



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2016 – 03:30 PM EDT

PDB ID : 5JEA  
Title : Structure of a cytoplasmic 11-subunit RNA exosome complex including Ski7,  
bound to RNA  
Authors : Kowalinski, E.; Ebert, J.; Stegmann, E.; Conti, E.  
Deposited on : 2016-04-18  
Resolution : 2.65 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

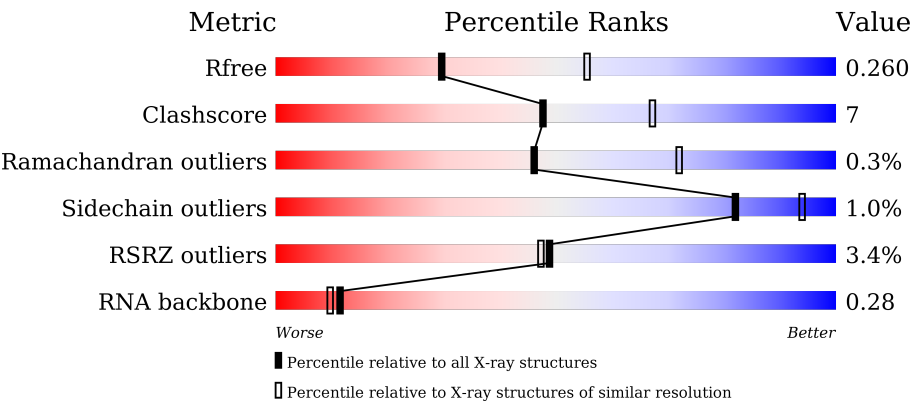
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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 <sub>free</sub>	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)
RNA backbone	2183	1001 (3.08-2.24)

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

Mol	Chain	Length	Quality of chain
1	A	305	<div><div>%</div><div>82%16%.</div></div>
2	B	249	<div><div>%</div><div>82%16%.</div></div>
3	C	394	<div><div>%</div><div>66%13%.20%</div></div>
4	D	226	<div><div></div><div>85%15%.</div></div>

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Mol	Chain	Length	Quality of chain
5	E	268	<p>78% 17% .</p>
6	F	250	<p>66% 18% 16%</p>
7	G	244	<p>80% 16% . .</p>
8	H	316	<p>77% 12% . 11%</p>
9	I	295	<p>68% 11% 20%</p>
10	J	1005	<p>76% 17% . 7%</p>
11	K	279	<p>15% 48% 16% . 34%</p>
12	R	46	<p>4% 13% 17% 26% . 41%</p>

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	A	401	-	-	-	X
13	MPD	A	402	-	-	-	X
13	MPD	G	301	-	-	-	X
13	MPD	G	302	-	-	-	X
13	MPD	J	1101	-	-	-	X
14	NA	F	301	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 27142 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	299	Total	C	N	O	S	0	0	0
			2291	1441	390	444	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1896	1185	337	366	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P46948
B	-1	PRO	-	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	314	Total	C	N	O	S	0	0	0
			2427	1536	415	466	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	SER	ALA	conflict	UNP P25359
C	363	MET	VAL	conflict	UNP P25359

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	224	Total	C	N	O	S	0	0	0
			1712	1076	290	336	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP P53256
D	-1	ALA	-	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	256	Total	C	N	O	S	0	0	0
			1960	1252	324	379	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q12277
E	-1	PRO	-	expression tag	UNP Q12277
E	0	HIS	-	expression tag	UNP Q12277
E	138	ILE	VAL	conflict	UNP Q12277

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	210	Total	C	N	O	S	0	0	0
			1592	999	269	314	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	161	THR	MET	conflict	UNP P48240

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	235	Total	C	N	O	S	0	0	0
			1810	1153	296	350	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	PRO	-	expression tag	UNP Q08285
G	-1	ASP	-	expression tag	UNP Q08285
G	0	SER	-	expression tag	UNP Q08285

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	282	Total	C	N	O	S	0	0	0
			2188	1366	392	418	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	44	THR	-	expression tag	UNP P38792
H	45	GLY	-	expression tag	UNP P38792
H	46	GLY	-	expression tag	UNP P38792
H	47	ARG	-	expression tag	UNP P38792
H	48	SER	-	expression tag	UNP P38792
H	49	MET	-	expression tag	UNP P38792

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	235	Total	C	N	O	S	0	0	0
			1737	1086	306	338	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	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 DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	936	Total	C	N	O	S	0	0	0
			7389	4679	1293	1382	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-3	GLY	-	expression tag	UNP Q08162
J	-2	PRO	-	expression tag	UNP Q08162
J	-1	ASP	-	expression tag	UNP Q08162
J	0	SER	-	expression tag	UNP Q08162
J	171	ASN	ASP	conflict	UNP Q08162
J	551	ASN	ASP	conflict	UNP Q08162

- Molecule 11 is a protein called Superciller protein 7,Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	185	Total	C	N	O	S	0	0	0
			1421	899	248	268	6			

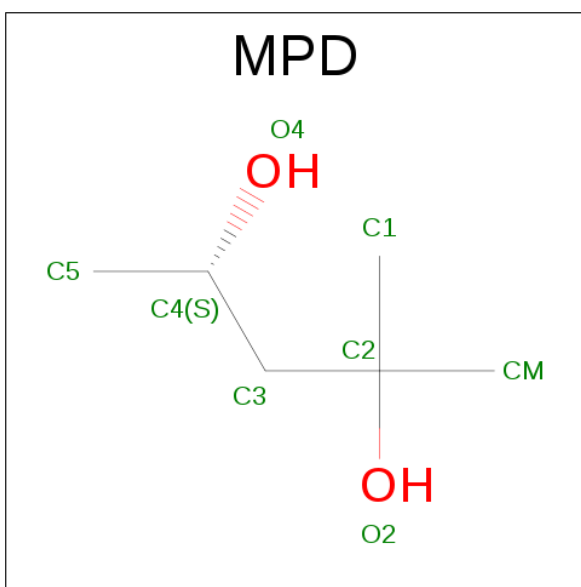
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	111	GLY	-	expression tag	UNP Q08491
K	112	PRO	-	expression tag	UNP Q08491
K	113	ASP	-	expression tag	UNP Q08491
K	114	SER	-	expression tag	UNP Q08491
K	115	MET	-	expression tag	UNP Q08491
K	237	GLY	ARG	conflict	UNP P00720
K	279	THR	CYS	conflict	UNP P00720
K	322	ALA	CYS	conflict	UNP P00720
K	362	ARG	ILE	conflict	UNP P00720
K	364	HIS	TYR	conflict	UNP P00720

- Molecule 12 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	R	27	Total	C	N	O	P	0	0	0
			524	231	81	186	26			

- Molecule 13 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			8	6	2		
13	A	1	Total	C	O	0	0
			8	6	2		
13	C	1	Total	C	O	0	0
			8	6	2		
13	D	1	Total	C	O	0	0
			8	6	2		
13	G	1	Total	C	O	0	0
			8	6	2		
13	G	1	Total	C	O	0	0
			8	6	2		
13	J	1	Total	C	O	0	0
			8	6	2		

- Molecule 14 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	2	Total	Na	0	0
			2	2		
14	J	1	Total	Na	0	0
			1	1		
14	F	1	Total	Na	0	0
			1	1		

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

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

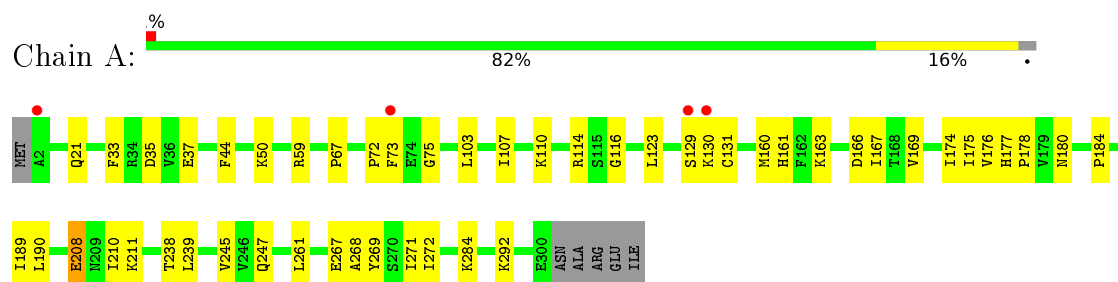
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	19	Total 19	O 19	0	0
16	B	13	Total 13	O 13	0	0
16	C	12	Total 12	O 12	0	0
16	D	14	Total 14	O 14	0	0
16	E	8	Total 8	O 8	0	0
16	F	6	Total 6	O 6	0	0
16	G	19	Total 19	O 19	0	0
16	H	15	Total 15	O 15	0	0
16	I	2	Total 2	O 2	0	0
16	J	26	Total 26	O 26	0	0

