Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 PM GMT

PDB ID	:	4K2J
Title	:	Decameric ring structure of KSHV (HHV-8) latency-associated nuclear antigen (LANA) DNA binding domain
Authors	:	Domsic, J.F.; Marmorstein, R.
Deposited on	:	2013-04-09
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

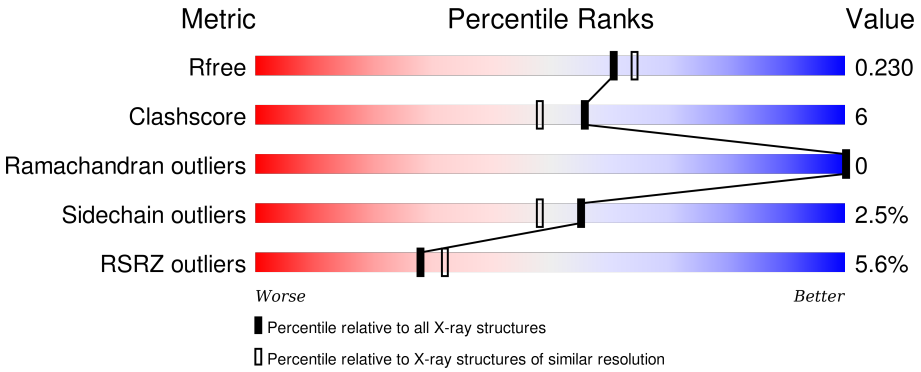
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 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	140	4% 84% 15%
1	B	140	3% 82% 14%
1	C	140	14% 85% 11%
1	D	140	11% 83% 11%
1	E	140	% 89% 9%

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Mol	Chain	Length	Quality of chain
1	F	140	95%
1	G	140	6% 80% 14%
1	H	140	9% 80% 16%
1	I	140	5% 84% 14%
1	J	140	% 79% 19%

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
2	FMT	C	1201	-	-	-	X
2	FMT	E	1202	-	-	-	X
2	FMT	I	1201	-	-	-	X
3	CL	I	1202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22577 atoms, of which 11029 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 KSHV (HHV-8) latency-associated nuclear antigen (LANA).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	138	Total	C	H	N	O	S	0	0	0
			2226	719	1113	201	187	6			
1	B	135	Total	C	H	N	O	S	0	0	0
			2183	705	1093	196	183	6			
1	C	135	Total	C	H	N	O	S	0	0	0
			2183	705	1093	196	183	6			
1	D	136	Total	C	H	N	O	S	0	0	0
			2197	710	1100	197	184	6			
1	E	137	Total	C	H	N	O	S	0	0	0
			2212	715	1108	198	185	6			
1	F	137	Total	C	H	N	O	S	0	0	0
			2204	712	1103	198	185	6			
1	G	135	Total	C	H	N	O	S	0	0	0
			2183	705	1093	196	183	6			
1	H	135	Total	C	H	N	O	S	0	0	0
			2183	705	1093	196	183	6			
1	I	138	Total	C	H	N	O	S	0	0	0
			2219	717	1111	199	186	6			
1	J	138	Total	C	H	N	O	S	0	0	0
			2226	719	1113	201	187	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
B	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
C	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
D	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
E	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
F	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
G	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
H	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0
I	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0

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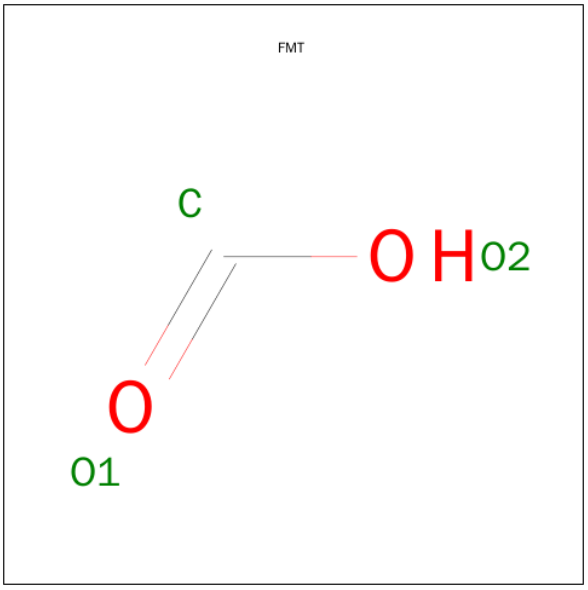
Chain	Residue	Modelled	Actual	Comment	Reference
J	1010	SER	-	EXPRESSION TAG	UNP Q9DUN0

