Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 06:53 AM EDT

PDB ID	:	4OO1
Title	:	Structure of an Rrp6-RNA exosome complex bound to poly(A) RNA
Authors	:	Lima, C.D.; Wasmuth, E.V.
Deposited on	:	2014-01-29
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 (i) 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 (i)) were used in the production of this report:

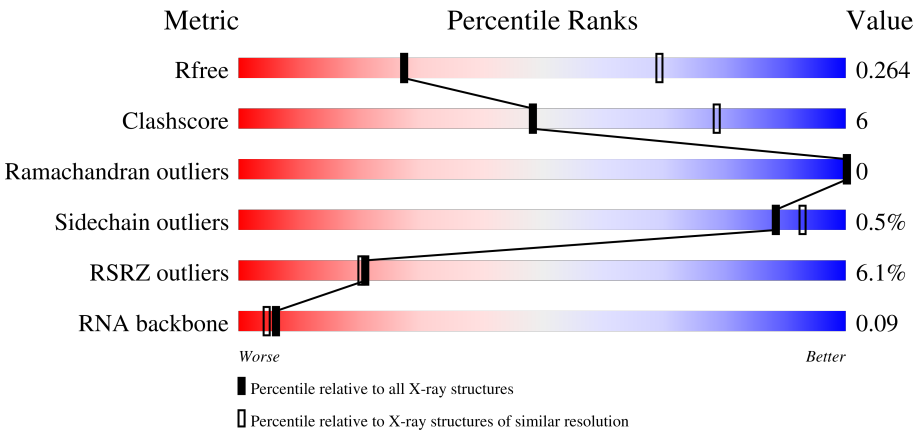
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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% 83% 13% •
2	B	250	% 79% 16% •
3	C	394	8% 63% 16% 21%
4	D	225	2% 79% 19% •

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Mol	Chain	Length	Quality of chain
5	E	269	4% 80% 14% • 5%
6	F	250	4% 68% 15% 17%
7	G	244	11% 70% 22% 7%
8	H	363	2% 69% 8% 23%
9	I	296	8% 60% 13% 27%
10	J	560	6% 74% 14% 12%
11	S	24	8% 17% 75%

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	MPD	E	302	-	-	-	X
14	MES	G	301	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 21590 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
			Total	C	N	O	S			
1	A	293	2282	1434	388	443	17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	239	1879	1176	334	361	8	0	0	0

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
			Total	C	N	O	S			
3	C	312	2425	1539	410	467	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	221	1689	1061	287	332	9	0	0	0

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
			Total	C	N	O	S			
5	E	255	1964	1255	326	379	4	0	0	0

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
			Total	C	N	O	S			
6	F	207	1600	1004	271	315	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	226	1763	1128	288	337	10	0	0	0

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
			Total	C	N	O	S			
8	H	279	2159	1350	389	408	12	0	0	0

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
			Total	C	N	O	S			
9	I	216	1650	1036	288	319	7	0	0	0

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
			Total	C	N	O	S			
10	J	493	4034	2577	693	754	10	0	0	0

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

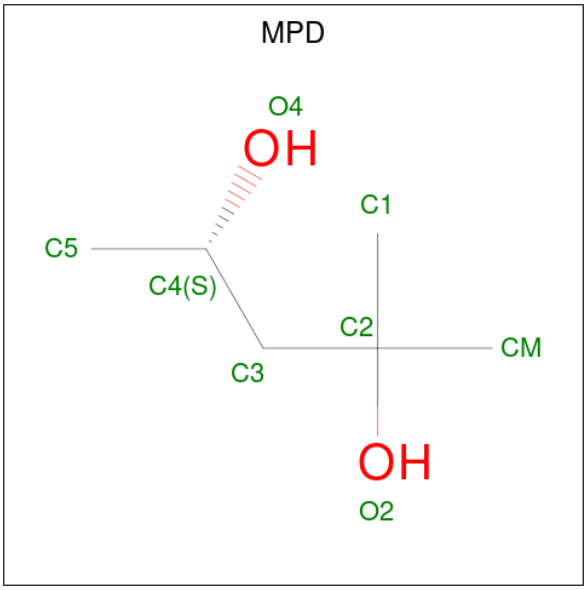
- Molecule 11 is a RNA chain called POLY A RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	S	6	119	55	25	34	5	0	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

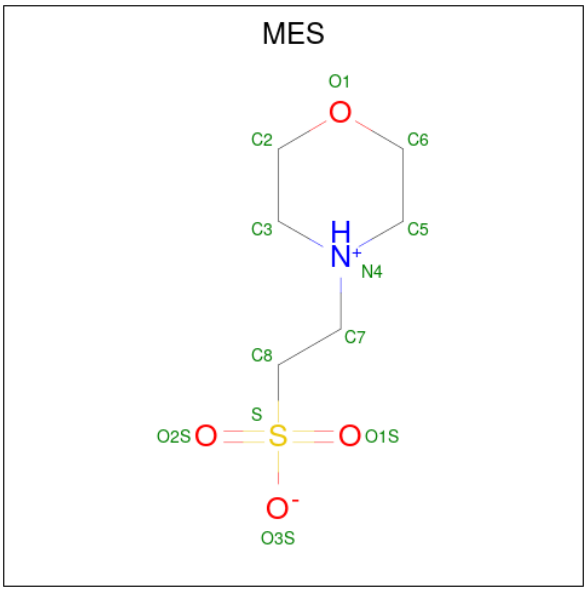
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
12	E	1	1	1	0	0
			Total	Mg		
12	S	1	1	1	0	0

- Molecule 13 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



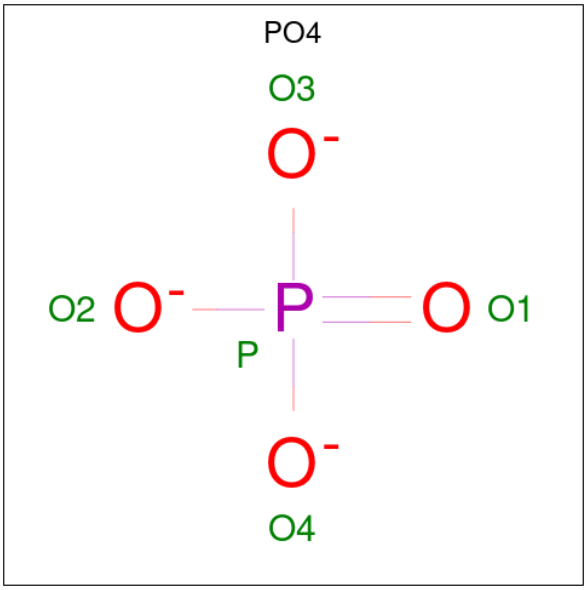
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	E	1	8	6	2	0	0

