Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 08:48 am GMT

PDB ID	:	5A76
Title	:	KSHV LANA (ORF73) C-terminal domain, open non-ring conformation: orthorhombic crystal form
Authors	:	Ponnusamy, R.; Mcvey, C.E.
Deposited on	:	2015-07-02
Resolution	:	3.80 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 (i) 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 (1)) were used in the production of this report:

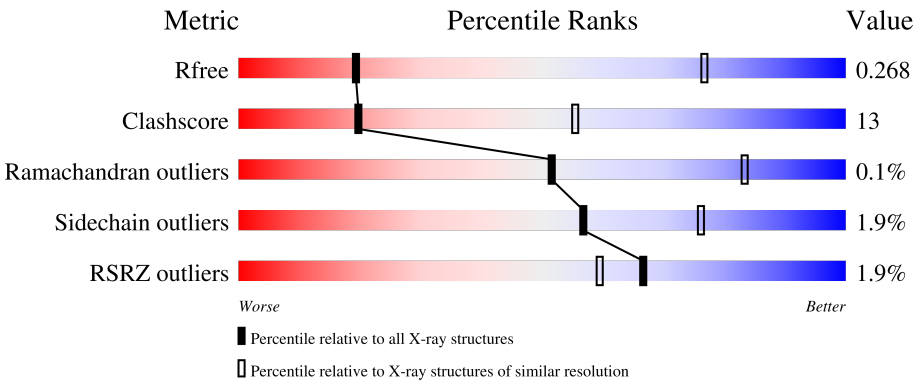
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 <=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	134	.% 63% 15% • • 19%
1	B	134	.% 69% 15% 16%
1	C	134	.% 64% 21% 15%
1	D	134	.% 72% 10% • 16%
1	E	134	3% 70% 15% • 13%

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Mol	Chain	Length	Quality of chain
1	F	134	2% 66% 22% 12%
1	G	134	4% 70% 15% 13%
1	H	134	71% 14% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7328 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 ORF 73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	109	876	575	156	140	5	0	0	0
1	B	113	909	592	164	148	5	0	0	0
1	C	114	918	597	165	151	5	0	0	0
1	D	113	905	593	162	146	4	0	0	0
1	E	116	929	606	167	151	5	0	0	0
1	F	118	943	613	169	156	5	0	0	0
1	G	116	927	604	166	152	5	0	0	0
1	H	114	917	597	165	150	5	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1017	GLY	-	expression tag	UNP Q76SB0
B	1017	GLY	-	expression tag	UNP Q76SB0
C	1017	GLY	-	expression tag	UNP Q76SB0
D	1017	GLY	-	expression tag	UNP Q76SB0
E	1017	GLY	-	expression tag	UNP Q76SB0
F	1017	GLY	-	expression tag	UNP Q76SB0
G	1017	GLY	-	expression tag	UNP Q76SB0
H	1017	GLY	-	expression tag	UNP Q76SB0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

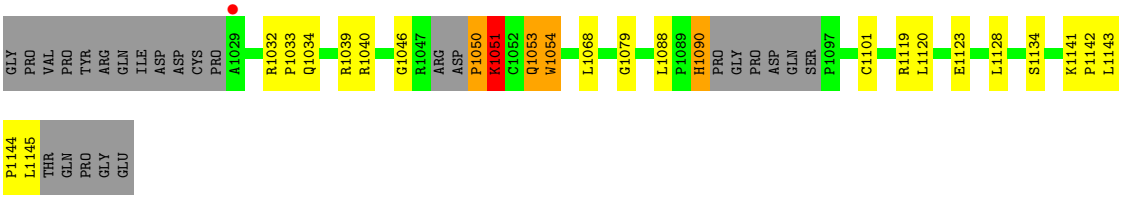
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
			Total	Mg		
2	C	1	1	1	0	0
			Total	Mg		
2	E	1	1	1	0	0
			Total	Mg		
2	G	1	1	1	0	0

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.

