



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2018 – 10:10 AM EDT

PDB ID : 6D8F  
Title : RsAgo Ternary Complex with Guide RNA and Target DNA Containing T-T  
Bulge Within the Seed Segment  
Authors : Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.  
Deposited on : 2018-04-26  
Resolution : 2.15 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

<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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

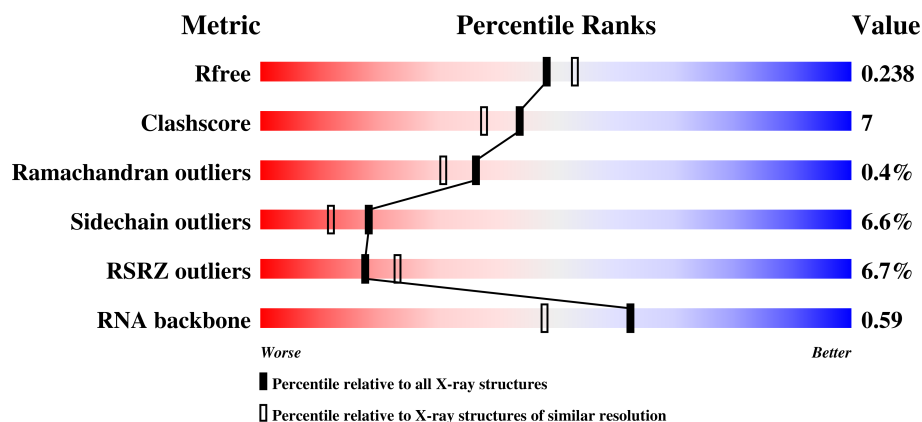
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	111664	1287 (2.16-2.16)
Clashscore	122126	1390 (2.16-2.16)
Ramachandran outliers	120053	1368 (2.16-2.16)
Sidechain outliers	120020	1367 (2.16-2.16)
RSRZ outliers	108989	1262 (2.16-2.16)
RNA backbone	2636	1006 (2.66-1.66)

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	791	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>
1	F	791	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
2	C	18	<div> <div></div> <div> <div>61%</div> <div>39%</div> </div> </div>
2	H	18	<div> <div></div> <div> <div>44%</div> <div>44%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	26	<div><div></div><div>8%</div><div>50%</div><div>19%</div><div>12%</div><div>19%</div></div>
3	J	26	<div><div></div><div>15%</div><div>54%</div><div>23%</div><div>8%</div><div>15%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26181 atoms, of which 12264 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	758	Total	C	H	N	O	S	1	0	0
			11604	3719	5749	1051	1069	16			
1	F	758	Total	C	H	N	O	S	0	0	0
			11365	3674	5594	1021	1060	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A4WYU7
A	-12	HIS	-	expression tag	UNP A4WYU7
A	-11	HIS	-	expression tag	UNP A4WYU7
A	-10	HIS	-	expression tag	UNP A4WYU7
A	-9	HIS	-	expression tag	UNP A4WYU7
A	-8	HIS	-	expression tag	UNP A4WYU7
A	-7	HIS	-	expression tag	UNP A4WYU7
A	-6	ASP	-	expression tag	UNP A4WYU7
A	-5	TYR	-	expression tag	UNP A4WYU7
A	-4	LYS	-	expression tag	UNP A4WYU7
A	-3	ASP	-	expression tag	UNP A4WYU7
A	-2	ASP	-	expression tag	UNP A4WYU7
A	-1	ASP	-	expression tag	UNP A4WYU7
A	0	ASP	-	expression tag	UNP A4WYU7
A	1	LYS	-	expression tag	UNP A4WYU7
F	-13	MET	-	initiating methionine	UNP A4WYU7
F	-12	HIS	-	expression tag	UNP A4WYU7
F	-11	HIS	-	expression tag	UNP A4WYU7
F	-10	HIS	-	expression tag	UNP A4WYU7
F	-9	HIS	-	expression tag	UNP A4WYU7
F	-8	HIS	-	expression tag	UNP A4WYU7
F	-7	HIS	-	expression tag	UNP A4WYU7
F	-6	ASP	-	expression tag	UNP A4WYU7
F	-5	TYR	-	expression tag	UNP A4WYU7
F	-4	LYS	-	expression tag	UNP A4WYU7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	ASP	-	expression tag	UNP A4WYU7
F	-2	ASP	-	expression tag	UNP A4WYU7
F	-1	ASP	-	expression tag	UNP A4WYU7
F	0	ASP	-	expression tag	UNP A4WYU7
F	1	LYS	-	expression tag	UNP A4WYU7

