Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 11:22 AM EDT

PDB ID	:	5VZJ
Title	:	STRUCTURE OF A TWELVE COMPONENT MPP6-NUCLEAR RNA EXOSOME COMPLEX BOUND TO RNA
Authors	:	Lima, C.D.; Wasmuth, E.V.
Deposited on	:	2017-05-28
Resolution	:	3.30 Å(reported)

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

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

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

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

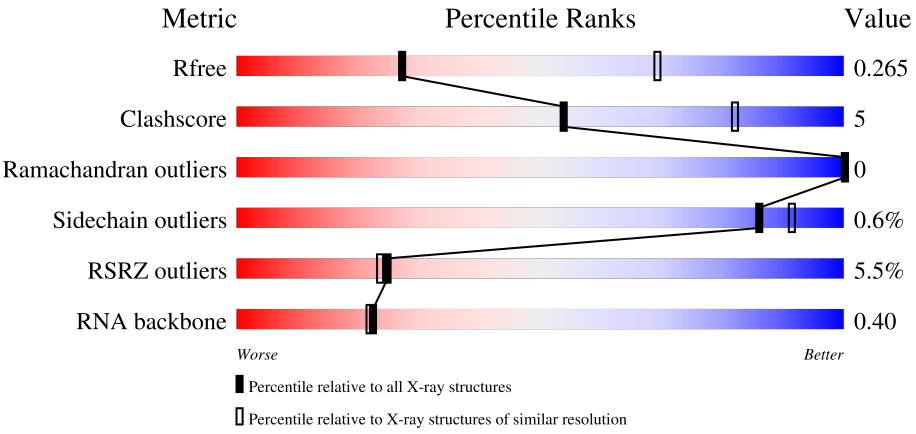
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	3% 87% 12%
2	B	250	% 81% 15%
3	C	394	8% 66% 10% 24%
4	D	225	3% 77% 21%

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Mol	Chain	Length	Quality of chain
5	E	269	4% 80% 15%
6	F	250	5% 68% 15% 17%
7	G	244	5% 81% 16%
8	H	363	9% 71% 9% 20%
9	I	296	14% 58% 11% 30%
10	J	559	4% 71% 11% 18%
11	K	1003	2% 82% 13% 5%
12	L	42	7% 64% 31%
13	M	11	9% 27% 18% 55%
14	N	19	11% 21% 16% 63%

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
15	SO4	G	302	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 29498 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	302	Total	C	N	O	S	0	0	0
			2350	1473	401	459	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1896	1186	338	363	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	299	Total	C	N	O	S	0	0	0
			2325	1482	397	436	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	222	Total	C	N	O	S	0	0	0
			1698	1068	288	333	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	257	Total	C	N	O	S	0	0	0
			1979	1262	328	385	4			

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	207	Total	C	N	O	S	0	0	0
			1589	998	265	316	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	236	Total	C	N	O	S	0	0	0
			1831	1169	302	349	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	291	Total	C	N	O	S	0	0	0
			2249	1411	401	425	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	207	Total	C	N	O	S	0	0	0
			1579	986	285	301	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	460	Total	C	N	O	S	0	0	0
			3784	2412	653	709	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	956	Total	C	N	O	S	0	0	0
			7645	4834	1345	1430	36			

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 protein called M-phase phosphoprotein 6 homolog.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	29	Total	C	N	O	0	0	0
			222	139	40	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	79	GLY	-	expression tag	UNP P53725
L	80	SER	-	expression tag	UNP P53725

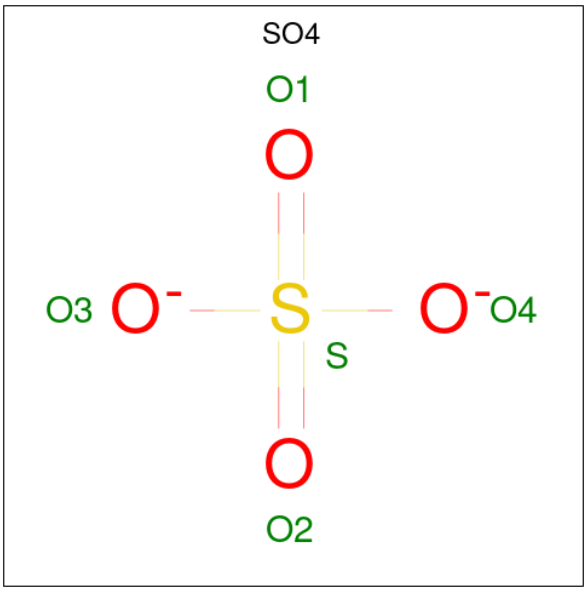
- Molecule 13 is a RNA chain called RNA (11-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	5	Total	C	N	O	P	0	0	0
			101	45	21	30	5			

- Molecule 14 is a RNA chain called RNA (19-MER).

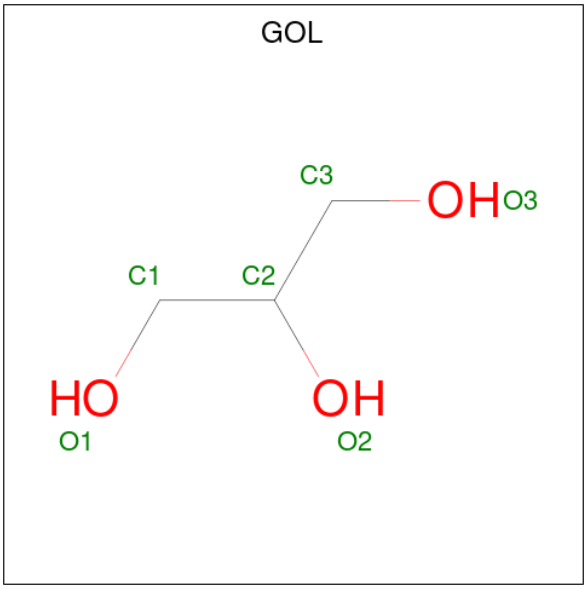
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	7	Total	C	N	O	P	0	0	0
			148	67	26	48	7			

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total O S 5 4 1	0	0
15	B	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	G	1	Total O S 5 4 1	0	0
15	K	1	Total O S 5 4 1	0	0

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

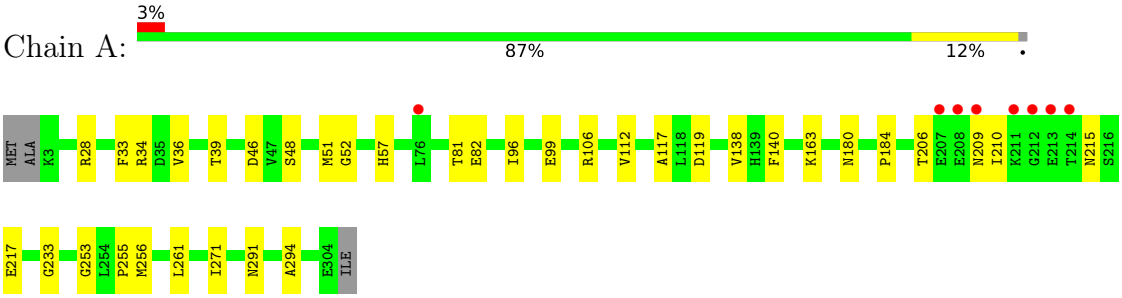
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	16	Total O 16 16	0	0
18	B	17	Total O 17 17	0	0
18	D	5	Total O 5 5	0	0
18	E	1	Total O 1 1	0	0
18	G	2	Total O 2 2	0	0
18	H	3	Total O 3 3	0	0
18	J	2	Total O 2 2	0	0
18	K	18	Total O 18 18	0	0

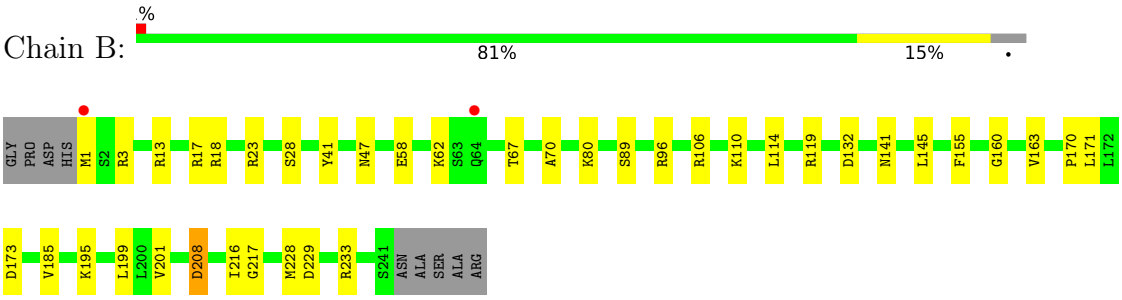
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