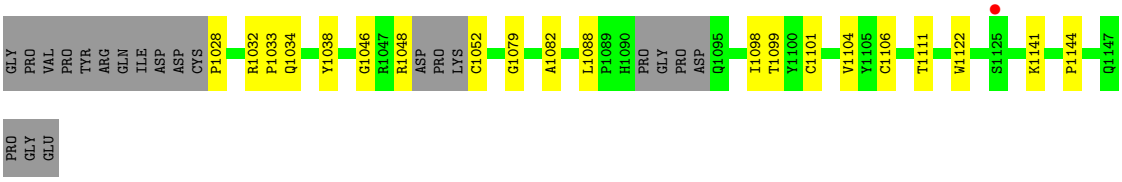
- Molecule 1: ORF 73

Chain A:



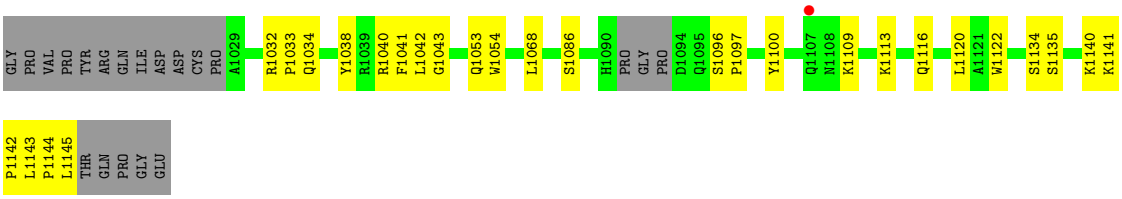
- Molecule 1: ORF 73

Chain B:



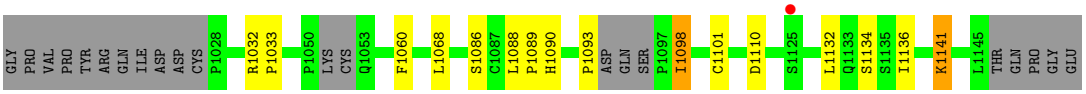
- Molecule 1: ORF 73

Chain C:



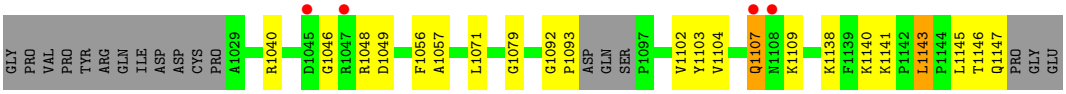
- Molecule 1: ORF 73

Chain D:



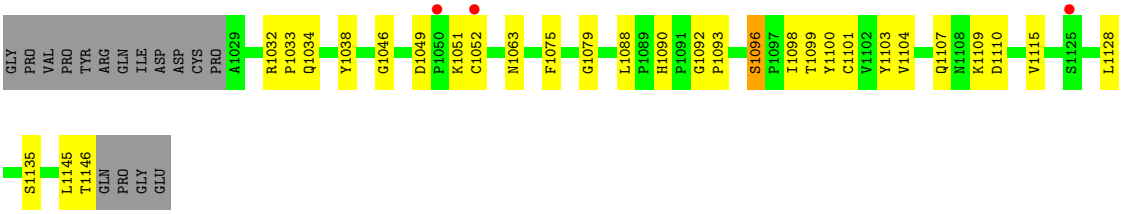
• Molecule 1: ORF 73

Chain E:



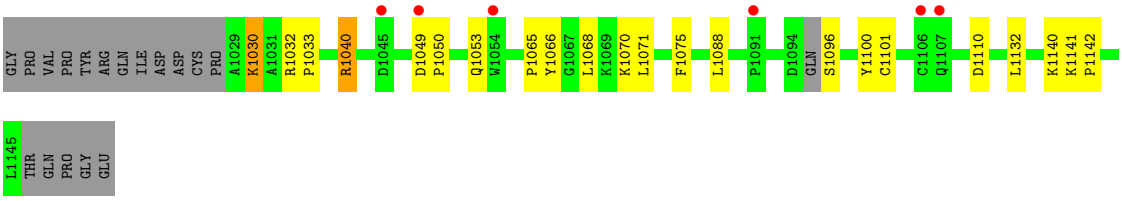
• Molecule 1: ORF 73

Chain F:



• Molecule 1: ORF 73

Chain G:



• Molecule 1: ORF 73

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	200.22Å 200.22Å 83.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.58 – 3.80 47.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (141.58-3.80) 98.8 (47.19-3.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.221 , 0.269 0.223 , 0.268	Depositor DCC
R_{free} test set	853 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	1.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.100 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7328	wwPDB-VP
Average B, all atoms (Å^2)	80.0	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 36.55 % 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 4.9116e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG

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	1.30	2/903 (0.2%)	0.92	5/1214 (0.4%)
1	B	0.59	0/936	0.66	1/1260 (0.1%)
1	C	0.62	0/946	0.68	0/1275
1	D	0.65	0/935	0.73	2/1261 (0.2%)
1	E	0.61	0/959	0.69	0/1294
1	F	0.58	0/974	0.75	2/1317 (0.2%)
1	G	0.64	0/957	0.66	2/1292 (0.2%)
1	H	0.58	0/945	0.67	2/1274 (0.2%)
All	All	0.73	2/7555 (0.0%)	0.72	14/10187 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1050	PRO	C-N	-29.28	0.66	1.34
1	A	1051	LYS	C-N	-18.24	0.92	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1051	LYS	C-N-CA	13.42	155.25	121.70
1	A	1051	LYS	O-C-N	-11.95	103.58	122.70
1	A	1128	LEU	CB-CG-CD2	-8.87	95.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1110	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	D	1110	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	1051	LYS	CA-C-N	7.51	133.73	117.20
1	F	1096	SER	C-N-CD	-6.92	105.38	120.60
1	H	1110	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	H	1141	LYS	CD-CE-NZ	6.11	125.76	111.70
1	B	1048	ARG	CB-CA-C	-5.61	99.19	110.40
1	G	1040	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	1141	LYS	CD-CE-NZ	5.36	124.03	111.70
1	G	1030	LYS	CB-CG-CD	5.08	124.80	111.60
1	A	1120	LEU	CB-CG-CD2	-5.04	102.42	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	LYS	Peptide

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	876	0	893	28	0
1	B	909	0	922	15	0
1	C	918	0	928	48	0
1	D	905	0	918	28	0
1	E	929	0	944	27	0
1	F	943	0	953	34	0
1	G	927	0	937	39	0
1	H	917	0	931	14	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
All	All	7328	0	7426	188	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 13.

