



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 09:43 pm BST

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 wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

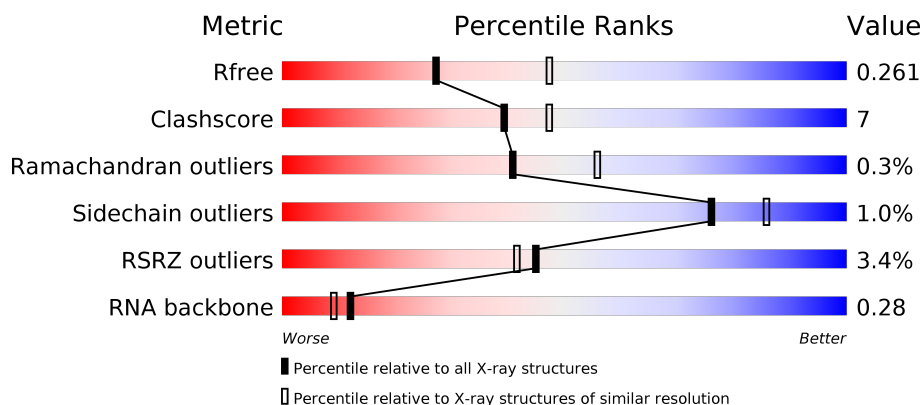
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)

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 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  $\leq 5\%$ . 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	
6	F	250	
7	G	244	
8	H	316	
9	I	295	
10	J	1005	

## 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 Superkiller 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			

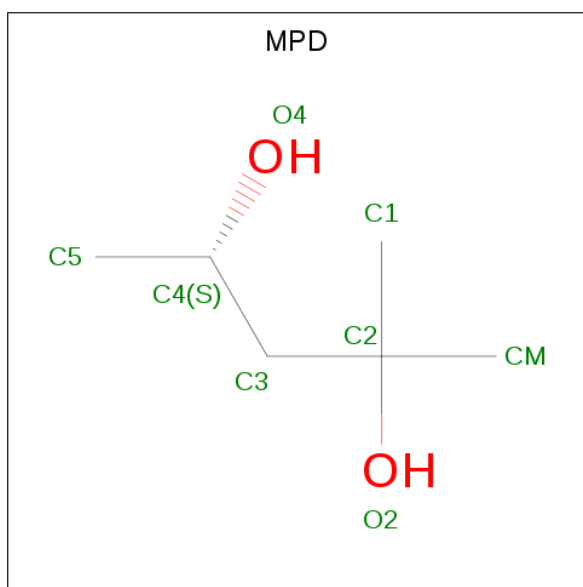
There are 10 discrepancies between the modelled and reference sequences:

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).




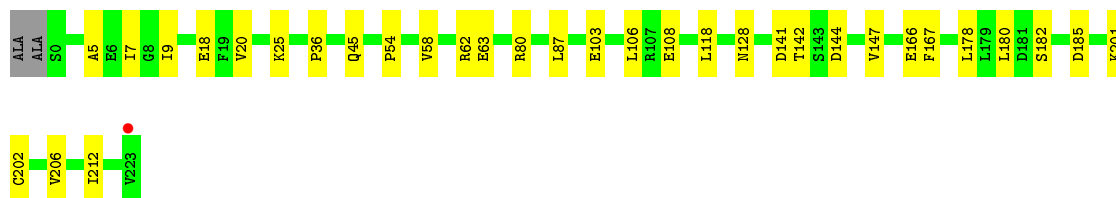
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total 1	Zn 1	0	0

- 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

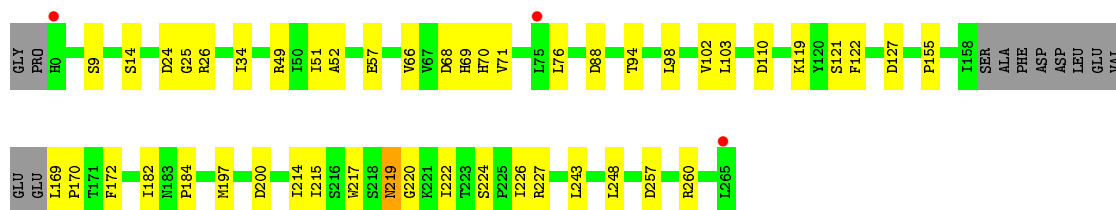


Chain D:  85% 15% .