- Molecule 14 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
14	G	1	6	2	3	1	0	0

- Molecule 15 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



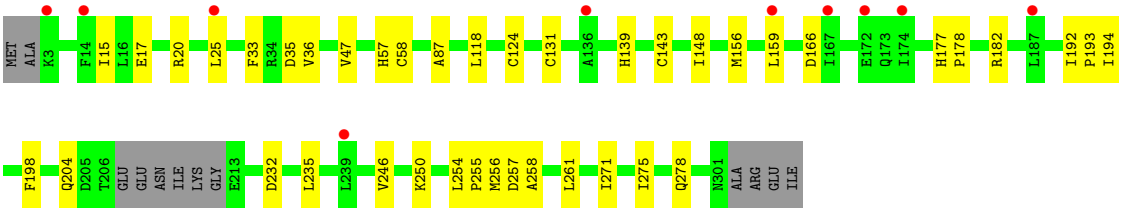
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
15	I	1	5	4	1		0	0
			Total	O	P			
15	S	1	5	4	1		0	0

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.

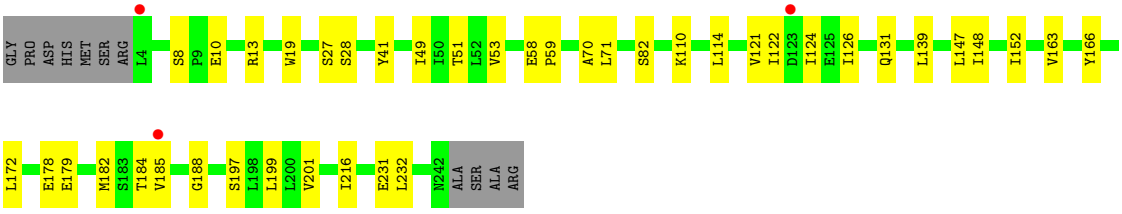
• Molecule 1: Exosome complex component RRP45

Chain A:



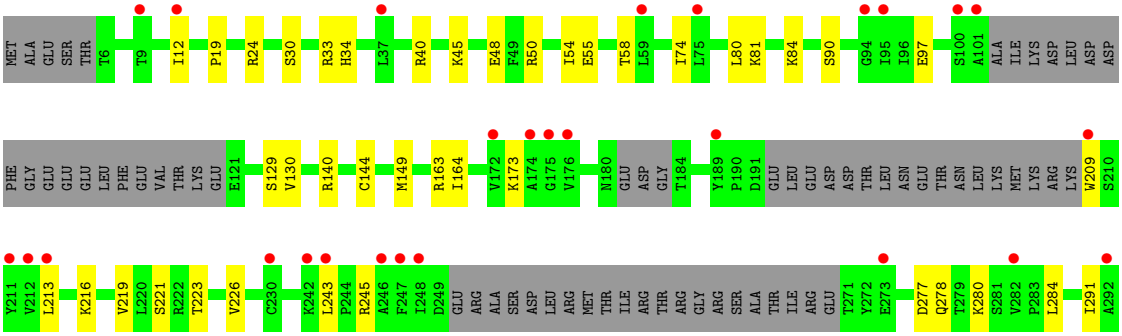
• Molecule 2: Exosome complex component SKI6

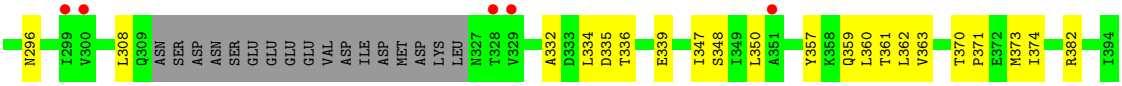
Chain B:



• Molecule 3: Exosome complex component RRP43

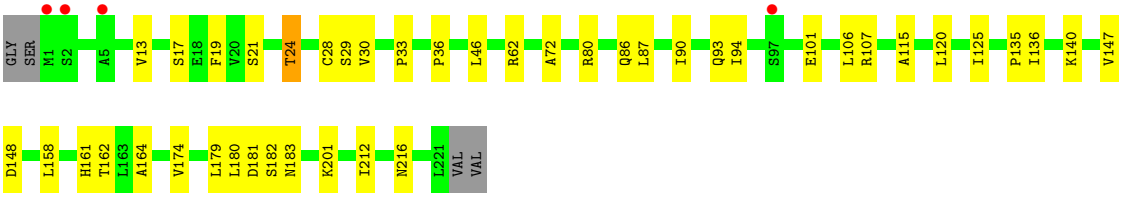
Chain C:





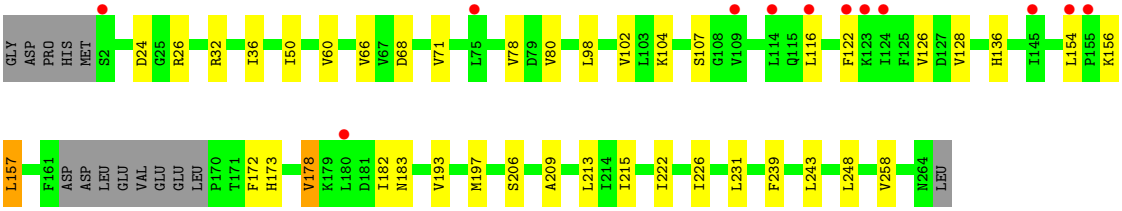
• Molecule 4: Exosome complex component RRP46

Chain D:



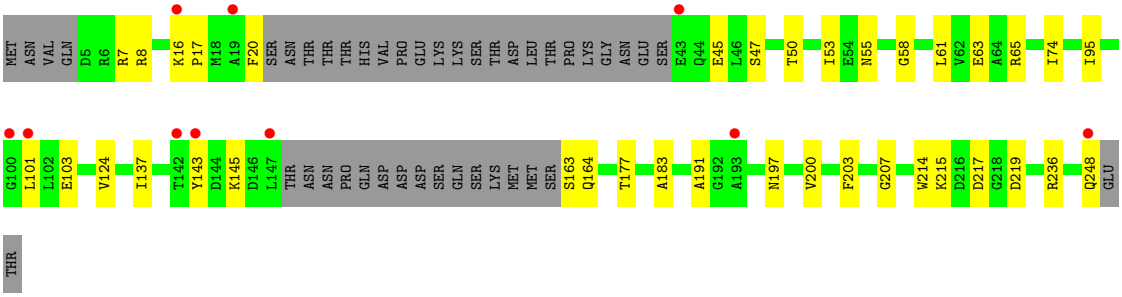
• Molecule 5: Exosome complex component RRP42

