Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:07 pm GMT

PDB ID	:	4CSG
Title	:	Structural insights into Toscana virus RNA encapsidation
Authors	:	Olal, D.; Daumke, O.
Deposited on	:	2014-03-07
Resolution	:	3.32 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:

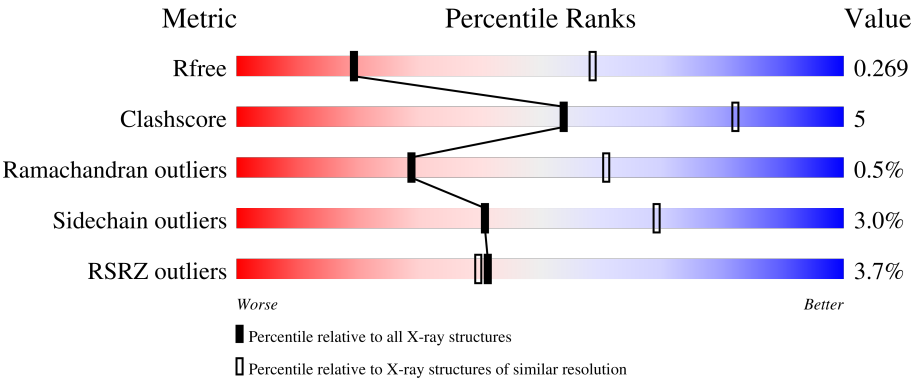
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	253	81% 15%
1	B	253	81% 15%
1	C	253	2% 83% 13%
1	D	253	3% 83% 14%
1	E	253	15% 83% 13%

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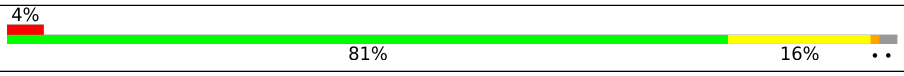
Mol	Chain	Length	Quality of chain
1	F	253	
1	H	253	
1	I	253	
1	J	253	
1	K	253	
1	L	253	
2	G	253	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22844 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 NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	1
			1889	1199	330	349	11			
1	B	248	Total	C	N	O	S	0	0	0
			1905	1208	332	354	11			
1	C	248	Total	C	N	O	S	0	0	1
			1901	1205	332	353	11			
1	D	249	Total	C	N	O	S	0	0	0
			1902	1207	332	352	11			
1	E	248	Total	C	N	O	S	0	0	0
			1905	1208	332	354	11			
1	F	248	Total	C	N	O	S	0	0	1
			1901	1205	332	353	11			
1	H	251	Total	C	N	O	S	0	0	0
			1927	1220	335	360	12			
1	I	248	Total	C	N	O	S	0	0	1
			1897	1203	332	351	11			
1	J	248	Total	C	N	O	S	0	0	0
			1901	1206	332	352	11			
1	K	249	Total	C	N	O	S	0	0	0
			1909	1210	333	355	11			
1	L	248	Total	C	N	O	S	0	0	1
			1901	1205	332	353	11			

- Molecule 2 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	248	Total	C	N	O	S	0	0	0
			1906	1209	332	354	11			

There is a discrepancy between the modelled and reference sequences:

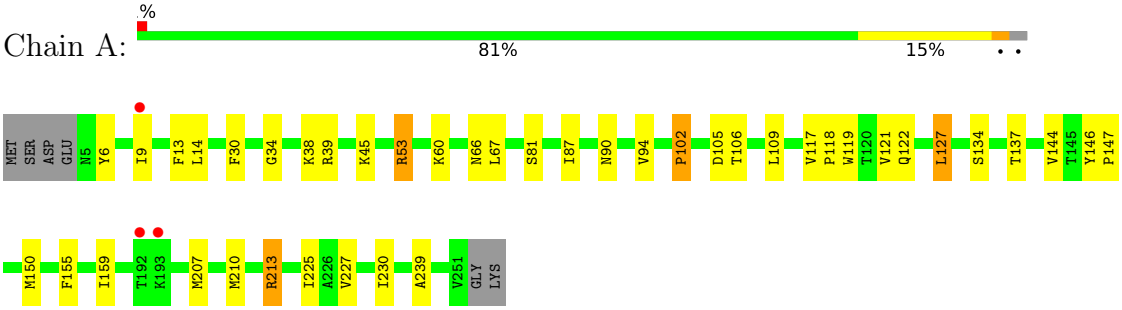
Chain	Residue	Modelled	Actual	Comment	Reference
G	41	ILE	VAL	conflict	UNP P21701

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.

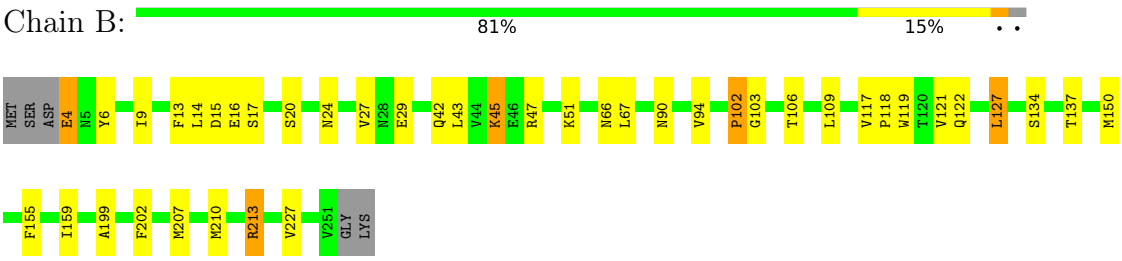
• Molecule 1: NUCLEOPROTEIN

Chain A:



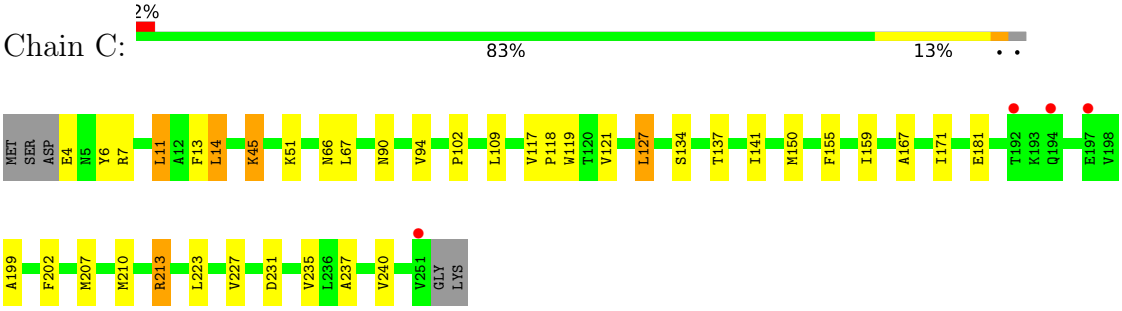
• Molecule 1: NUCLEOPROTEIN

Chain B:



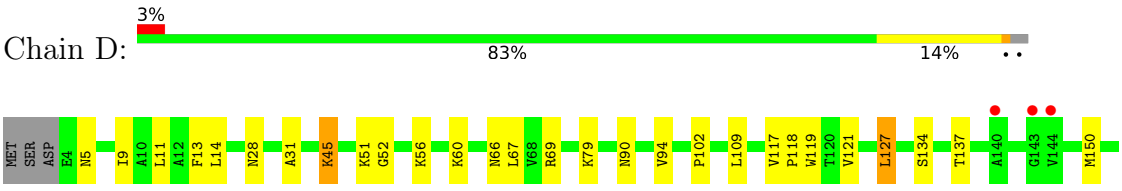
• Molecule 1: NUCLEOPROTEIN

Chain C:



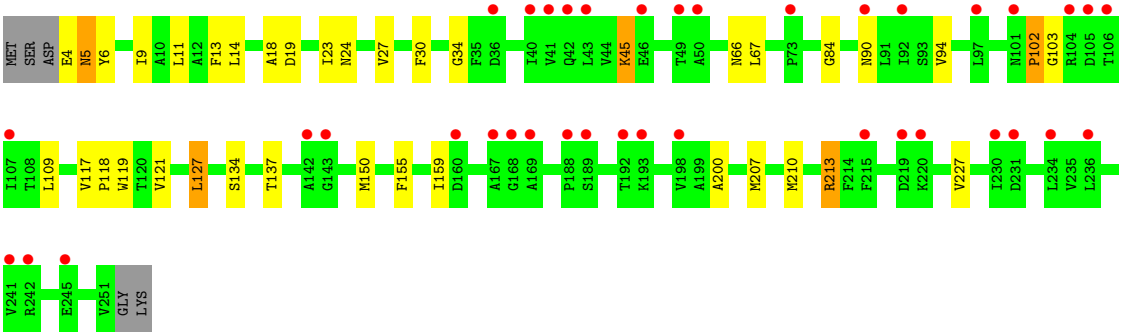
• Molecule 1: NUCLEOPROTEIN

Chain D:



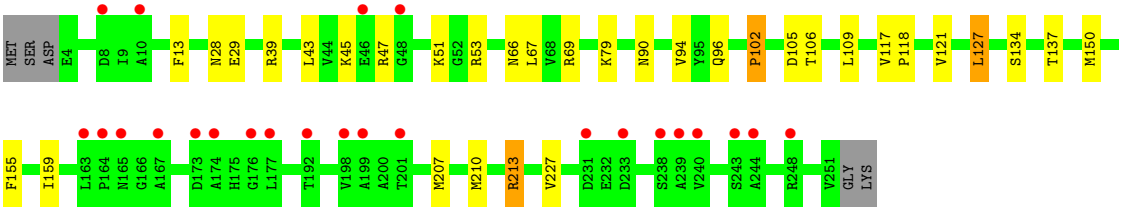
• Molecule 1: NUCLEOPROTEIN

Chain E:



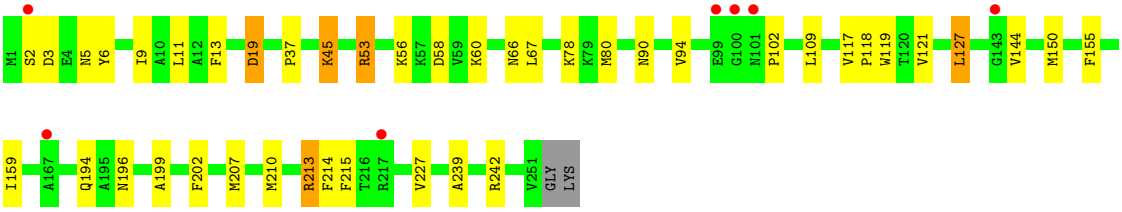
• Molecule 1: NUCLEOPROTEIN

Chain F:



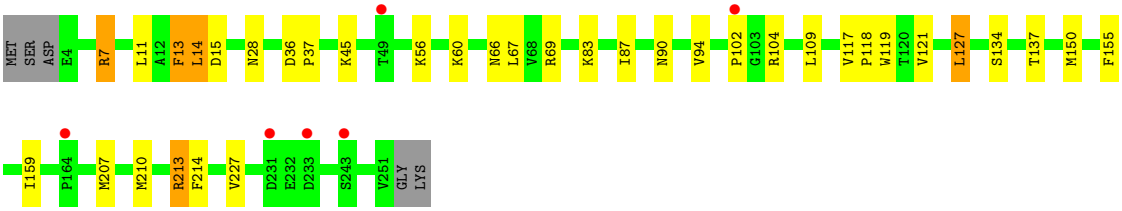
• Molecule 1: NUCLEOPROTEIN

Chain H:



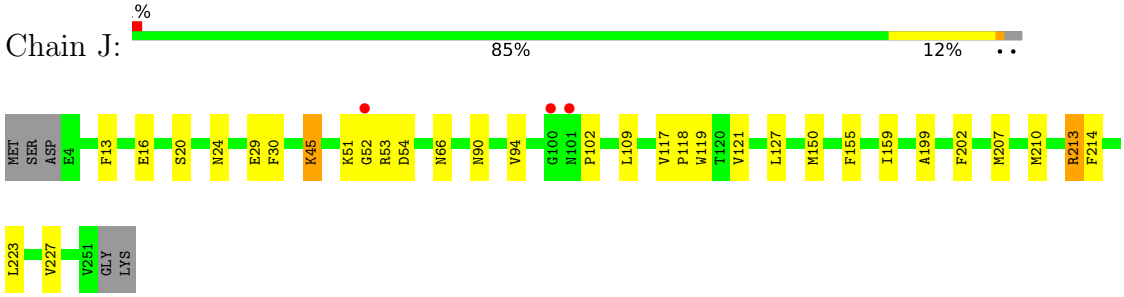
• Molecule 1: NUCLEOPROTEIN

Chain I:



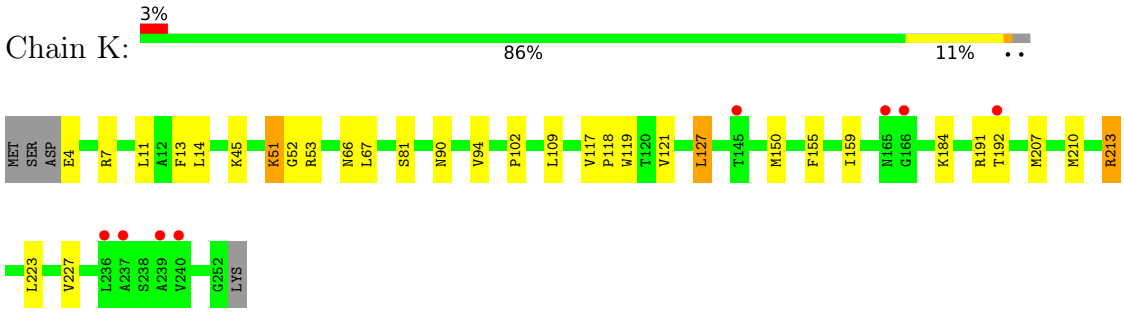
• Molecule 1: NUCLEOPROTEIN

Chain J:



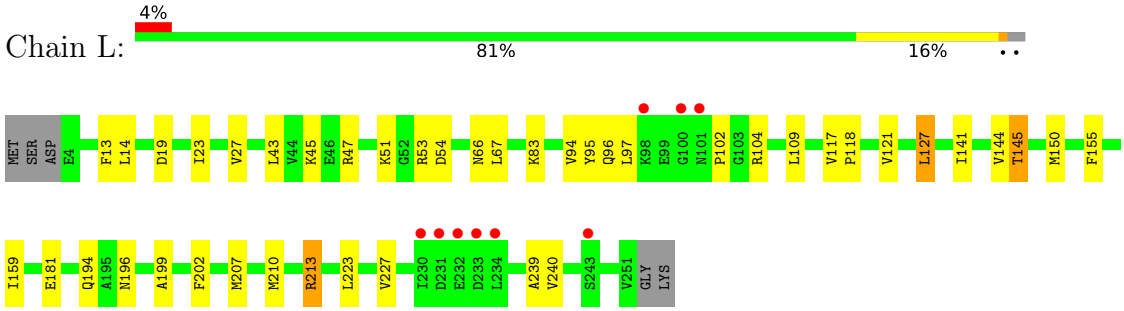
• Molecule 1: NUCLEOPROTEIN

Chain K:



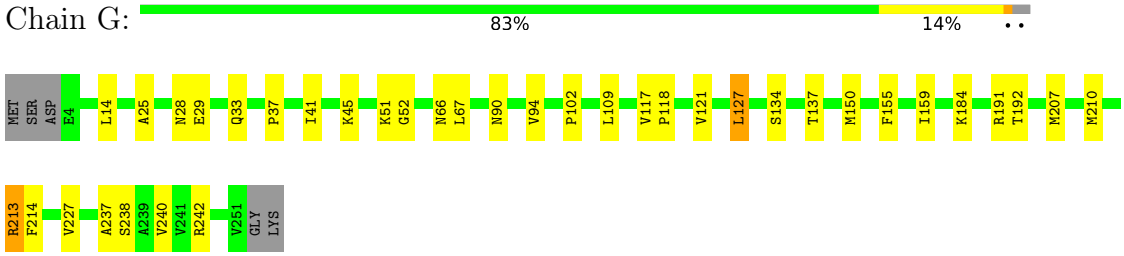
• Molecule 1: NUCLEOPROTEIN

Chain L:



• Molecule 2: NUCLEOPROTEIN

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	104.48Å 104.48Å 510.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.12 – 3.32 34.12 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.12-3.32) 99.2 (34.12-3.32)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.268 0.240 , 0.269	Depositor DCC
R_{free} test set	2295 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.095 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	22844	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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	0.26	0/1921	0.43	0/2593
1	B	0.24	0/1937	0.42	0/2614
1	C	0.25	0/1933	0.41	0/2609
1	D	0.23	0/1934	0.42	0/2610
1	E	0.23	0/1937	0.41	0/2614
1	F	0.25	0/1933	0.43	0/2609
1	H	0.23	0/1959	0.41	0/2643
1	I	0.25	0/1929	0.45	0/2604
1	J	0.23	0/1933	0.42	0/2609
1	K	0.22	0/1941	0.41	0/2619
1	L	0.25	0/1933	0.43	0/2609
2	G	0.25	0/1938	0.42	0/2615
All	All	0.24	0/23228	0.42	0/31348

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	1889	0	1937	32	0
1	B	1905	0	1949	30	1
1	C	1901	0	1947	22	0
1	D	1902	0	1944	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1905	0	1949	23	1
1	F	1901	0	1947	20	0
1	H	1927	0	1970	28	0
1	I	1897	0	1943	25	0
1	J	1901	0	1945	19	0
1	K	1909	0	1952	22	0
1	L	1901	0	1947	24	0
2	G	1906	0	1951	31	0
All	All	22844	0	23381	246	1