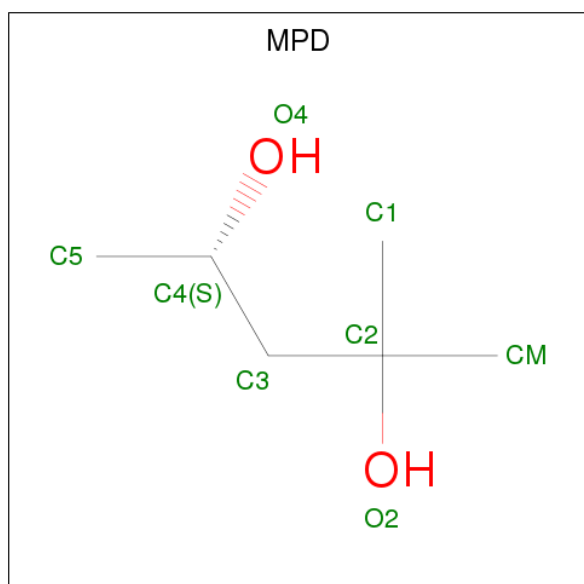
- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	H	N	O	P	0	0	0
			581	172	195	70	126	18			
2	H	18	Total	C	H	N	O	P	0	0	0
			581	172	195	70	126	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*TP\*TP\*TP\*AP\*AP\*C)-3').

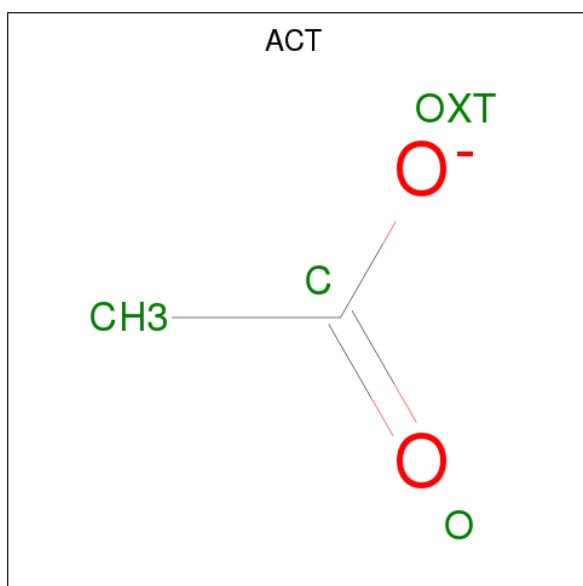
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	21	Total	C	H	N	O	P	0	0	0
			621	190	221	65	124	21			
3	J	22	Total	C	H	N	O	P	3	0	0
			667	204	237	73	131	22			

- Molecule 4 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
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	A	1	Total	C	H	O	0	0
			22	6	14	2		
4	F	1	Total	C	H	O	0	0
			22	6	14	2		
4	F	1	Total	C	H	O	0	0
			22	6	14	2		
4	J	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

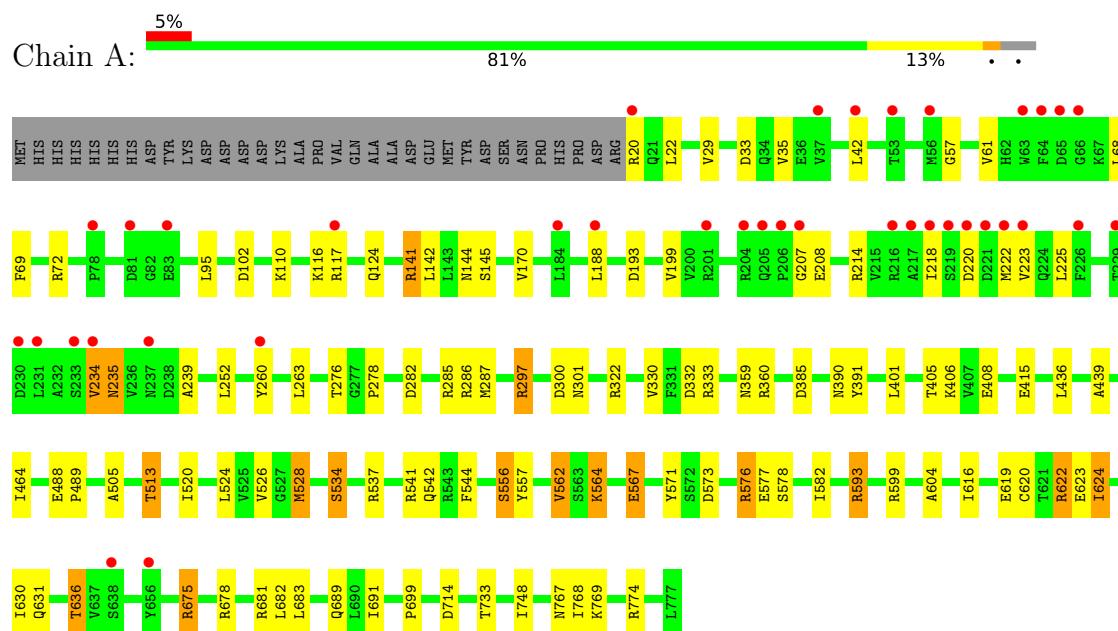
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	294	Total 294	O 294	0	0
7	C	40	Total 40	O 40	0	0
7	G	31	Total 31	O 31	0	0
7	F	214	Total 214	O 214	0	0
7	H	35	Total 35	O 35	0	0
7	J	28	Total 28	O 28	0	0

