



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:23 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

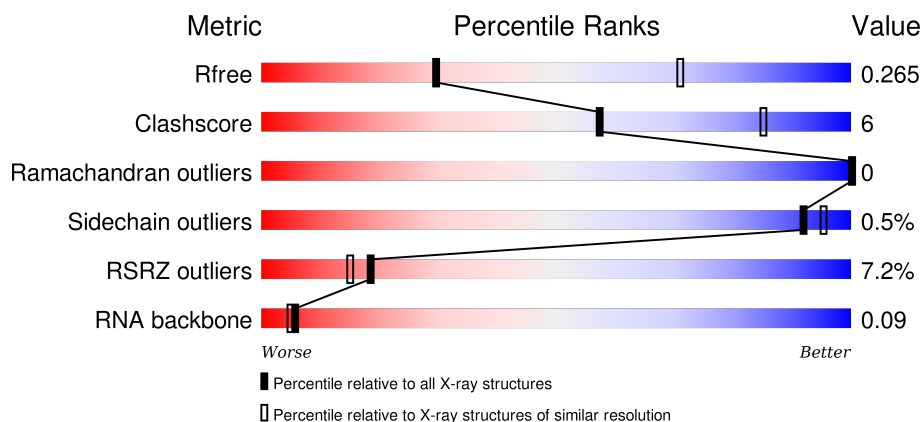
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.





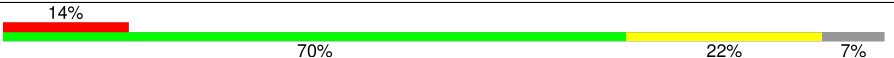
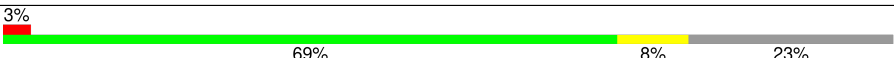
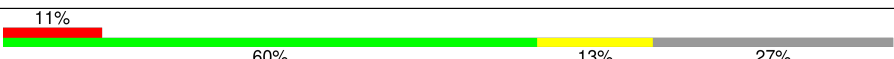
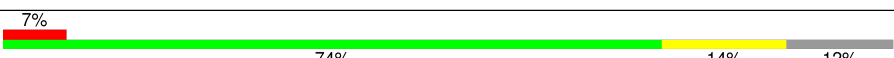
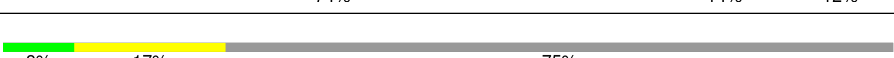
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
2	B	250	<div> <div>2%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
3	C	394	<div> <div>10%</div> <div>63%</div> <div>16%</div> <div>21%</div> </div>
4	D	225	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>

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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	560	
11	S	24	

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

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
1	A	293	Total	C	N	O	S	0	0	0
			2282	1434	388	443	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
			1879	1176	334	361	8			

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

- 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
			1689	1061	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	255	Total	C	N	O	S	0	0	0
			1964	1255	326	379	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
			1600	1004	271	315	10			

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

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

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	279	Total	C	N	O	S	0	0	0
			2159	1350	389	408	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	216	Total	C	N	O	S	0	0	0
			1650	1036	288	319	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	493	Total	C	N	O	S	0	0	0
			4034	2577	693	754	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

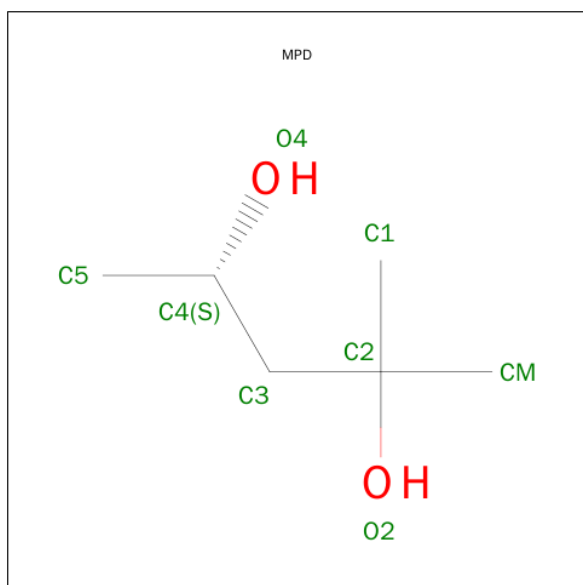
- Molecule 11 is a RNA chain called POLY A RNA.