Chain E:



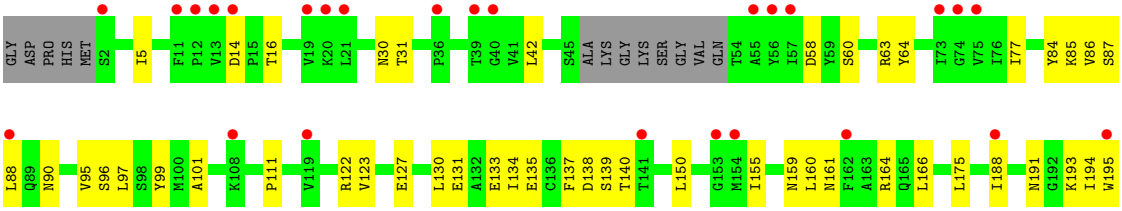
• Molecule 6: Exosome complex component MTR3

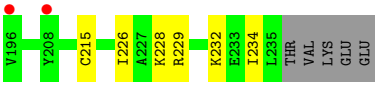
Chain F:



• Molecule 7: Exosome complex component RRP40

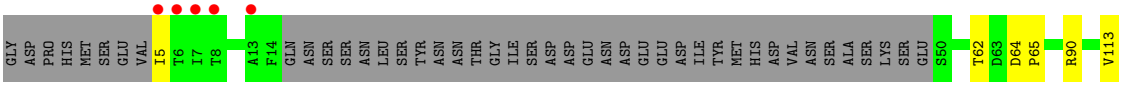
Chain G:

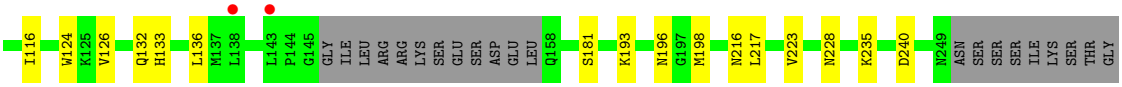


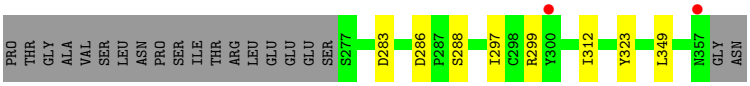


• Molecule 8: Exosome complex component RRP4

Chain H:

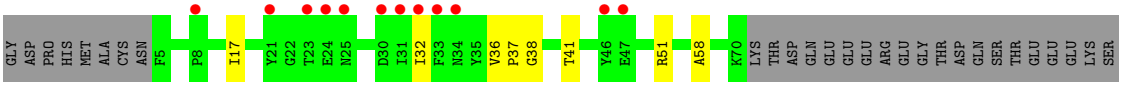


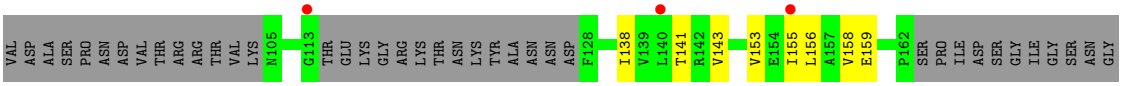


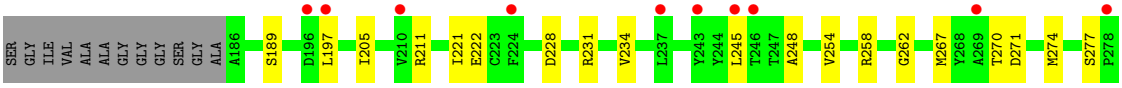


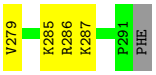
• Molecule 9: Exosome complex component CSL4

Chain I:



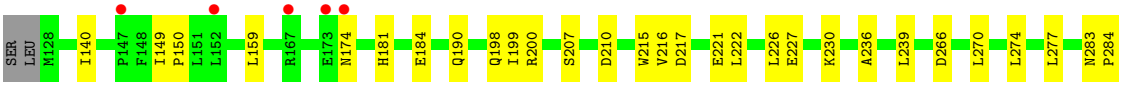


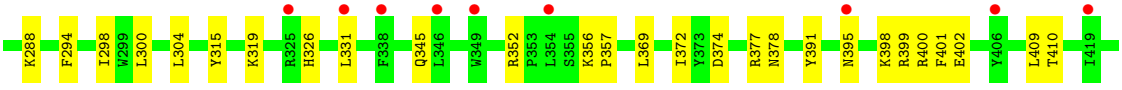


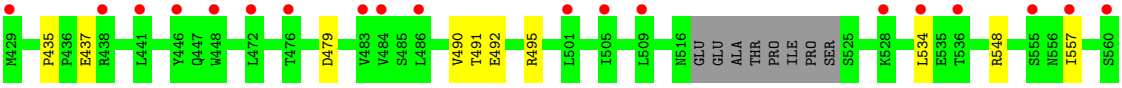


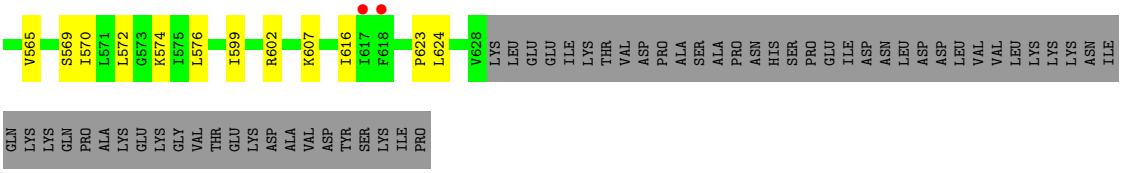
• Molecule 10: Exosome complex exonuclease RRP6

Chain J:









- Molecule 11: POLY A RNA

Chain S:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	193.29Å 200.08Å 97.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 3.30 48.43 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.43-3.30) 97.7 (48.43-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.227 , 0.265 0.227 , 0.264	Depositor DCC
R_{free} test set	2856 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	113.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 20.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21590	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, MG, PO4, MPD

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	0.21	0/2317	0.34	0/3125
2	B	0.20	0/1903	0.36	0/2563
3	C	0.20	0/2460	0.37	0/3334
4	D	0.20	0/1707	0.37	0/2316
5	E	0.21	0/2002	0.36	0/2720
6	F	0.21	0/1622	0.36	0/2186
7	G	0.21	0/1799	0.36	0/2439
8	H	0.21	0/2193	0.37	0/2962
9	I	0.20	0/1675	0.38	0/2269
10	J	0.20	0/4125	0.35	0/5599
11	S	0.16	0/134	0.61	0/207
All	All	0.21	0/21937	0.36	0/29720

