



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 08:02 AM JST

PDB ID : 7FCA
Title : PfkB(Mycobacterium marinum)
Authors : Li, J.; Gao, B.; Ji, R.
Deposited on : 2021-07-14
Resolution : 2.21 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

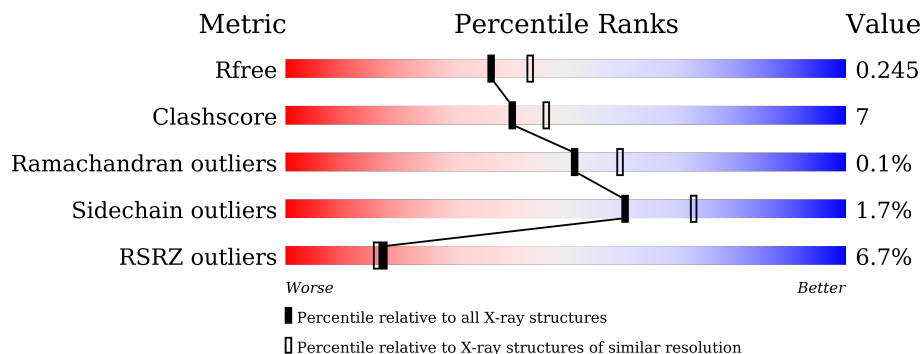
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	303	
1	B	303	
1	C	303	
1	E	303	
1	F	303	
2	D	291	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	401	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11955 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 Fructokinase, PfkB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	1991	1253	355	378	5	0	0	0
1	B	272	1937	1218	341	374	4	0	0	0
1	C	273	1929	1212	344	369	4	0	0	0
1	E	278	1966	1236	349	377	4	0	0	0
1	F	270	1905	1200	341	360	4	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	THR	ALA	conflict	UNP B2HEF4
B	108	THR	ALA	conflict	UNP B2HEF4
C	108	THR	ALA	conflict	UNP B2HEF4
E	108	THR	ALA	conflict	UNP B2HEF4
F	108	THR	ALA	conflict	UNP B2HEF4

- Molecule 2 is a protein called Fructokinase, PfkB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	282	2011	1264	359	384	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

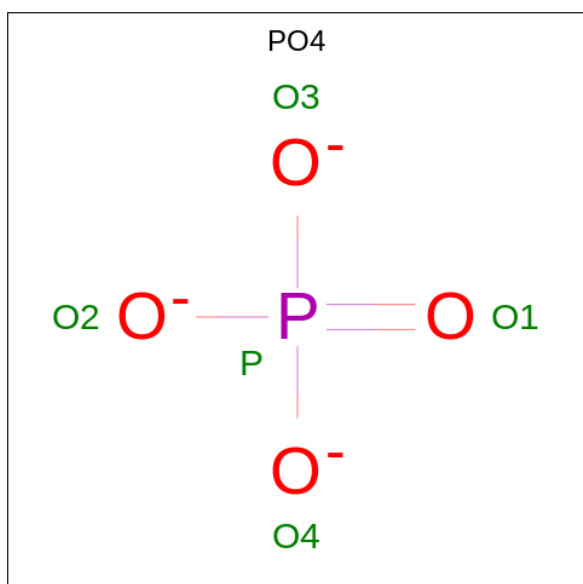
Chain	Residue	Modelled	Actual	Comment	Reference
D	161	ARG	GLU	conflict	UNP B2HEF4

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

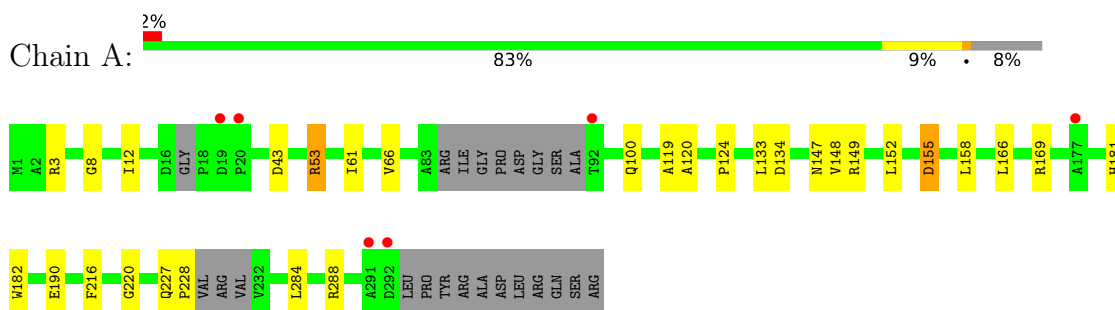
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	23	Total	O	0	0
			23	23		
5	C	17	Total	O	0	0
			17	17		
5	D	40	Total	O	0	0
			40	40		
5	E	18	Total	O	0	0
			18	18		
5	F	14	Total	O	0	0
			14	14		