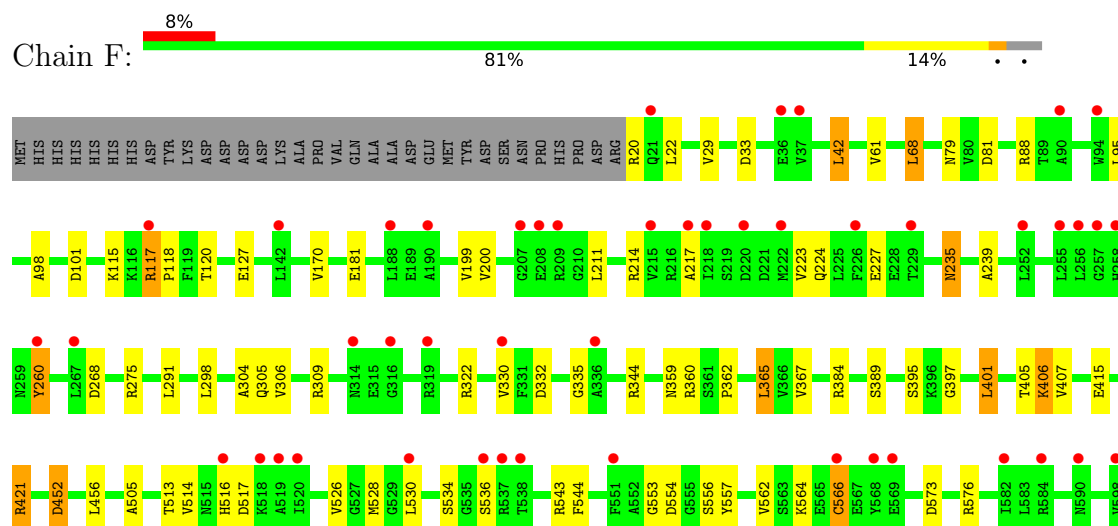
### 3 Residue-property plots

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

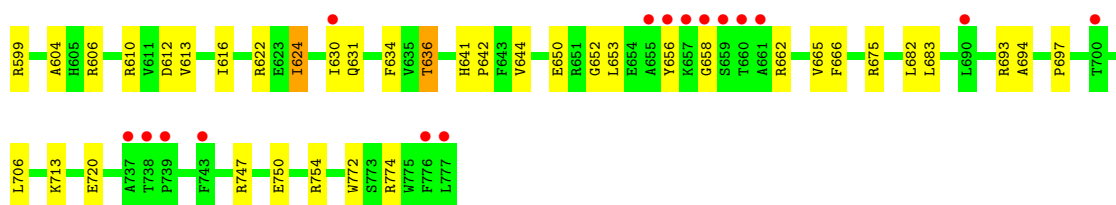
#### • Molecule 1: Uncharacterized protein



#### • Molecule 1: Uncharacterized protein







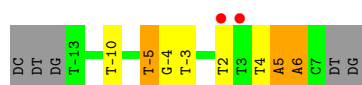
- Molecule 2: RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*C P\*GP\*A)-3')



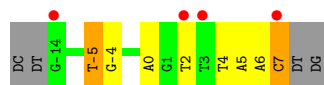
- Molecule 2: RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*C P\*GP\*A)-3')



- Molecule 3: DNA (5'-D(P\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*T P\*TP\*TP\*AP\*AP\*C)-3')



- Molecule 3: DNA (5'-D(P\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*T P\*TP\*TP\*AP\*AP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.04Å 118.31Å 117.67Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	42.30 – 2.15 42.35 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.30-2.15) 94.2 (42.35-2.15)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.16Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.201 , 0.240 0.197 , 0.238	Depositor DCC
$R_{free}$ test set	2000 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: MPD, MG, ACT

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	0.56	0/5984	0.62	1/8129 (0.0%)
1	F	0.50	0/5900	0.57	0/8029
2	C	1.30	2/431 (0.5%)	1.06	0/668
2	H	1.14	1/431 (0.2%)	1.06	0/668
3	G	1.49	3/446 (0.7%)	1.17	2/684 (0.3%)
3	J	1.56	2/480 (0.4%)	1.22	2/737 (0.3%)
All	All	0.70	8/13672 (0.1%)	0.70	5/18915 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	U	OP3-P	-12.70	1.46	1.61
2	H	1	U	OP3-P	-8.15	1.51	1.61
2	C	15	A	N3-C4	-6.36	1.31	1.34
3	G	-5	DT	C5-C7	-5.84	1.46	1.50
3	G	5	DA	C6-N6	5.33	1.38	1.33
3	G	-10	DT	C5-C7	-5.19	1.47	1.50
3	J	7	DC	C1'-N1	5.10	1.55	1.49
3	J	-5	DT	C5-C7	-5.06	1.47	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	7	DC	O4'-C4'-C3'	-6.90	101.74	104.50
1	A	714	ASP	CB-CG-OD1	5.20	122.98	118.30
3	G	6	DA	O4'-C1'-N9	5.15	111.61	108.00
3	G	-3	DT	N3-C4-O4	5.13	122.98	119.90
3	J	4	DT	N3-C4-O4	5.11	122.97	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	117	ARG	Peptide
1	F	566	CYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5855	5749	5748	74	1
1	F	5771	5594	5594	78	1
2	C	386	195	195	4	0
2	H	386	195	195	11	0
3	G	400	221	222	8	0
3	J	430	237	238	12	0
4	A	16	28	28	2	0
4	F	16	28	28	2	0
4	J	8	14	14	2	0
5	A	4	3	3	0	0
6	C	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
7	A	294	0	0	26	0
7	C	40	0	0	4	0
7	F	214	0	0	20	0
7	G	31	0	0	6	0
7	H	35	0	0	5	0
7	J	28	0	0	2	0
All	All	13917	12264	12265	183	1