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2276	24	0
2	B	1879	0	1930	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2425	0	2480	42	0
4	D	1689	0	1741	27	0
5	E	1964	0	1997	23	0
6	F	1600	0	1584	28	0
7	G	1763	0	1750	34	0
8	H	2159	0	2166	18	0
9	I	1650	0	1639	23	0
10	J	4034	0	4062	47	0
11	S	119	0	63	1	0
12	E	1	0	0	0	0
12	S	1	0	0	0	0
13	E	8	0	14	0	0
14	G	6	0	2	0	0
15	I	5	0	0	0	0
15	S	5	0	0	0	0
All	All	21590	0	21704	261	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 (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:GLU:HG2	2:B:184:THR:HG21	1.72	0.72
3:C:360:LEU:HB3	4:D:182:SER:HB2	1.72	0.70
10:J:181:HIS:HB3	10:J:184:GLU:HB2	1.75	0.69
4:D:33:PRO:HB2	4:D:86:GLN:HG2	1.75	0.69
2:B:70:ALA:H	2:B:114:LEU:HB3	1.56	0.69
6:F:236:ARG:HH22	10:J:565:VAL:HG21	1.58	0.69
9:I:267:MET:HG2	9:I:277:SER:HB3	1.76	0.67
4:D:46:LEU:H	4:D:80:ARG:HB3	1.60	0.66
9:I:143:VAL:HA	9:I:153:VAL:HG12	1.77	0.66
5:E:226:ILE:HB	6:F:215:LYS:HB3	1.80	0.64
3:C:363:VAL:HG11	4:D:72:ALA:HB1	1.78	0.64
3:C:81:LYS:NZ	10:J:576:LEU:O	2.26	0.64
3:C:24:ARG:HD2	9:I:156:LEU:HD22	1.79	0.63
3:C:350:LEU:HB2	3:C:359:GLN:H	1.64	0.63
6:F:200:VAL:HB	6:F:214:TRP:HB3	1.81	0.62
1:A:33:PHE:HB2	1:A:271:ILE:HD13	1.82	0.62
7:G:155:ILE:HD11	7:G:193:LYS:HB3	1.82	0.61
7:G:88:LEU:HB3	7:G:191:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:226:ILE:HG12	7:G:229:ARG:HH21	1.64	0.61
2:B:13:ARG:HH22	2:B:172:LEU:H	1.46	0.60
7:G:122:ARG:NH2	7:G:139:SER:OG	2.34	0.60
6:F:61:LEU:HD23	6:F:74:ILE:HG12	1.83	0.60
9:I:258:ARG:HB2	9:I:262:GLY:HA2	1.83	0.60
10:J:345:GLN:NE2	11:S:24:A:N7	2.50	0.59
10:J:374:ASP:O	10:J:378:ASN:ND2	2.34	0.59
1:A:57:HIS:HB3	1:A:139:HIS:HB2	1.85	0.59
6:F:47:SER:HB3	6:F:63:GLU:HB2	1.85	0.59
4:D:212:ILE:O	4:D:216:ASN:ND2	2.33	0.59
1:A:193:PRO:HB3	1:A:246:VAL:HG21	1.84	0.58
10:J:216:VAL:HG13	10:J:221:GLU:HG3	1.84	0.58
3:C:50:ARG:NH1	3:C:335:ASP:OD2	2.37	0.58
3:C:359:GLN:NE2	4:D:183:ASN:OD1	2.37	0.58
8:H:235:LYS:NZ	8:H:288:SER:O	2.36	0.58
10:J:222:LEU:HD22	10:J:270:LEU:HD23	1.85	0.58
8:H:217:LEU:HD11	8:H:223:VAL:HG12	1.85	0.57
10:J:198:GLN:O	10:J:377:ARG:NH1	2.37	0.57
9:I:228:ASP:OD2	9:I:286:ARG:NE	2.32	0.57
10:J:599:ILE:HA	10:J:602:ARG:HD2	1.86	0.57
3:C:348:SER:HB2	3:C:361:THR:HB	1.87	0.57
3:C:33:ARG:HD2	3:C:308:LEU:HD11	1.86	0.56
6:F:215:LYS:NZ	6:F:217:ASP:O	2.36	0.56
4:D:162:THR:HB	4:D:181:ASP:HB2	1.87	0.56
1:A:17:GLU:OE2	1:A:20:ARG:NH2	2.38	0.56
3:C:216:LYS:NZ	6:F:103:GLU:OE2	2.38	0.56
4:D:24:THR:HG22	4:D:107:ARG:HH21	1.71	0.56
10:J:435:PRO:HB2	10:J:437:GLU:HG2	1.87	0.55
2:B:51:THR:HG23	2:B:126:ILE:HG12	1.87	0.55
3:C:221:SER:HA	6:F:55:ASN:HB2	1.89	0.55
3:C:347:ILE:HG12	3:C:362:LEU:HG	1.87	0.55
10:J:400:ARG:NH1	10:J:402:GLU:OE1	2.40	0.55
5:E:68:ASP:HB3	5:E:71:VAL:HG22	1.89	0.54
6:F:65:ARG:HE	10:J:570:ILE:HG23	1.72	0.54
7:G:96:SER:HB3	7:G:133:GLU:HG2	1.90	0.54
8:H:132:GLN:OE1	8:H:181:SER:OG	2.26	0.54
10:J:490:VAL:HG13	10:J:495:ARG:HH21	1.72	0.54
5:E:60:VAL:HG22	5:E:128:VAL:HG22	1.89	0.54
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.89	0.54
7:G:166:LEU:HD11	7:G:175:LEU:HD13	1.90	0.54
9:I:138:ILE:HG21	9:I:231:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:211:ARG:NH2	9:I:248:ALA:O	2.41	0.54
6:F:143:TYR:OH	6:F:145:LYS:NZ	2.36	0.53
10:J:391:TYR:O	10:J:395:ASN:ND2	2.41	0.53
5:E:206:SER:HB3	5:E:231:LEU:HB3	1.91	0.53
2:B:122:ILE:HD13	2:B:152:ILE:HD13	1.91	0.53
9:I:38:GLY:H	9:I:41:THR:HG1	1.54	0.53
10:J:294:PHE:HB2	10:J:399:ARG:HH11	1.73	0.53
5:E:239:PHE:HB2	5:E:243:LEU:HD12	1.91	0.53
8:H:116:ILE:HD13	8:H:126:VAL:HG22	1.89	0.53
6:F:197:ASN:ND2	6:F:219:ASP:OD1	2.42	0.52
7:G:85:LYS:NZ	7:G:131:GLU:OE2	2.34	0.52
2:B:70:ALA:HB3	2:B:114:LEU:HD22	1.89	0.52
7:G:97:LEU:HD13	7:G:134:ILE:HG13	1.90	0.52
7:G:101:ALA:HB1	7:G:135:GLU:HA	1.91	0.52
10:J:174:ASN:HD22	10:J:410:THR:HB	1.73	0.52
2:B:27:SER:HB2	2:B:231:GLU:HG2	1.91	0.52
7:G:5:ILE:HG13	7:G:42:LEU:HB2	1.90	0.52
8:H:216:ASN:ND2	8:H:240:ASP:O	2.38	0.52
10:J:623:PRO:HG2	10:J:624:LEU:HD22	1.93	0.52
1:A:15:ILE:HG12	1:A:25:LEU:HD11	1.92	0.51
1:A:118:LEU:HD12	1:A:159:LEU:HD13	1.90	0.51
3:C:357:TYR:OH	3:C:382:ARG:NH2	2.43	0.51
4:D:93:GLN:NE2	4:D:94:ILE:O	2.43	0.51
9:I:17:ILE:HD11	9:I:58:ALA:HB2	1.91	0.51
2:B:49:ILE:HD13	2:B:139:LEU:HD23	1.92	0.51
6:F:63:GLU:OE1	10:J:572:LEU:N	2.35	0.51
2:B:148:ILE:HG21	2:B:232:LEU:HD21	1.93	0.51
4:D:135:PRO:HG2	4:D:148:ASP:HA	1.93	0.51