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

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

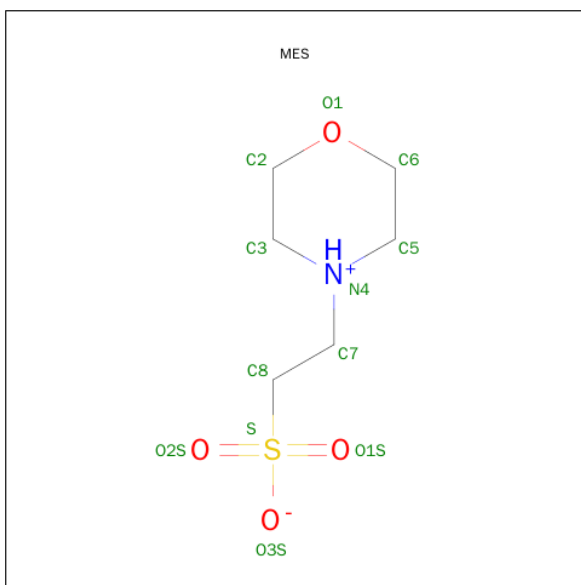
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	S	1	Total	Mg	0	0
			1	1		
12	E	1	Total	Mg	0	0
			1	1		

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



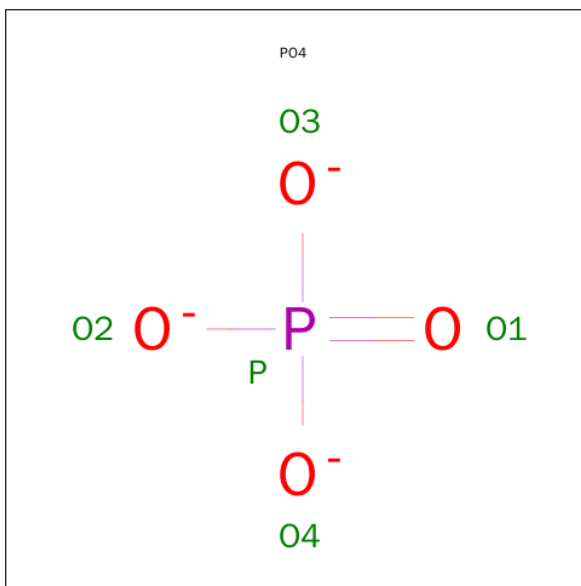
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	C	O	0	0
			8	6	2		

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



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

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

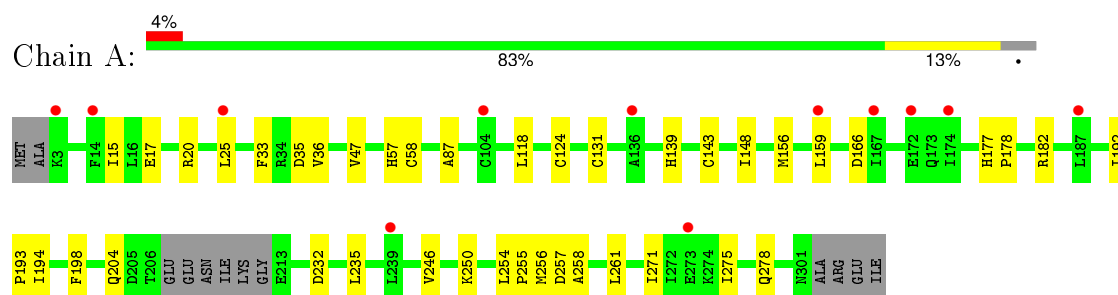


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	I	1	Total	O	P	0	0
			5	4	1		
15	S	1	Total	O	P	0	0
			5	4	1		

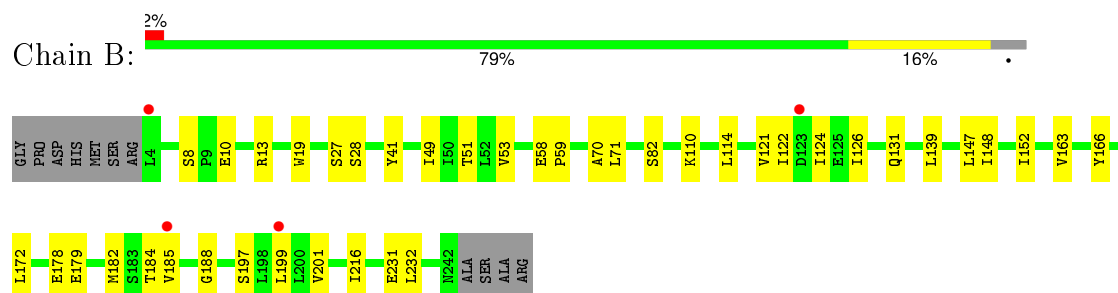
3 Residue-property plots [i](#)

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

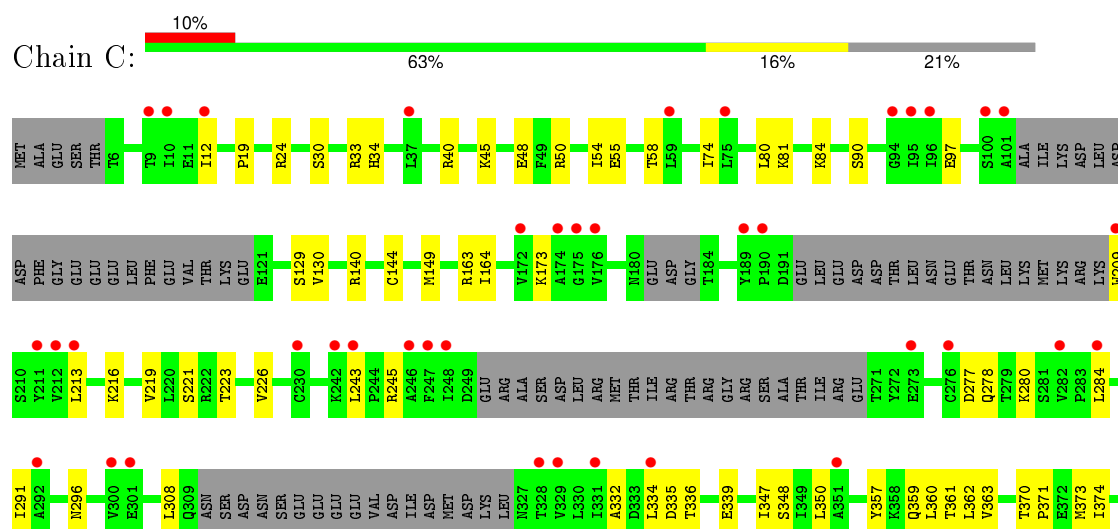
- Molecule 1: Exosome complex component RRP45