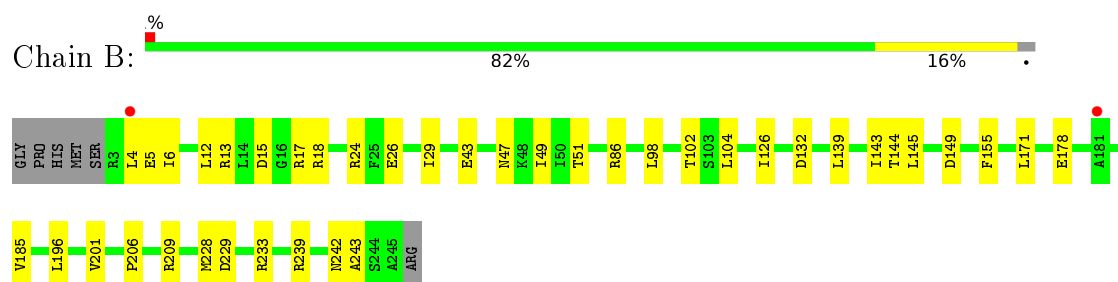
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

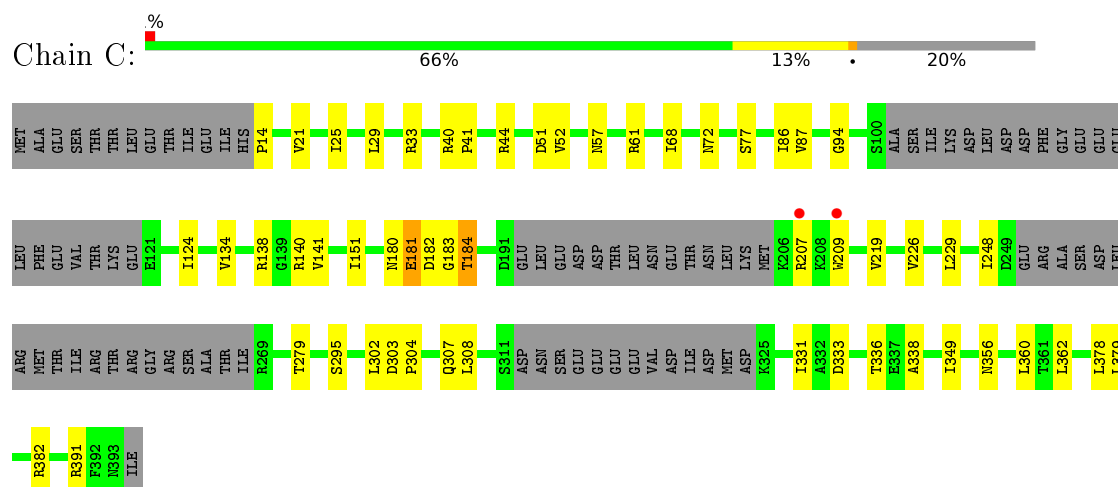
- Molecule 1: Exosome complex component RRP45



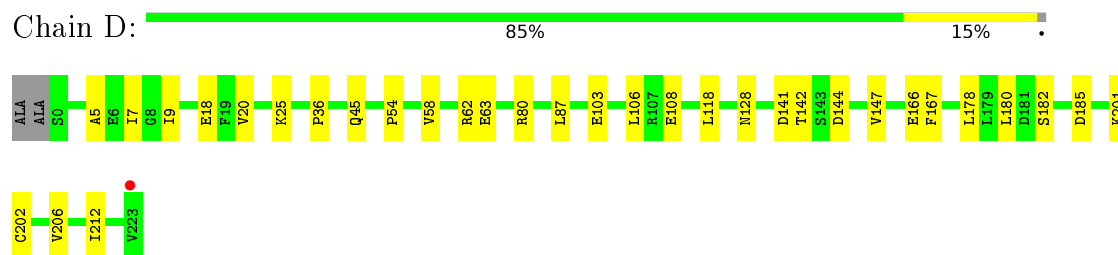
- Molecule 2: Exosome complex component SKI6



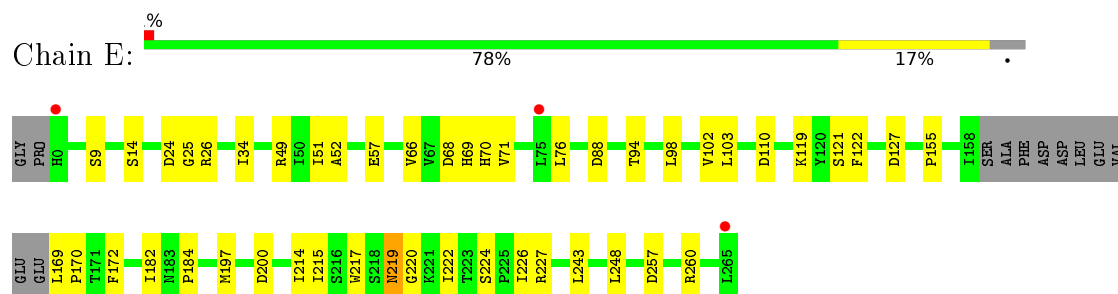
- Molecule 3: Exosome complex component RRP43



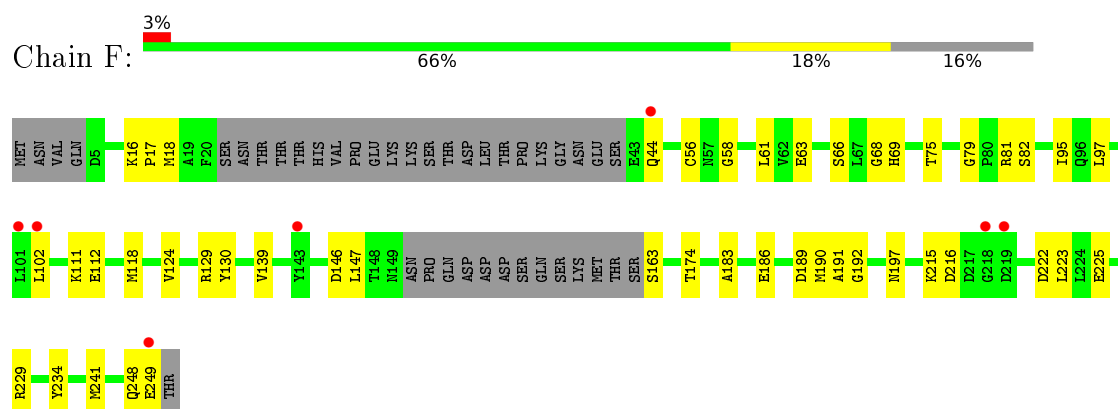
- Molecule 4: Exosome complex component RRP46



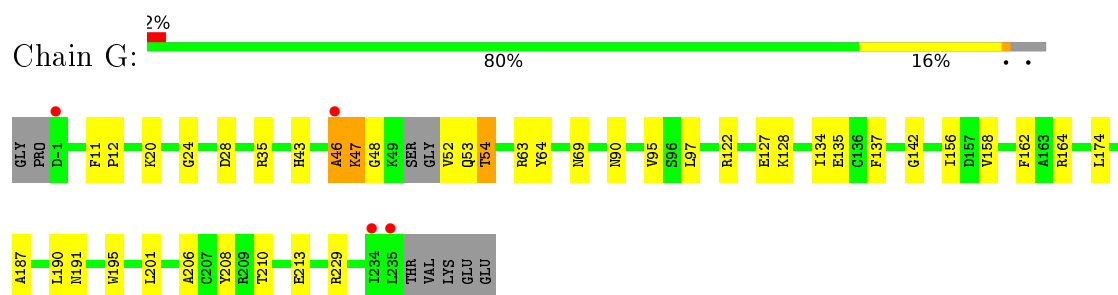
- Molecule 5: Exosome complex component RRP42



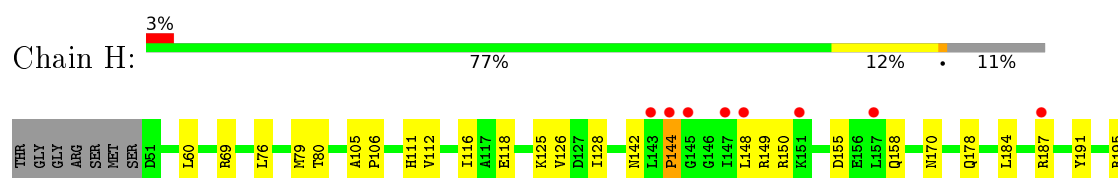
- Molecule 6: Exosome complex component MTR3

