



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 12:44 PM EDT

PDB ID : 9MIN / pdb_00009min
Title : Structure of a designed minibinder to NYESO1-A*02:01
Authors : Jude, K.M.; Householder, K.D.
Deposited on : 2024-12-13
Resolution : 2.05 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

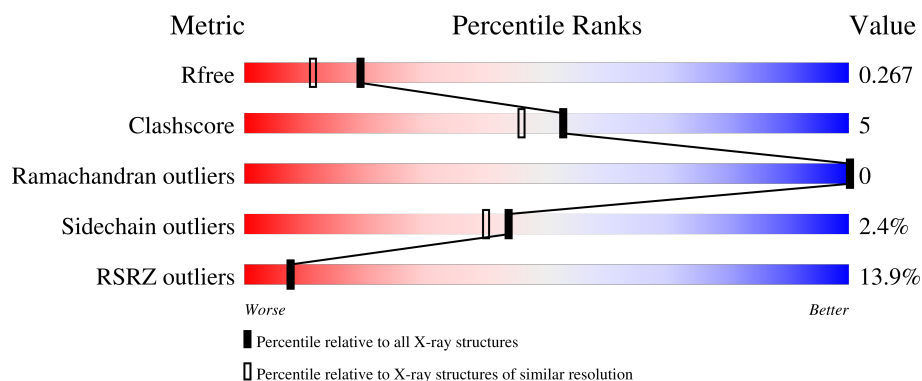
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	278	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	F	278	<div> <div>5%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
2	B	101	<div> <div>6%</div> <div>81%</div> <div>19%</div> </div>
2	G	101	<div> <div>5%</div> <div>89%</div> <div>11%</div> </div>
3	C	9	<div> <div>22%</div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	9	<div><div></div><div>11%</div><div>56%</div><div>44%</div></div>
4	D	136	<div><div></div><div>47%</div><div>79%</div><div>15%</div><div>6%</div></div>
4	I	136	<div><div></div><div>41%</div><div>75%</div><div>17%</div><div>7%</div></div>
5	E	119	<div><div></div><div>8%</div><div>86%</div><div>12%</div><div></div></div>
5	J	119	<div><div></div><div>6%</div><div>86%</div><div>11%</div><div></div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10482 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 HLA class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	F	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q53Z42
A	0	GLY	ALA	conflict	UNP Q53Z42
F	-1	MET	-	initiating methionine	UNP Q53Z42
F	0	GLY	ALA	conflict	UNP Q53Z42

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	1	0
			845	539	142	160	4			
2	G	101	Total	C	N	O	S	0	0	0
			841	535	142	160	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	initiating methionine	UNP P61769
B	0	GLY	-	expression tag	UNP P61769
G	-1	MET	-	initiating methionine	UNP P61769
G	0	GLY	-	expression tag	UNP P61769

- Molecule 3 is a protein called Cancer/testis antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			
3	H	9	Total	C	N	O	S	0	0	0
			76	51	11	13	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	CYS	engineered mutation	UNP P78358
H	9	VAL	CYS	engineered mutation	UNP P78358

- Molecule 4 is a protein called designed minibinder KH46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	128	Total	C	N	O	S	0	0	0
			1028	666	163	198	1			
4	I	127	Total	C	N	O	S	0	0	0
			1023	663	162	197	1			

- Molecule 5 is a protein called nanobody AD01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	116	Total	C	N	O	S	0	0	0
			864	534	148	178	4			
5	J	116	Total	C	N	O	S	0	0	0
			864	534	148	178	4			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

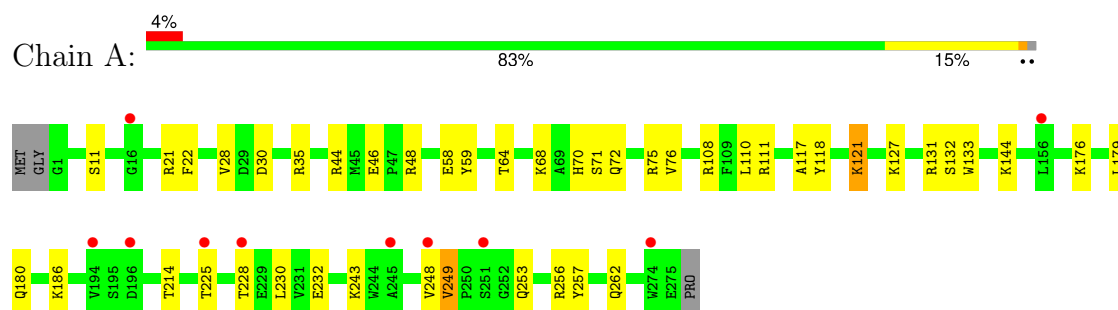
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		
7	B	56	Total	O	0	0
			56	56		
7	C	3	Total	O	0	0
			3	3		
7	E	29	Total	O	0	0
			29	29		
7	F	59	Total	O	0	0
			59	59		
7	G	42	Total	O	0	0
			42	42		
7	J	26	Total	O	0	0
			26	26		