10:J:491:THR:OG1	10:J:492:GLU:N	2.42	0.51
1:A:35:ASP:OD1	1:A:35:ASP:N	2.43	0.51
10:J:266:ASP:OD2	10:J:352:ARG:NH1	2.39	0.51
2:B:82:SER:HB2	2:B:131:GLN:HG2	1.93	0.50
5:E:215:ILE:HD13	5:E:248:LEU:HD23	1.93	0.50
7:G:60:SER:HA	7:G:161:ASN:HD21	1.76	0.50
3:C:40:ARG:NH1	3:C:332:ALA:O	2.42	0.50
7:G:99:TYR:HD1	7:G:111:PRO:HD2	1.76	0.50
9:I:51:ARG:HH11	10:J:548:ARG:HD2	1.76	0.50
7:G:159:ASN:ND2	7:G:215:CYS:SG	2.85	0.50
1:A:156:MET:HE2	1:A:192:ILE:HG13	1.94	0.50
1:A:194:ILE:HG21	1:A:275:ILE:HD11	1.94	0.50
5:E:104:LYS:HE3	5:E:107:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:TRP:HB2	8:H:136:LEU:HB3	1.93	0.50
10:J:356:LYS:HG3	10:J:357:PRO:HD3	1.93	0.50
10:J:227:GLU:HA	10:J:230:LYS:HE2	1.94	0.50
3:C:30:SER:O	3:C:34:HIS:ND1	2.38	0.49
3:C:173:LYS:NZ	3:C:245:ARG:HH12	2.10	0.49
9:I:271:ASP:HB3	9:I:274:MET:HB3	1.93	0.49
7:G:95:VAL:HG11	7:G:134:ILE:HG23	1.93	0.49
7:G:127:GLU:HB2	7:G:130:LEU:HB3	1.93	0.49
7:G:138:ASP:OD1	7:G:139:SER:N	2.45	0.49
3:C:164:ILE:HD12	3:C:291:ILE:HD13	1.93	0.49
7:G:58:ASP:OD1	7:G:164:ARG:NH1	2.46	0.49
2:B:13:ARG:HH21	2:B:19:TRP:HA	1.78	0.49
2:B:8:SER:OG	2:B:10:GLU:OE1	2.31	0.49
4:D:30:VAL:HG21	4:D:120:LEU:HD12	1.95	0.49
3:C:12:ILE:HD11	10:J:616:ILE:HB	1.94	0.49
3:C:362:LEU:HB2	4:D:180:LEU:HB3	1.93	0.49
8:H:124:TRP:O	8:H:136:LEU:N	2.42	0.49
4:D:13:VAL:HG11	4:D:29:SER:HB2	1.95	0.49
3:C:243:LEU:HD11	3:C:284:LEU:HD13	1.93	0.48
2:B:71:LEU:HB2	2:B:121:VAL:HG22	1.95	0.48
6:F:95:ILE:HG12	6:F:137:ILE:HB	1.95	0.48
10:J:331:LEU:HB3	10:J:372:ILE:HD13	1.95	0.48
5:E:197:MET:HE1	5:E:213:LEU:HD12	1.95	0.48
8:H:198:MET:HE2	8:H:297:ILE:HG22	1.96	0.48
9:I:141:THR:HG22	9:I:155:ILE:HA	1.95	0.48
2:B:185:VAL:HG22	2:B:201:VAL:HG22	1.94	0.48
5:E:36:ILE:HG12	5:E:50:ILE:HG12	1.96	0.48
10:J:239:LEU:HD11	10:J:300:LEU:HG	1.96	0.48
8:H:113:VAL:O	8:H:228:ASN:ND2	2.45	0.48
2:B:58:GLU:HG3	8:H:133:HIS:CG	2.49	0.47
2:B:188:GLY:O	2:B:197:SER:N	2.40	0.47
3:C:19:PRO:HG3	10:J:607:LYS:HG2	1.95	0.47
3:C:45:LYS:HB2	3:C:48:GLU:HG3	1.95	0.47
7:G:127:GLU:HG3	9:I:221:ILE:HD13	1.96	0.47
7:G:188:ILE:HG13	7:G:194:ILE:HG23	1.95	0.47
3:C:163:ARG:NH1	4:D:158:LEU:O	2.44	0.47
3:C:370:THR:H	3:C:373:MET:HE2	1.80	0.47
4:D:30:VAL:HG11	4:D:125:ILE:HD11	1.96	0.47
5:E:154:LEU:HB2	5:E:178:VAL:HG13	1.96	0.47
3:C:149:MET:HE2	6:F:7:ARG:HG3	1.97	0.47
4:D:28:CYS:SG	4:D:29:SER:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:161:ASN:OD1	7:G:164:ARG:NH1	2.47	0.47
1:A:148:ILE:HD12	1:A:148:ILE:H	1.80	0.47
1:A:261:LEU:HD13	2:B:199:LEU:HD22	1.97	0.47
9:I:254:VAL:N	9:I:287:LYS:O	2.36	0.47
10:J:149:ILE:HD12	10:J:150:PRO:HD2	1.96	0.47
6:F:124:VAL:HG21	6:F:191:ALA:HB2	1.97	0.46
4:D:164:ALA:HB3	4:D:179:LEU:HB3	1.96	0.46
3:C:371:PRO:HA	3:C:374:ILE:HD13	1.98	0.46
4:D:147:VAL:HG21	4:D:201:LYS:HG3	1.96	0.46
1:A:257:ASP:OD1	1:A:258:ALA:N	2.47	0.46
1:A:124:CYS:HA	1:A:131:CYS:HB2	1.98	0.46
3:C:296:ASN:OD1	3:C:334:LEU:N	2.40	0.46
9:I:159:GLU:OE1	9:I:231:ARG:NH2	2.49	0.46
2:B:28:SER:HB2	2:B:41:TYR:HB3	1.97	0.46
10:J:274:LEU:HD12	10:J:304:LEU:HD22	1.98	0.46
3:C:144:CYS:SG	6:F:8:ARG:NE	2.89	0.46
3:C:84:LYS:HE3	3:C:223:THR:HG21	1.98	0.45
4:D:30:VAL:HG22	4:D:90:ILE:HG12	1.98	0.45
6:F:45:GLU:HA	10:J:565:VAL:HG11	1.97	0.45
9:I:222:GLU:HB3	9:I:285:LYS:HD3	1.97	0.45
5:E:258:VAL:HA	8:H:5:ILE:HG21	1.97	0.45
10:J:315:TYR:CZ	10:J:319:LYS:HD2	2.51	0.45
3:C:55:GLU:HB3	3:C:58:THR:HG21	1.99	0.45
5:E:156:LYS:HA	5:E:178:VAL:HG12	1.99	0.45
2:B:163:VAL:HG22	2:B:172:LEU:HD12	1.99	0.45
5:E:193:VAL:HG22	5:E:209:ALA:HA	1.99	0.45
10:J:319:LYS:HG2	10:J:326:HIS:CE1	2.52	0.45
3:C:278:GLN:NE2	6:F:20:PHE:O	2.40	0.45
1:A:87:ALA:HB1	1:A:143:CYS:HB2	1.99	0.45
2:B:172:LEU:HD13	2:B:216:ILE:HG22	1.98	0.45
10:J:283:ASN:O	10:J:288:LYS:NZ	2.50	0.45
2:B:53:VAL:HG22	2:B:124:ILE:HG12	1.99	0.45
10:J:215:TRP:HE1	10:J:217:ASP:HB3	1.82	0.45
10:J:236:ALA:HB1	10:J:369:LEU:HD23	1.98	0.45
3:C:90:SER:HB3	6:F:101:LEU:HD22	1.99	0.44
8:H:312:ILE:HD12	8:H:349:LEU:HD21	1.98	0.44
10:J:569:SER:HB3	10:J:574:LYS:HG3	1.99	0.44
1:A:166:ASP:OD2	1:A:182:ARG:NH1	2.51	0.44
10:J:207:SER:HB3	10:J:210:ASP:HB2	1.98	0.44
1:A:20:ARG:NH1	1:A:204:GLN:O	2.50	0.44
1:A:232:ASP:O	2:B:110:LYS:NZ	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:LEU:HD22	5:E:157:LEU:HD23	2.00	0.44
10:J:298:ILE:HG23	10:J:401:PHE:HB2	2.00	0.44
1:A:198:PHE:HB2	1:A:235:LEU:HB3	2.00	0.44
5:E:66:VAL:HG11	5:E:172:PHE:HZ	1.82	0.44
6:F:163:SER:OG	6:F:164:GLN:N	2.51	0.44