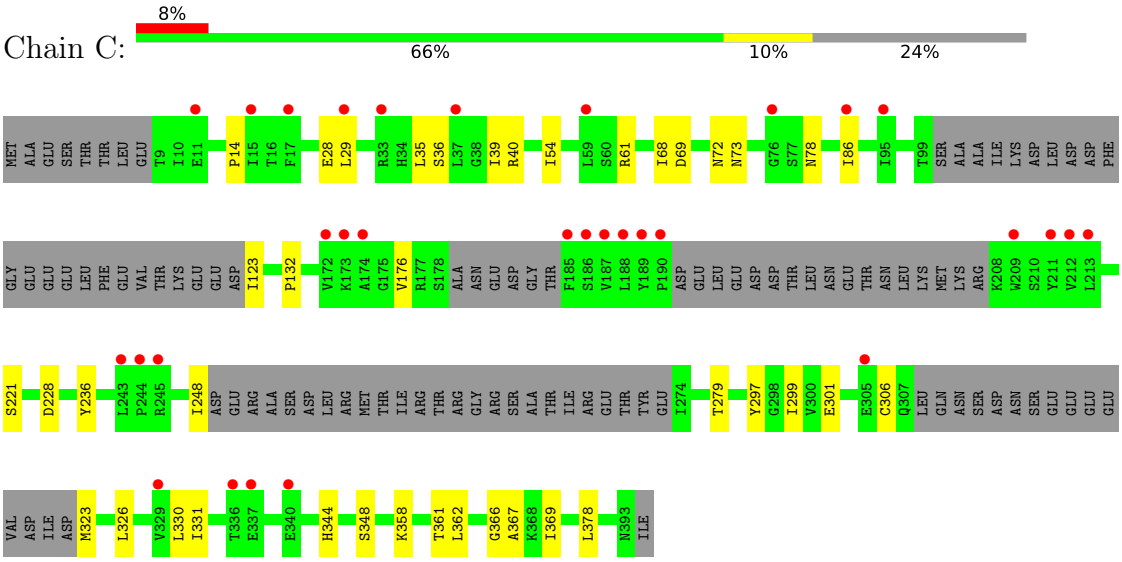
• Molecule 1: Exosome complex component RRP45



• Molecule 2: Exosome complex component SKI6

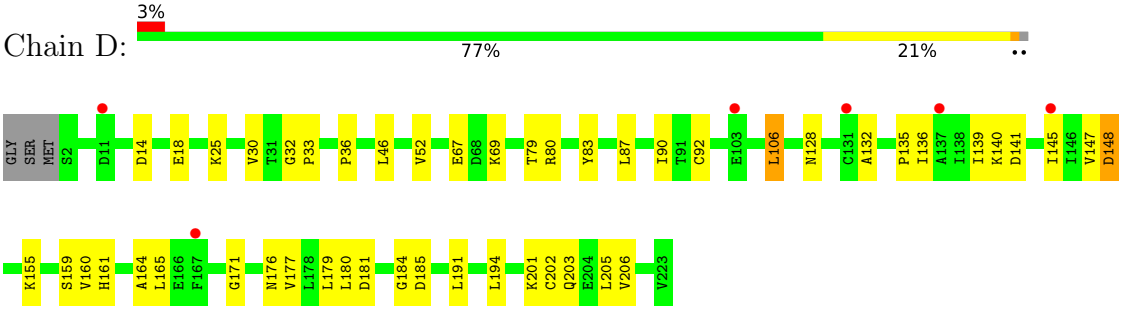


• Molecule 3: Exosome complex component RRP43



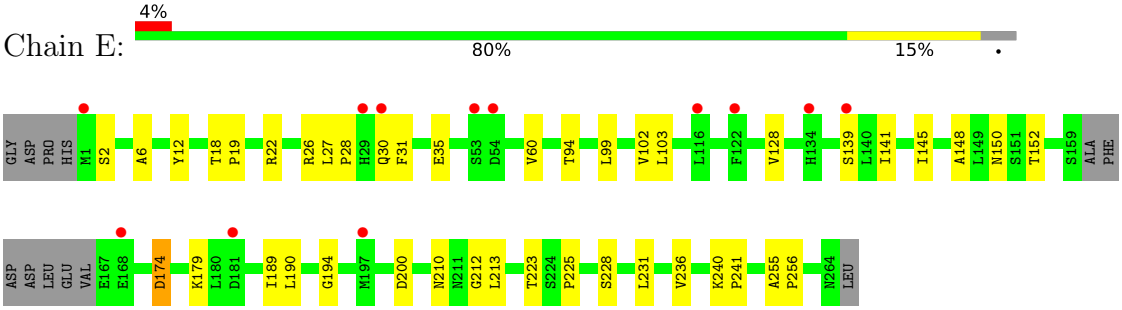
• Molecule 4: Exosome complex component RRP46

Chain D:



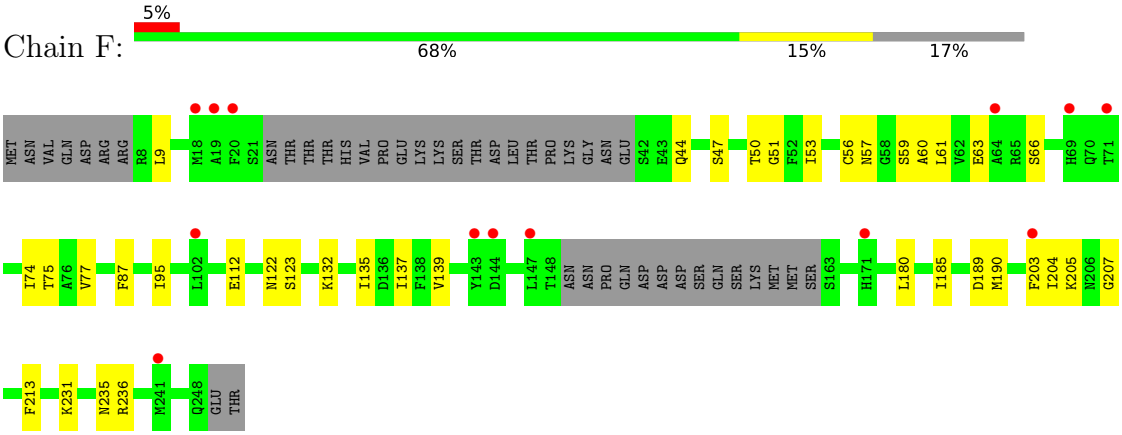
• Molecule 5: Exosome complex component RRP42

Chain E:



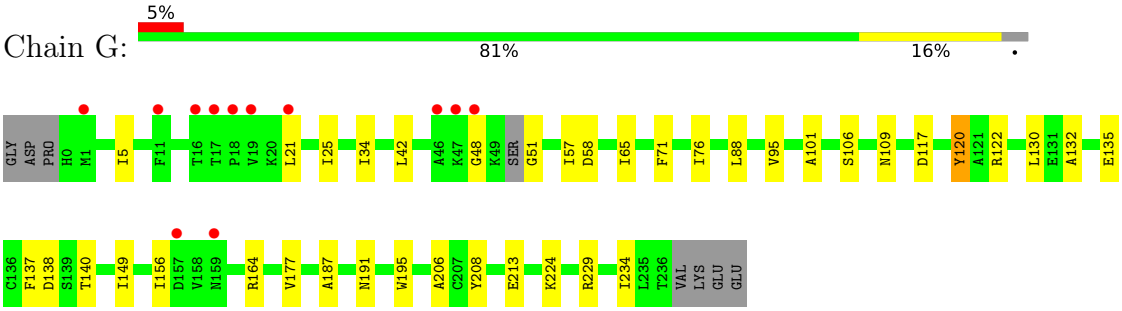
• Molecule 6: Exosome complex component MTR3

Chain F:



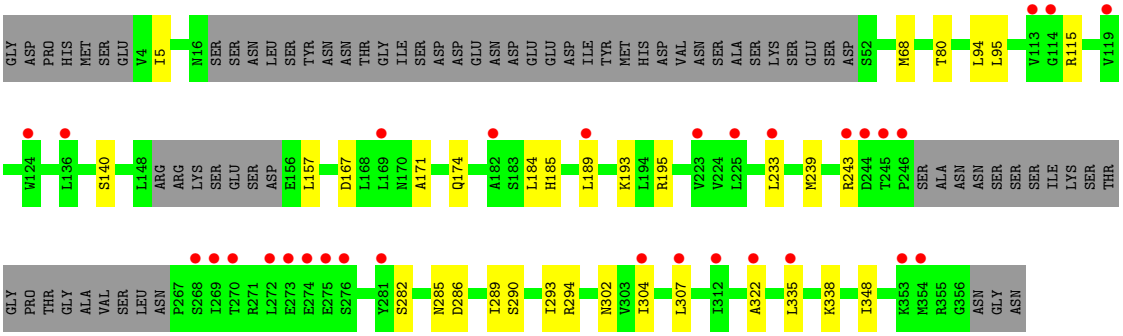
• Molecule 7: Exosome complex component RRP40

Chain G:



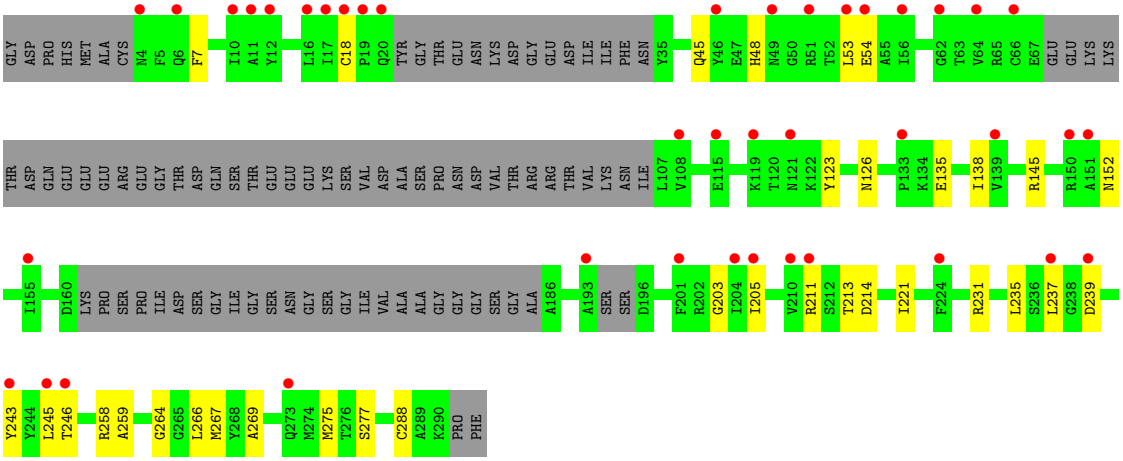
• Molecule 8: Exosome complex component RRP4

Chain H:



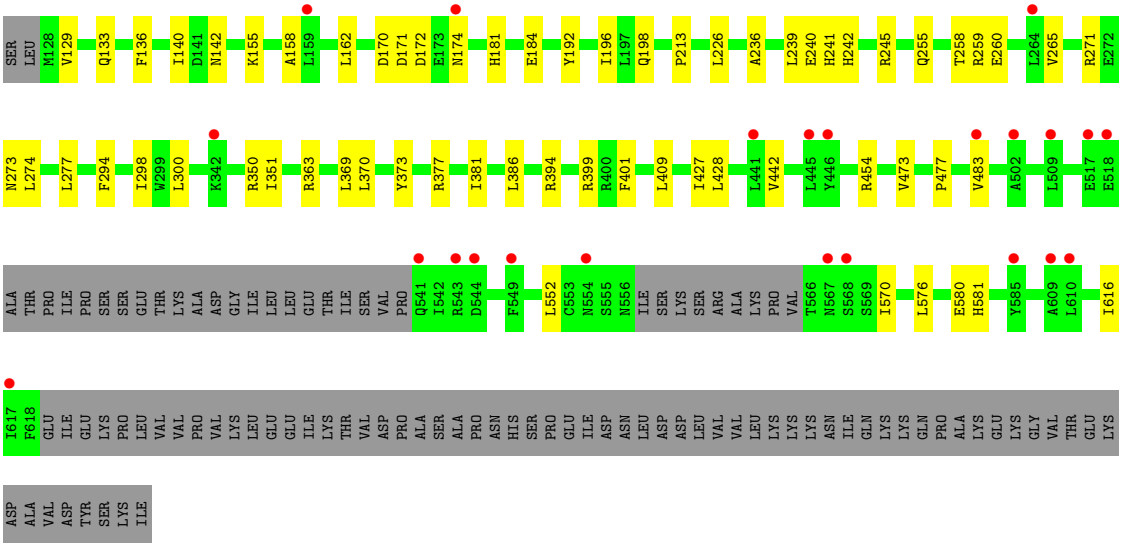
• Molecule 9: Exosome complex component CSL4

Chain I:



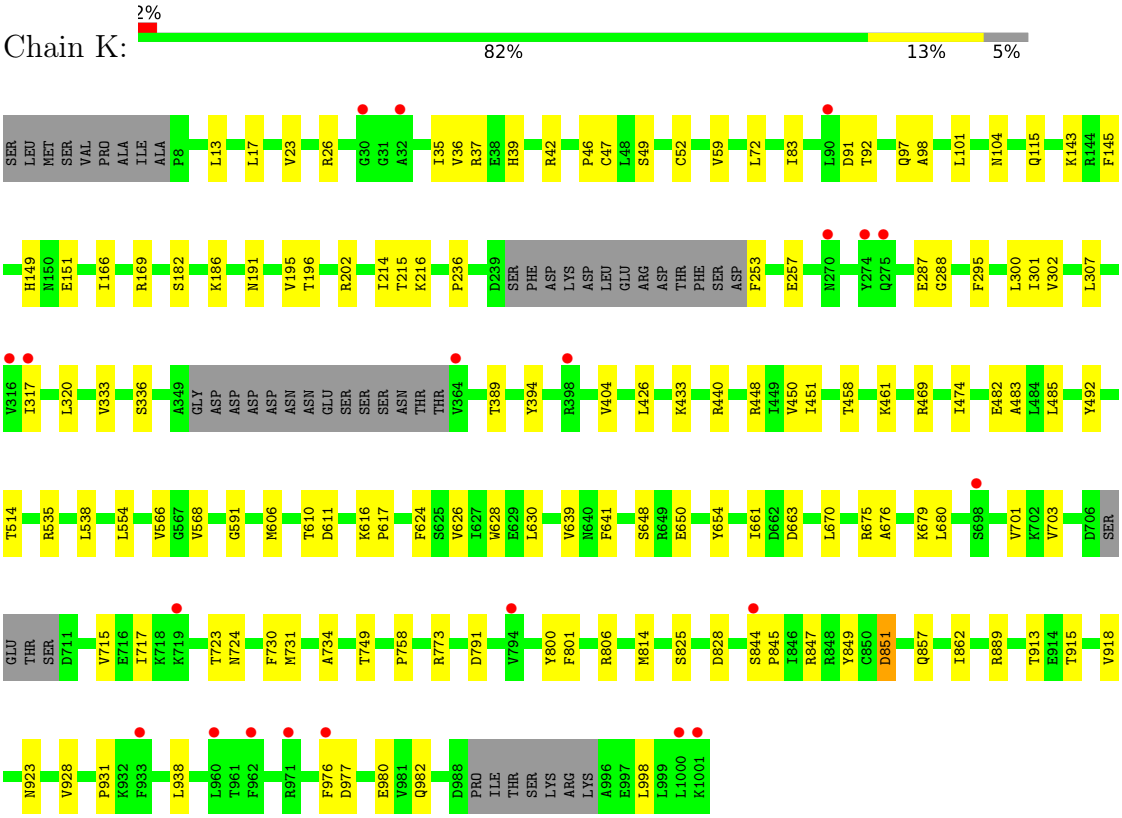
• Molecule 10: Exosome complex exonuclease RRP6

Chain J:



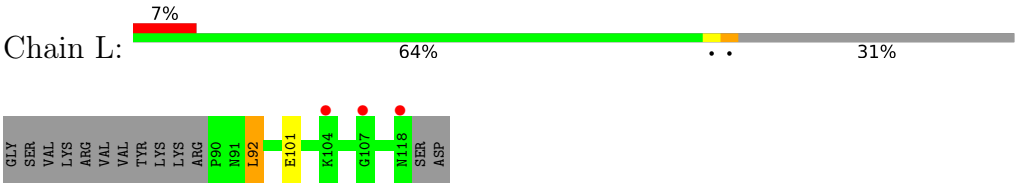
• Molecule 11: Exosome complex exonuclease DIS3

