



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:37 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](mailto: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.

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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

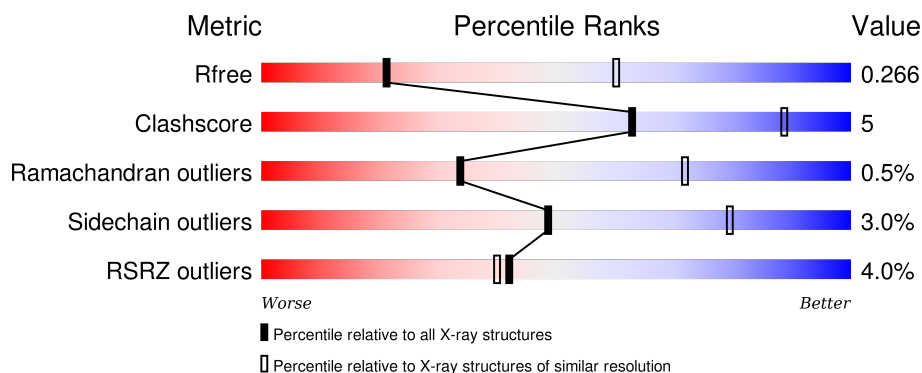
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	 2% 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	<div><div></div><div>11%</div><div>85%</div><div>12%</div><div>..</div></div>
1	H	253	<div><div></div><div>3%</div><div>82%</div><div>15%</div><div>..</div></div>
1	I	253	<div><div></div><div>3%</div><div>84%</div><div>12%</div><div>..</div></div>
1	J	253	<div><div></div><div>%</div><div>85%</div><div>12%</div><div>..</div></div>
1	K	253	<div><div></div><div>4%</div><div>86%</div><div>11%</div><div>..</div></div>
1	L	253	<div><div></div><div>4%</div><div>81%</div><div>16%</div><div>..</div></div>
2	G	253	<div><div></div><div></div><div>83%</div><div>14%</div><div>..</div></div>

## 2 Entry composition

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			

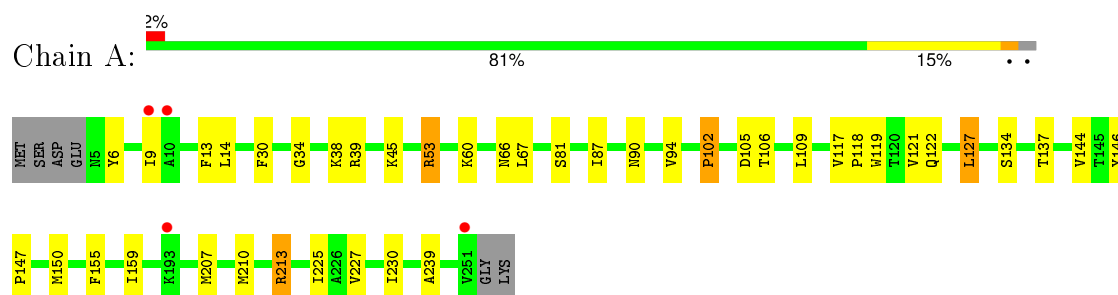
There is a discrepancy between the modelled and reference sequences:

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

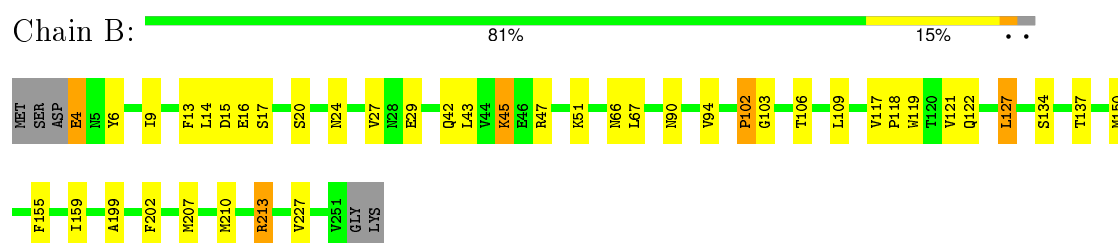
### 3 Residue-property plots

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.