- Molecule 2: Exosome complex component SKI6

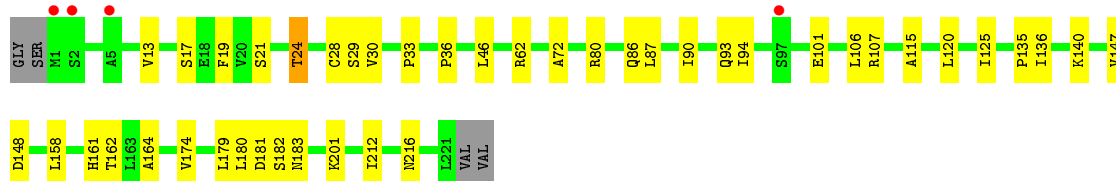
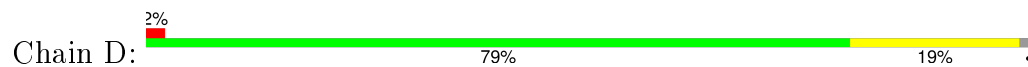


- Molecule 3: Exosome complex component RRP43

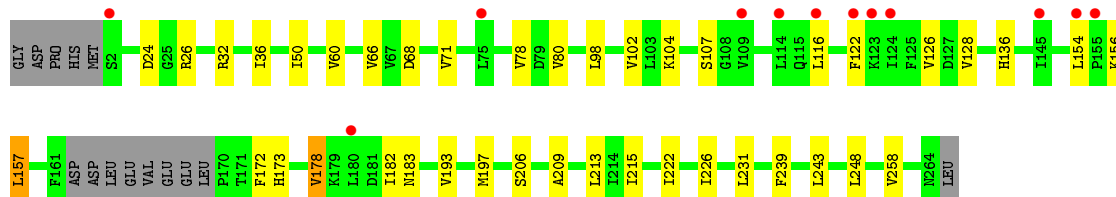
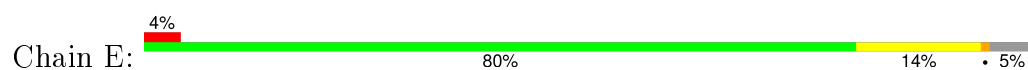




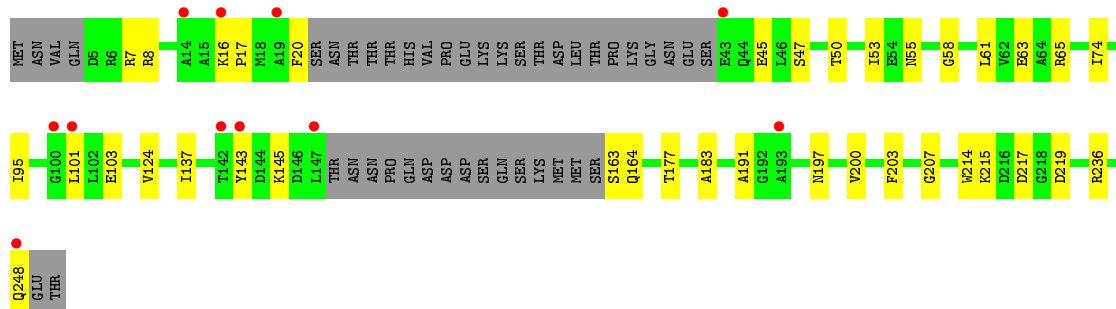
• Molecule 4: Exosome complex component RRP46



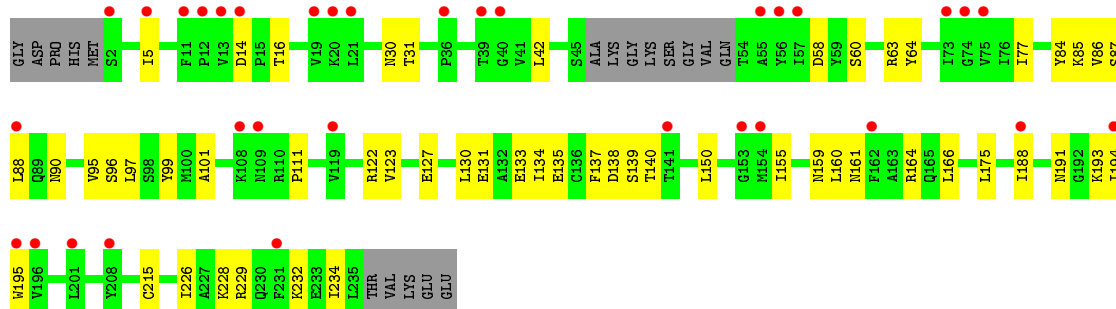
• Molecule 5: Exosome complex component RRP42