All (188) 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:1050:PRO:CA	1:A:1051:LYS:N	1.87	1.35
1:A:1050:PRO:C	1:A:1051:LYS:CA	1.93	1.34
1:A:1050:PRO:O	1:A:1051:LYS:N	1.71	1.20
1:D:1098:ILE:HG22	1:G:1040:ARG:HD2	1.27	1.10
1:C:1040:ARG:HG3	1:F:1098:ILE:CD1	1.82	1.08
1:C:1054:TRP:CG	1:C:1145:LEU:HD11	1.87	1.08
1:C:1054:TRP:CD2	1:C:1145:LEU:HD11	1.93	1.03
1:F:1049:ASP:OD2	1:F:1052:CYS:SG	2.18	1.02
1:C:1040:ARG:HD2	1:F:1098:ILE:HG12	1.40	1.01
1:C:1040:ARG:HG3	1:F:1098:ILE:HD11	1.01	0.99
1:B:1098:ILE:HD11	1:E:1040:ARG:HG3	1.43	0.98
1:D:1098:ILE:HG22	1:G:1040:ARG:CD	1.95	0.96
1:C:1054:TRP:CD2	1:C:1145:LEU:CD1	2.49	0.95
1:C:1040:ARG:CG	1:F:1098:ILE:HD11	1.96	0.95
1:A:1053:GLN:N	1:A:1053:GLN:OE1	2.03	0.91
1:C:1054:TRP:CG	1:C:1145:LEU:CD1	2.53	0.90
1:D:1093:PRO:CD	1:G:1040:ARG:HH22	1.85	0.89
1:E:1056:PHE:CE2	1:E:1109:LYS:HB2	2.08	0.88
1:D:1093:PRO:HD2	1:G:1040:ARG:HH22	1.39	0.86
1:E:1057:ALA:HB1	1:E:1104:VAL:O	1.76	0.86
1:G:1049:ASP:CG	1:G:1050:PRO:HD2	1.96	0.86
1:D:1098:ILE:H	1:D:1098:ILE:HD13	1.42	0.85
1:C:1054:TRP:CD1	1:C:1145:LEU:HD12	2.12	0.84
1:C:1034:GLN:HG2	1:C:1122:TRP:CZ2	2.12	0.84
1:G:1049:ASP:CG	1:G:1050:PRO:CD	2.46	0.84
1:E:1049:ASP:H	1:E:1107:GLN:HE22	1.29	0.81
1:G:1141:LYS:CE	1:H:1134:SER:O	2.29	0.81
1:C:1040:ARG:CD	1:F:1098:ILE:HG12	2.09	0.81
1:C:1054:TRP:CE2	1:C:1145:LEU:CD1	2.65	0.80
1:D:1093:PRO:HD2	1:G:1040:ARG:NH2	1.98	0.78
1:H:1145:LEU:O	1:H:1146:THR:OG1	2.02	0.76
1:E:1056:PHE:CD2	1:E:1109:LYS:N	2.54	0.76
1:G:1049:ASP:OD1	1:G:1050:PRO:CD	2.34	0.76
1:G:1141:LYS:HE3	1:H:1134:SER:O	1.87	0.74
1:G:1049:ASP:OD1	1:G:1050:PRO:HD3	1.88	0.73
1:C:1054:TRP:CD1	1:C:1145:LEU:CD1	2.69	0.73
1:E:1056:PHE:HD2	1:E:1109:LYS:N	1.87	0.72
1:A:1050:PRO:C	1:A:1051:LYS:N	0.66	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1066:TYR:CE1	1:G:1070:LYS:HE3	2.25	0.71
1:C:1034:GLN:HG2	1:C:1122:TRP:CE2	2.25	0.70
1:A:1050:PRO:CB	1:A:1051:LYS:N	2.57	0.68
1:C:1143:LEU:N	1:C:1143:LEU:HD23	2.11	0.65
1:C:1034:GLN:CG	1:C:1122:TRP:CZ2	2.79	0.65
1:E:1057:ALA:CB	1:E:1104:VAL:O	2.43	0.65
1:E:1141:LYS:HE2	1:F:1135:SER:HA	1.77	0.65
1:A:1050:PRO:O	1:A:1051:LYS:CA	2.33	0.65
1:E:1048:ARG:NH1	1:E:1146:THR:HG21	2.12	0.64
1:C:1054:TRP:CE2	1:C:1145:LEU:HD13	2.32	0.64
1:D:1093:PRO:HD3	1:G:1040:ARG:HH22	1.62	0.63
1:B:1098:ILE:HD12	1:B:1098:ILE:N	2.14	0.62
1:G:1071:LEU:C	1:G:1071:LEU:HD23	2.20	0.62
1:G:1049:ASP:OD1	1:G:1050:PRO:HD2	1.99	0.61
1:F:1063:ASN:OD1	1:F:1099:THR:HG22	2.00	0.61
1:F:1098:ILE:O	1:F:1098:ILE:HG22	2.01	0.61
1:D:1098:ILE:CG2	1:G:1040:ARG:HD2	2.17	0.60
1:C:1040:ARG:NH1	1:F:1096:SER:OG	2.35	0.60
1:C:1135:SER:HA	1:D:1141:LYS:HE2	1.83	0.60
1:B:1028:PRO:O	1:B:1032:ARG:N	2.35	0.60
1:F:1034:GLN:HG2	1:F:1038:TYR:CE2	2.36	0.59
1:D:1098:ILE:H	1:D:1098:ILE:CD1	2.14	0.59
1:C:1116:GLN:O	1:C:1120:LEU:HG	2.03	0.59
1:G:1141:LYS:HB2	1:H:1135:SER:HB2	1.84	0.58
1:D:1098:ILE:CG2	1:G:1040:ARG:CD	2.75	0.58
1:A:1088:LEU:CD1	1:A:1101:CYS:SG	2.92	0.58
1:C:1040:ARG:HH12	1:F:1090:HIS:HB2	1.69	0.58
1:E:1056:PHE:CD2	1:E:1109:LYS:CA	2.86	0.58