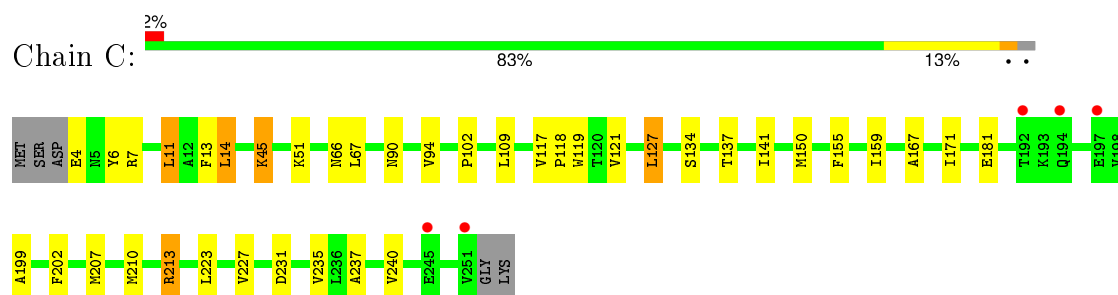
#### • Molecule 1: NUCLEOPROTEIN



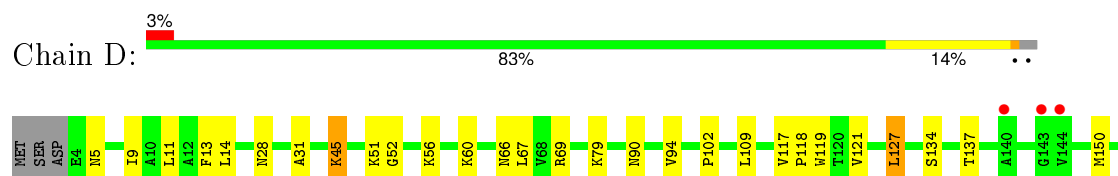
#### • Molecule 1: NUCLEOPROTEIN



#### • Molecule 1: NUCLEOPROTEIN

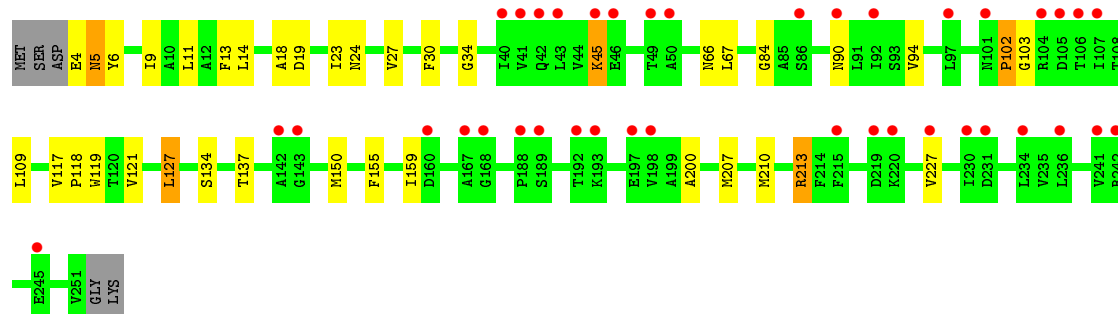
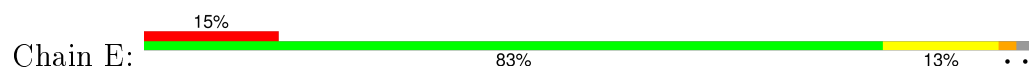


