Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 03:23 pm GMT

PDB ID	:	2YPZ
Title	:	KSHV LANA (ORF73) C-terminal domain, decameric ring: orthorhombic crystal form
Authors	:	Hellert, J.; Krausze, J.; Luhrs, T.
Deposited on	:	2012-11-02
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

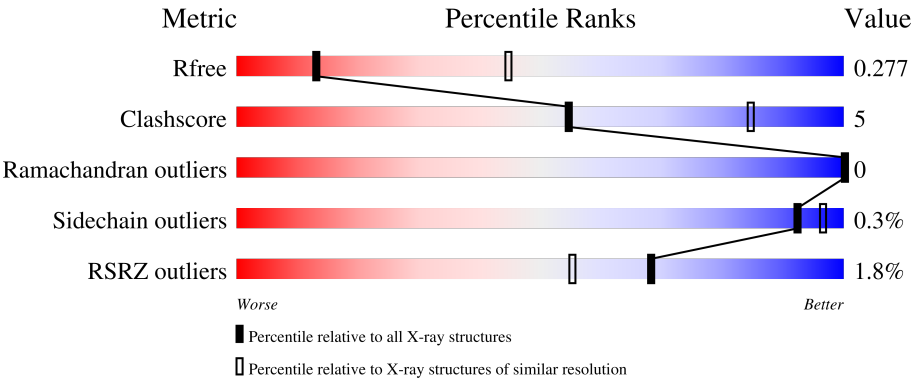
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	139	86% 12%
1	B	139	80% 17%
1	C	139	79% 18%
1	D	139	86% 11%
1	E	139	2% 86% 9%

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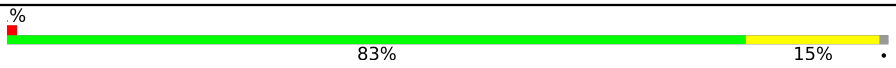
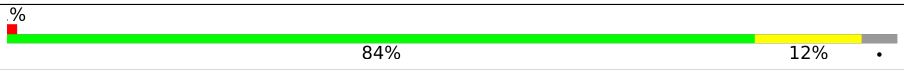
Mol	Chain	Length	Quality of chain
1	F	139	
1	G	139	
1	H	139	
1	I	139	
1	J	139	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10845 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 KSHV LANA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	6			
1	B	134	Total	C	N	O	S	0	0	0
			1079	699	192	182	6			
1	C	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	6			
1	D	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	6			
1	E	133	Total	C	N	O	S	0	0	0
			1069	695	190	178	6			
1	F	137	Total	C	N	O	S	0	0	0
			1103	713	198	186	6			
1	G	135	Total	C	N	O	S	0	1	0
			1094	708	195	185	6			
1	H	133	Total	C	N	O	S	0	0	0
			1070	694	190	180	6			
1	I	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	6			
1	J	135	Total	C	N	O	S	0	0	0
			1086	704	193	183	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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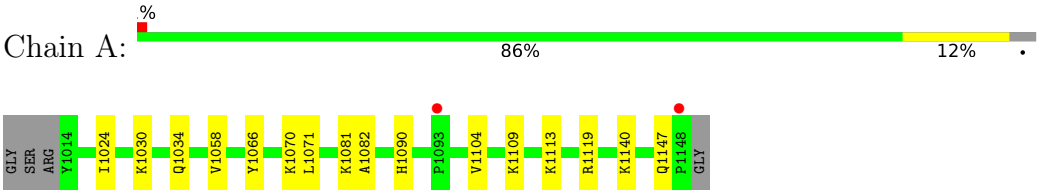
Chain	Residue	Modelled	Actual	Comment	Reference
E	1012	SER	-	expression tag	UNP Q76SB0
F	1011	GLY	-	expression tag	UNP Q76SB0
F	1012	SER	-	expression tag	UNP Q76SB0
G	1011	GLY	-	expression tag	UNP Q76SB0
G	1012	SER	-	expression tag	UNP Q76SB0
H	1011	GLY	-	expression tag	UNP Q76SB0
H	1012	SER	-	expression 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

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.