1:C:1140:LYS:HE2	1:D:1136:ILE:HD12	1.85	0.57
1:F:1052:CYS:HB2	1:F:1107:GLN:HE21	1.69	0.57
1:A:1053:GLN:H	1:A:1053:GLN:CD	2.08	0.57
1:C:1145:LEU:HD12	1:C:1145:LEU:C	2.24	0.57
1:C:1054:TRP:NE1	1:C:1145:LEU:HD12	2.20	0.57
1:B:1098:ILE:H	1:B:1098:ILE:CD1	2.18	0.56
1:A:1054:TRP:N	1:A:1054:TRP:CD1	2.72	0.56
1:C:1041:PHE:HA	1:F:1098:ILE:HD12	1.87	0.56
1:D:1089:PRO:O	1:D:1090:HIS:ND1	2.37	0.56
1:G:1049:ASP:OD2	1:G:1050:PRO:HD2	2.05	0.56
1:E:1147:GLN:O	1:E:1147:GLN:HG2	2.05	0.56
1:C:1145:LEU:HD23	1:D:1089:PRO:HD2	1.89	0.55
1:A:1050:PRO:O	1:A:1051:LYS:HA	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1053:GLN:HB3	1:C:1142:PRO:HB3	1.88	0.55
1:D:1093:PRO:HD2	1:G:1040:ARG:CZ	2.37	0.55
1:F:1075:PHE:HE2	1:F:1115:VAL:HG13	1.73	0.54
1:A:1090:HIS:CD2	1:A:1090:HIS:N	2.73	0.54
1:C:1034:GLN:HA	1:C:1122:TRP:CZ3	2.42	0.54
1:G:1071:LEU:CD2	1:G:1075:PHE:HD2	2.20	0.54
1:A:1143:LEU:HD12	1:A:1143:LEU:N	2.24	0.53
1:D:1093:PRO:HD2	1:G:1040:ARG:NH1	2.24	0.53
1:G:1071:LEU:HD23	1:G:1071:LEU:O	2.08	0.53
1:E:1143:LEU:CD1	1:E:1143:LEU:N	2.72	0.52
1:H:1096:SER:HB3	1:H:1097:PRO:HD2	1.90	0.52
1:C:1134:SER:O	1:D:1141:LYS:HE2	2.10	0.52
1:G:1068:LEU:HD11	1:G:1132:LEU:HD21	1.91	0.52
1:C:1040:ARG:CD	1:F:1098:ILE:CG1	2.85	0.52
1:B:1098:ILE:N	1:B:1098:ILE:CD1	2.73	0.51
1:H:1060:PHE:CD1	1:H:1134:SER:HB3	2.45	0.51
1:F:1051:LYS:NZ	1:F:1051:LYS:HB2	2.25	0.51
1:E:1048:ARG:HH12	1:E:1146:THR:HG21	1.76	0.51
1:G:1053:GLN:HB3	1:G:1142:PRO:HB3	1.92	0.50
1:C:1040:ARG:CG	1:F:1098:ILE:CD1	2.71	0.50
1:E:1056:PHE:CE2	1:E:1109:LYS:N	2.78	0.50
1:A:1090:HIS:CD2	1:A:1090:HIS:H	2.30	0.50
1:C:1054:TRP:CD2	1:C:1145:LEU:HD13	2.46	0.50
1:D:1093:PRO:HD2	1:G:1040:ARG:HH12	1.76	0.50
1:B:1098:ILE:HD12	1:B:1098:ILE:H	1.75	0.49
1:A:1068:LEU:HD12	1:A:1068:LEU:N	2.26	0.49
1:E:1092:GLY:N	1:E:1093:PRO:HD2	2.28	0.49
1:F:1145:LEU:O	1:F:1146:THR:HG22	2.13	0.49
1:C:1140:LYS:CE	1:D:1136:ILE:HD12	2.43	0.49
1:C:1040:ARG:HH12	1:F:1090:HIS:CB	2.26	0.49
1:F:1075:PHE:CE2	1:F:1115:VAL:HG13	2.47	0.49
1:C:1054:TRP:NE1	1:C:1145:LEU:CD1	2.76	0.48
1:D:1098:ILE:HD13	1:D:1098:ILE:N	2.17	0.48
1:A:1040:ARG:HH12	1:H:1095:GLN:HG2	1.79	0.48
1:A:1134:SER:O	1:B:1141:LYS:HE2	2.12	0.48
1:B:1082:ALA:HB2	1:B:1104:VAL:HG12	1.96	0.48
1:C:1109:LYS:HE2	1:C:1113:LYS:HE3	1.96	0.48
1:G:1140:LYS:HD2	1:H:1136:ILE:HD12	1.94	0.47
1:C:1086:SER:HB3	1:D:1086:SER:OG	2.14	0.47
1:E:1046:GLY:O	1:E:1079:GLY:N	2.47	0.47
1:D:1032:ARG:N	1:D:1033:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:GLN:HG2	1:B:1038:TYR:CE2	2.49	0.47
1:F:1088:LEU:HD11	1:F:1101:CYS:HB3	1.96	0.47
1:C:1144:PRO:O	1:C:1145:LEU:C	2.52	0.47
1:G:1066:TYR:CE1	1:G:1070:LYS:HG3	2.50	0.47
1:H:1060:PHE:HB3	1:H:1132:LEU:HD23	1.97	0.47
1:B:1032:ARG:N	1:B:1033:PRO:HD2	2.30	0.47
1:C:1145:LEU:HD22	1:D:1089:PRO:HG2	1.98	0.46
1:E:1146:THR:HG22	1:E:1147:GLN:N	2.30	0.46
1:E:1140:LYS:HE2	1:F:1109:LYS:NZ	2.30	0.46
1:B:1046:GLY:O	1:B:1079:GLY:N	2.48	0.46
1:E:1056:PHE:HE2	1:E:1109:LYS:H	1.62	0.46
1:F:1032:ARG:N	1:F:1033:PRO:HD2	2.31	0.46
