



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2025 – 01:58 PM EST

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	:	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

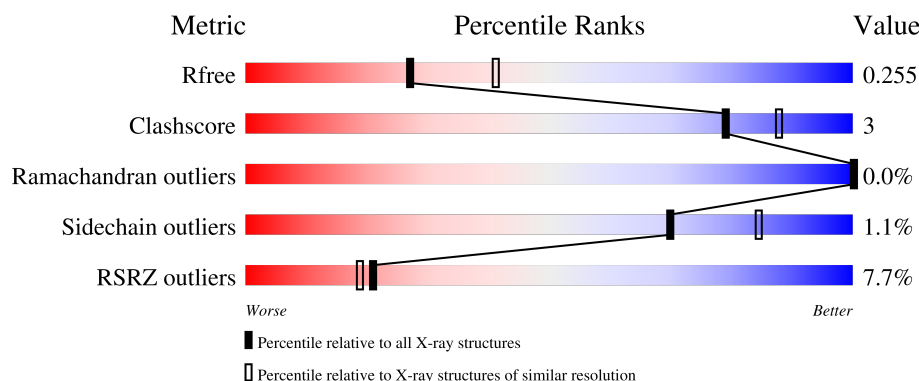
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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	<div> <div>2%</div> <div>84% 7% 8%</div> </div>
1	B	798	<div> <div>2%</div> <div>85% 5% 9%</div> </div>
1	C	798	<div> <div>16%</div> <div>79% 10% 10%</div> </div>
1	D	798	<div> <div>4%</div> <div>87% 5% 8%</div> </div>
1	E	798	<div> <div>2%</div> <div>85% 6% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	798	<div><div></div><div>15%</div><div>82%</div><div>9%</div><div>9%</div></div>

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).



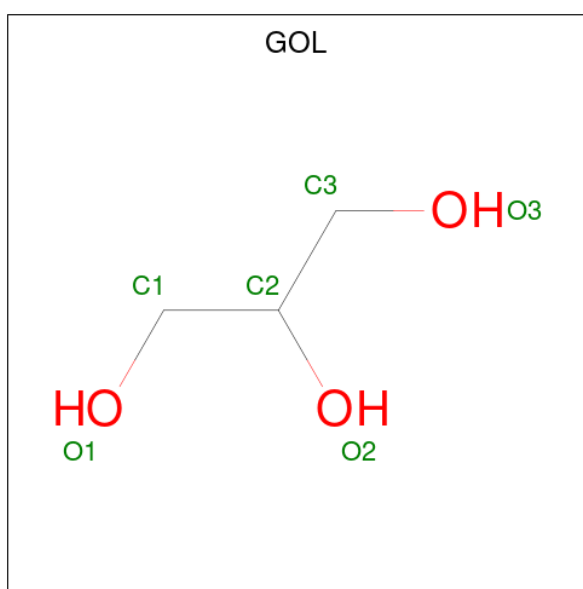
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	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		
2	D	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	E	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	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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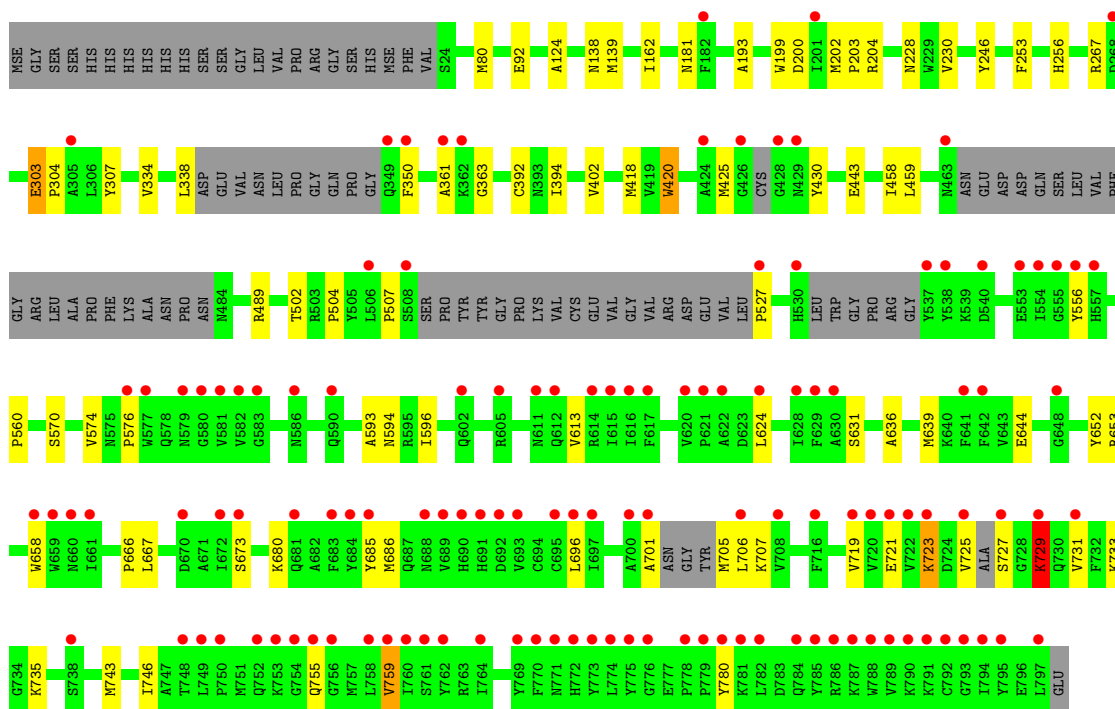
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

