Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2016 – 05:06 AM EDT

PDB ID	:	5F3W
Title	:	Structure of the ATPrS-Mre11/Rad50-DNA complex
Authors	:	Liu, Y.
Deposited on	:	2015-12-03
Resolution	:	3.11 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

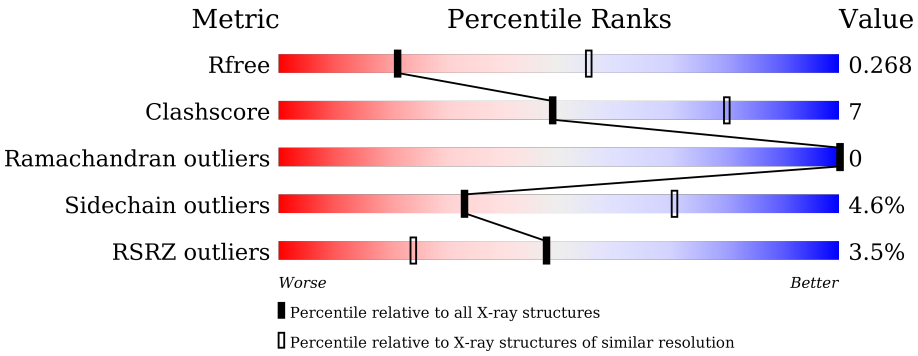
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	386	3% 77% 13% • 9%
1	C	386	4% 69% 20% • 9%
2	B	372	2% 76% 19% • •
2	D	372	4% 73% 21% • •
3	E	27	85% 7% 7%
4	F	27	67% 19% 15%

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
5	MG	A	401	-	-	-	X
5	MG	C	401	-	-	-	X
5	MG	C	402	-	-	-	X
6	AGS	D	1101	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12658 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 DNA double-strand break repair protein Mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2936	1895	493	538	10			
1	C	351	Total	C	N	O	S	0	0	0
			2919	1883	489	537	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q58719
A	-18	GLY	-	expression tag	UNP Q58719
A	-17	SER	-	expression tag	UNP Q58719
A	-16	SER	-	expression tag	UNP Q58719
A	-15	HIS	-	expression tag	UNP Q58719
A	-14	HIS	-	expression tag	UNP Q58719
A	-13	HIS	-	expression tag	UNP Q58719
A	-12	HIS	-	expression tag	UNP Q58719
A	-11	HIS	-	expression tag	UNP Q58719
A	-10	HIS	-	expression tag	UNP Q58719
A	-9	SER	-	expression tag	UNP Q58719
A	-8	SER	-	expression tag	UNP Q58719
A	-7	GLY	-	expression tag	UNP Q58719
A	-6	LEU	-	expression tag	UNP Q58719
A	-5	VAL	-	expression tag	UNP Q58719
A	-4	PRO	-	expression tag	UNP Q58719
A	-3	ARG	-	expression tag	UNP Q58719
A	-2	GLY	-	expression tag	UNP Q58719
A	-1	SER	-	expression tag	UNP Q58719
A	0	HIS	-	expression tag	UNP Q58719
C	-19	MET	-	expression tag	UNP Q58719
C	-18	GLY	-	expression tag	UNP Q58719
C	-17	SER	-	expression tag	UNP Q58719
C	-16	SER	-	expression tag	UNP Q58719
C	-15	HIS	-	expression tag	UNP Q58719

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q58719
C	-13	HIS	-	expression tag	UNP Q58719
C	-12	HIS	-	expression tag	UNP Q58719
C	-11	HIS	-	expression tag	UNP Q58719
C	-10	HIS	-	expression tag	UNP Q58719
C	-9	SER	-	expression tag	UNP Q58719
C	-8	SER	-	expression tag	UNP Q58719
C	-7	GLY	-	expression tag	UNP Q58719
C	-6	LEU	-	expression tag	UNP Q58719
C	-5	VAL	-	expression tag	UNP Q58719
C	-4	PRO	-	expression tag	UNP Q58719
C	-3	ARG	-	expression tag	UNP Q58719
C	-2	GLY	-	expression tag	UNP Q58719
C	-1	SER	-	expression tag	UNP Q58719
C	0	HIS	-	expression tag	UNP Q58719

- Molecule 2 is a protein called DNA double-strand break repair Rad50 ATPase,DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	359	Total	C	N	O	S	0	0	0
			2877	1844	490	534	9			
2	D	358	Total	C	N	O	S	0	0	0
			2874	1845	488	533	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	824	MET	-	linker	UNP Q58718
D	824	MET	-	linker	UNP Q58718