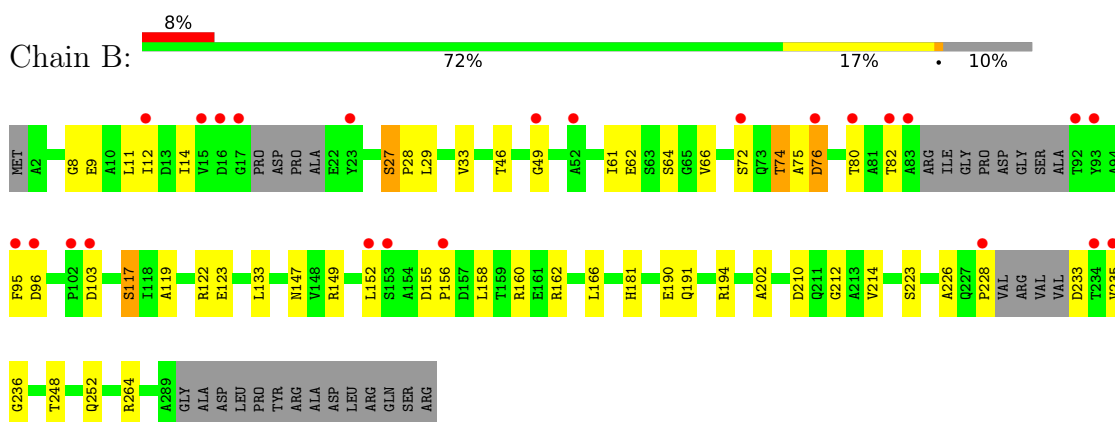
3 Residue-property plots [i](#)

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.

