



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2017 – 09:09 AM EDT

PDB ID : 5K36  
Title : Structure of an eleven component nuclear RNA exosome complex bound to RNA  
Authors : Lima, C.D.; Zinder, J.C.  
Deposited on : unknown  
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

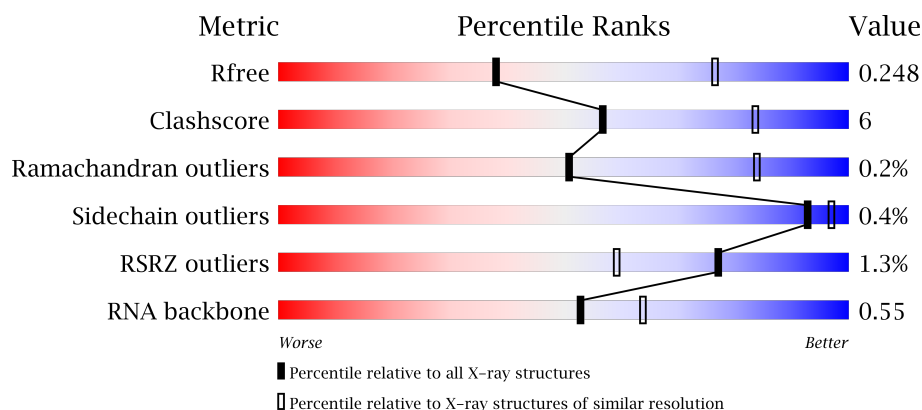
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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	305	
2	B	250	
3	C	394	
4	D	225	

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Mol	Chain	Length	Quality of chain
5	E	269	
6	F	250	
7	G	244	
8	H	363	
9	I	296	
10	J	559	
11	K	1003	
12	L	17	
12	M	17	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SO4	G	301	-	-	-	X
14	GOL	A	402	-	-	-	X
14	GOL	A	403	-	-	-	X
14	GOL	A	404	-	-	-	X
14	GOL	B	302	-	-	-	X
14	GOL	H	401	-	-	-	X
14	GOL	K	2004	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 30251 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 Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2255	1419	385	434	17			

- Molecule 2 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1883	1178	336	360	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P46948
B	-2	PRO	-	expression tag	UNP P46948
B	-1	ASP	-	expression tag	UNP P46948
B	0	HIS	-	expression tag	UNP P46948

- Molecule 3 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	340	Total	C	N	O	S	0	0	0
			2656	1683	446	516	11			

- Molecule 4 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	0	0	0
			1691	1063	287	332	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P53256
D	0	SER	-	expression tag	UNP P53256

- Molecule 5 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	259	Total	C	N	O	S	0	0	0
			1997	1275	330	387	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q12277
E	-2	ASP	-	expression tag	UNP Q12277
E	-1	PRO	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277

- Molecule 6 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	215	Total	C	N	O	S	0	0	0
			1651	1033	278	330	10			

- Molecule 7 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	232	Total	C	N	O	S	0	0	0
			1803	1152	295	345	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP Q08285
G	-2	ASP	-	expression tag	UNP Q08285
G	-1	PRO	-	expression tag	UNP Q08285
G	0	HIS	-	expression tag	UNP Q08285

- Molecule 8 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	289	Total	C	N	O	S	0	0	0
			2245	1404	406	423	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-3	GLY	-	expression tag	UNP P38792
H	-2	ASP	-	expression tag	UNP P38792
H	-1	PRO	-	expression tag	UNP P38792
H	0	HIS	-	expression tag	UNP P38792

- Molecule 9 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	224	Total	C	N	O	S	0	0	0
			1728	1079	305	337	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-3	GLY	-	expression tag	UNP P53859
I	-2	ASP	-	expression tag	UNP P53859
I	-1	PRO	-	expression tag	UNP P53859
I	0	HIS	-	expression tag	UNP P53859

- Molecule 10 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	467	Total	C	N	O	S	0	0	0
			3829	2445	659	715	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	126	SER	-	expression tag	UNP Q12149
J	127	LEU	-	expression tag	UNP Q12149
J	128	MET	-	expression tag	UNP Q12149
J	238	ASN	ASP	engineered mutation	UNP Q12149

- Molecule 11 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	955	Total	C	N	O	S	0	0	0
			7638	4829	1344	1430	35			

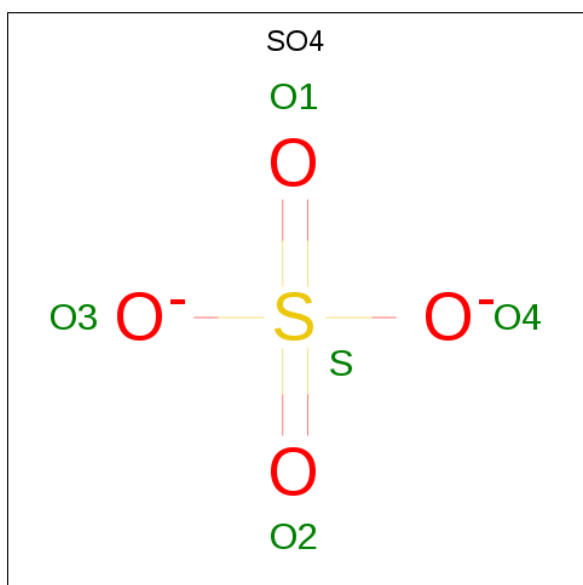
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	SER	-	expression tag	UNP Q08162
K	0	LEU	-	expression tag	UNP Q08162
K	171	ASN	ASP	engineered mutation	UNP Q08162
K	551	ASN	ASP	engineered mutation	UNP Q08162

- Molecule 12 is a RNA chain called RNA (17-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	7	Total	C	N	O	P	0	0	0
			148	67	26	48	7			
12	L	17	Total	C	N	O	P	0	0	0
			354	160	55	122	17			

- Molecule 13 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



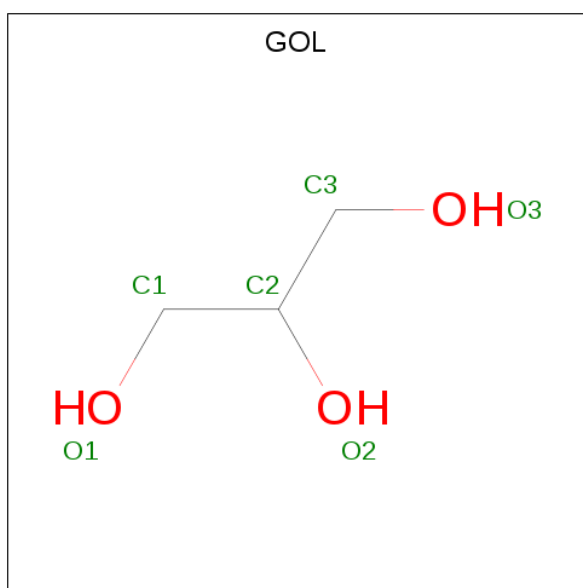
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	O	S	0	0
			5	4	1		
13	B	1	Total	O	S	0	0
			5	4	1		
13	D	1	Total	O	S	0	0
			5	4	1		
13	E	1	Total	O	S	0	0
			5	4	1		
13	F	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	G	1	Total	O	S	0	0
			5	4	1		
13	I	1	Total	O	S	0	0
			5	4	1		
13	K	1	Total	O	S	0	0
			5	4	1		
13	K	1	Total	O	S	0	0
			5	4	1		
13	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			6	3	3		
14	A	1	Total	C	O	0	0
			6	3	3		
14	A	1	Total	C	O	0	0
			6	3	3		
14	B	1	Total	C	O	0	0
			6	3	3		
14	H	1	Total	C	O	0	0
			6	3	3		
14	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Zn	0	0
			1	1		

