



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID : 3NVI  
Title : Structure of N-terminal truncated Nop56/58 bound with L7Ae and box C/D RNA  
Authors : Li, H.; Xue, S.; Wang, R.  
Deposited on : 2010-07-08  
Resolution : 2.71 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

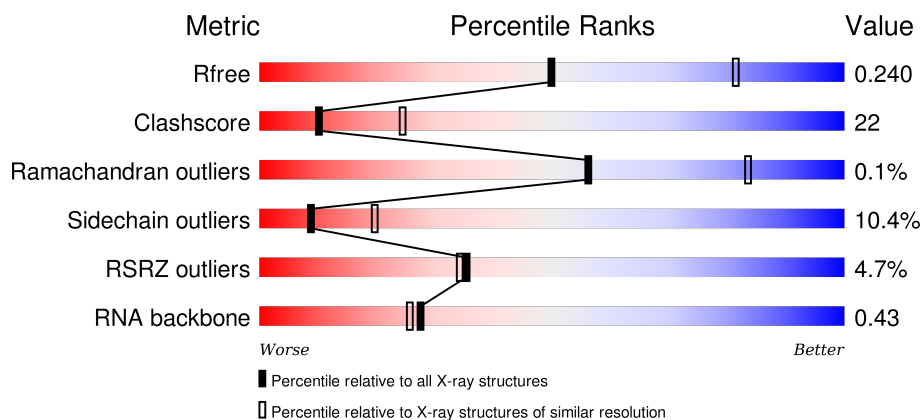
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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	379	<div> <div>3%</div> <div>38% 25% • 35%</div> </div>
1	C	379	<div> <div>2%</div> <div>39% 22% • 35%</div> </div>
2	B	129	<div> <div>4%</div> <div>55% 33% 6% 6%</div> </div>
2	D	129	<div> <div>9%</div> <div>56% 36% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	24	<div><div></div><div>4%</div><div>50%</div><div>21%</div><div>25%</div><div></div></div>
3	F	24	<div><div></div><div>4%</div><div>54%</div><div>33%</div><div>13%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6870 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 NOP5/NOP56 related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1990	1270	354	360	6			
1	C	247	Total	C	N	O	S	0	0	0
			1990	1270	354	360	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q8U4M1
A	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	0	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
A	2	VAL	-	EXPRESSION TAG	UNP Q8U4M1
A	3	MET	-	EXPRESSION TAG	UNP Q8U4M1
A	4	ILE	-	EXPRESSION TAG	UNP Q8U4M1
C	-5	MET	-	EXPRESSION TAG	UNP Q8U4M1
C	-4	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-3	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-2	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	-1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	0	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	1	HIS	-	EXPRESSION TAG	UNP Q8U4M1
C	2	VAL	-	EXPRESSION TAG	UNP Q8U4M1
C	3	MET	-	EXPRESSION TAG	UNP Q8U4M1
C	4	ILE	-	EXPRESSION TAG	UNP Q8U4M1

- Molecule 2 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			
2	D	121	Total	C	N	O	S	0	0	0
			926	591	153	179	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	EXPRESSION TAG	UNP Q8U160
B	-3	HIS	-	EXPRESSION TAG	UNP Q8U160
B	-2	HIS	-	EXPRESSION TAG	UNP Q8U160
B	-1	HIS	-	EXPRESSION TAG	UNP Q8U160