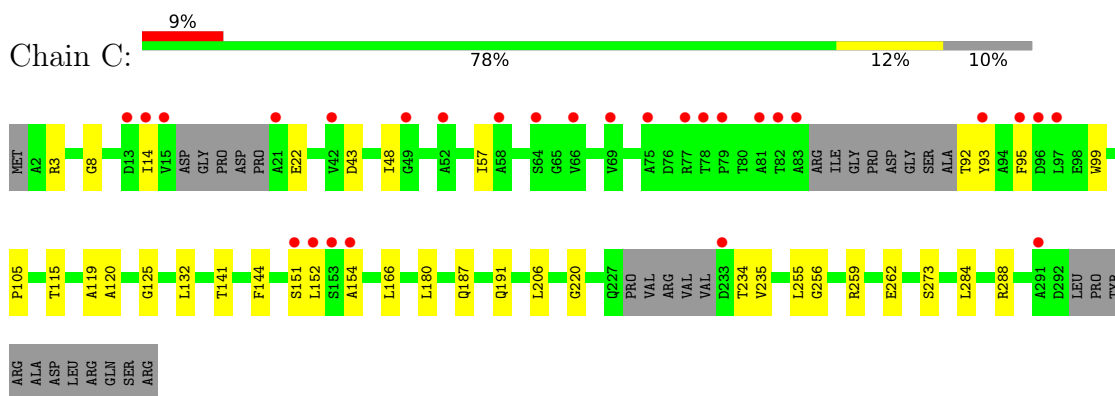
- Molecule 1: Fructokinase, PfkB



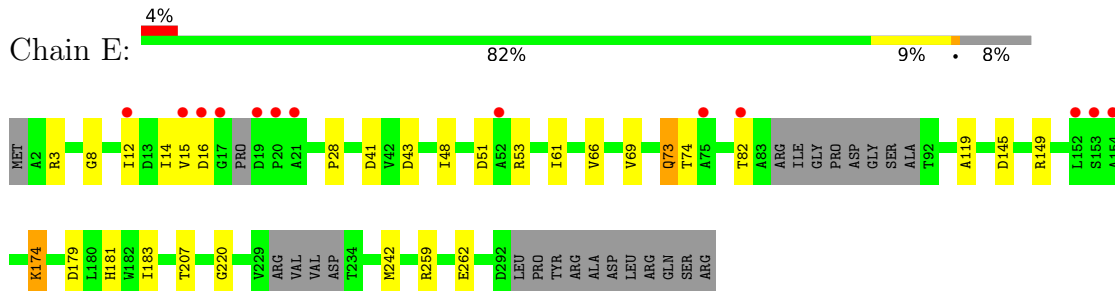
- Molecule 1: Fructokinase, PfkB



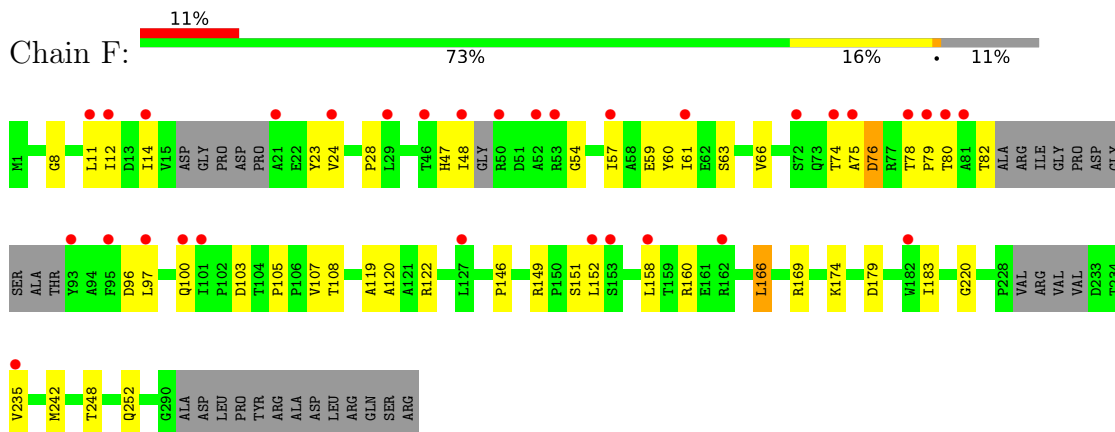
- Molecule 1: Fructokinase, PfkB



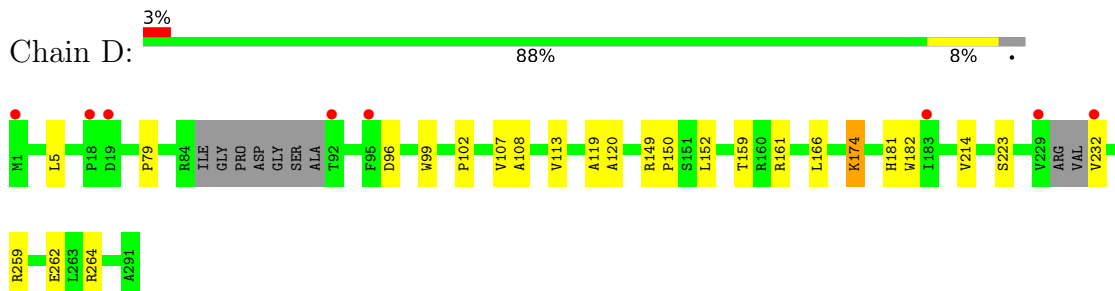
• Molecule 1: Fructokinase, PfkB



• Molecule 1: Fructokinase, PfkB



• Molecule 2: Fructokinase, PfkB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.41Å 125.41Å 137.52Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	66.92 – 2.21 66.92 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.8 (66.92-2.21) 99.8 (66.92-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.212 , 0.245 0.212 , 0.245	Depositor DCC
R_{free} test set	5123 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11955	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0880e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.52	0/2025	0.64	0/2774
1	B	0.52	0/1969	0.65	1/2699 (0.0%)
1	C	0.39	0/1960	0.56	0/2686
1	E	0.39	0/1999	0.57	0/2742
1	F	0.43	0/1935	0.59	0/2652
2	D	0.48	0/2046	0.62	1/2805 (0.0%)
All	All	0.46	0/11934	0.61	2/16358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	PRO	N-CA-CB	5.84	110.31	103.30
1	B	228	PRO	N-CA-CB	5.67	110.11	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts i

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	1991	0	1969	31	0
1	B	1937	0	1888	43	0
1	C	1929	0	1900	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1966	0	1935	23	0
1	F	1905	0	1878	39	0
2	D	2011	0	1993	19	0
3	A	6	0	8	1	0
3	B	12	0	16	5	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	49	0	0	1	0
5	B	23	0	0	1	0
5	C	17	0	0	0	0
5	D	40	0	0	1	0
5	E	18	0	0	1	0
5	F	14	0	0	0	0
All	All	11955	0	11603	168	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 7.