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 (183) 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)
1:A:769:LYS:NZ	7:A:901:HOH:O	1.81	1.14
1:A:287:MET:SD	7:A:1194:HOH:O	2.04	1.14
1:A:322:ARG:NH2	7:A:902:HOH:O	1.82	1.10
1:A:322:ARG:CZ	7:A:902:HOH:O	2.02	1.07
3:G:-5:DT:C2	7:G:601:HOH:O	2.15	0.98
3:J:7:DC:N3	4:J:102:MPD:O4	2.00	0.94
1:F:573:ASP:OD1	1:F:576:ARG:NH1	2.04	0.91
1:A:218:ILE:HG23	1:A:223:VAL:HG12	1.56	0.85
1:F:694:ALA:N	7:F:907:HOH:O	2.08	0.85
1:F:452:ASP:OD1	7:F:902:HOH:O	1.94	0.84
3:J:5:DA:N7	7:J:203:HOH:O	2.10	0.84
1:A:286:ARG:NH2	7:A:910:HOH:O	2.10	0.83
1:A:322:ARG:NH1	7:A:902:HOH:O	2.03	0.83
3:G:-5:DT:O2	7:G:601:HOH:O	1.94	0.83
1:F:513:THR:HG21	1:F:556:SER:HB3	1.62	0.82
1:A:333:ARG:NH1	7:A:911:HOH:O	2.11	0.82
1:A:390:ASN:OD1	7:A:903:HOH:O	1.98	0.81
1:F:61:VAL:HG13	1:F:68:LEU:HD21	1.64	0.80
1:F:227:GLU:OE1	7:F:903:HOH:O	2.01	0.79
1:A:207:GLY:O	7:A:905:HOH:O	2.01	0.78
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.64	0.78
1:A:57:GLY:O	7:A:906:HOH:O	2.02	0.78
1:A:116:LYS:O	7:A:904:HOH:O	2.01	0.77
1:F:675:ARG:HD2	7:F:962:HOH:O	1.84	0.77
1:F:181:GLU:OE1	7:F:904:HOH:O	2.03	0.76
1:A:322:ARG:NH2	7:A:914:HOH:O	2.15	0.76
1:F:513:THR:HG23	1:F:557:TYR:O	1.86	0.76
1:A:675:ARG:NH1	7:A:913:HOH:O	2.14	0.75
1:F:322:ARG:NH1	7:F:909:HOH:O	2.18	0.75
3:J:-4:DG:OP1	7:J:201:HOH:O	2.04	0.75
1:A:439:ALA:O	7:A:907:HOH:O	2.06	0.74
1:F:650:GLU:OE2	7:F:905:HOH:O	2.06	0.74
1:A:102:ASP:OD2	7:A:908:HOH:O	2.06	0.73
3:G:-4:DG:C8	7:G:601:HOH:O	2.42	0.73
1:A:110:LYS:O	1:A:124:GLN:NE2	2.22	0.72
1:A:385:ASP:OD2	7:A:909:HOH:O	2.08	0.71
3:G:-4:DG:C5	7:G:601:HOH:O	2.45	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:G:O3'	7:H:201:HOH:O	2.10	0.68
3:J:7:DC:O2	3:J:7:DC:H2'	1.93	0.68
1:A:599:ARG:NH1	1:A:631:GLN:OE1	2.28	0.67
1:A:297:ARG:HG3	7:A:934:HOH:O	1.95	0.67
1:F:309:ARG:O	7:F:908:HOH:O	2.13	0.67
1:F:79:ASN:ND2	7:F:912:HOH:O	2.29	0.66
1:F:260:TYR:OH	3:J:0:DA:OP1	2.12	0.66
1:A:359:ASN:OD1	7:A:912:HOH:O	2.13	0.66
1:F:115:LYS:HE2	7:F:1037:HOH:O	1.96	0.65
1:F:624:ILE:HD11	1:F:630:ILE:HD12	1.78	0.64
1:A:276:THR:HG22	1:A:278:PRO:HD2	1.78	0.64
4:A:801:MPD:O2	4:A:801:MPD:O4	1.97	0.64
1:F:384:ARG:NH2	4:F:802:MPD:H52	2.14	0.63
1:F:513:THR:HG22	1:F:514:VAL:N	2.14	0.63
1:A:513:THR:CG2	1:A:557:TYR:O	2.47	0.62
3:G:-4:DG:C4	7:G:601:HOH:O	2.52	0.62
1:A:567:GLU:HG2	7:A:926:HOH:O	1.98	0.62
1:A:360:ARG:HB3	1:A:405:THR:HG23	1.81	0.61
1:A:218:ILE:HD12	1:A:223:VAL:HG12	1.82	0.61
2:H:13:U:OP1	7:H:201:HOH:O	2.16	0.61
4:A:801:MPD:HO2	4:A:801:MPD:HO4	1.43	0.61
2:H:13:U:OP2	7:H:202:HOH:O	2.16	0.60
2:H:13:U:P	7:H:201:HOH:O	2.59	0.60