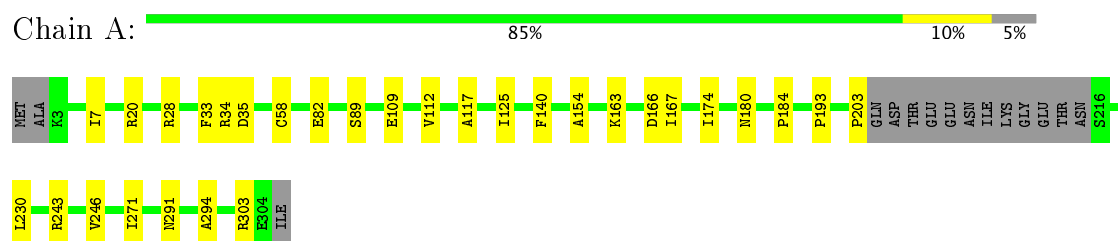
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	52	Total	O	0	0
			52	52		
16	B	32	Total	O	0	0
			32	32		
16	C	18	Total	O	0	0
			18	18		
16	D	27	Total	O	0	0
			27	27		
16	E	8	Total	O	0	0
			8	8		
16	F	9	Total	O	0	0
			9	9		
16	G	30	Total	O	0	0
			30	30		
16	H	11	Total	O	0	0
			11	11		
16	I	4	Total	O	0	0
			4	4		
16	J	23	Total	O	0	0
			23	23		
16	K	64	Total	O	0	0
			64	64		
16	L	2	Total	O	0	0
			2	2		

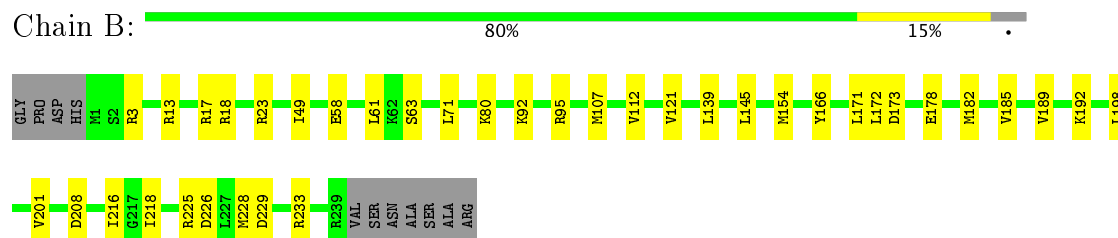
### 3 Residue-property plots

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.

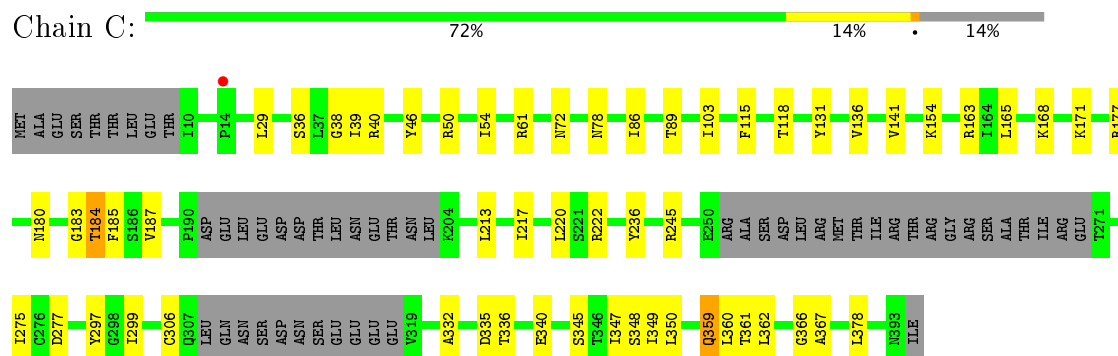
- Molecule 1: Exosome complex component RRP45



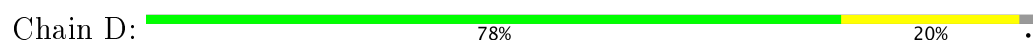
- Molecule 2: Exosome complex component SKI6

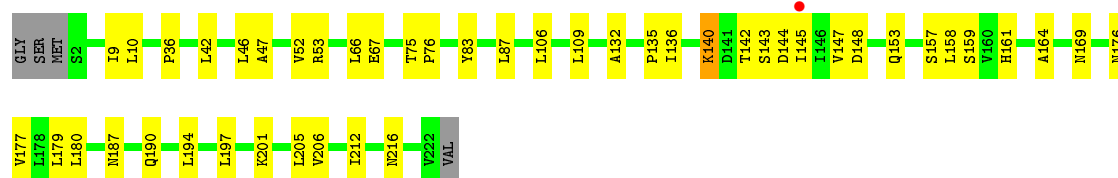


- Molecule 3: Exosome complex component RRP43

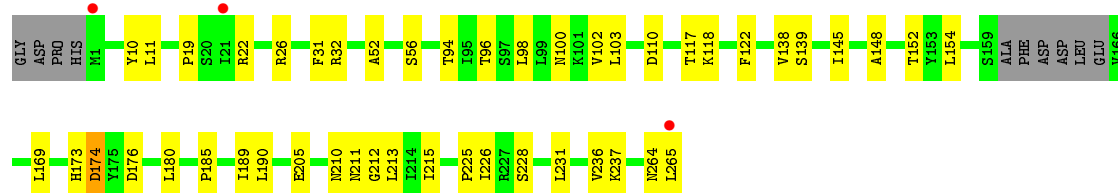
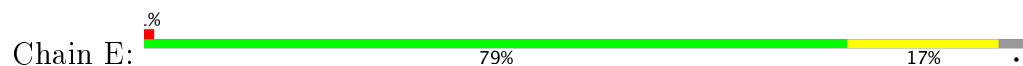


- Molecule 4: Exosome complex component RRP46

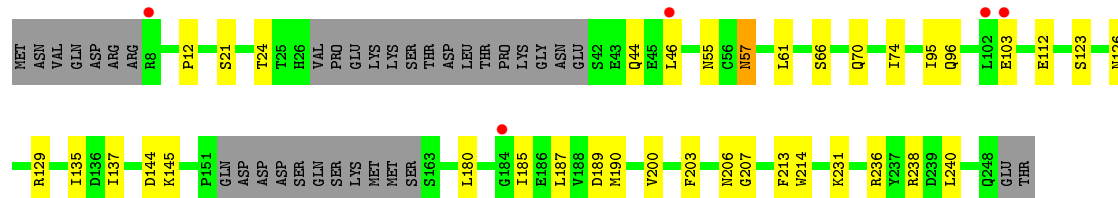




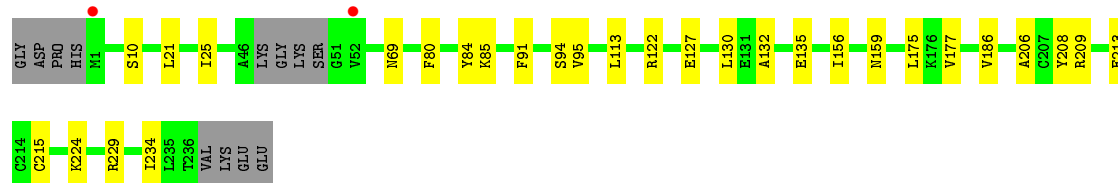
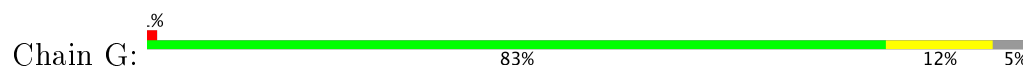
• Molecule 5: Exosome complex component RRP42