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			4	1	1	2		
2	C	1	Total	C	H	O	0	0
			4	1	1	2		
2	C	1	Total	C	H	O	0	0
			4	1	1	2		
2	E	1	Total	C	H	O	0	0
			4	1	1	2		
2	E	1	Total	C	H	O	0	0
			4	1	1	2		
2	G	1	Total	C	H	O	0	0
			4	1	1	2		
2	I	1	Total	C	H	O	0	0
			4	1	1	2		
2	J	1	Total	C	H	O	0	0
			4	1	1	2		
2	J	1	Total	C	H	O	0	0
			4	1	1	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	4	Total Cl 4 4	0	0
3	H	3	Total Cl 3 3	0	0
3	B	2	Total Cl 2 2	0	0
3	I	4	Total Cl 4 4	0	0
3	C	2	Total Cl 2 2	0	0
3	A	2	Total Cl 2 2	0	0
3	F	3	Total Cl 3 3	0	0

- Molecule 4 is water.

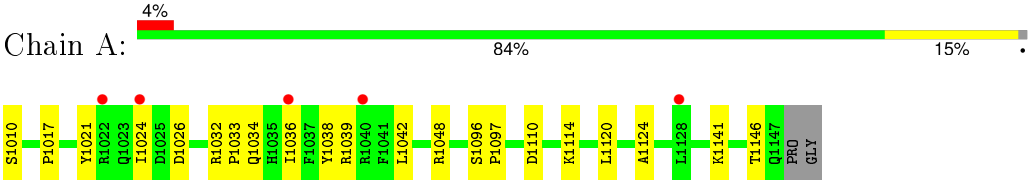
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	51	Total O 51 51	0	0
4	C	49	Total O 49 49	0	0
4	D	31	Total O 31 31	0	0
4	E	79	Total O 79 79	0	0
4	F	66	Total O 66 66	0	0
4	G	30	Total O 30 30	0	0
4	H	45	Total O 45 45	0	0
4	I	53	Total O 53 53	0	0
4	J	55	Total O 55 55	0	0

3 Residue-property plots (i)

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.

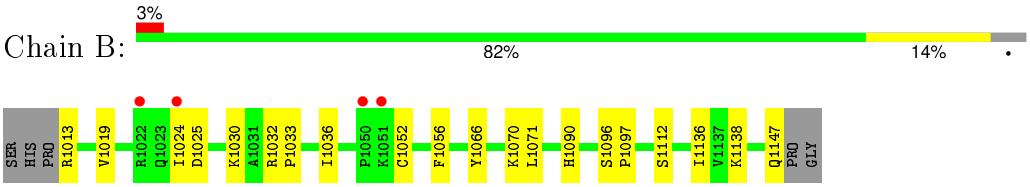
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain A:



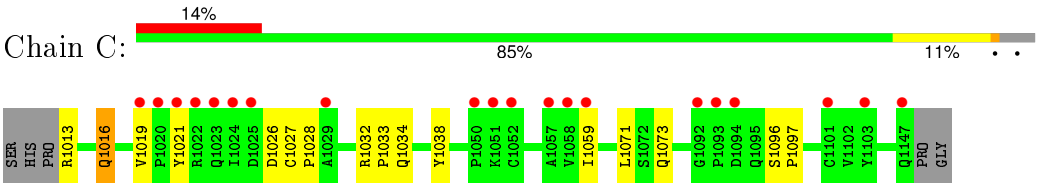
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain B:



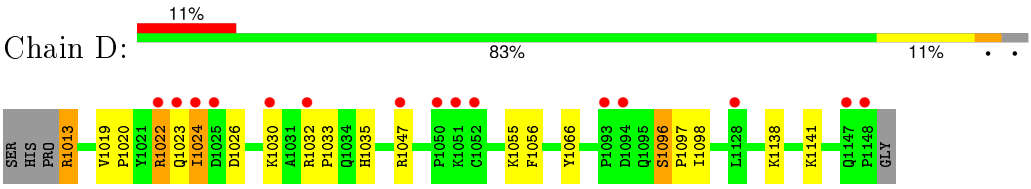
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain C:



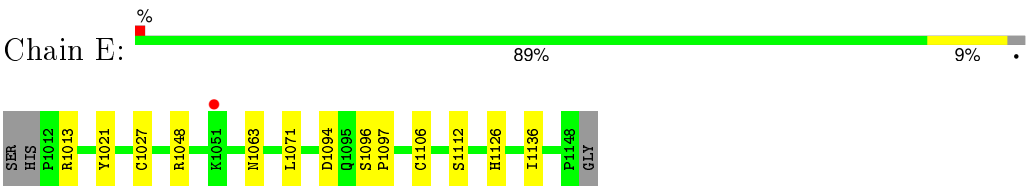
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain D:



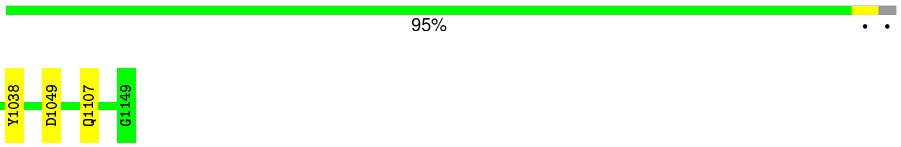
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain E:



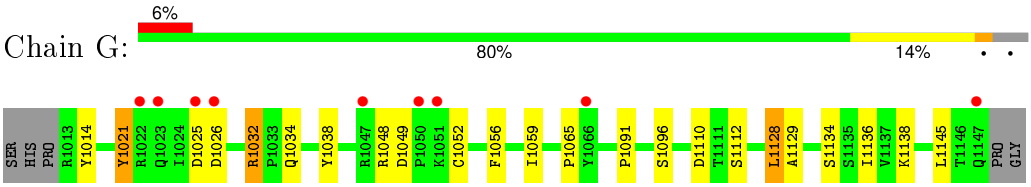
- Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain F:



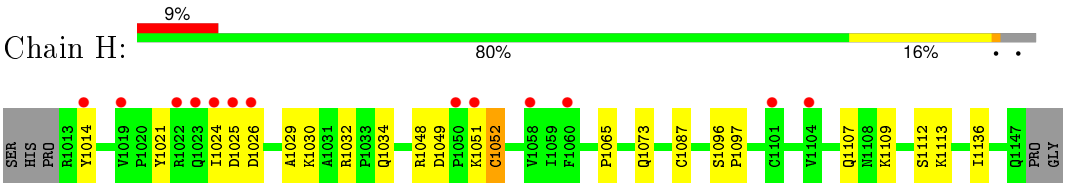
• Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain G:



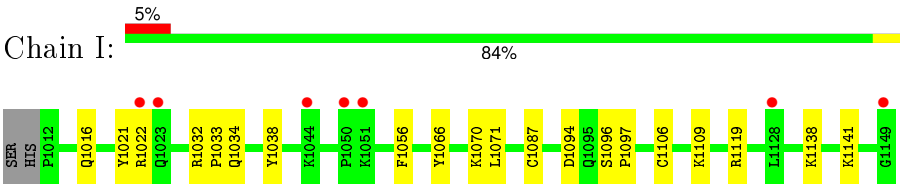
• Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain H:



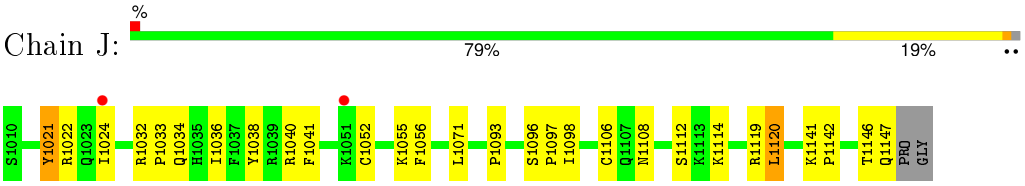
• Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain I:



• Molecule 1: KSHV (HHV-8) latency-associated nuclear antigen (LANA)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.44Å 175.18Å 97.06Å 90.00° 95.30° 90.00°	Depositor
Resolution (Å)	39.89 – 2.05 39.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.89-2.05) 95.3 (39.89-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.182 , 0.226 0.186 , 0.230	Depositor DCC
R_{free} test set	5076 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.3	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 101732 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22577	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: FMT, CL

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	0.63	0/1152	0.70	0/1563
1	B	0.69	0/1127	0.67	0/1528
1	C	0.63	0/1127	0.65	0/1528
1	D	0.72	0/1135	0.65	0/1540
1	E	0.81	1/1143 (0.1%)	0.71	0/1551
1	F	0.81	0/1139	0.70	0/1545
1	G	0.69	0/1127	0.69	0/1528
1	H	0.69	1/1127 (0.1%)	0.66	0/1528
1	I	0.71	2/1147 (0.2%)	0.69	0/1556
1	J	0.65	0/1152	0.69	0/1563
All	All	0.71	4/11376 (0.0%)	0.68	0/15430

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1087	CYS	CB-SG	-5.98	1.72	1.81
1	E	1106	CYS	CB-SG	-5.94	1.72	1.81
1	I	1087	CYS	CB-SG	-5.44	1.73	1.81
1	I	1106	CYS	CB-SG	-5.40	1.73	1.81