#### • Molecule 1: NUCLEOPROTEIN

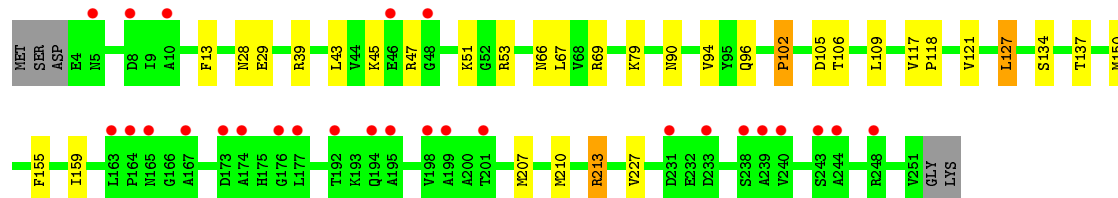
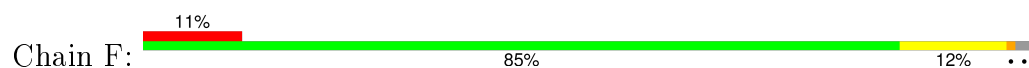




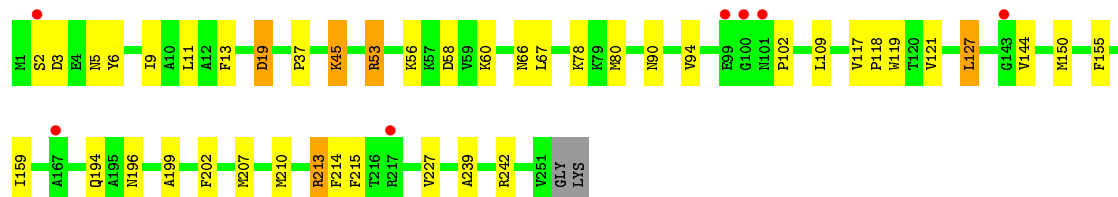
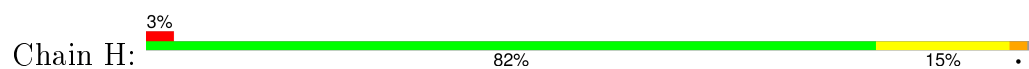
• Molecule 1: NUCLEOPROTEIN



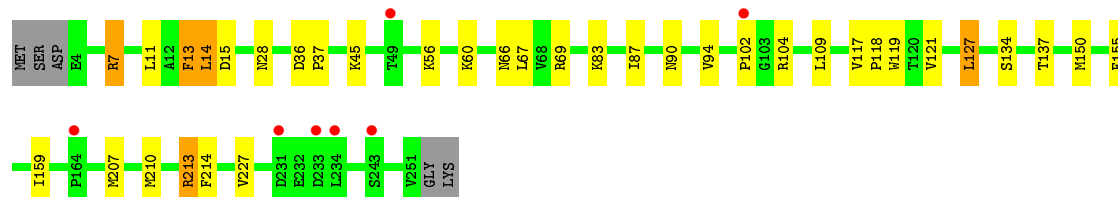
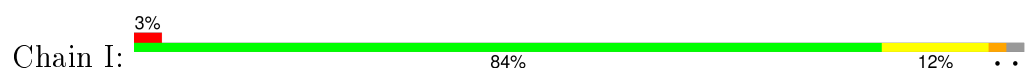
• Molecule 1: NUCLEOPROTEIN



