	A	807	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	C	812	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	D	808	-	5,5,5	0.35	0	5,5,5	0.42	0
2	PO4	F	801	-	4,4,4	1.59	1 (25%)	6,6,6	0.47	0
3	GOL	E	807	-	5,5,5	0.32	0	5,5,5	0.46	0
2	PO4	D	803	-	4,4,4	1.67	1 (25%)	6,6,6	0.50	0
3	GOL	E	811	-	5,5,5	0.36	0	5,5,5	0.47	0
3	GOL	C	808	-	5,5,5	0.34	0	5,5,5	0.41	0
3	GOL	F	807	-	5,5,5	0.31	0	5,5,5	0.42	0
2	PO4	E	803	-	4,4,4	1.56	1 (25%)	6,6,6	0.49	0
2	PO4	F	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.47	0
2	PO4	D	802	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
3	GOL	A	804	-	5,5,5	0.33	0	5,5,5	0.33	0
2	PO4	C	803	-	4,4,4	1.55	1 (25%)	6,6,6	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	804	-	4,4,4	1.55	1 (25%)	6,6,6	0.68	0
2	PO4	C	805	-	4,4,4	1.62	1 (25%)	6,6,6	0.45	0
3	GOL	D	809	-	5,5,5	0.33	0	5,5,5	0.43	0
2	PO4	B	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	GOL	D	805	-	5,5,5	0.33	0	5,5,5	0.41	0
3	GOL	C	807	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	D	807	-	5,5,5	0.33	0	5,5,5	0.44	0
3	GOL	E	809	-	5,5,5	0.34	0	5,5,5	0.44	0
2	PO4	C	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	GOL	C	811	-	5,5,5	0.33	0	5,5,5	0.39	0
3	GOL	A	806	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	C	809	-	5,5,5	0.35	0	5,5,5	0.36	0
2	PO4	B	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.47	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	GOL	B	807	-	-	0/4/4/4	-
3	GOL	B	809	-	-	2/4/4/4	-
3	GOL	D	806	-	-	2/4/4/4	-
3	GOL	C	810	-	-	2/4/4/4	-
3	GOL	F	810	-	-	2/4/4/4	-
3	GOL	B	810	-	-	0/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	B	806	-	-	0/4/4/4	-
3	GOL	B	805	-	-	0/4/4/4	-
3	GOL	B	808	-	-	0/4/4/4	-
3	GOL	F	804	-	-	2/4/4/4	-
3	GOL	B	811	-	-	2/4/4/4	-
3	GOL	E	808	-	-	2/4/4/4	-
3	GOL	F	809	-	-	0/4/4/4	-
3	GOL	F	805	-	-	0/4/4/4	-
3	GOL	E	810	-	-	0/4/4/4	-
3	GOL	F	806	-	-	2/4/4/4	-
3	GOL	F	808	-	-	2/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	812	-	-	0/4/4/4	-
3	GOL	D	808	-	-	0/4/4/4	-
3	GOL	E	807	-	-	0/4/4/4	-
3	GOL	E	811	-	-	2/4/4/4	-
3	GOL	C	808	-	-	0/4/4/4	-
3	GOL	F	807	-	-	0/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	D	809	-	-	4/4/4/4	-
3	GOL	D	805	-	-	0/4/4/4	-
3	GOL	C	807	-	-	3/4/4/4	-