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	1113	1113	1109	15	0
1	B	1090	1093	1090	18	0
1	C	1090	1093	1090	12	0
1	D	1097	1100	1097	21	0
1	E	1104	1108	1105	6	0
1	F	1101	1103	1100	3	0
1	G	1090	1093	1090	17	0
1	H	1090	1093	1090	15	0
1	I	1108	1111	1108	15	0
1	J	1113	1113	1109	24	0
2	A	3	1	1	0	0
2	C	6	2	2	1	0
2	E	6	2	2	1	0
2	G	3	1	1	0	0
2	I	3	1	1	0	0
2	J	6	2	2	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	E	4	0	0	2	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	1	0
3	I	4	0	0	2	0
3	J	1	0	0	0	0
4	A	43	0	0	2	0
4	B	51	0	0	0	0
4	C	49	0	0	1	0
4	D	31	0	0	1	0
4	E	79	0	0	1	0
4	F	66	0	0	1	0
4	G	30	0	0	0	0
4	H	45	0	0	0	0
4	I	53	0	0	1	0
4	J	55	0	0	1	0
All	All	11548	11029	10997	136	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 6.

All (136) 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:D:1030:LYS:HD2	1:D:1066:TYR:OH	1.47	1.15
1:D:1022:ARG:HG3	1:D:1026:ASP:OD2	1.86	0.76
1:G:1021:TYR:HB3	1:G:1026:ASP:HB2	1.68	0.75
2:C:1202:FMT:O2	4:C:1346:HOH:O	2.02	0.75
1:G:1048:ARG:NH2	1:G:1145:LEU:O	2.21	0.74
1:D:1030:LYS:CD	1:D:1066:TYR:OH	2.33	0.73
1:I:1016:GLN:OE1	1:J:1098:ILE:HD11	1.91	0.70
1:E:1048:ARG:NH1	4:E:1378:HOH:O	2.27	0.68
1:D:1030:LYS:HD2	1:D:1066:TYR:HH	1.59	0.66
3:C:1203:CL:CL	1:D:1141:LYS:HD3	2.33	0.66
1:F:1107:GLN:HB2	4:F:1306:HOH:O	1.95	0.65
1:J:1096:SER:HB2	1:J:1097:PRO:CD	2.25	0.65
1:B:1024:ILE:HD11	1:B:1036:ILE:CG1	2.27	0.65
1:B:1024:ILE:HD11	1:B:1036:ILE:HD11	1.79	0.63
1:C:1096:SER:HB2	1:C:1097:PRO:HD2	1.80	0.63
1:I:1056:PHE:CE2	1:I:1138:LYS:HD3	2.34	0.62
1:I:1022:ARG:HD3	1:J:1093:PRO:HB3	1.80	0.61
1:G:1128:LEU:HD22	1:G:1129:ALA:N	2.14	0.61
1:C:1021:TYR:HB2	1:C:1026:ASP:HB2	1.82	0.61
1:H:1021:TYR:HB2	1:H:1026:ASP:HB2	1.81	0.61
1:D:1022:ARG:CG	1:D:1026:ASP:OD2	2.47	0.61
2:E:1202:FMT:C	3:E:1206:CL:CL	2.85	0.61
1:H:1025:ASP:O	1:H:1032:ARG:NH2	2.34	0.61
1:D:1024:ILE:HG22	1:D:1032:ARG:HD3	1.82	0.60
1:C:1096:SER:HB2	1:C:1097:PRO:CD	2.32	0.59
1:I:1016:GLN:OE1	1:J:1098:ILE:CD1	2.51	0.58
1:G:1112:SER:HB3	1:G:1136:ILE:HD12	1.87	0.57
1:D:1056:PHE:CE1	1:D:1138:LYS:HD3	2.40	0.57
1:J:1024:ILE:O	1:J:1024:ILE:HG12	2.04	0.57
1:I:1141:LYS:HD3	3:I:1202:CL:CL	2.42	0.57
1:D:1013:ARG:HB3	1:D:1013:ARG:CZ	2.35	0.56
1:G:1091:PRO:O	1:H:1048:ARG:NH2	2.38	0.56
1:H:1112:SER:OG	1:H:1136:ILE:HD12	2.06	0.56
1:G:1056:PHE:CE1	1:G:1138:LYS:HD3	2.42	0.55
1:I:1066:TYR:CE2	1:I:1070:LYS:HE2	2.42	0.54
1:A:1021:TYR:HB2	1:A:1026:ASP:HB2	1.89	0.54
1:D:1019:VAL:HG12	1:D:1020:PRO:O	2.07	0.54
1:G:1021:TYR:HB3	1:G:1026:ASP:CB	2.36	0.53
1:G:1112:SER:CB	1:G:1136:ILE:HD12	2.39	0.53
1:B:1030:LYS:CG	1:B:1070:LYS:HD3	2.38	0.53
1:B:1024:ILE:HD11	1:B:1036:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1047:ARG:HD3	4:D:1331:HOH:O	2.09	0.52