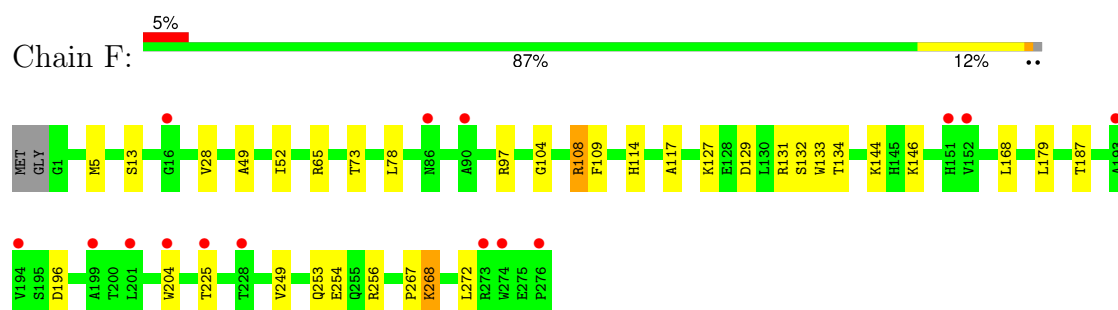
3 Residue-property plots [i](#)

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.

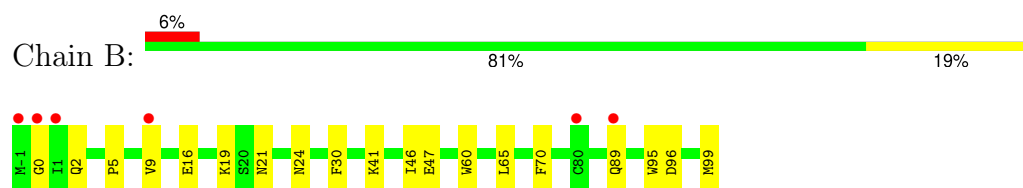
- Molecule 1: HLA class I antigen



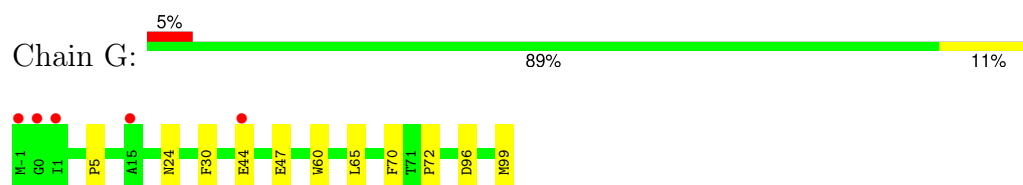
- Molecule 1: HLA class I antigen



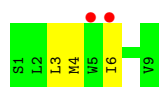
- Molecule 2: Beta-2-microglobulin



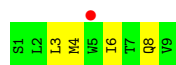
- Molecule 2: Beta-2-microglobulin



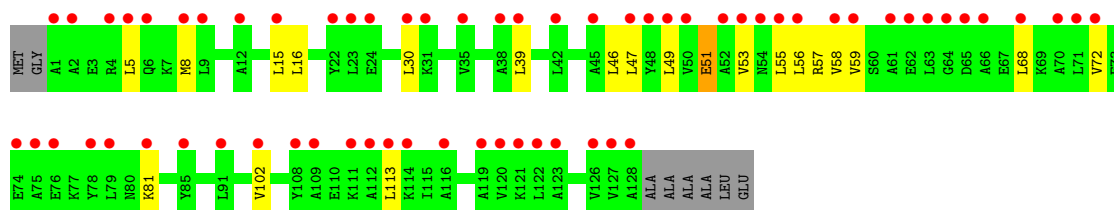
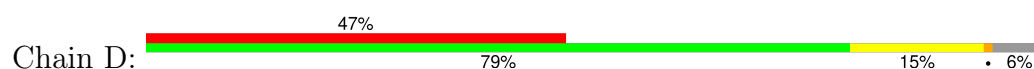
- Molecule 3: Cancer/testis antigen 1