- Molecule 3 is a DNA chain called 27-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	P	0	0	0
			517	246	99	147	25			

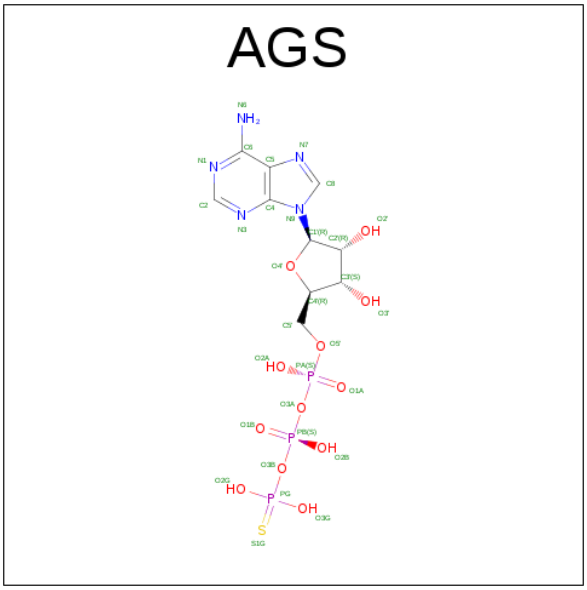
- Molecule 4 is a DNA chain called 27-MER DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	23	Total	C	N	O	P	0	0	0
			467	223	83	138	23			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P S 31 10 5 12 3 1	0	0
6	D	1	Total C N O P S 31 10 5 12 3 1	0	0

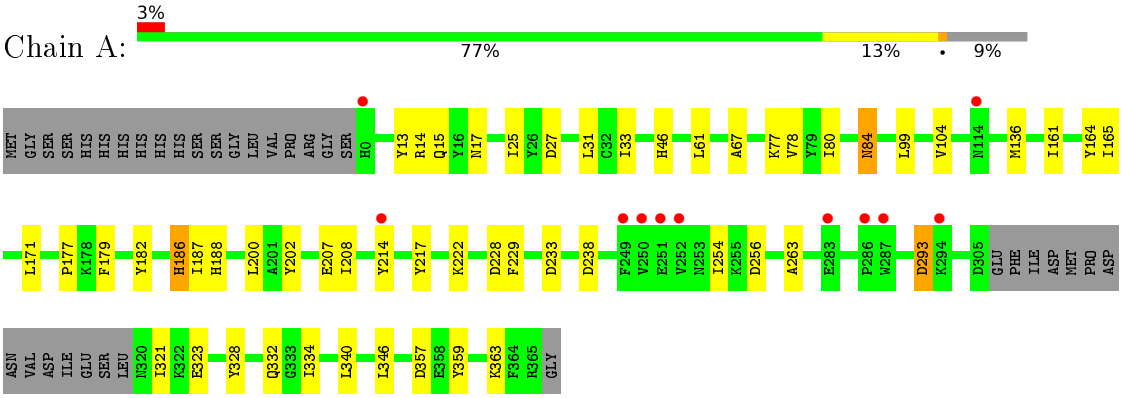
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0
7	C	1	Total O 1 1	0	0

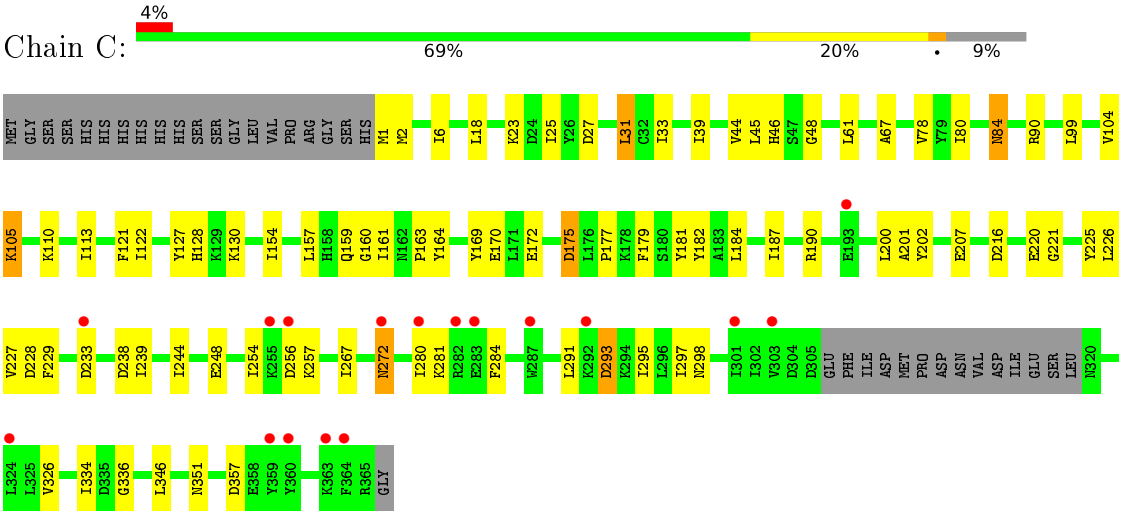
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