7:G:226:ILE:HA	7:G:229:ARG:HE	1.83	0.44
10:J:190:GLN:HG2	10:J:284:PRO:HG3	1.99	0.44
5:E:182:ILE:HG12	5:E:183:ASN:H	1.83	0.43
7:G:138:ASP:C	7:G:140:THR:HA	2.38	0.43
10:J:226:LEU:HD13	10:J:277:LEU:HD23	2.00	0.43
7:G:228:LYS:HG2	7:G:232:LYS:HE3	2.00	0.43
9:I:158:VAL:HG13	9:I:189:SER:HB2	1.98	0.43
6:F:177:THR:HG21	6:F:191:ALA:H	1.83	0.43
7:G:84:TYR:HB2	7:G:97:LEU:HB3	2.01	0.43
2:B:178:GLU:O	2:B:182:MET:HG2	2.19	0.43
9:I:32:ILE:HG21	10:J:534:LEU:HD13	1.99	0.43
7:G:86:VAL:HG11	7:G:134:ILE:HD11	1.99	0.43
4:D:62:ARG:HH12	4:D:101:GLU:HB2	1.84	0.43
4:D:136:ILE:HB	4:D:161:HIS:HB2	2.00	0.43
6:F:58:GLY:HA3	6:F:183:ALA:HB2	1.99	0.43
9:I:270:THR:OG1	9:I:271:ASP:N	2.50	0.43
6:F:50:THR:OG1	6:F:248:GLN:OE1	2.32	0.43
2:B:59:PRO:HG3	2:B:121:VAL:HG23	2.02	0.42
4:D:19:PHE:HE1	4:D:21:SER:HB2	1.84	0.42
3:C:40:ARG:NH2	3:C:339:GLU:OE1	2.43	0.42
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.02	0.42
6:F:53:ILE:HG22	6:F:55:ASN:H	1.84	0.42
10:J:140:ILE:H	10:J:140:ILE:HG13	1.58	0.42
4:D:120:LEU:HG	4:D:125:ILE:HD12	2.02	0.42
1:A:36:VAL:O	1:A:278:GLN:NE2	2.47	0.42
4:D:17:SER:OG	4:D:115:ALA:O	2.34	0.42
10:J:479:ASP:OD1	10:J:479:ASP:N	2.50	0.42
6:F:203:PHE:HB3	6:F:207:GLY:HA2	2.01	0.42
7:G:30:ASN:OD1	7:G:31:THR:N	2.50	0.42
1:A:47:VAL:HG13	1:A:58:CYS:HB3	2.01	0.42
1:A:250:LYS:HE2	1:A:256:MET:HG2	2.02	0.42
3:C:54:ILE:HG22	3:C:80:LEU:HD13	2.01	0.42
7:G:150:LEU:HD13	7:G:195:TRP:CD2	2.55	0.42
7:G:234:ILE:H	7:G:234:ILE:HG13	1.71	0.42
2:B:53:VAL:HG11	2:B:147:LEU:HD23	2.02	0.41
5:E:156:LYS:O	5:E:173:HIS:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:SER:N	7:G:140:THR:HA	2.34	0.41
8:H:64:ASP:HA	8:H:65:PRO:HD3	1.85	0.41
3:C:219:VAL:HG11	3:C:226:VAL:HG21	2.01	0.41
3:C:277:ASP:OD1	3:C:280:LYS:N	2.47	0.41
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.35	0.41
7:G:63:ARG:NH1	7:G:90:ASN:O	2.48	0.41
5:E:222:ILE:HD12	5:E:222:ILE:H	1.84	0.41
7:G:77:ILE:HD13	7:G:87:SER:HB2	2.03	0.41
9:I:205:ILE:HG12	9:I:245:LEU:HB2	2.02	0.41
9:I:221:ILE:H	9:I:221:ILE:HG13	1.73	0.41
10:J:200:ARG:HB2	10:J:377:ARG:HH22	1.84	0.41
1:A:177:HIS:HA	1:A:178:PRO:HD3	1.92	0.41
5:E:80:VAL:HA	5:E:128:VAL:HB	2.01	0.41
1:A:235:LEU:HD13	1:A:250:LYS:HB2	2.02	0.41
5:E:98:LEU:O	5:E:102:VAL:HG23	2.20	0.41
6:F:16:LYS:HA	6:F:17:PRO:HD3	1.94	0.41
7:G:64:TYR:HA	7:G:160:LEU:HD21	2.03	0.41
8:H:193:LYS:NZ	8:H:283:ASP:OD1	2.35	0.41
2:B:58:GLU:HG2	8:H:132:GLN:HA	2.03	0.41
3:C:74:ILE:HD11	6:F:101:LEU:HB3	2.03	0.41
8:H:299:ARG:HD2	8:H:323:TYR:CE1	2.55	0.41
9:I:36:VAL:HA	9:I:37:PRO:HD3	1.95	0.41
10:J:174:ASN:HA	10:J:409:LEU:HB2	2.03	0.41
10:J:557:ILE:H	10:J:557:ILE:HG13	1.72	0.41
3:C:130:VAL:HG12	3:C:213:LEU:HB2	2.03	0.41
10:J:395:ASN:HA	10:J:398:LYS:HG2	2.02	0.41
3:C:140:ARG:HD2	9:I:197:LEU:HD11	2.02	0.40
7:G:14:ASP:OD2	7:G:16:THR:OG1	2.39	0.40
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.56	0.40
3:C:278:GLN:HG3	6:F:20:PHE:HB3	2.03	0.40
4:D:140:LYS:HB2	4:D:158:LEU:HB2	2.03	0.40
4:D:106:LEU:HD21	4:D:183:ASN:HD22	1.85	0.40
5:E:24:ASP:OD2	5:E:26:ARG:NE	2.53	0.40
7:G:123:VAL:HG22	7:G:134:ILE:HG22	2.03	0.40
5:E:78:VAL:HG22	5:E:126:VAL:HB	2.04	0.40
8:H:62:THR:HB	8:H:90:ARG:HH22	1.86	0.40
8:H:196:ASN:ND2	8:H:286:ASP:HB2	2.36	0.40
3:C:129:SER:OG	3:C:130:VAL:N	2.54	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	289/305 (95%)	282 (98%)	7 (2%)	0	100	100
2	B	237/250 (95%)	227 (96%)	10 (4%)	0	100	100
3	C	300/394 (76%)	289 (96%)	11 (4%)	0	100	100
4	D	219/225 (97%)	207 (94%)	12 (6%)	0	100	100
5	E	251/269 (93%)	242 (96%)	9 (4%)	0	100	100
6	F	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
7	G	222/244 (91%)	209 (94%)	13 (6%)	0	100	100
8	H	271/363 (75%)	261 (96%)	10 (4%)	0	100	100
9	I	208/296 (70%)	196 (94%)	12 (6%)	0	100	100
10	J	489/560 (87%)	465 (95%)	24 (5%)	0	100	100
All	All	2687/3156 (85%)	2572 (96%)	115 (4%)	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	257/266 (97%)	257 (100%)	0	100	100
2	B	213/221 (96%)	212 (100%)	1 (0%)	88	93
3	C	274/349 (78%)	273 (100%)	1 (0%)	91	95
4	D	194/198 (98%)	192 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	230/243 (95%)	226 (98%)	4 (2%)	60	78
6	F	177/219 (81%)	177 (100%)	0	100	100
7	G	198/212 (93%)	197 (100%)	1 (0%)	88	93
8	H	238/314 (76%)	238 (100%)	0	100	100
9	I	177/243 (73%)	175 (99%)	2 (1%)	73	85
10	J	456/517 (88%)	454 (100%)	2 (0%)	91	95
All	All	2414/2782 (87%)	2401 (100%)	13 (0%)	88	93