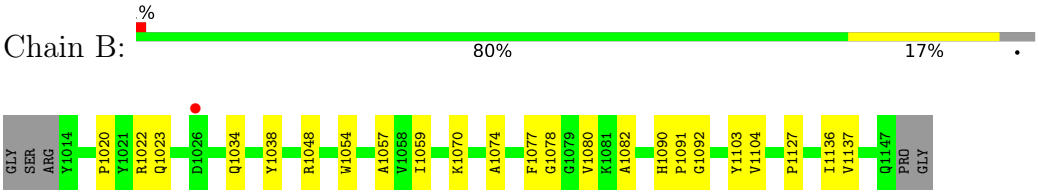
• Molecule 1: KSHV LANA

Chain A:



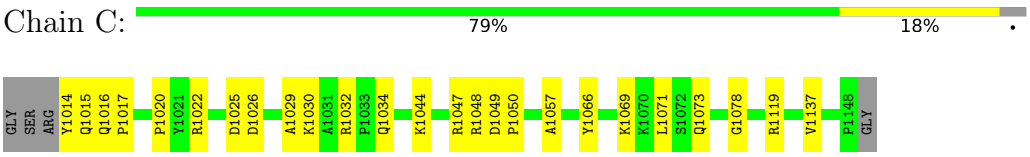
• Molecule 1: KSHV LANA

Chain B:



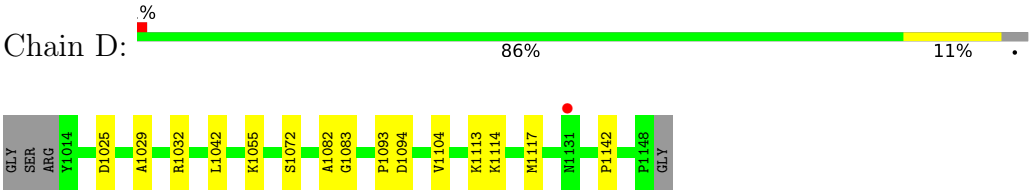
• Molecule 1: KSHV LANA

Chain C:



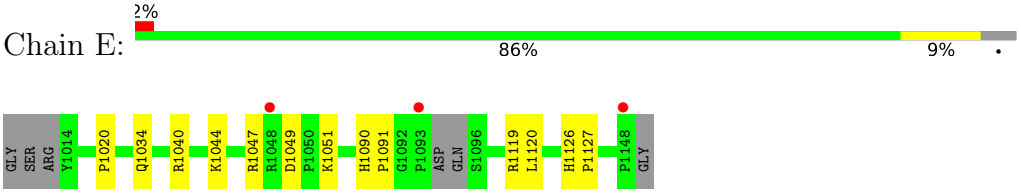
• Molecule 1: KSHV LANA

Chain D:



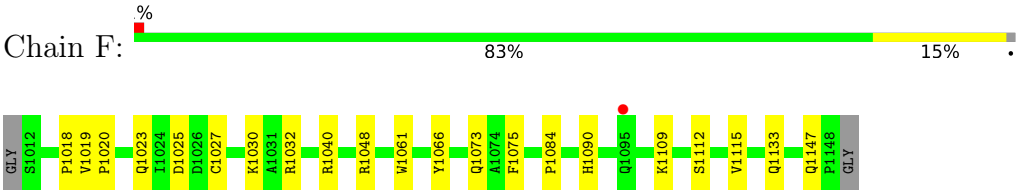
• Molecule 1: KSHV LANA

Chain E:



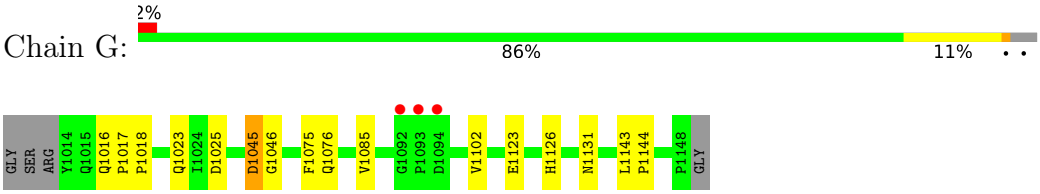
• Molecule 1: KSHV LANA

Chain F:



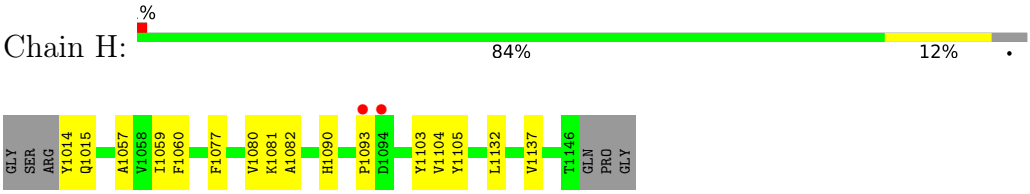
• Molecule 1: KSHV LANA

Chain G:



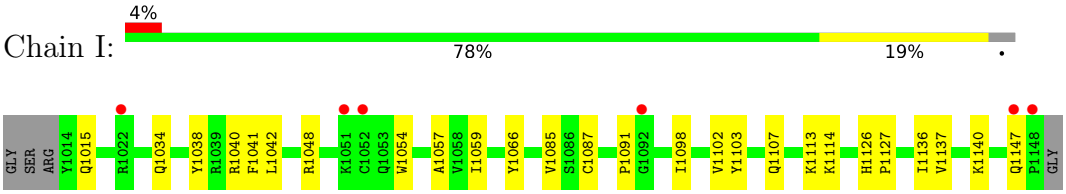
• Molecule 1: KSHV LANA

Chain H:



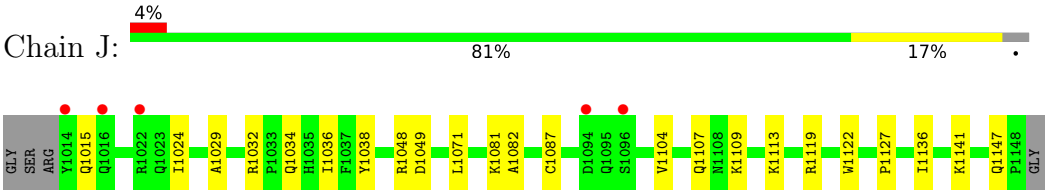
• Molecule 1: KSHV LANA

Chain I:



• Molecule 1: KSHV LANA

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.79Å 100.29Å 214.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.43 – 3.20 73.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.43-3.20) 97.5 (73.26-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.265 0.227 , 0.277	Depositor DCC
R_{free} test set	1373 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10845	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.22	0/1124	0.39	0/1526
1	B	0.22	0/1116	0.40	0/1514
1	C	0.22	0/1124	0.40	0/1526
1	D	0.22	0/1124	0.40	0/1526
1	E	0.23	0/1106	0.41	0/1500
1	F	0.22	0/1141	0.40	0/1548
1	G	0.22	0/1132	0.43	0/1537
1	H	0.22	0/1107	0.40	0/1502
1	I	0.22	0/1124	0.40	0/1526
1	J	0.22	0/1124	0.40	0/1526
All	All	0.22	0/11222	0.40	0/15231