• Molecule 6: Exosome complex component MTR3



• Molecule 7: Exosome complex component RRP40



Chain H:

Position	Amino Acid	Conservation (bits)
1	GLY	0.00
2	ASP	0.00
3	PRO	0.00
4	HIS	0.00
5	MET	0.00
6	SER	0.00
7	GLU	0.00
8	VAL	0.00
9	T5	0.00
10	T6	0.00
11	I7	0.00
12	T8	0.00
13	A13	0.00
14	F14	0.00
15	GLN	0.00
16	ASN	0.00
17	SER	0.00
18	SER	0.00
19	ASN	0.00
20	LEU	0.00
21	SER	0.00
22	TYR	0.00
23	ASN	0.00
24	ASN	0.00
25	THR	0.00
26	GLY	0.00
27	ILE	0.00
28	SER	0.00
29	ASP	0.00
30	ASP	0.00
31	GLU	0.00
32	ASN	0.00
33	ASP	0.00
34	GLU	0.00
35	GLU	0.00
36	ASP	0.00
37	GLU	0.00
38	ASP	0.00
39	ASP	0.00
40	ASP	0.00
41	ASP	0.00
42	ASP	0.00
43	ASP	0.00
44	ASP	0.00
45	ASP	0.00
46	ASP	0.00
47	ASP	0.00
48	ASP	0.00
49	ASP	0.00
50	ASP	0.00
51	ASP	0.00
52	ASP	0.00
53	ASP	0.00
54	ASP	0.00
55	ASP	0.00
56	ASP	0.00
57	ASP	0.00
58	ASP	0.00
59	ASP	0.00
60	ASP	0.00
61	ASP	0.00
62	ASP	0.00
63	ASP	0.00
64	ASP	0.00
65	ASP	0.00
66	ASP	0.00
67	ASP	0.00
68	ASP	0.00
69	ASP	0.00
70	ASP	0.00
71	ASP	0.00
72	ASP	0.00
73	ASP	0.00
74	ASP	0.00
75	ASP	0.00
76	ASP	0.00
77	ASP	0.00
78	ASP	0.00
79	ASP	0.00
80	ASP	0.00
81	ASP	0.00
82	ASP	0.00
83	ASP	0.00
84	ASP	0.00
85	ASP	0.00
86	ASP	0.00
87	ASP	0.00
88	ASP	0.00
89	ASP	0.00
90	ASP	0.00
91	ASP	0.00
92	ASP	0.00
93	ASP	0.00
94	ASP	0.00
95	ASP	0.00
96	ASP	0.00
97	ASP	0.00
98	ASP	0.00
99	ASP	0.00
100	ASP	0.00

Chain I:

11% 60% 13% 27%

GLY ASP PRQ HIS MET ALA CYS ASN F5 Q6 F7 F8 I17 Y21 G22 T23 E24 N25 D30 I31 I32 F33 N34 Y35 V36 P37 G38 T41 Y46 E47 R51 A58 F70 LYS THR ASP GLN GLU GLU ARG GLU GLY THR ASP GLN THR THR THR GLU GLU LYS SER PRO ILE ASP SER GLY ILE GLY ASN

SER VAL ASP ALA SER PRO ASN VAL THR ARG ARG THR VAL LYS H105 G113 THR GLU LYS ARG LYS THR ASN LYS TYR ALA ASN ASP ASP F128 I138 V139 L140 T141 R142 V143 V153 E154 I155 A156 A157 V158 E159 P162 SER PRO ILE ASP SER GLY ILE GLY ASN

GLY SER GLY ILE VAL ALA GLY GLY SER GLY ALA A186 S189 D196 L197 I205 V210 R211 I221 E222 G223 F224 D228 I229 V230 R231 V234 L237 V243 Y244 L245 T246 T247 A248 V254 R258 G262 M267 Y268 A269 T270 D271 M272 Q273 M274

S277 P278 V279 K285 R286 K287 P291 PHE

[illegible]