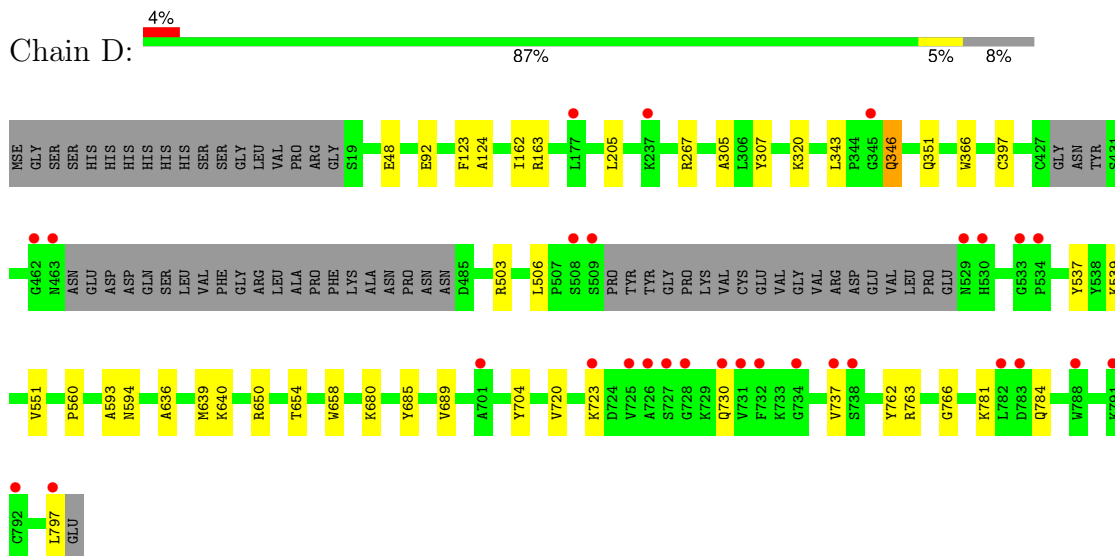
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	435	Total	O	0	0
			435	435		
4	B	407	Total	O	0	0
			407	407		
4	C	229	Total	O	0	0
			229	229		
4	D	419	Total	O	0	0
			419	419		
4	E	449	Total	O	0	0
			449	449		
4	F	265	Total	O	0	0
			265	265		