B	0	HIS	-	EXPRESSION TAG	UNP Q8U160
B	1	HIS	-	EXPRESSION TAG	UNP Q8U160
B	2	HIS	-	EXPRESSION TAG	UNP Q8U160
D	-4	MET	-	EXPRESSION TAG	UNP Q8U160
D	-3	HIS	-	EXPRESSION TAG	UNP Q8U160
D	-2	HIS	-	EXPRESSION TAG	UNP Q8U160
D	-1	HIS	-	EXPRESSION TAG	UNP Q8U160
D	0	HIS	-	EXPRESSION TAG	UNP Q8U160
D	1	HIS	-	EXPRESSION TAG	UNP Q8U160
D	2	HIS	-	EXPRESSION TAG	UNP Q8U160

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	24	Total	C	N	O	P	0	0	0
			513	230	96	164	23			
3	F	24	Total	C	N	O	P	0	0	0
			513	230	96	164	23			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	C	3	Total O 3 3	0	0
4	D	2	Total O 2 2	0	0
4	E	2	Total O 2 2	0	0

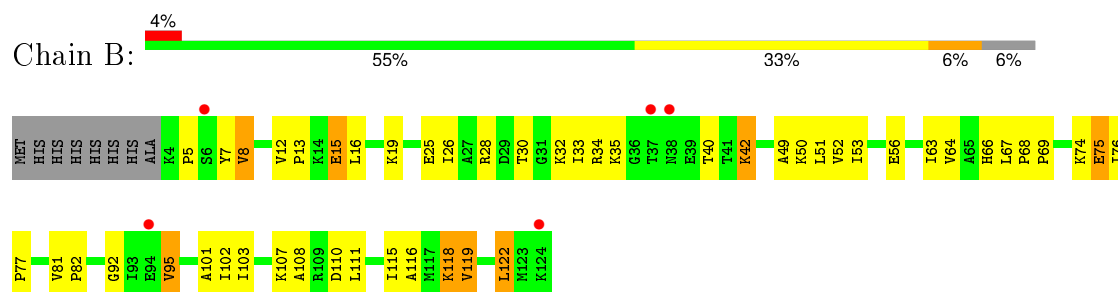
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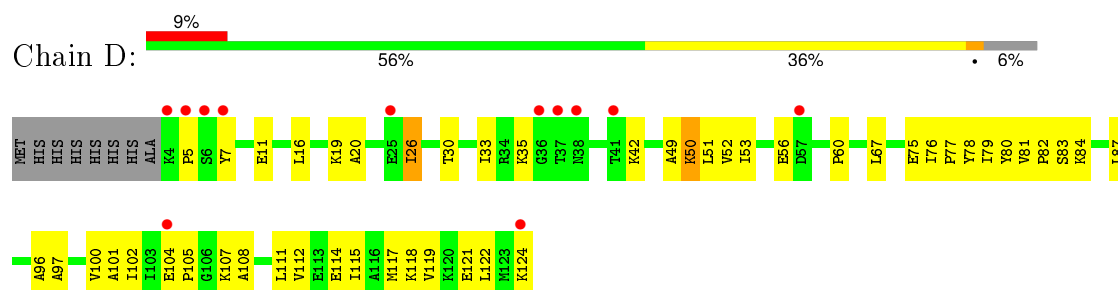
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	O	0	0
			1	1		



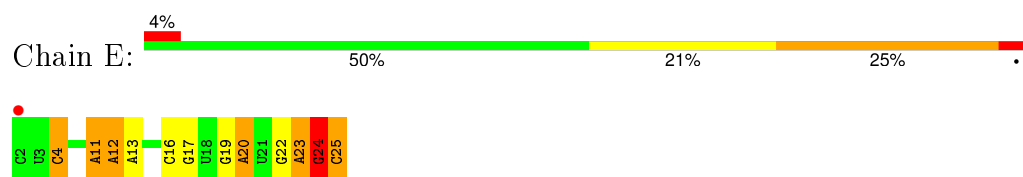
- Molecule 2: 50S ribosomal protein L7Ae



- Molecule 2: 50S ribosomal protein L7Ae



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.22Å 91.84Å 155.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.62 – 2.71 31.62 – 2.71	Depositor EDS
% Data completeness (in resolution range)	80.7 (31.62-2.71) 79.9 (31.62-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_589)	Depositor
R, $R_{free}$	0.208 , 0.249 0.199 , 0.240	Depositor DCC
$R_{free}$ test set	1371 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 43.4	EDS
Estimated twinning fraction	0.022 for k,h,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29881 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.57	0/2024	0.71	0/2724
1	C	0.51	0/2024	0.70	1/2724 (0.0%)
2	B	0.42	0/938	0.60	0/1264
2	D	0.45	0/938	0.62	0/1264
3	E	0.74	0/574	1.24	4/894 (0.4%)
3	F	0.64	0/574	1.24	4/894 (0.4%)
All	All	0.54	0/7072	0.81	9/9764 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	23	A	C5-N7-C8	-8.65	99.57	103.90
3	E	23	A	C8-N9-C4	-8.35	102.46	105.80
3	F	23	A	N7-C8-N9	7.88	117.74	113.80
3	E	23	A	C5-N7-C8	-6.45	100.67	103.90
3	E	23	A	N7-C8-N9	6.40	117.00	113.80
3	F	23	A	C4-C5-N7	6.36	113.88	110.70
1	C	190	ILE	CG1-CB-CG2	-6.08	98.03	111.40
3	F	23	A	C8-N9-C4	-5.95	103.42	105.80
3	E	24	G	N3-C4-C5	-5.04	126.08	128.60

There are no chirality outliers.