● Molecule 11: POLY A RNA



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.227 , 0.265 0.226 , 0.265	Depositor DCC
R_{free} test set	2855 reflections (5.07%)	DCC
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 , 20.7	EDS
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 56332 reflections (0.002%)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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:374:ASP:O	10:J:378:ASN:ND2	2.34	0.59
10:J:345:GLN:NE2	11:S:24:A:N7	2.50	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
10:J:198:GLN:O	10:J:377:ARG:NH1	2.37	0.57
8:H:217:LEU:HD11	8:H:223:VAL:HG12	1.85	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
4:D:24:THR:HG22	4:D:107:ARG:HH21	1.71	0.56
3:C:216:LYS:NZ	6:F:103:GLU:OE2	2.38	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
7:G:166:LEU:HD11	7:G:175:LEU:HD13	1.90	0.54
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.89	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
10:J:174:ASN:HD22	10:J:410:THR:HB	1.73	0.52
7:G:101:ALA:HB1	7:G:135:GLU:HA	1.91	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
10:J:623:PRO:HG2	10:J:624:LEU:HD22	1.93	0.52
8:H:216:ASN:ND2	8:H:240:ASP:O	2.38	0.52
3:C:357:TYR:OH	3:C:382:ARG:NH2	2.43	0.51
1:A:118:LEU:HD12	1:A:159:LEU:HD13	1.90	0.51
1:A:15:ILE:HG12	1:A:25:LEU:HD11	1.92	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
6:F:63:GLU:OE1	10:J:572:LEU:N	2.35	0.51
2:B:49:ILE:HD13	2:B:139:LEU:HD23	1.92	0.51
4:D:135:PRO:HG2	4:D:148:ASP:HA	1.93	0.51
2:B:148:ILE:HG21	2:B:232:LEU:HD21	1.93	0.51
10:J:491:THR:OG1	10:J:492:GLU:N	2.42	0.51
10:J:266:ASP:OD2	10:J:352:ARG:NH1	2.39	0.51
1:A:35:ASP:OD1	1:A:35:ASP:N	2.43	0.51
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
2:B:82:SER:HB2	2:B:131:GLN:HG2	1.93	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:194:ILE:HG21	1:A:275:ILE:HD11	1.94	0.50
1:A:156:MET:HE2	1:A:192:ILE:HG13	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)
10:J:356:LYS:HG3	10:J:357:PRO:HD3	1.93	0.50
8:H:124:TRP:HB2	8:H:136:LEU:HB3	1.93	0.50
10:J:227:GLU:HA	10:J:230:LYS:HE2	1.94	0.50
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
3:C:30:SER:O	3:C:34:HIS:ND1	2.38	0.49
7:G:95:VAL:HG11	7:G:134:ILE:HG23	1.93	0.49
7:G:138:ASP:OD1	7:G:139:SER:N	2.45	0.49
7:G:127:GLU:HB2	7:G:130:LEU:HB3	1.93	0.49
7:G:58:ASP:OD1	7:G:164:ARG:NH1	2.46	0.49
3:C:164:ILE:HD12	3:C:291:ILE:HD13	1.93	0.49
2:B:13:ARG:HH21	2:B:19:TRP:HA	1.78	0.49
4:D:30:VAL:HG21	4:D:120:LEU:HD12	1.95	0.49
2:B:8:SER:OG	2:B:10:GLU:OE1	2.31	0.49
3:C:362:LEU:HB2	4:D:180:LEU:HB3	1.93	0.49
3:C:12:ILE:HD11	10:J:616:ILE:HB	1.94	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
9:I:141:THR:HG22	9:I:155:ILE:HA	1.95	0.48
8:H:198:MET:HE2	8:H:297:ILE:HG22	1.96	0.48
2:B:185:VAL:HG22	2:B:201:VAL:HG22	1.94	0.48
10:J:239:LEU:HD11	10:J:300:LEU:HG	1.96	0.48
5:E:36:ILE:HG12	5:E:50:ILE:HG12	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
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:45:LYS:HB2	3:C:48:GLU:HG3	1.95	0.47
3:C:19:PRO:HG3	10:J:607:LYS:HG2	1.95	0.47
2:B:188:GLY:O	2:B:197:SER:N	2.40	0.47
4:D:30:VAL:HG11	4:D:125:ILE:HD11	1.96	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
5:E:154:LEU:HB2	5:E:178:VAL:HG13	1.96	0.47
4:D:28:CYS:SG	4:D:29:SER:N	2.88	0.47
3:C:149:MET:HE2	6:F:7:ARG:HG3	1.97	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:261:LEU:HD13	2:B:199:LEU:HD22	1.97	0.47
1:A:148:ILE:HD12	1:A:148:ILE:H	1.80	0.47
10:J:149:ILE:HD12	10:J:150:PRO:HD2	1.96	0.47
9:I:254:VAL:N	9:I:287:LYS:O	2.36	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
9:I:159:GLU:OE1	9:I:231:ARG:NH2	2.49	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
