Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:54 AM GMT

PDB ID	:	2YPY
Title	:	KSHV LANA (ORF73) C-terminal domain, decameric ring: monoclinic crystal form
Authors	:	Hellert, J.; Krausze, J.; Luhrs, T.
Deposited on	:	2012-11-02
Resolution	:	2.45 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 ⓘ) were used in the production of this report:

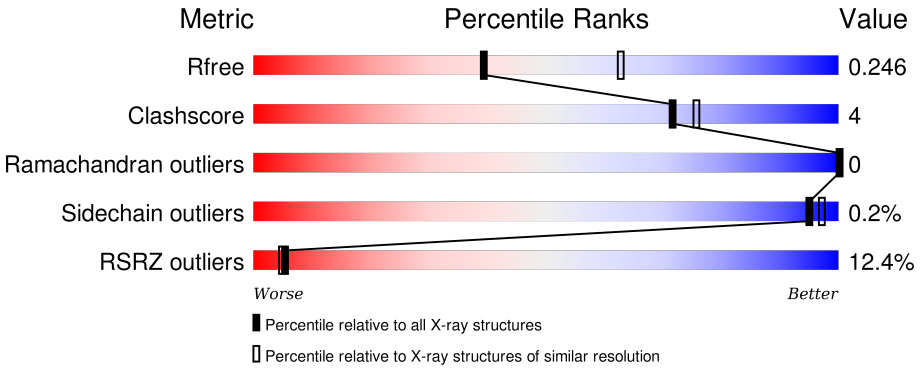
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	139	13% 85% 12%
1	B	139	4% 87% 10%
1	C	139	12% 86% 12%
1	D	139	11% 90% 7%
1	E	139	6% 88% 10%

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Mol	Chain	Length	Quality of chain
1	F	139	12% 86% 10%
1	G	139	25% 81% 14%
1	H	139	12% 84% 12%
1	I	139	12% 88% 9%
1	J	139	14% 81% 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
2	CL	B	2151	-	-	X	-
2	CL	G	2147	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11040 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
1	A	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			
1	B	136	Total	C	N	O	S	0	1	0
			1103	715	195	187	6			
1	C	135	Total	C	N	O	S	0	1	0
			1098	713	194	185	6			
1	D	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	6			
1	E	136	Total	C	N	O	S	0	1	0
			1103	715	195	187	6			
1	F	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			
1	G	133	Total	C	N	O	S	0	1	0
			1082	703	191	182	6			
1	H	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			
1	I	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			
1	J	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
A	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
B	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
B	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
C	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
C	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
D	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
D	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
E	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
F	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
F	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
G	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
G	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
H	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
H	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
I	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
I	1012	SER	-	EXPRESSION TAG	UNP Q76SB0
J	1011	GLY	-	EXPRESSION TAG	UNP Q76SB0
J	1012	SER	-	EXPRESSION TAG	UNP Q76SB0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	B	20	Total O 20 20	0	0

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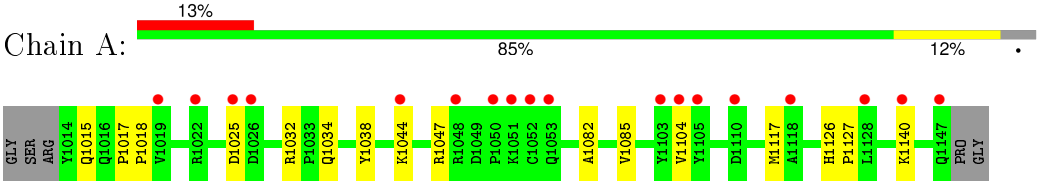
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	14	Total O 14 14	0	0
3	D	17	Total O 17 17	0	0
3	E	27	Total O 27 27	0	0
3	F	10	Total O 10 10	0	0
3	G	12	Total O 12 12	0	0
3	H	9	Total O 9 9	0	0
3	I	15	Total O 15 15	0	0
3	J	6	Total O 6 6	0	0

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.