All (168) 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:B:233:ASP:OD2	1:B:236:GLY:HA3	1.38	1.19
1:A:284:LEU:HD21	1:A:288:ARG:NH1	1.66	1.09
1:A:284:LEU:HD21	1:A:288:ARG:HH11	1.18	1.00
1:F:160:ARG:HG3	1:F:160:ARG:HH11	1.39	0.88
1:B:12:ILE:CD1	3:B:401:GOL:H12	2.04	0.87
1:E:12:ILE:HD13	1:E:53:ARG:HB3	1.59	0.84
1:B:12:ILE:HD11	3:B:401:GOL:H12	1.59	0.83
1:E:12:ILE:CD1	1:E:53:ARG:HB3	2.11	0.81
1:B:149:ARG:NH1	1:B:235:VAL:HG21	1.97	0.78
1:B:235:VAL:HG12	5:B:521:HOH:O	1.84	0.78
1:F:47:HIS:HD2	1:F:100:GLN:H	1.28	0.78
1:B:12:ILE:HD13	3:B:401:GOL:H32	1.68	0.75
1:E:12:ILE:HD13	1:E:53:ARG:HD2	1.69	0.75
1:B:76:ASP:OD1	1:B:76:ASP:N	2.09	0.74
1:F:48:ILE:HD11	1:F:57:ILE:HB	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:CD2	1:A:288:ARG:HH11	2.01	0.72
1:F:76:ASP:OD1	1:F:76:ASP:N	2.18	0.70
1:F:160:ARG:HG3	1:F:160:ARG:NH1	2.04	0.69
1:F:122:ARG:HD2	1:F:152:LEU:HD11	1.74	0.69
1:A:155:ASP:HB3	2:D:161:ARG:HG2	1.74	0.68
1:F:149:ARG:NH2	1:F:235:VAL:HG11	2.08	0.68
1:F:149:ARG:HH22	1:F:235:VAL:HG11	1.60	0.66
1:F:152:LEU:HD23	1:F:152:LEU:O	1.96	0.66
1:C:14:ILE:HG23	1:C:22:GLU:HG2	1.79	0.65
2:D:264:ARG:HH12	3:D:301:GOL:H11	1.62	0.65
1:A:149:ARG:O	1:A:152:LEU:HB3	1.97	0.65
1:B:12:ILE:CD1	3:B:401:GOL:H32	2.26	0.65
1:B:12:ILE:HD13	3:B:401:GOL:H12	1.79	0.65
1:B:133:LEU:HD12	1:B:166:LEU:HD22	1.80	0.62
1:A:12:ILE:HG13	1:A:53:ARG:HB3	1.81	0.62
1:A:181:HIS:CD2	1:C:220:GLY:HA2	2.35	0.62
1:F:80:THR:OG1	1:F:96:ASP:HB3	2.00	0.61
1:F:14:ILE:HB	1:F:82:THR:HA	1.83	0.60
1:B:46:THR:H	1:B:72:SER:HB2	1.67	0.60
1:C:3:ARG:NH1	1:C:43:ASP:OD1	2.36	0.59
1:E:179:ASP:O	1:E:183:ILE:HG12	2.02	0.59
1:B:80:THR:HG22	1:B:96:ASP:HB3	1.84	0.58
1:A:155:ASP:OD2	1:A:155:ASP:N	2.31	0.58
1:A:227:GLN:OE1	1:A:228:PRO:HD2	2.04	0.58
1:B:61:ILE:HG23	1:B:66:VAL:HB	1.84	0.58
1:B:27:SER:OG	1:B:147:ASN:ND2	2.36	0.57
1:F:47:HIS:HD2	1:F:100:GLN:N	2.02	0.57
1:A:155:ASP:CB	2:D:161:ARG:HG2	2.36	0.56
1:B:62:GLU:OE2	1:B:62:GLU:HA	2.07	0.55
2:D:181:HIS:CD2	1:E:220:GLY:HA2	2.43	0.54
1:F:11:LEU:HD21	1:F:97:LEU:HD12	1.90	0.54
1:A:147:ASN:OD1	3:A:401:GOL:O1	2.26	0.54
1:C:180:LEU:HD22	1:C:206:LEU:HD13	1.90	0.54
1:B:149:ARG:HH12	1:B:235:VAL:HG11	1.72	0.54
1:C:48:ILE:HG21	1:C:57:ILE:HG21	1.89	0.54
1:A:149:ARG:O	1:A:152:LEU:N	2.41	0.53
1:B:190:GLU:O	1:B:194:ARG:HG3	2.08	0.53
1:E:181:HIS:CE1	1:F:220:GLY:HA2	2.45	0.52
1:E:8:GLY:HA2	1:E:119:ALA:CB	2.40	0.52
1:C:120:ALA:HB1	1:C:166:LEU:HD12	1.91	0.52
2:D:174:LYS:NZ	5:D:403:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLY:HA2	1:E:119:ALA:HB2	1.91	0.51
1:B:122:ARG:HD3	1:B:152:LEU:HD21	1.92	0.51