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 (246) 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)
2:G:29:GLU:OE2	1:L:83:LYS:NZ	2.16	0.78
1:A:106:THR:HG23	2:G:242:ARG:HH12	1.49	0.76
1:H:2:SER:HB2	1:H:5:ASN:HB2	1.67	0.76
1:A:122:GLN:NE2	1:B:14:LEU:O	2.19	0.75
1:A:34:GLY:HA2	1:F:79:LYS:HD2	1.69	0.75
1:F:66:ASN:HB2	1:F:109:LEU:HB3	1.76	0.67
1:D:119:TRP:HB2	1:E:13:PHE:HB3	1.76	0.67
1:D:28:ASN:O	1:D:213:ARG:NH2	2.29	0.66
1:A:66:ASN:HB2	1:A:109:LEU:HB3	1.77	0.66
2:G:28:ASN:O	2:G:213:ARG:NH2	2.30	0.65
1:J:119:TRP:HB2	1:K:13:PHE:HB3	1.79	0.64
1:B:66:ASN:HB2	1:B:109:LEU:HB3	1.78	0.64
1:D:79:LYS:HD2	1:E:34:GLY:HA2	1.80	0.63
2:G:66:ASN:HB2	2:G:109:LEU:HB3	1.81	0.63
1:D:66:ASN:HB2	1:D:109:LEU:HB3	1.81	0.62
1:H:66:ASN:HB2	1:H:109:LEU:HB3	1.81	0.62
1:H:117:VAL:HG13	1:H:118:PRO:HD3	1.81	0.62
1:C:66:ASN:HB2	1:C:109:LEU:HB3	1.80	0.61
1:F:28:ASN:O	1:F:213:ARG:NH2	2.32	0.61
1:I:66:ASN:HB2	1:I:109:LEU:HB3	1.81	0.61
1:K:66:ASN:HB2	1:K:109:LEU:HB3	1.81	0.61
1:K:117:VAL:HG13	1:K:118:PRO:HD3	1.82	0.61
1:E:66:ASN:HB2	1:E:109:LEU:HB3	1.81	0.61
2:G:117:VAL:HG13	2:G:118:PRO:HD3	1.83	0.60
1:L:66:ASN:HB2	1:L:109:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:HG13	1:D:118:PRO:HD3	1.84	0.60
1:B:117:VAL:HG13	1:B:118:PRO:HD3	1.84	0.60
1:J:66:ASN:HB2	1:J:109:LEU:HB3	1.81	0.60
1:A:117:VAL:HG13	1:A:118:PRO:HD3	1.84	0.60
1:L:117:VAL:HG13	1:L:118:PRO:HD3	1.83	0.59
1:E:117:VAL:HG13	1:E:118:PRO:HD3	1.84	0.59
1:I:117:VAL:HG13	1:I:118:PRO:HD3	1.84	0.59
1:A:119:TRP:HD1	1:B:16:GLU:HB2	1.67	0.59
1:J:117:VAL:HG13	1:J:118:PRO:HD3	1.84	0.58
1:F:117:VAL:HG13	1:F:118:PRO:HD3	1.84	0.58
1:A:106:THR:HG23	2:G:242:ARG:NH1	2.18	0.58
2:G:191:ARG:HG2	1:H:196:ASN:HB3	1.85	0.58
1:K:7:ARG:O	1:K:11:LEU:HB2	2.02	0.58
1:A:105:ASP:HB2	2:G:242:ARG:HH11	1.68	0.57
1:C:117:VAL:HG13	1:C:118:PRO:HD3	1.84	0.57
1:K:51:LYS:O	1:K:53:ARG:HB2	2.06	0.56
1:D:134:SER:HG	1:D:137:THR:HG1	1.53	0.56
1:H:144:VAL:HG21	1:H:239:ALA:HA	1.88	0.55
1:B:4:GLU:OE1	1:B:4:GLU:N	2.39	0.55
1:K:119:TRP:HB2	1:L:13:PHE:HB3	1.89	0.55
1:K:191:ARG:HG2	1:L:196:ASN:HB3	1.88	0.54
1:B:159:ILE:HD11	1:B:210:MET:HG2	1.90	0.54
2:G:213:ARG:H	2:G:213:ARG:HD2	1.72	0.54
1:H:80:MET:H	1:I:104:ARG:HH21	1.55	0.54
1:K:223:LEU:HD23	1:L:14:LEU:HD11	1.90	0.54
1:J:159:ILE:HD11	1:J:210:MET:HG2	1.91	0.54
1:B:6:TYR:HA	1:B:9:ILE:HD13	1.89	0.53
1:A:106:THR:HG23	2:G:242:ARG:HH22	1.72	0.53
1:I:28:ASN:O	1:I:213:ARG:NH2	2.42	0.53
1:I:119:TRP:HD1	1:J:16:GLU:HG3	1.74	0.53
1:J:51:LYS:HD2	1:J:94:VAL:HG23	1.90	0.53
1:K:159:ILE:HD11	1:K:210:MET:HG2	1.91	0.53
1:A:159:ILE:HD11	1:A:210:MET:HG2	1.90	0.53
1:L:95:TYR:O	1:L:97:LEU:N	2.42	0.53
1:I:159:ILE:HD11	1:I:210:MET:HG2	1.91	0.52
1:H:53:ARG:NH1	1:H:58:ASP:OD1	2.42	0.52
1:L:159:ILE:HD11	1:L:210:MET:HG2	1.90	0.52
1:C:67:LEU:HD23	1:C:127:LEU:HD11	1.91	0.52
1:E:159:ILE:HD11	1:E:210:MET:HG2	1.91	0.52
1:E:213:ARG:H	1:E:213:ARG:HD2	1.75	0.52
1:K:213:ARG:H	1:K:213:ARG:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:ILE:HD11	1:F:210:MET:HG2	1.91	0.52
2:G:159:ILE:HD11	2:G:210:MET:HG2	1.91	0.52
1:H:159:ILE:HD11	1:H:210:MET:HG2	1.91	0.52
1:C:159:ILE:HD11	1:C:210:MET:HG2	1.91	0.51
1:C:213:ARG:H	1:C:213:ARG:HD2	1.75	0.51
1:B:134:SER:HG	1:B:137:THR:HG1	1.56	0.51
1:A:121:VAL:HG22	1:A:227:VAL:HG21	1.93	0.51
1:C:121:VAL:HG22	1:C:227:VAL:HG21	1.92	0.51
1:C:134:SER:HG	1:C:137:THR:HG1	1.55	0.51
1:D:159:ILE:HD11	1:D:210:MET:HG2	1.92	0.51
1:H:213:ARG:H	1:H:213:ARG:HD2	1.74	0.51
1:E:134:SER:HG	1:E:137:THR:HG1	1.57	0.51
1:A:119:TRP:CD1	1:B:16:GLU:HB2	2.45	0.51
1:F:121:VAL:HG22	1:F:227:VAL:HG21	1.93	0.51
1:I:121:VAL:HG22	1:I:227:VAL:HG21	1.93	0.51
1:L:121:VAL:HG22	1:L:227:VAL:HG21	1.93	0.51
1:L:213:ARG:H	1:L:213:ARG:HD2	1.75	0.51
1:A:213:ARG:H	1:A:213:ARG:HD2	1.76	0.50
1:D:121:VAL:HG22	1:D:227:VAL:HG21	1.93	0.50
1:I:213:ARG:H	1:I:213:ARG:HD2	1.75	0.50
2:G:28:ASN:HB3	2:G:213:ARG:HH21	1.75	0.50
2:G:121:VAL:HG22	2:G:227:VAL:HG21	1.94	0.50
1:J:213:ARG:H	1:J:213:ARG:HD2	1.76	0.50
1:F:213:ARG:H	1:F:213:ARG:HD2	1.77	0.50
2:G:184:LYS:HG2	2:G:191:ARG:HA	1.94	0.50
1:I:90:ASN:O	1:I:94:VAL:HG12	2.12	0.49
1:K:121:VAL:HG22	1:K:227:VAL:HG21	1.93	0.49
1:B:213:ARG:H	1:B:213:ARG:HD2	1.76	0.49
1:H:121:VAL:HG22	1:H:227:VAL:HG21	1.94	0.49
1:A:39:ARG:NH2	2:G:238:SER:OG	2.45	0.49
1:B:121:VAL:HG22	1:B:227:VAL:HG21	1.94	0.49
1:E:121:VAL:HG22	1:E:227:VAL:HG21	1.94	0.49
1:J:121:VAL:HG22	1:J:227:VAL:HG21	1.93	0.49
1:C:7:ARG:O	1:C:11:LEU:HD12	2.13	0.49
1:D:213:ARG:H	1:D:213:ARG:HD2	1.77	0.49
1:I:37:PRO:HB2	1:I:214:PHE:CD1	2.48	0.48
1:D:188:PRO:HB3	1:E:200:ALA:HB3	1.94	0.48
1:H:19:ASP:OD1	1:H:19:ASP:N	2.30	0.48
1:A:6:TYR:HA	1:A:9:ILE:HD13	1.95	0.48
1:K:90:ASN:O	1:K:94:VAL:HG12	2.12	0.48
1:E:6:TYR:HA	1:E:9:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD23	1:A:127:LEU:HD11	1.96	0.48
2:G:67:LEU:HD23	2:G:127:LEU:HD11	1.95	0.48
1:K:67:LEU:HD23	1:K:127:LEU:HD11	1.94	0.48
1:A:87:ILE:HA	1:A:90:ASN:ND2	2.29	0.48
1:A:134:SER:HG	1:A:137:THR:HG1	1.62	0.48
1:D:223:LEU:HD23	1:E:14:LEU:HD11	1.96	0.48
1:D:90:ASN:O	1:D:94:VAL:HG12	2.13	0.48
1:B:119:TRP:HB2	1:C:13:PHE:HB3	1.95	0.47
1:E:18:ALA:HB1	1:E:23:ILE:HD11	1.96	0.47
1:L:67:LEU:HD23	1:L:127:LEU:HD11	1.96	0.47
1:H:37:PRO:HB2	1:H:214:PHE:CD1	2.49	0.47
1:D:51:LYS:N	1:D:52:GLY:HA2	2.29	0.47
2:G:41:ILE:HD11	1:H:9:ILE:HG21	1.96	0.47
1:H:78:LYS:O	1:I:104:ARG:NE	2.44	0.47
1:E:24:ASN:HA	1:E:27:VAL:HG22	1.96	0.47