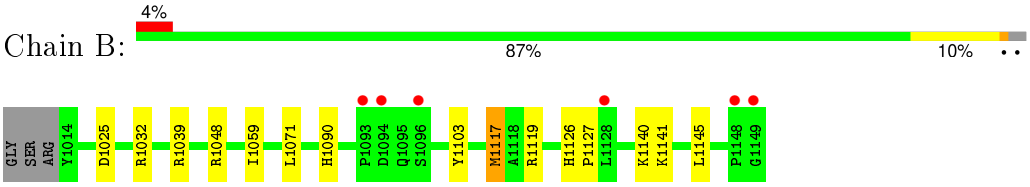
- Molecule 1: ORF 73

Chain A:



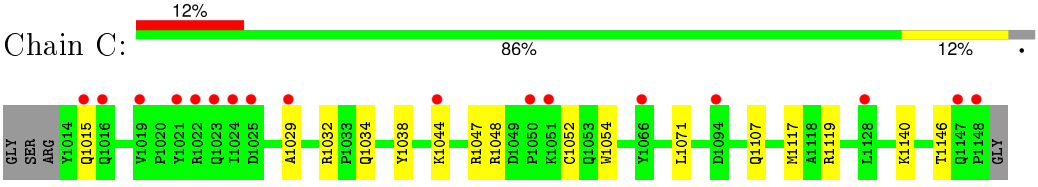
- Molecule 1: ORF 73

Chain B:



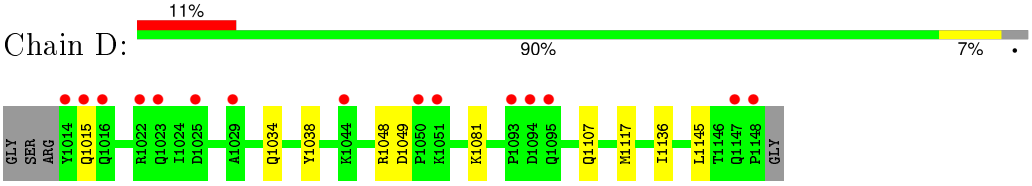
- Molecule 1: ORF 73

Chain C:



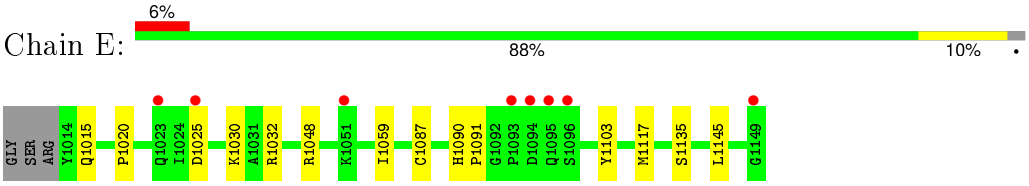
- Molecule 1: ORF 73

Chain D:



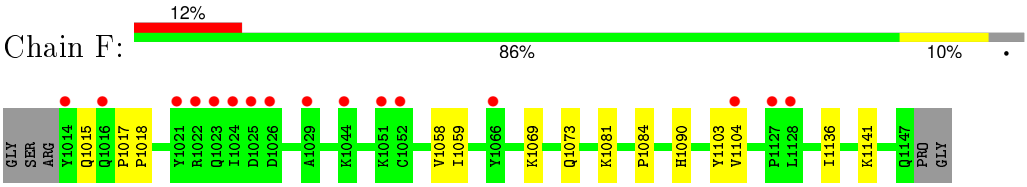
- Molecule 1: ORF 73

Chain E:



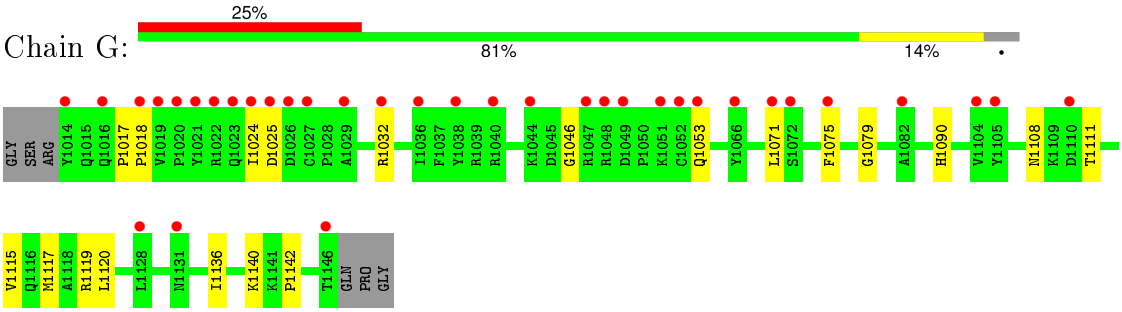
- Molecule 1: ORF 73

Chain F:



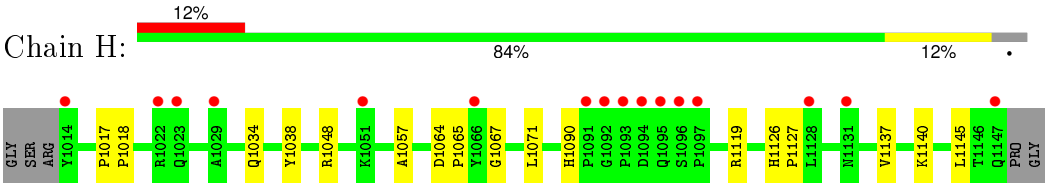
• Molecule 1: ORF 73

Chain G:



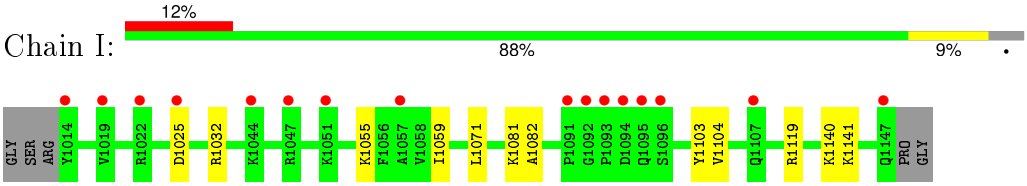
• Molecule 1: ORF 73

Chain H:



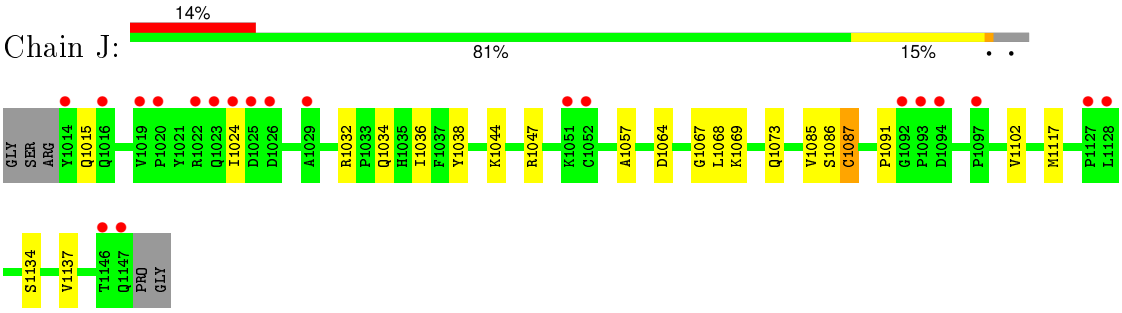
• Molecule 1: ORF 73

Chain I:



• Molecule 1: ORF 73

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	51.74Å 175.92Å 97.58Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	19.65 – 2.45 19.65 – 2.45	Depositor EDS
% Data completeness (in resolution range)	85.9 (19.65-2.45) 85.9 (19.65-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.46Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.252 0.213 , 0.246	Depositor DCC
R_{free} test set	2764 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 54311 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11040	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: 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	0.23	0/1116	0.38	0/1514
1	B	0.23	0/1142	0.38	0/1549
1	C	0.23	0/1137	0.38	0/1544
1	D	0.23	0/1124	0.39	0/1526
1	E	0.24	0/1142	0.40	0/1549
1	F	0.23	0/1116	0.37	0/1514
1	G	0.23	0/1120	0.38	0/1520
1	H	0.22	0/1116	0.37	0/1514
1	I	0.23	0/1116	0.38	0/1514
1	J	0.23	0/1116	0.38	0/1514
All	All	0.23	0/11245	0.38	0/15258