10:J:274:LEU:HD12	10:J:304:LEU:HD22	1.98	0.46
2:B:28:SER:HB2	2:B:41:TYR:HB3	1.97	0.46
3:C:144:CYS:SG	6:F:8:ARG:NE	2.89	0.46
6:F:45:GLU:HA	10:J:565:VAL:HG11	1.97	0.45
4:D:30:VAL:HG22	4:D:90:ILE:HG12	1.98	0.45
3:C:84:LYS:HE3	3:C:223:THR:HG21	1.98	0.45
9:I:222:GLU:HB3	9:I:285:LYS:HD3	1.97	0.45
10:J:315:TYR:CZ	10:J:319:LYS:HD2	2.51	0.45
5:E:258:VAL:HA	8:H:5:ILE:HG21	1.97	0.45
5:E:156:LYS:HA	5:E:178:VAL:HG12	1.99	0.45
3:C:55:GLU:HB3	3:C:58:THR:HG21	1.99	0.45
2:B:163:VAL:HG22	2:B:172:LEU:HD12	1.99	0.45
10:J:319:LYS:HG2	10:J:326:HIS:CE1	2.52	0.45
5:E:193:VAL:HG22	5:E:209:ALA:HA	1.99	0.45
3:C:278:GLN:NE2	6:F:20:PHE:O	2.40	0.45
2:B:172:LEU:HD13	2:B:216:ILE:HG22	1.98	0.45
1:A:87:ALA:HB1	1:A:143:CYS:HB2	1.99	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
8:H:312:ILE:HD12	8:H:349:LEU:HD21	1.98	0.44
3:C:90:SER:HB3	6:F:101:LEU:HD22	1.99	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)
10:J:298:ILE:HG23	10:J:401:PHE:HB2	2.00	0.44
5:E:116:LEU:HD22	5:E:157:LEU:HD23	2.00	0.44
7:G:226:ILE:HA	7:G:229:ARG:HE	1.83	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
1:A:198:PHE:HB2	1:A:235:LEU:HB3	2.00	0.44
10:J:190:GLN:HG2	10:J:284:PRO:HG3	1.99	0.44
7:G:138:ASP:C	7:G:140:THR:HA	2.38	0.43
5:E:182:ILE:HG12	5:E:183:ASN:H	1.83	0.43
10:J:226:LEU:HD13	10:J:277:LEU:HD23	2.00	0.43
9:I:158:VAL:HG13	9:I:189:SER:HB2	1.98	0.43
7:G:228:LYS:HG2	7:G:232:LYS:HE3	2.00	0.43
7:G:84:TYR:HB2	7:G:97:LEU:HB3	2.01	0.43
6:F:177:THR:HG21	6:F:191:ALA:H	1.83	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
9:I:270:THR:OG1	9:I:271:ASP:N	2.50	0.43
6:F:58:GLY:HA3	6:F:183:ALA:HB2	1.99	0.43
4:D:136:ILE:HB	4:D:161:HIS:HB2	2.00	0.43
4:D:62:ARG:HH12	4:D:101:GLU:HB2	1.84	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
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
1:A:254:LEU:HD12	1:A:255:PRO:HD2	2.02	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
10:J:479:ASP:OD1	10:J:479:ASP:N	2.50	0.42
4:D:17:SER:OG	4:D:115:ALA:O	2.34	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
7:G:150:LEU:HD13	7:G:195:TRP:CD2	2.55	0.42
7:G:234:ILE:HG13	7:G:234:ILE:H	1.71	0.42
3:C:54:ILE:HG22	3:C:80:LEU:HD13	2.01	0.42
5:E:156:LYS:O	5:E:173:HIS:N	2.49	0.41
2:B:53:VAL:HG11	2:B:147:LEU:HD23	2.02	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
7:G:63:ARG:NH1	7:G:90:ASN:O	2.48	0.41
5:E:26:ARG:NH1	5:E:32:ARG:HG3	2.35	0.41
10:J:200:ARG:HB2	10:J:377:ARG:HH22	1.84	0.41
9:I:221:ILE:H	9:I:221:ILE:HG13	1.73	0.41
9:I:205:ILE:HG12	9:I:245:LEU:HB2	2.02	0.41
7:G:77:ILE:HD13	7:G:87:SER:HB2	2.03	0.41
5:E:222:ILE:H	5:E:222:ILE:HD12	1.84	0.41
5:E:80:VAL:HA	5:E:128:VAL:HB	2.01	0.41
1:A:177:HIS:HA	1:A:178:PRO:HD3	1.92	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
8:H:193:LYS:NZ	8:H:283:ASP:OD1	2.35	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
2:B:58:GLU:HG2	8:H:132:GLN:HA	2.03	0.41
10:J:174:ASN:HA	10:J:409:LEU:HB2	2.03	0.41
3:C:74:ILE:HD11	6:F:101:LEU:HB3	2.03	0.41
9:I:36:VAL:HA	9:I:37:PRO:HD3	1.95	0.41
10:J:557:ILE:HG13	10:J:557:ILE:H	1.72	0.41
8:H:299:ARG:HD2	8:H:323:TYR:CE1	2.55	0.41
10:J:395:ASN:HA	10:J:398:LYS:HG2	2.02	0.41
3:C:130:VAL:HG12	3:C:213:LEU:HB2	2.03	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
4:D:140:LYS:HB2	4:D:158:LEU:HB2	2.03	0.40
3:C:278:GLN:HG3	6:F:20:PHE:HB3	2.03	0.40
3:C:97:GLU:HG2	3:C:209:TRP:CD1	2.56	0.40
4:D:106:LEU:HD21	4:D:183:ASN:HD22	1.85	0.40
7:G:123:VAL:HG22	7:G:134:ILE:HG22	2.03	0.40
5:E:24:ASP:OD2	5:E:26:ARG:NE	2.53	0.40
5:E:78:VAL:HG22	5:E:126:VAL:HB	2.04	0.40
8:H:196:ASN:ND2	8:H:286:ASP:HB2	2.36	0.40
8:H:62:THR:HB	8:H:90:ARG:HH22	1.86	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