1:C:1141:LYS:HE2	1:D:1134:SER:O	2.16	0.45
1:G:1065:PRO:HB3	1:G:1100:TYR:CD2	2.50	0.45
1:C:1034:GLN:HB3	1:C:1038:TYR:CE2	2.52	0.45
1:A:1032:ARG:N	1:A:1033:PRO:HD2	2.31	0.45
1:E:1057:ALA:CA	1:E:1104:VAL:O	2.65	0.45
1:A:1054:TRP:HE1	1:A:1145:LEU:HB2	1.82	0.45
1:B:1106:CYS:HB3	1:B:1111:THR:HG23	1.99	0.44
1:G:1071:LEU:C	1:G:1071:LEU:CD2	2.86	0.44
1:G:1066:TYR:CD1	1:G:1066:TYR:O	2.70	0.44
1:G:1141:LYS:HE2	1:H:1134:SER:O	2.12	0.44
1:A:1119:ARG:NE	1:A:1123:GLU:OE2	2.48	0.44
1:F:1075:PHE:CD2	1:F:1104:VAL:HG11	2.53	0.44
1:B:1098:ILE:HD11	1:E:1040:ARG:CG	2.30	0.44
1:D:1098:ILE:CD1	1:D:1098:ILE:N	2.78	0.44
1:F:1075:PHE:HD2	1:F:1104:VAL:HG11	1.83	0.43
1:C:1040:ARG:NH1	1:F:1090:HIS:HB2	2.31	0.43
1:D:1088:LEU:HD11	1:D:1101:CYS:HB3	2.00	0.43
1:D:1068:LEU:CD1	1:D:1132:LEU:HD21	2.48	0.43
1:H:1056:PHE:CE1	1:H:1138:LYS:HD3	2.54	0.43
1:A:1034:GLN:OE1	1:A:1119:ARG:NH1	2.51	0.43
1:B:1088:LEU:HD11	1:B:1101:CYS:HB3	2.01	0.43
1:E:1056:PHE:CE2	1:E:1109:LYS:CB	2.92	0.43
1:A:1053:GLN:HG2	1:A:1142:PRO:HB3	2.01	0.43
1:F:1092:GLY:N	1:F:1093:PRO:HD2	2.33	0.43
1:E:1056:PHE:CE1	1:E:1138:LYS:HD3	2.53	0.43
1:G:1066:TYR:CD1	1:G:1070:LYS:HE3	2.54	0.43
1:C:1040:ARG:C	1:F:1098:ILE:HD11	2.39	0.42
1:G:1088:LEU:HD11	1:G:1101:CYS:HB3	2.01	0.42
1:G:1071:LEU:HD23	1:G:1075:PHE:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1046:GLY:O	1:F:1079:GLY:N	2.52	0.42
1:F:1146:THR:O	1:F:1146:THR:OG1	2.32	0.42
1:F:1098:ILE:O	1:F:1100:TYR:CE1	2.72	0.42
1:C:1096:SER:N	1:C:1097:PRO:CD	2.83	0.42
1:D:1060:PHE:HB3	1:D:1132:LEU:HD23	2.01	0.42
1:C:1032:ARG:N	1:C:1033:PRO:HD2	2.34	0.42
1:G:1032:ARG:N	1:G:1033:PRO:HD2	2.35	0.42
1:G:1068:LEU:HD11	1:G:1132:LEU:CD2	2.50	0.42
1:E:1071:LEU:HD22	1:E:1102:VAL:HG11	2.01	0.42
1:A:1050:PRO:HB2	1:A:1051:LYS:N	2.33	0.41
1:H:1032:ARG:N	1:H:1033:PRO:HD2	2.35	0.41
1:E:1146:THR:CG2	1:E:1147:GLN:N	2.83	0.41
1:F:1145:LEU:C	1:F:1146:THR:CG2	2.87	0.41
1:E:1103:TYR:CE2	1:F:1103:TYR:CZ	3.08	0.41
1:A:1145:LEU:C	1:A:1145:LEU:HD23	2.41	0.41
1:A:1040:ARG:HD3	1:H:1090:HIS:CE1	2.56	0.40
1:A:1088:LEU:HD12	1:A:1101:CYS:SG	2.61	0.40
1:H:1088:LEU:HD11	1:H:1101:CYS:HB3	2.02	0.40
1:A:1046:GLY:O	1:A:1079:GLY:N	2.54	0.40
1:C:1068:LEU:HD12	1:C:1100:TYR:HB2	2.02	0.40
1:C:1145:LEU:CD1	1:C:1145:LEU:C	2.90	0.40
1:G:1066:TYR:O	1:G:1066:TYR:HD1	2.05	0.40
1:C:1042:LEU:O	1:C:1043:GLY:C	2.60	0.40
1:E:1145:LEU:HA	1:E:1145:LEU:HD13	1.70	0.40
1:A:1143:LEU:HB3	1:A:1144:PRO:HD2	2.03	0.40
1:B:1034:GLN:HA	1:B:1122:TRP:CZ3	2.56	0.40
1:G:1068:LEU:N	1:G:1068:LEU:HD12	2.36	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	103/134 (77%)	99 (96%)	4 (4%)	0	100	100
1	B	107/134 (80%)	105 (98%)	1 (1%)	1 (1%)	17	54
1	C	110/134 (82%)	108 (98%)	2 (2%)	0	100	100
1	D	107/134 (80%)	104 (97%)	3 (3%)	0	100	100
1	E	112/134 (84%)	110 (98%)	2 (2%)	0	100	100
1	F	116/134 (87%)	112 (97%)	4 (3%)	0	100	100
1	G	112/134 (84%)	109 (97%)	3 (3%)	0	100	100
1	H	110/134 (82%)	108 (98%)	2 (2%)	0	100	100
All	All	877/1072 (82%)	855 (98%)	21 (2%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1144	PRO