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	1079	0	1077	10	0
1	B	1103	0	1095	10	0
1	C	1098	0	1092	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1086	0	1084	10	0
1	E	1103	0	1095	14	0
1	F	1079	0	1077	13	0
1	G	1082	0	1077	13	0
1	H	1079	0	1077	11	0
1	I	1079	0	1077	7	0
1	J	1079	0	1077	13	0
2	A	2	0	0	1	0
2	B	4	0	0	3	0
2	C	2	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	1	0
2	F	2	0	0	1	0
2	G	2	0	0	2	0
2	H	1	0	0	1	0
2	I	3	0	0	0	0
2	J	1	0	0	0	0
3	A	19	0	0	0	0
3	B	20	0	0	0	0
3	C	14	0	0	0	0
3	D	17	0	0	1	0
3	E	27	0	0	0	0
3	F	10	0	0	0	0
3	G	12	0	0	0	0
3	H	9	0	0	0	0
3	I	15	0	0	0	0
3	J	6	0	0	0	0
All	All	11040	0	10828	94	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 4.

All (94) 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:C:1048:ARG:HH22	1:C:1146:THR:HA	1.38	0.87
1:D:1048:ARG:NH2	1:D:1145:LEU:O	2.24	0.71
1:H:1048:ARG:NH2	1:H:1145:LEU:O	2.29	0.66
1:B:1048:ARG:NH2	1:B:1145:LEU:O	2.28	0.66
1:E:1048:ARG:NH2	1:E:1145:LEU:O	2.31	0.64
1:G:1025:ASP:HA	1:G:1032:ARG:HH12	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:LYS:HD2	1:A:1047:ARG:HD3	1.80	0.62
1:J:1015:GLN:NE2	1:J:1085:VAL:O	2.33	0.61
1:C:1044:LYS:HD2	1:C:1047:ARG:HD2	1.83	0.61
1:D:1117:MET:HE1	1:E:1117:MET:HB3	1.82	0.60
1:C:1029:ALA:HA	1:C:1032:ARG:HG3	1.83	0.59
1:J:1024:ILE:HG12	1:J:1032:ARG:HD3	1.83	0.59
1:J:1064:ASP:OD2	1:J:1067:GLY:N	2.32	0.58
1:D:1049:ASP:H	1:D:1107:GLN:HE21	1.56	0.54
1:H:1064:ASP:OD2	1:H:1067:GLY:N	2.36	0.52
1:I:1025:ASP:O	1:I:1032:ARG:NH2	2.43	0.52
1:C:1048:ARG:NH2	1:C:1146:THR:HA	2.16	0.52
1:A:1017:PRO:HG2	1:B:1090:HIS:CE1	2.45	0.51
1:G:1140:LYS:HD3	2:H:2148:CL:CL	2.48	0.51
1:C:1048:ARG:NH2	1:C:1054:TRP:HE1	2.08	0.51
1:A:1117:MET:HG2	1:J:1117:MET:HG2	1.93	0.51
1:A:1025:ASP:HA	1:A:1032:ARG:HE	1.76	0.50
1:D:1049:ASP:O	1:D:1107:GLN:NE2	2.44	0.50
1:E:1059:ILE:HD12	1:E:1103:TYR:CZ	2.46	0.49
1:G:1024:ILE:O	1:G:1032:ARG:NH1	2.45	0.49
1:I:1082:ALA:HA	1:I:1104:VAL:HA	1.94	0.49
1:J:1044:LYS:HD2	1:J:1047:ARG:HD2	1.93	0.49
1:B:1117:MET:HE1	1:C:1117:MET:HG3	1.94	0.48
1:B:1039:ARG:NH1	2:B:2153:CL:CL	2.82	0.48