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	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

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%)	92	95
3	C	274/349 (78%)	273 (100%)	1 (0%)	93	96
4	D	194/198 (98%)	192 (99%)	2 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	230/243 (95%)	226 (98%)	4 (2%)	68	86
6	F	177/219 (81%)	177 (100%)	0	100	100
7	G	198/212 (93%)	197 (100%)	1 (0%)	92	95
8	H	238/314 (76%)	238 (100%)	0	100	100
9	I	177/243 (73%)	175 (99%)	2 (1%)	80	90
10	J	456/517 (88%)	454 (100%)	2 (0%)	93	96
All	All	2414/2782 (87%)	2401 (100%)	13 (0%)	92	95

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

Some 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 ⓘ

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 carbohydrates 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	$\# Z > 2$
13	MPD	E	302	-	6,7,7	0.31	0	7,10,10	0.53	0
14	MES	G	301	-	5,5,12	3.45	1 (20%)	6,7,16	1.98	2 (33%)
15	PO4	I	301	-	4,4,4	0.48	0	6,6,6	0.27	0
15	PO4	S	102	-	4,4,4	0.48	0	6,6,6	0.27	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	MPD	E	302	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MES	G	301	-	-	0/3/3/14	0/0/0/1
15	PO4	I	301	-	-	0/0/0/0	0/0/0/0
15	PO4	S	102	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	301	MES	C8-S	-7.52	1.66	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	301	MES	O1S-S-C8	3.02	109.48	106.91
14	G	301	MES	O2S-S-C8	3.10	109.55	106.91