3	GOL	D	807	-	-	0/4/4/4	-
3	GOL	E	809	-	-	0/4/4/4	-
3	GOL	C	811	-	-	0/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	C	809	-	-	1/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	803	PO4	P-O1	2.87	1.57	1.50
2	A	802	PO4	P-O1	2.82	1.57	1.50
2	C	805	PO4	P-O1	2.81	1.57	1.50
2	E	802	PO4	P-O1	2.80	1.57	1.50
2	E	805	PO4	P-O1	2.80	1.57	1.50
2	E	804	PO4	P-O1	2.79	1.57	1.50
2	D	804	PO4	P-O1	2.78	1.57	1.50
2	B	801	PO4	P-O1	2.78	1.57	1.50
2	D	801	PO4	P-O1	2.77	1.57	1.50
2	F	801	PO4	P-O1	2.76	1.57	1.50
2	B	802	PO4	P-O1	2.76	1.57	1.50
2	E	806	PO4	P-O1	2.75	1.57	1.50
2	F	802	PO4	P-O1	2.75	1.57	1.50
2	C	806	PO4	P-O1	2.75	1.57	1.50
2	C	802	PO4	P-O1	2.74	1.57	1.50
2	F	803	PO4	P-O1	2.73	1.57	1.50
2	A	803	PO4	P-O1	2.73	1.57	1.50
2	B	803	PO4	P-O1	2.73	1.57	1.50
2	C	804	PO4	P-O1	2.72	1.56	1.50
2	C	801	PO4	P-O1	2.71	1.56	1.50
2	E	801	PO4	P-O1	2.70	1.56	1.50
2	B	804	PO4	P-O1	2.70	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	803	PO4	P-O1	2.69	1.56	1.50
2	D	802	PO4	P-O1	2.68	1.56	1.50
2	A	801	PO4	P-O1	2.68	1.56	1.50
2	C	803	PO4	P-O1	2.65	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	805	GOL	O1-C1-C2-C3
3	A	807	GOL	C1-C2-C3-O3
3	C	807	GOL	O1-C1-C2-C3
3	C	810	GOL	O1-C1-C2-C3
3	D	806	GOL	C1-C2-C3-O3
3	D	809	GOL	O1-C1-C2-C3
3	D	809	GOL	C1-C2-C3-O3
3	D	809	GOL	O2-C2-C3-O3
3	E	808	GOL	O1-C1-C2-C3
3	F	806	GOL	O1-C1-C2-C3
3	F	808	GOL	O1-C1-C2-C3
3	A	804	GOL	C1-C2-C3-O3
3	B	809	GOL	O1-C1-C2-C3
3	B	811	GOL	C1-C2-C3-O3
3	C	809	GOL	O1-C1-C2-C3
3	E	811	GOL	O1-C1-C2-C3
3	F	804	GOL	C1-C2-C3-O3
3	F	810	GOL	O1-C1-C2-C3
3	A	805	GOL	O1-C1-C2-O2
3	A	807	GOL	O2-C2-C3-O3
3	B	809	GOL	O1-C1-C2-O2
3	C	810	GOL	O1-C1-C2-O2
3	D	809	GOL	O1-C1-C2-O2
3	F	806	GOL	O1-C1-C2-O2
3	F	808	GOL	O1-C1-C2-O2
3	E	808	GOL	O1-C1-C2-O2
3	D	806	GOL	O2-C2-C3-O3
3	A	804	GOL	O2-C2-C3-O3
3	C	807	GOL	O1-C1-C2-O2
3	E	811	GOL	O2-C2-C3-O3
3	F	810	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	811	GOL	O2-C2-C3-O3
3	A	806	GOL	O1-C1-C2-O2
3	C	807	GOL	C1-C2-C3-O3
3	F	804	GOL	O2-C2-C3-O3
3	A	806	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	806	GOL	1	0
3	B	811	GOL	1	0
3	E	807	GOL	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	713/798 (89%)	0.08	21 (2%) 53 50	27, 41, 75, 86	0