Chain K:



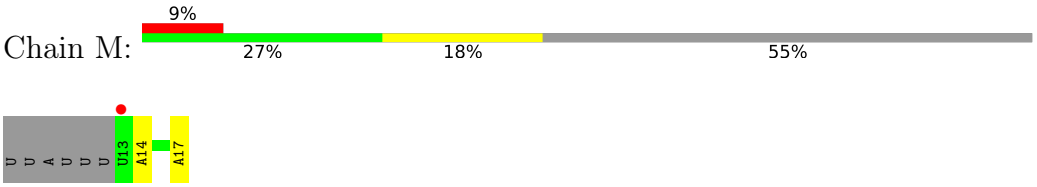
• Molecule 12: M-phase phosphoprotein 6 homolog

Chain L:



• Molecule 13: RNA (11-MER)

Chain M:



• Molecule 14: RNA (19-MER)

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.09Å 213.59Å 225.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.25 – 3.30 44.25 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.25-3.30) 97.4 (44.25-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.217 , 0.266 0.215 , 0.265	Depositor DCC
R_{free} test set	4993 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	100.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29498	wwPDB-VP
Average B, all atoms (Å^2)	138.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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

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

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	0/2386	0.39	0/3219
2	B	0.23	0/1920	0.40	0/2584
3	C	0.23	0/2359	0.41	0/3193
4	D	0.23	0/1716	0.42	0/2329
5	E	0.24	0/2016	0.41	0/2740
6	F	0.24	0/1611	0.43	0/2173
7	G	0.24	0/1868	0.41	0/2531
8	H	0.23	0/2284	0.42	0/3086
9	I	0.24	0/1599	0.43	0/2160
10	J	0.23	0/3869	0.38	0/5248
11	K	0.23	0/7794	0.39	0/10559
12	L	0.25	0/225	0.48	0/301
13	M	0.14	0/113	0.64	0/174
14	N	0.11	0/165	0.63	0/254
All	All	0.23	0/29925	0.41	0/40551

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2350	0	2335	22	0
2	B	1896	0	1954	29	0
3	C	2325	0	2408	27	0
4	D	1698	0	1754	31	0
5	E	1979	0	2010	27	0
6	F	1589	0	1571	27	0
7	G	1831	0	1819	24	0
8	H	2249	0	2263	21	0
9	I	1579	0	1584	22	0
10	J	3784	0	3776	36	0
11	K	7645	0	7684	79	0
12	L	222	0	225	3	0
13	M	101	0	52	1	0
14	N	148	0	75	2	0
15	A	5	0	0	0	0
15	B	5	0	0	0	0
15	G	10	0	0	0	0
15	K	5	0	0	0	0
16	A	6	0	8	0	0
16	K	6	0	8	1	0
17	K	1	0	0	0	0
18	A	16	0	0	0	0
18	B	17	0	0	1	0
18	D	5	0	0	0	0
18	E	1	0	0	0	0
18	G	2	0	0	0	0
18	H	3	0	0	0	0
18	J	2	0	0	0	0
18	K	18	0	0	1	0
All	All	29498	0	29526	313	0