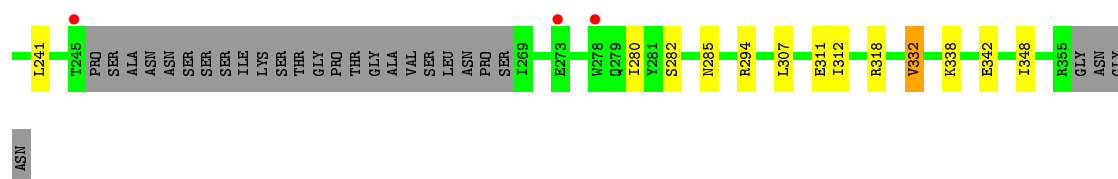


- Molecule 7: Exosome complex component RRP40

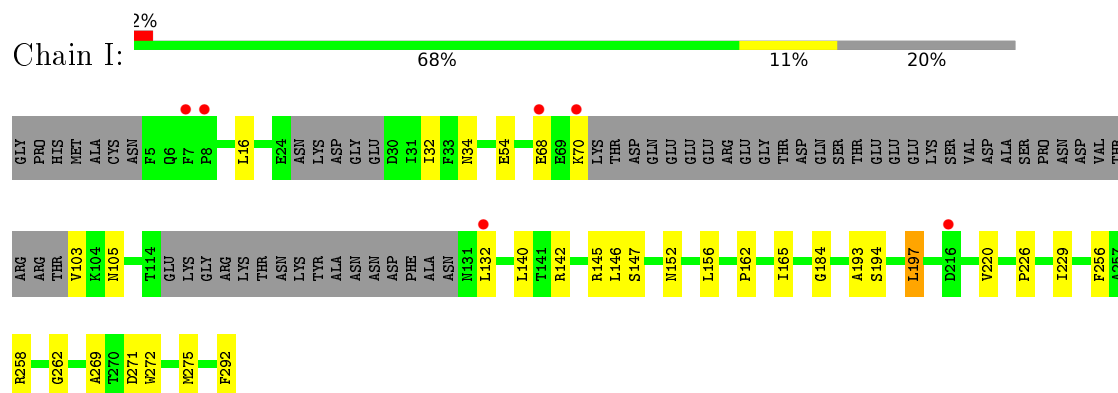


- Molecule 8: Exosome complex component RRP4

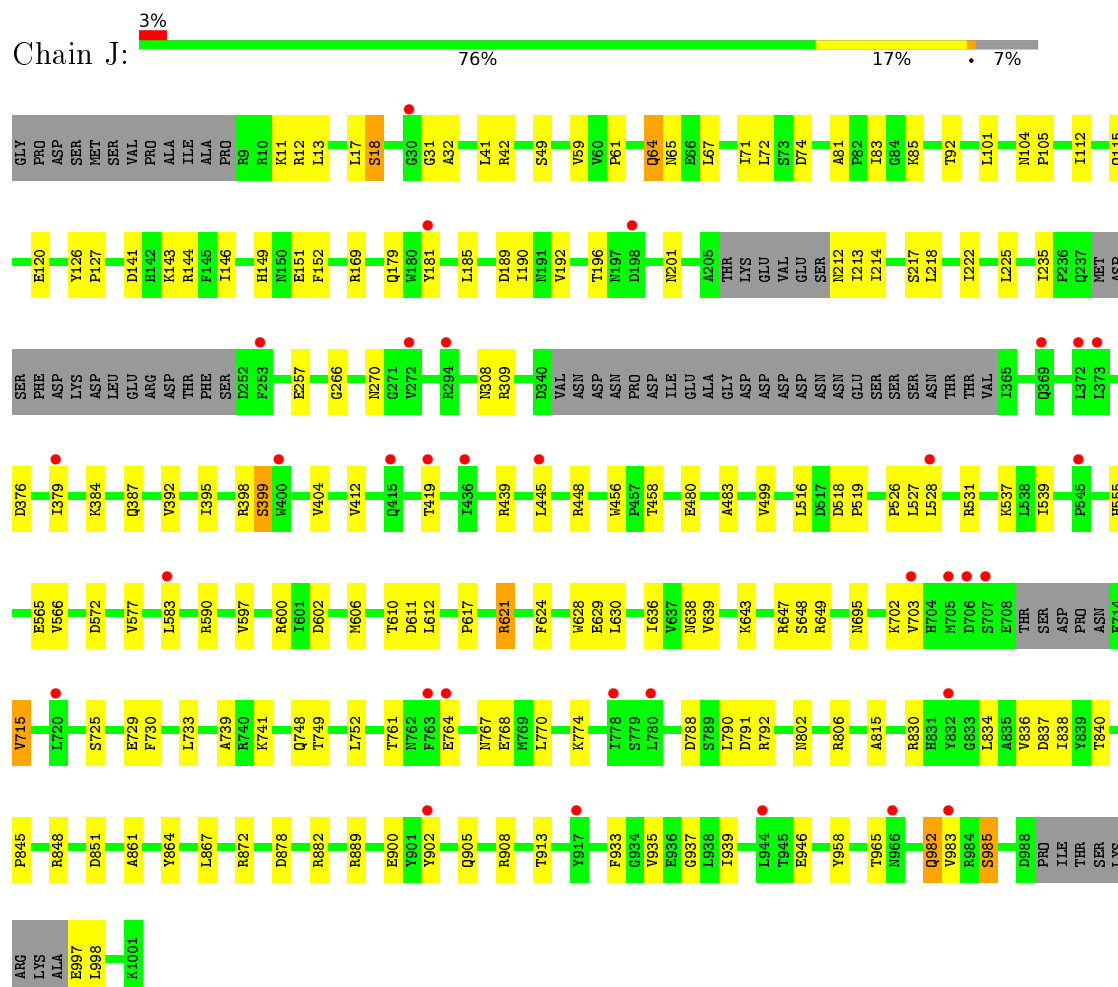




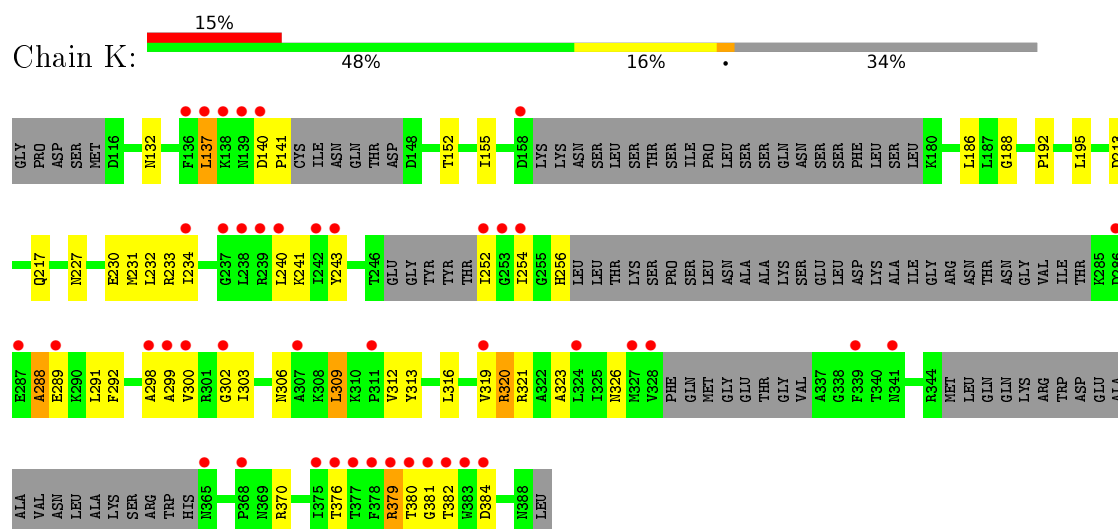
- Molecule 9: Exosome complex component CSL4



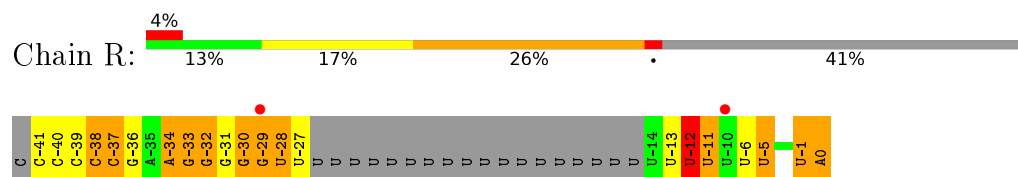
- Molecule 10: Exosome complex exonuclease DIS3



- Molecule 11: Superkiller protein 7, Endolysin



- Molecule 12: RNA (29-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.08Å 182.53Å 250.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.69 – 2.65 91.72 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.69-2.65) 100.0 (91.72-2.65)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.215 , 0.259 0.216 , 0.260	Depositor DCC
$R_{free}$ test set	7076 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, 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	0.25	0/2327	0.40	0/3144
2	B	0.23	0/1920	0.40	0/2588
3	C	0.26	0/2462	0.46	0/3332
4	D	0.24	0/1730	0.43	0/2347
5	E	0.25	0/1997	0.42	0/2718
6	F	0.25	0/1613	0.44	0/2178
7	G	0.25	0/1846	0.44	0/2505
8	H	0.24	0/2222	0.43	0/3002
9	I	0.23	0/1762	0.44	0/2387
10	J	0.25	0/7534	0.44	0/10226
11	K	0.31	0/1443	0.54	1/1956 (0.1%)
12	R	0.38	0/579	1.06	2/896 (0.2%)
All	All	0.25	0/27435	0.46	3/37279 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	137	LEU	CA-CB-CG	6.52	130.30	115.30
12	R	-12	U	N1-C2-O2	5.67	126.77	122.80
12	R	-12	U	N3-C2-O2	-5.33	118.47	122.20

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	2291	0	2263	29	0
2	B	1896	0	1935	24	0
3	C	2427	0	2472	39	0
4	D	1712	0	1771	21	0
5	E	1960	0	1982	34	0
6	F	1592	0	1554	29	0
7	G	1810	0	1771	24	0
8	H	2188	0	2188	29	0
9	I	1737	0	1724	25	0
10	J	7389	0	7324	120	0
11	K	1421	0	1316	45	0
12	R	524	0	268	23	0
13	A	16	0	28	3	0
13	C	8	0	14	0	0
13	D	8	0	14	1	0
13	G	16	0	28	2	0
13	J	8	0	14	1	0
14	B	2	0	0	0	0
14	F	1	0	0	0	0
14	J	1	0	0	0	0
15	J	1	0	0	0	0
16	A	19	0	0	2	0
16	B	13	0	0	0	0
16	C	12	0	0	0	0
16	D	14	0	0	0	0
16	E	8	0	0	0	0
16	F	6	0	0	0	0
16	G	19	0	0	0	0
16	H	15	0	0	0	0
16	I	2	0	0	0	0
16	J	26	0	0	0	0
All	All	27142	0	26666	398	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 7.