1:F:43:LEU:HD13	1:F:47:ARG:HH22	1.80	0.47
1:K:192:THR:HG22	1:L:194:GLN:NE2	2.30	0.47
2:G:184:LYS:HD3	2:G:191:ARG:HD3	1.97	0.47
1:A:30:PHE:O	1:F:69:ARG:HD3	2.14	0.46
1:F:67:LEU:HD23	1:F:127:LEU:HD11	1.96	0.46
1:J:13:PHE:HA	1:J:16:GLU:OE2	2.14	0.46
1:F:102:PRO:HG2	1:F:106:THR:OG1	2.15	0.46
2:G:192:THR:HG22	1:H:194:GLN:NE2	2.30	0.46
1:L:23:ILE:O	1:L:27:VAL:HG23	2.15	0.46
1:A:81:SER:OG	1:B:29:GLU:O	2.33	0.46
1:D:67:LEU:HD23	1:D:127:LEU:HD11	1.97	0.46
2:G:41:ILE:HG21	1:H:6:TYR:HD1	1.79	0.46
1:C:223:LEU:HD23	1:D:14:LEU:HD11	1.96	0.46
1:H:90:ASN:O	1:H:94:VAL:HG12	2.16	0.46
1:J:53:ARG:NH2	1:J:90:ASN:HB3	2.31	0.46
1:A:90:ASN:O	1:A:94:VAL:HG12	2.16	0.46
1:E:5:ASN:O	1:E:5:ASN:ND2	2.48	0.46
1:A:106:THR:CG2	2:G:242:ARG:HH22	2.29	0.46
1:C:90:ASN:O	1:C:94:VAL:HG12	2.15	0.46
1:B:90:ASN:O	1:B:94:VAL:HG12	2.15	0.45
1:E:84:GLY:HA2	1:F:29:GLU:HG2	1.98	0.45
1:I:134:SER:HG	1:I:137:THR:HG1	1.58	0.45
1:B:24:ASN:HA	1:B:27:VAL:HG22	1.99	0.45
1:I:87:ILE:HA	1:I:90:ASN:ND2	2.32	0.45
1:A:53:ARG:HH22	1:A:90:ASN:HB3	1.81	0.45
2:G:90:ASN:O	2:G:94:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:184:LYS:HG2	1:K:191:ARG:HA	1.98	0.45
1:C:119:TRP:HB2	1:D:13:PHE:HB3	1.99	0.45
2:G:14:LEU:HD11	1:L:223:LEU:HD23	1.99	0.45
2:G:150:MET:HG2	2:G:155:PHE:CE2	2.52	0.45
1:H:215:PHE:CD1	1:I:11:LEU:HD12	2.51	0.45
1:I:36:ASP:HB2	1:I:104:ARG:HH12	1.81	0.45
1:H:45:LYS:HB3	1:H:45:LYS:HE3	1.85	0.45
1:E:90:ASN:O	1:E:94:VAL:HG12	2.17	0.45
2:G:25:ALA:O	2:G:29:GLU:HG3	2.17	0.45
1:A:60:LYS:NZ	1:B:17:SER:OG	2.43	0.45
1:D:150:MET:HG2	1:D:155:PHE:CE2	2.52	0.45
1:H:150:MET:HG2	1:H:155:PHE:CE2	2.52	0.45
1:J:214:PHE:O	1:K:7:ARG:HD3	2.16	0.45
1:C:141:ILE:HD13	1:C:181:GLU:HG3	2.00	0.44
2:G:134:SER:HG	2:G:137:THR:HG1	1.60	0.44
1:A:14:LEU:HG	1:F:118:PRO:HB3	1.99	0.44
1:I:14:LEU:HD12	1:I:14:LEU:H	1.81	0.44
1:L:51:LYS:HD2	1:L:94:VAL:HG23	1.99	0.44
1:L:150:MET:HG2	1:L:155:PHE:CE2	2.52	0.44
1:I:150:MET:HG2	1:I:155:PHE:CE2	2.52	0.44
1:B:150:MET:HG2	1:B:155:PHE:CE2	2.52	0.44
1:E:84:GLY:CA	1:F:29:GLU:HG2	2.47	0.44
1:I:7:ARG:O	1:I:11:LEU:N	2.51	0.44
1:J:45:LYS:HE3	1:J:45:LYS:HB3	1.86	0.44
1:J:53:ARG:HG3	1:J:54:ASP:N	2.32	0.44
1:J:150:MET:HG2	1:J:155:PHE:CE2	2.52	0.44
1:C:51:LYS:HD2	1:C:94:VAL:HG23	1.99	0.44
1:C:150:MET:HG2	1:C:155:PHE:CE2	2.53	0.44
1:F:150:MET:HG2	1:F:155:PHE:CE2	2.53	0.44
1:A:150:MET:HG2	1:A:155:PHE:CE2	2.52	0.44
1:E:150:MET:HG2	1:E:155:PHE:CE2	2.52	0.44
1:D:5:ASN:O	1:D:9:ILE:HG12	2.17	0.43
1:D:45:LYS:HB3	1:D:45:LYS:HE3	1.83	0.43
1:F:90:ASN:O	1:F:94:VAL:HG12	2.19	0.43
1:F:134:SER:HG	1:F:137:THR:HG1	1.61	0.43
1:C:237:ALA:HB3	1:C:240:VAL:HG23	2.01	0.43
1:H:119:TRP:HB2	1:I:13:PHE:HD1	1.84	0.43
1:I:13:PHE:C	1:I:15:ASP:H	2.21	0.43
1:K:184:LYS:HD3	1:K:191:ARG:HD3	2.00	0.43
1:K:4:GLU:N	1:K:4:GLU:OE1	2.52	0.43
1:B:47:ARG:O	1:B:51:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ASN:HA	1:D:31:ALA:HB2	2.00	0.43
2:G:184:LYS:HB3	2:G:191:ARG:CZ	2.49	0.43
1:I:69:ARG:HD3	1:J:30:PHE:O	2.18	0.43
1:B:45:LYS:HE3	1:B:45:LYS:HB3	1.88	0.43
1:K:150:MET:HG2	1:K:155:PHE:CE2	2.53	0.43
1:D:56:LYS:O	1:D:60:LYS:HG3	2.19	0.43
1:J:20:SER:O	1:J:24:ASN:ND2	2.51	0.43
1:H:215:PHE:HD1	1:I:11:LEU:HD12	1.84	0.42
1:B:67:LEU:HD23	1:B:127:LEU:HD11	2.00	0.42
2:G:33:GLN:NE2	2:G:214:PHE:HZ	2.18	0.42
1:B:103:GLY:H	1:H:242:ARG:NH1	2.17	0.42
1:B:106:THR:CG2	1:H:144:VAL:HG12	2.50	0.42
1:E:119:TRP:HB2	1:F:13:PHE:HB3	2.01	0.42
1:L:43:LEU:HD13	1:L:47:ARG:HH22	1.84	0.42
1:C:167:ALA:O	1:C:171:ILE:HG13	2.20	0.42
1:C:45:LYS:HE3	1:C:45:LYS:HB3	1.88	0.42
1:K:81:SER:HA	1:L:104:ARG:NH2	2.35	0.42
1:A:102:PRO:HG2	1:A:106:THR:OG1	2.19	0.41
1:B:102:PRO:HG2	1:B:106:THR:OG1	2.19	0.41
1:D:51:LYS:HA	1:D:51:LYS:HD2	1.79	0.41
1:F:39:ARG:NE	1:F:105:ASP:OD2	2.52	0.41
1:A:144:VAL:HG21	1:A:239:ALA:HA	2.02	0.41
1:H:199:ALA:HA	1:H:202:PHE:CE2	2.56	0.41
1:H:56:LYS:O	1:H:60:LYS:HG3	2.20	0.41
1:K:52:GLY:HA3	1:K:53:ARG:CB	2.50	0.41
1:A:38:LYS:HD2	1:B:4:GLU:HA	2.02	0.41
1:E:67:LEU:HD23	1:E:127:LEU:HD11	2.02	0.41
1:H:67:LEU:HD23	1:H:127:LEU:HD11	2.03	0.41
1:E:45:LYS:HB3	1:E:45:LYS:HE3	1.86	0.41
1:A:146:TYR:HA	1:A:147:PRO:HD3	1.98	0.41
2:G:37:PRO:HD2	2:G:214:PHE:CZ	2.56	0.41
1:I:56:LYS:O	1:I:60:LYS:HG3	2.21	0.41
1:J:223:LEU:HD23	1:K:14:LEU:HD11	2.02	0.41
1:F:96:GLN:NE2	1:L:145:THR:HG21	2.35	0.41
1:I:67:LEU:HD23	1:I:127:LEU:HD11	2.02	0.41
1:L:199:ALA:HA	1:L:202:PHE:CE2	2.56	0.41
1:B:43:LEU:HD13	1:B:47:ARG:HH22	1.86	0.41
1:C:231:ASP:OD2	1:C:235:VAL:HB	2.20	0.41
1:D:184:LYS:HG2	1:D:191:ARG:HA	2.03	0.41
1:I:83:LYS:HG2	1:J:29:GLU:OE2	2.21	0.41
1:L:53:ARG:HG3	1:L:54:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:VAL:HG21	1:L:239:ALA:HA	2.03	0.41
1:B:42:GLN:HB2	1:C:6:TYR:CE2	2.56	0.40
1:L:150:MET:HE3	1:L:240:VAL:HG22	2.03	0.40
1:A:106:THR:HG23	2:G:242:ARG:NH2	2.34	0.40
1:A:225:ILE:HA	1:A:230:ILE:O	2.22	0.40
1:D:69:ARG:HD3	1:E:30:PHE:O	2.21	0.40
2:G:237:ALA:HB3	2:G:240:VAL:HG23	2.03	0.40
1:L:141:ILE:HD13	1:L:181:GLU:HG3	2.03	0.40
1:E:102:PRO:HB2	1:E:103:GLY:H	1.67	0.40
1:J:199:ALA:HA	1:J:202:PHE:CE2	2.57	0.40
1:B:13:PHE:HA	1:B:16:GLU:HG2	2.04	0.40
1:B:102:PRO:HB2	1:B:103:GLY:H	1.63	0.40
1:B:199:ALA:HA	1:B:202:PHE:CE2	2.57	0.40
1:C:199:ALA:HA	1:C:202:PHE:CE2	2.57	0.40
1:B:122:GLN:NE2	1:C:14:LEU:O	2.53	0.40
1:H:11:LEU:HD23	1:H:11:LEU:HA	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:SER:OG	1:E:19:ASP:OD1[1_545]	2.16	0.04