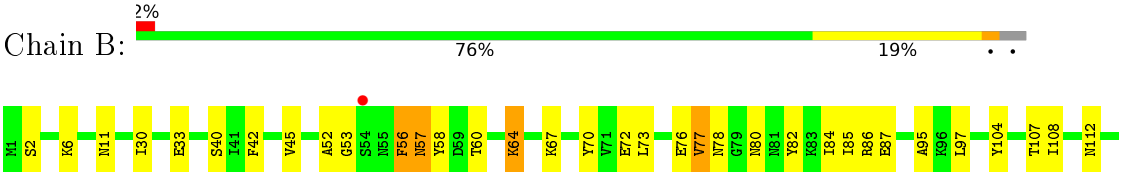
• Molecule 1: DNA double-strand break repair protein Mre11

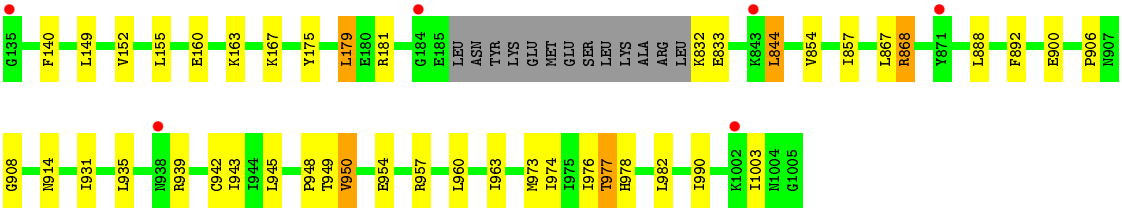


• Molecule 1: DNA double-strand break repair protein Mre11

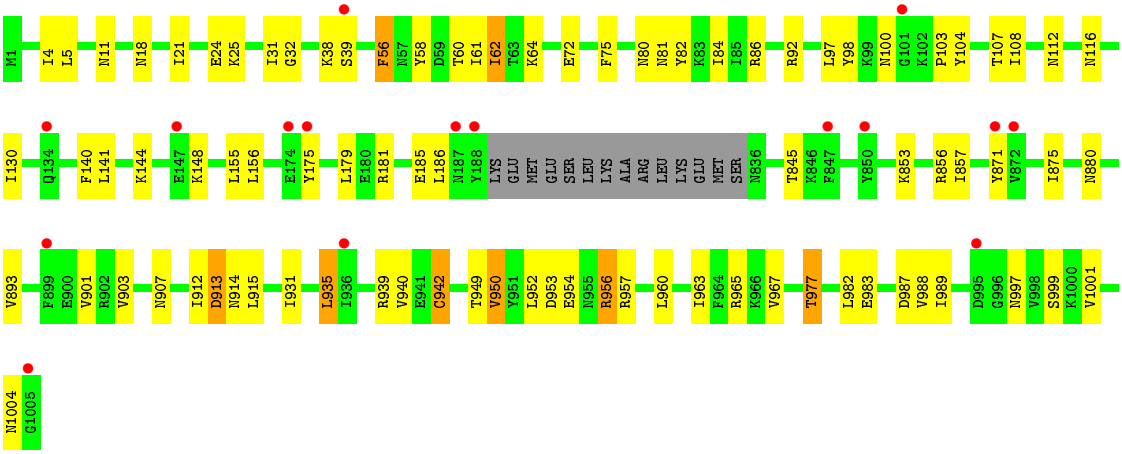


• Molecule 2: DNA double-strand break repair Rad50 ATPase,DNA double-strand break repair Rad50 ATPase

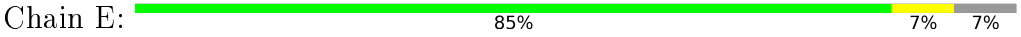


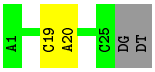


• Molecule 2: DNA double-strand break repair Rad50 ATPase,DNA double-strand break repair Rad50 ATPase