1:A:29:VAL:HG21	1:A:170:VAL:HG23	1.82	0.60
1:F:199:VAL:CG1	1:F:239:ALA:HB1	2.30	0.60
1:A:33:ASP:OD2	7:A:915:HOH:O	2.15	0.60
1:F:235:ASN:N	1:F:235:ASN:OD1	2.35	0.59
1:F:544:PHE:HD2	1:F:566:CYS:HB3	1.68	0.58
1:A:222:MET:HG2	1:A:235:ASN:HA	1.85	0.58
1:F:421:ARG:HG2	1:F:456:LEU:HD21	1.85	0.58
1:F:513:THR:HG21	1:F:556:SER:CB	2.33	0.58
1:F:720:GLU:OE1	7:F:909:HOH:O	2.17	0.57
3:J:6:DA:OP1	4:J:102:MPD:H11	2.04	0.57
1:A:208:GLU:HA	7:A:905:HOH:O	2.04	0.56
1:F:513:THR:HG22	1:F:514:VAL:H	1.70	0.56
1:A:282:ASP:OD1	1:A:285:ARG:NH1	2.32	0.56
1:F:624:ILE:HD11	1:F:630:ILE:CD1	2.35	0.56
1:A:513:THR:HG21	1:A:556:SER:HB3	1.89	0.55
1:F:652:GLY:O	1:F:653:LEU:HD12	2.07	0.54
3:J:5:DA:H4'	3:J:6:DA:OP2	2.06	0.54
1:F:332:ASP:OD1	1:F:335:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASN:OD1	7:A:916:HOH:O	2.18	0.54
1:F:543:ARG:NH2	2:H:14:G:OP1	2.39	0.54
1:F:606:ARG:NH1	7:F:915:HOH:O	2.33	0.53
3:G:-4:DG:N7	7:G:601:HOH:O	2.41	0.53
1:F:747:ARG:NH2	1:F:750:GLU:OE2	2.29	0.52
1:F:268:ASP:OD2	1:F:693:ARG:NH2	2.39	0.52
1:F:115:LYS:HB2	1:F:120:THR:HB	1.90	0.52
1:F:344:ARG:CB	3:J:7:DC:H41	2.23	0.52
2:C:8:A:N3	7:C:202:HOH:O	2.34	0.51
1:F:599:ARG:NH1	1:F:631:GLN:OE1	2.43	0.51
1:A:537:ARG:CD	7:C:214:HOH:O	2.59	0.51
1:A:576:ARG:HD3	1:A:619:GLU:HG3	1.92	0.51
1:A:29:VAL:CG2	1:A:170:VAL:HG23	2.41	0.51
1:A:576:ARG:HB2	1:A:616:ILE:HD12	1.93	0.51
1:F:630:ILE:HD13	1:F:630:ILE:N	2.26	0.51
1:F:362:PRO:HG2	1:F:407:VAL:HG22	1.94	0.50
1:F:624:ILE:CD1	1:F:630:ILE:HD12	2.40	0.50
1:A:391:TYR:CE1	1:A:489:PRO:HB2	2.47	0.50
1:F:275:ARG:HD2	1:F:697:PRO:HG3	1.94	0.50
1:A:68:LEU:HD23	1:A:69:PHE:N	2.27	0.49
1:F:536:SER:HB2	7:F:903:HOH:O	2.12	0.49
1:A:604:ALA:O	1:A:636:THR:HA	2.13	0.49
2:H:17:G:H8	2:H:17:G:H5''	1.78	0.49
1:F:613:VAL:HG13	1:F:634:PHE:CE1	2.47	0.49
1:F:706:LEU:HD21	1:F:713:LYS:HA	1.95	0.49
2:H:3:A:H2'	2:H:4:C:C6	2.48	0.48
1:A:235:ASN:ND2	1:A:235:ASN:H	2.11	0.48
1:A:218:ILE:HD12	1:A:223:VAL:CG1	2.43	0.48
1:A:408:GLU:OE1	7:A:917:HOH:O	2.20	0.48
1:F:747:ARG:HA	1:F:747:ARG:CZ	2.44	0.48
1:F:656:TYR:HB3	3:J:2:DT:H2''	1.95	0.48
2:C:3:A:H2'	2:C:4:C:C6	2.48	0.48
3:G:2:DT:O5'	3:G:4:DT:H5'	2.14	0.47
1:F:29:VAL:CG2	1:F:170:VAL:HG23	2.45	0.47
4:F:801:MPD:HM2	2:H:11:G:O6	2.14	0.47
1:A:193:ASP:O	7:A:918:HOH:O	2.20	0.47
1:F:604:ALA:O	1:F:636:THR:HA	2.14	0.47
1:F:772:TRP:NE1	7:F:918:HOH:O	2.35	0.47
1:A:534:SER:HB2	1:A:541:ARG:HG2	1.98	0.46
1:A:622:ARG:HG3	1:A:623:GLU:N	2.30	0.46
1:A:513:THR:HG22	1:A:557:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:VAL:HG12	1:F:211:LEU:HA	1.98	0.46
1:A:524:LEU:HD13	1:A:582:ILE:HG21	1.98	0.46
1:F:747:ARG:HA	1:F:747:ARG:NE	2.31	0.46