All (398) 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)
9:I:34:ASN:HB3	9:I:105:ASN:HB3	1.52	0.89
10:J:985:SER:HG	10:J:997:GLU:N	1.77	0.82
3:C:180:ASN:OD1	3:C:184:THR:N	2.12	0.81
3:C:181:GLU:HG2	3:C:182:ASP:H	1.45	0.80
12:R:-40:C:N4	12:R:-30:G:O6	2.12	0.79
8:H:118:GLU:HB3	8:H:125:LYS:HB2	1.66	0.77
10:J:257:GLU:HG3	10:J:458:THR:HG21	1.67	0.77
5:E:26:ARG:NH2	5:E:200:ASP:O	2.18	0.76
10:J:802:ASN:OD1	10:J:806:ARG:NH2	2.19	0.76
10:J:185:LEU:HB3	10:J:190:ILE:HB	1.67	0.76
9:I:70:LYS:H	9:I:70:LYS:HD2	1.51	0.75
12:R:-38:C:O2'	12:R:-37:C:O4'	2.05	0.73
8:H:144:PRO:HG2	8:H:149:ARG:HH12	1.54	0.72
10:J:764:GLU:HA	10:J:767:ASN:HB2	1.70	0.71
3:C:362:LEU:HB2	4:D:180:LEU:HB3	1.72	0.71
6:F:124:VAL:HG21	6:F:191:ALA:HB2	1.73	0.70
5:E:257:ASP:HA	5:E:260:ARG:HG2	1.73	0.70
2:B:24:ARG:NH2	2:B:43:GLU:OE1	2.24	0.69
4:D:45:GLN:OE1	4:D:80:ARG:NH1	2.24	0.69
9:I:145:ARG:HB2	9:I:152:ASN:HB2	1.75	0.69
5:E:66:VAL:HG21	10:J:31:GLY:HA2	1.77	0.67
12:R:-32:G:N1	12:R:-31:G:O6	2.28	0.67
1:A:35:ASP:H	13:A:402:MPD:H13	1.59	0.66
8:H:178:GLN:OE1	12:R:-29:G:N2	2.29	0.66
10:J:266:GLY:O	10:J:270:ASN:ND2	2.27	0.65
10:J:419:THR:OG1	10:J:439:ARG:NE	2.30	0.65
11:K:243:TYR:HB2	11:K:252:ILE:HD11	1.78	0.65
2:B:206:PRO:HG2	2:B:209:ARG:HH21	1.62	0.65
9:I:229:ILE:HB	9:I:256:PHE:HB2	1.78	0.65
3:C:124:ILE:HD13	4:D:103:GLU:HB3	1.79	0.64
6:F:129:ARG:NH1	6:F:186:GLU:OE2	2.30	0.64
10:J:222:ILE:HA	10:J:225:LEU:HD12	1.79	0.64
10:J:748:GLN:HG2	10:J:749:THR:HG23	1.78	0.64
4:D:7:ILE:HD11	4:D:118:LEU:HB3	1.80	0.64
11:K:192:PRO:HG2	11:K:195:LEU:HB2	1.78	0.64
6:F:75:THR:HG22	6:F:139:VAL:HG22	1.79	0.64
10:J:308:ASN:HB3	10:J:392:VAL:HG22	1.79	0.64
6:F:79:GLY:HA2	6:F:81:ARG:HG3	1.79	0.63
12:R:-41:C:H42	12:R:-30:G:H1	1.47	0.63
9:I:70:LYS:HD2	9:I:70:LYS:N	2.13	0.63
10:J:636:ILE:HD11	10:J:733:LEU:HD11	1.80	0.63
7:G:63:ARG:NH2	7:G:90:ASN:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:PRO:HB3	4:D:87:LEU:HB2	1.79	0.63
8:H:142:ASN:ND2	8:H:187:ARG:O	2.31	0.62
13:J:1101:MPD:O2	13:J:1101:MPD:O4	2.15	0.62
7:G:122:ARG:NH2	7:G:135:GLU:OE2	2.31	0.62
10:J:878:ASP:OD2	10:J:882:ARG:NH1	2.32	0.62
10:J:531:ARG:NH1	10:J:572:ASP:OD2	2.24	0.62
9:I:32:ILE:O	9:I:103:VAL:N	2.32	0.62
5:E:217:TRP:CZ2	5:E:220:GLY:HA2	2.34	0.61
6:F:44:GLN:HB3	6:F:66:SER:HB3	1.82	0.61
9:I:142:ARG:HB2	9:I:156:LEU:HD11	1.81	0.61
10:J:83:ILE:HG12	10:J:214:ILE:HD13	1.82	0.61
8:H:69:ARG:NH2	8:H:80:THR:OG1	2.33	0.61
1:A:239:LEU:HD23	1:A:245:VAL:HA	1.82	0.61
10:J:404:VAL:HG11	10:J:483:ALA:HB1	1.82	0.61
10:J:703:VAL:HG12	10:J:715:VAL:HA	1.82	0.61
2:B:13:ARG:HD3	2:B:171:LEU:HD13	1.82	0.61
5:E:9:SER:OG	8:H:285:ASN:ND2	2.33	0.60
8:H:307:LEU:HD21	8:H:348:ILE:HD12	1.84	0.60
10:J:790:LEU:HD13	10:J:806:ARG:HG2	1.83	0.60
2:B:86:ARG:NH1	5:E:127:ASP:OD1	2.34	0.60
5:E:68:ASP:OD1	5:E:70:HIS:ND1	2.22	0.60
8:H:338:LYS:NZ	8:H:342:GLU:OE2	2.35	0.60
10:J:617:PRO:HA	10:J:648:SER:HB3	1.84	0.60
10:J:900:GLU:HG2	10:J:935:VAL:HG13	1.83	0.60
6:F:69:HIS:HA	6:F:146:ASP:HA	1.84	0.59
3:C:25:ILE:HD11	9:I:140:LEU:HD13	1.84	0.59
10:J:629:GLU:HB3	10:J:638:ASN:HB3	1.83	0.59
1:A:269:TYR:HA	1:A:272:ILE:HG12	1.84	0.59
10:J:101:LEU:HD22	10:J:235:ILE:HD11	1.83	0.59
4:D:128:ASN:OD1	7:G:35:ARG:NH2	2.35	0.59
5:E:14:SER:OG	8:H:294:ARG:NH1	2.35	0.59
3:C:308:LEU:HD11	11:K:186:LEU:HB3	1.84	0.59
3:C:141:VAL:HG12	9:I:193:ALA:HB2	1.85	0.58
5:E:227:ARG:NH2	6:F:216:ASP:OD1	2.32	0.58
2:B:26:GLU:OE1	10:J:11:LYS:NZ	2.34	0.58
4:D:141:ASP:OD1	4:D:142:THR:N	2.36	0.58
10:J:201:ASN:HD21	10:J:212:ASN:HD21	1.51	0.58
1:A:67:PRO:HG3	1:A:131:CYS:HB3	1.85	0.58
5:E:68:ASP:HB3	5:E:71:VAL:HG22	1.85	0.58
9:I:269:ALA:HA	9:I:275:MET:HG2	1.84	0.58
5:E:49:ARG:HE	5:E:51:ILE:HD11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:ASP:OD2	2:B:233:ARG:NH2	2.36	0.58
3:C:134:VAL:HG21	3:C:151:ILE:HG22	1.86	0.58
10:J:12:ARG:NH2	10:J:18:SER:OG	2.37	0.57
10:J:13:LEU:HB2	10:J:17:LEU:HB3	1.86	0.57
10:J:384:LYS:O	10:J:387:GLN:NE2	2.37	0.57
10:J:59:VAL:HG13	10:J:67:LEU:HD22	1.86	0.57
10:J:761:THR:HA	10:J:764:GLU:OE1	2.05	0.57
9:I:32:ILE:H	9:I:103:VAL:HG23	1.67	0.57
10:J:179:GLN:HA	10:J:213:ILE:HD11	1.86	0.57
10:J:64:GLN:HG2	10:J:64:GLN:O	2.04	0.57
10:J:889:ARG:HH22	12:R:-6:U:H5"	1.67	0.56
3:C:226:VAL:HG23	3:C:229:LEU:HD12	1.88	0.56
13:D:301:MPD:O4	13:D:301:MPD:O2	2.17	0.56
3:C:219:VAL:HG11	3:C:226:VAL:HG21	1.88	0.56
7:G:69:ASN:OD1	7:G:122:ARG:NH1	2.35	0.56
11:K:309:LEU:H	11:K:309:LEU:HD12	1.71	0.56
1:A:267:GLU:OE1	13:A:401:MPD:O4	2.24	0.56
7:G:46:ALA:O	7:G:53:GLN:NE2	2.38	0.56
11:K:320:ARG:HH21	11:K:379:ARG:HA	1.70	0.56
2:B:29:ILE:HD12	2:B:149:ASP:HB2	1.87	0.56
11:K:227:ASN:HA	11:K:230:GLU:HG2	1.87	0.56
1:A:167:ILE:HG22	1:A:176:VAL:HA	1.88	0.56
3:C:356:ASN:ND2	4:D:185:ASP:OD1	2.38	0.56