1	B	705/798 (88%)	0.22	19 (2%) 56 52	29, 43, 66, 87	0
1	C	694/798 (86%)	0.99	134 (19%) 3 2	35, 60, 110, 121	0
1	D	714/798 (89%)	0.13	34 (4%) 35 32	27, 41, 75, 88	0
1	E	704/798 (88%)	0.15	18 (2%) 57 53	27, 40, 63, 84	0
1	F	703/798 (88%)	0.88	119 (16%) 4 3	34, 54, 106, 127	0
All	All	4233/4788 (88%)	0.41	345 (8%) 17 14	27, 46, 90, 127	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	673	SER	5.4
1	C	755	GLN	5.2
1	C	722	VAL	4.6
1	C	620	VAL	4.6
1	C	701	ALA	4.6
1	F	770	PHE	4.5
1	C	789	VAL	4.4
1	C	630	ALA	4.4
1	C	782	LEU	4.4
1	C	793	GLY	4.4
1	F	793	GLY	4.4
1	F	629	PHE	4.2
1	C	685	TYR	4.2
1	C	795	TYR	4.2
1	C	788	TRP	4.2
1	F	758	LEU	4.2
1	C	527	PRO	4.1
1	C	758	LEU	4.1
1	F	797	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	788	TRP	4.1
1	C	629	PHE	4.0
1	D	509	SER	4.0
1	E	427	CYS	4.0
1	F	782	LEU	4.0
1	F	612	GLN	4.0
1	F	620	VAL	4.0
1	C	463	ASN	3.9
1	F	611	ASN	3.9
1	D	533	GLY	3.9
1	F	536	GLY	3.9
1	C	754	GLY	3.9
1	C	785	TYR	3.9
1	C	612	GLN	3.8
1	C	769	TYR	3.8
1	C	794	ILE	3.8
1	C	581	VAL	3.8
1	F	617	PHE	3.8
1	F	795	TYR	3.8
1	F	628	ILE	3.8
1	F	538	TYR	3.8
1	C	774	LEU	3.8
1	C	781	LYS	3.7
1	B	427	CYS	3.7
1	C	760	ILE	3.7
1	A	529	ASN	3.7
1	F	785	TYR	3.7
1	C	615	ILE	3.7
1	C	779	PRO	3.7
1	C	780	TYR	3.7
1	D	725	VAL	3.6
1	C	426	GLY	3.6
1	D	797	LEU	3.6
1	E	347	PRO	3.6
1	D	728	GLY	3.6
1	F	725	VAL	3.6
1	F	426	GLY	3.6
1	C	770	PHE	3.6
1	F	764	ILE	3.6
1	C	759	VAL	3.5
1	C	727	SER	3.5
1	F	630	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	538	TYR	3.5
1	C	762	TYR	3.5
1	A	509	SER	3.5
1	F	753	LYS	3.5
1	C	771	ASN	3.5
1	F	722	VAL	3.5
1	C	621	PRO	3.5
1	F	556	TYR	3.5
1	F	780	TYR	3.5
1	C	616	ILE	3.5
1	C	738	SER	3.4
1	F	787	LYS	3.4
1	D	529	ASN	3.4
1	E	533	GLY	3.4
1	F	581	VAL	3.4
1	D	177	LEU	3.4
1	F	685	TYR	3.3
1	F	688	ASN	3.3
1	C	693	VAL	3.3
1	F	789	VAL	3.3
1	C	797	LEU	3.3
1	D	726	ALA	3.3
1	A	797	LEU	3.2
1	C	725	VAL	3.2
1	F	759	VAL	3.2
1	C	624	LEU	3.2
1	D	463	ASN	3.2
1	D	731	VAL	3.2
1	C	554	ILE	3.2
1	F	627	PHE	3.2
1	B	530	HIS	3.2
1	F	769	TYR	3.2
1	F	728	GLY	3.2
1	F	754	GLY	3.2
1	E	270	ARG	3.1
1	F	784	GLN	3.1
1	F	781	LYS	3.1
1	F	463	ASN	3.1
1	F	723	LYS	3.1
1	F	298	PRO	3.1
1	F	677	GLY	3.1
1	C	792	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	557	HIS	3.1
1	E	530	HIS	3.1
1	C	791	LYS	3.1