- Molecule 1: Glycoside hydrolase family 2

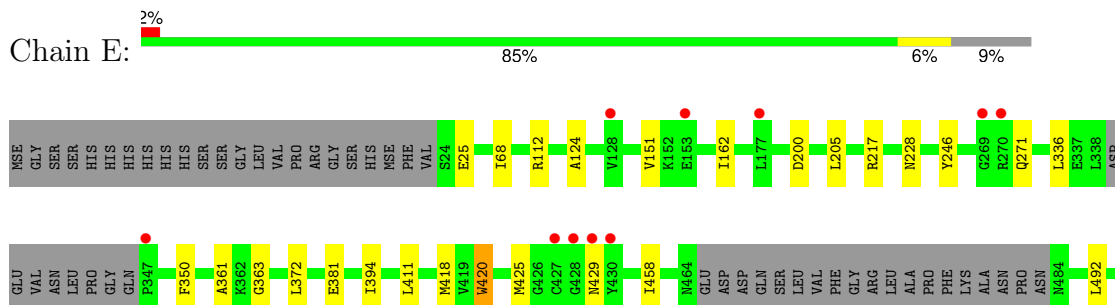




- Molecule 1: Glycoside hydrolase family 2

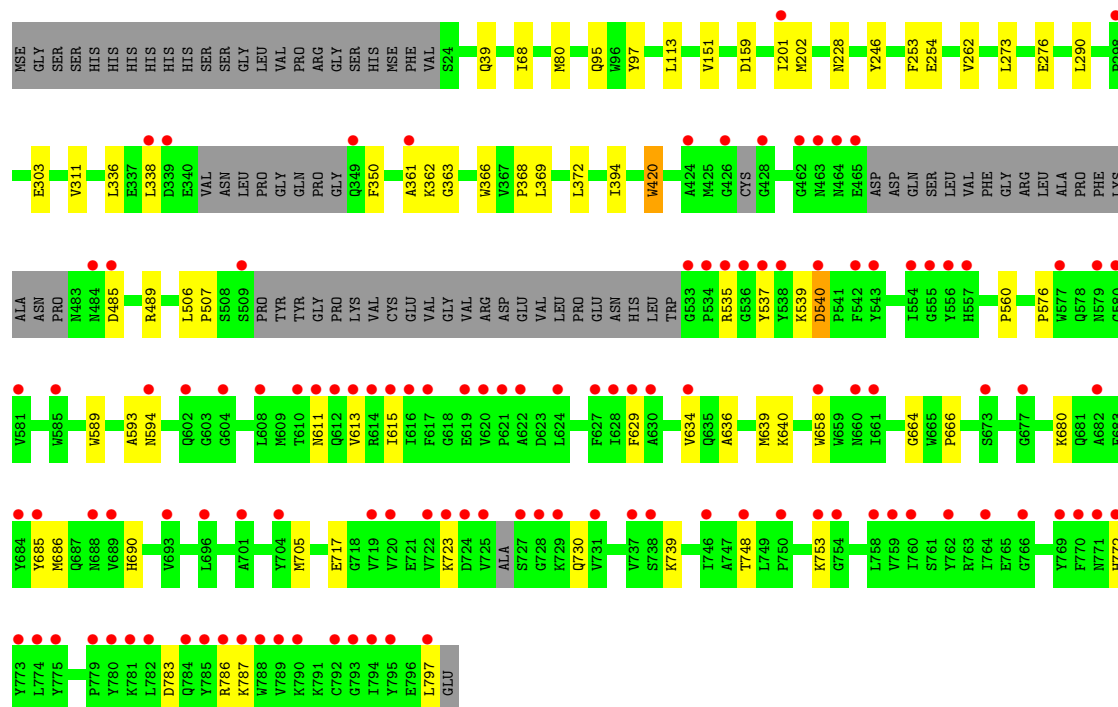
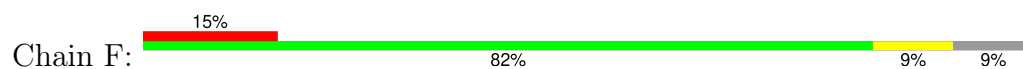


- Molecule 1: Glycoside hydrolase family 2





● 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	65
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%)	65	81
1	B	626/666 (94%)	622 (99%)	4 (1%)	84	92
1	C	620/666 (93%)	612 (99%)	8 (1%)	65	81
1	D	636/666 (96%)	630 (99%)	6 (1%)	75	88
1	E	625/666 (94%)	616 (99%)	9 (1%)	62	79
1	F	626/666 (94%)	618 (99%)	8 (1%)	65	81
All	All	3768/3996 (94%)	3725 (99%)	43 (1%)	70	84