There are no planarity outliers.

### 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	1990	0	2060	97	0
1	C	1990	0	2060	112	0
2	B	926	0	977	49	0
2	D	926	0	977	36	0
3	E	513	0	262	18	0
3	F	513	0	262	9	0
4	A	4	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
All	All	6870	0	6598	293	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 22.

All (293) 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:365:ARG:HH12	3:E:19:G:H5''	1.17	1.07
1:C:190:ILE:HG13	1:C:212:LYS:HE2	1.34	1.04
1:A:372:LYS:O	1:A:373:TYR:CD1	2.17	0.98
1:A:372:LYS:O	1:A:373:TYR:CG	2.16	0.98
1:C:195:LEU:HD21	1:C:208:ILE:HD11	1.47	0.94
2:B:26:ILE:HG13	2:B:108:ALA:HB2	1.52	0.91
2:B:5:PRO:HG2	2:B:7:TYR:CE2	2.05	0.91
1:C:190:ILE:CG1	1:C:212:LYS:HE2	2.03	0.86
2:B:26:ILE:O	2:B:30:THR:HG22	1.77	0.83
2:B:5:PRO:HG2	2:B:7:TYR:HE2	1.42	0.82
1:C:372:LYS:O	1:C:373:TYR:CG	2.33	0.82
1:C:203:GLU:HA	1:C:206:LYS:NZ	1.95	0.81
1:C:190:ILE:CD1	1:C:209:LEU:HD12	2.10	0.81
1:A:208:ILE:O	1:A:212:LYS:HB3	1.81	0.80
1:A:363:GLU:OE1	1:A:363:GLU:HA	1.83	0.79
1:A:163:HIS:HE1	1:A:187:ARG:H	1.30	0.79
1:C:190:ILE:HD11	1:C:209:LEU:HD12	1.63	0.78
2:B:15:GLU:HG2	2:B:16:LEU:N	1.96	0.77
1:A:212:LYS:HG3	1:A:213:GLU:N	2.00	0.77
2:B:26:ILE:CG1	2:B:108:ALA:HB2	2.14	0.76
1:A:195:LEU:CD1	1:A:209:LEU:HD11	2.15	0.76
2:B:68:PRO:HB2	2:B:69:PRO:HD3	1.67	0.76
1:A:141:ALA:HB2	1:C:155:ARG:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ARG:NH1	3:E:24:G:C5	2.54	0.75
1:C:180:PHE:O	1:C:184:VAL:HG12	1.87	0.74
2:B:25:GLU:HG3	2:B:28:ARG:HH21	1.53	0.74
1:A:210:GLU:CD	1:A:211:ALA:H	1.91	0.74
1:C:308:LYS:CE	3:F:23:A:H4'	2.18	0.73
1:C:201:SER:O	1:C:205:ILE:HG22	1.88	0.73
1:C:372:LYS:O	1:C:373:TYR:CD1	2.42	0.72
2:B:95:VAL:HG21	3:E:17:G:N2	2.04	0.72
1:A:210:GLU:OE2	1:A:210:GLU:N	2.22	0.72
2:B:30:THR:CG2	2:B:107:LYS:H	2.03	0.72
2:D:114:GLU:HA	2:D:117:MET:HG2	1.71	0.71
2:B:111:LEU:O	2:B:115:ILE:HG12	1.90	0.71
1:C:314:VAL:O	1:C:317:GLN:HG2	1.90	0.71
2:D:16:LEU:HA	2:D:19:LYS:NZ	2.07	0.70
1:C:210:GLU:C	1:C:214:LYS:HE3	2.12	0.70