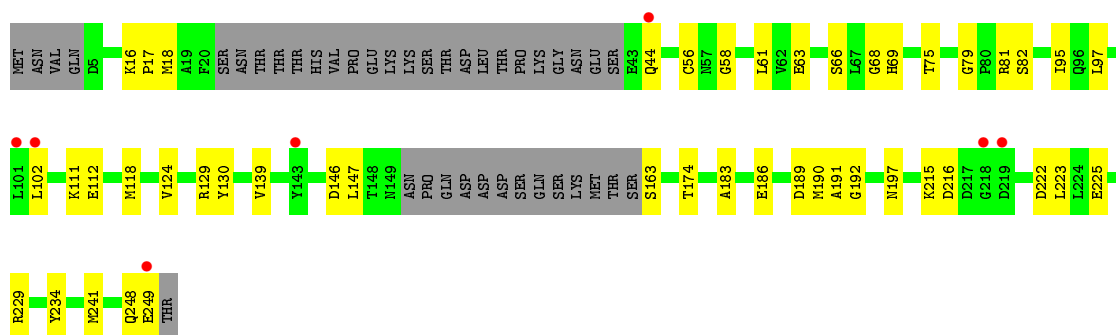
- Molecule 5: Exosome complex component RRP42

Chain E:  78% 17% .




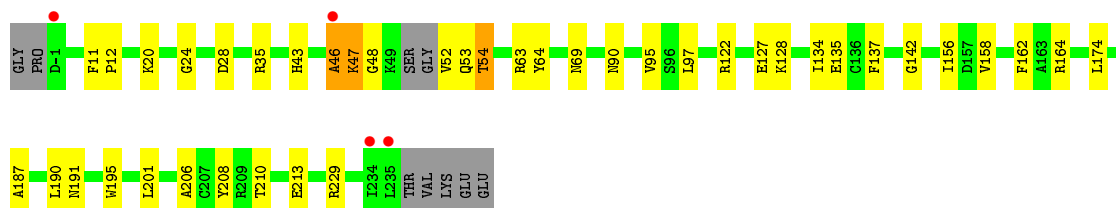
- Molecule 6: Exosome complex component MTR3

Chain F:  66% 18% 16% .




- Molecule 7: Exosome complex component RRP40

Chain G:  80% 16% . .