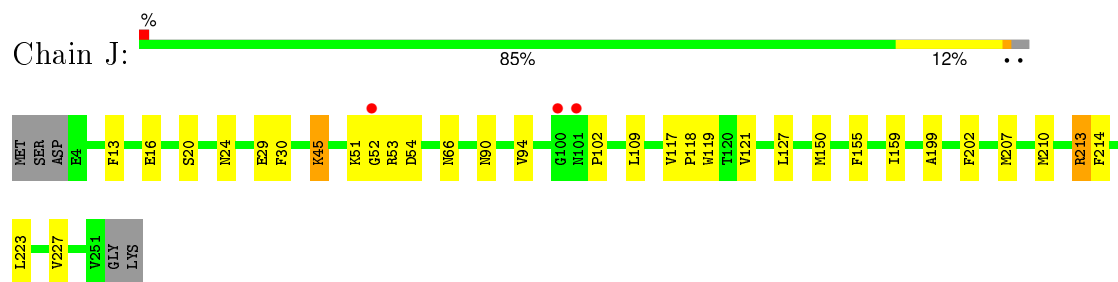
• Molecule 1: NUCLEOPROTEIN



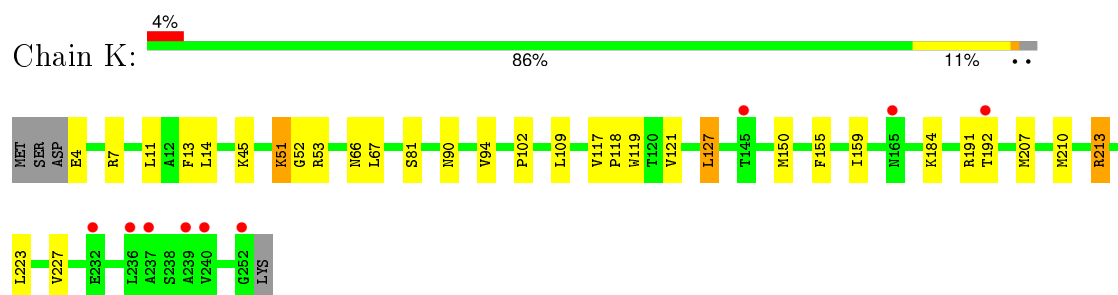
• Molecule 1: NUCLEOPROTEIN



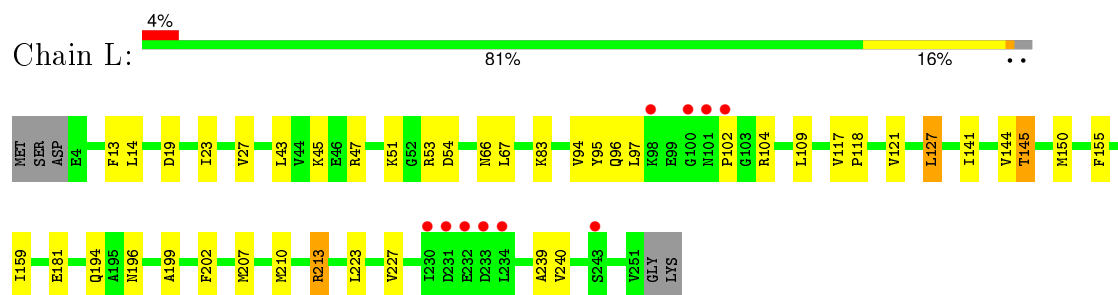
• Molecule 1: NUCLEOPROTEIN



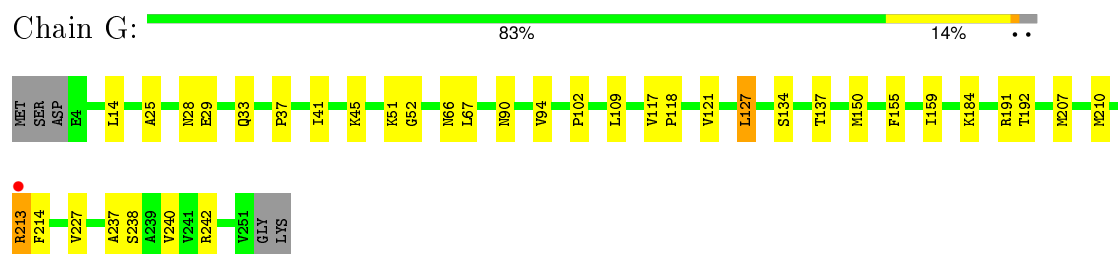
- Molecule 1: NUCLEOPROTEIN



- Molecule 1: NUCLEOPROTEIN



- Molecule 2: NUCLEOPROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.240 , 0.268 0.238 , 0.266	Depositor DCC
$R_{free}$ test set	2293 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.3	EDS
Estimated twinning fraction	0.095 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 45888 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	22844	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [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	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:H:66:ASN:HB2	1:H:109:LEU:HB3	1.81	0.62
1:D:66:ASN:HB2	1:D:109:LEU:HB3	1.81	0.62
1:H:117:VAL:HG13	1:H:118:PRO:HD3	1.81	0.62
1:I:66:ASN:HB2	1:I:109:LEU:HB3	1.81	0.61
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: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
1:L:66:ASN:HB2	1:L:109:LEU:HB3	1.82	0.60
2:G:117:VAL:HG13	2:G:118:PRO:HD3	1.83	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:N	1:B:4:GLU:OE1	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
2:G:213:ARG:HD2	2:G:213:ARG:H	1.72	0.54
1:B:159:ILE:HD11	1:B:210:MET:HG2	1.90	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:J:51:LYS:HD2	1:J:94:VAL:HG23	1.90	0.53
1:I:119:TRP:HD1	1:J:16:GLU:HG3	1.74	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:E:159:ILE:HD11	1:E:210:MET:HG2	1.91	0.52
1:C:67:LEU:HD23	1:C:127:LEU:HD11	1.91	0.52
1:K:213:ARG:HD2	1:K:213:ARG:H	1.74	0.52
1:E:213:ARG:H	1:E:213:ARG:HD2	1.75	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:D:159:ILE:HD11	1:D:210:MET:HG2	1.92	0.51