1:A:192:GLU:HG2	1:A:196:ARG:NH2	2.07	0.69
1:C:190:ILE:HD12	1:C:191:ASN:CA	2.22	0.69
2:B:30:THR:OG1	2:B:107:LYS:HG3	1.93	0.69
1:C:212:LYS:HB3	1:C:212:LYS:HZ2	1.56	0.69
1:C:328:GLN:OE1	1:C:370:LYS:HD3	1.93	0.69
2:B:53:ILE:N	2:B:53:ILE:HD12	2.07	0.69
1:A:309:PRO:HD2	3:E:23:A:H1'	1.75	0.68
1:C:190:ILE:HD12	1:C:191:ASN:N	2.09	0.68
1:C:319:PRO:HA	1:C:322:ASN:ND2	2.11	0.66
1:A:328:GLN:OE1	1:A:370:LYS:HD3	1.96	0.66
1:A:212:LYS:HG3	1:A:213:GLU:H	1.59	0.66
1:C:190:ILE:CG1	1:C:212:LYS:CE	2.73	0.65
1:C:187:ARG:O	1:C:190:ILE:HG23	1.95	0.65
1:C:203:GLU:HA	1:C:206:LYS:HZ1	1.60	0.65
1:A:163:HIS:CE1	1:A:187:ARG:H	2.14	0.65
1:A:191:ASN:OD1	1:A:194:VAL:HG23	1.96	0.65
1:A:205:ILE:O	1:A:209:LEU:HD13	1.97	0.65
2:D:87:LEU:HD23	2:D:97:ALA:O	1.97	0.65
2:D:51:LEU:HB3	2:D:102:ILE:HD12	1.78	0.65
1:A:163:HIS:CE1	1:A:187:ARG:HG3	2.32	0.64
2:B:49:ALA:O	2:B:76:ILE:HD12	1.98	0.64
2:B:95:VAL:HG21	3:E:17:G:H21	1.62	0.63
2:D:20:ALA:HB2	2:D:79:ILE:HD13	1.80	0.63
1:C:174:HIS:HB2	1:C:175:PRO:HD3	1.81	0.63
2:B:8:VAL:HG12	2:B:8:VAL:O	1.99	0.63
2:B:30:THR:HG23	2:B:107:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:HB2	1:A:175:PRO:HD3	1.80	0.62
1:A:208:ILE:HG22	1:A:209:LEU:HD12	1.81	0.62
2:B:56:GLU:HG2	2:B:82:PRO:HA	1.79	0.62
3:E:12:A:OP2	3:E:12:A:H8	1.83	0.62
1:A:365:ARG:NH1	3:E:19:G:H5''	2.02	0.62
1:C:280:ARG:O	1:C:284:MET:HG2	1.99	0.62
2:D:5:PRO:HB2	2:D:7:TYR:CE2	2.34	0.61
2:D:11:GLU:N	2:D:11:GLU:OE1	2.33	0.61
1:C:203:GLU:HA	1:C:206:LYS:HZ3	1.62	0.61
1:C:308:LYS:HE3	3:F:23:A:H4'	1.82	0.60
1:C:198:LEU:HD12	1:C:198:LEU:O	2.00	0.60
1:C:180:PHE:CE1	1:C:184:VAL:HG11	2.37	0.59
2:D:51:LEU:HD12	2:D:77:PRO:O	2.02	0.59
1:C:203:GLU:OE2	1:C:207:LYS:HE3	2.02	0.59
1:A:365:ARG:O	1:A:369:ILE:HG12	2.02	0.59
1:C:359:LYS:O	1:C:363:GLU:HG2	2.02	0.58
1:C:268:LEU:HD12	1:C:268:LEU:O	2.03	0.58
1:C:372:LYS:O	1:C:373:TYR:CD2	2.56	0.58
1:C:280:ARG:CZ	1:C:284:MET:HE2	2.33	0.58
2:B:40:THR:HG23	2:B:101:ALA:HB2	1.86	0.58
2:D:51:LEU:HB3	2:D:102:ILE:CD1	2.34	0.58
1:A:170:LEU:CD1	1:A:208:ILE:HG13	2.33	0.57
1:C:293:LEU:O	1:C:313:GLY:HA3	2.04	0.57