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	G	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1045	ASP	Peptide
1	G	1046	GLY	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	1086	0	1084	13	0
1	B	1079	0	1077	17	0
1	C	1086	0	1084	16	0
1	D	1086	0	1084	10	0
1	E	1069	0	1071	8	0
1	F	1103	0	1102	14	0
1	G	1094	0	1089	10	0
1	H	1070	0	1069	8	0
1	I	1086	0	1084	19	0
1	J	1086	0	1084	14	0
All	All	10845	0	10828	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (112) 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:J:1048:ARG:HH12	1:J:1147:GLN:HB3	1.34	0.92
1:I:1091:PRO:O	1:J:1081:LYS:NZ	2.05	0.90
1:I:1087:CYS:HB2	1:I:1098:ILE:HD11	1.72	0.70
1:D:1042:LEU:HA	1:D:1114:LYS:HE3	1.74	0.69
1:F:1040:ARG:NH2	1:G:1131[A]:ASN:OD1	2.24	0.69
1:I:1041:PHE:O	1:I:1114:LYS:NZ	2.33	0.61
1:J:1048:ARG:HH12	1:J:1147:GLN:CB	2.12	0.59
1:D:1029:ALA:HA	1:D:1032:ARG:NH1	2.18	0.59
1:J:1024:ILE:HD11	1:J:1036:ILE:HG12	1.85	0.58
1:I:1054:TRP:HA	1:I:1107:GLN:HA	1.84	0.58
1:J:1109:LYS:HE2	1:J:1113:LYS:HE3	1.86	0.58
1:B:1127:PRO:HG3	1:I:1040:ARG:NH2	2.20	0.56
1:G:1016:GLN:HG3	1:G:1017:PRO:HD2	1.87	0.56
1:B:1022:ARG:HG3	1:B:1023:GLN:H	1.71	0.56
1:D:1025:ASP:HA	1:D:1032:ARG:HE	1.70	0.56
1:A:1090:HIS:HD2	1:B:1020:PRO:HD3	1.70	0.55
1:C:1048:ARG:HB2	1:C:1078:GLY:C	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1127:PRO:HG3	1:I:1040:ARG:HH21	1.74	0.53
1:C:1022:ARG:NH2	1:D:1094:ASP:OD1	2.42	0.52
1:I:1048:ARG:NH2	1:I:1147:GLN:H	2.08	0.52
1:D:1072:SER:OG	1:D:1083:GLY:O	2.24	0.52
1:I:1042:LEU:HA	1:I:1114:LYS:HZ2	1.75	0.52
1:I:1085:VAL:HA	1:I:1102:VAL:HG22	1.92	0.52
1:F:1023:GLN:HG3	1:F:1025:ASP:H	1.74	0.52
1:F:1040:ARG:NH1	1:G:1126:HIS:O	2.44	0.50
1:F:1027:CYS:O	1:F:1032:ARG:NH2	2.44	0.50
1:A:1109:LYS:HG2	1:A:1113:LYS:HE3	1.93	0.50
1:J:1049:ASP:H	1:J:1107:GLN:HE22	1.59	0.50
1:A:1030:LYS:HG3	1:A:1070:LYS:HD3	1.93	0.50
1:C:1020:PRO:HB2	1:D:1093:PRO:HA	1.95	0.49
1:H:1082:ALA:HA	1:H:1104:VAL:HA	1.94	0.49
1:E:1020:PRO:HD3	1:F:1090:HIS:CD2	2.48	0.49
1:A:1081:LYS:NZ	1:B:1091:PRO:O	2.46	0.48
1:C:1022:ARG:N	1:C:1026:ASP:OD2	2.46	0.48
1:F:1040:ARG:NH1	1:G:1123:GLU:O	2.47	0.48
1:A:1140:LYS:NZ	1:B:1136:ILE:HD12	2.28	0.48
1:F:1030:LYS:NZ	1:F:1073:GLN:HE22	2.13	0.47
1:A:1058:VAL:HG13	1:A:1104:VAL:HB	1.95	0.47
1:E:1040:ARG:NH2	1:J:1127:PRO:HB3	2.29	0.47
1:A:1024:ILE:HD12	1:A:1024:ILE:H	1.79	0.47
1:I:1015:GLN:HE22	1:J:1015:GLN:HE22	1.63	0.47
1:C:1034:GLN:OE1	1:C:1119:ARG:NH1	2.48	0.47
1:B:1048:ARG:HB2	1:B:1078:GLY:C	2.34	0.47
1:J:1034:GLN:HG2	1:J:1038:TYR:CE2	2.49	0.47
1:H:1014:TYR:HB3	1:H:1015:GLN:H	1.55	0.46
1:H:1077:PHE:N	1:H:1080:VAL:O	2.47	0.46
1:I:1042:LEU:HA	1:I:1114:LYS:NZ	2.29	0.46
1:F:1061:TRP:NE1	1:F:1133:GLN:OE1	2.49	0.45
1:A:1030:LYS:HG2	1:A:1066:TYR:OH	2.17	0.45
1:E:1044:LYS:HA	1:E:1047:ARG:HG2	1.99	0.45
1:J:1029:ALA:HA	1:J:1032:ARG:HD3	1.98	0.45
1:C:1071:LEU:HD12	1:C:1119:ARG:HD3	1.97	0.45
1:G:1143:LEU:HA	1:G:1144:PRO:HD3	1.84	0.45
1:H:1059:ILE:HD12	1:H:1103:TYR:CZ	2.51	0.45
1:J:1071:LEU:HD12	1:J:1119:ARG:HD3	1.98	0.45
1:C:1025:ASP:HA	1:C:1032:ARG:HE	1.82	0.45
1:E:1049:ASP:OD1	1:E:1051:LYS:HG2	2.16	0.45
1:G:1023:GLN:NE2	1:G:1025:ASP:OD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1045:ASP:OD1	1:G:1045:ASP:N	2.50	0.45
1:E:1090:HIS:HA	1:E:1091:PRO:HD3	1.80	0.45
1:H:1090:HIS:HE1	1:H:1093:PRO:O	2.00	0.45
1:D:1029:ALA:HA	1:D:1032:ARG:HH12	1.82	0.45
1:D:1082:ALA:HA	1:D:1104:VAL:HA	1.99	0.44