1:A:100:GLN:HE21	1:A:124:PRO:HG2	1.74	0.51
1:C:95:PHE:CB	1:C:152:LEU:HD23	2.41	0.51
1:B:155:ASP:HB3	1:B:158:LEU:HB2	1.93	0.50
1:A:61:ILE:HG23	1:A:66:VAL:HB	1.92	0.50
1:E:145:ASP:HB2	1:E:242:MET:HE2	1.93	0.50
1:B:29:LEU:C	1:B:29:LEU:HD23	2.32	0.50
1:B:27:SER:HB3	1:B:28:PRO:HD3	1.94	0.49
1:E:259:ARG:NH2	1:E:262:GLU:HG2	2.28	0.49
1:F:152:LEU:HD23	1:F:152:LEU:C	2.32	0.49
1:F:47:HIS:CE1	1:F:74:THR:HG23	2.48	0.48
1:A:220:GLY:HA2	1:B:181:HIS:CD2	2.48	0.48
1:A:158:LEU:HD13	2:D:159:THR:HG21	1.94	0.48
2:D:99:TRP:CZ2	2:D:119:ALA:HB1	2.49	0.48
2:D:264:ARG:HH22	3:D:301:GOL:H2	1.78	0.48
1:F:105:PRO:HB2	1:F:107:VAL:HG23	1.95	0.48
1:B:149:ARG:HH11	1:B:235:VAL:HG21	1.78	0.48
1:F:48:ILE:O	1:F:75:ALA:HB3	2.14	0.48
1:F:79:PRO:HB3	1:F:97:LEU:CB	2.43	0.48
1:C:92:THR:C	1:C:93:TYR:HD2	2.17	0.47
1:B:14:ILE:CB	1:B:82:THR:HG22	2.44	0.47
1:C:8:GLY:HA2	1:C:119:ALA:CB	2.43	0.47
1:F:24:VAL:HG11	1:F:60:TYR:CD2	2.49	0.47
1:A:149:ARG:O	1:A:152:LEU:CB	2.61	0.47
1:F:54:GLY:CA	1:F:78:THR:HG21	2.45	0.47
1:E:3:ARG:NH1	1:E:41:ASP:HB3	2.30	0.47
2:D:107:VAL:HG12	2:D:108:ALA:O	2.15	0.47
1:F:107:VAL:HG12	1:F:108:THR:O	2.15	0.47
1:A:190:GLU:HG3	1:A:216:PHE:CZ	2.50	0.47
1:F:12:ILE:HD12	1:F:23:TYR:O	2.15	0.47
1:B:9:GLU:O	1:B:9:GLU:HG2	2.14	0.46
1:C:141:THR:HG23	1:C:256:GLY:N	2.31	0.46
2:D:152:LEU:HD11	2:D:182:TRP:CD1	2.51	0.46
1:E:8:GLY:HA3	1:E:28:PRO:HG2	1.96	0.46
1:B:8:GLY:HA3	1:B:28:PRO:HG2	1.97	0.46
1:B:191:GLN:NE2	1:C:191:GLN:HE21	2.14	0.46
1:E:51:ASP:N	1:E:51:ASP:OD1	2.50	0.45
1:B:123:GLU:OE2	1:B:162:ARG:NH1	2.33	0.45
1:E:43:ASP:HB3	1:E:69:VAL:CG2	2.46	0.45
1:F:59:GLU:O	1:F:63:SER:OG	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CD2	1:B:152:LEU:HB2	2.52	0.45
1:B:49:GLY:N	1:B:75:ALA:HB3	2.31	0.45
1:F:12:ILE:HG22	1:F:80:THR:HA	1.99	0.45
1:A:155:ASP:OD1	2:D:161:ARG:HG2	2.16	0.45
1:B:214:VAL:HG12	1:B:223:SER:HB3	1.99	0.45
1:C:141:THR:HG21	1:C:255:LEU:HA	1.99	0.45
2:D:262:GLU:OE1	2:D:262:GLU:N	2.46	0.45
1:C:187:GLN:NE2	1:C:191:GLN:HG2	2.31	0.44
1:F:12:ILE:CG2	1:F:80:THR:HG22	2.47	0.44
1:B:74:THR:O	1:B:74:THR:OG1	2.35	0.44
1:E:74:THR:HG22	1:E:74:THR:O	2.16	0.44
1:E:14:ILE:HD12	1:E:82:THR:HG22	1.99	0.44
1:F:160:ARG:NH1	1:F:160:ARG:CG	2.76	0.44
1:C:259:ARG:HA	1:C:262:GLU:OE2	2.18	0.44
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.79	0.44
2:D:259:ARG:HH21	2:D:262:GLU:HG2	1.83	0.44
1:F:169:ARG:HH21	1:F:169:ARG:HG3	1.83	0.44
1:B:11:LEU:HD12	1:B:11:LEU:C	2.38	0.44
1:B:27:SER:CB	1:B:28:PRO:HD3	2.47	0.44
2:D:214:VAL:HG12	2:D:223:SER:HB3	2.00	0.43
1:F:79:PRO:HB3	1:F:97:LEU:HA	1.99	0.43
