Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:16 am BST

PDB ID	:	4CSF
Title	:	Structural insights into Toscana virus RNA encapsidation
Authors	:	Olal, D.; Daumke, O.
Deposited on	:	2014-03-07
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

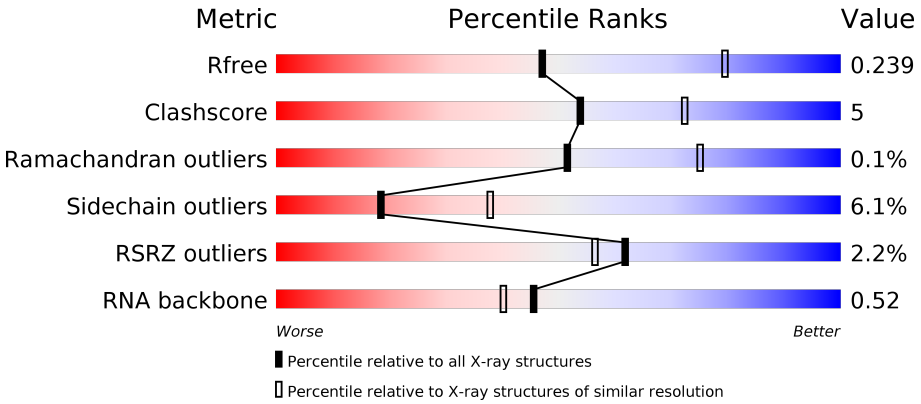
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 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	85% 13%
1	B	253	2% 81% 15%
1	D	253	4% 82% 13%
1	F	253	6% 82% 14%

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Mol	Chain	Length	Quality of chain
1	G	253	2% 83% 15%
1	H	253	81% 15%
1	I	253	81% 17%
1	J	253	6% 80% 15%
1	K	253	2% 81% 17%
1	L	253	2% 80% 16%
1	M	253	% 79% 17%
1	N	253	4% 83% 13%
1	O	253	% 81% 17%
1	P	253	3% 81% 15%
1	Q	253	87% 9%
1	R	253	3% 82% 14%
1	S	253	% 86% 11%
1	T	253	4% 83% 13%
1	U	253	84% 12%
1	V	253	% 82% 13%
1	W	253	2% 85% 11%
2	C	253	84% 14%
2	X	253	2% 81% 15%
3	E	253	5% 80% 17%
4	a	9	78% 22%
4	c	9	78% 22%
4	e	9	78% 22%
4	g	9	89% 11%
4	i	9	78% 22%

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Mol	Chain	Length	Quality of chain
4	k	9	78% 22%
4	m	9	78% 22%
4	o	9	78% 22%
4	q	9	89% 11%
4	s	9	78% 22%
4	u	9	78% 22%
4	w	9	89% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 49442 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	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	B	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	D	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	F	249	Total	C	N	O	S	0	0	0
			1904	1209	332	352	11			
1	G	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	H	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	I	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	J	249	Total	C	N	O	S	0	0	0
			1904	1209	332	352	11			
1	K	251	Total	C	N	O	S	0	0	0
			1921	1218	335	357	11			
1	L	250	Total	C	N	O	S	0	0	0
			1919	1216	334	358	11			
1	M	248	Total	C	N	O	S	0	0	0
			1899	1206	331	351	11			
1	N	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	O	248	Total	C	N	O	S	0	0	0
			1899	1206	331	351	11			
1	P	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	Q	249	Total	C	N	O	S	0	0	0
			1906	1210	333	352	11			
1	R	248	Total	C	N	O	S	0	0	0
			1902	1207	332	352	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	T	250	Total	C	N	O	S	0	0	0
			1916	1215	334	356	11			
1	U	247	Total	C	N	O	S	0	0	0
			1895	1204	330	350	11			
1	V	249	Total	C	N	O	S	0	0	0
			1907	1210	333	353	11			
1	W	250	Total	C	N	O	S	0	0	0
			1916	1215	334	356	11			

- Molecule 2 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1914	1215	332	356	11			
2	X	249	Total	C	N	O	S	0	0	0
			1902	1209	330	352	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	53	LYS	ARG	conflict	UNP P21701
X	53	LYS	ARG	conflict	UNP P21701

- Molecule 3 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	249	Total	C	N	O	S	0	0	0
			1904	1209	331	353	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	33	GLU	GLN	conflict	UNP P21701

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	c	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	e	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	g	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	i	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	k	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	m	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	o	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	q	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	s	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	u	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			
4	w	9	Total	C	N	O	P	0	0	0
			183	83	25	67	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	86	Total	O	0	0
			86	86		
5	C	103	Total	O	0	0
			103	103		
5	D	26	Total	O	0	0
			26	26		
5	E	38	Total	O	0	0
			38	38		
5	F	20	Total	O	0	0
			20	20		
5	G	73	Total	O	0	0
			73	73		
5	H	68	Total	O	0	0
			68	68		

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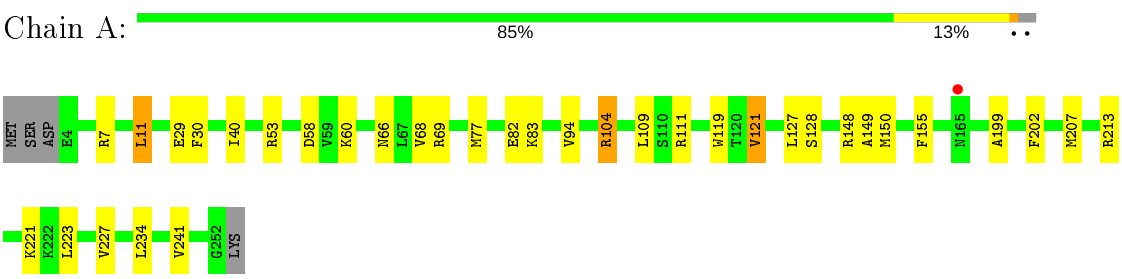
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	56	Total O 56 56	0	0
5	J	26	Total O 26 26	0	0
5	K	46	Total O 46 46	0	0
5	L	56	Total O 56 56	0	0
5	M	56	Total O 56 56	0	0
5	N	55	Total O 55 55	0	0
5	O	80	Total O 80 80	0	0
5	P	83	Total O 83 83	0	0
5	Q	86	Total O 86 86	0	0
5	R	31	Total O 31 31	0	0
5	S	67	Total O 67 67	0	0
5	T	87	Total O 87 87	0	0
5	U	84	Total O 84 84	0	0
5	V	65	Total O 65 65	0	0
5	W	62	Total O 62 62	0	0
5	X	41	Total O 41 41	0	0

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 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.

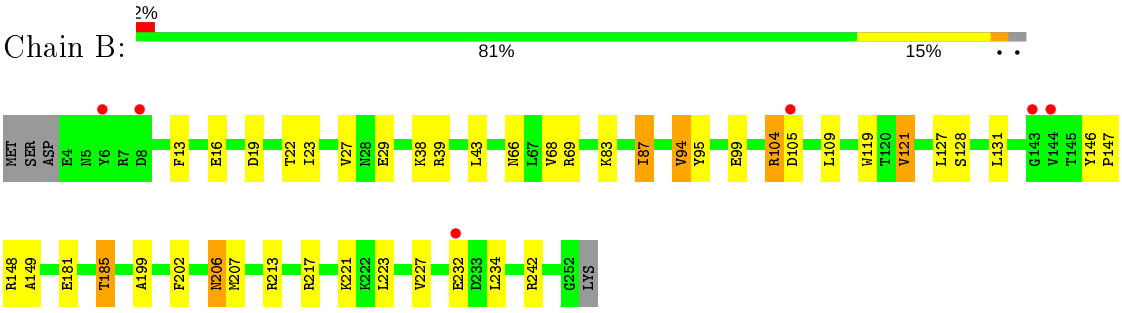
- Molecule 1: NUCLEOPROTEIN

Chain A:



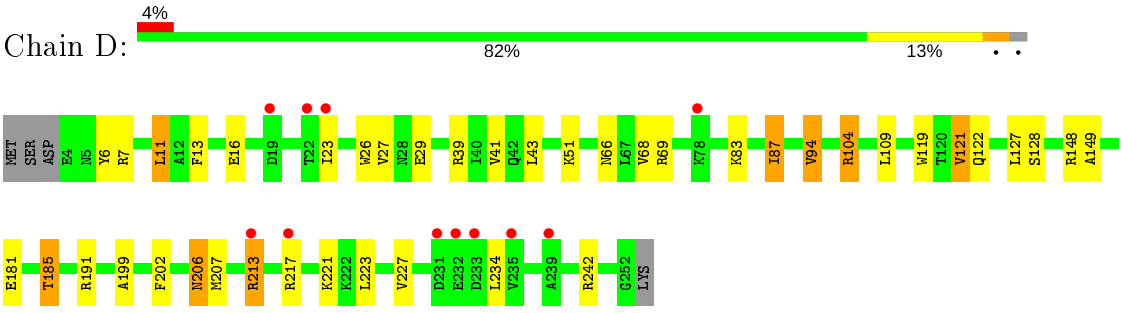
- Molecule 1: NUCLEOPROTEIN

Chain B:



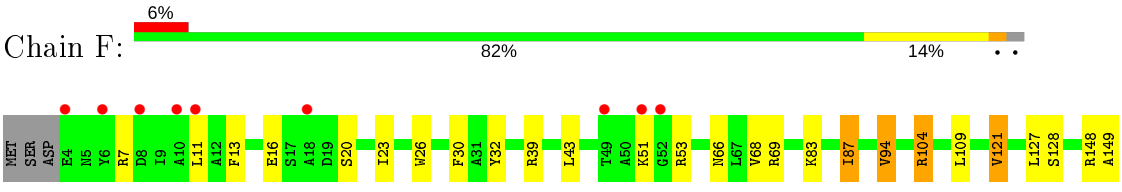
- Molecule 1: NUCLEOPROTEIN

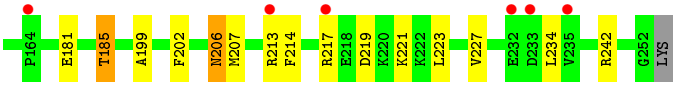
Chain D:



- Molecule 1: NUCLEOPROTEIN

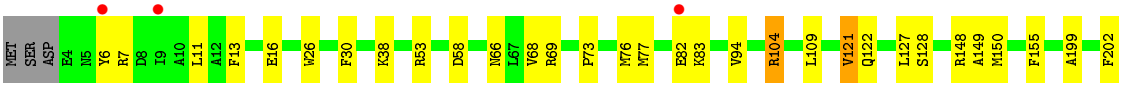
Chain F:

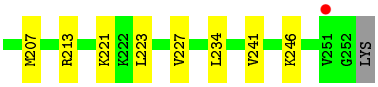




• Molecule 1: NUCLEOPROTEIN

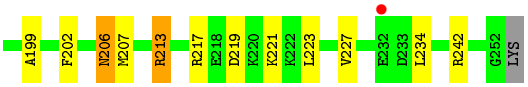
Chain G:





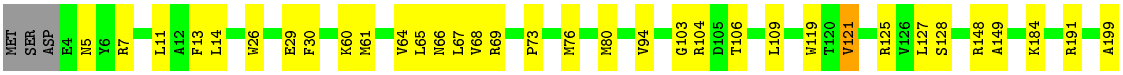
• Molecule 1: NUCLEOPROTEIN

Chain H:



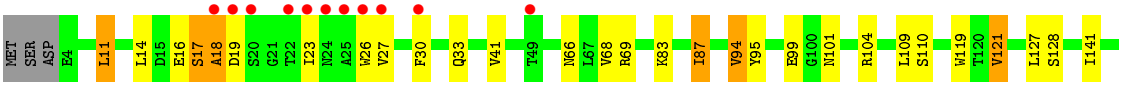
• Molecule 1: NUCLEOPROTEIN

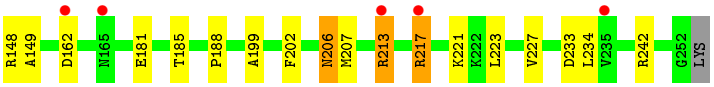
Chain I:



• Molecule 1: NUCLEOPROTEIN

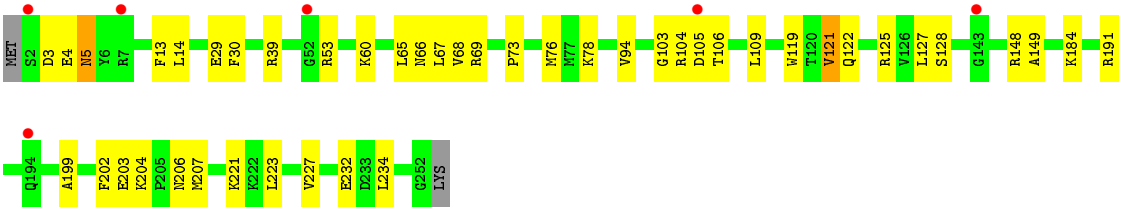
Chain J:



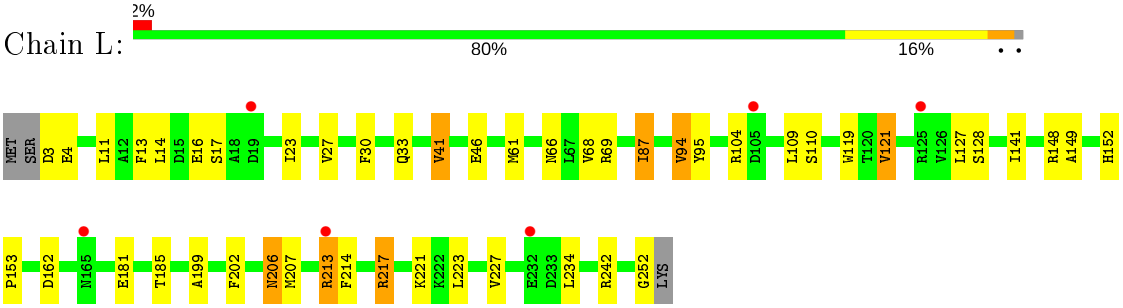


• Molecule 1: NUCLEOPROTEIN

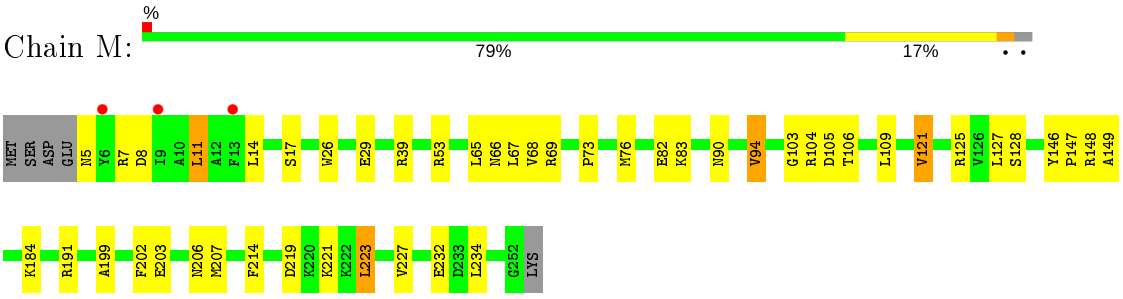
Chain K:



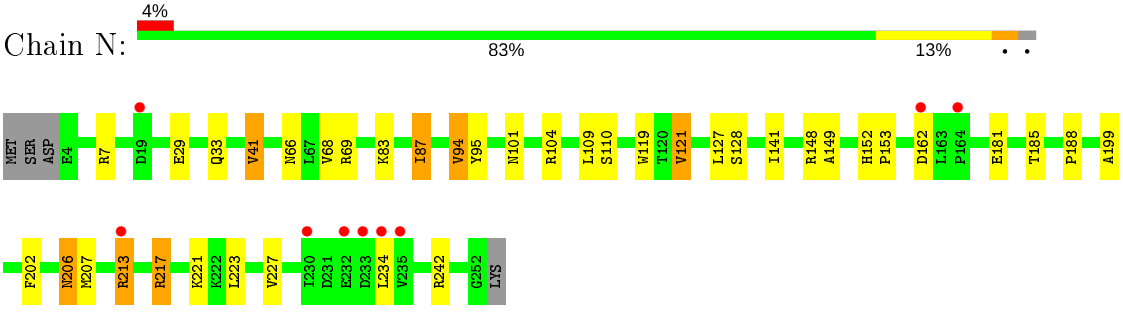
• Molecule 1: NUCLEOPROTEIN



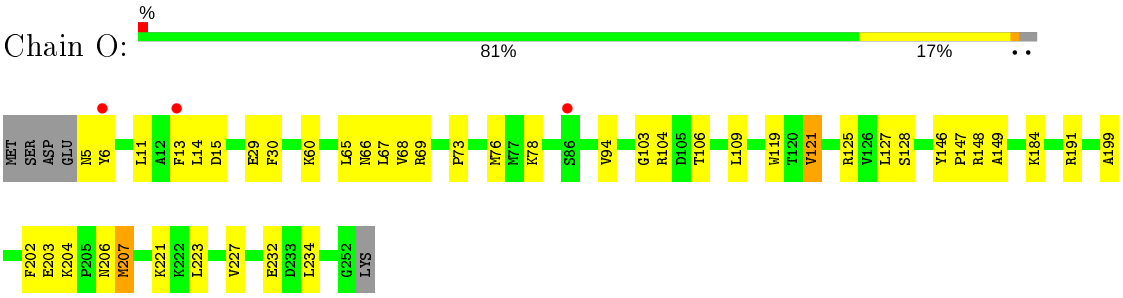
• Molecule 1: NUCLEOPROTEIN



• Molecule 1: NUCLEOPROTEIN

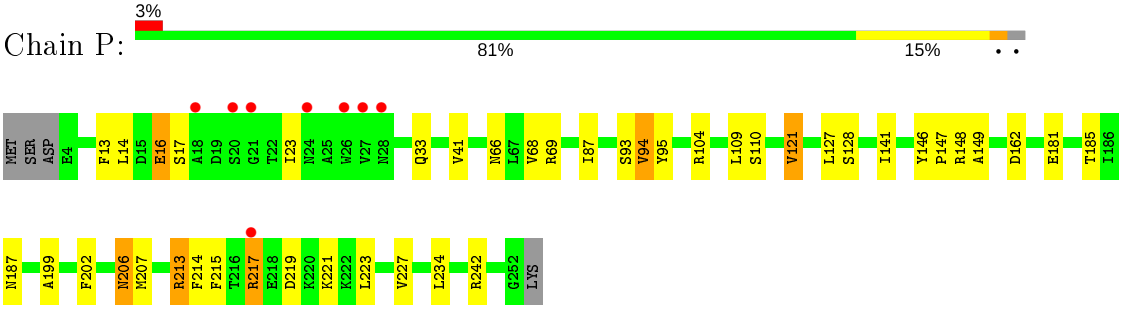


• Molecule 1: NUCLEOPROTEIN



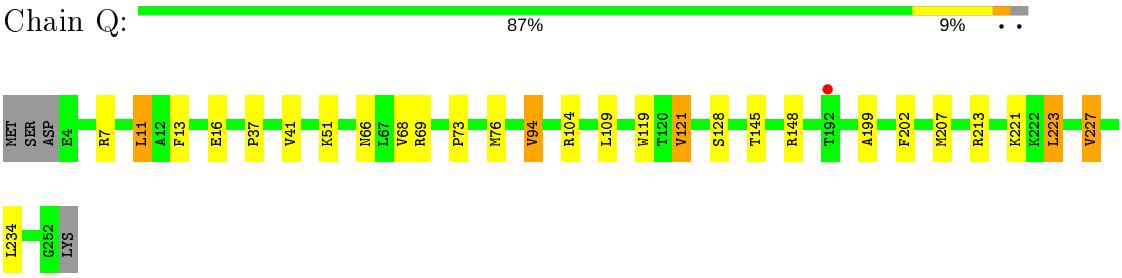
• Molecule 1: NUCLEOPROTEIN

Chain P:



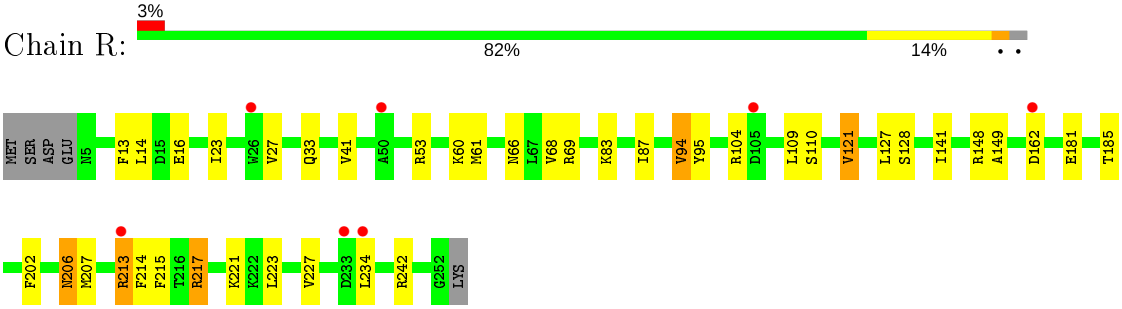
• Molecule 1: NUCLEOPROTEIN

Chain Q:



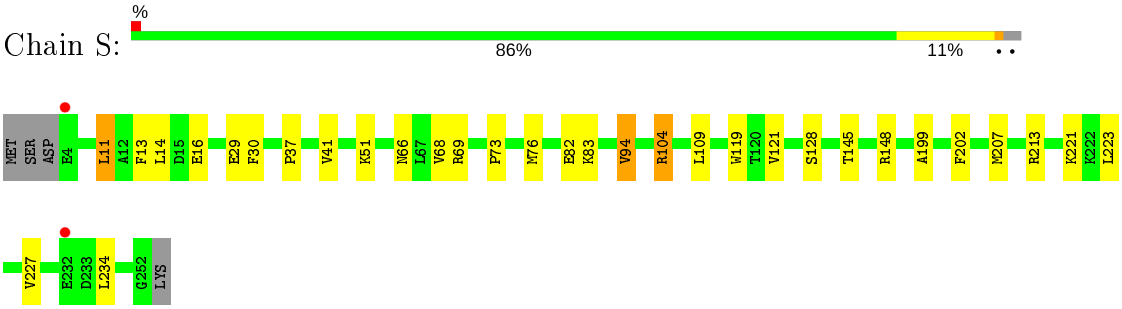
• Molecule 1: NUCLEOPROTEIN

Chain R:



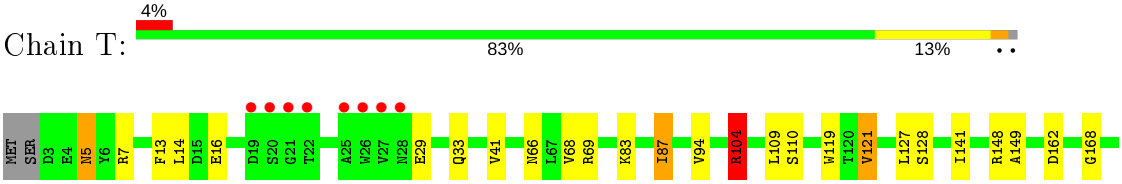
• Molecule 1: NUCLEOPROTEIN

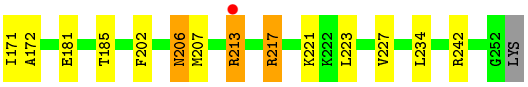
Chain S:



• Molecule 1: NUCLEOPROTEIN

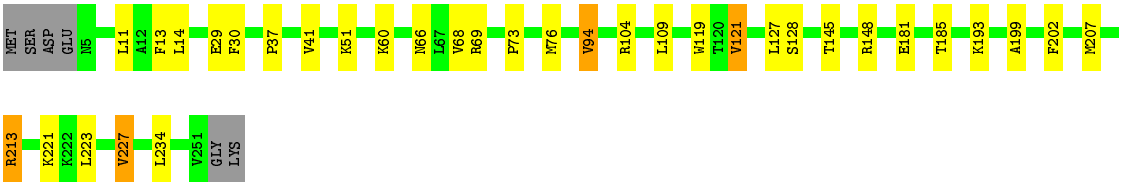
Chain T:





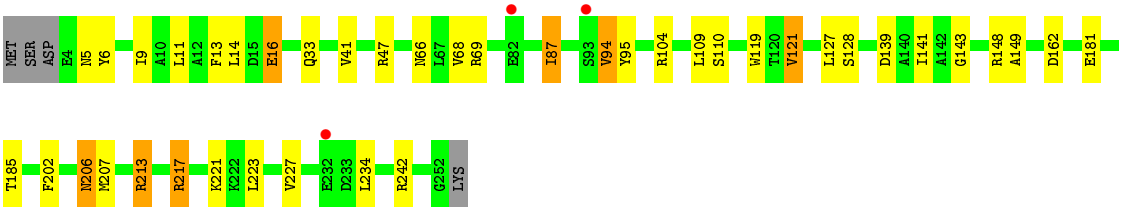
• Molecule 1: NUCLEOPROTEIN

Chain U:



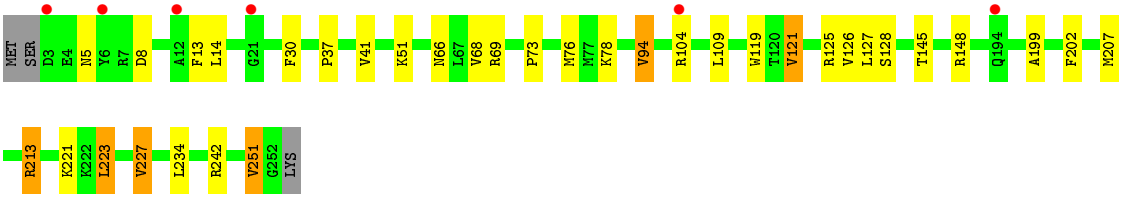
• Molecule 1: NUCLEOPROTEIN

Chain V:



• Molecule 1: NUCLEOPROTEIN

Chain W:

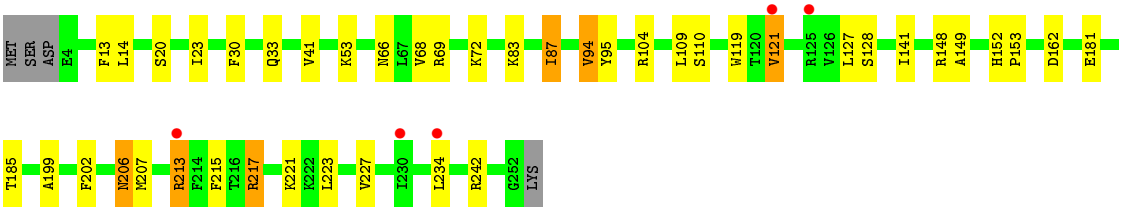


• Molecule 2: NUCLEOPROTEIN

Chain C:

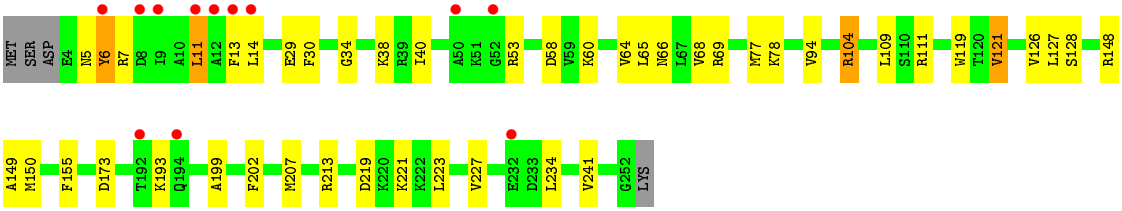
• Molecule 2: NUCLEOPROTEIN

Chain X:



• Molecule 3: NUCLEOPROTEIN

Chain E:



• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain a:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain c:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain e:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain g:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain i:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain k:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain m:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain o:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain q:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain s:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain u:

• Molecule 4: RNA (5'-R(*UP*GP*UP*GP*UP*UP*UP*CP*UP)-3')

Chain w:


U1
U9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.78Å 127.84Å 170.47Å 82.10° 79.75° 74.49°	Depositor
Resolution (Å)	34.47 – 2.60 34.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.47-2.60) 94.8 (34.48-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.240 0.203 , 0.239	Depositor DCC
R_{free} test set	11465 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49442	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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	0.29	0/1939	0.58	3/2617 (0.1%)
1	B	0.29	0/1939	0.48	0/2617
1	D	0.28	0/1939	0.48	1/2617 (0.0%)
1	F	0.28	0/1936	0.45	0/2613
1	G	0.29	0/1939	0.58	3/2617 (0.1%)
1	H	0.31	0/1939	0.49	2/2617 (0.1%)
1	I	0.28	0/1939	0.45	0/2617
1	J	0.29	0/1936	0.44	0/2613
1	K	0.28	0/1953	0.45	0/2636
1	L	0.29	0/1951	0.47	0/2633
1	M	0.28	0/1931	0.45	0/2606
1	N	0.28	0/1939	0.44	0/2617
1	O	0.28	0/1931	0.45	0/2606
1	P	0.31	0/1939	0.81	3/2617 (0.1%)
1	Q	0.30	0/1938	0.46	0/2616
1	R	0.28	0/1934	0.44	0/2610
1	S	0.28	0/1939	0.45	0/2617
1	T	0.30	0/1948	0.73	3/2629 (0.1%)
1	U	0.30	0/1927	0.46	0/2601
1	V	0.29	0/1939	0.44	0/2617
1	W	0.29	0/1948	0.49	1/2629 (0.0%)
2	C	0.30	0/1946	0.58	3/2626 (0.1%)
2	X	0.28	0/1934	0.44	0/2610
3	E	0.28	0/1936	0.58	3/2613 (0.1%)
4	a	0.40	0/202	0.86	0/312
4	c	0.37	0/202	0.89	0/312
4	e	0.30	0/202	0.77	0/312
4	g	0.38	0/202	0.83	0/312
4	i	0.40	0/202	0.82	0/312
4	k	0.37	0/202	0.79	0/312
4	m	0.38	0/202	0.86	0/312
4	o	0.39	0/202	0.74	0/312
4	q	0.41	0/202	0.87	0/312
4	s	0.36	0/202	0.82	0/312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
4	u	0.47	0/202	0.93	0/312
4	w	0.41	0/202	0.88	0/312
All	All	0.29	0/48963	0.54	22/66555 (0.0%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	217	ARG	NE-CZ-NH1	24.27	132.44	120.30
1	P	217	ARG	NE-CZ-NH2	-22.98	108.81	120.30
1	T	104	ARG	NE-CZ-NH1	20.51	130.55	120.30
1	T	104	ARG	NE-CZ-NH2	-20.06	110.27	120.30
2	C	104	ARG	NE-CZ-NH2	-12.87	113.87	120.30
3	E	104	ARG	NE-CZ-NH1	12.86	126.73	120.30
1	A	104	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	A	104	ARG	NE-CZ-NH2	-12.81	113.90	120.30
1	G	104	ARG	NE-CZ-NH2	-12.72	113.94	120.30
2	C	104	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	G	104	ARG	NE-CZ-NH1	12.63	126.62	120.30
3	E	104	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	P	217	ARG	CD-NE-CZ	9.52	136.93	123.60
1	T	104	ARG	CD-NE-CZ	8.50	135.50	123.60
1	H	104	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	C	104	ARG	CD-NE-CZ	5.71	131.60	123.60
1	A	104	ARG	CD-NE-CZ	5.69	131.56	123.60
1	G	104	ARG	CD-NE-CZ	5.68	131.55	123.60
3	E	104	ARG	CD-NE-CZ	5.57	131.40	123.60
1	D	213	ARG	CA-CB-CG	5.39	125.27	113.40
1	H	213	ARG	CA-CB-CG	5.36	125.19	113.40
1	W	251	VAL	CG1-CB-CG2	5.01	118.92	110.90