1:A:201:SER:O	1:A:205:ILE:HG22	2.05	0.57
2:B:95:VAL:CG2	3:E:17:G:N2	2.68	0.57
1:A:163:HIS:HE1	1:A:187:ARG:N	1.98	0.57
3:F:18:U:H4'	3:F:19:G:OP2	2.06	0.56
1:C:327:TRP:CZ2	1:C:373:TYR:O	2.59	0.56
1:C:221:ASP:OD2	1:C:223:THR:HG22	2.04	0.56
1:C:308:LYS:HE2	3:F:23:A:H4'	1.87	0.55
2:D:117:MET:HG3	2:D:118:LYS:N	2.22	0.55
1:A:209:LEU:N	1:A:209:LEU:HD12	2.22	0.55
2:D:121:GLU:HG3	2:D:122:LEU:N	2.21	0.55
1:A:308:LYS:HB3	3:E:23:A:O2'	2.06	0.55
1:C:211:ALA:HA	1:C:214:LYS:NZ	2.22	0.55
1:C:368:GLU:O	1:C:371:GLU:HB3	2.07	0.55
1:C:190:ILE:HD12	1:C:191:ASN:HA	1.87	0.54
1:C:208:ILE:HG13	1:C:209:LEU:N	2.22	0.54
1:A:213:GLU:OE1	1:A:214:LYS:N	2.39	0.54
2:B:5:PRO:CG	2:B:7:TYR:HE2	2.18	0.54
1:C:316:TYR:O	1:C:322:ASN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:THR:HG21	2:B:107:LYS:H	1.72	0.54
1:C:170:LEU:O	1:C:172:PRO:HD3	2.06	0.54
1:A:312:HIS:CD2	1:A:316:TYR:CD2	2.96	0.54
1:A:331:LYS:HE2	1:A:373:TYR:CZ	2.43	0.54
1:A:207:LYS:O	1:A:208:ILE:HB	2.07	0.54
1:C:185:GLY:HA3	1:C:229:ARG:HD2	1.90	0.53
2:B:25:GLU:HG3	2:B:28:ARG:NH2	2.21	0.53
2:D:111:LEU:O	2:D:115:ILE:HG13	2.09	0.53
3:F:24:G:H4'	3:F:25:C:OP1	2.09	0.53
1:A:259:ASN:ND2	1:A:347:ASP:OD1	2.42	0.53
2:D:105:PRO:HB3	2:D:112:VAL:HG21	1.90	0.53
1:A:346:VAL:HG21	1:A:354:ILE:HD13	1.89	0.53
1:C:210:GLU:OE2	1:C:214:LYS:HE2	2.08	0.53
2:D:121:GLU:HG3	2:D:122:LEU:H	1.74	0.53
1:C:156:LEU:O	1:C:156:LEU:HD22	2.10	0.52
1:A:169:GLU:HG2	1:A:170:LEU:N	2.23	0.52
2:D:30:THR:HG21	2:D:107:LYS:HD2	1.90	0.52
1:A:159:TRP:HA	1:C:137:GLN:HG3	1.91	0.52
2:D:16:LEU:HA	2:D:19:LYS:HZ1	1.73	0.52
1:A:170:LEU:CD2	1:A:204:LYS:HD2	2.40	0.52
1:C:365:ARG:NH1	1:C:369:ILE:HD11	2.25	0.52
1:A:314:VAL:O	1:A:317:GLN:HG2	2.10	0.52
1:C:190:ILE:HG12	1:C:212:LYS:CE	2.40	0.51
1:C:167:LEU:HD11	1:C:171:LEU:HD22	1.93	0.51
1:C:363:GLU:HA	1:C:363:GLU:OE1	2.10	0.51
1:C:204:LYS:O	1:C:208:ILE:HG23	2.10	0.51
1:C:331:LYS:HE2	3:F:22:G:OP2	2.10	0.51
1:C:210:GLU:O	1:C:214:LYS:HG2	2.11	0.51
1:A:212:LYS:CG	1:A:213:GLU:N	2.73	0.51
1:C:212:LYS:HB3	1:C:212:LYS:NZ	2.17	0.51