1	B	529	ASN	3.1
1	F	771	ASN	3.1
1	A	345	GLY	3.1
1	A	731	VAL	3.1
1	C	764	ILE	3.1
1	F	424	ALA	3.0
1	F	792	CYS	3.0
1	F	533	GLY	3.0
1	C	689	VAL	3.0
1	C	556	TYR	3.0
1	F	557	HIS	3.0
1	F	724	ASP	3.0
1	B	269	GLY	3.0
1	F	661	ILE	3.0
1	F	774	LEU	3.0
1	F	535	ARG	3.0
1	C	428	GLY	3.0
1	C	784	GLN	3.0
1	F	689	VAL	3.0
1	F	464	ASN	3.0
1	F	615	ILE	2.9
1	F	748	THR	2.9
1	D	783	ASP	2.9
1	F	462	GLY	2.9
1	F	779	PRO	2.9
1	F	790	LYS	2.9
1	C	673	SER	2.9
1	F	604	GLY	2.9
1	A	726	ALA	2.9
1	D	530	HIS	2.9
1	D	701	ALA	2.9
1	C	350	PHE	2.9
1	E	430	TYR	2.9
1	F	773	TYR	2.9
1	D	738	SER	2.8
1	C	530	HIS	2.8
1	C	690	HIS	2.8
1	C	537	TYR	2.8
1	F	537	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	543	TYR	2.8
1	E	428	GLY	2.8
1	A	508	SER	2.8
1	F	534	PRO	2.8
1	A	728	GLY	2.8
1	B	177	LEU	2.8
1	C	424	ALA	2.8
1	C	700	ALA	2.8
1	A	430	TYR	2.8
1	C	661	ILE	2.8
1	C	775	TYR	2.8
1	E	429	ASN	2.8
1	F	621	PRO	2.8
1	C	723	LYS	2.8
1	F	580	GLY	2.7
1	C	579	ASN	2.7
1	F	660	ASN	2.7
1	C	361	ALA	2.7
1	C	617	PHE	2.7
1	F	794	ILE	2.7
1	F	737	VAL	2.7
1	C	696	LEU	2.7
1	C	790	LYS	2.7
1	C	691	HIS	2.7
1	C	692	ASP	2.7
1	C	641	PHE	2.7
1	C	720	VAL	2.7
1	F	624	LEU	2.7
1	B	428	GLY	2.7
1	D	792	CYS	2.7
1	C	642	PHE	2.7
1	B	702	ASN	2.7
1	F	696	LEU	2.7
1	B	462	GLY	2.6
1	D	462	GLY	2.6
1	C	697	ILE	2.6
1	C	778	PRO	2.6
1	F	594	ASN	2.6
1	F	786	ARG	2.6
1	D	508	SER	2.6
1	F	762	TYR	2.6
1	C	659	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	787	LYS	2.6
1	C	305	ALA	2.6
1	F	585	TRP	2.6
1	C	776	GLY	2.6
1	C	576	PRO	2.6
1	C	605	ARG	2.6
1	C	695	CYS	2.6
1	C	614	ARG	2.6
1	F	616	ILE	2.6
1	C	731	VAL	2.6
1	F	361	ALA	2.6
1	F	772	HIS	2.6
1	F	729	LYS	2.6
1	F	577	TRP	2.5
1	F	608	LEU	2.5
1	C	611	ASN	2.5
1	A	488	SER	2.5
1	C	773	TYR	2.5
1	C	658	TRP	2.5
1	F	760	ILE	2.5
1	C	729	LYS	2.5
1	C	753	LYS	2.5
1	D	737	VAL	2.5
1	B	270	ARG	2.5
1	F	684	TYR	2.5
1	B	426	GLY	2.5
1	C	506	LEU	2.5
1	B	429	ASN	2.5
1	C	708	VAL	2.5
1	F	484	ASN	2.5
1	F	579	ASN	2.5
1	F	613	VAL	2.5
1	C	786	ARG	2.5
1	F	738	SER	2.5
1	C	756	GLY	2.5
1	D	345	GLY	2.5
1	B	430	TYR	2.5
1	C	540	ASP	2.5
1	F	775	TYR	2.5
1	F	542	PHE	2.5
1	C	772	HIS	2.5
1	F	720	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	583	GLY	2.4
1	A	532	TRP	2.4
1	F	634	VAL	2.4
1	F	727	SER	2.4
1	B	533	GLY	2.4
1	C	628	ILE	2.4