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	1907	0	1955	19	0
1	B	1907	0	1955	28	0
1	D	1907	0	1955	27	0
1	F	1904	0	1951	31	0
1	G	1907	0	1955	22	0
1	H	1907	0	1955	27	0
1	I	1907	0	1955	45	0
1	J	1904	0	1951	48	1
1	K	1921	0	1963	27	0
1	L	1919	0	1963	34	0
1	M	1899	0	1949	28	0
1	N	1907	0	1955	25	0
1	O	1899	0	1949	27	0
1	P	1907	0	1955	28	0
1	Q	1906	0	1952	16	0
1	R	1902	0	1953	21	1
1	S	1907	0	1955	20	0
1	T	1916	0	1961	26	0
1	U	1895	0	1946	20	0
1	V	1907	0	1955	21	0
1	W	1916	0	1961	23	0
2	C	1914	0	1961	29	0
2	X	1902	0	1951	27	0
3	E	1904	0	1949	35	0
4	a	183	0	95	0	0
4	c	183	0	95	0	0
4	e	183	0	95	0	0
4	g	183	0	95	0	0
4	i	183	0	95	0	0
4	k	183	0	95	0	0
4	m	183	0	95	0	0
4	o	183	0	95	0	0
4	q	183	0	95	0	0
4	s	183	0	95	0	0
4	u	183	0	95	0	0
4	w	183	0	95	0	0
5	A	80	0	0	0	0
5	B	86	0	0	4	0
5	C	103	0	0	2	0
5	D	26	0	0	0	0
5	E	38	0	0	4	0
5	F	20	0	0	0	0
5	G	73	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	68	0	0	4	0
5	I	56	0	0	1	0
5	J	26	0	0	1	0
5	K	46	0	0	0	0
5	L	56	0	0	4	0
5	M	56	0	0	1	0
5	N	55	0	0	0	0
5	O	80	0	0	2	0
5	P	83	0	0	1	0
5	Q	86	0	0	0	0
5	R	31	0	0	0	0
5	S	67	0	0	1	0
5	T	87	0	0	4	0
5	U	84	0	0	1	0
5	V	65	0	0	4	0
5	W	62	0	0	2	0
5	X	41	0	0	1	0
All	All	49442	0	48050	502	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 (502) 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:I:61:MET:HG2	1:J:26:TRP:CE2	2.01	0.95
1:T:168:GLY:O	5:T:2059:HOH:O	1.92	0.87
1:L:3:ASP:N	5:L:2001:HOH:O	2.10	0.84
1:S:83:LYS:NZ	1:T:29:GLU:OE2	2.13	0.81
3:E:119:TRP:HB2	1:F:13:PHE:HB3	1.64	0.80
1:K:60:LYS:NZ	1:L:17:SER:O	2.15	0.78
2:C:83:LYS:NZ	1:D:29:GLU:OE2	2.16	0.77
3:E:127:LEU:HD21	1:F:23:ILE:HG22	1.68	0.76
1:W:5:ASN:ND2	1:W:8:ASP:OD2	2.19	0.76
1:L:217:ARG:NH1	5:L:2051:HOH:O	2.19	0.74
1:T:172:ALA:N	5:T:2059:HOH:O	2.18	0.74
1:H:15:ASP:HB3	1:W:5:ASN:HB2	1.68	0.74
1:Q:221:LYS:HD2	1:Q:234:LEU:HD11	1.71	0.72
1:S:221:LYS:HD2	1:S:234:LEU:HD11	1.71	0.72
1:W:127:LEU:HD21	2:X:23:ILE:HG22	1.70	0.72
3:E:219:ASP:OD2	1:F:7:ARG:HD2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:221:LYS:HD2	1:U:234:LEU:HD11	1.70	0.72
1:K:69:ARG:NH1	1:L:30:PHE:O	2.22	0.72
1:L:162:ASP:OD2	1:L:217:ARG:NH2	2.23	0.72
1:V:47:ARG:NH1	5:V:2014:HOH:O	2.22	0.72
1:W:126:VAL:HG11	2:X:20:SER:HA	1.72	0.71
1:W:221:LYS:HD2	1:W:234:LEU:HD11	1.72	0.71
1:J:162:ASP:OD2	1:J:217:ARG:NH2	2.24	0.70
1:U:193:LYS:NZ	5:U:2071:HOH:O	2.24	0.70
1:U:66:ASN:HB2	1:U:109:LEU:HB3	1.74	0.70
2:X:162:ASP:OD2	2:X:217:ARG:NH2	2.25	0.70
2:C:221:LYS:HE3	2:C:234:LEU:HD11	1.74	0.70
1:V:162:ASP:OD2	1:V:217:ARG:NH2	2.24	0.69
1:A:221:LYS:HE3	1:A:234:LEU:HD11	1.73	0.69
2:C:56:LYS:NZ	1:P:217:ARG:HE	1.90	0.69
3:E:221:LYS:HE3	3:E:234:LEU:HD11	1.74	0.69
1:M:219:ASP:OD2	1:N:7:ARG:NH1	2.26	0.69
1:I:65:LEU:HD13	1:J:30:PHE:CG	2.27	0.69
1:R:162:ASP:OD2	1:R:217:ARG:NH2	2.26	0.68
1:Q:66:ASN:HB2	1:Q:109:LEU:HB3	1.74	0.68
1:G:221:LYS:HE3	1:G:234:LEU:HD11	1.74	0.68
1:N:162:ASP:OD2	1:N:217:ARG:NH2	2.26	0.68
1:T:162:ASP:OD2	1:T:217:ARG:NH2	2.27	0.68
1:J:17:SER:O	1:J:19:ASP:N	2.26	0.67
1:P:221:LYS:HD2	1:P:234:LEU:HD11	1.77	0.67
1:W:66:ASN:HB2	1:W:109:LEU:HB3	1.76	0.67
1:G:66:ASN:HB2	1:G:109:LEU:HB3	1.76	0.67
1:H:83:LYS:NZ	1:I:29:GLU:OE2	2.27	0.66
5:E:2014:HOH:O	1:F:32:TYR:OH	2.13	0.66
1:G:246:LYS:NZ	5:G:2073:HOH:O	2.26	0.66
1:A:66:ASN:HB2	1:A:109:LEU:HB3	1.76	0.66
1:I:64:VAL:HG22	1:J:23:ILE:HG23	1.76	0.66
1:S:66:ASN:HB2	1:S:109:LEU:HB3	1.76	0.66
1:D:68:VAL:HG23	1:D:69:ARG:HG2	1.78	0.66
5:I:2030:HOH:O	1:J:101:ASN:ND2	2.27	0.66
1:L:121:VAL:HG22	1:L:149:ALA:HB1	1.78	0.66
5:M:2025:HOH:O	1:N:101:ASN:ND2	2.28	0.65
1:N:221:LYS:HD2	1:N:234:LEU:HD11	1.79	0.65
1:V:121:VAL:HG22	1:V:149:ALA:HB1	1.78	0.65
1:P:121:VAL:HG22	1:P:149:ALA:HB1	1.78	0.65
1:J:221:LYS:HD2	1:J:234:LEU:HD11	1.79	0.65
1:T:33:GLN:OE1	1:T:104:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:66:ASN:HB2	3:E:109:LEU:HB3	1.78	0.65
1:O:68:VAL:HG23	1:O:69:ARG:HG2	1.78	0.65
1:T:221:LYS:HD2	1:T:234:LEU:HD11	1.77	0.65
1:L:221:LYS:HD2	1:L:234:LEU:HD11	1.79	0.65
1:B:68:VAL:HG23	1:B:69:ARG:HG2	1.78	0.65
1:D:66:ASN:HB2	1:D:109:LEU:HB3	1.79	0.65
3:E:193:LYS:NZ	5:E:2033:HOH:O	2.29	0.64
1:V:221:LYS:HD2	1:V:234:LEU:HD11	1.79	0.64
1:B:38:LYS:NZ	5:B:2009:HOH:O	2.23	0.64
1:J:121:VAL:HG22	1:J:149:ALA:HB1	1.79	0.64
1:M:68:VAL:HG23	1:M:69:ARG:HG2	1.79	0.64
1:I:64:VAL:CG2	1:J:23:ILE:HG23	2.27	0.64
1:F:68:VAL:HG23	1:F:69:ARG:HG2	1.78	0.64
1:R:221:LYS:HD2	1:R:234:LEU:HD11	1.80	0.64
2:C:66:ASN:HB2	2:C:109:LEU:HB3	1.78	0.64
2:X:221:LYS:HD2	2:X:234:LEU:HD11	1.78	0.64
1:I:61:MET:HG2	1:J:26:TRP:CZ2	2.31	0.64
1:N:119:TRP:HB2	1:O:13:PHE:HB3	1.80	0.64
1:H:66:ASN:HB2	1:H:109:LEU:HB3	1.79	0.64
1:L:252:GLY:O	5:L:2056:HOH:O	2.15	0.63
1:H:68:VAL:HG23	1:H:69:ARG:HG2	1.80	0.63
1:I:68:VAL:HG23	1:I:69:ARG:HG2	1.81	0.63
1:R:121:VAL:HG22	1:R:149:ALA:HB1	1.79	0.63
2:X:121:VAL:HG22	2:X:149:ALA:HB1	1.79	0.63
1:H:5:ASN:ND2	5:H:2004:HOH:O	2.30	0.63
1:N:121:VAL:HG22	1:N:149:ALA:HB1	1.80	0.63
1:H:5:ASN:ND2	5:H:2003:HOH:O	2.31	0.63
1:P:33:GLN:OE1	1:P:104:ARG:NH1	2.32	0.63
1:B:105:ASP:O	5:B:2011:HOH:O	2.15	0.63
3:E:60:LYS:HE2	1:F:16:GLU:HG2	1.81	0.62
1:K:68:VAL:HG23	1:K:69:ARG:HG2	1.81	0.62
1:B:66:ASN:HB2	1:B:109:LEU:HB3	1.80	0.62
2:C:68:VAL:HG23	2:C:69:ARG:HG2	1.82	0.62
1:K:119:TRP:HB2	1:L:13:PHE:HB3	1.81	0.62
2:C:82:GLU:HG3	1:D:104:ARG:HH12	1.65	0.62
1:I:66:ASN:HB2	1:I:109:LEU:HB3	1.82	0.62
1:O:5:ASN:N	5:O:2006:HOH:O	2.32	0.62
3:E:68:VAL:HG23	3:E:69:ARG:HG2	1.82	0.61
1:J:33:GLN:OE1	1:J:104:ARG:NH1	2.33	0.61
2:C:3:ASP:N	5:C:2002:HOH:O	2.33	0.61
1:G:68:VAL:HG23	1:G:69:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:33:GLN:OE1	1:N:104:ARG:NH1	2.33	0.61
1:V:33:GLN:OE1	1:V:104:ARG:NH1	2.33	0.61
1:F:66:ASN:HB2	1:F:109:LEU:HB3	1.82	0.61
1:O:66:ASN:HB2	1:O:109:LEU:HB3	1.83	0.61
1:I:60:LYS:HB2	1:J:26:TRP:CH2	2.37	0.60
1:T:121:VAL:HG22	1:T:149:ALA:HB1	1.81	0.60
1:M:83:LYS:NZ	1:N:29:GLU:OE2	2.34	0.60
2:X:33:GLN:OE1	2:X:104:ARG:NH1	2.34	0.60
1:V:68:VAL:HG23	1:V:69:ARG:HG2	1.83	0.60
1:K:66:ASN:HB2	1:K:109:LEU:HB3	1.82	0.60
1:L:33:GLN:OE1	1:L:104:ARG:NH1	2.34	0.60
1:M:66:ASN:HB2	1:M:109:LEU:HB3	1.83	0.60
1:F:121:VAL:HG22	1:F:149:ALA:HB1	1.84	0.60
3:E:127:LEU:HD21	1:F:23:ILE:CG2	2.32	0.60
1:R:33:GLN:OE1	1:R:104:ARG:NH1	2.34	0.59
1:H:121:VAL:HG22	1:H:149:ALA:HB1	1.84	0.59
1:P:68:VAL:HG23	1:P:69:ARG:HG2	1.85	0.59
1:A:68:VAL:HG23	1:A:69:ARG:HG2	1.83	0.59
3:E:78:LYS:O	1:F:104:ARG:HG2	2.02	0.59
1:L:68:VAL:HG23	1:L:69:ARG:HG2	1.84	0.59
1:M:7:ARG:HG3	1:R:214:PHE:O	2.02	0.59
2:X:68:VAL:HG23	2:X:69:ARG:HG2	1.84	0.59
1:A:83:LYS:NZ	1:B:29:GLU:OE2	2.27	0.59
1:D:119:TRP:HB2	3:E:13:PHE:HB3	1.84	0.59
1:S:119:TRP:HB2	1:T:13:PHE:HB3	1.82	0.59
1:O:119:TRP:HB2	1:P:13:PHE:HB3	1.85	0.59
1:G:128:SER:HB3	1:G:148:ARG:HG3	1.85	0.58
2:C:56:LYS:HZ1	1:P:217:ARG:HE	1.51	0.58
1:K:122:GLN:NE2	1:L:14:LEU:O	2.37	0.58
1:N:68:VAL:HG23	1:N:69:ARG:HG2	1.85	0.58
1:P:162:ASP:OD2	1:P:217:ARG:NH1	2.36	0.58
1:Q:128:SER:HB3	1:Q:148:ARG:HG3	1.86	0.58
1:D:121:VAL:HG22	1:D:149:ALA:HB1	1.85	0.58
3:E:128:SER:HB3	3:E:148:ARG:HG3	1.86	0.58
1:U:68:VAL:HG23	1:U:69:ARG:HG2	1.86	0.58
1:B:83:LYS:NZ	2:C:29:GLU:OE2	2.32	0.58
1:S:68:VAL:HG23	1:S:69:ARG:HG2	1.86	0.57
1:J:68:VAL:HG23	1:J:69:ARG:HG2	1.86	0.57
1:A:128:SER:HB3	1:A:148:ARG:HG3	1.85	0.57
1:L:66:ASN:HB2	1:L:109:LEU:HB3	1.87	0.57
1:T:68:VAL:HG23	1:T:69:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:69:ARG:NH1	2:X:30:PHE:O	2.29	0.57
1:D:41:VAL:HG11	3:E:6:TYR:HB3	1.87	0.57
1:J:66:ASN:HB2	1:J:109:LEU:HB3	1.86	0.57
1:Q:68:VAL:HG23	1:Q:69:ARG:HG2	1.87	0.57
1:B:121:VAL:HG22	1:B:149:ALA:HB1	1.87	0.57
1:J:16:GLU:O	1:J:18:ALA:N	2.36	0.57
1:M:29:GLU:OE2	1:R:83:LYS:NZ	2.32	0.57
1:I:69:ARG:NH1	1:J:30:PHE:O	2.34	0.57
1:V:119:TRP:HB2	1:W:13:PHE:HB3	1.86	0.57
1:W:128:SER:HB3	1:W:148:ARG:HG3	1.86	0.57
2:C:128:SER:HB3	2:C:148:ARG:HG3	1.86	0.56
3:E:126:VAL:HG11	1:F:20:SER:HA	1.86	0.56
1:I:61:MET:HG2	1:J:26:TRP:CD2	2.40	0.56
1:M:128:SER:HB3	1:M:148:ARG:HG3	1.88	0.56
1:P:214:PHE:O	1:Q:7:ARG:HG3	2.05	0.56
1:W:119:TRP:HB2	2:X:13:PHE:HB3	1.87	0.56
1:N:66:ASN:HB2	1:N:109:LEU:HB3	1.86	0.56
1:S:128:SER:HB3	1:S:148:ARG:HG3	1.86	0.56
1:R:68:VAL:HG23	1:R:69:ARG:HG2	1.87	0.56
1:T:87:ILE:HD11	1:U:30:PHE:HZ	1.69	0.56
1:P:215:PHE:CE1	1:Q:11:LEU:HD13	2.40	0.56
1:V:139:ASP:O	5:V:2039:HOH:O	2.18	0.56
1:R:66:ASN:HB2	1:R:109:LEU:HB3	1.87	0.56
1:M:11:LEU:HD13	1:R:215:PHE:CE1	2.41	0.56
1:O:128:SER:HB3	1:O:148:ARG:HG3	1.88	0.56
1:V:66:ASN:HB2	1:V:109:LEU:HB3	1.88	0.55
1:A:29:GLU:OE2	1:F:83:LYS:NZ	2.38	0.55
3:E:64:VAL:HG21	1:F:26:TRP:HE3	1.72	0.55
1:I:60:LYS:HE2	1:J:16:GLU:HG2	1.87	0.55
1:W:68:VAL:HG23	1:W:69:ARG:HG2	1.87	0.55
1:T:66:ASN:HB2	1:T:109:LEU:HB3	1.87	0.55
1:B:99:GLU:OE1	5:B:2030:HOH:O	2.17	0.55
1:B:119:TRP:HB2	2:C:13:PHE:HB3	1.88	0.55
1:K:128:SER:HB3	1:K:148:ARG:HG3	1.89	0.55
2:X:66:ASN:HB2	2:X:109:LEU:HB3	1.89	0.55
1:I:128:SER:HB3	1:I:148:ARG:HG3	1.89	0.55
1:H:188:PRO:HG2	1:I:204:LYS:HA	1.89	0.54
1:L:13:PHE:HA	1:L:16:GLU:HB2	1.89	0.54
1:L:46:GLU:OE1	5:L:2012:HOH:O	2.17	0.54
1:H:87:ILE:HD11	1:I:30:PHE:HZ	1.72	0.54
1:S:13:PHE:HB3	2:X:119:TRP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:73:PRO:HA	1:O:76:MET:HG2	1.90	0.54
2:C:82:GLU:HG3	1:D:104:ARG:NH1	2.21	0.54
1:U:128:SER:HB3	1:U:148:ARG:HG3	1.89	0.54
1:I:68:VAL:HG11	1:J:27:VAL:HG13	1.90	0.54
1:I:61:MET:HA	1:J:26:TRP:CE3	2.43	0.54
1:B:87:ILE:HD11	2:C:30:PHE:HZ	1.73	0.53
3:E:104:ARG:NH1	5:E:2008:HOH:O	2.36	0.53
1:P:66:ASN:HB2	1:P:109:LEU:HB3	1.88	0.53
1:I:73:PRO:HA	1:I:76:MET:HG2	1.91	0.53
1:M:17:SER:OG	1:R:60:LYS:NZ	2.42	0.53
3:E:34:GLY:O	5:E:2008:HOH:O	2.19	0.53
1:O:121:VAL:HG22	1:O:149:ALA:HB1	1.91	0.53
1:K:73:PRO:HA	1:K:76:MET:HG2	1.91	0.53
1:I:64:VAL:HG21	1:J:26:TRP:HE3	1.74	0.53
1:M:121:VAL:HG22	1:M:149:ALA:HB1	1.91	0.53
1:M:73:PRO:HA	1:M:76:MET:HG2	1.90	0.53
1:A:127:LEU:HD21	1:B:23:ILE:HG22	1.89	0.52
1:O:15:ASP:OD1	5:O:2011:HOH:O	2.18	0.52
1:O:199:ALA:HA	1:O:202:PHE:CE2	2.43	0.52
1:N:83:LYS:NZ	1:O:29:GLU:OE2	2.22	0.52
1:P:219:ASP:CG	1:Q:11:LEU:HD21	2.30	0.52
3:E:69:ARG:NH1	1:F:30:PHE:O	2.28	0.52
1:I:184:LYS:HD2	1:I:191:ARG:HA	1.92	0.52
1:N:87:ILE:HD11	1:O:30:PHE:HZ	1.73	0.52
1:M:103:GLY:N	1:M:106:THR:OG1	2.43	0.52
1:J:119:TRP:HB2	1:K:13:PHE:HB3	1.92	0.52
1:U:51:LYS:HG3	1:U:94:VAL:HB	1.92	0.52
1:I:103:GLY:N	1:I:106:THR:OG1	2.42	0.52
1:I:65:LEU:HB2	1:J:30:PHE:CE2	2.44	0.52
1:S:51:LYS:HG3	1:S:94:VAL:HB	1.92	0.52
1:D:83:LYS:NZ	3:E:29:GLU:OE2	2.30	0.51
5:T:2050:HOH:O	1:U:213:ARG:NH1	2.29	0.51
1:K:121:VAL:HG22	1:K:149:ALA:HB1	1.91	0.51
1:B:39:ARG:HH12	1:B:43:LEU:HD21	1.74	0.51
1:I:199:ALA:HA	1:I:202:PHE:CE2	2.46	0.51
1:U:60:LYS:HE2	1:V:16:GLU:HG2	1.92	0.51
1:K:199:ALA:HA	1:K:202:PHE:CE2	2.46	0.51
2:C:199:ALA:HA	2:C:202:PHE:CE2	2.46	0.51
3:E:65:LEU:HD13	1:F:30:PHE:CG	2.46	0.51
1:K:67:LEU:HD12	1:K:127:LEU:HD12	1.93	0.51
1:Q:51:LYS:HG3	1:Q:94:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:GLU:CG	1:D:104:ARG:HH12	2.22	0.51
1:M:199:ALA:HA	1:M:202:PHE:CE2	2.45	0.51
1:S:82:GLU:HG3	1:T:104:ARG:CZ	2.41	0.51
1:K:184:LYS:HD2	1:K:191:ARG:HA	1.93	0.51
1:I:121:VAL:HG22	1:I:149:ALA:HB1	1.93	0.51
1:O:184:LYS:HD2	1:O:191:ARG:HA	1.93	0.51
1:V:87:ILE:HD11	1:W:30:PHE:HZ	1.76	0.51
1:U:199:ALA:HA	1:U:202:PHE:CE2	2.46	0.51
1:S:30:PHE:HZ	2:X:87:ILE:HD11	1.75	0.50
1:V:143:GLY:HA3	5:V:2041:HOH:O	2.11	0.50
1:H:5:ASN:HB2	5:H:2002:HOH:O	2.10	0.50
1:M:184:LYS:HD2	1:M:191:ARG:HA	1.93	0.50
1:O:60:LYS:HE2	1:P:16:GLU:HG2	1.94	0.50
1:M:7:ARG:HA	1:R:214:PHE:CZ	2.46	0.50
1:P:93:SER:OG	1:T:83:LYS:HB2	2.12	0.50
3:E:219:ASP:CG	1:F:7:ARG:HH11	2.16	0.50
5:V:2037:HOH:O	1:W:213:ARG:NH1	2.44	0.50
2:C:125:ARG:HD2	5:C:2094:HOH:O	2.12	0.49
1:D:221:LYS:HE3	1:D:234:LEU:HD11	1.94	0.49
1:I:65:LEU:HD11	1:I:76:MET:SD	2.52	0.49
1:I:119:TRP:CZ2	1:J:23:ILE:HD11	2.47	0.49
1:K:103:GLY:N	1:K:106:THR:OG1	2.45	0.49
1:M:82:GLU:HG3	1:N:104:ARG:NH2	2.27	0.49
1:G:199:ALA:HA	1:G:202:PHE:CE2	2.47	0.49
1:W:51:LYS:HG3	1:W:94:VAL:HB	1.92	0.49
1:D:128:SER:HB3	1:D:148:ARG:HG3	1.95	0.49
1:F:128:SER:HB3	1:F:148:ARG:HG3	1.95	0.49
1:H:128:SER:HB3	1:H:148:ARG:HG3	1.94	0.49
1:D:87:ILE:HD11	3:E:30:PHE:HZ	1.77	0.49
3:E:121:VAL:HG22	3:E:149:ALA:HB1	1.95	0.49
1:K:5:ASN:N	1:K:5:ASN:OD1	2.46	0.49
1:I:5:ASN:N	1:I:5:ASN:OD1	2.44	0.49
1:L:141:ILE:HD13	1:L:181:GLU:HG3	1.94	0.49
1:M:5:ASN:N	1:M:8:ASP:OD2	2.46	0.49
1:M:26:TRP:CE2	1:R:61:MET:HG2	2.47	0.49
1:B:128:SER:HB3	1:B:148:ARG:HG3	1.95	0.49
1:B:221:LYS:HE3	1:B:234:LEU:HD11	1.95	0.49
2:C:121:VAL:HG22	2:C:149:ALA:HB1	1.95	0.49
3:E:199:ALA:HA	3:E:202:PHE:CE2	2.47	0.49
1:F:13:PHE:HA	1:F:16:GLU:HB2	1.94	0.49
1:L:128:SER:HB3	1:L:148:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:67:LEU:HD12	1:M:127:LEU:HD12	1.95	0.49
1:O:103:GLY:N	1:O:106:THR:OG1	2.45	0.49
1:G:83:LYS:NZ	1:H:29:GLU:OE2	2.43	0.48
1:N:41:VAL:CG2	1:O:6:TYR:HB3	2.43	0.48
1:O:221:LYS:HE3	1:O:234:LEU:HD11	1.95	0.48
1:W:199:ALA:HA	1:W:202:PHE:CE2	2.48	0.48
1:R:202:PHE:O	1:R:206:ASN:HB2	2.13	0.48
1:S:104:ARG:NH2	5:S:2026:HOH:O	2.46	0.48
1:U:60:LYS:CE	1:V:16:GLU:HG2	2.43	0.48
1:G:7:ARG:HG3	1:L:214:PHE:O	2.12	0.48
1:I:67:LEU:HD12	1:I:127:LEU:HD12	1.94	0.48
1:S:199:ALA:HA	1:S:202:PHE:CE2	2.48	0.48
1:T:128:SER:HB3	1:T:148:ARG:HG3	1.96	0.48
1:A:30:PHE:HZ	1:F:87:ILE:HD11	1.79	0.48
1:T:119:TRP:HB2	1:U:13:PHE:HB3	1.93	0.48
1:U:73:PRO:HA	1:U:76:MET:HG2	1.96	0.48
1:A:121:VAL:HG22	1:A:149:ALA:HB1	1.96	0.48
1:G:121:VAL:HG22	1:G:149:ALA:HB1	1.96	0.48
1:K:221:LYS:HE3	1:K:234:LEU:HD11	1.96	0.48
1:O:67:LEU:HD12	1:O:127:LEU:HD12	1.95	0.48
1:R:128:SER:HB3	1:R:148:ARG:HG3	1.95	0.48
1:G:6:TYR:HB3	1:L:41:VAL:HG22	1.94	0.48
1:J:128:SER:HB3	1:J:148:ARG:HG3	1.96	0.48
1:M:221:LYS:HE3	1:M:234:LEU:HD11	1.95	0.48
1:V:141:ILE:HD13	1:V:181:GLU:HG3	1.96	0.48
1:P:141:ILE:HD13	1:P:181:GLU:HG3	1.96	0.47
1:Q:199:ALA:HA	1:Q:202:PHE:CE2	2.48	0.47
2:X:213:ARG:HD2	2:X:213:ARG:H	1.79	0.47
1:R:13:PHE:HA	1:R:16:GLU:HB2	1.96	0.47
1:J:202:PHE:O	1:J:206:ASN:HB2	2.13	0.47
1:V:128:SER:HB3	1:V:148:ARG:HG3	1.96	0.47
2:X:141:ILE:HD13	2:X:181:GLU:HG3	1.96	0.47
1:J:83:LYS:NZ	1:K:29:GLU:OE2	2.33	0.47
1:K:65:LEU:HD11	1:K:76:MET:SD	2.54	0.47
1:P:213:ARG:HD2	1:P:213:ARG:H	1.79	0.47
1:T:202:PHE:O	1:T:206:ASN:HB2	2.14	0.47
1:A:7:ARG:HG3	1:F:214:PHE:O	2.15	0.47
1:O:127:LEU:HD21	1:P:23:ILE:CG2	2.44	0.47
1:F:221:LYS:HE3	1:F:234:LEU:HD11	1.97	0.47
1:H:13:PHE:HA	1:H:16:GLU:HB2	1.97	0.47
1:J:141:ILE:HD13	1:J:181:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:213:ARG:H	1:T:213:ARG:HD2	1.80	0.47
1:D:13:PHE:HA	1:D:16:GLU:HB2	1.95	0.47
1:J:87:ILE:HD11	1:K:30:PHE:HZ	1.79	0.47
1:N:141:ILE:HD13	1:N:181:GLU:HG3	1.97	0.47
1:R:213:ARG:HD2	1:R:213:ARG:H	1.80	0.47
1:W:127:LEU:HD21	2:X:23:ILE:CG2	2.40	0.47
2:X:202:PHE:O	2:X:206:ASN:HB2	2.15	0.47
1:A:199:ALA:HA	1:A:202:PHE:CE2	2.50	0.47
1:R:141:ILE:HD13	1:R:181:GLU:HG3	1.97	0.47
2:X:128:SER:HB3	2:X:148:ARG:HG3	1.97	0.47
1:J:99:GLU:OE1	5:J:2013:HOH:O	2.20	0.47
1:T:141:ILE:HD13	1:T:181:GLU:HG3	1.96	0.47
1:B:13:PHE:HA	1:B:16:GLU:HB2	1.97	0.46
1:Q:73:PRO:HA	1:Q:76:MET:HG2	1.97	0.46
1:W:242:ARG:NH2	5:W:2062:HOH:O	2.48	0.46
1:A:82:GLU:HG3	1:B:104:ARG:HH12	1.80	0.46
1:G:30:PHE:HZ	1:L:87:ILE:HD11	1.80	0.46
1:P:202:PHE:O	1:P:206:ASN:HB2	2.15	0.46
1:H:221:LYS:HE3	1:H:234:LEU:HD11	1.97	0.46
1:J:213:ARG:H	1:J:213:ARG:HD2	1.80	0.46
1:G:122:GLN:NE2	5:G:2044:HOH:O	2.48	0.46
1:L:202:PHE:O	1:L:206:ASN:HB2	2.15	0.46
1:N:128:SER:HB3	1:N:148:ARG:HG3	1.97	0.46
1:O:60:LYS:CE	1:P:16:GLU:HG2	2.46	0.46
2:C:56:LYS:HZ2	1:P:217:ARG:HE	1.64	0.46
1:I:60:LYS:HB3	1:J:26:TRP:HZ3	1.80	0.46
1:N:213:ARG:H	1:N:213:ARG:HD2	1.80	0.46
1:O:78:LYS:O	1:P:104:ARG:HG2	2.16	0.46
1:H:199:ALA:HA	1:H:202:PHE:CE2	2.51	0.45
1:I:221:LYS:HE3	1:I:234:LEU:HD11	1.97	0.45
1:T:13:PHE:HA	1:T:16:GLU:HB2	1.98	0.45
1:V:213:ARG:HD2	1:V:213:ARG:H	1.81	0.45
1:W:125:ARG:HD2	5:W:2056:HOH:O	2.16	0.45
1:K:65:LEU:HD13	1:L:30:PHE:CG	2.51	0.45
1:F:202:PHE:O	1:F:206:ASN:HB2	2.17	0.45
1:W:78:LYS:O	2:X:104:ARG:HG2	2.17	0.45
1:N:202:PHE:O	1:N:206:ASN:HB2	2.17	0.45
1:P:128:SER:HB3	1:P:148:ARG:HG3	1.98	0.45
1:B:199:ALA:HA	1:B:202:PHE:CE2	2.52	0.45
1:J:17:SER:C	1:J:19:ASP:N	2.69	0.45
1:I:60:LYS:CB	1:J:26:TRP:CZ3	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:LEU:HD11	1:M:76:MET:SD	2.57	0.45
1:S:73:PRO:HA	1:S:76:MET:HG2	1.98	0.45
1:W:37:PRO:O	1:W:41:VAL:HG12	2.17	0.45
3:E:38:LYS:HE3	3:E:38:LYS:HB2	1.78	0.45
1:N:181:GLU:O	1:N:185:THR:HG23	2.16	0.45
1:V:202:PHE:O	1:V:206:ASN:HB2	2.16	0.45
1:T:181:GLU:O	1:T:185:THR:HG23	2.17	0.44
1:G:13:PHE:HB3	1:L:119:TRP:HB2	2.00	0.44
1:H:119:TRP:HB2	1:I:13:PHE:HB3	2.00	0.44
1:D:202:PHE:O	1:D:206:ASN:HB2	2.18	0.44
1:G:26:TRP:CE2	1:L:61:MET:HG2	2.53	0.44
1:K:78:LYS:O	1:L:104:ARG:HG2	2.17	0.44
1:S:37:PRO:O	1:S:41:VAL:HG12	2.17	0.44
1:H:129:GLU:OE1	5:H:2034:HOH:O	2.21	0.44
1:U:119:TRP:HB2	1:V:13:PHE:HB3	1.98	0.44
1:G:38:LYS:HB2	1:G:38:LYS:HE3	1.78	0.44
1:L:213:ARG:HD2	1:L:213:ARG:H	1.83	0.44
1:P:214:PHE:CZ	1:Q:7:ARG:HA	2.52	0.44
3:E:219:ASP:OD1	1:F:7:ARG:NH1	2.51	0.44
1:P:187:ASN:HB2	5:P:2060:HOH:O	2.17	0.44
1:U:37:PRO:O	1:U:41:VAL:HG12	2.17	0.44
1:H:39:ARG:HH12	1:H:43:LEU:HD21	1.83	0.44
1:K:68:VAL:HG11	1:L:27:VAL:HG13	2.00	0.44
1:O:65:LEU:HD11	1:O:76:MET:SD	2.57	0.43
1:T:171:ILE:HB	5:T:2059:HOH:O	2.17	0.43
1:A:60:LYS:HE2	1:B:16:GLU:HG2	2.00	0.43
1:S:29:GLU:OE2	2:X:83:LYS:NZ	2.28	0.43
1:I:127:LEU:CD2	1:J:27:VAL:HG21	2.48	0.43
2:X:199:ALA:HA	2:X:202:PHE:CE2	2.53	0.43
1:F:199:ALA:HA	1:F:202:PHE:CE2	2.54	0.43
1:H:202:PHE:O	1:H:206:ASN:HB2	2.18	0.43
1:A:53:ARG:HD3	1:A:58:ASP:OD2	2.19	0.43
1:D:191:ARG:NH2	3:E:173:ASP:OD1	2.47	0.43
3:E:5:ASN:O	3:E:7:ARG:N	2.51	0.43
2:C:36:ASP:O	2:C:40:ILE:HG12	2.19	0.43
1:D:199:ALA:HA	1:D:202:PHE:CE2	2.54	0.43
1:I:203:GLU:HA	1:I:206:ASN:HB3	2.01	0.43
1:Q:13:PHE:HA	1:Q:16:GLU:HB2	2.01	0.43
2:C:214:PHE:CZ	1:D:7:ARG:HA	2.53	0.43
1:H:181:GLU:O	1:H:185:THR:HG23	2.19	0.43
1:P:94:VAL:HG22	1:P:95:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:223:LEU:HD12	1:Q:223:LEU:HA	1.92	0.43
1:W:73:PRO:HA	1:W:76:MET:HG2	2.00	0.43
1:I:119:TRP:NE1	1:J:18:ALA:HA	2.34	0.43
1:M:203:GLU:HA	1:M:206:ASN:HB3	2.01	0.43
1:V:6:TYR:HA	1:V:9:ILE:HD12	2.01	0.43
1:B:131:LEU:O	2:C:213:ARG:NH2	2.50	0.43
2:C:61:MET:HG2	1:D:26:TRP:CD2	2.54	0.43
1:Q:119:TRP:HB2	1:R:13:PHE:HB3	2.00	0.43
1:R:181:GLU:O	1:R:185:THR:HG23	2.19	0.43
1:D:181:GLU:O	1:D:185:THR:HG23	2.19	0.42
1:I:64:VAL:HG11	1:J:26:TRP:HB2	2.00	0.42
1:B:146:TYR:HA	1:B:147:PRO:HD3	1.94	0.42
2:C:38:LYS:HG2	1:D:6:TYR:HB2	2.00	0.42
2:X:94:VAL:HG22	2:X:95:TYR:CD2	2.54	0.42
1:G:127:LEU:HD22	1:H:27:VAL:HG21	2.00	0.42
1:I:60:LYS:HB2	1:J:26:TRP:HH2	1.81	0.42
1:J:11:LEU:HA	1:J:11:LEU:HD12	1.87	0.42
1:M:39:ARG:NH2	1:M:105:ASP:OD1	2.46	0.42
1:A:11:LEU:HD21	1:F:219:ASP:CG	2.40	0.42
1:W:223:LEU:HD12	1:W:223:LEU:HA	1.92	0.42
2:C:38:LYS:HE3	2:C:38:LYS:HB2	1.78	0.42
2:C:53:LYS:HB3	2:C:53:LYS:HE2	1.94	0.42
1:H:61:MET:HG2	1:I:26:TRP:CE2	2.54	0.42
1:I:127:LEU:HA	1:I:127:LEU:HD23	1.76	0.42
1:U:127:LEU:HD23	1:U:127:LEU:HA	1.77	0.42
1:V:181:GLU:O	1:V:185:THR:HG23	2.19	0.42
2:X:72:LYS:HB2	5:X:2012:HOH:O	2.20	0.42
1:F:181:GLU:O	1:F:185:THR:HG23	2.19	0.42
1:L:181:GLU:O	1:L:185:THR:HG23	2.19	0.42
1:P:199:ALA:HA	1:P:202:PHE:CE2	2.55	0.42
1:U:121:VAL:HG22	1:U:227:VAL:HG21	2.01	0.42
1:A:150:MET:HG2	1:A:155:PHE:CE2	2.54	0.42
1:O:203:GLU:HA	1:O:206:ASN:HB3	2.02	0.42
1:V:94:VAL:HG22	1:V:95:TYR:CD2	2.54	0.42
1:B:181:GLU:O	1:B:185:THR:HG23	2.20	0.42
3:E:53:ARG:HD3	3:E:58:ASP:OD2	2.20	0.42
1:I:80:MET:O	1:J:104:ARG:NH1	2.51	0.42
1:L:199:ALA:HA	1:L:202:PHE:CE2	2.54	0.42
1:T:87:ILE:HD11	1:U:30:PHE:CZ	2.51	0.42
2:C:150:MET:HG2	2:C:155:PHE:CE2	2.55	0.42
1:F:39:ARG:HH12	1:F:43:LEU:HD21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ARG:HD3	1:G:58:ASP:OD2	2.20	0.42
1:R:94:VAL:HG22	1:R:95:TYR:CD2	2.55	0.42
1:T:5:ASN:O	1:T:7:ARG:N	2.45	0.42
1:J:181:GLU:O	1:J:185:THR:HG23	2.19	0.41
1:J:94:VAL:HG22	1:J:95:TYR:CD2	2.55	0.41
1:N:199:ALA:HA	1:N:202:PHE:CE2	2.55	0.41
1:B:94:VAL:HG22	1:B:95:TYR:CD2	2.55	0.41
1:G:150:MET:HG2	1:G:155:PHE:CE2	2.55	0.41
1:O:146:TYR:HA	1:O:147:PRO:HD3	1.96	0.41
1:T:83:LYS:NZ	1:U:29:GLU:OE2	2.35	0.41
3:E:150:MET:HG2	3:E:155:PHE:CE2	2.54	0.41
3:E:219:ASP:OD2	1:F:7:ARG:NH1	2.49	0.41
1:A:30:PHE:CZ	1:F:87:ILE:HD11	2.55	0.41
1:L:94:VAL:HG22	1:L:95:TYR:CD2	2.55	0.41
1:B:202:PHE:O	1:B:206:ASN:HB2	2.19	0.41
1:B:23:ILE:O	1:B:27:VAL:HG23	2.21	0.41
1:I:65:LEU:HD13	1:J:30:PHE:CD1	2.55	0.41
1:K:39:ARG:NH2	1:K:105:ASP:OD1	2.45	0.41
1:M:146:TYR:HA	1:M:147:PRO:HD3	1.95	0.41
1:M:90:ASN:O	1:M:94:VAL:HG12	2.20	0.41
1:N:152:HIS:CD2	1:N:153:PRO:HD2	2.55	0.41
1:S:11:LEU:HD13	2:X:215:PHE:CE1	2.55	0.41
1:D:51:LYS:HG3	1:D:94:VAL:HB	2.03	0.41
2:C:215:PHE:CE1	1:D:11:LEU:HD13	2.54	0.41
1:D:39:ARG:HH12	1:D:43:LEU:HD21	1.85	0.41
3:E:11:LEU:HD12	3:E:11:LEU:HA	1.88	0.41
1:I:127:LEU:HD22	1:J:27:VAL:HG21	2.02	0.41
1:K:203:GLU:HA	1:K:206:ASN:HB3	2.02	0.41
1:K:60:LYS:HE2	1:L:16:GLU:HG2	2.03	0.41
1:L:152:HIS:CD2	1:L:153:PRO:HD2	2.56	0.41
1:U:181:GLU:O	1:U:185:THR:HG23	2.21	0.41
2:X:181:GLU:O	2:X:185:THR:HG23	2.20	0.41
1:D:23:ILE:O	1:D:27:VAL:HG23	2.21	0.41
1:M:223:LEU:HA	1:M:223:LEU:HD12	1.93	0.41
1:J:199:ALA:HA	1:J:202:PHE:CE2	2.55	0.41
1:M:73:PRO:HG3	1:M:109:LEU:HD11	2.02	0.41
1:M:214:PHE:CZ	1:N:7:ARG:HA	2.56	0.41
1:O:127:LEU:HD23	1:O:127:LEU:HA	1.69	0.41
1:N:188:PRO:HG3	1:O:207:MET:HG3	2.03	0.41
1:P:146:TYR:HA	1:P:147:PRO:HD3	1.96	0.41
1:R:23:ILE:O	1:R:27:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:121:VAL:HG22	1:W:227:VAL:HG21	2.02	0.41
1:A:119:TRP:HB2	1:B:13:PHE:HB3	2.02	0.41
1:B:232:GLU:OE1	5:B:2078:HOH:O	2.22	0.41
1:B:87:ILE:HD11	2:C:30:PHE:CZ	2.54	0.41
1:G:13:PHE:HA	1:G:16:GLU:HB2	2.03	0.41
1:G:82:GLU:HG3	1:H:104:ARG:NH1	2.36	0.41
1:G:7:ARG:HA	1:L:214:PHE:CZ	2.56	0.41
1:Q:121:VAL:HG22	1:Q:227:VAL:HG21	2.01	0.41
1:S:30:PHE:CZ	2:X:87:ILE:HD11	2.55	0.41
1:S:83:LYS:HD3	1:T:29:GLU:HG2	2.03	0.41
1:A:40:ILE:HD12	1:A:111:ARG:HB3	2.03	0.40
1:D:122:GLN:NE2	3:E:14:LEU:HD22	2.36	0.40
1:D:87:ILE:HD11	3:E:30:PHE:CZ	2.56	0.40
1:F:53:ARG:HB3	1:F:53:ARG:HE	1.71	0.40
1:H:219:ASP:OD2	1:I:7:ARG:HD3	2.21	0.40
1:H:51:LYS:HG3	1:H:94:VAL:HB	2.03	0.40
1:I:119:TRP:NE1	1:J:18:ALA:CA	2.84	0.40
1:K:127:LEU:HD21	1:L:23:ILE:HG22	2.04	0.40
3:E:40:ILE:HD12	3:E:111:ARG:HB3	2.03	0.40
1:H:23:ILE:O	1:H:27:VAL:HG23	2.21	0.40
1:J:188:PRO:HG2	1:K:204:LYS:HA	2.03	0.40
1:P:181:GLU:O	1:P:185:THR:HG23	2.21	0.40
2:C:40:ILE:HD12	2:C:111:ARG:HB3	2.03	0.40
1:I:65:LEU:HD13	1:J:30:PHE:CD2	2.56	0.40
2:X:152:HIS:CD2	2:X:153:PRO:HD2	2.56	0.40
2:X:53:LYS:HE2	2:X:53:LYS:HB3	1.97	0.40
1:F:51:LYS:HG3	1:F:94:VAL:HB	2.04	0.40
1:H:63:ILE:O	1:H:67:LEU:HG	2.22	0.40
1:N:94:VAL:HG22	1:N:95:TYR:CD2	2.57	0.40
1:Q:37:PRO:O	1:Q:41:VAL:HG12	2.21	0.40
1:S:13:PHE:HA	1:S:16:GLU:HB2	2.03	0.40
1:B:19:ASP:OD2	1:B:22:THR:HG23	2.21	0.40
1:G:73:PRO:HA	1:G:76:MET:HG2	2.03	0.40
1:N:188:PRO:HG2	1:O:204:LYS:HA	2.03	0.40
1:S:82:GLU:HG3	1:T:104:ARG:NH1	2.36	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:J:233:ASP:OD2	1:R:53:ARG:NH2[1_564]	2.17	0.03