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

All (313) 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)
4:D:145:ILE:HG12	4:D:194:LEU:HB3	1.67	0.76
9:I:203:GLY:HA2	9:I:243:TYR:H	1.49	0.76
10:J:140:ILE:HD11	10:J:271:ARG:HH12	1.54	0.73
3:C:362:LEU:HB3	4:D:180:LEU:HB3	1.71	0.72
11:K:91:ASP:HB2	11:K:196:THR:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:VAL:HG21	4:D:201:LYS:HE2	1.73	0.70
10:J:259:ARG:HE	10:J:370:LEU:HB3	1.57	0.69
11:K:115:GLN:HB2	11:K:149:HIS:HA	1.74	0.69
10:J:213:PRO:HG3	10:J:363:ARG:HD2	1.74	0.68
3:C:61:ARG:HG3	3:C:69:ASP:HB2	1.78	0.66
9:I:205:ILE:HG12	9:I:245:LEU:HB2	1.77	0.66
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.78	0.66
3:C:301:GLU:HB2	3:C:367:ALA:HB2	1.78	0.65
4:D:132:ALA:HB2	4:D:206:VAL:HG13	1.78	0.65
4:D:135:PRO:HG2	4:D:148:ASP:HA	1.80	0.64
8:H:171:ALA:HB3	8:H:184:LEU:HD23	1.79	0.64
1:A:99:GLU:OE1	2:B:106:ARG:NH2	2.31	0.64
11:K:617:PRO:HA	11:K:648:SER:HB3	1.78	0.64
2:B:17:ARG:HH12	2:B:173:ASP:HB3	1.64	0.63
11:K:915:THR:HG22	11:K:980:GLU:HG2	1.80	0.63
3:C:176:VAL:HG22	3:C:248:ILE:HB	1.81	0.62
10:J:181:HIS:HB3	10:J:184:GLU:HB2	1.82	0.62
1:A:209:ASN:ND2	1:A:217:GLU:OE2	2.33	0.61
11:K:514:THR:HA	11:K:535:ARG:HH12	1.66	0.61
11:K:404:VAL:HG11	11:K:483:ALA:HB1	1.82	0.61
9:I:135:GLU:HG2	9:I:237:LEU:HD13	1.83	0.61
10:J:192:TYR:HB3	10:J:196:ILE:HD11	1.82	0.61
9:I:211:ARG:NH2	9:I:213:THR:O	2.34	0.60
7:G:122:ARG:NH1	7:G:135:GLU:OE1	2.35	0.60
11:K:913:THR:HG22	11:K:982:GLN:HG2	1.84	0.60
11:K:469:ARG:NH2	11:K:482:GLU:OE2	2.35	0.59
2:B:18:ARG:HH11	11:K:42:ARG:HH21	1.51	0.58
3:C:123:ILE:N	4:D:155:LYS:O	2.36	0.58
7:G:187:ALA:HB3	7:G:195:TRP:HB3	1.86	0.58
8:H:302:ASN:HD22	8:H:335:LEU:HB2	1.66	0.58
5:E:2:SER:O	8:H:115:ARG:NH1	2.36	0.58
6:F:61:LEU:HD22	10:J:576:LEU:HD12	1.83	0.58
5:E:236:VAL:HG21	6:F:122:ASN:HB3	1.85	0.58
11:K:13:LEU:HB2	11:K:17:LEU:HB3	1.85	0.58
5:E:94:THR:HG22	6:F:112:GLU:HA	1.84	0.58
6:F:95:ILE:HA	6:F:137:ILE:HB	1.86	0.58
10:J:294:PHE:O	10:J:399:ARG:NH1	2.36	0.57
1:A:291:ASN:HB3	1:A:294:ALA:HB2	1.86	0.57
5:E:212:GLY:HA3	5:E:231:LEU:HD13	1.85	0.57
2:B:145:LEU:HD21	2:B:228:MET:HB3	1.85	0.57
3:C:323:MET:SD	3:C:323:MET:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:95:VAL:HG12	7:G:132:ALA:HB3	1.85	0.57
11:K:448:ARG:HH21	11:K:474:ILE:HG23	1.69	0.57
11:K:791:ASP:OD1	11:K:806:ARG:NH1	2.37	0.57
11:K:287:GLU:HG3	11:K:302:VAL:HG22	1.85	0.57
3:C:362:LEU:HD11	3:C:369:ILE:HG21	1.87	0.57
4:D:139:ILE:HG22	4:D:141:ASP:H	1.70	0.57
6:F:135:ILE:HD13	6:F:185:ILE:HD13	1.87	0.57
11:K:918:VAL:HG12	11:K:928:VAL:HG22	1.87	0.56
6:F:61:LEU:HD13	6:F:74:ILE:HG12	1.86	0.56
3:C:36:SER:OG	3:C:306:CYS:O	2.19	0.56
10:J:133:GLN:NE2	10:J:245:ARG:O	2.38	0.55
10:J:442:VAL:HG12	10:J:473:VAL:HG11	1.88	0.55
8:H:68:MET:HB3	8:H:94:LEU:HA	1.89	0.55
4:D:147:VAL:HG11	4:D:201:LYS:HG3	1.88	0.55
1:A:215:ASN:OD1	2:B:195:LYS:NZ	2.40	0.55
10:J:171:ASP:OD2	10:J:171:ASP:N	2.40	0.55
10:J:241:HIS:N	13:M:17:A:O3'	2.39	0.55
4:D:106:LEU:HD13	4:D:160:VAL:HB	1.88	0.55
8:H:289:ILE:HB	8:H:294:ARG:HE	1.72	0.55
2:B:3:ARG:NH2	18:B:403:HOH:O	2.40	0.54
6:F:231:LYS:O	6:F:235:ASN:ND2	2.41	0.54
9:I:123:TYR:HB3	9:I:126:ASN:HB2	1.90	0.54
11:K:47:CYS:SG	11:K:52:CYS:HB2	2.48	0.54
9:I:267:MET:HG2	9:I:277:SER:HB2	1.89	0.54
11:K:83:ILE:HG12	11:K:214:ILE:HD13	1.89	0.54
2:B:70:ALA:H	2:B:114:LEU:HB3	1.73	0.54
11:K:800:TYR:CZ	11:K:931:PRO:HB3	2.43	0.54
2:B:13:ARG:HD3	2:B:171:LEU:HD22	1.89	0.54
11:K:307:LEU:HD13	16:K:2003:GOL:H31	1.90	0.54
8:H:286:ASP:HB3	8:H:289:ILE:HD11	1.89	0.53
5:E:139:SER:HB2	5:E:189:ILE:HG13	1.90	0.53
4:D:79:THR:OG1	4:D:128:ASN:OD1	2.20	0.53
8:H:167:ASP:HB3	8:H:193:LYS:HE3	1.90	0.53
8:H:290:SER:HB2	8:H:293:ILE:HB	1.91	0.53
10:J:265:VAL:HG11	10:J:274:LEU:HD21	1.91	0.53
4:D:159:SER:HB3	4:D:185:ASP:H	1.74	0.53
10:J:226:LEU:HD12	10:J:277:LEU:HD23	1.90	0.53
3:C:54:ILE:HB	3:C:78:ASN:HD21	1.74	0.52
6:F:51:GLY:O	6:F:59:SER:OG	2.26	0.52
8:H:157:LEU:H	8:H:157:LEU:HD23	1.75	0.52
11:K:49:SER:HA	11:K:72:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HG22	1:A:138:VAL:HB	1.92	0.52
7:G:130:LEU:HD11	9:I:221:ILE:HB	1.92	0.52
3:C:35:LEU:HD21	3:C:331:ILE:HD11	1.91	0.52
3:C:132:PRO:HD2	6:F:9:LEU:HD12	1.92	0.52
4:D:132:ALA:HB1	4:D:205:LEU:HD23	1.92	0.52
11:K:749:THR:O	11:K:857:GLN:NE2	2.42	0.52
8:H:195:ARG:NH1	8:H:282:SER:O	2.42	0.52
11:K:83:ILE:O	11:K:191:ASN:ND2	2.43	0.51
2:B:70:ALA:HB3	2:B:114:LEU:HD22	1.93	0.51
7:G:106:SER:OG	7:G:109:ASN:OD1	2.23	0.51
11:K:46:PRO:HG3	11:K:59:VAL:HG12	1.91	0.51
11:K:641:PHE:HB2	11:K:862:ILE:HD11	1.91	0.51
2:B:185:VAL:HG22	2:B:201:VAL:HG22	1.92	0.51
7:G:48:GLY:HA2	7:G:51:GLY:HA2	1.93	0.51
10:J:580:GLU:O	10:J:581:HIS:ND1	2.44	0.51
11:K:23:VAL:HG22	11:K:36:VAL:HG12	1.91	0.51
3:C:39:ILE:HG12	3:C:40:ARG:H	1.75	0.51
10:J:129:VAL:HG21	10:J:351:ILE:HG22	1.91	0.51
5:E:236:VAL:HG12	6:F:123:SER:HB2	1.93	0.51
10:J:198:GLN:O	10:J:377:ARG:NH2	2.43	0.51
9:I:259:ALA:HB3	9:I:264:GLY:HA3	1.94	0.50
1:A:261:LEU:HD23	2:B:199:LEU:HD22	1.93	0.50
4:D:136:ILE:O	4:D:161:HIS:N	2.44	0.50
11:K:98:ALA:HB1	11:K:101:LEU:HB3	1.93	0.50