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	245/253 (97%)	232 (95%)	12 (5%)	1 (0%)	34	66
1	B	246/253 (97%)	236 (96%)	9 (4%)	1 (0%)	34	66
1	C	246/253 (97%)	230 (94%)	15 (6%)	1 (0%)	34	66
1	D	247/253 (98%)	236 (96%)	10 (4%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	246/253 (97%)	235 (96%)	10 (4%)	1 (0%)	34	66
1	F	246/253 (97%)	235 (96%)	10 (4%)	1 (0%)	34	66
1	H	249/253 (98%)	237 (95%)	11 (4%)	1 (0%)	34	66
1	I	246/253 (97%)	234 (95%)	11 (4%)	1 (0%)	34	66
1	J	246/253 (97%)	232 (94%)	12 (5%)	2 (1%)	19	51
1	K	247/253 (98%)	235 (95%)	11 (4%)	1 (0%)	34	66
1	L	246/253 (97%)	232 (94%)	12 (5%)	2 (1%)	19	51
2	G	246/253 (97%)	235 (96%)	9 (4%)	2 (1%)	19	51
All	All	2956/3036 (97%)	2809 (95%)	132 (4%)	15 (0%)	29	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	GLN
1	A	102	PRO
1	B	102	PRO
1	C	102	PRO
1	D	102	PRO
1	E	102	PRO
1	F	102	PRO
2	G	102	PRO
1	H	102	PRO
1	I	102	PRO
1	J	52	GLY
1	J	102	PRO
1	K	102	PRO
1	L	102	PRO
2	G	52	GLY