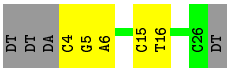


• Molecule 3: 27-MER DNA





• Molecule 4: 27-MER DNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.30Å 130.11Å 166.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.87 – 3.11 40.86 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.87-3.11) 95.8 (40.86-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10-2152_1069: ???)	Depositor
R, R_{free}	0.222 , 0.269 0.221 , 0.268	Depositor DCC
R_{free} test set	1636 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	95.3	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 32232 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, AGS

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	0.25	0/2997	0.41	0/4025
1	C	0.25	0/2979	0.43	0/4002
2	B	0.29	1/2920 (0.0%)	0.44	0/3913
2	D	0.25	0/2918	0.41	0/3913
3	E	0.53	0/581	0.89	0/895
4	F	0.53	0/522	0.91	0/802
All	All	0.29	1/12917 (0.0%)	0.49	0/17550

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	888	LEU	C-N	8.19	1.49	1.34

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	2936	0	2956	32	0
1	C	2919	0	2929	51	0
2	B	2877	0	2959	52	0
2	D	2874	0	2952	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	517	0	282	1	0
4	F	467	0	260	5	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	B	31	0	12	1	0
6	D	31	0	12	2	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
All	All	12658	0	12362	179	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 (179) 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)
3:E:19:DC:H2"	3:E:20:DA:H5"	1.65	0.76
2:D:84:ILE:HG12	2:D:97:LEU:HD13	1.71	0.71
1:A:165:ILE:HD11	1:A:187:ILE:HB	1.73	0.71
1:C:175:ASP:OD1	1:C:175:ASP:N	2.25	0.70
2:D:949:THR:HG21	2:D:982:LEU:HD11	1.74	0.69
2:D:62:ILE:O	6:D:1101:AGS:N6	2.27	0.66
2:D:86:ARG:NH2	2:D:112:ASN:OD1	2.28	0.66
1:C:281:LYS:HB3	1:C:284:PHE:HD2	1.63	0.64
1:C:326:VAL:HG13	1:C:336:GLY:HA3	1.78	0.64
2:D:112:ASN:O	2:D:116:ASN:ND2	2.31	0.64
2:B:45:VAL:HG13	2:B:73:LEU:HD11	1.81	0.63
2:D:935:LEU:HD13	2:D:939:ARG:HB3	1.79	0.63
2:D:141:LEU:HD13	2:D:912:ILE:HD13	1.80	0.62
1:C:122:ILE:HG12	1:C:154:ILE:HD11	1.82	0.62
2:B:908:GLY:HA3	2:D:64:LYS:HB3	1.81	0.62
2:D:92:ARG:HH22	4:F:4:DC:H41	1.48	0.61
2:D:977:THR:HG21	2:D:982:LEU:HD13	1.83	0.60
1:C:216:ASP:O	1:C:220:GLU:N	2.26	0.60
1:A:182:TYR:HB2	1:A:200:LEU:HA	1.84	0.60
1:A:33:ILE:HG13	1:A:67:ALA:HB1	1.83	0.59
1:C:90:ARG:NH2	2:D:983:GLU:OE1	2.34	0.59
1:C:154:ILE:HG22	1:C:181:TYR:HB3	1.82	0.59
2:D:21:ILE:HG12	2:D:1001:VAL:HG11	1.83	0.59
2:D:913:ASP:OD1	2:D:913:ASP:N	2.30	0.59
2:B:149:LEU:HD22	2:B:868:ARG:HE	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:THR:HG21	2:B:982:LEU:HD11	1.84	0.59
1:C:228:ASP:HB3	1:C:238:ASP:HB2	1.84	0.58
1:C:2:MET:HG2	1:C:228:ASP:HA	1.86	0.57
1:C:182:TYR:HB2	1:C:200:LEU:HA	1.86	0.57
2:B:977:THR:HG21	2:B:982:LEU:HD13	1.86	0.56
1:A:25:ILE:HD13	1:A:207:GLU:HB3	1.86	0.56
1:C:161:ILE:HB	1:C:164:TYR:HD2	1.70	0.56
1:C:177:PRO:HG2	1:C:179:PHE:HE1	1.70	0.56
2:B:950:VAL:HG22	2:D:950:VAL:HG22	1.87	0.56
1:A:177:PRO:HG2	1:A:179:PHE:HE1	1.71	0.56
2:D:903:VAL:HG21	2:D:915:LEU:HD11	1.87	0.56
2:B:155:LEU:HD13	2:B:931:ILE:HD13	1.88	0.56
1:A:228:ASP:HB3	1:A:238:ASP:HB2	1.87	0.55
1:A:334:ILE:HG21	2:B:854:VAL:HG22	1.88	0.55
1:C:357:ASP:OD1	2:D:175:TYR:OH	2.23	0.55