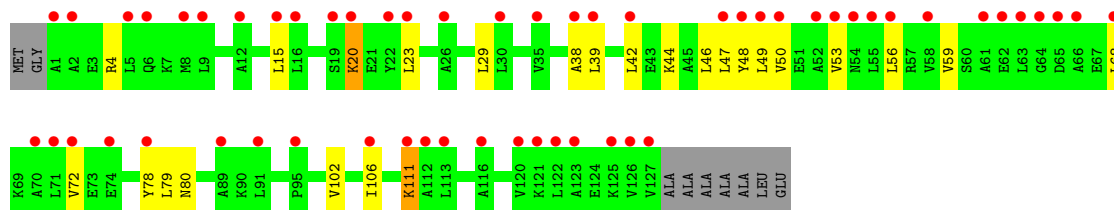
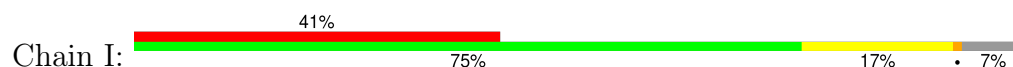
- Molecule 3: Cancer/testis antigen 1



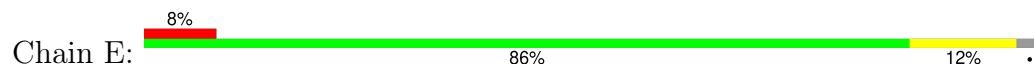
- Molecule 4: designed minibinder KH46



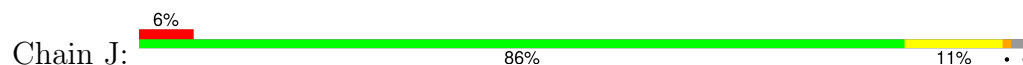
- Molecule 4: designed minibinder KH46



- Molecule 5: nanobody AD01



- Molecule 5: nanobody AD01



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.45Å 98.54Å 155.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 2.05 49.27 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.27-2.05) 88.9 (49.27-2.05)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.255 , 0.267 0.255 , 0.267	Depositor DCC
R_{free} test set	1394 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10482	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.07 % 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 3.8705e-07. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/2311	0.29	0/3137
1	F	0.13	0/2319	0.31	0/3149
2	B	0.12	0/871	0.35	0/1177
2	G	0.14	0/864	0.36	0/1167
3	C	0.14	0/77	0.37	0/103
3	H	0.15	0/77	0.40	0/103
4	D	0.09	0/1036	0.23	0/1382
4	I	0.09	0/1031	0.24	0/1375
5	E	0.14	0/879	0.35	0/1191
5	J	0.15	0/879	0.35	0/1191
All	All	0.12	0/10344	0.31	0/13975

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	2246	0	2096	22	0
1	F	2253	0	2103	20	0
2	B	845	0	815	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	841	0	806	7	0
3	C	76	0	83	5	0
3	H	76	0	83	6	0
4	D	1028	0	1112	14	0
4	I	1023	0	1107	14	0
5	E	864	0	817	8	0
5	J	864	0	817	8	0
6	A	30	0	40	3	0
6	B	24	0	32	0	0
6	E	6	0	8	1	0
6	F	18	0	24	1	0
6	G	12	0	16	0	0
6	J	6	0	8	0	0
7	A	55	0	0	0	0
7	B	56	0	0	0	0
7	C	3	0	0	0	0
7	E	29	0	0	0	0
7	F	59	0	0	0	0
7	G	42	0	0	0	0
7	J	26	0	0	0	0
All	All	10482	0	9967	99	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 5.