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

Mol	Chain	Res	Type
2	B	166	TYR
3	C	336	THR
4	D	24	THR
4	D	174	VAL
5	E	122	PHE
5	E	136	HIS
5	E	157	LEU
5	E	178	VAL
7	G	137	PHE
9	I	234	VAL
9	I	279	VAL
10	J	159	LEU
10	J	199	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
2	B	101	GLN
7	G	159	ASN
10	J	345	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	S	5/24 (20%)	3 (60%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	S	20	A
11	S	21	A
11	S	22	A

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	PO4	S	102	-	4,4,4	0.91	0	6,6,6	0.43	0
13	MPD	E	302	-	7,7,7	0.31	0	9,10,10	0.34	0
15	PO4	I	301	-	4,4,4	0.92	0	6,6,6	0.43	0
14	MES	G	301	-	5,5,12	1.51	1 (20%)	7,7,16	1.65	3 (42%)

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	MPD	E	302	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MES	G	301	-	-	0/3/3/14	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	301	MES	C8-S	-2.89	1.66	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	301	MES	O3S-S-C8	2.28	109.45	105.77
14	G	301	MES	O2S-S-C8	2.19	109.55	106.92
14	G	301	MES	O1S-S-C8	2.13	109.48	106.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	293/305 (96%)	0.08	10 (3%) 45 43	80, 122, 175, 265	0
2	B	239/250 (95%)	-0.01	3 (1%) 77 77	55, 91, 152, 185	0
3	C	312/394 (79%)	0.44	32 (10%) 6 6	70, 130, 166, 185	0
4	D	221/225 (98%)	0.32	4 (1%) 68 67	89, 125, 172, 193	0
5	E	255/269 (94%)	0.20	12 (4%) 31 29	68, 98, 167, 196	0
6	F	207/250 (82%)	0.15	10 (4%) 30 28	65, 93, 154, 178	0
7	G	226/244 (92%)	0.60	28 (12%) 4 3	89, 140, 201, 265	0
8	H	279/363 (76%)	0.13	9 (3%) 47 46	62, 95, 176, 239	0
9	I	216/296 (72%)	0.50	25 (11%) 4 4	94, 135, 207, 278	0
10	J	493/560 (88%)	0.32	35 (7%) 16 16	72, 141, 197, 234	0
11	S	6/24 (25%)	0.43	0 100 100	131, 140, 205, 208	0
All	All	2747/3180 (86%)	0.27	168 (6%) 21 20	55, 122, 181, 278	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	122	PHE	6.3
8	H	13	ALA	6.3
3	C	95	ILE	6.2
6	F	100	GLY	5.9
9	I	113	GLY	5.5
7	G	21	LEU	5.2
7	G	11	PHE	5.1
7	G	19	VAL	4.8
9	I	24	GLU	4.7
7	G	13	VAL	4.7
10	J	472	LEU	4.5
7	G	2	SER	4.4