2:D:155:LEU:HD23	2:D:931:ILE:HD13	1.89	0.55
2:B:949:THR:HB	2:B:957:ARG:HG2	1.89	0.55
2:B:86:ARG:NH2	2:B:112:ASN:OD1	2.30	0.54
2:D:901:VAL:HB	2:D:912:ILE:HD11	1.88	0.54
1:C:127:TYR:HA	1:C:159:GLN:HE22	1.72	0.54
1:A:357:ASP:OD1	2:B:175:TYR:OH	2.24	0.54
2:B:978:HIS:CD2	2:B:978:HIS:H	2.27	0.53
2:D:11:ASN:OD1	2:D:18:ASN:ND2	2.42	0.53
2:D:156:LEU:HD21	2:D:875:ILE:HD11	1.90	0.53
1:A:14:ARG:HG2	1:A:17:ASN:HA	1.91	0.52
1:C:254:ILE:HB	1:C:280:ILE:HA	1.91	0.52
2:B:11:ASN:HB2	2:B:70:TYR:HB3	1.92	0.51
1:C:46:HIS:O	1:C:80:ILE:HA	2.10	0.51
1:C:248:GLU:H	1:C:272:ASN:HD21	1.58	0.51
2:D:92:ARG:NH2	4:F:4:DC:H41	2.08	0.51
2:D:965:ARG:NH2	2:D:987:ASP:OD1	2.40	0.51
2:B:40:SER:OG	6:B:1101:AGS:O1A	2.23	0.50
2:B:149:LEU:HD13	2:B:868:ARG:HH11	1.76	0.50
2:D:853:LYS:HA	2:D:856:ARG:HD3	1.94	0.50
2:D:181:ARG:NH1	2:D:185:GLU:OE2	2.44	0.50
1:A:186:HIS:O	1:A:186:HIS:ND1	2.45	0.50
2:D:98:TYR:HA	2:D:103:PRO:HA	1.94	0.49
2:B:6:LYS:HD2	2:B:76:GLU:HG3	1.93	0.49
2:B:954:GLU:HG3	2:B:957:ARG:NH1	2.27	0.49
2:B:95:ALA:HB3	2:B:108:ILE:HA	1.94	0.49
1:C:130:LYS:HD3	1:C:169:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:LYS:NZ	1:C:27:ASP:OD2	2.40	0.48
1:A:321:ILE:HG22	2:B:867:LEU:HD11	1.95	0.48
1:C:113:ILE:HD13	1:C:122:ILE:HD11	1.95	0.48
1:C:110:LYS:HB2	1:C:121:PHE:HE1	1.78	0.48
2:B:155:LEU:HD13	2:B:931:ILE:HG21	1.95	0.48
2:D:144:LYS:O	2:D:148:LYS:N	2.41	0.48
2:D:949:THR:HG22	2:D:960:LEU:HD23	1.96	0.47
2:B:868:ARG:HH21	2:B:868:ARG:CG	2.27	0.47
2:D:24:GLU:HG3	2:D:988:VAL:HG21	1.95	0.47
1:C:187:ILE:HG22	1:C:202:TYR:CD1	2.50	0.47
1:C:45:LEU:HD11	1:C:154:ILE:HD12	1.96	0.47
2:B:77:VAL:HG22	2:B:78:ASN:ND2	2.28	0.47
1:A:161:ILE:HB	1:A:164:TYR:HD2	1.79	0.47
2:B:30:ILE:HB	2:B:976:ILE:HG12	1.96	0.47
1:C:254:ILE:HD12	1:C:280:ILE:HG12	1.97	0.47
1:C:84:ASN:HD22	1:C:84:ASN:H	1.62	0.47
2:D:949:THR:HB	2:D:957:ARG:HG2	1.96	0.47
1:C:256:ASP:OD1	1:C:256:ASP:N	2.48	0.47
1:C:33:ILE:HG13	1:C:67:ALA:HB1	1.96	0.46
4:F:5:DG:H2"	4:F:6:DA:C8	2.51	0.46
2:D:31:ILE:HD13	2:D:989:ILE:HG13	1.96	0.46
2:D:58:TYR:HA	2:D:61:ILE:HG12	1.96	0.46
2:D:56:PHE:HD1	2:D:56:PHE:HA	1.68	0.46
1:C:128:HIS:H	1:C:159:GLN:HE22	1.62	0.46
2:D:989:ILE:HG23	2:D:1004:ASN:HB2	1.98	0.46
2:B:914:ASN:HD22	2:D:60:THR:HG23	1.81	0.46
1:C:190:ARG:NH2	1:C:221:GLY:O	2.39	0.46
1:A:217:TYR:HD1	1:A:222:LYS:HG3	1.81	0.46
1:A:256:ASP:OD1	1:A:256:ASP:N	2.49	0.46
2:B:949:THR:HG22	2:B:960:LEU:HD23	1.97	0.46
1:C:31:LEU:HB3	1:C:244:ILE:HD11	1.96	0.46
2:D:880:ASN:HD21	2:D:893:VAL:H	1.64	0.46
2:B:64:LYS:HA	2:B:64:LYS:HD2	1.77	0.45
2:B:868:ARG:HG2	2:B:868:ARG:HH21	1.81	0.45
1:C:293:ASP:OD1	1:C:293:ASP:N	2.50	0.45
2:B:179:LEU:HG	2:B:844:LEU:HD13	1.98	0.45
2:B:33:GLU:OE1	2:D:956:ARG:NH2	2.46	0.45
2:D:81:ASN:HD22	2:D:100:ASN:ND2	2.13	0.45
2:B:57:ASN:HD22	2:B:58:TYR:N	2.13	0.45
2:B:2:SER:HB3	2:B:78:ASN:HA	1.98	0.45
1:C:227:VAL:HG13	1:C:239:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:953:ASP:OD2	2:D:956:ARG:NH1	2.49	0.45
2:D:954:GLU:HG3	2:D:957:ARG:NH1	2.31	0.45
2:D:86:ARG:HH12	2:D:108:ILE:HG23	1.81	0.45
2:B:149:LEU:HA	2:B:152:VAL:HB	1.99	0.44
1:A:46:HIS:O	1:A:80:ILE:HA	2.17	0.44
1:C:46:HIS:HD1	1:C:48:GLY:H	1.65	0.44
1:A:293:ASP:OD1	1:A:293:ASP:N	2.51	0.44
1:A:136:MET:HG2	1:A:171:LEU:HD11	2.00	0.43