1:H:1048:ARG:NH1	3:H:1202:CL:CL	2.79	0.52
1:A:1096:SER:HB2	1:A:1097:PRO:CD	2.40	0.52
1:A:1110:ASP:O	1:A:1114:LYS:HG2	2.10	0.52
1:D:1024:ILE:HD13	1:D:1035:HIS:HD2	1.75	0.52
1:D:1013:ARG:HB3	1:D:1013:ARG:NH1	2.24	0.52
1:A:1024:ILE:HD11	1:A:1039:ARG:HD3	1.92	0.52
1:J:1096:SER:HB2	1:J:1097:PRO:HD2	1.91	0.51
1:A:1141:LYS:NZ	4:A:1324:HOH:O	2.42	0.51
1:I:1096:SER:HB2	1:I:1097:PRO:CD	2.40	0.51
1:A:1034:GLN:HG2	1:A:1038:TYR:CE2	2.46	0.51
1:J:1071:LEU:HD12	1:J:1119:ARG:HD3	1.92	0.51
1:B:1030:LYS:HG2	1:B:1070:LYS:HD3	1.93	0.50
1:A:1032:ARG:N	1:A:1033:PRO:CD	2.74	0.50
1:D:1024:ILE:CG2	1:D:1032:ARG:HD3	2.42	0.50
1:C:1016:GLN:HG2	1:D:1098:ILE:HD11	1.93	0.50
1:J:1056:PHE:CD2	1:J:1108:ASN:HA	2.47	0.50
1:F:1049:ASP:OD1	1:F:1049:ASP:O	2.30	0.50
1:I:1094:ASP:OD1	1:J:1022:ARG:NH2	2.45	0.49
1:H:1096:SER:HB3	1:H:1097:PRO:CD	2.43	0.49
1:H:1029:ALA:HA	1:H:1032:ARG:HH11	1.77	0.49
1:C:1071:LEU:HD23	1:C:1071:LEU:C	2.33	0.49
1:B:1024:ILE:CD1	1:B:1036:ILE:HG12	2.43	0.49
1:F:1034:GLN:HG2	1:F:1038:TYR:CE2	2.48	0.48
1:G:1128:LEU:HD13	1:G:1128:LEU:H	1.77	0.48
1:G:1034:GLN:HG2	1:G:1038:TYR:CE2	2.49	0.48
1:B:1024:ILE:CD1	1:B:1036:ILE:CG1	2.92	0.48
1:A:1124:ALA:O	1:J:1040:ARG:HD2	2.13	0.48
1:C:1021:TYR:CB	1:C:1026:ASP:HB2	2.44	0.48
1:I:1109:LYS:NZ	4:I:1320:HOH:O	2.45	0.48
1:G:1025:ASP:HA	1:G:1032:ARG:NH1	2.29	0.48
1:H:1030:LYS:HE2	1:H:1073:GLN:OE1	2.13	0.47
1:E:1071:LEU:C	1:E:1071:LEU:HD23	2.35	0.47
1:B:1024:ILE:CD1	1:B:1036:ILE:HD11	2.44	0.47
1:I:1021:TYR:CD1	1:I:1021:TYR:O	2.67	0.47
1:H:1096:SER:HB3	1:H:1097:PRO:HD2	1.95	0.47
1:G:1128:LEU:H	1:G:1128:LEU:CD1	2.28	0.47
1:B:1032:ARG:N	1:B:1033:PRO:HD2	2.30	0.47
1:J:1106:CYS:SG	1:J:1112:SER:HB3	2.56	0.46
1:J:1024:ILE:HD11	1:J:1036:ILE:HD11	1.98	0.46
1:H:1109:LYS:HE2	1:H:1113:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1032:ARG:N	1:D:1033:PRO:CD	2.78	0.46
1:H:1049:ASP:OD1	1:H:1051:LYS:HG2	2.16	0.45
1:C:1059:ILE:O	1:C:1059:ILE:HG23	2.15	0.45
1:E:1112:SER:HB3	1:E:1136:ILE:HD12	1.99	0.45
1:I:1022:ARG:CD	1:J:1093:PRO:HB3	2.46	0.45
1:G:1065:PRO:HB2	1:H:1014:TYR:CD2	2.52	0.45
1:B:1096:SER:HB2	1:B:1097:PRO:CD	2.46	0.45
1:B:1024:ILE:HD12	1:B:1036:ILE:HG12	1.99	0.44
1:D:1055:LYS:O	1:D:1138:LYS:HD2	2.17	0.44
1:B:1030:LYS:HG2	1:B:1066:TYR:OH	2.17	0.44
1:G:1049:ASP:OD1	1:G:1049:ASP:C	2.55	0.44
1:G:1025:ASP:HA	1:G:1032:ARG:HH11	1.82	0.44
1:I:1034:GLN:HG2	1:I:1038:TYR:CE2	2.53	0.44
1:G:1014:TYR:CE1	1:H:1065:PRO:HB2	2.52	0.44
1:J:1034:GLN:NE2	1:J:1038:TYR:OH	2.43	0.44
1:A:1038:TYR:O	1:A:1042:LEU:HD23	2.18	0.43
1:C:1032:ARG:N	1:C:1033:PRO:CD	2.81	0.43
1:H:1024:ILE:HG22	1:H:1024:ILE:O	2.17	0.43
1:C:1021:TYR:OH	1:C:1073:GLN:O	2.33	0.43
1:J:1032:ARG:N	1:J:1033:PRO:CD	2.81	0.43
1:H:1052:CYS:HB3	1:H:1107:GLN:HB3	2.00	0.43