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Mol	Chain	Res	Type	RSRZ
10	J	617	ILE	4.2
3	C	209	TRP	4.2
3	C	246	ALA	4.1
7	G	39	THR	4.1
10	J	476	THR	4.1
10	J	534	LEU	4.1
10	J	441	LEU	3.8
3	C	351	ALA	3.8
1	A	172	GLU	3.8
6	F	101	LEU	3.8
8	H	7	ILE	3.7
10	J	346	LEU	3.7
9	I	246	THR	3.7
6	F	143	TYR	3.7
7	G	154	MET	3.7
5	E	155	PRO	3.6
10	J	501	LEU	3.6
4	D	1	MET	3.6
9	I	243	TYR	3.6
8	H	6	THR	3.6
10	J	173	GLU	3.5
10	J	448	TRP	3.5
5	E	75	LEU	3.5
2	B	4	LEU	3.5
10	J	618	PHE	3.5
9	I	8	PRO	3.5
7	G	75	VAL	3.5
9	I	196	ASP	3.4
7	G	57	ILE	3.4
7	G	14	ASP	3.4
3	C	243	LEU	3.3
3	C	211	TYR	3.3
9	I	47	GLU	3.3
9	I	34	ASN	3.3
9	I	31	ILE	3.2
5	E	109	VAL	3.2
9	I	245	LEU	3.2
7	G	208	TYR	3.2
1	A	14	PHE	3.1
3	C	94	GLY	3.1
3	C	273	GLU	3.1
3	C	174	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	2	SER	3.1
2	B	123	ASP	3.0
10	J	147	PRO	3.0
1	A	3	LYS	3.0
1	A	136	ALA	3.0
9	I	30	ASP	3.0
7	G	73	ILE	3.0
5	E	2	SER	3.0
10	J	167	ARG	3.0
3	C	37	LEU	3.0
3	C	175	GLY	2.9
5	E	114	LEU	2.9
1	A	187	LEU	2.9
1	A	25	LEU	2.9
3	C	213	LEU	2.9
10	J	354	LEU	2.8
9	I	33	PHE	2.8
6	F	19	ALA	2.8
9	I	46	TYR	2.8
8	H	357	ASN	2.8
9	I	21	TYR	2.8
9	I	140	LEU	2.8
7	G	119	VAL	2.8
6	F	43	GLU	2.7
8	H	143	LEU	2.7
9	I	224	PHE	2.7
9	I	32	ILE	2.7
3	C	189	TYR	2.7
3	C	242	LYS	2.7
10	J	528	LYS	2.7
3	C	101	ALA	2.7
7	G	196	VAL	2.7
10	J	325	ARG	2.6
3	C	212	VAL	2.6
10	J	509	LEU	2.6
8	H	5	ILE	2.6
5	E	123	LYS	2.6
1	A	167	ILE	2.6
7	G	188	ILE	2.6
10	J	557	ILE	2.6
10	J	555	SER	2.6
10	J	505	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
7	G	195	TRP	2.6
8	H	8	THR	2.6
3	C	328	THR	2.6
3	C	300	VAL	2.5
3	C	248	ILE	2.5
10	J	406	TYR	2.5
3	C	172	VAL	2.5
6	F	248	GLN	2.5
1	A	239	LEU	2.5
7	G	74	GLY	2.5
9	I	210	VAL	2.5
5	E	154	LEU	2.5
6	F	16	LYS	2.5
4	D	5	ALA	2.5
7	G	153	GLY	2.5
9	I	197	LEU	2.5
4	D	97	SER	2.5
5	E	180	LEU	2.4
10	J	152	LEU	2.4
7	G	20	LYS	2.4
9	I	269	ALA	2.4
7	G	40	GLY	2.4
9	I	155	ILE	2.4
6	F	193	ALA	2.4
7	G	56	TYR	2.4
6	F	147	LEU	2.4
8	H	138	LEU	2.4
5	E	124	ILE	2.4
3	C	100	SER	2.4
10	J	429	MET	2.4
10	J	349	TRP	2.3
10	J	174	ASN	2.3
7	G	162	PHE	2.3
3	C	59	LEU	2.3
9	I	237	LEU	2.3
9	I	23	THR	2.3
1	A	159	LEU	2.2
5	E	116	LEU	2.2
7	G	36	PRO	2.2
3	C	12	ILE	2.2
5	E	145	ILE	2.2
10	J	331	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	230	CYS	2.2
2	B	185	VAL	2.2
10	J	484	VAL	2.2
10	J	446	TYR	2.1
10	J	560	SER	2.1
3	C	9	THR	2.1
3	C	176	VAL	2.1
3	C	329	VAL	2.1
3	C	75	LEU	2.1
7	G	108	LYS	2.1
10	J	438	ARG	2.1
10	J	483	VAL	2.1
7	G	12	PRO	2.1
3	C	299	ILE	2.1
6	F	142	THR	2.1
9	I	25	ASN	2.1
3	C	282	VAL	2.1
9	I	278	PRO	2.1
10	J	338	PHE	2.1
10	J	536	THR	2.1
10	J	395	ASN	2.0
10	J	419	ILE	2.0
1	A	174	ILE	2.0
7	G	88	LEU	2.0
3	C	292	ALA	2.0
7	G	55	ALA	2.0
7	G	141	THR	2.0
8	H	300	TYR	2.0
3	C	247	PHE	2.0
10	J	486	LEU	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, 95th 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
14	MES	G	301	6/12	0.59	0.55	136,164,166,170	0
13	MPD	E	302	8/8	0.71	0.53	78,95,113,115	0
15	PO4	I	301	5/5	0.76	0.35	165,172,186,193	0
15	PO4	S	102	5/5	0.81	0.18	153,157,178,180	0
12	MG	S	101	1/1	0.84	0.13	135,135,135,135	0
12	MG	E	301	1/1	0.86	0.24	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.