1:C:157:LEU:O	1:C:184:LEU:HA	2.18	0.43
1:C:25:ILE:HD13	1:C:207:GLU:HB3	2.00	0.43
2:B:53:GLY:H	2:B:56:PHE:HB3	1.83	0.43
1:A:61:LEU:HD22	1:A:99:LEU:HD12	2.00	0.43
2:B:943:ILE:O	2:B:973:MET:HA	2.18	0.43
2:B:914:ASN:ND2	2:D:60:THR:HG23	2.34	0.43
1:A:84:ASN:HD22	1:A:84:ASN:H	1.67	0.43
1:C:257:LYS:HA	1:C:284:PHE:CZ	2.54	0.43
2:D:25:LYS:HE3	2:D:25:LYS:HB2	1.88	0.43
1:A:27:ASP:O	1:A:31:LEU:HG	2.19	0.43
1:A:161:ILE:HB	1:A:164:TYR:CD2	2.54	0.43
2:B:80:ASN:HB2	2:B:82:TYR:CE1	2.54	0.43
1:A:334:ILE:HD12	2:B:857:ILE:HD11	2.00	0.43
2:D:39:SER:N	6:D:1101:AGS:O2A	2.52	0.43
2:B:906:PRO:HD2	2:D:997:ASN:HD21	1.84	0.43
1:A:328:TYR:O	1:A:332:GLN:HG2	2.19	0.43
2:B:868:ARG:HB3	2:B:868:ARG:HH21	1.82	0.43
2:D:130:ILE:HD12	2:D:942:CYS:O	2.18	0.43
1:A:13:TYR:CE2	1:A:15:GLN:HB2	2.54	0.43
1:C:161:ILE:HG22	1:C:163:PRO:HD2	2.00	0.43
1:C:6:ILE:O	1:C:46:HIS:HA	2.19	0.43
2:B:160:GLU:HA	2:B:163:LYS:HD2	2.00	0.42
1:C:172:GLU:HB2	1:C:175:ASP:OD1	2.19	0.42
2:D:72:GLU:HA	2:D:84:ILE:O	2.18	0.42
1:C:105:LYS:HA	1:C:105:LYS:HD3	1.96	0.42
2:D:179:LEU:HD11	2:D:845:THR:HG22	2.01	0.42
1:A:78:VAL:HB	1:A:104:VAL:HG22	2.00	0.42
2:B:84:ILE:HG12	2:B:97:LEU:HD13	2.02	0.42
2:D:5:LEU:HD23	2:D:75:PHE:HB3	2.02	0.42
2:B:72:GLU:HA	2:B:84:ILE:O	2.19	0.42
1:C:46:HIS:HB3	1:C:80:ILE:HG13	2.02	0.42
2:D:64:LYS:HA	2:D:64:LYS:HD3	1.84	0.42
2:D:32:GLY:N	2:D:38:LYS:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ALA:HB1	1:C:225:TYR:HE2	1.85	0.42
1:C:39:ILE:HD13	1:C:226:LEU:HD22	2.00	0.42
2:D:963:ILE:O	2:D:967:VAL:HG23	2.20	0.42
1:A:254:ILE:HD11	1:A:263:ALA:HB2	2.02	0.41
2:B:990:ILE:HG12	2:B:1003:ILE:HG23	2.02	0.41
2:B:945:LEU:HB3	2:B:948:PRO:HG3	2.01	0.41
2:D:80:ASN:HB2	2:D:82:TYR:CE1	2.54	0.41
1:A:187:ILE:HG22	1:A:202:TYR:CD1	2.56	0.41
1:A:346:LEU:HD23	2:B:167:LYS:HB3	2.02	0.41
2:B:60:THR:HG23	2:D:914:ASN:ND2	2.36	0.41
1:C:267:ILE:HD13	1:C:295:ILE:HD11	2.01	0.41
1:C:44:VAL:HB	1:C:78:VAL:HG22	2.01	0.41
1:C:61:LEU:HD22	1:C:99:LEU:HD12	2.01	0.41
4:F:15:DC:H2"	4:F:16:DT:O4'	2.21	0.41
2:B:52:ALA:HB1	2:B:56:PHE:O	2.20	0.41
1:C:160:GLY:H	1:C:170:GLU:HG2	1.85	0.41
2:B:179:LEU:HD11	2:B:844:LEU:HD22	2.03	0.41
2:B:960:LEU:HA	2:B:963:ILE:HD12	2.02	0.41
2:B:72:GLU:HB3	2:B:85:ILE:HG12	2.02	0.41
1:C:334:ILE:HD12	2:D:857:ILE:HD11	2.03	0.41
1:C:78:VAL:HB	1:C:104:VAL:HG22	2.03	0.41
1:A:208:ILE:HD13	1:A:214:TYR:HD1	1.86	0.41
1:A:188:HIS:CD2	1:A:188:HIS:N	2.88	0.40
1:A:77:LYS:HD2	1:A:77:LYS:HA	1.81	0.40
2:B:42:PHE:HZ	2:B:974:ILE:HG21	1.85	0.40
2:B:906:PRO:HD2	2:D:997:ASN:ND2	2.36	0.40
2:D:92:ARG:HH22	4:F:4:DC:N4	2.16	0.40
1:A:359:TYR:HA	1:A:363:LYS:HG3	2.03	0.40
1:C:298:ASN:OD1	1:C:298:ASN:N	2.54	0.40
2:D:952:LEU:O	2:D:957:ARG:NH2	2.54	0.40
1:C:18:LEU:HD22	1:C:297:ILE:HD13	2.03	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	348/386 (90%)	323 (93%)	25 (7%)	0	100	100
1	C	347/386 (90%)	322 (93%)	25 (7%)	0	100	100
2	B	355/372 (95%)	331 (93%)	24 (7%)	0	100	100
2	D	354/372 (95%)	328 (93%)	26 (7%)	0	100	100
All	All	1404/1516 (93%)	1304 (93%)	100 (7%)	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	322/352 (92%)	315 (98%)	7 (2%)	60	86
1	C	319/352 (91%)	307 (96%)	12 (4%)	40	76
2	B	312/325 (96%)	290 (93%)	22 (7%)	18	54
2	D	311/325 (96%)	294 (94%)	17 (6%)	27	64
All	All	1264/1354 (93%)	1206 (95%)	58 (5%)	33	70