1:H:213:ARG:HD2	1:H:213:ARG:H	1.74	0.51
1:C:134:SER:HG	1:C:137:THR:HG1	1.55	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:HD2	1:L:213:ARG:H	1.75	0.51
1:I:213:ARG:H	1:I:213:ARG:HD2	1.75	0.50
1:D:121:VAL:HG22	1:D:227:VAL:HG21	1.93	0.50
1:A:213:ARG:HD2	1:A:213:ARG:H	1.76	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:HD2	1:F:213:ARG:H	1.77	0.50
2:G:184:LYS:HG2	2:G:191:ARG:HA	1.94	0.50
1:K:121:VAL:HG22	1:K:227:VAL:HG21	1.93	0.49
1:I:90:ASN:O	1:I:94:VAL:HG12	2.12	0.49
1:B:213:ARG:HD2	1:B:213:ARG:H	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:J:121:VAL:HG22	1:J:227:VAL:HG21	1.93	0.49
1:E:121:VAL:HG22	1:E:227:VAL:HG21	1.94	0.49
1:D:213:ARG:H	1:D:213:ARG:HD2	1.77	0.49
1:C:7:ARG:O	1:C:11:LEU:HD12	2.13	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)
2:G:67:LEU:HD23	2:G:127:LEU:HD11	1.95	0.48
1:A:67:LEU:HD23	1:A:127:LEU:HD11	1.96	0.48
1:K:67:LEU:HD23	1:K:127:LEU:HD11	1.94	0.48
1:D:223:LEU:HD23	1:E:14:LEU:HD11	1.96	0.48
1:A:134:SER:HG	1:A:137:THR:HG1	1.62	0.48
1:A:87:ILE:HA	1:A:90:ASN:ND2	2.29	0.48
1:D:90:ASN:O	1:D:94:VAL:HG12	2.13	0.48
1:L:67:LEU:HD23	1:L:127:LEU:HD11	1.96	0.47
1:E:18:ALA:HB1	1:E:23:ILE:HD11	1.96	0.47
1:B:119:TRP:HB2	1:C:13:PHE:HB3	1.95	0.47
1:H:37:PRO:HB2	1:H:214:PHE:CD1	2.49	0.47
1:H:78:LYS:O	1:I:104:ARG:NE	2.44	0.47
2:G:41:ILE:HD11	1:H:9:ILE:HG21	1.96	0.47
1:D:51:LYS:N	1:D:52:GLY:HA2	2.29	0.47
1:F:43:LEU:HD13	1:F:47:ARG:HH22	1.80	0.47
1:E:24:ASN:HA	1:E:27:VAL:HG22	1.96	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:J:13:PHE:HA	1:J:16:GLU:OE2	2.14	0.46
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: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
2:G:41:ILE:HG21	1:H:6:TYR:HD1	1.79	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
1:J:53:ARG:NH2	1:J:90:ASN:HB3	2.31	0.46
1:H:90:ASN:O	1:H:94:VAL:HG12	2.16	0.46
1:C:223:LEU:HD23	1:D:14:LEU:HD11	1.96	0.46