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	$\# Z > 2$
3	GOL	C	811	-	5,5,5	0.33	0	5,5,5	0.39	0
3	GOL	F	807	-	5,5,5	0.31	0	5,5,5	0.42	0
2	PO4	A	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.51	0
2	PO4	C	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	GOL	B	806	-	5,5,5	0.34	0	5,5,5	0.39	0
3	GOL	B	809	-	5,5,5	0.30	0	5,5,5	0.37	0
3	GOL	E	809	-	5,5,5	0.34	0	5,5,5	0.44	0
3	GOL	F	806	-	5,5,5	0.33	0	5,5,5	0.38	0
2	PO4	F	803	-	4,4,4	1.57	1 (25%)	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	804	-	5,5,5	0.36	0	5,5,5	0.48	0
2	PO4	E	804	-	4,4,4	1.61	1 (25%)	6,6,6	0.47	0
3	GOL	C	807	-	5,5,5	0.34	0	5,5,5	0.37	0
2	PO4	D	801	-	4,4,4	1.60	1 (25%)	6,6,6	0.53	0
2	PO4	E	806	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	GOL	C	812	-	5,5,5	0.34	0	5,5,5	0.38	0
2	PO4	C	805	-	4,4,4	1.62	1 (25%)	6,6,6	0.45	0
2	PO4	A	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.44	0
3	GOL	A	807	-	5,5,5	0.32	0	5,5,5	0.34	0
3	GOL	E	811	-	5,5,5	0.36	0	5,5,5	0.47	0
2	PO4	C	803	-	4,4,4	1.55	1 (25%)	6,6,6	0.54	0
2	PO4	D	802	-	4,4,4	1.56	1 (25%)	6,6,6	0.48	0
3	GOL	F	810	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	B	807	-	5,5,5	0.37	0	5,5,5	0.51	0
2	PO4	D	803	-	4,4,4	1.67	1 (25%)	6,6,6	0.50	0
3	GOL	C	808	-	5,5,5	0.34	0	5,5,5	0.41	0
2	PO4	E	801	-	4,4,4	1.55	1 (25%)	6,6,6	0.47	0
2	PO4	C	806	-	4,4,4	1.58	1 (25%)	6,6,6	0.47	0
3	GOL	F	808	-	5,5,5	0.32	0	5,5,5	0.35	0
3	GOL	D	805	-	5,5,5	0.33	0	5,5,5	0.41	0
3	GOL	D	807	-	5,5,5	0.33	0	5,5,5	0.44	0
3	GOL	A	806	-	5,5,5	0.34	0	5,5,5	0.37	0
2	PO4	A	803	-	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	0.51	0
3	GOL	F	809	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	C	810	-	5,5,5	0.33	0	5,5,5	0.42	0
2	PO4	C	804	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
2	PO4	B	801	-	4,4,4	1.61	1 (25%)	6,6,6	0.46	0
2	PO4	F	801	-	4,4,4	1.59	1 (25%)	6,6,6	0.47	0
2	PO4	E	803	-	4,4,4	1.56	1 (25%)	6,6,6	0.49	0
3	GOL	A	804	-	5,5,5	0.33	0	5,5,5	0.33	0
2	PO4	B	804	-	4,4,4	1.55	1 (25%)	6,6,6	0.68	0
2	PO4	B	803	-	4,4,4	1.57	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	D	806	-	5,5,5	0.35	0	5,5,5	0.39	0
2	PO4	E	802	-	4,4,4	1.62	1 (25%)	6,6,6	0.50	0
3	GOL	E	808	-	5,5,5	0.32	0	5,5,5	0.49	0
3	GOL	B	811	-	5,5,5	0.35	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	802	-	4,4,4	1.60	1 (25%)	6,6,6	0.50	0
3	GOL	D	809	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	C	809	-	5,5,5	0.35	0	5,5,5	0.36	0
3	GOL	B	805	-	5,5,5	0.33	0	5,5,5	0.37	0
3	GOL	B	808	-	5,5,5	0.33	0	5,5,5	0.43	0
3	GOL	B	810	-	5,5,5	0.35	0	5,5,5	0.36	0
2	PO4	C	801	-	4,4,4	1.57	1 (25%)	6,6,6	0.51	0
3	GOL	E	807	-	5,5,5	0.32	0	5,5,5	0.46	0
2	PO4	F	802	-	4,4,4	1.58	1 (25%)	6,6,6	0.47	0
3	GOL	E	810	-	5,5,5	0.34	0	5,5,5	0.40	0
2	PO4	D	804	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	0
3	GOL	D	808	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	F	805	-	5,5,5	0.31	0	5,5,5	0.37	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	C	811	-	-	0/4/4/4	-
3	GOL	F	807	-	-	0/4/4/4	-
3	GOL	B	806	-	-	0/4/4/4	-
3	GOL	B	809	-	-	2/4/4/4	-
3	GOL	E	809	-	-	0/4/4/4	-
3	GOL	F	806	-	-	2/4/4/4	-
3	GOL	F	804	-	-	2/4/4/4	-
3	GOL	C	807	-	-	3/4/4/4	-
3	GOL	E	811	-	-	2/4/4/4	-
3	GOL	C	812	-	-	0/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	F	810	-	-	2/4/4/4	-
3	GOL	B	807	-	-	0/4/4/4	-
3	GOL	C	808	-	-	0/4/4/4	-
3	GOL	F	808	-	-	2/4/4/4	-
3	GOL	D	805	-	-	0/4/4/4	-
3	GOL	D	807	-	-	0/4/4/4	-
3	GOL	A	806	-	-	2/4/4/4	-
3	GOL	F	809	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	810	-	-	2/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	D	806	-	-	2/4/4/4	-
3	GOL	A	805	-	-	2/4/4/4	-
3	GOL	E	808	-	-	2/4/4/4	-
3	GOL	B	811	-	-	2/4/4/4	-
3	GOL	D	809	-	-	4/4/4/4	-
3	GOL	C	809	-	-	1/4/4/4	-
3	GOL	B	805	-	-	0/4/4/4	-
3	GOL	B	808	-	-	0/4/4/4	-
3	GOL	B	810	-	-	0/4/4/4	-
3	GOL	E	807	-	-	0/4/4/4	-
3	GOL	E	810	-	-	0/4/4/4	-
3	GOL	D	808	-	-	0/4/4/4	-
3	GOL	F	805	-	-	0/4/4/4	-