1:G:1017:PRO:HG2	1:H:1090:HIS:NE2	2.29	0.48
2:G:2147:CL:CL	1:H:1140:LYS:HD3	2.51	0.48
1:A:1015:GLN:NE2	1:A:1085:VAL:O	2.46	0.48
1:B:1071:LEU:HD12	1:B:1119:ARG:HD3	1.96	0.47
1:B:1025:ASP:O	1:B:1032:ARG:NH1	2.47	0.47
1:E:1025:ASP:HA	1:E:1032:ARG:HE	1.78	0.47
1:G:1117:MET:HA	1:G:1120:LEU:HD12	1.97	0.47
1:C:1015:GLN:HG2	1:D:1015:GLN:HE21	1.79	0.47
1:C:1071:LEU:HD12	1:C:1119:ARG:HD3	1.97	0.47
2:E:2150:CL:CL	1:F:1141:LYS:HD2	2.51	0.47
1:A:1034:GLN:HG2	1:A:1038:TYR:CE2	2.51	0.46
1:E:1015:GLN:OE1	1:F:1015:GLN:NE2	2.48	0.45
1:J:1034:GLN:HG2	1:J:1038:TYR:CE2	2.51	0.45
1:E:1090:HIS:CE1	1:F:1017:PRO:HG2	2.51	0.45
1:J:1086:SER:OG	1:J:1087:CYS:N	2.49	0.45
1:H:1057:ALA:HB3	1:H:1137:VAL:HB	1.99	0.45
1:H:1071:LEU:HD12	1:H:1119:ARG:HD3	1.99	0.45
1:G:1090:HIS:NE2	1:H:1017:PRO:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1090:HIS:NE2	1:F:1017:PRO:HG2	2.32	0.45
1:J:1032:ARG:O	1:J:1036:ILE:HG13	2.17	0.44
1:F:1058:VAL:HG13	1:F:1104:VAL:HB	2.00	0.44
1:G:1053:GLN:HB3	1:G:1142:PRO:HB3	2.00	0.44
1:B:1140:LYS:HD3	2:B:2151:CL:CL	2.55	0.44
1:F:1136:ILE:HG12	2:F:2148:CL:CL	2.55	0.44
1:E:1135:SER:HB2	1:F:1141:LYS:HB2	1.99	0.44
1:I:1055:LYS:NZ	1:I:1140:LYS:O	2.51	0.43
1:G:1071:LEU:HD12	1:G:1119:ARG:HD3	1.98	0.43
1:D:1117:MET:HE1	1:E:1117:MET:CB	2.46	0.43
1:I:1071:LEU:HD12	1:I:1119:ARG:HD3	2.00	0.43
1:I:1081:LYS:NZ	1:J:1091:PRO:O	2.52	0.43
1:D:1117:MET:HB3	1:D:1117:MET:HE3	1.59	0.43
1:F:1017:PRO:HA	1:F:1018:PRO:HD3	1.91	0.43
1:A:1082:ALA:HA	1:A:1104:VAL:HA	1.99	0.43
1:I:1059:ILE:HD12	1:I:1103:TYR:CZ	2.54	0.43
1:A:1140:LYS:HD3	2:A:2148:CL:CL	2.56	0.43
1:C:1140:LYS:HD2	1:D:1136:ILE:HD11	2.01	0.42
1:E:1020:PRO:HD3	1:F:1090:HIS:CD2	2.54	0.42
1:G:1075:PHE:CZ	1:G:1115:VAL:HG13	2.55	0.42
1:G:1017:PRO:HA	1:G:1018:PRO:HD3	1.95	0.42
1:D:1034:GLN:HG2	1:D:1038:TYR:CE2	2.54	0.42
1:E:1030:LYS:HE3	1:E:1030:LYS:HB2	1.84	0.42
1:A:1017:PRO:HA	1:A:1018:PRO:HD3	1.92	0.42
1:I:1141:LYS:HD2	1:J:1134:SER:O	2.19	0.42
1:G:1108:ASN:OD1	1:G:1111:THR:N	2.47	0.42
1:J:1069:LYS:HE3	1:J:1073:GLN:NE2	2.35	0.42
1:E:1091:PRO:O	1:F:1081:LYS:NZ	2.49	0.42
1:C:1034:GLN:HG2	1:C:1038:TYR:CE2	2.55	0.42