1:A:90:ASN:O	1:A:94:VAL:HG12	2.16	0.46
1:E:5:ASN:ND2	1:E:5:ASN:O	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:I:87:ILE:HA	1:I:90:ASN:ND2	2.32	0.45
1:B:24:ASN:HA	1:B:27:VAL:HG22	1.99	0.45
1:K:184:LYS:HG2	1:K:191:ARG:HA	1.98	0.45
1:A:53:ARG:HH22	1:A:90:ASN:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:90:ASN:O	2:G:94:VAL:HG12	2.17	0.45
1:I:36:ASP:HB2	1:I:104:ARG:HH12	1.81	0.45
1:H:215:PHE:CD1	1:I:11:LEU:HD12	2.51	0.45
1:C:119:TRP:HB2	1:D:13:PHE:HB3	1.99	0.45
2:G:150:MET:HG2	2:G:155:PHE:CE2	2.52	0.45
2:G:14:LEU:HD11	1:L:223:LEU:HD23	1.99	0.45
1:H:45:LYS:HE3	1:H:45:LYS:HB3	1.85	0.45
2:G:25:ALA:O	2:G:29:GLU:HG3	2.17	0.45
1:E:90:ASN:O	1:E:94:VAL:HG12	2.17	0.45
1:J:214:PHE:O	1:K:7:ARG:HD3	2.16	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: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:L:51:LYS:HD2	1:L:94:VAL:HG23	1.99	0.44
1:I:14:LEU:HD12	1:I:14:LEU:H	1.81	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: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:HB3	1:J:45:LYS:HE3	1.86	0.44
1:B:150:MET:HG2	1:B:155:PHE:CE2	2.52	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:E:150:MET:HG2	1:E:155:PHE:CE2	2.52	0.44
1:A:150:MET:HG2	1:A:155:PHE:CE2	2.52	0.44
1:D:45:LYS:HE3	1:D:45:LYS:HB3	1.83	0.43
1:D:5:ASN:O	1:D:9:ILE:HG12	2.17	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:K:184:LYS:HD3	1:K:191:ARG:HD3	2.00	0.43
1:I:13:PHE:C	1:I:15:ASP:H	2.21	0.43
1:H:119:TRP:HB2	1:I:13:PHE:HD1	1.84	0.43
1:K:4:GLU:OE1	1:K:4:GLU:N	2.52	0.43
1:D:28:ASN:HA	1:D:31:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:184:LYS:HB3	2:G:191:ARG:CZ	2.49	0.43
1:B:47:ARG:O	1:B:51:LYS:HB2	2.19	0.43
1:I:69:ARG:HD3	1:J:30:PHE:O	2.18	0.43
1:K:150:MET:HG2	1:K:155:PHE:CE2	2.53	0.43
1:B:45:LYS:HE3	1:B:45:LYS:HB3	1.88	0.43
1:J:20:SER:O	1:J:24:ASN:ND2	2.51	0.43