6:F:44:GLN:HA	6:F:66:SER:HB3	1.93	0.50
11:K:731:MET:HG3	14:N:16:A:H5'	1.94	0.50
10:J:381:ILE:HG12	10:J:386:LEU:HD22	1.94	0.50
11:K:300:LEU:HB2	11:K:389:THR:HG22	1.94	0.49
4:D:46:LEU:HB2	4:D:83:TYR:HB2	1.94	0.49
5:E:102:VAL:HA	5:E:225:PRO:HG3	1.95	0.49
5:E:150:ASN:O	5:E:179:LYS:NZ	2.41	0.49
5:E:194:GLY:N	5:E:210:ASN:OD1	2.38	0.49
11:K:253:PHE:HE1	11:K:461:LYS:HD2	1.78	0.49
4:D:52:VAL:HG12	4:D:67:GLU:HG3	1.94	0.49
11:K:333:VAL:HG11	11:K:938:LEU:HD21	1.93	0.49
12:L:92:LEU:H	12:L:92:LEU:HD12	1.78	0.49
10:J:298:ILE:HG23	10:J:401:PHE:HB2	1.95	0.49
7:G:71:PHE:HB3	7:G:120:TYR:CE2	2.48	0.49
7:G:138:ASP:OD1	7:G:140:THR:OG1	2.27	0.49
6:F:203:PHE:HB3	6:F:207:GLY:HA2	1.95	0.48
2:B:17:ARG:NH1	2:B:23:ARG:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:156:ILE:HG12	7:G:208:TYR:HD1	1.78	0.48
11:K:538:LEU:HD23	11:K:670:LEU:HB2	1.93	0.48
3:C:378:LEU:HD11	4:D:191:LEU:HD13	1.95	0.48
11:K:91:ASP:OD1	11:K:92:THR:N	2.42	0.48
6:F:189:ASP:OD1	6:F:190:MET:N	2.47	0.48
7:G:206:ALA:HB2	7:G:234:ILE:HD13	1.94	0.48
10:J:170:ASP:OD1	10:J:170:ASP:N	2.46	0.48
11:K:202:ARG:HG2	11:K:215:THR:HB	1.95	0.48
1:A:256:MET:HB2	1:A:261:LEU:HD11	1.94	0.48
8:H:174:GLN:HB2	8:H:185:HIS:HD2	1.78	0.48
9:I:267:MET:HB3	9:I:275:MET:HG2	1.95	0.48
11:K:758:PRO:HA	11:K:814:MET:HG2	1.96	0.48
3:C:301:GLU:HG2	3:C:326:LEU:HD11	1.96	0.47
8:H:307:LEU:HD21	8:H:348:ILE:HD12	1.96	0.47
3:C:68:ILE:HG21	3:C:279:THR:HG22	1.95	0.47
5:E:35:GLU:OE2	8:H:338:LYS:NZ	2.46	0.47
11:K:851:ASP:N	11:K:851:ASP:OD1	2.47	0.47
3:C:358:LYS:NZ	4:D:185:ASP:OD1	2.44	0.47
9:I:269:ALA:HB1	9:I:288:CYS:HB3	1.94	0.47
10:J:155:LYS:HG2	10:J:158:ALA:HB2	1.95	0.47
11:K:703:VAL:HG12	11:K:715:VAL:HA	1.97	0.47
1:A:39:THR:HB	1:A:48:SER:HB2	1.96	0.47
4:D:33:PRO:HG2	7:G:65:ILE:HD11	1.96	0.47
11:K:336:SER:HB2	11:K:433:LYS:HG3	1.96	0.47
7:G:58:ASP:OD1	7:G:164:ARG:NH1	2.48	0.47
1:A:33:PHE:HB2	1:A:271:ILE:HD13	1.96	0.47
5:E:102:VAL:HG23	5:E:103:LEU:HG	1.97	0.47
8:H:140:SER:HB3	8:H:185:HIS:HA	1.96	0.47
2:B:80:LYS:NZ	2:B:89:SER:O	2.46	0.47
3:C:348:SER:OG	3:C:361:THR:OG1	2.29	0.47
7:G:21:LEU:HD22	7:G:25:ILE:HG21	1.96	0.47
8:H:322:ALA:HB2	8:H:348:ILE:HD11	1.96	0.47
11:K:115:GLN:NE2	18:K:2101:HOH:O	2.46	0.47
7:G:213:GLU:OE2	7:G:229:ARG:NH2	2.48	0.47
10:J:192:TYR:HE2	10:J:394:ARG:HH21	1.61	0.47
7:G:156:ILE:HG12	7:G:208:TYR:CD1	2.49	0.47
11:K:39:HIS:NE2	11:K:151:GLU:O	2.40	0.47
11:K:26:ARG:HE	11:K:35:ILE:HD11	1.81	0.46
11:K:801:PHE:HE1	11:K:976:PHE:HB3	1.80	0.46
6:F:44:GLN:H	6:F:236:ARG:HH22	1.63	0.46
5:E:240:LYS:HD2	5:E:241:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:288:GLY:O	11:K:301:ILE:N	2.44	0.46
11:K:317:ILE:HB	11:K:394:TYR:HB3	1.96	0.46
5:E:18:THR:OG1	5:E:19:PRO:HD3	2.16	0.46
11:K:628:TRP:HD1	11:K:639:VAL:HG22	1.80	0.46
10:J:477:PRO:HB2	10:J:483:VAL:HG13	1.97	0.46
2:B:170:PRO:HG2	2:B:216:ILE:HD12	1.98	0.46
9:I:235:LEU:HD11	9:I:246:THR:HB	1.98	0.46
1:A:106:ARG:HE	2:B:96:ARG:HA	1.80	0.46
2:B:67:THR:HA	2:B:119:ARG:HG2	1.97	0.46
11:K:257:GLU:HG2	11:K:458:THR:HG21	1.98	0.46
10:J:240:GLU:OE2	10:J:255:GLN:NE2	2.49	0.46
1:A:233:GLY:HA2	1:A:253:GLY:HA3	1.98	0.46
12:L:101:GLU:OE1	12:L:101:GLU:N	2.43	0.46
11:K:143:LYS:HD2	11:K:145:PHE:HE1	1.80	0.45
4:D:69:LYS:NZ	4:D:181:ASP:OD2	2.40	0.45
6:F:47:SER:HB3	6:F:63:GLU:HB2	1.98	0.45
4:D:14:ASP:OD2	4:D:32:GLY:N	2.46	0.45
9:I:138:ILE:HD11	9:I:231:ARG:HG2	1.97	0.45
1:A:28:ARG:NH2	1:A:34:ARG:HG3	2.32	0.45
11:K:998:LEU:H	11:K:998:LEU:HD23	1.80	0.45
3:C:86:ILE:HD13	10:J:576:LEU:HD22	1.98	0.45
5:E:22:ARG:HH11	5:E:28:PRO:HA	1.82	0.45
5:E:148:ALA:O	5:E:152:THR:OG1	2.29	0.45
4:D:136:ILE:HB	4:D:161:HIS:HB2	1.97	0.45
4:D:164:ALA:HB3	4:D:179:LEU:HB3	1.99	0.45
1:A:255:PRO:HB2	2:B:195:LYS:HB3	1.99	0.44
7:G:177:VAL:HG21	7:G:224:LYS:HA	1.99	0.44
10:J:133:GLN:HA	10:J:136:PHE:CD2	2.51	0.44
1:A:82:GLU:HG2	1:A:96:ILE:HG23	1.99	0.44
3:C:344:HIS:O	3:C:366:GLY:N	2.47	0.44
10:J:239:LEU:HD11	10:J:300:LEU:HG	1.98	0.44
11:K:104:ASN:O	11:K:143:LYS:NZ	2.48	0.44
2:B:208:ASP:OD1	2:B:208:ASP:N	2.50	0.44
4:D:18:GLU:OE2	4:D:25:LYS:NZ	2.50	0.44
11:K:47:CYS:SG	11:K:52:CYS:CB	3.05	0.44
11:K:918:VAL:HG22	11:K:977:ASP:H	1.81	0.44
1:A:210:ILE:HG21	2:B:155:PHE:HB3	1.99	0.44
7:G:71:PHE:HB3	7:G:120:TYR:HE2	1.82	0.44
2:B:58:GLU:OE1	2:B:62:LYS:NZ	2.49	0.44
11:K:654:TYR:HD2	11:K:723:THR:HG23	1.82	0.44
5:E:228:SER:OG	6:F:213:PHE:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:626:VAL:HG22	11:K:641:PHE:HD1	1.83	0.44
11:K:630:LEU:HD22	11:K:680:LEU:HD13	2.00	0.44
3:C:29:LEU:HD13	9:I:266:LEU:HD21	2.00	0.43
3:C:297:TYR:HB3	3:C:330:LEU:HD21	2.00	0.43
7:G:101:ALA:HA	7:G:137:PHE:HE1	1.83	0.43
11:K:844:SER:HB3	11:K:847:ARG:HD3	2.00	0.43
11:K:845:PRO:HA	11:K:851:ASP:HB2	1.99	0.43
11:K:566:VAL:HG11	11:K:730:PHE:CE1	2.53	0.43
1:A:119:ASP:OD1	11:K:440:ARG:NH2	2.50	0.43
10:J:174:ASN:HB3	10:J:409:LEU:HD12	2.01	0.43
10:J:427:ILE:HG13	10:J:428:LEU:HD12	1.99	0.43
3:C:14:PRO:HD3	10:J:616:ILE:HG12	2.00	0.43
3:C:72:ASN:OD1	3:C:73:ASN:N	2.52	0.43
7:G:5:ILE:HG12	7:G:42:LEU:HB2	2.00	0.43
8:H:239:MET:HG3	8:H:243:ARG:HH11	1.83	0.43
11:K:611:ASP:HA	11:K:616:LYS:HD2	2.00	0.43