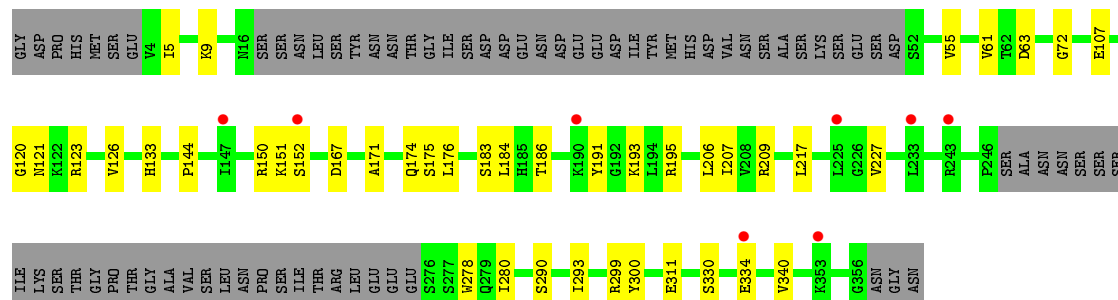
• Molecule 6: Exosome complex component MTR3



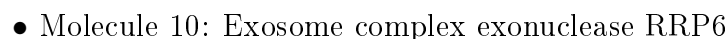
• Molecule 7: Exosome complex component RRP40



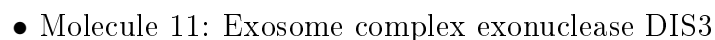
• Molecule 8: Exosome complex component RRP4



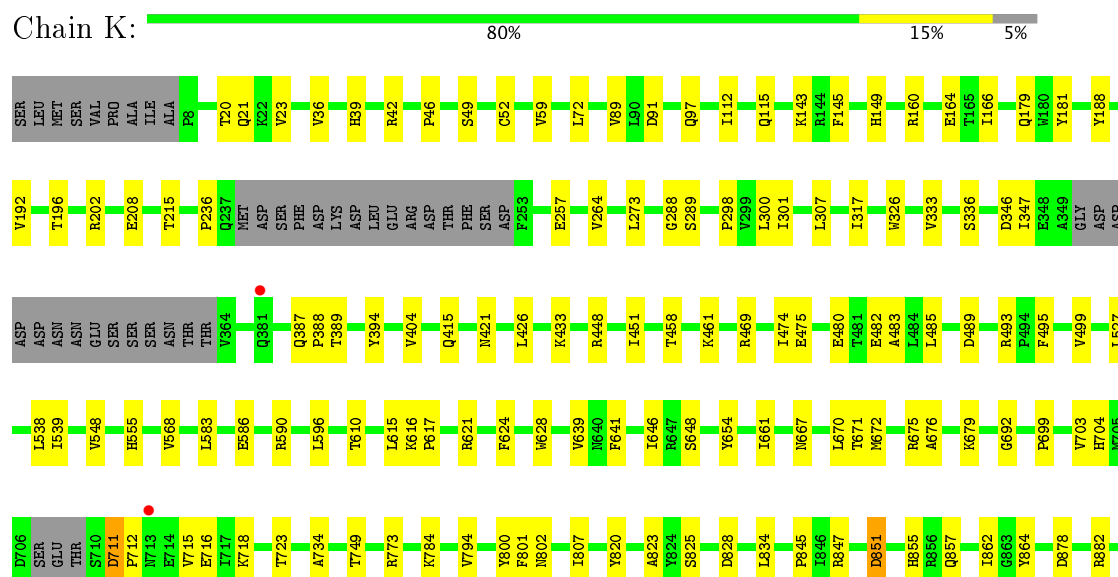
Chain I:



## Chain J:

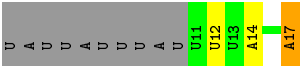
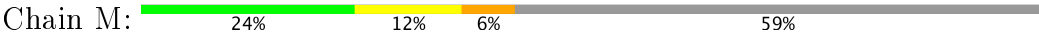


Chain K:

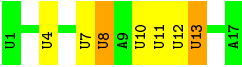




● Molecule 12: RNA (17-MER)



● Molecule 12: RNA (17-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.70Å 212.26Å 218.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.13 – 3.10 106.13 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (106.13-3.10) 97.6 (106.13-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.201 , 0.249 0.199 , 0.248	Depositor DCC
$R_{free}$ test set	5765 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.8	Xtriage
Anisotropy	0.662	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/2290	0.40	0/3088
2	B	0.23	0/1907	0.41	0/2566
3	C	0.23	0/2695	0.42	0/3647
4	D	0.23	0/1709	0.42	0/2319
5	E	0.24	0/2034	0.41	0/2764
6	F	0.24	0/1675	0.44	0/2263
7	G	0.24	0/1839	0.41	0/2493
8	H	0.24	0/2280	0.42	0/3078
9	I	0.24	0/1751	0.43	0/2366
10	J	0.23	0/3914	0.39	0/5310
11	K	0.23	0/7787	0.40	0/10550
12	L	0.21	0/394	0.92	3/609 (0.5%)
12	M	0.13	0/165	0.65	0/254
All	All	0.23	0/30440	0.42	3/41307 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	12	U	C2-N1-C1'	7.33	126.49	117.70
12	L	12	U	N1-C2-O2	6.95	127.67	122.80
12	L	12	U	N3-C2-O2	-6.43	117.70	122.20