1:E:1126:HIS:HB3	3:E:1205:CL:CL	2.56	0.43
1:A:1017:PRO:HG2	1:B:1090:HIS:NE2	2.34	0.43
1:J:1032:ARG:N	1:J:1033:PRO:HD2	2.34	0.43
1:G:1059:ILE:O	1:G:1134:SER:HA	2.19	0.43
1:C:1016:GLN:HG2	1:D:1098:ILE:CD1	2.49	0.43
1:J:1024:ILE:HD11	1:J:1036:ILE:CG1	2.49	0.42
1:C:1027:CYS:O	1:C:1028:PRO:C	2.56	0.42
1:J:1041:PHE:O	1:J:1114:LYS:HE2	2.19	0.42
1:B:1030:LYS:HG3	1:B:1070:LYS:HD3	2.01	0.42
1:J:1141:LYS:NZ	4:J:1353:HOH:O	2.50	0.42
1:A:1034:GLN:CG	1:A:1038:TYR:CE2	3.03	0.42
1:D:1056:PHE:CZ	1:D:1138:LYS:HD3	2.54	0.42
1:A:1096:SER:O	1:A:1097:PRO:C	2.58	0.42
1:D:1096:SER:CB	1:D:1097:PRO:CD	2.98	0.42
1:A:1024:ILE:HD13	1:A:1036:ILE:HG12	2.02	0.41
1:C:1034:GLN:HG2	1:C:1038:TYR:CE2	2.54	0.41
1:A:1048:ARG:NH1	4:A:1320:HOH:O	2.50	0.41
1:I:1141:LYS:CD	3:I:1202:CL:CL	3.05	0.41
1:E:1096:SER:HB2	1:E:1097:PRO:HD2	2.01	0.41
1:B:1056:PHE:CE2	1:B:1138:LYS:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:ARG:NH1	1:D:1013:ARG:CB	2.83	0.41
1:B:1112:SER:HB3	1:B:1136:ILE:HD12	2.03	0.41
1:J:1024:ILE:CD1	1:J:1036:ILE:HG12	2.51	0.41
1:I:1071:LEU:HD12	1:I:1119:ARG:HD3	2.02	0.41
1:B:1019:VAL:O	1:B:1019:VAL:HG23	2.21	0.41
1:B:1071:LEU:HD23	1:B:1071:LEU:C	2.40	0.41
1:I:1032:ARG:N	1:I:1033:PRO:CD	2.85	0.40
1:J:1146:THR:O	1:J:1147:GLN:C	2.59	0.40
1:J:1021:TYR:CD1	1:J:1021:TYR:N	2.88	0.40
1:J:1120:LEU:O	1:J:1120:LEU:HD13	2.22	0.40
1:A:1096:SER:HB2	1:A:1097:PRO:HD2	2.03	0.40
1:E:1021:TYR:CE2	1:E:1027:CYS:HB2	2.57	0.40
1:J:1055:LYS:HG2	1:J:1142:PRO:HA	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	136/140 (97%)	130 (96%)	6 (4%)	0	100	100
1	B	133/140 (95%)	128 (96%)	5 (4%)	0	100	100
1	C	133/140 (95%)	130 (98%)	3 (2%)	0	100	100
1	D	134/140 (96%)	129 (96%)	5 (4%)	0	100	100
1	E	135/140 (96%)	133 (98%)	2 (2%)	0	100	100
1	F	135/140 (96%)	133 (98%)	2 (2%)	0	100	100
1	G	133/140 (95%)	131 (98%)	2 (2%)	0	100	100
1	H	133/140 (95%)	129 (97%)	4 (3%)	0	100	100
1	I	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
1	J	136/140 (97%)	133 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1344/1400 (96%)	1309 (97%)	35 (3%)	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	120/121 (99%)	117 (98%)	3 (2%)	55 48
1	B	117/121 (97%)	113 (97%)	4 (3%)	44 36
1	C	117/121 (97%)	114 (97%)	3 (3%)	54 47
1	D	118/121 (98%)	113 (96%)	5 (4%)	36 28
1	E	119/121 (98%)	116 (98%)	3 (2%)	55 48
1	F	118/121 (98%)	118 (100%)	0	100 100
1	G	117/121 (97%)	111 (95%)	6 (5%)	29 19
1	H	117/121 (97%)	115 (98%)	2 (2%)	68 65
1	I	119/121 (98%)	119 (100%)	0	100 100
1	J	120/121 (99%)	117 (98%)	3 (2%)	55 48
All	All	1182/1210 (98%)	1153 (98%)	29 (2%)	55 48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	SER
1	A	1120	LEU
1	A	1146	THR
1	B	1013	ARG
1	B	1025	ASP
1	B	1052	CYS
1	B	1147	GLN
1	C	1013	ARG
1	C	1016	GLN