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	92/114 (81%)	86 (94%)	6 (6%)	17	48
1	B	96/114 (84%)	94 (98%)	2 (2%)	53	74
1	C	97/114 (85%)	97 (100%)	0	100	100
1	D	95/114 (83%)	94 (99%)	1 (1%)	73	85
1	E	98/114 (86%)	96 (98%)	2 (2%)	55	75
1	F	100/114 (88%)	99 (99%)	1 (1%)	76	86
1	G	98/114 (86%)	95 (97%)	3 (3%)	40	65
1	H	97/114 (85%)	97 (100%)	0	100	100
All	All	773/912 (85%)	758 (98%)	15 (2%)	57	76

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1039	ARG
1	A	1051	LYS
1	A	1053	GLN
1	A	1054	TRP
1	A	1090	HIS
1	A	1141	LYS
1	B	1052	CYS
1	B	1099	THR
1	D	1098	ILE
1	E	1107	GLN
1	E	1143	LEU
1	F	1128	LEU
1	G	1030	LYS
1	G	1096	SER
1	G	1110	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1090	HIS
1	D	1063	ASN
1	E	1107	GLN
1	E	1147	GLN
1	F	1107	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1051:LYS	C	1052:CYS	N	0.92
1	A	1050:PRO	C	1051:LYS	N	0.66