1:F:576:ARG:HB3	1:F:616:ILE:CD1	2.47	0.45
2:C:7:C:H2'	2:C:8:A:C8	2.52	0.45
2:H:6:G:H2'	2:H:7:C:O4'	2.16	0.45
1:A:537:ARG:HD3	7:C:214:HOH:O	2.15	0.45
1:F:291:LEU:HB3	1:F:306:VAL:HG21	1.98	0.45
1:A:142:LEU:O	1:A:145:SER:OG	2.30	0.44
1:F:29:VAL:HG21	1:F:170:VAL:HG23	1.98	0.44
1:A:225:LEU:HD11	1:A:234:VAL:HG22	2.00	0.44
1:A:675:ARG:HG3	1:A:681:ARG:CZ	2.48	0.44
1:A:95:LEU:C	1:A:95:LEU:HD13	2.37	0.44
1:A:573:ASP:OD1	1:A:576:ARG:NH1	2.48	0.44
1:F:298:LEU:HD11	1:F:304:ALA:HB2	1.99	0.44
1:F:641:HIS:HB2	1:F:642:PRO:HD2	2.00	0.44
1:F:754:ARG:NH1	7:F:906:HOH:O	2.08	0.44
1:A:252:LEU:HD13	1:A:263:LEU:HD23	2.00	0.44
1:F:344:ARG:CB	3:J:7:DC:N4	2.81	0.44
1:F:360:ARG:HB3	1:F:405:THR:HG23	2.00	0.44
1:A:301:ASN:OD1	1:A:301:ASN:N	2.40	0.43
1:F:95:LEU:C	1:F:95:LEU:HD13	2.38	0.43
1:A:505:ALA:HB1	1:A:774:ARG:HG3	1.98	0.43
1:F:772:TRP:CD1	7:F:918:HOH:O	2.69	0.43
1:F:530:LEU:HD12	1:F:544:PHE:O	2.17	0.43
1:F:553:GLY:N	1:F:556:SER:O	2.44	0.43
1:F:747:ARG:NH1	7:F:925:HOH:O	2.44	0.43
1:F:665:VAL:O	1:F:666:PHE:HB2	2.18	0.43
3:G:5:DA:H4'	3:G:6:DA:OP2	2.18	0.43
3:J:-5:DT:H2''	3:J:-4:DG:H5'	2.00	0.43
1:A:528:MET:CE	1:A:571:TYR:HB2	2.49	0.43
1:A:620:CYS:O	1:A:624:ILE:HG23	2.18	0.42
1:A:141:ARG:HG3	1:A:141:ARG:H	1.63	0.42
1:A:678:ARG:HD3	7:A:1110:HOH:O	2.19	0.42
1:F:199:VAL:HG11	1:F:239:ALA:HB1	2.00	0.42
1:F:365:LEU:HD13	1:F:367:VAL:CG2	2.50	0.42
2:H:13:U:H5'	7:H:201:HOH:O	2.20	0.42
1:A:562:VAL:HG21	1:A:748:ILE:HD11	2.01	0.42
1:F:98:ALA:O	1:F:101:ASP:HB2	2.20	0.42
1:A:542:GLN:HG3	1:A:544:PHE:CE1	2.55	0.42
1:F:612:ASP:O	1:F:616:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:VAL:CG1	1:A:239:ALA:HB1	2.50	0.42
1:F:397:GLY:O	1:F:401:LEU:HB2	2.20	0.42
1:A:564:LYS:HB3	7:A:1129:HOH:O	2.19	0.41
1:A:464:ILE:HD12	1:A:464:ILE:HA	1.88	0.41
1:F:610:ARG:NH1	2:H:17:G:OP1	2.46	0.41
1:F:513:THR:CG2	1:F:514:VAL:N	2.83	0.41
1:A:691:ILE:HD11	1:A:699:PRO:HG3	2.02	0.41
2:C:10:A:OP2	7:C:201:HOH:O	2.22	0.41
1:F:217:ALA:O	1:F:224:GLN:N	2.46	0.41
1:F:530:LEU:HD11	1:F:543:ARG:HD2	2.02	0.41
3:J:5:DA:C4'	3:J:6:DA:OP2	2.67	0.41
1:F:305:GLN:HA	7:F:959:HOH:O	2.20	0.41
1:A:300:ASP:N	1:A:300:ASP:OD1	2.53	0.41
1:F:652:GLY:C	1:F:653:LEU:HD12	2.40	0.41
1:F:693:ARG:HB3	7:F:907:HOH:O	2.20	0.41
1:A:505:ALA:HB1	1:A:774:ARG:CG	2.50	0.41
1:A:576:ARG:HB2	1:A:616:ILE:CD1	2.51	0.41
1:A:188:LEU:HD11	1:A:218:ILE:HG13	2.03	0.40
1:F:42:LEU:HB2	1:F:68:LEU:HB2	2.04	0.40
1:F:505:ALA:HB1	1:F:774:ARG:CG	2.51	0.40
1:A:225:LEU:HD11	1:A:234:VAL:CG2	2.51	0.40
1:A:391:TYR:CZ	1:A:489:PRO:HB2	2.56	0.40
1:F:406:LYS:HB2	7:F:1043:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ARG:HH22	1:F:81:ASP:OD1[1_565]	1.44	0.16