All (99) 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:A:253:GLN:HB3	1:A:256:ARG:HD3	1.73	0.70
4:D:15:LEU:HD13	4:D:51:GLU:HB3	1.73	0.70
4:D:5:LEU:HD11	4:D:59:VAL:HG22	1.74	0.69
5:E:21:ARG:HH12	6:E:201:GOL:H32	1.58	0.68
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.79	0.65
2:G:96:ASP:HB3	2:G:99:MET:HB2	1.79	0.63
1:A:228:THR:HG21	6:A:301:GOL:H32	1.80	0.62
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.83	0.60
5:J:21:ARG:NH1	5:J:83:GLN:HG2	2.17	0.60
1:A:30:ASP:HA	6:A:302:GOL:H11	1.84	0.58
5:E:84:MET:HE2	5:E:87:LEU:HD21	1.86	0.57
2:G:44:GLU:HG3	5:J:34:ASN:ND2	2.20	0.56
1:A:70:HIS:HA	3:C:6:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HD2	1:A:48:ARG:HD3	1.88	0.56
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.89	0.54
1:A:75:ARG:HH12	4:D:58:VAL:HG13	1.71	0.54
5:J:84:MET:HE2	5:J:87:LEU:HD21	1.90	0.53
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.89	0.53
4:D:68:LEU:O	4:D:72:VAL:HG23	2.09	0.53
4:I:23:LEU:HD22	4:I:106:ILE:HG23	1.89	0.53
4:D:56:LEU:HA	4:D:59:VAL:HB	1.91	0.53
1:F:133:TRP:HB2	1:F:144:LYS:HG3	1.89	0.53
4:I:68:LEU:O	4:I:72:VAL:HG23	2.09	0.52
3:H:4:MET:HE3	4:I:47:LEU:HD23	1.93	0.51
4:I:78:TYR:CE2	4:I:111:LYS:HD2	2.46	0.51
5:J:41:GLN:HB2	5:J:47:ARG:HB3	1.92	0.51
1:F:13:SER:HB3	1:F:78:LEU:HD13	1.93	0.51
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.47	0.50
1:A:35:ARG:HG2	1:A:46:GLU:HB2	1.92	0.50
1:F:28:VAL:HG11	1:F:179:LEU:HD13	1.93	0.49
4:I:56:LEU:HA	4:I:59:VAL:HB	1.93	0.49
1:F:249:VAL:HG21	1:F:254:GLU:HG3	1.95	0.49
4:I:49:LEU:O	4:I:53:VAL:HG23	2.13	0.49
1:F:253:GLN:HB3	1:F:256:ARG:HD3	1.93	0.49
1:A:214:THR:HB	1:A:262:GLN:HB2	1.93	0.49
5:J:26:ALA:HB3	5:J:78:ASN:HB3	1.94	0.49
1:F:73:THR:HG21	3:H:6:ILE:HG22	1.95	0.48
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.96	0.48
5:J:21:ARG:HH11	5:J:83:GLN:HG2	1.77	0.48
4:D:49:LEU:O	4:D:53:VAL:HG23	2.14	0.48
1:A:110:LEU:HG	1:A:111:ARG:HG3	1.96	0.47
1:A:76:VAL:HG21	4:D:57:ARG:HG2	1.95	0.47
1:F:204:TRP:CZ3	6:F:303:GOL:H2	2.50	0.47
1:F:104:GLY:HA3	1:F:108:ARG:HH21	1.80	0.46
3:H:4:MET:HE2	3:H:4:MET:HB3	1.70	0.46
4:I:42:LEU:HD13	4:I:106:ILE:HG12	1.98	0.46
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.96	0.45
1:F:187:THR:HB	1:F:272:LEU:HD21	1.97	0.45
1:F:108:ARG:HG2	1:F:109:PHE:N	2.30	0.45
4:D:39:LEU:HD13	4:D:102:VAL:HG22	1.99	0.45
1:A:44:ARG:HD2	1:A:64:THR:HG21	2.00	0.44
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.99	0.44
4:D:8:MET:HE3	4:D:55:LEU:HD22	1.98	0.44
4:D:16:LEU:HD22	4:D:113:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:PRO:HB2	1:F:268:LYS:HE3	1.98	0.44
5:J:15:GLN:HG2	5:J:16:PRO:HD2	2.00	0.44
3:C:4:MET:HE3	4:D:47:LEU:HD23	2.00	0.44
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.53	0.44