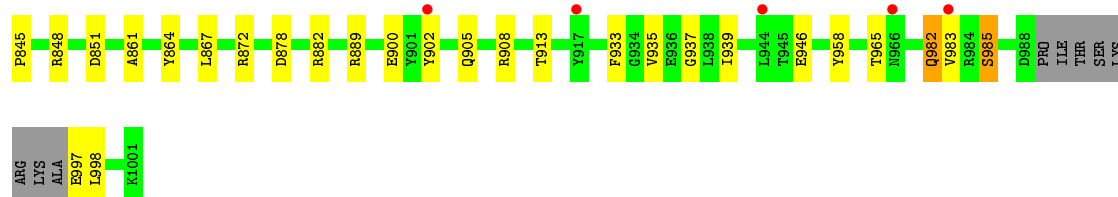


- Molecule 8: Exosome complex component RRP4

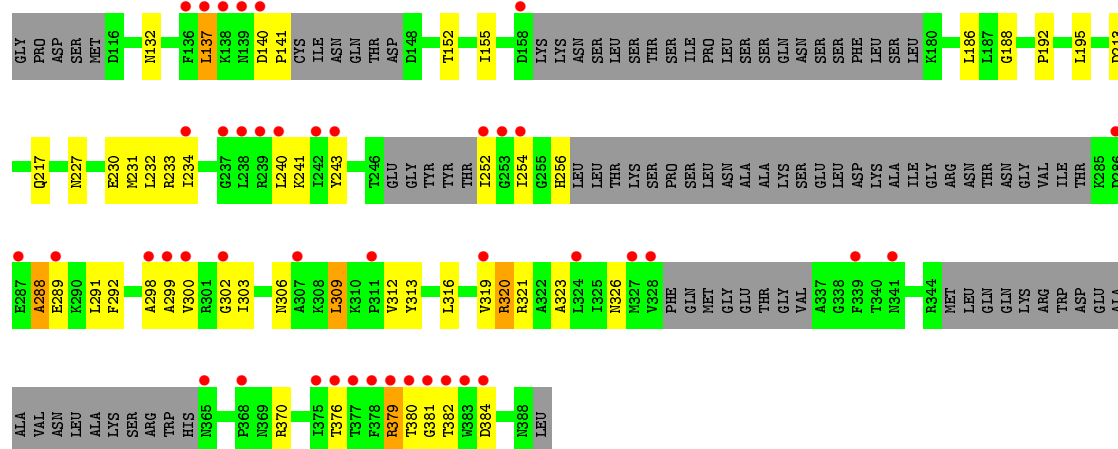
Chain H:  77% 12% 11% .



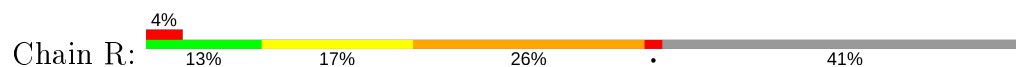




• Molecule 11: Superciller protein 7,Endolysin



• 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 1.9_1692	Depositor
R, $R_{free}$	0.215 , 0.259 0.218 , 0.261	Depositor DCC
$R_{free}$ test set	7077 reflections (5.00%)	wwPDB-VP
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.

The worst 5 of 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

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%)	34	48
3	C	304/394 (77%)	295 (97%)	8 (3%)	1 (0%)	41	56
4	D	222/226 (98%)	217 (98%)	5 (2%)	0	100	100
5	E	252/268 (94%)	243 (96%)	8 (3%)	1 (0%)	34	48
6	F	204/250 (82%)	198 (97%)	6 (3%)	0	100	100
7	G	231/244 (95%)	220 (95%)	9 (4%)	2 (1%)	17	26
8	H	278/316 (88%)	274 (99%)	3 (1%)	1 (0%)	34	48
9	I	227/295 (77%)	220 (97%)	7 (3%)	0	100	100
10	J	924/1005 (92%)	896 (97%)	26 (3%)	2 (0%)	47	64
11	K	171/279 (61%)	165 (96%)	5 (3%)	1 (1%)	25	37
All	All	3351/3831 (88%)	3250 (97%)	92 (3%)	9 (0%)	41	56

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	GLU
3	C	181	GLU

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Mol	Chain	Res	Type
5	E	219	ASN
10	J	399	SER
7	G	46	ALA

### 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%)	71	84
2	B	213/220 (97%)	213 (100%)	0	100	100
3	C	271/350 (77%)	268 (99%)	3 (1%)	73	85
4	D	198/198 (100%)	197 (100%)	1 (0%)	88	94
5	E	228/242 (94%)	227 (100%)	1 (0%)	91	95
6	F	172/219 (78%)	171 (99%)	1 (1%)	86	92
7	G	200/212 (94%)	197 (98%)	3 (2%)	65	80
8	H	241/270 (89%)	238 (99%)	3 (1%)	71	84
9	I	183/242 (76%)	181 (99%)	2 (1%)	73	85
10	J	814/904 (90%)	807 (99%)	7 (1%)	78	87
11	K	142/245 (58%)	138 (97%)	4 (3%)	43	61
All	All	2914/3368 (86%)	2886 (99%)	28 (1%)	76	86