1:B:1090:HIS:HA	1:B:1091:PRO:HD3	1.89	0.44
1:B:1059:ILE:HD12	1:B:1103:TYR:CZ	2.53	0.44
1:G:1075:PHE:O	1:G:1076:GLN:NE2	2.51	0.44
1:A:1082:ALA:HA	1:A:1104:VAL:HA	1.99	0.43
1:C:1025:ASP:O	1:C:1032:ARG:NH2	2.46	0.43
1:C:1030:LYS:HD3	1:C:1066:TYR:OH	2.18	0.43
1:I:1140:LYS:HE3	1:J:1136:ILE:HG13	1.99	0.43
1:F:1019:VAL:HA	1:F:1020:PRO:HD3	1.91	0.43
1:I:1034:GLN:HG2	1:I:1038:TYR:CE2	2.54	0.43
1:C:1016:GLN:HA	1:C:1017:PRO:HD3	1.92	0.43
1:I:1057:ALA:HB3	1:I:1137:VAL:HB	2.01	0.43
1:A:1090:HIS:CD2	1:B:1020:PRO:HD3	2.53	0.42
1:C:1069:LYS:O	1:C:1073:GLN:HG2	2.19	0.42
1:D:1113:LYS:O	1:D:1117:MET:HG2	2.19	0.42
1:E:1126:HIS:HA	1:E:1127:PRO:HD2	1.91	0.42
1:F:1075:PHE:CZ	1:F:1115:VAL:HG13	2.54	0.42
1:C:1014:TYR:HB3	1:C:1015:GLN:H	1.70	0.42
1:F:1048:ARG:HD2	1:F:1147:GLN:HG3	2.00	0.42
1:I:1048:ARG:HH21	1:I:1147:GLN:H	1.65	0.42
1:A:1071:LEU:HD12	1:A:1119:ARG:HD3	2.02	0.42
1:A:1147:GLN:HE21	1:B:1092:GLY:HA3	1.84	0.42
1:B:1034:GLN:HG2	1:B:1038:TYR:CE2	2.55	0.42
1:C:1057:ALA:HB3	1:C:1137:VAL:HB	2.02	0.42
1:G:1085:VAL:HA	1:G:1102:VAL:HG22	2.02	0.42
1:I:1113:LYS:HG3	1:I:1136:ILE:HD11	2.01	0.42
1:B:1082:ALA:HA	1:B:1104:VAL:HA	2.01	0.41
1:F:1030:LYS:HD2	1:F:1066:TYR:OH	2.21	0.41
1:C:1029:ALA:HA	1:C:1032:ARG:NH1	2.35	0.41
1:C:1049:ASP:HA	1:C:1050:PRO:HD3	1.93	0.41
1:F:1018:PRO:HD3	1:F:1084:PRO:HD3	2.03	0.41
1:H:1081:LYS:O	1:H:1105:TYR:N	2.48	0.41
1:I:1059:ILE:HD12	1:I:1103:TYR:CZ	2.56	0.41
1:J:1082:ALA:HA	1:J:1104:VAL:HA	2.02	0.41
1:B:1070:LYS:O	1:B:1074:ALA:HB2	2.21	0.41
1:F:1109:LYS:O	1:F:1112:SER:OG	2.30	0.41
1:H:1057:ALA:HB3	1:H:1137:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1077:PHE:N	1:B:1080:VAL:O	2.53	0.40
1:C:1044:LYS:HG2	1:C:1047:ARG:NH2	2.35	0.40
1:J:1034:GLN:HG3	1:J:1122:TRP:CD2	2.56	0.40
1:B:1054:TRP:CD1	1:B:1054:TRP:N	2.89	0.40
1:E:1034:GLN:OE1	1:E:1119:ARG:NH1	2.54	0.40
1:I:1126:HIS:HA	1:I:1127:PRO:HD2	1.94	0.40
1:G:1017:PRO:HA	1:G:1018:PRO:HD3	2.00	0.40
1:A:1034:GLN:OE1	1:A:1119:ARG:NH1	2.54	0.40
1:E:1120:LEU:HD23	1:E:1120:LEU:HA	1.95	0.40
1:I:1087:CYS:CB	1:I:1098:ILE:HD11	2.45	0.40
1:B:1057:ALA:HB3	1:B:1137:VAL:HB	2.03	0.40
1:D:1055:LYS:HE2	1:D:1142:PRO:HD3	2.04	0.40
1:H:1060:PHE:HB3	1:H:1132:LEU: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	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
1	B	132/139 (95%)	128 (97%)	4 (3%)	0	100	100
1	C	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
1	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
1	E	129/139 (93%)	126 (98%)	3 (2%)	0	100	100
1	F	135/139 (97%)	132 (98%)	3 (2%)	0	100	100
1	G	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
1	H	131/139 (94%)	126 (96%)	5 (4%)	0	100	100
1	I	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
1	J	133/139 (96%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1326/1390 (95%)	1298 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/119 (98%)	117 (100%)	0	100	100
1	B	116/119 (98%)	116 (100%)	0	100	100
1	C	117/119 (98%)	117 (100%)	0	100	100
1	D	117/119 (98%)	117 (100%)	0	100	100
1	E	115/119 (97%)	115 (100%)	0	100	100
1	F	119/119 (100%)	119 (100%)	0	100	100
1	G	118/119 (99%)	118 (100%)	0	100	100
1	H	115/119 (97%)	115 (100%)	0	100	100
1	I	117/119 (98%)	116 (99%)	1 (1%)	78	91
1	J	117/119 (98%)	115 (98%)	2 (2%)	60	83
All	All	1168/1190 (98%)	1165 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	1066	TYR
1	J	1087	CYS
1	J	1141	LYS