1:A:3:ARG:NH1	1:A:43:ASP:OD1	2.51	0.43
1:E:174:LYS:NZ	5:E:503:HOH:O	2.40	0.43
1:A:8:GLY:HA2	1:A:119:ALA:CB	2.48	0.43
1:A:133:LEU:HD12	1:A:166:LEU:HD22	2.01	0.43
1:C:93:TYR:O	1:C:151:SER:HB3	2.18	0.43
1:F:54:GLY:N	1:F:78:THR:HG21	2.33	0.43
1:F:61:ILE:HG23	1:F:66:VAL:HB	1.99	0.43
1:B:156:PRO:HB2	1:B:160:ARG:HH12	1.83	0.43
1:A:148:VAL:HG23	1:A:148:VAL:O	2.18	0.43
2:D:149:ARG:N	2:D:150:PRO:HD2	2.33	0.43
1:B:212:GLY:N	1:B:226:ALA:HB2	2.34	0.43
2:D:120:ALA:HB1	2:D:166:LEU:HD12	2.01	0.43
1:B:33:VAL:HG13	1:B:64:SER:CB	2.49	0.43
2:D:5:LEU:O	2:D:113:VAL:HA	2.19	0.43
1:B:191:GLN:NE2	1:C:187:GLN:OE1	2.51	0.43
1:A:100:GLN:NE2	1:A:124:PRO:HG2	2.34	0.42
1:A:149:ARG:O	1:A:152:LEU:HD23	2.19	0.42
1:A:152:LEU:HD13	1:A:182:TRP:CZ2	2.54	0.42
1:C:8:GLY:HA2	1:C:119:ALA:HB2	2.01	0.42
1:F:179:ASP:O	1:F:183:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLY:HA2	1:A:119:ALA:HB2	2.01	0.42
1:E:207:THR:HB	3:E:401:GOL:H31	2.01	0.42
1:F:248:THR:O	1:F:252:GLN:HG3	2.19	0.42
1:B:9:GLU:OE1	1:B:117:SER:HB3	2.20	0.42
1:E:15:VAL:HG12	1:E:16:ASP:N	2.35	0.42
1:A:120:ALA:HB1	1:A:166:LEU:HD12	2.02	0.41
1:A:134:ASP:OD2	1:A:169:ARG:NH2	2.53	0.41
2:D:120:ALA:HB1	2:D:166:LEU:CD1	2.50	0.41
1:F:146:PRO:HD2	1:F:174:LYS:O	2.20	0.41
1:A:100:GLN:NE2	1:A:100:GLN:HA	2.35	0.41
1:C:105:PRO:HA	1:C:132:LEU:HD21	2.01	0.41
1:F:79:PRO:HB3	1:F:97:LEU:HB2	2.02	0.41
1:A:53:ARG:HG3	5:A:535:HOH:O	2.19	0.41
1:B:8:GLY:HA2	1:B:119:ALA:HB2	2.02	0.41
1:E:14:ILE:HB	1:E:82:THR:HG22	2.01	0.41
1:E:61:ILE:HG23	1:E:66:VAL:HB	2.03	0.41
1:F:8:GLY:HA3	1:F:28:PRO:HG2	2.02	0.41
1:F:169:ARG:HH21	1:F:169:ARG:CG	2.34	0.41
1:E:149:ARG:HD3	1:E:149:ARG:HA	1.89	0.41
1:B:191:GLN:HE21	1:C:191:GLN:HE21	1.67	0.41
1:B:248:THR:O	1:B:252:GLN:HG3	2.20	0.41
1:E:48:ILE:O	1:E:73:GLN:HA	2.21	0.41
1:F:8:GLY:HA2	1:F:119:ALA:CB	2.51	0.41
1:B:202:ALA:HB1	1:B:264:ARG:HA	2.01	0.41
1:C:284:LEU:HG	1:C:288:ARG:HD2	2.02	0.41
1:C:115:THR:O	1:C:144:PHE:HA	2.21	0.41
1:F:120:ALA:HB1	1:F:166:LEU:HD12	2.04	0.40
1:C:99:TRP:CD1	1:C:125:GLY:HA3	2.56	0.40
1:C:234:THR:HG22	1:C:235:VAL:H	1.86	0.40
2:D:79:PRO:HA	2:D:96:ASP:O	2.21	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	272/303 (90%)	267 (98%)	5 (2%)	0	100	100
1	B	264/303 (87%)	257 (97%)	7 (3%)	0	100	100
1	C	265/303 (88%)	253 (96%)	11 (4%)	1 (0%)	34	37
1	E	270/303 (89%)	265 (98%)	5 (2%)	0	100	100
1	F	260/303 (86%)	254 (98%)	6 (2%)	0	100	100
2	D	276/291 (95%)	270 (98%)	6 (2%)	0	100	100
All	All	1607/1806 (89%)	1566 (97%)	40 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154	ALA