1:D:56:LYS:O	1:D:60:LYS:HG3	2.19	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:L:43:LEU:HD13	1:L:47:ARG:HH22	1.84	0.42
1:E:119:TRP:HB2	1:F:13:PHE:HB3	2.01	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:HD2	1:D:51:LYS:HA	1.79	0.41
1:F:39:ARG:NE	1:F:105:ASP:OD2	2.52	0.41
1:H:199:ALA:HA	1:H:202:PHE:CE2	2.56	0.41
1:A:144:VAL:HG21	1:A:239:ALA:HA	2.02	0.41
1:K:52:GLY:HA3	1:K:53:ARG:CB	2.50	0.41
1:H:56:LYS:O	1:H:60:LYS:HG3	2.20	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
2:G:37:PRO:HD2	2:G:214:PHE:CZ	2.56	0.41
1:J:223:LEU:HD23	1:K:14:LEU:HD11	2.02	0.41
1:I:56:LYS:O	1:I:60:LYS:HG3	2.21	0.41
1:A:146:TYR:HA	1:A:147:PRO:HD3	1.98	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:L:144:VAL:HG21	1:L:239:ALA:HA	2.03	0.41
1:C:231:ASP:OD2	1:C:235:VAL:HB	2.20	0.41
1:L:53:ARG:HG3	1:L:54:ASP:N	2.36	0.41
1:D:184:LYS:HG2	1:D:191:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:LYS:HG2	1:J:29:GLU:OE2	2.21	0.41
1:L:150:MET:HE3	1:L:240:VAL:HG22	2.03	0.40
1:B:42:GLN:HB2	1:C:6:TYR:CE2	2.56	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:C:199:ALA:HA	1:C:202:PHE:CE2	2.57	0.40
1:B:199:ALA:HA	1:B: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:HA	1:H:11:LEU:HD23	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%)	39 76
1	B	246/253 (97%)	236 (96%)	9 (4%)	1 (0%)	39 76
1	C	246/253 (97%)	230 (94%)	15 (6%)	1 (0%)	39 76
1	D	247/253 (98%)	236 (96%)	10 (4%)	1 (0%)	39 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	246/253 (97%)	235 (96%)	10 (4%)	1 (0%)	39	76
1	F	246/253 (97%)	235 (96%)	10 (4%)	1 (0%)	39	76
1	H	249/253 (98%)	237 (95%)	11 (4%)	1 (0%)	39	76
1	I	246/253 (97%)	234 (95%)	11 (4%)	1 (0%)	39	76
1	J	246/253 (97%)	232 (94%)	12 (5%)	2 (1%)	24	63
1	K	247/253 (98%)	235 (95%)	11 (4%)	1 (0%)	39	76
1	L	246/253 (97%)	232 (94%)	12 (5%)	2 (1%)	24	63
2	G	246/253 (97%)	235 (96%)	9 (4%)	2 (1%)	24	63
All	All	2956/3036 (97%)	2809 (95%)	132 (4%)	15 (0%)	34	72