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%)	-0.03	19 (2%) 56 53	27, 41, 75, 86	0
1	B	705/798 (88%)	0.12	18 (2%) 57 54	29, 43, 66, 87	0
1	C	694/798 (86%)	0.90	127 (18%) 4 4	35, 60, 110, 121	0
1	D	714/798 (89%)	0.02	29 (4%) 42 39	27, 41, 75, 88	0
1	E	704/798 (88%)	0.05	16 (2%) 61 58	27, 40, 63, 84	0
1	F	703/798 (88%)	0.79	116 (16%) 5 5	34, 54, 106, 127	0
All	All	4233/4788 (88%)	0.31	325 (7%) 21 19	27, 46, 90, 127	0

All (325) 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	4.5
1	C	789	VAL	4.4
1	C	630	ALA	4.4
1	C	793	GLY	4.4
1	F	770	PHE	4.3
1	F	793	GLY	4.3
1	C	782	LEU	4.3
1	C	685	TYR	4.1
1	C	795	TYR	4.1
1	C	527	PRO	4.1
1	F	629	PHE	4.1
1	F	758	LEU	4.1
1	C	788	TRP	4.0
1	C	758	LEU	4.0
1	F	797	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	509	SER	4.0
1	F	612	GLN	4.0
1	F	788	TRP	3.9
1	C	463	ASN	3.9
1	F	611	ASN	3.9
1	C	629	PHE	3.9
1	F	620	VAL	3.9
1	D	533	GLY	3.9
1	F	536	GLY	3.9
1	F	782	LEU	3.9
1	C	754	GLY	3.9
1	E	427	CYS	3.8
1	C	612	GLN	3.8
1	C	785	TYR	3.8
1	C	781	LYS	3.8
1	C	581	VAL	3.7
1	C	794	ILE	3.7
1	C	769	TYR	3.7
1	F	628	ILE	3.7
1	F	795	TYR	3.7
1	C	774	LEU	3.7
1	F	617	PHE	3.7
1	F	538	TYR	3.7
1	A	529	ASN	3.6
1	C	779	PRO	3.6
1	C	760	ILE	3.6
1	E	347	PRO	3.6
1	C	426	GLY	3.6
1	D	725	VAL	3.6
1	F	785	TYR	3.6
1	C	615	ILE	3.6
1	D	728	GLY	3.6
1	C	780	TYR	3.6
1	D	797	LEU	3.5
1	B	427	CYS	3.5
1	F	426	GLY	3.5
1	F	725	VAL	3.5
1	F	764	ILE	3.5
1	F	753	LYS	3.5
1	C	727	SER	3.5
1	C	759	VAL	3.5
1	F	630	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	770	PHE	3.5
1	F	787	LYS	3.5
1	C	771	ASN	3.4
1	A	509	SER	3.4
1	C	538	TYR	3.4
1	C	621	PRO	3.4
1	F	722	VAL	3.4
1	C	762	TYR	3.4
1	D	529	ASN	3.4
1	C	616	ILE	3.4
1	C	738	SER	3.4
1	F	556	TYR	3.4
1	F	780	TYR	3.4
1	E	533	GLY	3.4
1	F	581	VAL	3.3
1	F	688	ASN	3.3
1	D	177	LEU	3.3
1	C	693	VAL	3.3
1	F	789	VAL	3.3
1	F	685	TYR	3.3
1	C	797	LEU	3.2
1	D	726	ALA	3.2
1	E	270	ARG	3.2
1	C	725	VAL	3.2
1	F	759	VAL	3.2
1	F	781	LYS	3.2
1	A	797	LEU	3.1
1	D	463	ASN	3.1
1	F	723	LYS	3.1
1	C	624	LEU	3.1
1	D	731	VAL	3.1
1	B	530	HIS	3.1
1	F	784	GLN	3.1
1	C	554	ILE	3.1
1	F	728	GLY	3.1
1	F	754	GLY	3.1
1	F	463	ASN	3.1