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	247/253 (98%)	240 (97%)	7 (3%)	0	100	100
1	B	247/253 (98%)	238 (96%)	9 (4%)	0	100	100
1	D	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	F	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	G	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	H	247/253 (98%)	237 (96%)	10 (4%)	0	100	100
1	I	247/253 (98%)	239 (97%)	8 (3%)	0	100	100
1	J	247/253 (98%)	240 (97%)	5 (2%)	2 (1%)	19	39
1	K	249/253 (98%)	239 (96%)	9 (4%)	1 (0%)	34	57
1	L	248/253 (98%)	241 (97%)	6 (2%)	1 (0%)	34	57
1	M	246/253 (97%)	238 (97%)	8 (3%)	0	100	100
1	N	247/253 (98%)	241 (98%)	6 (2%)	0	100	100
1	O	246/253 (97%)	239 (97%)	7 (3%)	0	100	100
1	P	247/253 (98%)	240 (97%)	7 (3%)	0	100	100
1	Q	247/253 (98%)	242 (98%)	5 (2%)	0	100	100
1	R	246/253 (97%)	240 (98%)	6 (2%)	0	100	100
1	S	247/253 (98%)	243 (98%)	4 (2%)	0	100	100
1	T	248/253 (98%)	241 (97%)	7 (3%)	0	100	100
1	U	245/253 (97%)	241 (98%)	4 (2%)	0	100	100
1	V	247/253 (98%)	241 (98%)	6 (2%)	0	100	100
1	W	248/253 (98%)	243 (98%)	5 (2%)	0	100	100
2	C	248/253 (98%)	241 (97%)	7 (3%)	0	100	100
2	X	247/253 (98%)	240 (97%)	7 (3%)	0	100	100
3	E	247/253 (98%)	238 (96%)	8 (3%)	1 (0%)	34	57
All	All	5929/6072 (98%)	5759 (97%)	165 (3%)	5 (0%)	51	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	6	TYR
1	J	18	ALA
1	J	17	SER
1	L	4	GLU
1	K	3	ASP