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	193/228 (85%)	191 (99%)	2 (1%)	76	85
1	B	186/228 (82%)	180 (97%)	6 (3%)	39	49
1	C	186/228 (82%)	185 (100%)	1 (0%)	88	94
1	E	190/228 (83%)	188 (99%)	2 (1%)	73	84
1	F	182/228 (80%)	176 (97%)	6 (3%)	38	47
2	D	196/216 (91%)	194 (99%)	2 (1%)	76	85
All	All	1133/1356 (84%)	1114 (98%)	19 (2%)	60	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG

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Mol	Chain	Res	Type
1	A	155	ASP
1	B	27	SER
1	B	74	THR
1	B	76	ASP
1	B	103	ASP
1	B	117	SER
1	B	210	ASP
1	C	273	SER
2	D	174	LYS
2	D	232	VAL
1	E	73	GLN
1	E	174	LYS
1	F	76	ASP
1	F	103	ASP
1	F	151	SER
1	F	158	LEU
1	F	166	LEU
1	F	242	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	C	191	GLN
1	F	47	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

10 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
4	PO4	B	403	-	4,4,4	0.81	0	6,6,6	0.58	0
4	PO4	A	402	-	4,4,4	0.80	0	6,6,6	0.76	0
3	GOL	D	301	-	5,5,5	0.90	0	5,5,5	1.00	0
3	GOL	B	402	-	5,5,5	0.75	0	5,5,5	1.14	0
3	GOL	A	401	-	5,5,5	1.22	0	5,5,5	0.95	0
4	PO4	E	402	-	4,4,4	0.81	0	6,6,6	0.52	0
3	GOL	B	401	-	5,5,5	0.88	0	5,5,5	1.08	0
4	PO4	D	302	-	4,4,4	0.84	0	6,6,6	0.45	0
3	GOL	E	401	-	5,5,5	0.95	0	5,5,5	0.96	0
4	PO4	F	401	-	4,4,4	0.81	0	6,6,6	0.43	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	D	301	-	-	2/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-
3	GOL	B	401	-	-	1/4/4/4	-
3	GOL	E	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	E	401	GOL	O1-C1-C2-C3
3	A	401	GOL	O2-C2-C3-O3
3	D	301	GOL	C1-C2-C3-O3
3	E	401	GOL	O1-C1-C2-O2
3	D	301	GOL	O2-C2-C3-O3
3	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	GOL	2	0
3	A	401	GOL	1	0
3	B	401	GOL	5	0
3	E	401	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	280/303 (92%)	0.53	6 (2%) 63 61	34, 48, 83, 99	0
1	B	272/303 (89%)	0.65	24 (8%) 10 8	43, 59, 90, 101	0
1	C	273/303 (90%)	0.58	28 (10%) 6 5	44, 65, 91, 105	0
1	E	278/303 (91%)	0.47	13 (4%) 31 29	46, 60, 86, 105	0
1	F	270/303 (89%)	0.70	32 (11%) 4 3	42, 62, 97, 104	0
2	D	282/291 (96%)	0.53	8 (2%) 53 51	36, 52, 78, 108	0
All	All	1655/1806 (91%)	0.57	111 (6%) 17 16	34, 58, 91, 108	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	ALA	6.2
1	B	52	ALA	5.6
1	F	11	LEU	5.2
1	C	93	TYR	5.1
1	F	75	ALA	5.0
1	B	93	TYR	5.0
1	B	235	VAL	4.9