1:H:1064:ASP:HA	1:H:1065:PRO:HD2	1.95	0.42
1:G:1136:ILE:HG12	2:G:2147:CL:CL	2.57	0.41
1:E:1087:CYS:SG	1:F:1084:PRO:HG3	2.60	0.41
1:F:1059:ILE:HD12	1:F:1103:TYR:CZ	2.54	0.41
1:C:1052:CYS:HB3	1:C:1107:GLN:HB3	2.02	0.41
1:H:1034:GLN:HG2	1:H:1038:TYR:CE2	2.55	0.41
1:B:1059:ILE:HD12	1:B:1103:TYR:CZ	2.54	0.41
1:J:1057:ALA:HB3	1:J:1137:VAL:HB	2.01	0.41
1:B:1126:HIS:HA	1:B:1127:PRO:HD2	1.96	0.41
1:F:1069:LYS:HE3	1:F:1073:GLN:NE2	2.35	0.41
1:E:1025:ASP:O	1:E:1032:ARG:NH2	2.37	0.41
1:B:1141:LYS:HE3	2:B:2151:CL:CL	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1017:PRO:HA	1:H:1018:PRO:HD3	1.97	0.41
1:G:1046:GLY:O	1:G:1079:GLY:N	2.50	0.40
1:H:1126:HIS:HA	1:H:1127:PRO:HD2	1.96	0.40
1:D:1081:LYS:NZ	3:D:2008:HOH:O	2.49	0.40
1:J:1068:LEU:HB3	1:J:1102:VAL:HG23	2.03	0.40
1:A:1126:HIS:HA	1:A:1127:PRO:HD2	1.93	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	132/139 (95%)	129 (98%)	3 (2%)	0	100	100
1	B	135/139 (97%)	135 (100%)	0	0	100	100
1	C	134/139 (96%)	133 (99%)	1 (1%)	0	100	100
1	D	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
1	E	135/139 (97%)	134 (99%)	1 (1%)	0	100	100
1	F	132/139 (95%)	130 (98%)	2 (2%)	0	100	100
1	G	132/139 (95%)	131 (99%)	1 (1%)	0	100	100
1	H	132/139 (95%)	131 (99%)	1 (1%)	0	100	100
1	I	132/139 (95%)	132 (100%)	0	0	100	100
1	J	132/139 (95%)	132 (100%)	0	0	100	100
All	All	1329/1390 (96%)	1319 (99%)	10 (1%)	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	116/119 (98%)	116 (100%)	0	100 100
1	B	118/119 (99%)	117 (99%)	1 (1%)	86 92
1	C	118/119 (99%)	118 (100%)	0	100 100
1	D	117/119 (98%)	117 (100%)	0	100 100
1	E	118/119 (99%)	118 (100%)	0	100 100
1	F	116/119 (98%)	116 (100%)	0	100 100
1	G	116/119 (98%)	116 (100%)	0	100 100
1	H	116/119 (98%)	116 (100%)	0	100 100
1	I	116/119 (98%)	116 (100%)	0	100 100
1	J	116/119 (98%)	115 (99%)	1 (1%)	84 91
All	All	1167/1190 (98%)	1165 (100%)	2 (0%)	95 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1117	MET
1	J	1087	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1073	GLN
1	B	1090	HIS
1	C	1015	GLN
1	D	1107	GLN
1	E	1023	GLN
1	E	1073	GLN
1	E	1095	GLN