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	2255	0	2251	20	0
2	B	1883	0	1940	26	0
3	C	2656	0	2705	39	0
4	D	1691	0	1745	27	0
5	E	1997	0	2037	31	0
6	F	1651	0	1624	27	0
7	G	1803	0	1794	18	0
8	H	2245	0	2265	27	0
9	I	1728	0	1729	22	0
10	J	3829	0	3839	46	0
11	K	7638	0	7678	89	0
12	L	354	0	178	4	0
12	M	148	0	75	3	0
13	A	5	0	0	0	0
13	B	5	0	0	0	0
13	D	5	0	0	0	0
13	E	5	0	0	0	0
13	F	5	0	0	0	0
13	G	5	0	0	1	0
13	I	5	0	0	0	0
13	K	10	0	0	0	0
13	M	5	0	0	0	0
14	A	18	0	24	2	0
14	B	6	0	8	0	0
14	H	6	0	8	1	0
14	K	12	0	16	3	0
15	K	1	0	0	0	0
16	A	52	0	0	1	0
16	B	32	0	0	1	0
16	C	18	0	0	0	0
16	D	27	0	0	0	0
16	E	8	0	0	0	0
16	F	9	0	0	1	0
16	G	30	0	0	0	0
16	H	11	0	0	0	0
16	I	4	0	0	0	0
16	J	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	64	0	0	0	0
16	L	2	0	0	0	0
All	All	30251	0	29916	343	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (343) 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)
3:C:362:LEU:HB3	4:D:180:LEU:HB3	1.69	0.74
9:I:51:ARG:HB3	10:J:548:ARG:HH22	1.56	0.70
8:H:144:PRO:HB3	8:H:278:TRP:HB3	1.73	0.69
11:K:878:ASP:OD2	11:K:882:ARG:NH1	2.27	0.67
5:E:215:ILE:HA	5:E:226:ILE:HG22	1.77	0.65
9:I:211:ARG:NH2	9:I:213:THR:O	2.29	0.65
4:D:46:LEU:HB2	4:D:83:TYR:HB2	1.77	0.65
1:A:33:PHE:HB2	1:A:271:ILE:HD13	1.78	0.65
11:K:404:VAL:HG11	11:K:483:ALA:HB1	1.79	0.64
11:K:913:THR:HG22	11:K:982:GLN:HG2	1.78	0.64
4:D:52:VAL:HG12	4:D:67:GLU:HG3	1.78	0.64
8:H:126:VAL:HG11	8:H:184:LEU:HD22	1.80	0.64
4:D:132:ALA:HB2	4:D:206:VAL:HG13	1.78	0.63
10:J:259:ARG:HE	10:J:370:LEU:HB3	1.63	0.63
4:D:147:VAL:HG11	4:D:201:LYS:HG3	1.79	0.62
11:K:911:GLU:OE2	11:K:984:ARG:NH1	2.33	0.62
3:C:50:ARG:NH1	3:C:335:ASP:OD2	2.32	0.62
11:K:336:SER:HB2	11:K:433:LYS:HG3	1.80	0.62
6:F:207:GLY:HA3	6:F:231:LYS:HE3	1.80	0.62
9:I:145:ARG:HB3	9:I:152:ASN:HB2	1.81	0.62
10:J:294:PHE:O	10:J:399:ARG:NH1	2.32	0.62
11:K:300:LEU:HB2	11:K:389:THR:HG22	1.82	0.62
5:E:94:THR:HG22	6:F:112:GLU:HA	1.82	0.62
11:K:426:LEU:HD21	11:K:451:ILE:HD11	1.81	0.62
3:C:86:ILE:HB	3:C:220:LEU:HB2	1.82	0.61
4:D:159:SER:HG	4:D:161:HIS:HE2	1.49	0.61
5:E:190:LEU:HB2	5:E:213:LEU:HB2	1.83	0.61
6:F:44:GLN:O	6:F:236:ARG:NH2	2.33	0.61
7:G:21:LEU:HA	7:G:25:ILE:HD11	1.81	0.61
10:J:195:GLU:O	10:J:200:ARG:NH1	2.32	0.61
1:A:243:ARG:NH1	16:A:502:HOH:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:173:HIS:HD2	5:E:176:ASP:H	1.49	0.61
2:B:92:LYS:HZ2	2:B:95:ARG:HD2	1.66	0.61
1:A:180:ASN:ND2	3:C:118:THR:O	2.34	0.60
6:F:203:PHE:HB3	6:F:207:GLY:HA2	1.83	0.60
11:K:179:GLN:NE2	11:K:208:GLU:OE1	2.34	0.60
10:J:213:PRO:HG3	10:J:363:ARG:HD2	1.84	0.60
11:K:115:GLN:HB2	11:K:149:HIS:HA	1.83	0.60
11:K:617:PRO:HA	11:K:648:SER:HB3	1.84	0.60
2:B:17:ARG:HH12	2:B:173:ASP:HB3	1.66	0.59
4:D:147:VAL:HG21	4:D:201:LYS:HE2	1.82	0.59
10:J:442:VAL:HG12	10:J:473:VAL:HG11	1.82	0.59
10:J:549:PHE:HA	10:J:552:LEU:HD23	1.84	0.59
5:E:102:VAL:HG12	5:E:225:PRO:HD2	1.83	0.59
10:J:539:VAL:H	10:J:540:PRO:HD2	1.68	0.59
10:J:208:TRP:HE3	10:J:367:HIS:HD1	1.50	0.59
10:J:545:VAL:HA	10:J:548:ARG:HD2	1.85	0.59
11:K:616:LYS:HD3	11:K:621:ARG:HH11	1.68	0.59
10:J:227:GLU:HA	10:J:230:LYS:HE2	1.85	0.58
11:K:918:VAL:HG12	11:K:928:VAL:HG22	1.85	0.58
2:B:172:LEU:HD11	2:B:216:ILE:HG22	1.84	0.58
5:E:210:ASN:HB3	5:E:237:LYS:HB2	1.86	0.58
7:G:69:ASN:OD1	7:G:122:ARG:NH2	2.33	0.58
1:A:82:GLU:OE1	4:D:53:ARG:NH2	2.37	0.58
9:I:25:ASN:ND2	9:I:30:ASP:OD1	2.37	0.57
9:I:205:ILE:HG12	9:I:245:LEU:HB2	1.86	0.57
11:K:469:ARG:NH2	11:K:482:GLU:OE2	2.36	0.57
10:J:298:ILE:HG23	10:J:401:PHE:HB2	1.86	0.57
4:D:136:ILE:HB	4:D:161:HIS:HB2	1.86	0.57
6:F:46:LEU:O	10:J:567:ASN:ND2	2.38	0.57
6:F:200:VAL:HB	6:F:214:TRP:HB3	1.87	0.57
11:K:49:SER:HA	11:K:72:LEU:HB2	1.86	0.57
11:K:847:ARG:NH1	12:M:17:A:OP2	2.38	0.57
1:A:166:ASP:OD2	11:K:493:ARG:NH1	2.35	0.56
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.86	0.56
10:J:192:TYR:HE1	10:J:394:ARG:HE	1.52	0.56
11:K:21:GLN:HE21	11:K:36:VAL:HB	1.71	0.56
6:F:21:SER:OG	6:F:24:THR:OG1	2.23	0.56
11:K:800:TYR:CZ	11:K:931:PRO:HB3	2.40	0.56
11:K:903:VAL:HG21	11:K:933:PHE:HB3	1.87	0.56
5:E:22:ARG:NH2	5:E:205:GLU:OE1	2.38	0.56
5:E:139:SER:HB2	5:E:189:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:107:GLU:HA	8:H:176:LEU:HD11	1.88	0.56
11:K:346:ASP:HB3	11:K:421:ASN:HD22	1.71	0.56
9:I:19:PRO:HA	9:I:55:ALA:HA	1.88	0.55
11:K:46:PRO:HG3	11:K:59:VAL:HG12	1.87	0.55
7:G:206:ALA:HB2	7:G:234:ILE:HD13	1.88	0.55
6:F:61:LEU:HD13	6:F:74:ILE:HG12	1.89	0.55
1:A:109:GLU:OE1	2:B:92:LYS:NZ	2.39	0.55
11:K:307:LEU:HD13	14:K:2004:GOL:H31	1.88	0.55
11:K:495:PHE:HD1	11:K:586:GLU:HG2	1.71	0.55
7:G:159:ASN:ND2	7:G:215:CYS:SG	2.80	0.54
2:B:208:ASP:N	2:B:208:ASP:OD1	2.40	0.54
3:C:222:ARG:H	6:F:55:ASN:HD21	1.55	0.54
9:I:258:ARG:HB3	9:I:262:GLY:HA2	1.89	0.54
8:H:334:GLU:O	8:H:340:VAL:HG21	2.07	0.54
11:K:641:PHE:HB2	11:K:862:ILE:HD11	1.89	0.54
7:G:94:SER:OG	12:L:8:U:O2	2.25	0.54
9:I:141:THR:HG22	9:I:155:ILE:HA	1.90	0.54
3:C:36:SER:OG	3:C:306:CYS:O	2.24	0.54
11:K:181:TYR:HB3	11:K:192:VAL:HG21	1.89	0.54
4:D:132:ALA:HB1	4:D:205:LEU:HD23	1.89	0.53
7:G:175:LEU:HD11	7:G:186:VAL:HG11	1.89	0.53
7:G:177:VAL:HG21	7:G:224:LYS:HA	1.91	0.53
4:D:212:ILE:O	4:D:216:ASN:ND2	2.40	0.53
11:K:89:VAL:HG22	11:K:112:ILE:HB	1.91	0.53
11:K:317:ILE:HB	11:K:394:TYR:HB3	1.91	0.53
5:E:110:ASP:OD2	5:E:110:ASP:N	2.42	0.53
8:H:171:ALA:HB3	8:H:184:LEU:HD23	1.90	0.53
2:B:166:TYR:HB2	2:B:182:MET:HE2	1.91	0.53
10:J:258:THR:HG23	10:J:260:GLU:H	1.73	0.53
10:J:409:LEU:H	10:J:409:LEU:HD23	1.73	0.52
5:E:96:THR:O	5:E:100:ASN:ND2	2.34	0.52
2:B:189:VAL:HG21	2:B:218:ILE:HA	1.91	0.52
2:B:3:ARG:NH2	16:B:401:HOH:O	2.37	0.52
4:D:142:THR:O	4:D:144:ASP:N	2.42	0.52
6:F:189:ASP:OD1	6:F:190:MET:N	2.42	0.52
3:C:183:GLY:O	3:C:185:PHE:N	2.42	0.52
7:G:209:ARG:NH1	13:G:301:SO4:O4	2.39	0.52
8:H:55:VAL:HG11	8:H:61:VAL:HG12	1.91	0.52
8:H:175:SER:OG	12:L:13:U:O4	2.27	0.52
7:G:213:GLU:OE2	7:G:229:ARG:NH2	2.43	0.52
11:K:143:LYS:HD2	11:K:145:PHE:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LEU:HD21	3:C:213:LEU:HD12	1.91	0.51
11:K:91:ASP:HB3	11:K:196:THR:HG22	1.92	0.51
11:K:704:HIS:NE2	11:K:716:GLU:OE1	2.38	0.51
3:C:180:ASN:HD21	3:C:183:GLY:HA3	1.76	0.51
5:E:154:LEU:HD13	5:E:180:LEU:HB2	1.93	0.51
8:H:195:ARG:NH1	8:H:280:ILE:O	2.43	0.51
10:J:181:HIS:HB2	10:J:400:ARG:HB2	1.92	0.51
11:K:699:PRO:HG3	11:K:807:ILE:HD13	1.92	0.51
11:K:548:VAL:HB	11:K:610:THR:HG23	1.93	0.51
2:B:225:ARG:NH2	2:B:226:ASP:OD1	2.44	0.50
5:E:236:VAL:HG12	6:F:123:SER:HB2	1.94	0.50
11:K:97:GLN:NE2	11:K:236:PRO:O	2.43	0.50
1:A:112:VAL:HA	1:A:117:ALA:HB3	1.92	0.50
1:A:291:ASN:HB3	1:A:294:ALA:HB2	1.93	0.50
8:H:206:LEU:HD21	8:H:311:GLU:HA	1.91	0.50
10:J:226:LEU:HD23	10:J:277:LEU:HD23	1.93	0.50
11:K:918:VAL:HG22	11:K:977:ASP:H	1.76	0.50
3:C:39:ILE:HG12	3:C:40:ARG:H	1.77	0.50
4:D:135:PRO:HG2	4:D:148:ASP:HA	1.93	0.50
11:K:20:THR:HG23	11:K:39:HIS:HB3	1.93	0.50
2:B:61:LEU:HG	2:B:63:SER:H	1.77	0.50
5:E:265:LEU:HD23	8:H:9:LYS:HD3	1.93	0.50
10:J:478:THR:O	10:J:506:ARG:NE	2.45	0.50
3:C:345:SER:HB2	3:C:366:GLY:H	1.77	0.50
11:K:448:ARG:HH21	11:K:474:ILE:HG23	1.77	0.50
11:K:749:THR:O	11:K:857:GLN:NE2	2.45	0.50
2:B:185:VAL:HG22	2:B:201:VAL:HG22	1.94	0.49
4:D:106:LEU:H	4:D:106:LEU:HD23	1.77	0.49
8:H:150:ARG:HB3	8:H:151:LYS:HA	1.93	0.49
10:J:222:LEU:HD12	10:J:270:LEU:HG	1.94	0.49
3:C:335:ASP:OD1	3:C:336:THR:N	2.43	0.49
2:B:18:ARG:HH11	11:K:42:ARG:HH21	1.59	0.49
1:A:125:ILE:HA	14:A:403:GOL:H32	1.95	0.49
2:B:145:LEU:HD21	2:B:228:MET:HB3	1.93	0.49
11:K:489:ASP:O	11:K:887:LYS:NZ	2.45	0.49
3:C:348:SER:OG	3:C:361:THR:OG1	2.30	0.49
3:C:349:ILE:HD13	3:C:378:LEU:HD23	1.93	0.49
11:K:568:VAL:HG21	11:K:734:ALA:HB2	1.94	0.49
3:C:177:ARG:HB2	3:C:187:VAL:HG22	1.94	0.49
11:K:715:VAL:HG21	11:K:903:VAL:HG23	1.94	0.49
3:C:349:ILE:HG12	3:C:360:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:180:LEU:HB3	6:F:187:LEU:HD11	1.95	0.49
4:D:145:ILE:HD13	4:D:194:LEU:HB3	1.95	0.48
7:G:122:ARG:NH1	7:G:135:GLU:OE1	2.46	0.48
5:E:228:SER:OG	6:F:213:PHE:N	2.44	0.48
8:H:299:ARG:NH1	8:H:330:SER:O	2.46	0.48
10:J:222:LEU:HD11	10:J:274:LEU:HD23	1.96	0.48
10:J:331:LEU:HB3	10:J:372:ILE:HD13	1.95	0.48
6:F:44:GLN:HG3	6:F:66:SER:HB3	1.96	0.48
11:K:834:LEU:HD23	14:K:2005:GOL:H12	1.96	0.48
1:A:7:ILE:HG21	1:A:230:LEU:HD21	1.96	0.48
7:G:95:VAL:HG12	7:G:132:ALA:HB3	1.95	0.48
3:C:54:ILE:HB	3:C:78:ASN:HD21	1.77	0.48
5:E:52:ALA:HB3	5:E:56:SER:HB2	1.95	0.48
10:J:211:SER:OG	10:J:363:ARG:NH2	2.43	0.48
14:K:2005:GOL:H31	12:M:14:A:H1'	1.95	0.48
11:K:851:ASP:N	11:K:851:ASP:OD1	2.47	0.48