8:H:111:HIS:NE2	8:H:170:ASN:OD1	2.39	0.55
5:E:110:ASP:H	5:E:182:ILE:HD11	1.70	0.55
9:I:258:ARG:HB2	9:I:262:GLY:HA2	1.88	0.55
3:C:86:ILE:HD11	11:K:155:ILE:HG23	1.89	0.55
12:R:-37:C:O2	12:R:-34:A:N6	2.39	0.55
11:K:326:ASN:OD1	11:K:370:ARG:NH1	2.39	0.55
11:K:376:THR:O	11:K:380:THR:HG22	2.06	0.55
10:J:768:GLU:OE1	10:J:958:TYR:OH	2.24	0.55
10:J:141:ASP:O	10:J:144:ARG:NH2	2.40	0.55
11:K:254:ILE:HD13	11:K:292:PHE:HB2	1.88	0.55
1:A:110:LYS:HA	1:A:114:ARG:HG2	1.89	0.54
2:B:18:ARG:NE	10:J:42:ARG:HH12	2.06	0.54
4:D:20:VAL:HG22	4:D:25:LYS:HG3	1.89	0.54
6:F:189:ASP:OD1	6:F:190:MET:N	2.40	0.54
10:J:889:ARG:NH2	12:R:-6:U:OP1	2.39	0.54
8:H:195:ARG:HH11	8:H:282:SER:N	2.06	0.54
10:J:597:VAL:HG12	10:J:703:VAL:HG22	1.89	0.54
11:K:306:ASN:HB3	11:K:309:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:695:ASN:HD21	10:J:834:LEU:HD23	1.71	0.54
5:E:88:ASP:O	6:F:111:LYS:NZ	2.41	0.54
3:C:181:GLU:HG2	3:C:182:ASP:N	2.17	0.53
10:J:412:VAL:HG21	10:J:445:LEU:HD11	1.89	0.53
10:J:848:ARG:HB2	10:J:851:ASP:OD2	2.07	0.53
3:C:33:ARG:NH2	11:K:188:GLY:O	2.37	0.53
10:J:638:ASN:OD1	10:J:639:VAL:N	2.41	0.53
5:E:69:HIS:NE2	5:E:121:SER:HB2	2.24	0.53
10:J:788:ASP:O	10:J:792:ARG:HG2	2.08	0.53
8:H:155:ASP:HA	8:H:158:GLN:HG2	1.90	0.53
5:E:51:ILE:HG12	5:E:57:GLU:HG3	1.91	0.53
7:G:164:ARG:HG2	7:G:190:LEU:HD22	1.90	0.53
11:K:213:ASP:O	11:K:217:GLN:HB2	2.09	0.53
3:C:44:ARG:NH2	3:C:333:ASP:O	2.41	0.52
11:K:241:LYS:H	11:K:252:ILE:HG21	1.74	0.52
3:C:349:ILE:HD13	3:C:378:LEU:HD23	1.90	0.52
7:G:20:LYS:HE2	7:G:54:THR:OG1	2.09	0.52
9:I:54:GLU:OE1	9:I:54:GLU:N	2.42	0.52
2:B:12:LEU:HD13	10:J:152:PHE:HD2	1.74	0.52
10:J:908:ARG:HD2	10:J:985:SER:HB2	1.91	0.52
8:H:116:ILE:HD13	8:H:126:VAL:HG22	1.92	0.52
11:K:298:ALA:O	11:K:302:GLY:N	2.37	0.52
2:B:239:ARG:NH1	8:H:311:GLU:OE1	2.42	0.52
12:R:-6:U:O2'	12:R:-5:U:H5'	2.10	0.52
11:K:309:LEU:HD12	11:K:309:LEU:N	2.25	0.52
5:E:98:LEU:O	5:E:102:VAL:HG23	2.10	0.51
11:K:232:LEU:HD12	11:K:292:PHE:HE2	1.74	0.51
3:C:183:GLY:O	3:C:184:THR:HG23	2.10	0.51
3:C:51:ASP:OD1	3:C:391:ARG:NH2	2.43	0.51
10:J:181:TYR:HB3	10:J:192:VAL:HG11	1.92	0.51
1:A:160:MET:HG2	1:A:189:ILE:HG12	1.93	0.51
3:C:140:ARG:NH2	9:I:184:GLY:O	2.43	0.51
6:F:56:CYS:HA	9:I:165:ILE:HG21	1.92	0.51
1:A:211:LYS:NZ	16:A:503:HOH:O	2.36	0.51
3:C:21:VAL:HG12	9:I:162:PRO:HD3	1.91	0.51
11:K:240:LEU:HG	11:K:241:LYS:HG3	1.92	0.51
6:F:225:GLU:H	6:F:225:GLU:CD	2.13	0.51
11:K:323:ALA:O	11:K:326:ASN:HB3	2.11	0.51
6:F:222:ASP:OD1	6:F:223:LEU:N	2.42	0.51
5:E:224:SER:HA	5:E:226:ILE:HD12	1.93	0.51
1:A:210:ILE:HG21	2:B:155:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:748:GLN:N	10:J:748:GLN:OE1	2.42	0.50
10:J:703:VAL:HG11	10:J:902:TYR:CE1	2.46	0.50
10:J:539:ILE:HG12	10:J:555:HIS:HB3	1.93	0.50
11:K:380:THR:HG23	11:K:382:THR:H	1.76	0.50
11:K:231:MET:HE1	11:K:326:ASN:HB2	1.94	0.50
4:D:142:THR:HB	4:D:144:ASP:OD2	2.12	0.50
3:C:138:ARG:HB3	9:I:197:LEU:HD21	1.92	0.50
1:A:59:ARG:NH1	16:A:505:HOH:O	2.45	0.50
13:A:401:MPD:O4	13:A:401:MPD:O2	2.29	0.49
2:B:185:VAL:HG22	2:B:201:VAL:HG22	1.92	0.49
3:C:68:ILE:HG21	3:C:279:THR:HG22	1.93	0.49
10:J:611:ASP:OD1	10:J:621:ARG:NH1	2.44	0.49
3:C:360:LEU:HB3	4:D:182:SER:HB2	1.93	0.49
5:E:98:LEU:HD21	5:E:214:ILE:HG21	1.93	0.49
2:B:144:THR:HB	2:B:228:MET:HE1	1.95	0.49
8:H:195:ARG:HH12	8:H:280:ILE:C	2.15	0.49
11:K:186:LEU:H	11:K:186:LEU:HD23	1.77	0.49
10:J:702:LYS:HE3	12:R:-1:U:O2	2.12	0.49
4:D:147:VAL:HG21	4:D:201:LYS:HG3	1.94	0.49
10:J:791:ASP:OD1	10:J:806:ARG:NH1	2.45	0.49
11:K:306:ASN:HB3	11:K:309:LEU:CD1	2.42	0.49
3:C:61:ARG:HB3	3:C:72:ASN:HB3	1.95	0.49
6:F:197:ASN:OD1	6:F:229:ARG:NH2	2.45	0.49
5:E:226:ILE:HB	6:F:215:LYS:HB3	1.94	0.49
10:J:74:ASP:N	10:J:74:ASP:OD1	2.46	0.49
10:J:115:GLN:HB2	10:J:149:HIS:HA	1.95	0.49
10:J:577:VAL:HG12	10:J:583:LEU:HD22	1.95	0.49
12:R:-38:C:HO2'	12:R:-37:C:H6	1.59	0.49
1:A:72:PRO:HG2	1:A:73:PHE:HD2	1.77	0.49
2:B:29:ILE:HD11	2:B:145:LEU:HB3	1.95	0.48
5:E:182:ILE:O	5:E:184:PRO:HD3	2.13	0.48
6:F:95:ILE:H	6:F:118:MET:HE2	1.78	0.48
10:J:104:ASN:O	10:J:143:LYS:NZ	2.31	0.48
10:J:49:SER:HA	10:J:72:LEU:HB2	1.95	0.48
11:K:232:LEU:HD12	11:K:292:PHE:CE2	2.48	0.48
10:J:81:ALA:HA	10:J:83:ILE:H	1.78	0.48
10:J:499:VAL:HG13	10:J:583:LEU:HA	1.95	0.48
10:J:537:LYS:NZ	10:J:565:GLU:OE1	2.36	0.48
10:J:606:MET:O	10:J:610:THR:HG22	2.14	0.48
1:A:75:GLY:HA3	1:A:123:LEU:HB2	1.96	0.48
1:A:103:LEU:O	1:A:107:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:ALA:HB3	7:G:195:TRP:HB3	1.95	0.48
8:H:112:VAL:HG21	8:H:128:ILE:HD13	1.95	0.48
10:J:612:LEU:HA	10:J:621:ARG:HH11	1.77	0.48
11:K:230:GLU:O	11:K:234:ILE:HG13	2.13	0.48
5:E:68:ASP:HA	5:E:119:LYS:O	2.14	0.48
3:C:41:PRO:HB2	3:C:336:THR:HG21	1.96	0.48
5:E:76:LEU:HD22	5:E:103:LEU:HB3	1.96	0.48
11:K:256:HIS:ND1	11:K:291:LEU:HD11	2.28	0.48