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Mol	Chain	Res	Type
1	C	1019	VAL
1	D	1013	ARG
1	D	1022	ARG
1	D	1023	GLN
1	D	1024	ILE
1	D	1096	SER
1	E	1013	ARG
1	E	1063	ASN
1	E	1094	ASP
1	G	1021	TYR
1	G	1032	ARG
1	G	1052	CYS
1	G	1096	SER
1	G	1110	ASP
1	G	1128	LEU
1	H	1034	GLN
1	H	1052	CYS
1	J	1021	TYR
1	J	1052	CYS
1	J	1120	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1126	HIS
1	J	1034	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 23 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	FMT	A	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	C	1202	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	E	1202	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	G	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	I	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	J	1201	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	J	1202	-	0,2,2	0.00	-	0,1,1	0.00	-

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
2	FMT	A	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	C	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	C	1202	-	-	0/0/0/0	0/0/0/0
2	FMT	E	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	E	1202	-	-	0/0/0/0	0/0/0/0
2	FMT	G	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	I	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	J	1201	-	-	0/0/0/0	0/0/0/0
2	FMT	J	1202	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1202	FMT	1	0
2	E	1202	FMT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	138/140 (98%)	0.23	5 (3%) 46 53	31, 49, 83, 92	0
1	B	135/140 (96%)	0.11	4 (2%) 54 61	30, 41, 71, 90	0
1	C	135/140 (96%)	0.71	20 (14%) 3 3	33, 45, 82, 104	0
1	D	136/140 (97%)	0.50	15 (11%) 7 8	33, 48, 78, 100	0
1	E	137/140 (97%)	0.03	1 (0%) 89 91	25, 38, 66, 94	0
1	F	137/140 (97%)	0.01	0 100 100	25, 38, 65, 79	0
1	G	135/140 (96%)	0.18	9 (6%) 21 24	32, 47, 82, 99	0
1	H	135/140 (96%)	0.69	13 (9%) 10 11	31, 45, 77, 91	0
1	I	138/140 (98%)	0.15	7 (5%) 32 36	26, 41, 73, 86	0
1	J	138/140 (98%)	0.04	2 (1%) 78 82	29, 45, 79, 94	0
All	All	1364/1400 (97%)	0.26	76 (5%) 28 32	25, 44, 76, 104	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1148	PRO	5.6
1	D	1147	GLN	5.4
1	D	1051	LYS	5.3
1	C	1025	ASP	5.0
1	C	1051	LYS	5.0
1	H	1050	PRO	5.0
1	C	1022	ARG	4.8
1	C	1050	PRO	4.8
1	C	1024	ILE	4.6
1	D	1050	PRO	4.5
1	D	1022	ARG	4.4
1	D	1024	ILE	4.3
1	J	1051	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	1051	LYS	4.2
1	H	1022	ARG	4.2
1	H	1025	ASP	4.1
1	B	1050	PRO	3.8
1	H	1024	ILE	3.8
1	G	1050	PRO	3.7
1	G	1022	ARG	3.7
1	E	1051	LYS	3.6
1	C	1023	GLN	3.6
1	G	1023	GLN	3.6
1	I	1050	PRO	3.4
1	D	1128	LEU	3.3
1	I	1051	LYS	3.3