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	186	HIS
1	A	229	PHE
1	A	233	ASP
1	A	293	ASP
1	A	323	GLU
1	A	340	LEU
2	B	56	PHE
2	B	57	ASN
2	B	64	LYS

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Mol	Chain	Res	Type
2	B	67	LYS
2	B	77	VAL
2	B	87	GLU
2	B	104	TYR
2	B	107	THR
2	B	140	PHE
2	B	179	LEU
2	B	181	ARG
2	B	832	LYS
2	B	833	GLU
2	B	844	LEU
2	B	868	ARG
2	B	892	PHE
2	B	900	GLU
2	B	935	LEU
2	B	939	ARG
2	B	942	CYS
2	B	950	VAL
2	B	977	THR
1	C	1	MET
1	C	31	LEU
1	C	84	ASN
1	C	105	LYS
1	C	175	ASP
1	C	229	PHE
1	C	233	ASP
1	C	272	ASN
1	C	291	LEU
1	C	293	ASP
1	C	346	LEU
1	C	351	ASN
2	D	4	ILE
2	D	56	PHE
2	D	62	ILE
2	D	104	TYR
2	D	107	THR
2	D	140	PHE
2	D	186	LEU
2	D	871	TYR
2	D	907	ASN
2	D	913	ASP
2	D	935	LEU