## 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	756/791 (96%)	732 (97%)	22 (3%)	2 (0%)	43	39
1	F	756/791 (96%)	717 (95%)	35 (5%)	4 (0%)	31	24
All	All	1512/1582 (96%)	1449 (96%)	57 (4%)	6 (0%)	36	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	ARG
1	F	658	GLY
1	F	118	PRO
1	A	220	ASP
1	F	554	ASP
1	A	768	ILE

### 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	603/672 (90%)	560 (93%)	43 (7%)	16	10
1	F	585/672 (87%)	550 (94%)	35 (6%)	21	16
All	All	1188/1344 (88%)	1110 (93%)	78 (7%)	18	12

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	22	LEU
1	A	35	VAL
1	A	42	LEU
1	A	72	ARG
1	A	117	ARG
1	A	141	ARG
1	A	144	ASN
1	A	214	ARG
1	A	234	VAL

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	260	TYR
1	A	297	ARG
1	A	330	VAL
1	A	332	ASP
1	A	401	LEU
1	A	406	LYS
1	A	415	GLU
1	A	436	LEU
1	A	488	GLU
1	A	513	THR
1	A	520	ILE
1	A	526	VAL
1	A	528	MET
1	A	534	SER
1	A	556	SER
1	A	562	VAL
1	A	564	LYS
1	A	567	GLU
1	A	576	ARG
1	A	577	GLU
1	A	578	SER
1	A	593	ARG
1	A	622	ARG
1	A	624	ILE
1	A	630	ILE
1	A	636	THR
1	A	675	ARG
1	A	682	LEU
1	A	683	LEU
1	A	689	GLN
1	A	733	THR
1	A	767	ASN
1	F	20	ARG
1	F	22	LEU
1	F	33	ASP
1	F	42	LEU
1	F	68	LEU
1	F	88	ARG
1	F	127	GLU
1	F	214	ARG
1	F	223	VAL

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Mol	Chain	Res	Type
1	F	235	ASN
1	F	260	TYR
1	F	330	VAL
1	F	359	ASN
1	F	365	LEU
1	F	389	SER
1	F	395	SER
1	F	401	LEU
1	F	406	LYS
1	F	415	GLU
1	F	421	ARG
1	F	452	ASP
1	F	516	HIS
1	F	517	ASP
1	F	526	VAL
1	F	528	MET
1	F	534	SER
1	F	562	VAL
1	F	564	LYS
1	F	622	ARG
1	F	624	ILE
1	F	636	THR
1	F	644	VAL
1	F	662	ARG
1	F	682	LEU
1	F	683	LEU

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	H	17/18 (94%)	2 (11%)	0
All	All	34/36 (94%)	2 (5%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	11	G

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Mol	Chain	Res	Type
2	H	17	G

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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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
4	MPD	A	801	-	7,7,7	0.33	0	9,10,10	0.30	0
4	MPD	A	802	-	7,7,7	0.27	0	9,10,10	0.44	0
5	ACT	A	803	-	1,3,3	6.85	1 (100%)	0,3,3	0.00	-
4	MPD	F	801	-	7,7,7	0.24	0	9,10,10	0.59	0
4	MPD	F	802	-	7,7,7	0.36	0	9,10,10	0.36	0
4	MPD	J	102	-	7,7,7	0.27	0	9,10,10	0.62	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
4	MPD	A	801	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	A	802	-	-	0/5/5/5	0/0/0/0
5	ACT	A	803	-	-	0/0/0/0	0/0/0/0
4	MPD	F	801	-	-	0/5/5/5	0/0/0/0
4	MPD	F	802	-	-	0/5/5/5	0/0/0/0
4	MPD	J	102	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	803	ACT	CH3-C	6.85	1.57	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	MPD	2	0
4	F	801	MPD	1	0
4	F	802	MPD	1	0
4	J	102	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