1	C	791	LYS	3.1
1	F	298	PRO	3.1
1	F	769	TYR	3.1
1	F	627	PHE	3.0
1	F	677	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	557	HIS	3.0
1	E	530	HIS	3.0
1	F	535	ARG	3.0
1	F	724	ASP	3.0
1	B	529	ASN	3.0
1	F	771	ASN	3.0
1	A	345	GLY	3.0
1	A	731	VAL	3.0
1	F	424	ALA	3.0
1	C	764	ILE	3.0
1	F	533	GLY	3.0
1	C	689	VAL	3.0
1	F	557	HIS	3.0
1	C	792	CYS	2.9
1	B	269	GLY	2.9
1	D	783	ASP	2.9
1	C	784	GLN	2.9
1	C	556	TYR	2.9
1	F	790	LYS	2.9
1	C	428	GLY	2.9
1	F	661	ILE	2.9
1	F	689	VAL	2.9
1	F	464	ASN	2.9
1	F	774	LEU	2.9
1	F	792	CYS	2.9
1	F	748	THR	2.9
1	F	615	ILE	2.9
1	F	462	GLY	2.9
1	F	779	PRO	2.9
1	F	604	GLY	2.8
1	C	673	SER	2.8
1	A	726	ALA	2.8
1	D	530	HIS	2.8
1	D	701	ALA	2.8
1	C	530	HIS	2.8
1	C	690	HIS	2.8
1	D	738	SER	2.8
1	E	428	GLY	2.8
1	F	534	PRO	2.8
1	A	508	SER	2.8
1	C	723	LYS	2.8
1	E	430	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	773	TYR	2.8
1	A	728	GLY	2.7
1	C	350	PHE	2.7
1	C	537	TYR	2.7
1	F	537	TYR	2.7
1	F	543	TYR	2.7
1	C	424	ALA	2.7
1	C	700	ALA	2.7
1	E	429	ASN	2.7
1	F	621	PRO	2.7
1	C	790	LYS	2.7
1	B	177	LEU	2.7
1	C	692	ASP	2.7
1	C	579	ASN	2.7
1	F	660	ASN	2.7
1	C	661	ILE	2.7
1	F	580	GLY	2.7
1	A	430	TYR	2.7
1	C	361	ALA	2.7
1	C	775	TYR	2.7
1	F	786	ARG	2.7
1	F	737	VAL	2.6
1	C	691	HIS	2.6
1	F	794	ILE	2.6
1	C	605	ARG	2.6
1	C	696	LEU	2.6
1	C	720	VAL	2.6
1	C	787	LYS	2.6
1	B	702	ASN	2.6
1	B	428	GLY	2.6
1	C	617	PHE	2.6
1	C	614	ARG	2.6
1	F	624	LEU	2.6
1	C	778	PRO	2.6
1	F	594	ASN	2.6
1	B	462	GLY	2.6
1	D	462	GLY	2.6
1	C	641	PHE	2.6
1	F	696	LEU	2.6
1	D	508	SER	2.6
1	C	697	ILE	2.6
1	C	642	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	729	LYS	2.5
1	C	305	ALA	2.5
1	C	576	PRO	2.5
1	F	762	TYR	2.5
1	C	776	GLY	2.5
1	D	792	CYS	2.5
1	B	270	ARG	2.5
1	C	786	ARG	2.5
1	C	729	LYS	2.5
1	C	753	LYS	2.5
1	F	772	HIS	2.5
1	C	659	TRP	2.5
1	C	731	VAL	2.5
1	F	361	ALA	2.5
1	F	616	ILE	2.5
1	C	611	ASN	2.5
1	F	585	TRP	2.5
1	A	488	SER	2.5
1	C	540	ASP	2.5
1	F	608	LEU	2.4
1	C	695	CYS	2.4
1	D	737	VAL	2.4
1	F	760	ILE	2.4
1	B	426	GLY	2.4
1	B	429	ASN	2.4
1	F	484	ASN	2.4
1	F	579	ASN	2.4
1	C	773	TYR	2.4
1	C	708	VAL	2.4
1	F	613	VAL	2.4
1	F	465	GLU	2.4
1	F	577	TRP	2.4