1	C	1094	ASP	3.3
1	H	1058	VAL	3.2
1	A	1036	ILE	3.2
1	D	1094	ASP	3.1
1	H	1023	GLN	3.1
1	C	1021	TYR	3.1
1	B	1051	LYS	3.0
1	C	1019	VAL	3.0
1	H	1060	PHE	3.0
1	G	1026	ASP	3.0
1	I	1149	GLY	2.9
1	B	1022	ARG	2.9
1	I	1022	ARG	2.9
1	A	1128	LEU	2.8
1	H	1026	ASP	2.7
1	D	1047	ARG	2.7
1	A	1040	ARG	2.7
1	C	1103	TYR	2.7
1	C	1058	VAL	2.7
1	D	1025	ASP	2.6
1	D	1052	CYS	2.6
1	I	1128	LEU	2.6
1	C	1093	PRO	2.6
1	H	1019	VAL	2.6
1	D	1093	PRO	2.5
1	H	1101	CYS	2.4
1	J	1024	ILE	2.3
1	C	1092	GLY	2.3
1	D	1023	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1147	GLN	2.3
1	G	1147	GLN	2.3
1	H	1014	TYR	2.2
1	A	1022	ARG	2.2
1	G	1025	ASP	2.2
1	C	1052	CYS	2.2
1	A	1024	ILE	2.2
1	G	1051	LYS	2.2
1	D	1032	ARG	2.2
1	D	1030	LYS	2.2
1	C	1020	PRO	2.2
1	C	1057	ALA	2.1
1	G	1047	ARG	2.1
1	G	1066	TYR	2.1
1	H	1104	VAL	2.1
1	C	1059	ILE	2.1
1	C	1101	CYS	2.1
1	B	1024	ILE	2.1
1	I	1023	GLN	2.1
1	C	1029	ALA	2.0
1	I	1044	LYS	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 (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. 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
2	FMT	I	1201	3/3	0.81	0.26	5.63	50,51,55,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FMT	E	1202	3/3	0.84	0.16	2.15	39,42,42,50	0
2	FMT	C	1201	3/3	0.97	0.24	2.09	38,39,40,49	0
3	CL	E	1206	1/1	0.98	0.12	0.48	46,46,46,46	0
2	FMT	G	1201	3/3	0.99	0.15	0.40	32,33,34,40	0
3	CL	F	1203	1/1	0.96	0.11	0.38	46,46,46,46	0
2	FMT	A	1201	3/3	0.98	0.14	0.20	32,34,34,38	0
2	FMT	J	1202	3/3	0.97	0.11	0.09	43,45,54,64	0
2	FMT	E	1201	3/3	0.99	0.15	-0.00	30,32,33,40	0
3	CL	A	1202	1/1	0.94	0.13	-0.09	63,63,63,63	0
3	CL	H	1202	1/1	0.95	0.12	-0.70	67,67,67,67	0
3	CL	H	1203	1/1	0.97	0.14	-0.71	58,58,58,58	0
2	FMT	C	1202	3/3	0.96	0.09	-0.83	35,54,55,67	0
3	CL	F	1201	1/1	0.99	0.09	-1.03	36,36,36,36	0
3	CL	H	1201	1/1	1.00	0.16	-1.10	44,44,44,44	0
3	CL	I	1202	1/1	0.99	0.08	-1.15	40,40,40,40	0
3	CL	I	1204	1/1	0.98	0.05	-1.16	53,53,53,53	0
3	CL	D	1201	1/1	0.99	0.10	-1.26	41,41,41,41	0
3	CL	B	1202	1/1	0.97	0.06	-1.39	66,66,66,66	0
3	CL	A	1203	1/1	0.97	0.08	-1.48	43,43,43,43	0
3	CL	C	1204	1/1	0.94	0.07	-1.59	70,70,70,70	0
3	CL	B	1201	1/1	0.98	0.06	-1.84	42,42,42,42	0
3	CL	E	1203	1/1	0.98	0.08	-2.15	35,35,35,35	0
3	CL	E	1204	1/1	0.99	0.07	-2.39	50,50,50,50	0
3	CL	G	1202	1/1	0.99	0.05	-2.49	41,41,41,41	0
3	CL	I	1203	1/1	0.98	0.08	-2.75	41,41,41,41	0
2	FMT	J	1201	3/3	0.98	0.08	-2.82	32,34,36,43	0
3	CL	J	1203	1/1	1.00	0.07	-2.83	48,48,48,48	0
3	CL	C	1203	1/1	0.99	0.10	-8.25	42,42,42,42	0
3	CL	F	1202	1/1	0.96	0.14	-	55,55,55,55	0
3	CL	E	1205	1/1	0.98	0.06	-	56,56,56,56	0
3	CL	I	1205	1/1	0.92	0.12	-	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.