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	201/206 (98%)	191 (95%)	10 (5%)	24	47
1	B	201/206 (98%)	188 (94%)	13 (6%)	17	34
1	D	201/206 (98%)	187 (93%)	14 (7%)	15	30
1	F	200/206 (97%)	186 (93%)	14 (7%)	15	30
1	G	201/206 (98%)	191 (95%)	10 (5%)	24	47
1	H	201/206 (98%)	187 (93%)	14 (7%)	15	30
1	I	201/206 (98%)	191 (95%)	10 (5%)	24	47
1	J	200/206 (97%)	185 (92%)	15 (8%)	13	27
1	K	202/206 (98%)	190 (94%)	12 (6%)	19	39
1	L	203/206 (98%)	189 (93%)	14 (7%)	15	31
1	M	200/206 (97%)	189 (94%)	11 (6%)	21	43
1	N	201/206 (98%)	188 (94%)	13 (6%)	17	34
1	O	200/206 (97%)	190 (95%)	10 (5%)	24	47
1	P	201/206 (98%)	186 (92%)	15 (8%)	13	27
1	Q	200/206 (97%)	191 (96%)	9 (4%)	27	52
1	R	201/206 (98%)	187 (93%)	14 (7%)	15	30
1	S	201/206 (98%)	191 (95%)	10 (5%)	24	47
1	T	202/206 (98%)	186 (92%)	16 (8%)	12	24
1	U	200/206 (97%)	190 (95%)	10 (5%)	24	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	V	201/206 (98%)	184 (92%)	17 (8%)	10 21
1	W	202/206 (98%)	192 (95%)	10 (5%)	24 47
2	C	202/206 (98%)	194 (96%)	8 (4%)	31 57
2	X	200/206 (97%)	186 (93%)	14 (7%)	15 30
3	E	200/206 (97%)	191 (96%)	9 (4%)	27 52
All	All	4822/4944 (98%)	4530 (94%)	292 (6%)	18 38