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 ⓘ

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, 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%)	0.11	12 (4%) 41 34	80, 122, 175, 265	0
2	B	239/250 (95%)	0.02	4 (1%) 73 67	55, 91, 152, 185	0
3	C	312/394 (79%)	0.49	39 (12%) 5 4	70, 130, 166, 185	0
4	D	221/225 (98%)	0.35	4 (1%) 71 65	89, 125, 172, 193	0
5	E	255/269 (94%)	0.25	12 (4%) 35 29	68, 98, 167, 196	0
6	F	207/250 (82%)	0.19	11 (5%) 30 24	65, 93, 154, 178	0
7	G	226/244 (92%)	0.65	33 (14%) 3 3	89, 140, 201, 265	0
8	H	279/363 (76%)	0.17	11 (3%) 43 36	62, 95, 176, 239	0
9	I	216/296 (72%)	0.55	32 (14%) 3 3	94, 135, 207, 278	0
10	J	493/560 (88%)	0.37	41 (8%) 14 11	72, 141, 197, 234	0
11	S	6/24 (25%)	0.52	0 100 100	131, 140, 205, 208	0
All	All	2747/3180 (86%)	0.31	199 (7%) 18 15	55, 122, 181, 278	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	95	ILE	6.6
5	E	122	PHE	6.6
6	F	100	GLY	6.0
8	H	13	ALA	6.0
9	I	113	GLY	5.6
7	G	21	LEU	5.4
7	G	11	PHE	5.1
7	G	13	VAL	5.0
9	I	24	GLU	4.9
7	G	19	VAL	4.5
3	C	246	ALA	4.4
10	J	472	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
10	J	476	THR	4.3
3	C	209	TRP	4.2
10	J	534	LEU	4.2
8	H	7	ILE	4.2
8	H	6	THR	4.1
1	A	172	GLU	4.0
10	J	617	ILE	4.0
7	G	39	THR	4.0
7	G	2	SER	4.0
3	C	351	ALA	3.9
10	J	441	LEU	3.9
6	F	143	TYR	3.9
10	J	346	LEU	3.9
7	G	57	ILE	3.8
7	G	14	ASP	3.8
6	F	101	LEU	3.8
7	G	75	VAL	3.7
10	J	173	GLU	3.7
10	J	448	TRP	3.7
7	G	154	MET	3.7
9	I	243	TYR	3.7
10	J	501	LEU	3.7
10	J	618	PHE	3.6
9	I	196	ASP	3.6
4	D	1	MET	3.6
9	I	246	THR	3.6
5	E	155	PRO	3.6
2	B	4	LEU	3.5
8	H	5	ILE	3.4
3	C	174	ALA	3.4
2	B	123	ASP	3.4
5	E	109	VAL	3.4
3	C	94	GLY	3.4
7	G	208	TYR	3.4
9	I	34	ASN	3.4
5	E	114	LEU	3.4
5	E	75	LEU	3.3
9	I	245	LEU	3.3
3	C	273	GLU	3.3
3	C	243	LEU	3.3
3	C	211	TYR	3.3
9	I	47	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	PHE	3.2
5	E	2	SER	3.2
4	D	2	SER	3.2
9	I	8	PRO	3.2
9	I	31	ILE	3.2
3	C	175	GLY	3.2
9	I	30	ASP	3.1
1	A	3	LYS	3.1
10	J	354	LEU	3.1
3	C	37	LEU	3.1
7	G	73	ILE	3.1
10	J	147	PRO	3.1
9	I	21	TYR	3.1
1	A	187	LEU	3.0
1	A	136	ALA	3.0
10	J	509	LEU	3.0
1	A	25	LEU	3.0
6	F	43	GLU	3.0
7	G	188	ILE	2.9
10	J	167	ARG	2.9
8	H	357	ASN	2.9
3	C	213	LEU	2.9
9	I	224	PHE	2.9
9	I	33	PHE	2.9
9	I	140	LEU	2.9
9	I	46	TYR	2.8
10	J	528	LYS	2.8
3	C	189	TYR	2.8
10	J	555	SER	2.8
3	C	172	VAL	2.8
8	H	8	THR	2.8
3	C	212	VAL	2.8
6	F	16	LYS	2.8
10	J	557	ILE	2.8
5	E	123	LYS	2.8
10	J	174	ASN	2.7
6	F	19	ALA	2.7
1	A	167	ILE	2.7
5	E	154	LEU	2.7
7	G	119	VAL	2.7
8	H	143	LEU	2.7
4	D	97	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	300	VAL	2.7
7	G	195	TRP	2.7
7	G	74	GLY	2.6
9	I	23	THR	2.6
10	J	325	ARG	2.6
9	I	155	ILE	2.6
5	E	180	LEU	2.6
7	G	40	GLY	2.6
9	I	6	GLN	2.6
3	C	328	THR	2.6
8	H	138	LEU	2.5
10	J	505	ILE	2.5
3	C	242	LYS	2.5
3	C	248	ILE	2.5
10	J	483	VAL	2.5
9	I	32	ILE	2.5
7	G	108	LYS	2.5
7	G	153	GLY	2.5
9	I	210	VAL	2.5
6	F	248	GLN	2.5
9	I	197	LEU	2.5
10	J	406	TYR	2.5
1	A	239	LEU	2.5
10	J	349	TRP	2.4
10	J	338	PHE	2.4
3	C	59	LEU	2.4
5	E	124	ILE	2.4
7	G	196	VAL	2.4
6	F	193	ALA	2.4
10	J	429	MET	2.4
10	J	152	LEU	2.4
9	I	269	ALA	2.4
7	G	56	TYR	2.4
5	E	145	ILE	2.3
1	A	159	LEU	2.3
9	I	237	LEU	2.3
3	C	301	GLU	2.3
5	E	116	LEU	2.3
6	F	147	LEU	2.3
10	J	486	LEU	2.3
3	C	101	ALA	2.3
7	G	141	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	75	LEU	2.3
9	I	244	TYR	2.3
1	A	174	ILE	2.3
9	I	272	TRP	2.3
10	J	484	VAL	2.3
9	I	25	ASN	2.2
3	C	12	ILE	2.2
10	J	419	ILE	2.2
7	G	88	LEU	2.2
10	J	331	LEU	2.2
4	D	5	ALA	2.2
3	C	329	VAL	2.2
8	H	300	TYR	2.2
3	C	230	CYS	2.2
7	G	162	PHE	2.2
3	C	10	ILE	2.2
9	I	162	PRO	2.2
8	H	278	TRP	2.2
3	C	190	PRO	2.2
10	J	344	TYR	2.2
3	C	9	THR	2.2
10	J	613	LEU	2.2
10	J	438	ARG	2.2
3	C	100	SER	2.2
7	G	36	PRO	2.2
2	B	199	LEU	2.1
9	I	231	ARG	2.1
9	I	278	PRO	2.1
7	G	5	ILE	2.1
9	I	230	VAL	2.1
3	C	284	LEU	2.1
3	C	276	CYS	2.1
10	J	477	PRO	2.1
6	F	142	THR	2.1
10	J	536	THR	2.1
7	G	201	LEU	2.1
7	G	109	ASN	2.1
7	G	20	LYS	2.1
10	J	446	TYR	2.1
10	J	395	ASN	2.1
3	C	292	ALA	2.1
2	B	185	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	176	VAL	2.1
10	J	487	THR	2.1
3	C	247	PHE	2.1
3	C	334	LEU	2.1
7	G	231	PHE	2.1
1	A	273	GLU	2.1
3	C	282	VAL	2.1
10	J	473	VAL	2.1
10	J	464	MET	2.0
10	J	560	SER	2.0
6	F	14	ALA	2.0
7	G	12	PRO	2.0
7	G	194	ILE	2.0
9	I	35	TYR	2.0
7	G	55	ALA	2.0
8	H	52	SER	2.0
3	C	96	ILE	2.0
1	A	104	CYS	2.0
3	C	331	ILE	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, 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	LLDF	B-factors(Å ²)	Q<0.9
13	MPD	E	302	8/8	0.70	0.54	5.97	78,95,113,115	0
14	MES	G	301	6/12	0.56	0.55	1.41	136,164,166,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	MG	E	301	1/1	0.87	0.24	0.38	76,76,76,76	0
12	MG	S	101	1/1	0.84	0.13	-1.48	135,135,135,135	0
15	PO4	I	301	5/5	0.77	0.36	-	165,172,186,193	0
15	PO4	S	102	5/5	0.80	0.19	-	153,157,178,180	0

6.5 Other polymers [i](#)

There are no such residues in this entry.