9:I:267:MET:HB3	9:I:275:MET:HG2	1.95	0.48
5:E:98:LEU:HD23	5:E:138:VAL:HG21	1.95	0.47
6:F:206:ASN:OD1	6:F:238:ARG:NH2	2.46	0.47
8:H:63:ASP:N	8:H:63:ASP:OD1	2.47	0.47
10:J:488:ASN:N	10:J:488:ASN:OD1	2.41	0.47
3:C:61:ARG:HG3	3:C:72:ASN:HB3	1.95	0.47
7:G:80:PHE:HE2	7:G:85:LYS:HB2	1.80	0.47
11:K:539:ILE:HG12	11:K:555:HIS:HB3	1.97	0.47
1:A:303:ARG:NH1	11:K:596:LEU:O	2.42	0.47
1:A:167:ILE:HG23	1:A:174:ILE:HG23	1.97	0.47
6:F:70:GLN:O	6:F:145:LYS:N	2.48	0.47
9:I:216:ASP:OD2	9:I:217:ARG:N	2.48	0.47
7:G:130:LEU:HD11	9:I:221:ILE:HB	1.95	0.47
11:K:23:VAL:HG22	11:K:36:VAL:HG12	1.96	0.47
5:E:122:PHE:CD2	5:E:154:LEU:HD23	2.50	0.47
9:I:203:GLY:HA2	9:I:243:TYR:H	1.79	0.47
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.30	0.47
9:I:239:ASP:N	9:I:239:ASP:OD1	2.46	0.47
6:F:135:ILE:HD13	6:F:185:ILE:HD13	1.96	0.46
6:F:70:GLN:HB3	6:F:145:LYS:HB3	1.98	0.46
3:C:103:ILE:HD12	3:C:115:PHE:HB2	1.97	0.46
5:E:102:VAL:HG23	5:E:103:LEU:HG	1.96	0.46
5:E:169:LEU:H	5:E:169:LEU:HD12	1.81	0.46
10:J:155:LYS:HG2	10:J:158:ALA:HB2	1.96	0.46
11:K:52:CYS:HA	11:K:188:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:138:VAL:HG12	5:E:189:ILE:HD11	1.96	0.46
11:K:794:VAL:HG23	11:K:802:ASN:HB2	1.96	0.46
5:E:212:GLY:HA3	5:E:231:LEU:HD13	1.98	0.46
10:J:164:GLU:HB2	10:J:167:ARG:HH12	1.81	0.46
10:J:170:ASP:HB3	10:J:177:SER:HB3	1.98	0.46
11:K:820:TYR:CZ	11:K:823:ALA:HB2	2.51	0.46
9:I:150:ARG:HH12	12:L:7:U:H3'	1.81	0.46
4:D:140:LYS:HA	4:D:158:LEU:HG	1.98	0.46
11:K:667:ASN:HA	11:K:672:MET:HE3	1.99	0.45
11:K:703:VAL:HG12	11:K:715:VAL:HG13	1.98	0.45
3:C:347:ILE:HG12	3:C:362:LEU:HD12	1.98	0.45
8:H:290:SER:HB2	8:H:293:ILE:HD13	1.97	0.45
11:K:834:LEU:HD21	12:M:14:A:H4'	1.99	0.45
4:D:42:LEU:HG	4:D:47:ALA:HB2	1.99	0.45
4:D:66:LEU:HD11	4:D:109:LEU:HB2	1.99	0.45
9:I:267:MET:HG2	9:I:277:SER:HB2	1.99	0.45
10:J:183:TYR:CD1	10:J:186:GLU:HG3	2.52	0.45
1:A:35:ASP:HA	14:A:402:GOL:H32	1.98	0.45
11:K:615:LEU:HD22	11:K:646:ILE:HD11	1.99	0.45
4:D:176:ASN:OD1	4:D:177:VAL:N	2.48	0.45
2:B:58:GLU:HG3	8:H:133:HIS:CG	2.51	0.45
10:J:501:LEU:O	10:J:505:ILE:HG22	2.16	0.45
10:J:479:ASP:OD1	10:J:479:ASP:N	2.50	0.45
5:E:174:ASP:N	5:E:174:ASP:OD1	2.50	0.45
10:J:183:TYR:HD1	10:J:186:GLU:HG3	1.82	0.44
11:K:485:LEU:HD21	11:K:596:LEU:HD21	1.99	0.44
5:E:10:TYR:HD1	5:E:11:LEU:HD22	1.82	0.44
6:F:61:LEU:HD22	10:J:576:LEU:HD12	1.98	0.44
2:B:49:ILE:HD13	2:B:139:LEU:HD23	1.99	0.44
10:J:265:VAL:HG11	10:J:274:LEU:HD21	1.99	0.44
4:D:9:ILE:HG13	4:D:10:LEU:HG	1.99	0.44
3:C:39:ILE:HD12	10:J:602:ARG:HB3	2.00	0.44
11:K:654:TYR:O	11:K:723:THR:HG21	2.17	0.44
2:B:166:TYR:OH	11:K:415:GLN:NE2	2.51	0.44
2:B:192:LYS:HE2	2:B:225:ARG:NH2	2.32	0.44
4:D:197:LEU:O	4:D:201:LYS:HG2	2.18	0.44
7:G:156:ILE:HG12	7:G:208:TYR:HD2	1.82	0.44
11:K:166:ILE:H	11:K:166:ILE:HD12	1.83	0.44
11:K:914:GLU:HG3	11:K:933:PHE:CE2	2.52	0.44
3:C:222:ARG:NH2	3:C:340:GLU:OE2	2.51	0.44
11:K:298:PRO:O	11:K:387:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:167:ASP:HB3	8:H:193:LYS:HE3	1.99	0.44
11:K:527:LEU:HD23	11:K:864:TYR:CE1	2.53	0.44
11:K:915:THR:HG22	11:K:980:GLU:HG2	2.00	0.44
11:K:346:ASP:HB3	11:K:421:ASN:ND2	2.32	0.43
3:C:136:VAL:HG11	3:C:222:ARG:HD2	2.00	0.43
4:D:187:ASN:OD1	4:D:190:GLN:HG3	2.19	0.43
5:E:148:ALA:O	5:E:152:THR:OG1	2.35	0.43
3:C:29:LEU:HD13	9:I:266:LEU:HD21	1.99	0.43
11:K:538:LEU:HD23	11:K:670:LEU:HB2	2.00	0.43
11:K:628:TRP:HD1	11:K:639:VAL:HG22	1.83	0.43
11:K:676:ALA:HA	11:K:679:LYS:HG2	2.01	0.43
3:C:184:THR:HG22	3:C:185:PHE:CD2	2.53	0.43
3:C:154:LYS:HE2	3:C:154:LYS:HB3	1.89	0.43
9:I:32:ILE:HD13	10:J:542:ILE:HG13	2.00	0.43
11:K:289:SER:HB2	11:K:298:PRO:HB2	2.00	0.43
11:K:493:ARG:O	11:K:590:ARG:NH2	2.52	0.43
1:A:20:ARG:HD3	1:A:203:PRO:HB3	2.01	0.43
2:B:80:LYS:HG2	2:B:80:LYS:H	1.68	0.43
6:F:95:ILE:HA	6:F:137:ILE:HB	2.00	0.43
2:B:17:ARG:NH1	2:B:23:ARG:HG3	2.33	0.43
11:K:347:ILE:HG23	11:K:461:LYS:HB3	2.00	0.43
2:B:112:VAL:HG22	2:B:154:MET:HG2	2.01	0.43
2:B:178:GLU:O	2:B:182:MET:HG2	2.19	0.43
4:D:75:THR:HB	4:D:76:PRO:HD3	2.01	0.43
11:K:288:GLY:O	11:K:301:ILE:N	2.50	0.43
11:K:903:VAL:HG11	11:K:935:VAL:HG11	2.01	0.43
3:C:245:ARG:O	3:C:277:ASP:N	2.44	0.43
5:E:102:VAL:O	5:E:185:PRO:HG2	2.19	0.43
8:H:150:ARG:NH1	8:H:151:LYS:HG2	2.34	0.43
5:E:31:PHE:HB2	8:H:5:ILE:HG12	1.99	0.43
11:K:773:ARG:HD2	11:K:773:ARG:HA	1.80	0.43
1:A:163:LYS:HB3	1:A:184:PRO:HB2	2.01	0.42
3:C:141:VAL:HG12	6:F:96:GLN:HE22	1.84	0.42
11:K:825:SER:OG	11:K:828:ASP:OD2	2.37	0.42
11:K:661:ILE:HG23	11:K:675:ARG:HD3	2.01	0.42
5:E:211:ASN:OD1	5:E:212:GLY:N	2.45	0.42
8:H:123:ARG:NH2	12:L:11:U:OP2	2.52	0.42
9:I:233:GLN:OE1	9:I:249:ARG:NH1	2.52	0.42
3:C:168:LYS:HA	3:C:171:LYS:HE3	2.01	0.42
3:C:299:ILE:HG22	3:C:367:ALA:HB3	2.00	0.42
11:K:475:GLU:OE1	11:K:908:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:576:LEU:HB2	10:J:577:PRO:HD3	2.01	0.42
11:K:264:VAL:HA	11:K:273:LEU:HD12	2.02	0.42
3:C:54:ILE:HG21	3:C:236:TYR:CD2	2.55	0.42
4:D:153:GLN:O	4:D:157:SER:OG	2.28	0.42
8:H:217:LEU:HD13	8:H:300:TYR:CE1	2.55	0.42
10:J:252:CYS:O	10:J:352:ARG:NH2	2.53	0.42
5:E:103:LEU:HD11	5:E:145:ILE:HD13	2.01	0.42
7:G:84:TYR:CZ	7:G:113:LEU:HB2	2.55	0.42
5:E:264:ASN:HB3	8:H:9:LYS:HZ2	1.85	0.42
11:K:499:VAL:HG13	11:K:583:LEU:HD13	2.01	0.42
3:C:275:ILE:HG21	6:F:21:SER:HB3	2.01	0.42
6:F:46:LEU:HD23	6:F:240:LEU:HD23	2.00	0.42
10:J:342:LYS:HD2	10:J:361:TYR:HE1	1.84	0.42
1:A:193:PRO:HB3	1:A:246:VAL:HG21	2.02	0.41
1:A:28:ARG:NH2	1:A:34:ARG:HG3	2.35	0.41
9:I:20:GLN:HG3	9:I:21:TYR:CD2	2.54	0.41
9:I:237:LEU:HD12	9:I:237:LEU:H	1.85	0.41
3:C:38:GLY:HA2	3:C:46:TYR:CZ	2.55	0.41
5:E:117:THR:HG22	5:E:118:LYS:H	1.83	0.41
3:C:86:ILE:HD13	10:J:576:LEU:HD22	2.02	0.41
11:K:202:ARG:HG2	11:K:215:THR:HB	2.02	0.41
11:K:718:LYS:HD2	11:K:718:LYS:HA	1.89	0.41
3:C:297:TYR:HD1	3:C:332:ALA:HA	1.85	0.41
11:K:568:VAL:HG13	11:K:628:TRP:HZ3	1.85	0.41
11:K:801:PHE:HE1	11:K:976:PHE:HB3	1.84	0.41
2:B:71:LEU:HB2	2:B:121:VAL:HG23	2.02	0.41
11:K:326:TRP:CD2	11:K:388:PRO:HA	2.55	0.41
11:K:711:ASP:HB2	11:K:712:PRO:HD3	2.02	0.41
10:J:412:SER:HB3	10:J:415:VAL:HG12	2.03	0.41
2:B:13:ARG:NH2	2:B:172:LEU:O	2.48	0.41
10:J:408:PRO:HG2	10:J:415:VAL:HG11	2.03	0.41
11:K:333:VAL:HG11	11:K:938:LEU:HD21	2.03	0.41
7:G:127:GLU:HB2	7:G:130:LEU:HB2	2.02	0.41
9:I:147:SER:HB3	9:I:150:ARG:HG2	2.01	0.41
11:K:448:ARG:NE	11:K:480:GLU:OE2	2.52	0.41
11:K:692:GLY:HA2	11:K:784:LYS:HB2	2.02	0.41
2:B:107:MET:HE2	2:B:198:LEU:HD13	2.03	0.41
6:F:236:ARG:NH1	16:F:401:HOH:O	2.54	0.41
8:H:120:GLY:HA3	8:H:123:ARG:CZ	2.51	0.41
2:B:229:ASP:O	2:B:233:ARG:HG2	2.21	0.41
6:F:57:ASN:OD1	6:F:57:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:174:GLN:N	8:H:183:SER:O	2.47	0.41
8:H:207:ILE:HG21	8:H:227:VAL:HA	2.03	0.41
6:F:103:GLU:HB3	6:F:144:ASP:HB3	2.03	0.41
10:J:170:ASP:N	10:J:170:ASP:OD1	2.53	0.41
9:I:21:TYR:HB3	10:J:542:ILE:HD12	2.02	0.41
1:A:58:CYS:HB2	1:A:154:ALA:HB1	2.03	0.40
3:C:89:THR:HG23	3:C:217:ILE:HG12	2.02	0.40
8:H:186:THR:HG23	8:H:191:TYR:HB2	2.03	0.40
11:K:671:THR:O	11:K:675:ARG:HG2	2.21	0.40
3:C:131:TYR:CZ	6:F:12:PRO:HD3	2.55	0.40
8:H:121:ASN:O	8:H:123:ARG:HG3	2.21	0.40
10:J:229:LEU:HB3	10:J:280:VAL:HG11	2.04	0.40
10:J:506:ARG:O	10:J:510:ARG:HG2	2.21	0.40
11:K:257:GLU:HG2	11:K:458:THR:HG21	2.04	0.40
3:C:350:LEU:HD12	3:C:359:GLN:HB3	2.03	0.40
3:C:359:GLN:HE21	3:C:359:GLN:HB3	1.65	0.40
1:A:89:SER:HB2	7:G:91:PHE:CD2	2.56	0.40
8:H:72:GLY:N	14:H:401:GOL:H31	2.36	0.40
11:K:845:PRO:HG3	11:K:855:HIS:NE2	2.37	0.40
1:A:28:ARG:CZ	1:A:34:ARG:HG3	2.51	0.40
2:B:13:ARG:HD3	2:B:171:LEU:HD22	2.03	0.40
4:D:164:ALA:HB3	4:D:179:LEU:HB3	2.04	0.40
4:D:169:ASN:ND2	7:G:10:SER:HB3	2.37	0.40
10:J:254:MET:HB3	10:J:265:VAL:HB	2.03	0.40
11:K:160:ARG:NH2	11:K:164:GLU:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	286/305 (94%)	277 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	237/250 (95%)	226 (95%)	11 (5%)	0	100	100
3	C	332/394 (84%)	306 (92%)	25 (8%)	1 (0%)	44	79
4	D	219/225 (97%)	211 (96%)	7 (3%)	1 (0%)	32	71
5	E	255/269 (95%)	240 (94%)	14 (6%)	1 (0%)	38	75
6	F	209/250 (84%)	190 (91%)	19 (9%)	0	100	100
7	G	228/244 (93%)	216 (95%)	12 (5%)	0	100	100
8	H	283/363 (78%)	266 (94%)	16 (6%)	1 (0%)	38	75
9	I	216/296 (73%)	201 (93%)	15 (7%)	0	100	100
10	J	459/559 (82%)	438 (95%)	20 (4%)	1 (0%)	51	84
11	K	945/1003 (94%)	900 (95%)	44 (5%)	1 (0%)	55	88
All	All	3669/4158 (88%)	3471 (95%)	192 (5%)	6 (0%)	51	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	184	THR
11	K	711	ASP
4	D	143	SER
8	H	152	SER
10	J	539	VAL
5	E	19	PRO