1	F	738	SER	2.4
1	C	756	GLY	2.4
1	D	345	GLY	2.4
1	C	506	LEU	2.4
1	C	772	HIS	2.4
1	F	684	TYR	2.4
1	F	720	VAL	2.4
1	C	658	TRP	2.4
1	C	583	GLY	2.4
1	B	430	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	775	TYR	2.4
1	F	634	VAL	2.4
1	C	681	GLN	2.4
1	F	727	SER	2.4
1	B	533	GLY	2.4
1	F	542	PHE	2.3
1	A	719	VAL	2.3
1	C	582	VAL	2.3
1	B	271	GLN	2.3
1	C	602	GLN	2.3
1	C	628	ILE	2.3
1	C	580	GLY	2.3
1	D	782	LEU	2.3
1	F	338	LEU	2.3
1	A	791	LYS	2.3
1	C	553	GLU	2.3
1	F	619	GLU	2.3
1	A	532	TRP	2.3
1	D	732	PHE	2.3
1	D	723	LYS	2.3
1	C	719	VAL	2.3
1	C	201	ILE	2.3
1	C	622	ALA	2.3
1	F	509	SER	2.3
1	C	182	PHE	2.3
1	D	788	TRP	2.3
1	D	730	GLN	2.3
1	A	720	VAL	2.3
1	C	555	GLY	2.2
1	D	734	GLY	2.2
1	C	748	THR	2.2
1	C	716	PHE	2.2
1	F	540	ASP	2.2
1	B	710	ASN	2.2
1	C	586	ASN	2.2
1	C	752	GLN	2.2
1	F	554	ILE	2.2
1	E	177	LEU	2.2
1	D	791	LYS	2.2
1	D	727	SER	2.2
1	F	485	ASP	2.2
1	C	688	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	201	ILE	2.2
1	C	749	LEU	2.2
1	F	610	THR	2.2
1	A	485	ASP	2.2
1	A	534	PRO	2.2
1	C	670	ASP	2.2
1	F	750	PRO	2.2
1	F	731	VAL	2.2
1	F	701	ALA	2.2
1	B	698	ASN	2.2
1	C	660	ASN	2.2
1	C	577	TRP	2.2
1	C	672	ILE	2.2
1	A	725	VAL	2.2
1	F	682	ALA	2.2
1	C	684	TYR	2.1
1	E	269	GLY	2.1
1	F	766	GLY	2.1
1	A	792	CYS	2.1
1	C	508	SER	2.1
1	E	153	GLU	2.1
1	F	719	VAL	2.1
1	E	701	ALA	2.1
1	F	622	ALA	2.1
1	B	112	ARG	2.1
1	C	761	SER	2.1
1	D	534	PRO	2.1
1	C	590	GLN	2.1
1	F	349	GLN	2.1
1	F	602	GLN	2.1
1	C	429	ASN	2.1
1	D	237	LYS	2.1
1	E	746	ILE	2.1
1	E	128	VAL	2.1
1	F	704	TYR	2.1
1	C	750	PRO	2.1
1	E	699	PRO	2.1
1	C	349	GLN	2.1
1	B	268	ASP	2.1
1	A	701	ALA	2.1
1	F	614	ARG	2.1
1	C	648	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	362	LYS	2.1
1	E	747	ALA	2.0
1	F	658	TRP	2.0
1	C	683	PHE	2.0
1	F	746	ILE	2.0
1	C	268	ASP	2.0
1	F	339	ASP	2.0
1	C	706	LEU	2.0
1	F	693	VAL	2.0
1	F	428	GLY	2.0
1	F	555	GLY	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 [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(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

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

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