### 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	758/791 (95%)	0.32	38 (5%)	29	37	19, 37, 77, 137	1 (0%)
1	F	758/791 (95%)	0.61	63 (8%)	11	15	20, 46, 75, 173	3 (0%)
2	C	18/18 (100%)	-0.50	0	100	100	22, 34, 61, 85	0
2	H	18/18 (100%)	-0.42	0	100	100	29, 37, 52, 65	0
3	G	21/26 (80%)	0.31	2 (9%)	8	11	31, 45, 86, 108	1 (4%)
3	J	22/26 (84%)	0.49	4 (18%)	1	1	31, 49, 85, 113	1 (4%)
All	All	1595/1670 (95%)	0.45	107 (6%)	18	23	19, 42, 77, 173	6 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	GLU	24.0
1	F	207	GLY	9.9
1	A	206	PRO	9.1
1	F	656	TYR	8.5
1	F	218	ILE	8.3
1	F	658	GLY	8.1
1	A	218	ILE	8.1
1	A	207	GLY	6.8
1	F	660	THR	6.6
1	F	519	ALA	5.8
1	A	231	LEU	5.7
1	A	188	LEU	5.4
1	A	42	LEU	5.1
1	F	538	THR	5.0
1	A	220	ASP	4.7
1	F	536	SER	4.5
1	F	655	ALA	4.4
3	J	3	DT	4.3
1	F	520	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	566	CYS	4.0
1	A	223	VAL	4.0
1	F	260	TYR	4.0
1	A	234	VAL	4.0
1	F	661	ALA	3.9
1	A	204	ARG	3.8
1	F	215	VAL	3.7
1	F	659	SER	3.6
1	F	217	ALA	3.6
1	A	219	SER	3.6
1	F	316	GLY	3.5
1	F	252	LEU	3.5
1	F	256	LEU	3.2
1	F	220	ASP	3.2
1	F	226	PHE	3.2
1	A	217	ALA	3.2
1	F	190	ALA	3.2
1	F	188	LEU	3.1
1	F	330	VAL	3.1
1	F	117	ARG	3.1
1	A	20	ARG	3.1
1	F	743	PHE	3.1
1	F	319	ARG	3.1
3	G	2	DT	3.0
1	A	205	GLN	3.0
1	A	222	MET	3.0
1	F	267	LEU	3.0
1	F	537	ARG	2.9
1	A	53	THR	2.9
1	A	656	TYR	2.9
1	F	90	ALA	2.9
1	F	229	THR	2.9
1	A	64	PHE	2.8
1	A	216	ARG	2.8
1	F	518	LYS	2.8
1	A	230	ASP	2.8
1	A	56	MET	2.8
1	A	63	TRP	2.7
1	F	336	ALA	2.7
1	F	738	THR	2.7
1	F	257	GLY	2.6
1	F	737	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	J	7	DC	2.6
1	A	260	TYR	2.6
3	G	3	DT	2.6
1	A	184	LEU	2.5
1	F	37	VAL	2.5
3	J	-14	DG	2.5
1	A	229	THR	2.5
1	F	314	ASN	2.5
1	F	516	HIS	2.5
1	F	700	THR	2.4
1	F	582	ILE	2.4
1	F	630	ILE	2.4
1	F	590	ASN	2.4
1	F	258	HIS	2.4
1	F	209	ARG	2.4
1	F	36	GLU	2.3
1	A	37	VAL	2.3
1	A	65	ASP	2.3
1	A	221	ASP	2.3
1	A	83	GLU	2.3
1	F	569	GLU	2.2
1	A	237	ASN	2.2
1	F	739	PRO	2.2
3	J	2	DT	2.2
1	F	142	LEU	2.2
1	F	255	LEU	2.2
1	F	777	LEU	2.2
1	A	117	ARG	2.2
1	F	21	GLN	2.1
1	F	568	TYR	2.1
1	A	81	ASP	2.1
1	F	530	LEU	2.1
1	A	226	PHE	2.1
1	A	78	PRO	2.1
1	F	222	MET	2.1
1	F	776	PHE	2.1
1	A	66	GLY	2.1
1	A	233	SER	2.1
1	F	598	VAL	2.1
1	F	584	ARG	2.1
1	F	690	LEU	2.1
1	F	657	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	201	ARG	2.0
1	A	638	SER	2.0
1	F	551	PHE	2.0
1	F	94	TRP	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. 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
6	MG	J	101	1/1	0.62	0.16	43,43,43,43	0
4	MPD	J	102	8/8	0.65	0.23	51,69,78,84	0
4	MPD	A	802	8/8	0.71	0.16	64,93,111,112	0
5	ACT	A	803	4/4	0.83	0.18	44,52,57,57	0
4	MPD	F	802	8/8	0.85	0.44	56,67,80,80	0
4	MPD	F	801	8/8	0.89	0.22	45,56,79,80	0
6	MG	C	101	1/1	0.92	0.18	22,22,22,22	0
4	MPD	A	801	8/8	0.93	0.20	44,55,62,66	0
6	MG	H	101	1/1	0.97	0.17	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.