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	199/206 (97%)	193 (97%)	6 (3%)	41	69
1	B	201/206 (98%)	195 (97%)	6 (3%)	41	69
1	C	201/206 (98%)	194 (96%)	7 (4%)	36	66
1	D	199/206 (97%)	194 (98%)	5 (2%)	47	73
1	E	201/206 (98%)	194 (96%)	7 (4%)	36	66
1	F	201/206 (98%)	195 (97%)	6 (3%)	41	69
1	H	204/206 (99%)	196 (96%)	8 (4%)	32	63
1	I	200/206 (97%)	193 (96%)	7 (4%)	36	66
1	J	200/206 (97%)	196 (98%)	4 (2%)	55	77
1	K	201/206 (98%)	196 (98%)	5 (2%)	47	73
1	L	201/206 (98%)	195 (97%)	6 (3%)	41	69
2	G	201/206 (98%)	196 (98%)	5 (2%)	47	73
All	All	2409/2472 (98%)	2337 (97%)	72 (3%)	41	69

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	45	LYS
1	A	53	ARG
1	A	127	LEU
1	A	207	MET
1	A	213	ARG
1	B	4	GLU
1	B	15	ASP
1	B	45	LYS
1	B	127	LEU
1	B	207	MET
1	B	213	ARG
1	C	4	GLU
1	C	11	LEU
1	C	14	LEU
1	C	45	LYS
1	C	127	LEU
1	C	207	MET
1	C	213	ARG
1	D	11	LEU
1	D	45	LYS
1	D	127	LEU