1:C:139:ILE:HG13	1:C:270:ALA:HB3	1.93	0.51
1:A:187:ARG:HD3	1:A:215:THR:HG21	1.92	0.50
2:D:124:LYS:HG2	2:D:124:LYS:O	2.10	0.50
1:A:205:ILE:HG12	1:A:205:ILE:O	2.11	0.50
1:C:372:LYS:C	1:C:373:TYR:CG	2.84	0.50
2:B:16:LEU:HA	2:B:19:LYS:NZ	2.26	0.50
1:C:346:VAL:HG21	1:C:354:ILE:HD13	1.92	0.50
2:D:33:ILE:HG22	2:D:102:ILE:HA	1.92	0.50
1:A:316:TYR:O	1:A:322:ASN:HB3	2.11	0.50
1:A:230:GLN:HG3	1:C:244:LYS:HD3	1.94	0.50
1:C:316:TYR:CE1	3:F:25:C:N4	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLU:C	1:C:203:GLU:OE2	2.50	0.49
1:A:280:ARG:HG3	1:A:348:TYR:CZ	2.47	0.49
2:B:51:LEU:HD12	2:B:77:PRO:O	2.12	0.49
1:A:369:ILE:O	1:A:373:TYR:HD1	1.95	0.49
2:D:26:ILE:CG1	2:D:108:ALA:HB2	2.42	0.49
1:A:334:ARG:NH1	3:E:20:A:OP2	2.45	0.49
1:A:271:ARG:O	1:A:275:LEU:HD22	2.11	0.49
1:C:262:ALA:HB3	1:C:355:ALA:HB1	1.94	0.49
2:D:53:ILE:N	2:D:53:ILE:HD12	2.27	0.49
1:A:165:PRO:HD3	1:A:217:GLY:HA3	1.95	0.48
2:D:16:LEU:HA	2:D:19:LYS:HZ3	1.79	0.48
1:A:127:GLN:O	1:A:129:GLY:N	2.46	0.48
1:C:353:TYR:CZ	1:C:355:ALA:HB3	2.48	0.48
2:D:56:GLU:HG2	2:D:81:VAL:O	2.14	0.48
1:A:210:GLU:O	1:A:213:GLU:OE1	2.31	0.48
2:B:66:HIS:H	2:B:66:HIS:HD1	1.62	0.48
1:C:316:TYR:CE1	3:F:25:C:C4	3.02	0.47
1:A:237:ARG:HB2	1:C:234:GLU:OE1	2.14	0.47
1:A:286:PRO:CG	2:B:42:LYS:HD3	2.43	0.47
1:A:170:LEU:HD21	1:A:204:LYS:HD2	1.95	0.47
1:C:167:LEU:HD22	1:C:180:PHE:CE1	2.50	0.47
1:C:371:GLU:HG2	1:C:372:LYS:HG3	1.95	0.47
2:D:26:ILE:HG13	2:D:108:ALA:HB2	1.96	0.47
1:C:280:ARG:CZ	1:C:284:MET:CE	2.93	0.47
1:C:191:ASN:O	1:C:195:LEU:HD13	2.14	0.47
1:A:334:ARG:HG2	1:A:334:ARG:HH11	1.78	0.47
1:C:203:GLU:O	1:C:203:GLU:OE2	2.33	0.47
1:C:202:GLU:CD	1:C:202:GLU:H	2.18	0.47
2:B:30:THR:HG21	2:B:107:LYS:HB2	1.97	0.47
1:C:167:LEU:CD2	1:C:180:PHE:CE1	2.98	0.47
2:D:67:LEU:HA	2:D:67:LEU:HD23	1.77	0.47
2:B:32:LYS:HA	2:B:32:LYS:HD2	1.78	0.47
2:B:26:ILE:CD1	2:B:108:ALA:HB2	2.45	0.47
1:A:170:LEU:HD13	1:A:208:ILE:HG13	1.96	0.47
2:B:115:ILE:O	2:B:119:VAL:HB	2.15	0.47
1:C:195:LEU:HB2	1:C:205:ILE:HD12	1.97	0.46
1:A:363:GLU:OE1	1:A:363:GLU:CA	2.58	0.46