2:B:41:LYS:HB2	2:B:46:ILE:HD11	1.99	0.44
1:F:127:LYS:HB3	1:F:127:LYS:HE2	1.79	0.44
2:B:16:GLU:HB2	2:B:19:LYS:HG3	1.99	0.44
4:I:39:LEU:HD13	4:I:102:VAL:HG22	1.99	0.43
5:E:15:GLN:HG2	5:E:16:PRO:HD2	2.00	0.43
1:F:146:LYS:HE3	3:H:8:GLN:HG3	2.01	0.43
4:I:29:LEU:HB2	4:I:38:ALA:HB2	2.00	0.43
1:A:59:TYR:HA	6:A:305:GOL:H12	2.00	0.43
1:F:49:ALA:O	1:F:52:ILE:HG22	2.18	0.43
1:A:22:PHE:CD2	1:A:71:SER:HB3	2.53	0.43
2:B:47:GLU:HB2	2:G:47:GLU:HG3	2.01	0.43
5:E:41:GLN:HB2	5:E:47:ARG:HB3	2.00	0.43
1:A:249:VAL:HB	1:A:257:TYR:CE1	2.54	0.42
2:B:89:GLN:HG2	5:E:47:ARG:NH1	2.34	0.42
1:A:127:LYS:HD3	1:A:132:SER:OG	2.20	0.42
4:D:30:LEU:HD11	4:D:102:VAL:HG12	2.00	0.42
1:A:11:SER:HA	1:A:21:ARG:O	2.19	0.42
3:C:4:MET:HB3	3:C:4:MET:HE2	1.71	0.42
1:F:5:MET:HB2	1:F:168:LEU:HD13	2.01	0.42
2:G:70:PHE:CZ	2:G:72:PRO:HG3	2.54	0.42
4:I:44:LYS:O	4:I:48:TYR:HD1	2.03	0.42
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.55	0.42
3:C:4:MET:HE1	4:D:46:LEU:HB3	2.01	0.42
2:B:9[B]:VAL:HG23	2:B:95:TRP:HA	2.02	0.41
1:F:127:LYS:HD3	1:F:132:SER:OG	2.20	0.41
5:E:35:THR:HA	5:E:54:SER:HA	2.03	0.41
4:I:50:VAL:HG22	4:I:79:LEU:HD21	2.01	0.41
3:H:4:MET:HE1	4:I:46:LEU:HB3	2.01	0.41
1:F:65:ARG:HH22	4:I:15:LEU:HD22	1.85	0.41
5:E:22:LEU:HB2	5:E:82:LEU:HB3	2.02	0.41
5:J:61:TYR:HB2	5:J:66:LYS:HG2	2.03	0.41
2:G:5:PRO:HB3	2:G:30:PHE:HB3	2.01	0.41
3:H:3:LEU:HD23	3:H:6:ILE:HD13	2.02	0.41
4:I:20:LYS:NZ	4:I:20:LYS:HB2	2.35	0.41
3:C:4:MET:HE1	4:D:46:LEU:CB	2.52	0.40
5:E:89:PRO:HA	5:E:116:VAL:HB	2.03	0.40
1:A:176:LYS:HA	1:A:180:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:0:GLY:C	2:B:2:GLN:H	2.28	0.40
1:F:97:ARG:HH11	1:F:114:HIS:CE1	2.40	0.40
1:A:118:TYR:O	1:A:121:LYS:HG3	2.22	0.40
1:F:129:ASP:O	1:F:131:ARG:HG3	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	273/278 (98%)	268 (98%)	5 (2%)	0	100	100
1	F	274/278 (99%)	269 (98%)	5 (2%)	0	100	100
2	B	100/101 (99%)	97 (97%)	3 (3%)	0	100	100
2	G	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
4	D	126/136 (93%)	126 (100%)	0	0	100	100
4	I	125/136 (92%)	125 (100%)	0	0	100	100
5	E	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
5	J	114/119 (96%)	113 (99%)	1 (1%)	0	100	100
All	All	1239/1286 (96%)	1221 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	231/233 (99%)	220 (95%)	11 (5%)	21	15
1	F	232/233 (100%)	227 (98%)	5 (2%)	47	43
2	B	96/95 (101%)	96 (100%)	0	100	100
2	G	95/95 (100%)	95 (100%)	0	100	100
3	C	9/9 (100%)	8 (89%)	1 (11%)	5	1
3	H	9/9 (100%)	9 (100%)	0	100	100
4	D	107/110 (97%)	105 (98%)	2 (2%)	52	50
4	I	107/110 (97%)	103 (96%)	4 (4%)	29	23
5	E	93/98 (95%)	92 (99%)	1 (1%)	70	71
5	J	93/98 (95%)	91 (98%)	2 (2%)	47	43
All	All	1072/1090 (98%)	1046 (98%)	26 (2%)	44	40