5:E:60:VAL:HG11	5:E:145:ILE:HG22	2.01	0.43
10:J:236:ALA:HB1	10:J:369:LEU:HD23	2.00	0.43
11:K:97:GLN:HG2	11:K:236:PRO:HG2	1.99	0.43
11:K:404:VAL:HG22	11:K:450:VAL:HG22	2.01	0.43
7:G:88:LEU:HB3	7:G:191:ASN:HD22	1.83	0.43
1:A:34:ARG:HD2	1:A:52:GLY:HA3	2.00	0.43
7:G:5:ILE:HD11	7:G:57:ILE:HD13	2.00	0.43
11:K:661:ILE:HG23	11:K:675:ARG:HD3	2.00	0.43
5:E:190:LEU:HB2	5:E:213:LEU:HB2	2.00	0.43
9:I:145:ARG:HB2	9:I:152:ASN:HB2	2.01	0.43
2:B:28:SER:HB2	2:B:41:TYR:HB3	2.00	0.42
6:F:44:GLN:O	6:F:236:ARG:NH2	2.52	0.42
9:I:239:ASP:OD1	9:I:239:ASP:N	2.52	0.42
1:A:112:VAL:HA	1:A:117:ALA:HB3	2.00	0.42
4:D:159:SER:HA	4:D:184:GLY:HA3	2.01	0.42
6:F:204:ILE:HG23	6:F:205:LYS:HG3	2.00	0.42
2:B:145:LEU:HD11	2:B:228:MET:HG2	2.01	0.42
3:C:54:ILE:HG21	3:C:236:TYR:CD2	2.54	0.42
5:E:6:ALA:O	8:H:285:ASN:ND2	2.36	0.42
11:K:648:SER:OG	11:K:650:GLU:O	2.37	0.42
11:K:663:ASP:O	11:K:675:ARG:NH2	2.52	0.42
1:A:163:LYS:HB3	1:A:184:PRO:HB2	2.01	0.42
1:A:206:THR:HG23	2:B:110:LYS:HE3	2.02	0.42
3:C:221:SER:HB2	6:F:53:ILE:HD13	2.01	0.42
8:H:80:THR:HG21	8:H:95:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:ASN:OD1	4:D:177:VAL:N	2.53	0.42
9:I:48:HIS:HB2	10:J:552:LEU:HD13	2.02	0.42
11:K:295:PHE:HZ	11:K:320:LEU:HD21	1.84	0.42
11:K:825:SER:OG	11:K:828:ASP:OD2	2.37	0.42
3:C:299:ILE:HG22	3:C:367:ALA:HB3	2.00	0.42
2:B:163:VAL:HG21	2:B:217:GLY:HA2	2.01	0.42
10:J:142:ASN:HD22	10:J:454:ARG:HA	1.85	0.42
11:K:554:LEU:HG	11:K:568:VAL:HG12	2.01	0.42
6:F:132:LYS:NZ	9:I:239:ASP:OD2	2.53	0.41
8:H:233:LEU:HD11	8:H:304:ILE:HD12	2.01	0.41
11:K:591:GLY:O	11:K:849:TYR:N	2.50	0.41
4:D:52:VAL:HG23	4:D:92:CYS:HB2	2.02	0.41
4:D:171:GLY:O	4:D:203:GLN:NE2	2.53	0.41
10:J:258:THR:HG23	10:J:260:GLU:H	1.85	0.41
11:K:568:VAL:HG21	11:K:734:ALA:HB2	2.02	0.41
11:K:654:TYR:HE2	11:K:724:ASN:HA	1.85	0.41
2:B:80:LYS:H	2:B:80:LYS:HG2	1.71	0.41
11:K:195:VAL:HA	11:K:216:LYS:O	2.20	0.41
11:K:426:LEU:HD21	11:K:451:ILE:HD11	2.02	0.41
6:F:77:VAL:HG11	6:F:180:LEU:HD23	2.02	0.41
9:I:45:GLN:NE2	9:I:54:GLU:OE2	2.52	0.41
11:K:606:MET:O	11:K:610:THR:HB	2.20	0.41
5:E:223:THR:HG23	5:E:225:PRO:HD2	2.02	0.41
12:L:92:LEU:HD12	12:L:92:LEU:N	2.36	0.41
5:E:174:ASP:N	5:E:174:ASP:OD1	2.53	0.41
6:F:56:CYS:HB2	6:F:77:VAL:O	2.21	0.41
1:A:46:ASP:OD1	1:A:57:HIS:NE2	2.38	0.41
2:B:1:MET:SD	11:K:37:ARG:HG3	2.61	0.41
6:F:47:SER:HB2	10:J:570:ILE:HG13	2.02	0.41
6:F:57:ASN:HB3	9:I:126:ASN:OD1	2.20	0.41
6:F:75:THR:HG23	6:F:139:VAL:HG22	2.03	0.41
7:G:117:ASP:HB3	7:G:149:ILE:HD13	2.02	0.41
9:I:211:ARG:HH22	9:I:214:ASP:HB3	1.86	0.41
10:J:242:HIS:CD2	10:J:350:ARG:HD3	2.56	0.41
11:K:676:ALA:HA	11:K:679:LYS:HG2	2.02	0.41
1:A:36:VAL:HG12	1:A:51:MET:HB3	2.03	0.41
5:E:27:LEU:HB2	5:E:30:GLN:HG3	2.02	0.41
5:E:99:LEU:HA	5:E:102:VAL:HG22	2.01	0.41
7:G:76:ILE:HD12	7:G:117:ASP:HB2	2.03	0.41
8:H:189:LEU:HD12	8:H:189:LEU:H	1.86	0.41
10:J:155:LYS:HD2	10:J:162:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASN:OD1	2:B:160:GLY:N	2.40	0.40
4:D:30:VAL:HG22	4:D:90:ILE:HG12	2.03	0.40
5:E:255:ALA:N	5:E:256:PRO:HD2	2.36	0.40
6:F:50:THR:HA	6:F:60:ALA:HA	2.03	0.40
7:G:21:LEU:HD11	7:G:34:ILE:HG12	2.03	0.40
9:I:7:PHE:CE1	9:I:18:CYS:HB3	2.56	0.40
11:K:485:LEU:HD13	11:K:492:TYR:HB3	2.03	0.40
2:B:229:ASP:O	2:B:233:ARG:HG2	2.20	0.40
11:K:889:ARG:NH1	14:N:11:U:O4	2.54	0.40
3:C:28:GLU:HG2	9:I:258:ARG:HH12	1.86	0.40
4:D:46:LEU:H	4:D:80:ARG:HB3	1.86	0.40
5:E:31:PHE:HB2	8:H:5:ILE:HG12	2.04	0.40
11:K:182:SER:O	11:K:186:LYS:HG2	2.21	0.40
11:K:773:ARG:HA	11:K:773:ARG:HD2	1.85	0.40
4:D:165:LEU:HD12	4:D:202:CYS:HB2	2.04	0.40
5:E:128:VAL:HG11	5:E:141:ILE:HD13	2.03	0.40
11:K:166:ILE:H	11:K:166:ILE:HD12	1.85	0.40
11:K:701:VAL:HG12	11:K:717:ILE:HA	2.03	0.40
2:B:47:ASN:OD1	2:B:132:ASP:N	2.55	0.40
5:E:26:ARG:NH2	5:E:200:ASP:O	2.55	0.40
6:F:87:PHE:HA	6:F:132:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/305 (98%)	284 (95%)	16 (5%)	0	100	100
2	B	239/250 (96%)	226 (95%)	13 (5%)	0	100	100
3	C	287/394 (73%)	266 (93%)	21 (7%)	0	100	100
4	D	220/225 (98%)	207 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	253/269 (94%)	238 (94%)	15 (6%)	0	100	100
6	F	201/250 (80%)	185 (92%)	16 (8%)	0	100	100
7	G	232/244 (95%)	222 (96%)	10 (4%)	0	100	100
8	H	283/363 (78%)	264 (93%)	19 (7%)	0	100	100
9	I	197/296 (67%)	172 (87%)	25 (13%)	0	100	100
10	J	454/559 (81%)	424 (93%)	30 (7%)	0	100	100
11	K	946/1003 (94%)	891 (94%)	55 (6%)	0	100	100
12	L	27/42 (64%)	24 (89%)	3 (11%)	0	100	100
All	All	3639/4200 (87%)	3403 (94%)	236 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/266 (99%)	261 (99%)	2 (1%)	81	89
2	B	215/221 (97%)	214 (100%)	1 (0%)	88	93
3	C	263/349 (75%)	262 (100%)	1 (0%)	91	95
4	D	196/198 (99%)	193 (98%)	3 (2%)	65	81
5	E	232/243 (96%)	230 (99%)	2 (1%)	78	87
6	F	177/219 (81%)	177 (100%)	0	100	100
7	G	204/212 (96%)	203 (100%)	1 (0%)	88	93
8	H	248/314 (79%)	248 (100%)	0	100	100
9	I	168/243 (69%)	167 (99%)	1 (1%)	86	91
10	J	425/516 (82%)	422 (99%)	3 (1%)	84	90
11	K	857/903 (95%)	853 (100%)	4 (0%)	88	93
12	L	25/37 (68%)	24 (96%)	1 (4%)	31	61
All	All	3273/3721 (88%)	3254 (99%)	19 (1%)	86	91