1	C	681	GLN	2.4
1	D	782	LEU	2.4
1	F	338	LEU	2.4
1	D	732	PHE	2.4
1	A	719	VAL	2.4
1	C	582	VAL	2.4
1	D	788	TRP	2.4
1	F	465	GLU	2.4
1	C	580	GLY	2.4
1	B	271	GLN	2.4
1	C	602	GLN	2.4
1	C	182	PHE	2.4
1	C	201	ILE	2.4
1	C	716	PHE	2.4
1	C	719	VAL	2.4
1	C	622	ALA	2.4
1	F	509	SER	2.3
1	A	720	VAL	2.3
1	A	791	LYS	2.3
1	C	748	THR	2.3
1	C	555	GLY	2.3
1	D	734	GLY	2.3
1	D	730	GLN	2.3
1	E	177	LEU	2.3
1	F	554	ILE	2.3
1	D	723	LYS	2.3
1	C	553	GLU	2.3
1	F	619	GLU	2.3
1	B	710	ASN	2.3
1	C	586	ASN	2.3
1	C	577	TRP	2.3
1	C	752	GLN	2.3
1	D	727	SER	2.3
1	C	749	LEU	2.3
1	F	201	ILE	2.3
1	A	792	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	688	ASN	2.3
1	F	610	THR	2.3
1	F	540	ASP	2.3
1	F	731	VAL	2.3
1	A	534	PRO	2.3
1	F	750	PRO	2.3
1	C	684	TYR	2.3
1	F	701	ALA	2.2
1	C	672	ILE	2.2
1	D	791	LYS	2.2
1	F	485	ASP	2.2
1	A	725	VAL	2.2
1	B	698	ASN	2.2
1	C	660	ASN	2.2
1	F	682	ALA	2.2
1	E	269	GLY	2.2
1	F	766	GLY	2.2
1	C	508	SER	2.2
1	A	485	ASP	2.2
1	C	670	ASP	2.2
1	F	719	VAL	2.2
1	E	701	ALA	2.2
1	F	622	ALA	2.2
1	F	704	TYR	2.2
1	E	746	ILE	2.2
1	C	761	SER	2.2
1	F	658	TRP	2.2
1	D	534	PRO	2.2
1	E	128	VAL	2.2
1	C	429	ASN	2.2
1	C	590	GLN	2.2
1	F	349	GLN	2.2
1	F	602	GLN	2.2
1	C	750	PRO	2.2
1	E	699	PRO	2.2
1	C	683	PHE	2.2
1	A	701	ALA	2.1
1	C	349	GLN	2.1
1	C	648	GLY	2.1
1	E	153	GLU	2.1
1	D	237	LYS	2.1
1	E	747	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	706	LEU	2.1
1	F	746	ILE	2.1
1	B	112	ARG	2.1
1	F	695	CYS	2.1
1	B	268	ASP	2.1
1	C	732	PHE	2.1
1	D	716	PHE	2.1
1	F	693	VAL	2.1
1	F	428	GLY	2.1
1	F	555	GLY	2.1
1	C	362	LYS	2.1
1	C	542	PHE	2.1
1	D	720	VAL	2.1
1	C	604	GLY	2.1
1	D	426	GLY	2.1
1	E	703	GLY	2.1
1	F	614	ARG	2.1
1	C	268	ASP	2.1
1	F	339	ASP	2.1
1	E	99	SER	2.1
1	D	507	PRO	2.1
1	C	687	GLN	2.0
1	F	755	GLN	2.0
1	A	487	VAL	2.0
1	C	634	VAL	2.0
1	D	789	VAL	2.0
1	F	700	ALA	2.0
1	C	737	VAL	2.0
1	A	700	ALA	2.0
1	B	700	ALA	2.0
1	C	338	LEU	2.0
1	C	721	GLU	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	F	802	5/5	0.49	0.19	81,88,91,99	5
2	PO4	F	803	5/5	0.54	0.12	101,106,112,123	0
3	GOL	D	808	6/6	0.55	0.15	74,76,77,78	0
3	GOL	E	809	6/6	0.55	0.15	83,86,90,92	0
2	PO4	A	802	5/5	0.60	0.17	51,54,71,83	5
3	GOL	F	806	6/6	0.63	0.20	60,74,78,79	0
2	PO4	E	805	5/5	0.64	0.26	69,78,91,104	0
2	PO4	C	804	5/5	0.64	0.20	90,91,103,104	0