### 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	252/266 (95%)	251 (100%)	1 (0%)	93	97
2	B	213/221 (96%)	213 (100%)	0	100	100
3	C	299/349 (86%)	297 (99%)	2 (1%)	87	95
4	D	195/198 (98%)	194 (100%)	1 (0%)	91	96
5	E	235/243 (97%)	234 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	185/219 (84%)	182 (98%)	3 (2%)	68	89
7	G	202/212 (95%)	202 (100%)	0	100	100
8	H	248/314 (79%)	247 (100%)	1 (0%)	93	97
9	I	187/243 (77%)	187 (100%)	0	100	100
10	J	431/516 (84%)	429 (100%)	2 (0%)	91	96
11	K	857/903 (95%)	855 (100%)	2 (0%)	94	98
All	All	3304/3684 (90%)	3291 (100%)	13 (0%)	93	97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	PHE
3	C	163	ARG
3	C	359	GLN
4	D	140	LYS
5	E	174	ASP
6	F	57	ASN
6	F	126	ASN
6	F	129	ARG
8	H	209	ARG
10	J	260	GLU
10	J	409	LEU
11	K	624	PHE
11	K	851	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	278	GLN
3	C	67	ASN
3	C	278	GLN
3	C	359	GLN
4	D	86	GLN
5	E	173	HIS
6	F	55	ASN
6	F	96	GLN
6	F	126	ASN
7	G	159	ASN