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	PHE
1	A	180	ASN
2	B	208	ASP
3	C	228	ASP
4	D	106	LEU
4	D	140	LYS
4	D	148	ASP
5	E	12	TYR
5	E	174	ASP
7	G	120	TYR
9	I	53	LEU
10	J	172	ASP
10	J	273	ASN
10	J	373	TYR
11	K	169	ARG
11	K	624	PHE
11	K	851	ASP
11	K	923	ASN
12	L	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	M	4/11 (36%)	1 (25%)	0
14	N	6/19 (31%)	1 (16%)	0
All	All	10/30 (33%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	M	14	A
14	N	12	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
15	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	G	301	-	4,4,4	0.15	0	6,6,6	0.04	0
15	SO4	K	2002	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.06	0
16	GOL	K	2003	-	5,5,5	0.37	0	5,5,5	0.26	0
16	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.28	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
16	GOL	A	402	-	-	2/4/4/4	-
16	GOL	K	2003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	2003	GOL	O1-C1-C2-C3
16	A	402	GOL	O1-C1-C2-C3
16	A	402	GOL	O1-C1-C2-O2
16	K	2003	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	2003	GOL	1	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^{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	302/305 (99%)	-0.04	8 (2%) 56 53	61, 98, 184, 237	0
2	B	241/250 (96%)	-0.08	2 (0%) 86 86	48, 83, 150, 194	0
3	C	299/394 (75%)	0.50	31 (10%) 6 6	125, 177, 245, 299	0
4	D	222/225 (98%)	0.09	6 (2%) 54 52	87, 132, 197, 240	0
5	E	257/269 (95%)	0.23	12 (4%) 31 29	81, 144, 202, 248	0
6	F	207/250 (82%)	0.28	13 (6%) 20 20	120, 170, 223, 254	0
7	G	236/244 (96%)	0.20	12 (5%) 28 26	72, 115, 206, 266	0
8	H	291/363 (80%)	0.44	31 (10%) 6 5	77, 160, 218, 260	0
9	I	207/296 (69%)	1.01	41 (19%) 1 1	94, 185, 257, 286	0
10	J	460/559 (82%)	0.14	23 (5%) 28 27	86, 128, 218, 288	0
11	K	956/1003 (95%)	-0.01	21 (2%) 62 60	74, 114, 189, 245	0
12	L	29/42 (69%)	0.72	3 (10%) 6 6	113, 180, 246, 276	0
13	M	5/11 (45%)	0.54	1 (20%) 1 1	129, 134, 180, 235	0
14	N	7/19 (36%)	1.62	2 (28%) 0 0	105, 108, 134, 203	0
All	All	3719/4230 (87%)	0.20	206 (5%) 25 23	48, 132, 217, 299	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	11	ALA	8.6
9	I	16	LEU	7.6
3	C	172	VAL	6.4
6	F	18	MET	6.0
8	H	233	LEU	5.9
9	I	54	GLU	5.9
9	I	19	PRO	5.2
3	C	244	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
5	E	1	MET	4.7
3	C	173	LYS	4.5
8	H	245	THR	4.4
9	I	64	VAL	4.3
3	C	189	TYR	4.2
3	C	187	VAL	4.1
9	I	205	ILE	4.1
12	L	107	GLY	4.0
9	I	201	PHE	4.0
7	G	21	LEU	3.9
9	I	17	ILE	3.9
9	I	239	ASP	3.9
8	H	312	ILE	3.8
12	L	104	LYS	3.8
5	E	122	PHE	3.7
5	E	29	HIS	3.7
9	I	10	ILE	3.7
3	C	17	PHE	3.7
6	F	143	TYR	3.7
9	I	243	TYR	3.6
9	I	224	PHE	3.6
9	I	20	GLN	3.6
5	E	116	LEU	3.6
8	H	225	LEU	3.5
9	I	53	LEU	3.5
3	C	211	TYR	3.5
3	C	243	LEU	3.5
6	F	19	ALA	3.5
8	H	124	TRP	3.5
3	C	209	TRP	3.5
6	F	147	LEU	3.5
6	F	144	ASP	3.4
8	H	354	MET	3.4
10	J	543	ARG	3.4
1	A	213	GLU	3.4
10	J	610	LEU	3.4
8	H	270	THR	3.4
9	I	155	ILE	3.4
8	H	243	ARG	3.4
4	D	145	ILE	3.4
9	I	49	ASN	3.4
1	A	212	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
10	J	518	GLU	3.3
7	G	46	ALA	3.3
10	J	342	LYS	3.3
3	C	190	PRO	3.3
3	C	76	GLY	3.3
10	J	568	SER	3.2
11	K	270	ASN	3.2
3	C	37	LEU	3.2
8	H	276	SER	3.2
1	A	211	LYS	3.2
8	H	114	GLY	3.2
11	K	274	TYR	3.2
9	I	121	ASN	3.1
4	D	131	CYS	3.1
10	J	544	ASP	3.1
9	I	108	VAL	3.1
9	I	115	GLU	3.1
7	G	48	GLY	3.1
10	J	567	ASN	3.0
8	H	119	VAL	3.0
9	I	62	GLY	3.0
9	I	273	GLN	3.0
7	G	18	PRO	3.0
4	D	103	GLU	2.9
5	E	134	HIS	2.9
9	I	204	ILE	2.9
10	J	549	PHE	2.9
9	I	51	ARG	2.9
2	B	1	MET	2.9
3	C	188	LEU	2.9
9	I	66	CYS	2.9
8	H	274	GLU	2.9
11	K	933	PHE	2.9
5	E	168	GLU	2.9
1	A	208	GLU	2.9
11	K	719	LYS	2.8
9	I	56	ILE	2.8
9	I	119	LYS	2.8
9	I	12	TYR	2.8
11	K	1001	LYS	2.8
9	I	150	ARG	2.7
3	C	86	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
10	J	554	ASN	2.7
8	H	244	ASP	2.7
11	K	698	SER	2.7
8	H	304	ILE	2.7
8	H	136	LEU	2.7
11	K	960	LEU	2.7
9	I	133	PRO	2.7
10	J	445	LEU	2.7
6	F	69	HIS	2.7
6	F	203	PHE	2.7
8	H	307	LEU	2.7
9	I	6	GLN	2.7
8	H	269	ILE	2.7
8	H	273	GLU	2.6
11	K	398	ARG	2.6
8	H	189	LEU	2.6
11	K	976	PHE	2.6
8	H	353	LYS	2.6
3	C	245	ARG	2.6
8	H	322	ALA	2.5
6	F	102	LEU	2.5
11	K	317	ILE	2.5
5	E	30	GLN	2.5
6	F	171	HIS	2.5
8	H	281	TYR	2.5
9	I	237	LEU	2.5
4	D	167	PHE	2.5
8	H	113	VAL	2.5
9	I	210	VAL	2.5
3	C	336	THR	2.5
5	E	54	ASP	2.5
7	G	1	MET	2.5
10	J	585	TYR	2.5
3	C	15	ILE	2.5
8	H	169	LEU	2.5
9	I	245	LEU	2.5
8	H	275	GLU	2.5
10	J	509	LEU	2.4
10	J	264	LEU	2.4
1	A	207	GLU	2.4
10	J	159	LEU	2.4
9	I	151	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	59	LEU	2.4
11	K	1000	LEU	2.4
11	K	971	ARG	2.4
8	H	246	PRO	2.4
9	I	18	CYS	2.3
3	C	337	GLU	2.3
2	B	64	GLN	2.3
11	K	90	LEU	2.3
1	A	214	THR	2.3
11	K	794	VAL	2.3
8	H	272	LEU	2.3
11	K	275	GLN	2.3
1	A	76	LEU	2.3
3	C	186	SER	2.3
3	C	29	LEU	2.3
11	K	32	ALA	2.3
5	E	181	ASP	2.3
12	L	118	ASN	2.3
9	I	46	TYR	2.3
14	N	11	U	2.2
3	C	174	ALA	2.2
7	G	47	LYS	2.2
8	H	335	LEU	2.2
3	C	305	GLU	2.2
6	F	71	THR	2.2
11	K	962	PHE	2.2
5	E	53	SER	2.2
1	A	209	ASN	2.2
7	G	159	ASN	2.2
5	E	139	SER	2.2
6	F	20	PHE	2.2
3	C	213	LEU	2.2
7	G	16	THR	2.2
6	F	64	ALA	2.2
9	I	139	VAL	2.2
8	H	268	SER	2.1
10	J	617	ILE	2.1
9	I	4	ASN	2.1
10	J	609	ALA	2.1
10	J	517	GLU	2.1
11	K	364	VAL	2.1
11	K	844	SER	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	17	THR	2.1
3	C	212	VAL	2.1
9	I	193	ALA	2.1
10	J	174	ASN	2.1
11	K	316	VAL	2.1
3	C	340	GLU	2.1
6	F	241	MET	2.1
3	C	185	PHE	2.1
10	J	502	ALA	2.1
4	D	137	ALA	2.1
3	C	95	ILE	2.1
3	C	329	VAL	2.1
4	D	11	ASP	2.1
7	G	157	ASP	2.1
14	N	16	A	2.1
8	H	182	ALA	2.1
9	I	246	THR	2.1
3	C	33	ARG	2.1
8	H	223	VAL	2.0
10	J	483	VAL	2.0
11	K	30	GLY	2.0
13	M	13	U	2.0
5	E	197	MET	2.0
10	J	541	GLN	2.0
10	J	441	LEU	2.0
9	I	211	ARG	2.0
10	J	446	TYR	2.0
7	G	11	PHE	2.0
3	C	11	GLU	2.0
7	G	19	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
15	SO4	G	302	5/5	0.77	0.47	174,187,192,199	0
16	GOL	A	402	6/6	0.85	0.66	73,108,120,124	0
15	SO4	K	2002	5/5	0.86	0.14	166,179,188,209	0
15	SO4	B	301	5/5	0.86	0.17	171,175,177,186	0
15	SO4	G	301	5/5	0.90	0.32	130,142,158,175	0
15	SO4	A	401	5/5	0.93	0.29	75,87,114,122	0
16	GOL	K	2003	6/6	0.93	0.68	72,97,98,104	0
17	ZN	K	2001	1/1	0.99	0.20	125,125,125,125	0

6.5 Other polymers (i)

There are no such residues in this entry.