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	77	MET
1	A	94	VAL
1	A	104	ARG
1	A	121	VAL
1	A	207	MET
1	A	213	ARG
1	A	223	LEU
1	A	227	VAL
1	A	241	VAL
1	B	87	ILE
1	B	94	VAL
1	B	104	ARG
1	B	121	VAL
1	B	127	LEU
1	B	185	THR
1	B	206	ASN
1	B	207	MET
1	B	213	ARG
1	B	217	ARG
1	B	223	LEU
1	B	227	VAL
1	B	242	ARG
2	C	11	LEU
2	C	77	MET
2	C	94	VAL
2	C	121	VAL
2	C	207	MET
2	C	213	ARG
2	C	223	LEU

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Mol	Chain	Res	Type
2	C	227	VAL
1	D	11	LEU
1	D	87	ILE
1	D	94	VAL
1	D	104	ARG
1	D	121	VAL
1	D	127	LEU
1	D	185	THR
1	D	206	ASN
1	D	207	MET
1	D	213	ARG
1	D	217	ARG
1	D	223	LEU
1	D	227	VAL
1	D	242	ARG
3	E	11	LEU
3	E	77	MET
3	E	94	VAL
3	E	121	VAL
3	E	207	MET
3	E	213	ARG
3	E	223	LEU
3	E	227	VAL
3	E	241	VAL
1	F	11	LEU
1	F	87	ILE
1	F	94	VAL
1	F	104	ARG
1	F	121	VAL
1	F	127	LEU
1	F	185	THR
1	F	206	ASN
1	F	207	MET
1	F	213	ARG
1	F	217	ARG
1	F	223	LEU
1	F	227	VAL
1	F	242	ARG
1	G	11	LEU
1	G	77	MET
1	G	94	VAL
1	G	104	ARG

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Mol	Chain	Res	Type
1	G	121	VAL
1	G	207	MET
1	G	213	ARG
1	G	223	LEU
1	G	227	VAL
1	G	241	VAL
1	H	11	LEU
1	H	87	ILE
1	H	94	VAL
1	H	104	ARG
1	H	121	VAL
1	H	127	LEU
1	H	185	THR
1	H	206	ASN
1	H	207	MET
1	H	213	ARG
1	H	217	ARG
1	H	223	LEU
1	H	227	VAL
1	H	242	ARG
1	I	11	LEU
1	I	14	LEU
1	I	94	VAL
1	I	104	ARG
1	I	121	VAL
1	I	125	ARG
1	I	207	MET
1	I	223	LEU
1	I	227	VAL
1	I	232	GLU
1	J	11	LEU
1	J	14	LEU
1	J	41	VAL
1	J	87	ILE
1	J	94	VAL
1	J	110	SER
1	J	121	VAL
1	J	127	LEU
1	J	206	ASN
1	J	207	MET
1	J	213	ARG
1	J	217	ARG

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Mol	Chain	Res	Type
1	J	223	LEU
1	J	227	VAL
1	J	242	ARG
1	K	4	GLU
1	K	5	ASN
1	K	14	LEU
1	K	53	ARG
1	K	94	VAL
1	K	104	ARG
1	K	121	VAL
1	K	125	ARG
1	K	207	MET
1	K	223	LEU
1	K	227	VAL
1	K	232	GLU
1	L	11	LEU
1	L	41	VAL
1	L	87	ILE
1	L	94	VAL
1	L	110	SER
1	L	121	VAL
1	L	127	LEU
1	L	206	ASN
1	L	207	MET
1	L	213	ARG
1	L	217	ARG
1	L	223	LEU
1	L	227	VAL
1	L	242	ARG
1	M	11	LEU
1	M	14	LEU
1	M	53	ARG
1	M	94	VAL
1	M	104	ARG
1	M	121	VAL
1	M	125	ARG
1	M	207	MET
1	M	223	LEU
1	M	227	VAL
1	M	232	GLU
1	N	41	VAL
1	N	87	ILE