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Mol	Chain	Res	Type
2	D	940	VAL
2	D	942	CYS
2	D	950	VAL
2	D	956	ARG
2	D	977	THR
2	D	999	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	128	HIS
2	B	57	ASN
2	B	78	ASN
2	B	81	ASN
2	B	914	ASN
1	C	9	ASN
1	C	84	ASN
1	C	186	HIS
1	C	261	ASN
1	C	272	ASN
1	C	330	ASN
1	C	348	ASN
2	D	81	ASN
2	D	880	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	AGS	B	1101	-	26,33,33	0.79	1 (3%)	24,52,52	0.91	1 (4%)
6	AGS	D	1101	-	26,33,33	0.79	1 (3%)	24,52,52	0.99	1 (4%)

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	AGS	B	1101	-	-	0/17/38/38	0/3/3/3
6	AGS	D	1101	-	-	0/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1101	AGS	PG-S1G	2.56	1.95	1.90
6	B	1101	AGS	PG-S1G	2.59	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1101	AGS	PB-O3B-PG	-4.25	117.30	132.71
6	B	1101	AGS	PB-O3B-PG	-3.23	120.99	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1101	AGS	1	0
6	D	1101	AGS	2	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, 95^{th} 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	352/386 (91%)	0.15	11 (3%) 52 28	56, 109, 172, 199	0
1	C	351/386 (90%)	0.21	17 (4%) 34 15	54, 102, 178, 217	0
2	B	359/372 (96%)	0.05	7 (1%) 70 48	54, 95, 145, 176	0
2	D	358/372 (96%)	0.27	16 (4%) 37 17	68, 112, 160, 196	0
3	E	25/27 (92%)	0.44	0 100 100	122, 149, 193, 199	0
4	F	23/27 (85%)	0.10	0 100 100	91, 155, 187, 197	0
All	All	1468/1570 (93%)	0.17	51 (3%) 48 24	54, 105, 170, 217	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	184	GLY	5.6
1	A	283	GLU	5.0
2	D	188	TYR	4.8
1	C	287	TRP	4.8
1	A	287	TRP	4.4
2	D	187	ASN	4.2
2	D	134	GLN	4.2
2	B	54	SER	4.2
1	A	252	VAL	3.9
2	D	871	TYR	3.9
1	C	283	GLU	3.5
1	C	193	GLU	3.4
2	D	899	PHE	3.4
1	C	256	ASP	3.3
1	A	249	PHE	3.2
1	A	214	TYR	3.1
2	B	135	GLY	3.0
1	C	359	TYR	3.0
2	D	850	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	255	LYS	2.9
1	C	303	VAL	2.9
2	D	174	GLU	2.8
1	A	0	HIS	2.7
2	D	847	PHE	2.7
1	C	364	PHE	2.6
1	A	250	VAL	2.6
2	D	175	TYR	2.6
2	D	1005	GLY	2.5
2	B	843	LYS	2.5
1	C	324	LEU	2.5
1	C	280	ILE	2.5
2	D	995	ASP	2.4
1	C	360	TYR	2.4
2	D	39	SER	2.4
2	D	872	VAL	2.3
1	C	233	ASP	2.3
1	A	286	PRO	2.3
1	A	251	GLU	2.3
2	D	147	GLU	2.2
2	B	1002	LYS	2.2
1	C	363	LYS	2.2
1	C	292	LYS	2.2
1	A	114	ASN	2.1
2	B	938	ASN	2.1
2	B	871	TYR	2.1
1	C	272	ASN	2.1
1	C	282	ARG	2.1
1	A	294	LYS	2.0
2	D	101	GLY	2.0
2	D	936	ILE	2.0
1	C	301	ILE	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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	MG	C	402	1/1	0.97	0.42	4.12	85,85,85,85	0
5	MG	A	401	1/1	0.73	0.30	2.34	95,95,95,95	0
5	MG	C	401	1/1	0.90	0.34	2.26	93,93,93,93	0
6	AGS	D	1101	31/31	0.61	0.40	1.33	53,69,371,416	0
5	MG	A	402	1/1	0.82	0.26	1.04	80,80,80,80	0
6	AGS	B	1101	31/31	0.87	0.23	0.28	29,83,238,292	0

6.5 Other polymers

There are no such residues in this entry.