10:J:739:ALA:HB2	10:J:840:THR:HG22	1.96	0.47
7:G:95:VAL:HG11	7:G:134:ILE:HG23	1.95	0.47
4:D:9:ILE:HD13	4:D:18:GLU:HB2	1.95	0.47
7:G:47:LYS:HA	7:G:53:GLN:HG2	1.96	0.47
10:J:71:ILE:HD11	10:J:146:ILE:HG22	1.97	0.47
6:F:63:GLU:OE1	11:K:152:THR:HG23	2.14	0.47
8:H:195:ARG:HH11	8:H:282:SER:H	1.61	0.47
10:J:770:LEU:O	10:J:774:LYS:N	2.44	0.47
10:J:939:ILE:HG12	10:J:998:LEU:HB3	1.96	0.47
1:A:129:SER:OG	1:A:130:LYS:NZ	2.47	0.47
1:A:33:PHE:HB2	1:A:271:ILE:HD13	1.95	0.47
5:E:215:ILE:HD13	5:E:248:LEU:HD23	1.96	0.47
5:E:222:ILE:HG21	5:E:248:LEU:HD22	1.97	0.47
7:G:48:GLY:O	7:G:52:VAL:N	2.48	0.47
4:D:54:PRO:HD3	4:D:63:GLU:HG2	1.97	0.47
3:C:25:ILE:HG23	9:I:229:ILE:HG13	1.95	0.47
10:J:85:LYS:HE2	10:J:190:ILE:HG12	1.96	0.47
10:J:85:LYS:O	10:J:190:ILE:HA	2.14	0.47
10:J:85:LYS:HB3	10:J:190:ILE:HA	1.96	0.46
10:J:741:LYS:HE3	10:J:861:ALA:HB1	1.97	0.46
8:H:128:ILE:HD11	8:H:184:LEU:HD11	1.97	0.46
10:J:308:ASN:OD1	10:J:309:ARG:NH1	2.49	0.46
10:J:112:ILE:HG21	10:J:181:TYR:CE2	2.51	0.46
3:C:302:LEU:HB3	3:C:307:GLN:HE22	1.81	0.46
4:D:166:GLU:HB2	4:D:178:LEU:HG	1.97	0.46
5:E:94:THR:HG23	6:F:112:GLU:HG3	1.97	0.46
10:J:18:SER:HB2	10:J:41:LEU:HB2	1.98	0.46
10:J:647:ARG:O	10:J:649:ARG:NH2	2.49	0.46
1:A:169:VAL:HG22	1:A:174:ILE:HG22	1.98	0.46
1:A:37:GLU:HB2	1:A:50:LYS:HB3	1.97	0.46
11:K:382:THR:OG1	11:K:384:ASP:OD2	2.30	0.46
6:F:248:GLN:O	6:F:249:GLU:HB2	2.15	0.46
1:A:261:LEU:HD12	2:B:196:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:O	1:A:177:HIS:HD2	1.99	0.46
10:J:845:PRO:HA	10:J:851:ASP:HB2	1.97	0.46
12:R:-40:C:O5'	12:R:-40:C:H6	1.99	0.46
9:I:146:LEU:HD12	9:I:226:PRO:HD3	1.98	0.46
10:J:715:VAL:HG21	10:J:933:PHE:HE2	1.81	0.46
13:G:302:MPD:HM2	13:G:302:MPD:H4	1.78	0.45
5:E:172:PHE:CD2	10:J:32:ALA:HB2	2.51	0.45
6:F:61:LEU:HD21	11:K:152:THR:HA	1.98	0.45
10:J:61:PRO:HB2	10:J:65:ASN:HA	1.99	0.45
11:K:319:VAL:HG21	11:K:381:GLY:C	2.35	0.45
10:J:516:LEU:HD22	10:J:528:LEU:HD11	1.99	0.45
10:J:590:ARG:NH1	10:J:602:ASP:O	2.48	0.45
2:B:13:ARG:HD2	2:B:178:GLU:OE1	2.16	0.45
4:D:62:ARG:NH2	4:D:108:GLU:OE1	2.48	0.45
5:E:122:PHE:CZ	5:E:155:PRO:HG2	2.52	0.45
7:G:28:ASP:HB2	7:G:35:ARG:HD3	1.98	0.45
10:J:12:ARG:NH2	10:J:17:LEU:O	2.49	0.45
10:J:527:LEU:HD12	10:J:527:LEU:H	1.82	0.45
11:K:312:VAL:O	11:K:316:LEU:HG	2.17	0.45
10:J:218:LEU:O	10:J:222:ILE:HG12	2.16	0.45
10:J:445:LEU:HA	10:J:445:LEU:HD12	1.77	0.45
10:J:905:GLN:OE1	10:J:908:ARG:NH2	2.50	0.45
10:J:913:THR:HG22	10:J:982:GLN:NE2	2.32	0.45
11:K:320:ARG:NH2	11:K:379:ARG:HA	2.32	0.45
3:C:207:ARG:HG3	3:C:209:TRP:CH2	2.52	0.45
10:J:628:TRP:HB3	10:J:630:LEU:HD22	1.97	0.45
1:A:21:GLN:CD	7:G:201:LEU:HD23	2.37	0.45
10:J:376:ASP:HA	10:J:379:ILE:HG22	1.99	0.45
12:R:-32:G:N1	12:R:-31:G:C6	2.84	0.45
4:D:202:CYS:O	4:D:206:VAL:HG23	2.17	0.45
3:C:14:PRO:N	9:I:292:PHE:HA	2.32	0.44
3:C:51:ASP:OD1	3:C:52:VAL:N	2.50	0.44
11:K:300:VAL:O	11:K:303:ILE:HG22	2.17	0.44
11:K:299:ALA:O	11:K:303:ILE:N	2.50	0.44
8:H:148:LEU:HA	11:K:379:ARG:HH22	1.81	0.44
2:B:51:THR:HG23	2:B:126:ILE:HG12	1.99	0.44
10:J:815:ALA:HB2	12:R:-6:U:H5'	1.99	0.44
2:B:47:ASN:OD1	2:B:132:ASP:N	2.48	0.44
4:D:167:PHE:CD1	4:D:206:VAL:HG21	2.53	0.44
7:G:213:GLU:OE2	7:G:229:ARG:NH1	2.48	0.44
11:K:289:GLU:O	11:K:292:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:ALA:HB3	4:D:212:ILE:HD13	2.00	0.44
5:E:169:LEU:HA	5:E:170:PRO:HD3	1.80	0.44
9:I:271:ASP:OD2	9:I:272:TRP:N	2.46	0.44
10:J:85:LYS:HD3	10:J:189:ASP:HB3	1.98	0.44
11:K:288:ALA:O	11:K:291:LEU:HB3	2.17	0.44
10:J:448:ARG:HE	10:J:480:GLU:CD	2.20	0.44
10:J:725:SER:O	10:J:729:GLU:HG2	2.18	0.44
10:J:983:VAL:HG22	10:J:998:LEU:HD12	1.99	0.44
1:A:163:LYS:HB3	1:A:184:PRO:HB2	1.99	0.44
11:K:230:GLU:HB2	11:K:233:ARG:NH1	2.33	0.44
11:K:309:LEU:H	11:K:309:LEU:CD1	2.29	0.44
12:R:-12:U:O2	12:R:-12:U:H2'	2.17	0.44
8:H:148:LEU:HA	11:K:379:ARG:NH2	2.33	0.43
6:F:130:TYR:HA	9:I:132:LEU:HD22	1.99	0.43
10:J:395:ILE:HG21	10:J:398:ARG:HE	1.83	0.43
10:J:715:VAL:HG21	10:J:933:PHE:CE2	2.52	0.43
10:J:985:SER:OG	10:J:997:GLU:N	2.44	0.43
12:R:-40:C:H2'	12:R:-39:C:O4'	2.18	0.43
1:A:44:PHE:HA	1:A:161:HIS:CE1	2.53	0.43
4:D:141:ASP:OD1	4:D:142:THR:HG23	2.19	0.43
6:F:174:THR:HG23	6:F:241:MET:SD	2.58	0.43
7:G:97:LEU:HD13	7:G:134:ILE:HG13	1.99	0.43
10:J:566:VAL:HG11	10:J:730:PHE:CE1	2.53	0.43
10:J:600:ARG:NH1	12:R:0:A:OP2	2.49	0.43
10:J:218:LEU:HD21	10:J:235:ILE:HD12	2.00	0.43
10:J:752:LEU:HD21	10:J:838:ILE:HD11	1.99	0.43
3:C:87:VAL:HG22	3:C:219:VAL:HG22	2.00	0.43
3:C:336:THR:O	3:C:338:ALA:N	2.47	0.43
6:F:68:GLY:O	6:F:147:LEU:N	2.50	0.43
6:F:82:SER:O	9:I:194:SER:OG	2.32	0.43
7:G:64:TYR:CG	7:G:191:ASN:HA	2.54	0.43
10:J:526:PRO:HG2	10:J:527:LEU:HD12	2.01	0.43
3:C:40:ARG:HD2	3:C:331:ILE:HD12	2.01	0.43
10:J:185:LEU:HD13	10:J:190:ILE:HG21	1.99	0.43