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Mol	Chain	Res	Type
8	H	291	ASN
9	I	125	ASN
9	I	242	ASN
10	J	395	ASN
10	J	496	GLN
11	K	21	GLN
11	K	275	GLN
11	K	279	GLN
11	K	315	GLN
11	K	387	GLN
11	K	415	GLN
11	K	667	ASN
11	K	923	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	L	16/17 (94%)	4 (25%)	0
12	M	6/17 (35%)	2 (33%)	0
All	All	22/34 (64%)	6 (27%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	M	12	U
12	M	17	A
12	L	4	U
12	L	8	U
12	L	10	U
12	L	13	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.06	0
14	GOL	A	402	-	5,5,5	0.34	0	5,5,5	0.24	0
14	GOL	A	403	-	5,5,5	0.36	0	5,5,5	0.25	0
14	GOL	A	404	-	5,5,5	0.34	0	5,5,5	0.25	0
13	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.05	0
14	GOL	B	302	-	5,5,5	0.34	0	5,5,5	0.27	0
13	SO4	D	301	-	4,4,4	0.15	0	6,6,6	0.06	0
13	SO4	E	301	-	4,4,4	0.15	0	6,6,6	0.05	0
13	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.06	0
13	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.05	0
14	GOL	H	401	-	5,5,5	0.35	0	5,5,5	0.23	0
13	SO4	I	301	-	4,4,4	0.15	0	6,6,6	0.06	0
13	SO4	K	2002	-	4,4,4	0.14	0	6,6,6	0.06	0
13	SO4	K	2003	-	4,4,4	0.14	0	6,6,6	0.06	0
14	GOL	K	2004	-	5,5,5	0.35	0	5,5,5	0.22	0
14	GOL	K	2005	-	5,5,5	0.35	0	5,5,5	0.19	0
13	SO4	M	101	-	4,4,4	0.15	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SO4	A	401	-	-	0/0/0/0	0/0/0/0
14	GOL	A	402	-	-	0/4/4/4	0/0/0/0
14	GOL	A	403	-	-	0/4/4/4	0/0/0/0
14	GOL	A	404	-	-	0/4/4/4	0/0/0/0
13	SO4	B	301	-	-	0/0/0/0	0/0/0/0
14	GOL	B	302	-	-	0/4/4/4	0/0/0/0
13	SO4	D	301	-	-	0/0/0/0	0/0/0/0
13	SO4	E	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SO4	F	301	-	-	0/0/0/0	0/0/0/0
13	SO4	G	301	-	-	0/0/0/0	0/0/0/0
14	GOL	H	401	-	-	0/4/4/4	0/0/0/0
13	SO4	I	301	-	-	0/0/0/0	0/0/0/0
13	SO4	K	2002	-	-	0/0/0/0	0/0/0/0
13	SO4	K	2003	-	-	0/0/0/0	0/0/0/0
14	GOL	K	2004	-	-	0/4/4/4	0/0/0/0
14	GOL	K	2005	-	-	0/4/4/4	0/0/0/0
13	SO4	M	101	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	402	GOL	1	0
14	A	403	GOL	1	0
13	G	301	SO4	1	0
14	H	401	GOL	1	0
14	K	2004	GOL	1	0
14	K	2005	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.





