2	D	18	PRO	4.8
1	B	234	THR	4.5
1	F	21	ALA	4.4
1	E	19	ASP	4.1
1	C	14	ILE	4.1
1	F	57	ILE	4.1
1	F	235	VAL	4.1
1	C	152	LEU	4.1
1	B	152	LEU	4.0
1	B	49	GLY	3.9
1	F	153	SER	3.9
1	F	12	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	15	VAL	3.7
1	C	81	ALA	3.7
1	F	50	ARG	3.7
1	B	23	TYR	3.6
1	B	228	PRO	3.6
1	F	46	THR	3.6
1	C	75	ALA	3.5
1	C	233	ASP	3.5
1	C	15	VAL	3.5
1	F	95	PHE	3.5
1	E	20	PRO	3.5
1	B	76	ASP	3.4
1	C	95	PHE	3.4
1	C	291	ALA	3.4
1	C	83	ALA	3.4
1	C	79	PRO	3.4
1	F	53	ARG	3.3
1	E	17	GLY	3.3
1	A	92	THR	3.3
1	E	154	ALA	3.3
1	C	153	SER	3.2
1	F	127	LEU	3.2
1	F	48	ILE	3.2
1	B	153	SER	3.1
1	C	151	SER	3.1
1	B	83	ALA	3.1
1	E	75	ALA	3.1
1	E	153	SER	3.1
1	B	17	GLY	3.1
1	B	72	SER	3.0
1	F	79	PRO	3.0
1	E	152	LEU	3.0
1	E	21	ALA	3.0
1	C	82	THR	3.0
1	B	156	PRO	2.9
1	C	21	ALA	2.9
2	D	1	MET	2.8
1	F	24	VAL	2.8
1	F	81	ALA	2.8
1	B	96	ASP	2.8
1	B	16	ASP	2.8
1	F	158	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	232	VAL	2.7
1	B	82	THR	2.7
1	B	102	PRO	2.7
1	C	52	ALA	2.7
1	A	292	ASP	2.7
1	F	101	ILE	2.6
1	C	77	ARG	2.6
1	C	69	VAL	2.6
2	D	19	ASP	2.6
1	F	152	LEU	2.6
1	B	92	THR	2.5
1	F	93	TYR	2.5
1	A	291	ALA	2.5
1	F	80	THR	2.5
2	D	229	VAL	2.5
1	E	16	ASP	2.5
1	C	154	ALA	2.4
1	C	78	THR	2.4
1	F	14	ILE	2.4
1	F	74	THR	2.4
1	C	64	SER	2.4
1	B	95	PHE	2.3
1	E	12	ILE	2.3
1	C	97	LEU	2.3
1	F	52	ALA	2.3
1	F	61	ILE	2.3
1	A	177	ALA	2.3
1	A	19	ASP	2.2
1	C	66	VAL	2.2
2	D	92	THR	2.2
1	F	29	LEU	2.2
1	F	162	ARG	2.2
1	E	82	THR	2.2
1	F	78	THR	2.2
1	F	182	TRP	2.2
1	F	97	LEU	2.2
1	F	72	SER	2.2
1	C	96	ASP	2.1
1	C	42	VAL	2.1
1	B	103	ASP	2.1
1	E	15	VAL	2.1
1	F	100	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	20	PRO	2.1
1	B	12	ILE	2.1
2	D	95	PHE	2.1
1	C	58	ALA	2.0
2	D	183	ILE	2.0
1	C	49	GLY	2.0
1	B	80	THR	2.0
1	C	13	ASP	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 monosaccharides 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
3	GOL	B	401	6/6	0.79	0.13	77,86,89,90	0
3	GOL	A	401	6/6	0.82	0.23	48,60,67,68	0
3	GOL	B	402	6/6	0.83	0.30	72,78,83,84	0
3	GOL	E	401	6/6	0.85	0.15	65,68,70,72	0
3	GOL	D	301	6/6	0.87	0.11	67,71,76,80	0
4	PO4	B	403	5/5	0.91	0.13	79,90,94,95	0
4	PO4	F	401	5/5	0.91	0.18	96,100,110,111	0
4	PO4	D	302	5/5	0.93	0.16	69,75,76,81	0
4	PO4	A	402	5/5	0.93	0.19	68,68,74,81	0
4	PO4	E	402	5/5	0.97	0.08	77,79,82,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.