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Mol	Chain	Res	Type
1	D	207	MET
1	D	213	ARG
1	E	4	GLU
1	E	5	ASN
1	E	11	LEU
1	E	45	LYS
1	E	127	LEU
1	E	207	MET
1	E	213	ARG
1	F	45	LYS
1	F	51	LYS
1	F	53	ARG
1	F	127	LEU
1	F	207	MET
1	F	213	ARG
2	G	45	LYS
2	G	51	LYS
2	G	127	LEU
2	G	207	MET
2	G	213	ARG
1	H	3	ASP
1	H	13	PHE
1	H	19	ASP
1	H	45	LYS
1	H	53	ARG
1	H	127	LEU
1	H	207	MET
1	H	213	ARG
1	I	7	ARG
1	I	13	PHE
1	I	14	LEU
1	I	45	LYS
1	I	127	LEU
1	I	207	MET
1	I	213	ARG
1	J	45	LYS
1	J	127	LEU
1	J	207	MET
1	J	213	ARG
1	K	45	LYS
1	K	51	LYS
1	K	127	LEU

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Mol	Chain	Res	Type
1	K	207	MET
1	K	213	ARG
1	L	19	ASP
1	L	45	LYS
1	L	127	LEU
1	L	145	THR
1	L	207	MET
1	L	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	247/253 (97%)	-0.09	3 (1%) 79 79	29, 58, 100, 126	0
1	B	248/253 (98%)	-0.21	0 100 100	35, 56, 85, 106	0
1	C	248/253 (98%)	-0.04	4 (1%) 72 70	35, 62, 101, 136	0
1	D	249/253 (98%)	0.14	7 (2%) 53 51	32, 74, 130, 150	0
1	E	248/253 (98%)	0.88	38 (15%) 2 1	44, 105, 128, 144	0
1	F	248/253 (98%)	0.68	24 (9%) 7 8	52, 105, 138, 158	0
1	H	251/253 (99%)	0.02	7 (2%) 53 51	35, 72, 101, 133	0
1	I	248/253 (98%)	0.30	6 (2%) 59 57	52, 86, 113, 128	0
1	J	248/253 (98%)	-0.12	3 (1%) 79 79	36, 64, 93, 110	0
1	K	249/253 (98%)	0.09	8 (3%) 47 46	35, 75, 121, 149	0
1	L	248/253 (98%)	0.11	9 (3%) 42 41	37, 74, 123, 161	0
2	G	248/253 (98%)	-0.14	0 100 100	33, 57, 87, 98	0
All	All	2980/3036 (98%)	0.13	109 (3%) 41 40	29, 72, 121, 161	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	GLU	5.2
1	F	233	ASP	5.1
1	E	42	GLN	5.1
1	E	143	GLY	4.8
1	F	192	THR	4.4
1	L	101	ASN	4.3
1	C	192	THR	4.0
1	E	41	VAL	3.9
1	E	192	THR	3.8
1	E	105	ASP	3.8
1	D	230	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	100	GLY	3.7
1	D	144	VAL	3.6
1	F	231	ASP	3.6
1	E	230	ILE	3.6
1	F	10	ALA	3.6
1	E	107	ILE	3.6
1	F	163	LEU	3.5
1	E	90	ASN	3.5
1	E	40	ILE	3.5
1	F	8	ASP	3.5
1	E	189	SER	3.4
1	A	193	LYS	3.4
1	F	164	PRO	3.4
1	E	92	ILE	3.4
1	L	234	LEU	3.3
1	F	198	VAL	3.3
1	F	176	GLY	3.3
1	F	239	ALA	3.2
1	E	167	ALA	3.2
1	I	233	ASP	3.1
1	E	43	LEU	3.1
1	F	173	ASP	3.1
1	H	100	GLY	3.1
1	E	220	LYS	3.1
1	C	194	GLN	3.0
1	F	244	ALA	2.9
1	F	238	SER	2.9
1	D	143	GLY	2.9
1	F	240	VAL	2.9
1	H	101	ASN	2.9
1	D	140	ALA	2.9
1	E	104	ARG	2.8
1	F	243	SER	2.8
1	L	98	LYS	2.7
1	K	239	ALA	2.7
1	E	236	LEU	2.7
1	E	97	LEU	2.7
1	L	230	ILE	2.7
1	E	168	GLY	2.7
1	E	50	ALA	2.7
1	L	243	SER	2.6
1	E	160	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	167	ALA	2.6
1	E	193	LYS	2.6
1	E	234	LEU	2.6
1	F	174	ALA	2.6
1	K	237	ALA	2.6
1	E	219	ASP	2.6
1	E	242	ARG	2.5
1	J	101	ASN	2.5
1	L	232	GLU	2.5
1	H	143	GLY	2.5
1	K	165	ASN	2.5
1	I	231	ASP	2.5
1	C	251	VAL	2.5
1	E	106	THR	2.5
1	J	52	GLY	2.4
1	E	215	PHE	2.4
1	E	241	VAL	2.4
1	L	100	GLY	2.4
1	K	192	THR	2.4
1	L	231	ASP	2.4
1	K	166	GLY	2.4
1	E	198	VAL	2.4
1	F	248	ARG	2.4
1	C	197	GLU	2.4
1	F	177	LEU	2.4
1	F	199	ALA	2.3
1	H	2	SER	2.3
1	D	168	GLY	2.3
1	A	9	ILE	2.3
1	H	217	ARG	2.3
1	I	102	PRO	2.3
1	E	169	ALA	2.2
1	L	233	ASP	2.2
1	D	167	ALA	2.2
1	H	99	GLU	2.2
1	K	236	LEU	2.2
1	I	49	THR	2.2
1	E	231	ASP	2.2
1	F	165	ASN	2.2
1	I	164	PRO	2.2
1	D	241	VAL	2.2
1	E	142	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	46	GLU	2.1
1	I	243	SER	2.1
1	E	101	ASN	2.1
1	K	240	VAL	2.1
1	K	145	THR	2.1
1	E	245	GLU	2.1
1	F	48	GLY	2.1
1	E	49	THR	2.1
1	E	73	PRO	2.0
1	E	36	ASP	2.0
1	E	188	PRO	2.0
1	A	192	THR	2.0
1	F	201	THR	2.0
1	H	167	ALA	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.