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

Of 24 ligands modelled in this entry, 24 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

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	134/139 (96%)	0.62	18 (13%) 4 4	37, 74, 115, 129	0
1	B	136/139 (97%)	0.29	6 (4%) 38 41	28, 53, 89, 132	0
1	C	135/139 (97%)	0.59	17 (12%) 5 4	36, 59, 119, 144	0
1	D	135/139 (97%)	0.41	15 (11%) 7 7	34, 56, 125, 137	0
1	E	136/139 (97%)	0.15	8 (5%) 26 28	31, 50, 89, 132	0
1	F	134/139 (96%)	0.43	16 (11%) 6 5	33, 65, 110, 138	0
1	G	133/139 (95%)	1.16	35 (26%) 1 1	50, 86, 139, 155	0
1	H	134/139 (96%)	0.61	16 (11%) 6 5	51, 74, 106, 137	0
1	I	134/139 (96%)	0.67	16 (11%) 6 5	45, 73, 118, 144	0
1	J	134/139 (96%)	0.90	20 (14%) 3 3	56, 83, 131, 149	0
All	All	1345/1390 (96%)	0.58	167 (12%) 5 5	28, 68, 120, 155	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1024	ILE	9.0
1	I	1094	ASP	7.5
1	G	1022	ARG	7.3
1	D	1148	PRO	6.6
1	I	1093	PRO	5.9
1	I	1051	LYS	5.8
1	C	1148	PRO	5.6
1	J	1147	GLN	5.5
1	D	1094	ASP	5.5
1	F	1025	ASP	5.3
1	I	1014	TYR	5.3
1	I	1095	GLN	5.3
1	C	1022	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	1029	ALA	5.2
1	J	1029	ALA	5.1
1	J	1024	ILE	5.1
1	B	1149	GLY	4.9
1	H	1051	LYS	4.7
1	A	1051	LYS	4.7
1	H	1022	ARG	4.7
1	B	1093	PRO	4.7
1	G	1044	LYS	4.5
1	J	1025	ASP	4.4
1	J	1019	VAL	4.4
1	H	1092	GLY	4.4
1	A	1044	LYS	4.4
1	B	1148	PRO	4.3
1	F	1024	ILE	4.3
1	F	1128	LEU	4.3
1	I	1022	ARG	4.3
1	J	1051	LYS	4.3
1	E	1149	GLY	4.2
1	I	1092	GLY	4.2
1	G	1051	LYS	4.2
1	D	1095	GLN	4.2
1	I	1147	GLN	4.1
1	D	1093	PRO	4.0
1	E	1096	SER	3.9
1	H	1093	PRO	3.9
1	C	1050	PRO	3.9
1	H	1091	PRO	3.9
1	G	1014	TYR	3.8
1	C	1019	VAL	3.8
1	G	1075	PHE	3.7
1	G	1021	TYR	3.7
1	J	1127	PRO	3.7
1	G	1128	LEU	3.6
1	G	1029	ALA	3.6
1	A	1048	ARG	3.6
1	G	1047	ARG	3.6
1	C	1051	LYS	3.6
1	G	1023	GLN	3.5
1	G	1027	CYS	3.5
1	B	1128	LEU	3.5
1	J	1094	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	1097	PRO	3.5
1	I	1019	VAL	3.4
1	J	1026	ASP	3.4
1	C	1025	ASP	3.4
1	G	1049	ASP	3.4
1	A	1052	CYS	3.4
1	C	1023	GLN	3.3
1	G	1025	ASP	3.3
1	I	1047	ARG	3.3
1	G	1048	ARG	3.3
1	I	1044	LYS	3.2
1	D	1023	GLN	3.2
1	J	1128	LEU	3.2
1	C	1094	ASP	3.2
1	H	1014	TYR	3.2
1	G	1146	THR	3.2
1	F	1021	TYR	3.2
1	G	1040	ARG	3.1
1	D	1051	LYS	3.1
1	I	1091	PRO	3.0
1	C	1024	ILE	3.0
1	F	1026	ASP	3.0
1	G	1066[A]	TYR	3.0
1	A	1050	PRO	3.0
1	A	1110	ASP	2.9
1	D	1025	ASP	2.9
1	A	1147	GLN	2.9
1	C	1128	LEU	2.9
1	G	1016	GLN	2.8
1	A	1026	ASP	2.8
1	G	1105	TYR	2.8
1	E	1094	ASP	2.8
1	H	1128	LEU	2.7
1	G	1026	ASP	2.7
1	H	1147	GLN	2.7
1	F	1066	TYR	2.7
1	A	1128	LEU	2.7
1	G	1020	PRO	2.7
1	F	1051	LYS	2.7