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Mol	Chain	Res	Type
1	N	94	VAL
1	N	110	SER
1	N	121	VAL
1	N	127	LEU
1	N	206	ASN
1	N	207	MET
1	N	213	ARG
1	N	217	ARG
1	N	223	LEU
1	N	227	VAL
1	N	242	ARG
1	O	11	LEU
1	O	14	LEU
1	O	94	VAL
1	O	104	ARG
1	O	121	VAL
1	O	125	ARG
1	O	207	MET
1	O	223	LEU
1	O	227	VAL
1	O	232	GLU
1	P	14	LEU
1	P	16	GLU
1	P	17	SER
1	P	41	VAL
1	P	87	ILE
1	P	94	VAL
1	P	110	SER
1	P	121	VAL
1	P	127	LEU
1	P	206	ASN
1	P	207	MET
1	P	213	ARG
1	P	223	LEU
1	P	227	VAL
1	P	242	ARG
1	Q	11	LEU
1	Q	94	VAL
1	Q	104	ARG
1	Q	121	VAL
1	Q	145	THR
1	Q	207	MET

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Mol	Chain	Res	Type
1	Q	213	ARG
1	Q	223	LEU
1	Q	227	VAL
1	R	14	LEU
1	R	41	VAL
1	R	87	ILE
1	R	94	VAL
1	R	110	SER
1	R	121	VAL
1	R	127	LEU
1	R	206	ASN
1	R	207	MET
1	R	213	ARG
1	R	217	ARG
1	R	223	LEU
1	R	227	VAL
1	R	242	ARG
1	S	11	LEU
1	S	14	LEU
1	S	94	VAL
1	S	104	ARG
1	S	121	VAL
1	S	145	THR
1	S	207	MET
1	S	213	ARG
1	S	223	LEU
1	S	227	VAL
1	T	5	ASN
1	T	14	LEU
1	T	41	VAL
1	T	87	ILE
1	T	94	VAL
1	T	104	ARG
1	T	110	SER
1	T	121	VAL
1	T	127	LEU
1	T	206	ASN
1	T	207	MET
1	T	213	ARG
1	T	217	ARG
1	T	223	LEU
1	T	227	VAL

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Mol	Chain	Res	Type
1	T	242	ARG
1	U	11	LEU
1	U	14	LEU
1	U	94	VAL
1	U	104	ARG
1	U	121	VAL
1	U	145	THR
1	U	207	MET
1	U	213	ARG
1	U	223	LEU
1	U	227	VAL
1	V	5	ASN
1	V	11	LEU
1	V	14	LEU
1	V	16	GLU
1	V	41	VAL
1	V	87	ILE
1	V	94	VAL
1	V	110	SER
1	V	121	VAL
1	V	127	LEU
1	V	206	ASN
1	V	207	MET
1	V	213	ARG
1	V	217	ARG
1	V	223	LEU
1	V	227	VAL
1	V	242	ARG
1	W	14	LEU
1	W	94	VAL
1	W	104	ARG
1	W	121	VAL
1	W	145	THR
1	W	207	MET
1	W	213	ARG
1	W	223	LEU
1	W	227	VAL
1	W	251	VAL
2	X	14	LEU
2	X	41	VAL
2	X	87	ILE
2	X	94	VAL

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Mol	Chain	Res	Type
2	X	110	SER
2	X	121	VAL
2	X	127	LEU
2	X	206	ASN
2	X	207	MET
2	X	213	ARG
2	X	217	ARG
2	X	223	LEU
2	X	227	VAL
2	X	242	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	ASN
1	G	33	GLN
1	H	101	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	a	8/9 (88%)	2 (25%)	0
4	c	8/9 (88%)	2 (25%)	0
4	e	8/9 (88%)	2 (25%)	0
4	g	8/9 (88%)	1 (12%)	0
4	i	8/9 (88%)	2 (25%)	0
4	k	8/9 (88%)	2 (25%)	0
4	m	8/9 (88%)	2 (25%)	0
4	o	8/9 (88%)	2 (25%)	0
4	q	8/9 (88%)	1 (12%)	0
4	s	8/9 (88%)	2 (25%)	0
4	u	8/9 (88%)	2 (25%)	0
4	w	8/9 (88%)	1 (12%)	0
All	All	96/108 (88%)	21 (21%)	0

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	a	3	U
4	a	9	U

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Mol	Chain	Res	Type
4	c	3	U
4	c	9	U
4	e	3	U
4	e	9	U
4	g	9	U
4	i	3	U
4	i	9	U
4	k	2	G
4	k	3	U
4	m	3	U
4	m	9	U
4	o	3	U
4	o	9	U
4	q	9	U
4	s	3	U
4	s	9	U
4	u	3	U
4	u	9	U
4	w	9	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

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	249/253 (98%)	-0.04	1 (0%) 92 91	34, 48, 77, 112	0
1	B	249/253 (98%)	-0.07	6 (2%) 59 53	30, 44, 76, 103	0
1	D	249/253 (98%)	0.32	11 (4%) 34 27	37, 68, 96, 126	0
1	F	249/253 (98%)	0.33	15 (6%) 21 16	42, 66, 97, 122	0
1	G	249/253 (98%)	0.00	4 (1%) 72 68	29, 45, 70, 102	0
1	H	249/253 (98%)	-0.05	1 (0%) 92 91	31, 49, 72, 98	0
1	I	249/253 (98%)	-0.19	0 100 100	34, 50, 70, 92	0
1	J	249/253 (98%)	0.42	16 (6%) 19 14	39, 62, 96, 126	0
1	K	251/253 (99%)	0.19	6 (2%) 59 53	37, 56, 79, 122	0
1	L	250/253 (98%)	0.12	6 (2%) 59 53	27, 46, 78, 100	0
1	M	248/253 (98%)	0.06	3 (1%) 79 76	35, 51, 75, 105	0
1	N	249/253 (98%)	0.04	9 (3%) 42 35	38, 55, 82, 103	0
1	O	248/253 (98%)	0.09	3 (1%) 79 76	33, 50, 77, 101	0
1	P	249/253 (98%)	-0.02	8 (3%) 47 40	26, 42, 77, 100	0
1	Q	249/253 (98%)	-0.03	1 (0%) 92 91	27, 44, 67, 87	0
1	R	248/253 (98%)	0.17	7 (2%) 53 46	38, 58, 85, 109	0
1	S	249/253 (98%)	-0.03	2 (0%) 86 84	36, 51, 74, 101	0
1	T	250/253 (98%)	0.01	9 (3%) 42 35	28, 45, 83, 117	0
1	U	247/253 (97%)	-0.24	0 100 100	24, 39, 62, 74	0
1	V	249/253 (98%)	0.04	3 (1%) 79 76	32, 52, 80, 105	0
1	W	250/253 (98%)	0.07	6 (2%) 59 53	31, 49, 74, 110	0
2	C	250/253 (98%)	-0.14	0 100 100	26, 44, 68, 124	0
2	X	249/253 (98%)	0.14	5 (2%) 65 60	34, 53, 82, 104	0
3	E	249/253 (98%)	0.49	12 (4%) 30 24	47, 66, 99, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
4	a	9/9 (100%)	-0.67	0	100	100	42, 48, 58, 63	0
4	c	9/9 (100%)	-0.60	0	100	100	38, 42, 64, 76	0
4	e	9/9 (100%)	-0.59	0	100	100	55, 61, 78, 82	0
4	g	9/9 (100%)	-0.76	0	100	100	34, 43, 56, 69	0
4	i	9/9 (100%)	-0.76	0	100	100	38, 46, 56, 80	0
4	k	9/9 (100%)	-0.82	0	100	100	44, 51, 68, 73	0
4	m	9/9 (100%)	-0.77	0	100	100	44, 49, 64, 67	0
4	o	9/9 (100%)	-0.48	0	100	100	39, 48, 55, 62	0
4	q	9/9 (100%)	-0.77	0	100	100	35, 41, 61, 69	0
4	s	9/9 (100%)	-0.64	0	100	100	47, 50, 61, 63	0
4	u	9/9 (100%)	-0.83	0	100	100	33, 36, 50, 57	0
4	w	9/9 (100%)	-0.47	0	100	100	38, 46, 59, 78	0
All	All	6085/6180 (98%)	0.06	134 (2%)	62	56	24, 51, 83, 134	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	23	ILE	6.6
1	P	20	SER	5.9
1	J	22	THR	5.8
1	J	213	ARG	5.2
1	J	235	VAL	5.2
1	N	234	LEU	5.1
1	J	26	TRP	5.0
3	E	9	ILE	4.8
1	T	22	THR	4.5
3	E	6	TYR	4.4
1	O	6	TYR	4.2
1	T	25	ALA	4.0
1	T	26	TRP	3.9
1	G	6	TYR	3.8
1	J	20	SER	3.8
1	J	18	ALA	3.6
1	N	233	ASP	3.6
1	P	24	ASN	3.6
1	D	22	THR	3.6
1	J	24	ASN	3.5
1	M	6	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	R	105	ASP	3.4
1	F	51	LYS	3.4
1	J	19	ASP	3.4
1	J	30	PHE	3.4
1	D	235	VAL	3.4
1	R	234	LEU	3.4
1	J	27	VAL	3.3
1	G	251	VAL	3.3
3	E	13	PHE	3.2
1	W	3	ASP	3.2
1	Q	192	THR	3.2
1	P	18	ALA	3.1
1	P	21	GLY	3.0
1	D	19	ASP	3.0
1	L	105	ASP	3.0
1	V	232	GLU	3.0
3	E	12	ALA	2.9
1	F	232	GLU	2.9
1	J	165	ASN	2.9
1	J	25	ALA	2.9
1	F	233	ASP	2.8
3	E	8	ASP	2.8
1	M	13	PHE	2.8
1	O	86	SER	2.8
1	G	82	GLU	2.8
1	T	19	ASP	2.8
1	W	12	ALA	2.7
1	F	4	GLU	2.7
1	N	230	ILE	2.7
1	N	213	ARG	2.7
3	E	50	ALA	2.7
1	L	165	ASN	2.7
1	D	213	ARG	2.7
1	P	27	VAL	2.6
1	B	6	TYR	2.6
1	F	213	ARG	2.6
1	W	194	GLN	2.6
1	B	8	ASP	2.6
1	T	213	ARG	2.6
1	T	21	GLY	2.6
3	E	11	LEU	2.6
1	F	235	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	235	VAL	2.6
1	F	52	GLY	2.5
1	D	232	GLU	2.5
1	F	6	TYR	2.5
1	T	28	ASN	2.5
1	N	162	ASP	2.5
1	K	52	GLY	2.5
1	D	23	ILE	2.4
1	M	9	ILE	2.4
1	R	213	ARG	2.4
1	F	10	ALA	2.4
1	D	233	ASP	2.4
1	F	49	THR	2.4
1	N	232	GLU	2.4
1	L	125	ARG	2.4
1	P	26	TRP	2.4
1	F	217	ARG	2.4
1	L	19	ASP	2.4
3	E	192	THR	2.4
3	E	14	LEU	2.4
1	K	2	SER	2.3
1	D	78	LYS	2.3
1	S	232	GLU	2.3
1	L	232	GLU	2.3
1	R	26	TRP	2.3
1	G	9	ILE	2.3
2	X	125	ARG	2.2
1	B	144	VAL	2.2
2	X	121	VAL	2.2
1	S	4	GLU	2.2
2	X	234	LEU	2.2
1	N	164	PRO	2.2
1	B	232	GLU	2.2
1	B	105	ASP	2.2
1	D	217	ARG	2.2
1	K	194	GLN	2.2
1	F	164	PRO	2.2
1	W	104	ARG	2.2
1	B	143	GLY	2.2
1	W	6	TYR	2.2
3	E	232	GLU	2.2
1	F	18	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	162	ASP	2.2
3	E	194	GLN	2.1
1	K	7	ARG	2.1
1	V	82	GLU	2.1
1	F	11	LEU	2.1
1	D	231	ASP	2.1
1	L	213	ARG	2.1
1	T	27	VAL	2.1
1	H	232	GLU	2.1
1	J	162	ASP	2.1
1	R	233	ASP	2.1
2	X	230	ILE	2.1
1	K	105	ASP	2.1
1	P	28	ASN	2.1
1	J	217	ARG	2.1
1	D	239	ALA	2.1
1	P	217	ARG	2.1
1	R	50	ALA	2.1
1	W	21	GLY	2.1
2	X	213	ARG	2.1
1	J	49	THR	2.0
1	V	93	SER	2.0
1	O	13	PHE	2.0
1	F	8	ASP	2.0
1	N	19	ASP	2.0
1	A	165	ASN	2.0
3	E	52	GLY	2.0
1	K	143	GLY	2.0
1	T	20	SER	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.