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	68	LYS
1	A	72	GLN
1	A	108	ARG
1	A	121	LYS
1	A	131	ARG
1	A	186	LYS
1	A	225	THR
1	A	232	GLU
1	A	248	VAL
1	A	249	VAL
3	C	3	LEU
4	D	51	GLU
4	D	81	LYS
5	E	30	ILE
1	F	108	ARG
1	F	134	THR
1	F	196	ASP
1	F	225	THR
1	F	268	LYS

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Mol	Chain	Res	Type
4	I	4	ARG
4	I	20	LYS
4	I	80	ASN
4	I	111	LYS
5	J	30	ILE
5	J	83	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	72	GLN
1	A	151	HIS
2	B	13	HIS
4	D	80	ASN
1	F	43	GLN
1	F	86	ASN
1	F	93	HIS
1	F	155	GLN
2	G	13	HIS
4	I	6	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](#)

16 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
6	GOL	A	305	-	5,5,5	0.34	0	5,5,5	0.54	0
6	GOL	B	102	-	5,5,5	0.36	0	5,5,5	0.45	0
6	GOL	A	304	-	5,5,5	0.36	0	5,5,5	0.46	0
6	GOL	A	303	-	5,5,5	0.35	0	5,5,5	0.37	0
6	GOL	F	301	-	5,5,5	0.34	0	5,5,5	0.40	0
6	GOL	A	301	-	5,5,5	0.37	0	5,5,5	0.36	0
6	GOL	E	201	-	5,5,5	0.32	0	5,5,5	0.40	0
6	GOL	G	201	-	5,5,5	0.38	0	5,5,5	0.55	0
6	GOL	G	202	-	5,5,5	0.35	0	5,5,5	0.37	0
6	GOL	B	101	-	5,5,5	0.35	0	5,5,5	0.35	0
6	GOL	A	302	-	5,5,5	0.34	0	5,5,5	0.37	0
6	GOL	B	104	-	5,5,5	0.38	0	5,5,5	0.63	0
6	GOL	J	201	-	5,5,5	0.33	0	5,5,5	0.34	0
6	GOL	B	103	-	5,5,5	0.34	0	5,5,5	0.32	0
6	GOL	F	302	-	5,5,5	0.35	0	5,5,5	0.43	0
6	GOL	F	303	-	5,5,5	0.36	0	5,5,5	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
6	GOL	A	305	-	-	2/4/4/4	-
6	GOL	B	102	-	-	4/4/4/4	-
6	GOL	A	304	-	-	2/4/4/4	-
6	GOL	A	303	-	-	2/4/4/4	-
6	GOL	F	301	-	-	3/4/4/4	-
6	GOL	A	301	-	-	0/4/4/4	-
6	GOL	E	201	-	-	3/4/4/4	-
6	GOL	G	201	-	-	0/4/4/4	-
6	GOL	G	202	-	-	2/4/4/4	-
6	GOL	B	101	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	302	-	-	0/4/4/4	-
6	GOL	B	104	-	-	0/4/4/4	-
6	GOL	J	201	-	-	4/4/4/4	-
6	GOL	B	103	-	-	1/4/4/4	-
6	GOL	F	302	-	-	0/4/4/4	-
6	GOL	F	303	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	304	GOL	C1-C2-C3-O3
6	A	305	GOL	C1-C2-C3-O3
6	B	102	GOL	C1-C2-C3-O3
6	E	201	GOL	O1-C1-C2-O2
6	E	201	GOL	O1-C1-C2-C3
6	F	303	GOL	O1-C1-C2-C3
6	G	202	GOL	O1-C1-C2-O2
6	G	202	GOL	O1-C1-C2-C3
6	A	303	GOL	O1-C1-C2-C3
6	B	102	GOL	O1-C1-C2-C3
6	F	301	GOL	C1-C2-C3-O3
6	F	303	GOL	C1-C2-C3-O3
6	J	201	GOL	O1-C1-C2-C3
6	A	304	GOL	O2-C2-C3-O3
6	B	102	GOL	O2-C2-C3-O3
6	F	301	GOL	O2-C2-C3-O3
6	F	303	GOL	O2-C2-C3-O3
6	A	305	GOL	O2-C2-C3-O3