## 5.8 Polymer linkage issues [i](#)

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	290/305 (95%)	-0.17	0  	28, 47, 83, 114	0
2	B	239/250 (95%)	-0.01	0  	25, 50, 102, 137	0
3	C	340/394 (86%)	0.06	1 (0%)  	50, 83, 127, 173	0
4	D	221/225 (98%)	-0.11	1 (0%)  	36, 59, 87, 121	0
5	E	259/269 (96%)	-0.01	3 (1%)  	43, 91, 125, 145	0
6	F	215/250 (86%)	0.27	5 (2%)  	62, 99, 144, 162	0
7	G	232/244 (95%)	-0.03	2 (0%)  	36, 62, 119, 157	0
8	H	289/363 (79%)	0.20	8 (2%)  	48, 104, 147, 181	0
9	I	224/296 (75%)	0.76	22 (9%)  	55, 114, 171, 194	0
10	J	467/559 (83%)	-0.00	4 (0%)  	50, 84, 160, 183	0
11	K	955/1003 (95%)	-0.02	4 (0%)  	30, 65, 124, 163	0
12	L	17/17 (100%)	0.52	0  	65, 128, 149, 166	0
12	M	7/17 (41%)	-0.09	0  	61, 63, 86, 116	0
All	All	3755/4192 (89%)	0.05	50 (1%)  	25, 75, 141, 194	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	25	ASN	4.1
9	I	109	SER	3.9
9	I	106	ILE	3.6
6	F	103	GLU	3.5
9	I	21	TYR	3.2
8	H	152	SER	3.1
9	I	24	GLU	3.1
6	F	8	ARG	3.0
8	H	243	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	265	LEU	2.9
11	K	985	SER	2.8
9	I	108	VAL	2.8
9	I	66	CYS	2.8
9	I	231	ARG	2.8
10	J	505	ILE	2.8
6	F	102	LEU	2.8
9	I	33	PHE	2.6
5	E	21	ILE	2.6
9	I	23	THR	2.6
10	J	617	ILE	2.6
8	H	334	GLU	2.6
11	K	381	GLN	2.6
8	H	353	LYS	2.6
7	G	1	MET	2.5
8	H	225	LEU	2.5
9	I	104	LYS	2.5
10	J	616	ILE	2.4
9	I	48	HIS	2.4
9	I	9	GLU	2.4
8	H	147	ILE	2.4
9	I	233	GLN	2.3
6	F	46	LEU	2.3
9	I	210	VAL	2.2
8	H	190	LYS	2.2
9	I	6	GLN	2.2
9	I	35	TYR	2.2
9	I	62	GLY	2.2
3	C	14	PRO	2.2
5	E	1	MET	2.2
9	I	196	ASP	2.1
10	J	610	LEU	2.1
9	I	201	PHE	2.1
9	I	22	GLY	2.1
6	F	184	GLY	2.1
9	I	215	ARG	2.1
8	H	233	LEU	2.1
11	K	933	PHE	2.0
7	G	52	VAL	2.0
4	D	145	ILE	2.0
11	K	713	ASN	2.0



## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	GOL	B	302	6/6	0.88	0.40	10.89	68,72,79,90	0
13	SO4	G	301	5/5	0.85	0.46	6.24	105,105,132,150	0
14	GOL	A	404	6/6	0.86	0.36	4.46	81,85,87,92	0
14	GOL	A	402	6/6	0.95	0.35	3.14	57,63,81,87	0
14	GOL	K	2004	6/6	0.92	0.34	3.13	45,59,75,76	0
14	GOL	A	403	6/6	0.90	0.28	2.54	56,66,78,80	0
14	GOL	H	401	6/6	0.92	0.32	2.43	55,75,90,92	0
14	GOL	K	2005	6/6	0.94	0.31	0.66	58,66,83,90	0
13	SO4	M	101	5/5	0.91	0.22	-0.23	95,102,122,122	0
13	SO4	A	401	5/5	0.99	0.19	-0.68	45,54,64,66	0
13	SO4	D	301	5/5	0.94	0.17	-0.75	82,86,114,127	0
13	SO4	K	2003	5/5	0.92	0.19	-0.86	84,88,113,113	0
13	SO4	I	301	5/5	0.90	0.20	-1.18	109,120,154,155	0
13	SO4	B	301	5/5	0.95	0.14	-3.82	98,99,127,134	0
13	SO4	F	301	5/5	0.89	0.19	-	107,147,152,155	0
13	SO4	K	2002	5/5	0.85	0.14	-	98,104,145,151	0
13	SO4	E	301	5/5	0.78	0.12	-	124,141,148,155	0
15	ZN	K	2001	1/1	1.00	0.20	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.