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 ⓘ

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%)	48	79
1	B	201/206 (98%)	195 (97%)	6 (3%)	48	79
1	C	201/206 (98%)	194 (96%)	7 (4%)	43	76
1	D	199/206 (97%)	194 (98%)	5 (2%)	55	82
1	E	201/206 (98%)	194 (96%)	7 (4%)	43	76
1	F	201/206 (98%)	195 (97%)	6 (3%)	48	79
1	H	204/206 (99%)	196 (96%)	8 (4%)	39	74
1	I	200/206 (97%)	193 (96%)	7 (4%)	43	76
1	J	200/206 (97%)	196 (98%)	4 (2%)	63	85
1	K	201/206 (98%)	196 (98%)	5 (2%)	55	82
1	L	201/206 (98%)	195 (97%)	6 (3%)	48	79
2	G	201/206 (98%)	196 (98%)	5 (2%)	55	82
All	All	2409/2472 (98%)	2337 (97%)	72 (3%)	48	79

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

Some 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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	247/253 (97%)	-0.06	4 (1%) 74 73	29, 58, 100, 127	0
1	B	248/253 (98%)	-0.19	0 100 100	35, 56, 85, 106	0
1	C	248/253 (98%)	-0.02	5 (2%) 68 67	35, 62, 101, 136	0
1	D	249/253 (98%)	0.16	7 (2%) 56 56	32, 74, 130, 150	0
1	E	248/253 (98%)	0.91	39 (15%) 3 3	44, 105, 128, 144	0
1	F	248/253 (98%)	0.72	27 (10%) 7 7	52, 105, 138, 158	0
1	H	251/253 (99%)	0.05	7 (2%) 56 56	35, 72, 101, 133	0
1	I	248/253 (98%)	0.33	7 (2%) 56 56	52, 86, 113, 128	0
1	J	248/253 (98%)	-0.10	3 (1%) 81 81	36, 64, 93, 110	0
1	K	249/253 (98%)	0.11	9 (3%) 46 45	35, 75, 121, 149	0
1	L	248/253 (98%)	0.13	10 (4%) 42 40	37, 74, 123, 161	0
2	G	248/253 (98%)	-0.11	1 (0%) 93 93	33, 57, 87, 98	0
All	All	2980/3036 (98%)	0.16	119 (3%) 42 40	29, 72, 121, 161	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	GLU	5.7
1	F	233	ASP	5.3
1	E	42	GLN	5.0
1	E	143	GLY	4.9
1	F	192	THR	4.4
1	L	101	ASN	4.3
1	J	100	GLY	3.9
1	E	192	THR	3.7
1	F	231	ASP	3.7
1	E	41	VAL	3.7
1	L	234	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	10	ALA	3.7
1	C	194	GLN	3.7
1	F	163	LEU	3.6
1	E	40	ILE	3.6
1	E	189	SER	3.6
1	H	100	GLY	3.6
1	F	164	PRO	3.6
1	C	192	THR	3.6
1	E	90	ASN	3.6
1	E	105	ASP	3.6
1	D	230	ILE	3.6
1	E	230	ILE	3.5
1	E	107	ILE	3.4
1	E	92	ILE	3.4
1	E	167	ALA	3.3
1	A	193	LYS	3.3
1	F	239	ALA	3.3
1	E	236	LEU	3.3
1	F	8	ASP	3.2
1	F	176	GLY	3.2
1	F	173	ASP	3.2
1	D	144	VAL	3.2
1	H	101	ASN	3.1
1	E	43	LEU	3.1
1	F	198	VAL	3.1
1	I	233	ASP	3.1
1	F	243	SER	3.1
1	F	244	ALA	3.1
1	F	238	SER	3.1
1	D	140	ALA	3.0
1	E	97	LEU	2.9
1	E	220	LYS	2.9
1	E	104	ARG	2.9
1	L	98	LYS	2.9
1	L	243	SER	2.9
1	D	143	GLY	2.8
1	E	50	ALA	2.8
1	E	160	ASP	2.8
1	F	240	VAL	2.8
1	E	242	ARG	2.7
1	J	101	ASN	2.7
1	K	237	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	230	ILE	2.7
1	K	239	ALA	2.7
1	L	232	GLU	2.7
1	E	234	LEU	2.6
1	F	174	ALA	2.6
1	H	143	GLY	2.6
1	C	251	VAL	2.6
1	H	217	ARG	2.6
1	E	219	ASP	2.6
1	I	164	PRO	2.6
1	I	231	ASP	2.5
1	E	193	LYS	2.5
1	F	167	ALA	2.5
1	E	245	GLU	2.5
1	E	106	THR	2.5
1	E	168	GLY	2.5
1	K	145	THR	2.5
1	H	2	SER	2.4
1	F	199	ALA	2.4
1	F	248	ARG	2.4
1	L	231	ASP	2.4
1	E	215	PHE	2.4
1	F	177	LEU	2.4
1	J	52	GLY	2.4
1	L	100	GLY	2.4
1	E	198	VAL	2.4
1	A	9	ILE	2.3
1	I	49	THR	2.3
1	K	165	ASN	2.3
1	K	236	LEU	2.3
1	I	102	PRO	2.3
1	C	197	GLU	2.3
1	F	194	GLN	2.3
1	I	243	SER	2.3
1	E	142	ALA	2.2
1	L	233	ASP	2.2
1	E	231	ASP	2.2
1	E	241	VAL	2.2
1	K	240	VAL	2.2
1	E	188	PRO	2.2
1	H	99	GLU	2.2
1	E	227	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	192	THR	2.2
1	F	201	THR	2.2
1	F	165	ASN	2.2
2	G	213	ARG	2.2
1	E	45	LYS	2.2
1	F	48	GLY	2.2
1	F	46	GLU	2.1
1	K	252	GLY	2.1
1	D	167	ALA	2.1
1	F	5	ASN	2.1
1	H	167	ALA	2.1
1	D	241	VAL	2.1
1	E	197	GLU	2.1
1	E	101	ASN	2.1
1	F	195	ALA	2.1
1	A	251	VAL	2.1
1	E	49	THR	2.0
1	C	245	GLU	2.0
1	L	102	PRO	2.0
1	D	168	GLY	2.0
1	I	234	LEU	2.0
1	K	232	GLU	2.0
1	E	86	SER	2.0
1	A	10	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 carbohydrates 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.