1	J	1022	ARG	2.7
1	H	1023	GLN	2.7
1	H	1094	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	1107	GLN	2.6
1	G	1082	ALA	2.6
1	G	1104	VAL	2.6
1	J	1097	PRO	2.6
1	J	1014	TYR	2.6
1	G	1071	LEU	2.6
1	G	1110	ASP	2.6
1	G	1052	CYS	2.6
1	J	1023	GLN	2.6
1	I	1025	ASP	2.5
1	F	1127	PRO	2.5
1	J	1020	PRO	2.5
1	D	1050	PRO	2.5
1	G	1018	PRO	2.5
1	D	1014	TYR	2.5
1	I	1096	SER	2.5
1	D	1015	GLN	2.5
1	A	1022	ARG	2.5
1	F	1029	ALA	2.5
1	J	1016	GLN	2.5
1	D	1016	GLN	2.5
1	D	1022	ARG	2.5
1	F	1044	LYS	2.4
1	A	1053	GLN	2.4
1	H	1095	GLN	2.4
1	C	1066[A]	TYR	2.4
1	F	1014	TYR	2.4
1	J	1092	GLY	2.4
1	C	1044	LYS	2.4
1	E	1025	ASP	2.4
1	G	1053	GLN	2.4
1	A	1140	LYS	2.4
1	A	1118	ALA	2.4
1	H	1029	ALA	2.4
1	F	1022	ARG	2.4
1	J	1093	PRO	2.4
1	A	1104	VAL	2.4
1	D	1147	GLN	2.3
1	C	1015	GLN	2.3
1	B	1094	ASP	2.3
1	A	1105	TYR	2.3
1	G	1019	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	1131	ASN	2.3
1	J	1146	THR	2.3
1	C	1016	GLN	2.3
1	A	1025	ASP	2.3
1	F	1052	CYS	2.3
1	H	1096	SER	2.2
1	G	1072	SER	2.2
1	G	1038	TYR	2.2
1	D	1029	ALA	2.2
1	A	1103	TYR	2.2
1	C	1021	TYR	2.2
1	D	1044	LYS	2.2
1	B	1096	SER	2.1
1	I	1057	ALA	2.1
1	F	1023	GLN	2.1
1	J	1052	CYS	2.1
1	G	1131	ASN	2.1
1	E	1095	GLN	2.1
1	A	1019	VAL	2.1
1	G	1032	ARG	2.1
1	C	1147	GLN	2.1
1	E	1023	GLN	2.1
1	F	1016	GLN	2.0
1	E	1051	LYS	2.0
1	F	1104	VAL	2.0
1	E	1093	PRO	2.0
1	H	1066	TYR	2.0
1	G	1036	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 (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	CL	D	2151	1/1	0.95	0.15	0.30	81,81,81,81	0
2	CL	H	2148	1/1	0.91	0.16	-0.20	76,76,76,76	0
2	CL	I	2149	1/1	0.87	0.10	-0.90	101,101,101,101	0
2	CL	G	2147	1/1	0.97	0.12	-0.95	57,57,57,57	1
2	CL	E	2151	1/1	0.94	0.10	-1.06	68,68,68,68	0
2	CL	A	2148	1/1	0.91	0.11	-1.11	68,68,68,68	0
2	CL	B	2151	1/1	0.89	0.09	-1.21	71,71,71,71	0
2	CL	B	2153	1/1	0.88	0.07	-1.46	79,79,79,79	0
2	CL	I	2148	1/1	0.98	0.09	-1.49	61,61,61,61	0
2	CL	E	2150	1/1	0.97	0.08	-1.53	55,55,55,55	0
2	CL	A	2149	1/1	0.98	0.06	-1.67	70,70,70,70	0
2	CL	J	2148	1/1	0.98	0.07	-1.75	58,58,58,58	1
2	CL	D	2149	1/1	0.98	0.05	-1.79	40,40,40,40	1
2	CL	F	2148	1/1	0.98	0.04	-2.09	39,39,39,39	1
2	CL	C	2149	1/1	0.98	0.05	-2.35	48,48,48,48	0
2	CL	B	2152	1/1	0.96	0.04	-2.98	52,52,52,52	0
2	CL	D	2150	1/1	0.95	0.08	-	75,75,75,75	0
2	CL	I	2150	1/1	0.74	0.15	-	84,84,84,84	0
2	CL	D	2152	1/1	0.96	0.06	-	75,75,75,75	0
2	CL	G	2148	1/1	0.95	0.08	-	67,67,67,67	0
2	CL	F	2149	1/1	0.96	0.06	-	73,73,73,73	0
2	CL	E	2152	1/1	0.97	0.07	-	75,75,75,75	0
2	CL	B	2154	1/1	0.81	0.11	-	90,90,90,90	0
2	CL	C	2150	1/1	0.82	0.16	-	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.