10:J:946:GLU:N	10:J:965:THR:HG22	2.33	0.43
12:R:-33:G:H2'	12:R:-32:G:C8	2.53	0.43
1:A:178:PRO:HB2	1:A:180:ASN:OD1	2.19	0.43
10:J:201:ASN:HD21	10:J:212:ASN:ND2	2.17	0.43
7:G:206:ALA:O	7:G:210:THR:HG22	2.19	0.43
10:J:92:THR:OG1	10:J:120:GLU:OE1	2.24	0.43
10:J:518:ASP:HA	10:J:519:PRO:HD2	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:140:ASP:HA	11:K:141:PRO:HD3	1.81	0.43
3:C:379:LEU:HD12	3:C:382:ARG:HH22	1.84	0.42
6:F:58:GLY:HA3	6:F:183:ALA:HB2	2.01	0.42
7:G:24:GLY:H	13:G:302:MPD:H32	1.84	0.42
10:J:703:VAL:HG21	10:J:902:TYR:CZ	2.54	0.42
10:J:309:ARG:HD2	10:J:456:TRP:CD1	2.54	0.42
8:H:76:LEU:HA	8:H:76:LEU:HD22	1.75	0.42
10:J:151:GLU:CD	10:J:169:ARG:HH22	2.23	0.42
10:J:643:LYS:HD2	10:J:864:TYR:CZ	2.55	0.42
10:J:104:ASN:HA	10:J:105:PRO:HD3	1.82	0.42
7:G:162:PHE:HZ	7:G:174:LEU:HD13	1.84	0.42
8:H:60:LEU:HD13	8:H:79:MET:HG3	2.01	0.42
10:J:830:ARG:HG3	10:J:836:VAL:O	2.20	0.42
1:A:238:THR:HB	1:A:247:GLN:HG3	2.00	0.42
6:F:97:LEU:HD23	6:F:139:VAL:HB	2.01	0.42
10:J:867:LEU:HD23	10:J:872:ARG:HG3	2.01	0.42
5:E:214:ILE:HB	5:E:227:ARG:HB2	2.01	0.42
7:G:128:LYS:HB2	7:G:128:LYS:HE3	1.91	0.42
1:A:208:GLU:OE1	8:H:76:LEU:HD21	2.20	0.42
10:J:126:TYR:N	10:J:127:PRO:HD2	2.35	0.42
2:B:4:LEU:O	2:B:6:ILE:N	2.53	0.42
3:C:302:LEU:HB3	3:C:307:GLN:NE2	2.35	0.42
1:A:268:ALA:O	1:A:272:ILE:HG23	2.19	0.42
8:H:148:LEU:H	8:H:148:LEU:HD12	1.85	0.42
8:H:312:ILE:HG23	8:H:318:ARG:HH11	1.85	0.42
10:J:937:GLY:HA3	10:J:998:LEU:HD22	2.02	0.42
4:D:106:LEU:H	4:D:106:LEU:HD23	1.85	0.41
6:F:163:SER:O	6:F:163:SER:OG	2.35	0.41
9:I:147:SER:O	9:I:220:VAL:HG21	2.20	0.41
12:R:-12:U:H4'	12:R:-11:U:OP2	2.17	0.41
7:G:11:PHE:HA	7:G:12:PRO:HD3	1.78	0.41
11:K:313:TYR:CE1	11:K:321:ARG:HG2	2.56	0.41
11:K:316:LEU:HD22	11:K:320:ARG:HD3	2.02	0.41
12:R:-38:C:C4	12:R:-32:G:N2	2.86	0.41
1:A:116:GLY:O	1:A:190:LEU:HD12	2.20	0.41
5:E:197:MET:HE2	5:E:243:LEU:HB3	2.01	0.41
11:K:300:VAL:HA	11:K:303:ILE:HG22	2.03	0.41
3:C:303:ASP:HA	3:C:304:PRO:HD3	1.91	0.41
3:C:57:ASN:HA	3:C:77:SER:HB3	2.01	0.41
2:B:104:LEU:HD13	2:B:143:ILE:HD11	2.01	0.41
2:B:98:LEU:O	2:B:102:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:GLY:HA2	6:F:18:MET:HG3	2.03	0.41
9:I:16:LEU:O	11:K:132:ASN:ND2	2.40	0.41
1:A:284:LYS:HA	1:A:284:LYS:HD3	1.81	0.41
6:F:16:LYS:HA	6:F:17:PRO:HD3	1.96	0.41
6:F:192:GLY:HA3	6:F:234:TYR:HD1	1.85	0.41
7:G:156:ILE:HG12	7:G:208:TYR:CD2	2.56	0.41
10:J:531:ARG:NH1	10:J:643:LYS:HD3	2.36	0.41
3:C:29:LEU:O	3:C:33:ARG:HB2	2.20	0.41
5:E:24:ASP:OD2	5:E:26:ARG:HD3	2.20	0.41
5:E:34:ILE:HG22	5:E:52:ALA:HA	2.03	0.41
8:H:105:ALA:HA	8:H:106:PRO:HD2	1.94	0.41
5:E:25:GLY:HA3	8:H:332:VAL:HG13	2.03	0.41
12:R:-37:C:C2	12:R:-34:A:N6	2.89	0.41
8:H:312:ILE:HG23	8:H:318:ARG:NH1	2.36	0.41
7:G:158:VAL:HG21	7:G:162:PHE:CD2	2.56	0.41
10:J:85:LYS:HE2	10:J:85:LYS:HB3	1.91	0.41
2:B:49:ILE:HD13	2:B:139:LEU:HD23	2.03	0.40
2:B:242:ASN:OD1	2:B:243:ALA:N	2.54	0.40
10:J:112:ILE:HD13	10:J:181:TYR:CE2	2.56	0.40
10:J:112:ILE:HG21	10:J:181:TYR:HE2	1.87	0.40
12:R:-29:G:H4'	12:R:-28:U:C5'	2.50	0.40
12:R:-34:A:O2'	12:R:-33:G:H8	2.03	0.40
7:G:137:PHE:HD1	7:G:142:GLY:HA2	1.87	0.40
8:H:170:ASN:ND2	8:H:191:TYR:HD1	2.19	0.40
10:J:837:ASP:N	10:J:837:ASP:OD1	2.47	0.40
2:B:15:ASP:OD2	2:B:17:ARG:NE	2.38	0.40
10:J:196:THR:O	10:J:217:SER:HA	2.21	0.40
5:E:257:ASP:N	5:E:257:ASP:OD1	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	297/305 (97%)	288 (97%)	9 (3%)	0	100	100
2	B	241/249 (97%)	234 (97%)	6 (2%)	1 (0%)	39	65
3	C	304/394 (77%)	295 (97%)	8 (3%)	1 (0%)	46	72
4	D	222/226 (98%)	217 (98%)	5 (2%)	0	100	100
5	E	252/268 (94%)	243 (96%)	8 (3%)	1 (0%)	39	65
6	F	204/250 (82%)	198 (97%)	6 (3%)	0	100	100
7	G	231/244 (95%)	220 (95%)	9 (4%)	2 (1%)	21	44
8	H	278/316 (88%)	274 (99%)	3 (1%)	1 (0%)	39	65
9	I	227/295 (77%)	220 (97%)	7 (3%)	0	100	100
10	J	924/1005 (92%)	896 (97%)	26 (3%)	2 (0%)	52	77
11	K	171/279 (61%)	165 (96%)	5 (3%)	1 (1%)	30	54
All	All	3351/3831 (88%)	3250 (97%)	92 (3%)	9 (0%)	46	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	GLU
3	C	181	GLU
5	E	219	ASN
10	J	399	SER
7	G	46	ALA
7	G	47	LYS
8	H	144	PRO
11	K	288	ALA
10	J	715	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/266 (95%)	249 (99%)	3 (1%)	78	92
2	B	213/220 (97%)	213 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	271/350 (77%)	268 (99%)	3 (1%)	80	93
4	D	198/198 (100%)	197 (100%)	1 (0%)	92	98
5	E	228/242 (94%)	227 (100%)	1 (0%)	93	98
6	F	172/219 (78%)	171 (99%)	1 (1%)	90	97
7	G	200/212 (94%)	197 (98%)	3 (2%)	72	90
8	H	241/270 (89%)	238 (99%)	3 (1%)	78	92
9	I	183/242 (76%)	181 (99%)	2 (1%)	80	93
10	J	814/904 (90%)	807 (99%)	7 (1%)	84	95
11	K	142/245 (58%)	138 (97%)	4 (3%)	51	79
All	All	2914/3368 (86%)	2886 (99%)	28 (1%)	82	94