6	J	201	GOL	O1-C1-C2-O2
6	E	201	GOL	O2-C2-C3-O3
6	F	301	GOL	O1-C1-C2-C3
6	F	303	GOL	O1-C1-C2-O2
6	B	102	GOL	O1-C1-C2-O2
6	J	201	GOL	C1-C2-C3-O3
6	A	303	GOL	O1-C1-C2-O2
6	J	201	GOL	O2-C2-C3-O3
6	B	103	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	305	GOL	1	0
6	A	301	GOL	1	0
6	E	201	GOL	1	0
6	A	302	GOL	1	0
6	F	303	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	275/278 (98%)	0.82	10 (3%) 46 48	27, 47, 82, 127	0
1	F	276/278 (99%)	0.82	15 (5%) 32 34	27, 47, 93, 138	0
2	B	101/101 (100%)	0.50	6 (5%) 29 31	25, 32, 54, 86	1 (0%)
2	G	101/101 (100%)	0.45	5 (4%) 35 38	26, 33, 49, 99	0
3	C	9/9 (100%)	1.13	2 (22%) 3 2	39, 48, 64, 74	0
3	H	9/9 (100%)	1.10	1 (11%) 12 12	39, 45, 65, 66	0
4	D	128/136 (94%)	2.30	64 (50%) 0 0	71, 125, 170, 184	0
4	I	127/136 (93%)	2.10	56 (44%) 1 0	51, 113, 155, 185	0
5	E	116/119 (97%)	0.70	9 (7%) 20 22	23, 40, 69, 115	0
5	J	116/119 (97%)	0.77	7 (6%) 29 30	25, 40, 67, 116	0
All	All	1258/1286 (97%)	1.03	175 (13%) 7 7	23, 47, 139, 185	1 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	63	LEU	5.7
4	D	123	ALA	5.0
4	I	63	LEU	5.0
5	J	30	ILE	4.9
4	D	120	VAL	4.9
4	D	54	ASN	4.7
4	I	35	VAL	4.6
4	I	1	ALA	4.5
4	D	48	TYR	4.5
4	D	15	LEU	4.4
4	D	75	ALA	4.4
4	D	35	VAL	4.4
4	D	127	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
4	D	12	ALA	4.3
4	I	2	ALA	4.3
4	I	120	VAL	4.3
4	I	15	LEU	4.3
4	I	16	LEU	4.3
4	I	127	VAL	4.2
4	I	30	LEU	4.2
4	I	64	GLY	4.2
4	D	112	ALA	4.1
4	I	122	LEU	4.1
4	I	5	LEU	4.1
4	D	8	MET	4.1
5	E	30	ILE	4.0
1	F	276	PRO	4.0
4	I	91	LEU	4.0
4	D	52	ALA	4.0
5	J	29	SER	3.9
4	I	126	VAL	3.9
4	D	64	GLY	3.9
4	D	78	TYR	3.9
4	I	56	LEU	3.8
4	D	2	ALA	3.8
4	I	65	ASP	3.8
2	G	1	ILE	3.7
4	I	49	LEU	3.7
4	D	1	ALA	3.7
4	I	23	LEU	3.6
1	F	194	VAL	3.6
4	D	30	LEU	3.6
4	I	12	ALA	3.6
4	D	91	LEU	3.6
4	D	128	ALA	3.5
4	I	62	GLU	3.5
4	D	72	VAL	3.5
1	F	274	TRP	3.5
1	A	196	ASP	3.5
5	E	29	SER	3.5
4	D	126	VAL	3.5
4	D	58	VAL	3.4
4	I	53	VAL	3.4
4	D	47	LEU	3.4
4	I	123	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	65	ASP	3.4
4	I	55	LEU	3.3
4	D	53	VAL	3.3
4	I	72	VAL	3.3
4	D	55	LEU	3.3
2	B	-1	MET	3.3
4	D	111	LYS	3.3
4	D	74	GLU	3.3
4	D	9	LEU	3.3
2	G	0	GLY	3.2
4	I	39	LEU	3.2
4	I	95	PRO	3.2
2	B	1	ILE	3.2
2	B	9[A]	VAL	3.2
4	D	62	GLU	3.2
4	I	58	VAL	3.1
4	D	116	ALA	3.1
4	I	116	ALA	3.1
4	D	4	ARG	3.1
4	D	71	LEU	3.1
4	I	125	LYS	3.0
4	D	56	LEU	3.0
4	D	122	LEU	3.0