3	GOL	C	809	6/6	0.65	0.16	76,84,87,93	0
2	PO4	A	803	5/5	0.66	0.18	75,89,103,103	0
2	PO4	C	806	5/5	0.66	0.23	80,91,98,103	0
2	PO4	C	802	5/5	0.66	0.23	79,81,103,104	0
3	GOL	C	811	6/6	0.68	0.15	69,75,79,79	0
2	PO4	E	802	5/5	0.69	0.27	49,61,86,90	0
2	PO4	E	804	5/5	0.69	0.20	91,92,97,108	0
3	GOL	C	812	6/6	0.71	0.17	57,61,64,66	0
3	GOL	A	807	6/6	0.71	0.14	63,72,76,78	0
2	PO4	B	803	5/5	0.73	0.24	74,78,84,95	0
3	GOL	F	809	6/6	0.74	0.16	53,66,72,72	0
2	PO4	B	802	5/5	0.75	0.27	75,77,82,91	0
3	GOL	E	808	6/6	0.76	0.19	43,47,53,54	0
3	GOL	C	807	6/6	0.76	0.19	61,65,69,72	0
3	GOL	E	810	6/6	0.76	0.12	58,65,67,70	0
3	GOL	C	808	6/6	0.76	0.15	57,73,79,79	0
3	GOL	B	808	6/6	0.76	0.15	49,58,62,63	0
3	GOL	A	806	6/6	0.77	0.18	54,57,58,71	0
2	PO4	C	805	5/5	0.77	0.21	72,74,93,93	0
2	PO4	F	801	5/5	0.78	0.26	76,79,83,86	0
3	GOL	D	806	6/6	0.79	0.18	44,51,53,59	0
3	GOL	B	810	6/6	0.79	0.16	53,59,64,65	0
3	GOL	D	809	6/6	0.79	0.10	69,74,77,79	0
3	GOL	B	809	6/6	0.79	0.21	51,57,62,63	0
3	GOL	F	805	6/6	0.80	0.16	47,49,54,56	0
3	GOL	C	810	6/6	0.81	0.13	66,68,72,74	0
3	GOL	B	806	6/6	0.81	0.17	59,66,68,76	0
3	GOL	A	804	6/6	0.82	0.17	33,38,41,49	0
3	GOL	E	807	6/6	0.82	0.16	41,44,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	D	802	5/5	0.82	0.18	49,72,86,96	0
3	GOL	F	807	6/6	0.82	0.11	53,63,66,67	0
3	GOL	F	808	6/6	0.82	0.16	46,57,63,67	0
2	PO4	D	803	5/5	0.82	0.22	34,40,57,77	0
2	PO4	D	804	5/5	0.83	0.17	37,40,48,51	5
3	GOL	B	811	6/6	0.83	0.13	57,59,61,62	0
2	PO4	C	803	5/5	0.84	0.17	41,46,55,62	5
3	GOL	F	810	6/6	0.84	0.11	59,68,70,70	0
3	GOL	B	807	6/6	0.85	0.16	47,50,52,54	0
3	GOL	D	807	6/6	0.85	0.15	53,55,63,63	0
3	GOL	E	811	6/6	0.85	0.14	50,59,66,66	0
2	PO4	B	801	5/5	0.86	0.21	63,64,92,97	0
3	GOL	A	805	6/6	0.87	0.10	44,51,53,57	0
2	PO4	E	806	5/5	0.87	0.23	64,69,74,79	0
3	GOL	F	804	6/6	0.87	0.13	41,50,56,63	0
2	PO4	B	804	5/5	0.88	0.18	61,61,67,71	0
3	GOL	D	805	6/6	0.88	0.14	50,52,53,59	0
2	PO4	E	801	5/5	0.88	0.14	44,44,46,53	5
2	PO4	E	803	5/5	0.89	0.21	64,74,81,85	0
3	GOL	B	805	6/6	0.90	0.14	40,45,51,53	0
2	PO4	C	801	5/5	0.91	0.14	46,57,67,70	0
2	PO4	A	801	5/5	0.92	0.10	35,40,45,52	5
2	PO4	D	801	5/5	0.92	0.18	46,56,69,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.