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	109/134 (81%)	0.22	1 (0%)	84	79	43, 70, 113, 149	0
1	B	113/134 (84%)	0.29	1 (0%)	84	79	50, 79, 122, 151	0
1	C	114/134 (85%)	0.27	1 (0%)	84	79	45, 70, 129, 153	0
1	D	113/134 (84%)	0.26	1 (0%)	84	79	47, 72, 114, 144	0
1	E	116/134 (86%)	0.19	4 (3%)	45	37	50, 72, 136, 165	0
1	F	118/134 (88%)	0.34	3 (2%)	57	49	54, 84, 132, 153	0
1	G	116/134 (86%)	0.24	6 (5%)	27	24	47, 73, 127, 159	0
1	H	114/134 (85%)	0.25	0	100	100	50, 76, 122, 140	0
All	All	913/1072 (85%)	0.26	17 (1%)	66	59	43, 75, 129, 165	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1125	SER	3.8
1	G	1107	GLN	2.9
1	D	1125	SER	2.7
1	F	1125	SER	2.6
1	E	1047	ARG	2.4
1	G	1106	CYS	2.4
1	C	1107	GLN	2.3
1	F	1052	CYS	2.2
1	A	1029	ALA	2.2
1	E	1045	ASP	2.2
1	F	1050	PRO	2.2
1	G	1049	ASP	2.2
1	G	1045	ASP	2.1
1	E	1108	ASN	2.1
1	G	1054	TRP	2.1
1	E	1107	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	1091	PRO	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
2	MG	A	2146	1/1	0.82	0.27	19,19,19,19	0
2	MG	C	2146	1/1	0.86	0.29	26,26,26,26	0
2	MG	E	2146	1/1	0.90	0.19	12,12,12,12	0
2	MG	G	2146	1/1	0.90	0.34	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.