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	150	ARG
9	I	68	GLU
11	K	309	LEU
8	H	241	LEU
8	H	332	VAL

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 [i](#)

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

5 of 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

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	G	301	-	7,7,7	0.28	0	9,10,10	0.21	0
13	MPD	C	401	-	7,7,7	0.29	0	9,10,10	0.22	0
13	MPD	A	401	-	7,7,7	0.27	0	9,10,10	0.21	0
13	MPD	J	1101	-	7,7,7	0.28	0	9,10,10	0.19	0
13	MPD	A	402	-	7,7,7	0.27	0	9,10,10	0.20	0
13	MPD	D	301	-	7,7,7	0.26	0	9,10,10	0.17	0
13	MPD	G	302	-	7,7,7	0.28	0	9,10,10	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	G	301	-	-	4/5/5/5	-
13	MPD	C	401	-	-	0/5/5/5	-
13	MPD	A	401	-	-	1/5/5/5	-
13	MPD	J	1101	-	-	4/5/5/5	-
13	MPD	A	402	-	-	0/5/5/5	-
13	MPD	D	301	-	-	2/5/5/5	-
13	MPD	G	302	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	401	MPD	O2-C2-C3-C4
13	G	301	MPD	C2-C3-C4-C5
13	J	1101	MPD	C2-C3-C4-C5
13	D	301	MPD	C2-C3-C4-C5
13	J	1101	MPD	C2-C3-C4-O4

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	J	1101	MPD	1	0
13	A	402	MPD	1	0
13	D	301	MPD	1	0
13	G	302	MPD	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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%) 77 75	43, 58, 132, 165	0
2	B	243/249 (97%)	0.13	2 (0%) 86 85	43, 54, 96, 144	0
3	C	314/394 (79%)	0.14	2 (0%) 89 89	48, 67, 133, 205	0
4	D	224/226 (99%)	0.19	1 (0%) 92 93	43, 55, 88, 126	0
5	E	256/268 (95%)	0.06	3 (1%) 79 77	50, 69, 111, 142	0
6	F	210/250 (84%)	0.42	7 (3%) 46 43	50, 69, 138, 167	0
7	G	235/244 (96%)	0.18	4 (1%) 70 67	46, 61, 115, 169	0
8	H	282/316 (89%)	0.23	11 (3%) 39 35	48, 68, 121, 149	0
9	I	235/295 (79%)	0.25	6 (2%) 56 52	45, 70, 122, 171	0
10	J	936/1005 (93%)	0.27	33 (3%) 44 40	59, 82, 120, 201	0
11	K	185/279 (66%)	0.98	43 (23%) 0 0	67, 118, 157, 173	0
12	R	27/46 (58%)	0.29	2 (7%) 14 12	66, 155, 186, 200	0
All	All	3446/3877 (88%)	0.26	118 (3%) 45 41	43, 72, 132, 205	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	145	GLY	5.5
6	F	101	LEU	5.5
11	K	242	ILE	5.5
11	K	380	THR	4.9
11	K	365	ASN	4.9

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
13	MPD	A	402	8/8	0.79	0.27	75,95,102,114	0
13	MPD	J	1101	8/8	0.82	0.43	80,96,104,110	0
14	NA	F	301	1/1	0.82	0.48	84,84,84,84	0
13	MPD	D	301	8/8	0.88	0.20	71,86,92,94	0
13	MPD	C	401	8/8	0.89	0.24	78,94,103,105	0
13	MPD	G	301	8/8	0.89	0.35	71,73,81,89	0
14	NA	B	301	1/1	0.91	0.15	57,57,57,57	0
14	NA	B	302	1/1	0.92	0.42	64,64,64,64	0
13	MPD	A	401	8/8	0.94	0.23	77,87,91,100	0
13	MPD	G	302	8/8	0.94	0.28	76,85,111,111	0
15	ZN	J	1102	1/1	0.97	0.16	74,74,74,74	0
14	NA	J	1103	1/1	0.98	0.20	67,67,67,67	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.