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ILE
1	A	208	GLU
1	A	292	LYS
3	C	184	THR
3	C	248	ILE
3	C	295	SER
4	D	58	VAL
5	E	219	ASN
6	F	102	LEU
7	G	43	HIS
7	G	54	THR
7	G	127	GLU
8	H	150	ARG
8	H	241	LEU
8	H	332	VAL
9	I	68	GLU
9	I	197	LEU
10	J	18	SER
10	J	64	GLN
10	J	399	SER
10	J	621	ARG
10	J	624	PHE
10	J	982	GLN
10	J	985	SER
11	K	137	LEU

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Mol	Chain	Res	Type
11	K	309	LEU
11	K	320	ARG
11	K	379	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	HIS
8	H	170	ASN
10	J	201	ASN
10	J	943	ASN
10	J	982	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	23/46 (50%)	15 (65%)	3 (13%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	-38	C
12	R	-37	C
12	R	-36	G
12	R	-34	A
12	R	-33	G
12	R	-32	G
12	R	-30	G
12	R	-29	G
12	R	-28	U
12	R	-27	U
12	R	-13	U
12	R	-12	U
12	R	-11	U
12	R	-5	U
12	R	0	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	R	-33	G
12	R	-12	U
12	R	-1	U

## 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 12 ligands modelled in this entry, 5 are 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	$\# Z  > 2$
13	MPD	A	401	-	6,7,7	0.28	0	6,10,10	0.12	0
13	MPD	A	402	-	6,7,7	0.28	0	6,10,10	0.16	0
13	MPD	C	401	-	6,7,7	0.27	0	6,10,10	0.14	0
13	MPD	D	301	-	6,7,7	0.29	0	6,10,10	0.14	0
13	MPD	G	301	-	6,7,7	0.30	0	6,10,10	0.19	0
13	MPD	G	302	-	6,7,7	0.28	0	6,10,10	0.15	0
13	MPD	J	1101	-	6,7,7	0.30	0	6,10,10	0.16	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	A	401	-	-	0/5/5/5	0/0/0/0
13	MPD	A	402	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MPD	C	401	-	-	0/5/5/5	0/0/0/0
13	MPD	D	301	-	-	0/5/5/5	0/0/0/0
13	MPD	G	301	-	-	0/5/5/5	0/0/0/0
13	MPD	G	302	-	-	0/5/5/5	0/0/0/0
13	MPD	J	1101	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	401	MPD	2	0
13	A	402	MPD	1	0
13	D	301	MPD	1	0
13	G	302	MPD	2	0
13	J	1101	MPD	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	299/305 (98%)	0.17	4 (1%) 79 79	43, 58, 132, 165	0
2	B	243/249 (97%)	0.13	2 (0%) 87 87	43, 54, 96, 144	0
3	C	314/394 (79%)	0.14	2 (0%) 90 91	48, 67, 133, 205	0
4	D	224/226 (99%)	0.19	1 (0%) 93 94	43, 55, 88, 126	0
5	E	256/268 (95%)	0.05	3 (1%) 81 80	50, 69, 111, 142	0
6	F	210/250 (84%)	0.42	7 (3%) 50 48	50, 69, 138, 167	0
7	G	235/244 (96%)	0.18	4 (1%) 73 72	46, 61, 115, 169	0
8	H	282/316 (89%)	0.23	11 (3%) 43 41	48, 68, 121, 149	0
9	I	235/295 (79%)	0.25	6 (2%) 59 58	45, 70, 122, 171	0
10	J	936/1005 (93%)	0.27	33 (3%) 48 46	59, 82, 120, 201	0
11	K	185/279 (66%)	0.98	43 (23%) 1 1	67, 118, 157, 173	0
12	R	27/46 (58%)	0.29	2 (7%) 17 14	66, 155, 186, 200	0
All	All	3446/3877 (88%)	0.26	118 (3%) 49 47	43, 72, 132, 205	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	145	GLY	5.6
11	K	242	ILE	5.5
6	F	101	LEU	5.5
11	K	380	THR	4.9
11	K	365	ASN	4.8
7	G	46	ALA	4.7
10	J	294	ARG	4.7
11	K	311	PRO	4.6
11	K	239	ARG	4.3
5	E	0	HIS	4.3
11	K	136	PHE	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	F	102	LEU	4.0
8	H	148	LEU	4.0
11	K	382	THR	4.0
11	K	375	ILE	3.9
10	J	707	SER	3.9
6	F	219	ASP	3.8
1	A	2	ALA	3.8
3	C	209	TRP	3.8
1	A	129	SER	3.8
11	K	138	LYS	3.8
11	K	137	LEU	3.8
6	F	249	GLU	3.7
8	H	157	LEU	3.6
11	K	139	ASN	3.6
11	K	234	ILE	3.6
10	J	369	GLN	3.6
10	J	445	LEU	3.5
9	I	7	PHE	3.4
11	K	140	ASP	3.4
1	A	130	LYS	3.4
11	K	368	PRO	3.3
8	H	278	TRP	3.3
11	K	377	THR	3.2
10	J	372	LEU	3.2
10	J	198	ASP	3.1
11	K	237	GLY	3.1
11	K	324	LEU	3.1
1	A	73	PHE	3.1
6	F	218	GLY	3.1
11	K	381	GLY	3.0
8	H	147	ILE	3.0
12	R	-29	G	3.0
11	K	378	PHE	3.0
11	K	302	GLY	3.0
11	K	376	THR	2.9
11	K	238	LEU	2.9
12	R	-10	U	2.9
9	I	216	ASP	2.9
11	K	289	GLU	2.9
4	D	223	VAL	2.8
10	J	966	ASN	2.8
10	J	272	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
10	J	379	ILE	2.8
11	K	286	ASP	2.8
10	J	705	MET	2.8
10	J	944	LEU	2.7
11	K	254	ILE	2.7
11	K	307	ALA	2.7
10	J	400	TRP	2.7
11	K	240	LEU	2.7
10	J	778	ILE	2.6
9	I	68	GLU	2.6
11	K	158	ASP	2.6
7	G	234	ILE	2.6
10	J	415	GLN	2.6
7	G	-1	ASP	2.5
11	K	383	TRP	2.5
3	C	207	ARG	2.5
11	K	327	MET	2.5
11	K	379	ARG	2.5
10	J	764	GLU	2.5
10	J	30	GLY	2.5
8	H	187	ARG	2.5
2	B	4	LEU	2.5
9	I	132	LEU	2.4
6	F	143	TYR	2.4
8	H	144	PRO	2.4
9	I	8	PRO	2.4
10	J	373	LEU	2.4
10	J	583	LEU	2.4
11	K	287	GLU	2.4
11	K	299	ALA	2.4
9	I	70	LYS	2.4
8	H	143	LEU	2.3
10	J	917	TYR	2.3
11	K	243	TYR	2.3
10	J	983	VAL	2.3
10	J	832	TYR	2.3
10	J	528	LEU	2.3
10	J	181	TYR	2.3
11	K	298	ALA	2.3
10	J	419	THR	2.2
11	K	328	VAL	2.2
11	K	384	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
11	K	341	ASN	2.2
10	J	253	PHE	2.2
5	E	265	LEU	2.2
2	B	181	ALA	2.2
11	K	253	GLY	2.2
11	K	252	ILE	2.2
6	F	44	GLN	2.2
8	H	273	GLU	2.2
10	J	780	LEU	2.2
10	J	763	PHE	2.2
10	J	706	ASP	2.1
5	E	75	LEU	2.1
8	H	151	LYS	2.1
11	K	319	VAL	2.1
8	H	245	THR	2.1
7	G	235	LEU	2.1
10	J	720	LEU	2.1
10	J	436	ILE	2.1
11	K	339	PHE	2.1
10	J	545	PRO	2.1
10	J	902	TYR	2.0
11	K	300	VAL	2.0
10	J	703	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
13	MPD	J	1101	8/8	0.83	0.43	12.44	80,96,104,110	0
13	MPD	G	302	8/8	0.94	0.28	8.17	76,85,111,111	0
14	NA	F	301	1/1	0.82	0.48	5.58	84,84,84,84	0
13	MPD	G	301	8/8	0.89	0.35	4.60	71,73,81,89	0
13	MPD	A	402	8/8	0.79	0.27	3.33	75,95,102,114	0
13	MPD	A	401	8/8	0.94	0.23	2.04	77,87,91,100	0
13	MPD	C	401	8/8	0.89	0.25	1.44	78,94,103,105	0
13	MPD	D	301	8/8	0.88	0.20	-0.23	71,86,92,94	0
15	ZN	J	1102	1/1	0.97	0.16	-0.29	74,74,74,74	0
14	NA	B	301	1/1	0.91	0.15	-1.02	57,57,57,57	0
14	NA	J	1103	1/1	0.98	0.20	-	67,67,67,67	0
14	NA	B	302	1/1	0.92	0.42	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.