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

Mol	Chain	Res	Type
1	A	1147	GLN

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Mol	Chain	Res	Type
1	B	1023	GLN
1	B	1034	GLN
1	B	1073	GLN
1	F	1095	GLN
1	G	1034	GLN
1	G	1073	GLN
1	G	1116	GLN
1	I	1015	GLN
1	J	1015	GLN
1	J	1107	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	135/139 (97%)	0.14	2 (1%)	73	61	24, 41, 78, 99	0
1	B	134/139 (96%)	0.12	1 (0%)	87	81	25, 43, 80, 88	0
1	C	135/139 (97%)	0.16	0	100	100	20, 39, 70, 91	0
1	D	135/139 (97%)	0.16	1 (0%)	87	81	22, 41, 77, 95	0
1	E	133/139 (95%)	0.33	3 (2%)	60	47	28, 51, 89, 108	0
1	F	137/139 (98%)	0.29	1 (0%)	87	81	35, 56, 85, 109	0
1	G	135/139 (97%)	0.20	3 (2%)	62	48	27, 43, 80, 133	0
1	H	133/139 (95%)	0.19	2 (1%)	73	61	20, 43, 77, 89	0
1	I	135/139 (97%)	0.50	6 (4%)	34	21	34, 60, 100, 120	0
1	J	135/139 (97%)	0.37	5 (3%)	41	26	36, 52, 88, 103	0
All	All	1347/1390 (96%)	0.25	24 (1%)	68	55	20, 47, 86, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1093	PRO	4.7
1	I	1148	PRO	4.1
1	I	1147	GLN	3.7
1	I	1051	LYS	3.6
1	G	1094	ASP	3.5
1	A	1148	PRO	3.4
1	H	1094	ASP	3.2
1	G	1092	GLY	2.7
1	J	1014	TYR	2.7
1	D	1131	ASN	2.6
1	E	1148	PRO	2.5
1	A	1093	PRO	2.5
1	J	1016	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	1092	GLY	2.3
1	B	1026	ASP	2.3
1	J	1022	ARG	2.3
1	F	1095	GLN	2.3
1	I	1052	CYS	2.1
1	J	1096	SER	2.1
1	E	1048	ARG	2.1
1	J	1094	ASP	2.1
1	E	1093	PRO	2.1
1	H	1093	PRO	2.1
1	I	1022	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.