4	I	48	TYR	3.0
1	A	228	THR	3.0
4	I	71	LEU	3.0
4	D	119	ALA	2.9
4	I	52	ALA	2.9
4	D	22	TYR	2.9
4	I	54	ASN	2.9
4	I	68	LEU	2.8
4	D	70	ALA	2.8
4	I	42	LEU	2.8
4	D	109	ALA	2.8
1	F	204	TRP	2.8
4	D	102	VAL	2.8
4	D	108	TYR	2.7
1	F	199	ALA	2.7
4	I	38	ALA	2.7
4	D	5	LEU	2.7
4	I	113	LEU	2.7
5	E	118	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	193	ALA	2.7
1	A	225	THR	2.7
4	D	39	LEU	2.6
4	D	6	GLN	2.6
4	D	24	GLU	2.6
3	C	5	TRP	2.6
1	A	16	GLY	2.6
4	D	61	ALA	2.6
4	I	70	ALA	2.6
5	E	31	PHE	2.6
3	C	6	ILE	2.6
1	A	156	LEU	2.6
5	J	31	PHE	2.5
4	I	19	SER	2.5
4	D	121	LYS	2.5
4	D	38	ALA	2.5
1	A	248	VAL	2.5
4	I	106	ILE	2.5
1	A	274	TRP	2.5
4	I	66	ALA	2.5
5	J	78	ASN	2.5
4	D	42	LEU	2.5
5	J	100	LEU	2.5
1	F	90	ALA	2.5
5	J	86	SER	2.4
4	I	6	GLN	2.4
4	D	66	ALA	2.4
1	F	228	THR	2.4
4	D	85	TYR	2.4
4	D	49	LEU	2.4
4	D	50	VAL	2.4
4	I	8	MET	2.4
4	D	68	LEU	2.3
1	F	16	GLY	2.3
4	I	78	TYR	2.3
4	D	79	LEU	2.3
4	I	20	LYS	2.3
4	I	61	ALA	2.3
4	I	89	ALA	2.3
4	I	121	LYS	2.3
4	I	112	ALA	2.3
4	D	59	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
4	I	74	GLU	2.3
3	H	5	TRP	2.3
4	I	22	TYR	2.3
5	E	16	PRO	2.2
4	D	113	LEU	2.2
2	B	89	GLN	2.2
2	G	15	ALA	2.2
5	E	12	GLY	2.2
1	F	152	VAL	2.2
1	F	273	ARG	2.2
4	I	26	ALA	2.2
4	I	111	LYS	2.2
5	E	4	VAL	2.2
4	D	45	ALA	2.2
5	J	77	LYS	2.2
1	F	151	HIS	2.2
2	B	80	CYS	2.2
1	F	201	LEU	2.1
4	I	9	LEU	2.1
1	A	245	ALA	2.1
1	A	194	VAL	2.1
4	I	50	VAL	2.1
2	G	44	GLU	2.1
5	E	13	LEU	2.1
4	D	81	LYS	2.1
5	E	86	SER	2.1
4	D	31	LYS	2.1
1	A	251	SER	2.1
4	D	23	LEU	2.1
1	F	225	THR	2.1
1	F	86	ASN	2.0
2	G	-1	MET	2.0
4	I	47	LEU	2.0
2	B	0	GLY	2.0
4	D	76	GLU	2.0
4	D	114	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
6	GOL	B	102	6/6	0.75	0.17	51,55,59,62	0
6	GOL	A	301	6/6	0.78	0.16	63,71,76,87	0
6	GOL	F	301	6/6	0.79	0.17	55,60,67,70	0
6	GOL	A	302	6/6	0.80	0.16	40,44,50,58	0
6	GOL	F	302	6/6	0.81	0.14	45,51,57,65	0
6	GOL	B	101	6/6	0.82	0.13	44,53,55,58	0
6	GOL	A	303	6/6	0.83	0.14	45,54,57,57	0
6	GOL	A	305	6/6	0.83	0.19	57,68,80,90	0
6	GOL	F	303	6/6	0.83	0.16	35,46,56,59	0
6	GOL	G	202	6/6	0.84	0.15	33,51,56,57	0
6	GOL	E	201	6/6	0.86	0.13	42,46,56,56	0
6	GOL	J	201	6/6	0.86	0.13	36,45,57,58	0
6	GOL	A	304	6/6	0.87	0.13	52,61,69,70	0
6	GOL	B	103	6/6	0.87	0.14	49,50,55,56	0
6	GOL	B	104	6/6	0.87	0.14	36,44,51,63	0
6	GOL	G	201	6/6	0.90	0.14	37,39,42,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.