1:A:131:ARG:HD3	1:A:255:ASP:OD2	2.15	0.46
1:C:212:LYS:CB	1:C:212:LYS:HZ2	2.21	0.46
2:D:56:GLU:HG2	2:D:82:PRO:HA	1.96	0.46
1:A:308:LYS:HA	1:A:309:PRO:HD3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD12	1:A:209:LEU:HD11	1.96	0.46
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.74	0.46
1:C:210:GLU:O	1:C:213:GLU:HG2	2.16	0.46
1:C:323:ARG:O	1:C:323:ARG:HG3	2.16	0.46
1:C:302:HIS:CE1	1:C:309:PRO:HG3	2.51	0.46
1:C:281:GLU:O	1:C:285:MET:HG3	2.16	0.46
1:A:179:ALA:O	1:A:183:THR:HG23	2.16	0.46
1:C:169:GLU:HG2	1:C:170:LEU:N	2.30	0.45
1:C:180:PHE:C	1:C:184:VAL:HG12	2.37	0.45
2:D:75:GLU:OE1	2:D:75:GLU:N	2.49	0.45
1:C:300:PHE:O	1:C:304:ARG:HG3	2.16	0.45
1:A:357:GLU:HG2	1:A:358:LEU:N	2.30	0.45
1:A:208:ILE:N	1:A:210:GLU:OE2	2.49	0.45
2:B:53:ILE:N	2:B:53:ILE:CD1	2.76	0.45
1:A:372:LYS:NZ	3:E:12:A:N6	2.63	0.45
1:A:302:HIS:HE1	3:E:4:C:O2'	1.99	0.45
1:C:365:ARG:CZ	1:C:369:ILE:HD11	2.46	0.45
3:F:10:G:C2	3:F:14:G:C6	3.04	0.45
1:C:315:ILE:O	1:C:321:ILE:HD12	2.16	0.45
1:C:180:PHE:CD1	1:C:184:VAL:CG1	3.00	0.45
1:C:211:ALA:N	1:C:214:LYS:HE3	2.31	0.45
1:A:207:LYS:C	1:A:209:LEU:H	2.19	0.45
1:A:359:LYS:HE3	1:A:359:LYS:HB2	1.65	0.45
1:C:325:PRO:HB2	1:C:327:TRP:HD1	1.82	0.45
1:C:249:ILE:O	1:C:253:MET:HB2	2.17	0.45
1:C:167:LEU:HD21	1:C:180:PHE:CD1	2.51	0.45
1:C:242:ARG:HG2	1:C:242:ARG:HH11	1.82	0.45
1:A:210:GLU:CD	1:A:211:ALA:N	2.68	0.44
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.55	0.44
1:A:302:HIS:CD2	1:A:309:PRO:HG3	2.53	0.44
2:B:12:VAL:HA	2:B:13:PRO:HD3	1.87	0.44
2:B:33:ILE:HG22	2:B:102:ILE:HG23	1.98	0.44
1:A:298:ALA:HB3	1:A:310:PRO:HG3	2.00	0.44
1:C:180:PHE:CD1	1:C:184:VAL:HG11	2.51	0.44
1:A:170:LEU:O	1:A:172:PRO:HD3	2.17	0.44
2:B:7:TYR:OH	2:B:56:GLU:HA	2.18	0.44
1:A:309:PRO:HD2	3:E:23:A:O2'	2.18	0.44
2:B:16:LEU:HA	2:B:19:LYS:HZ3	1.83	0.44
1:A:372:LYS:O	1:A:373:TYR:CD2	2.70	0.43
1:A:293:LEU:O	1:A:313:GLY:HA3	2.17	0.43
2:D:50:LYS:HD3	2:D:50:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:O	1:A:323:ARG:HG2	2.18	0.43
2:B:68:PRO:HB2	2:B:69:PRO:CD	2.41	0.43
1:A:301:ARG:NH1	3:E:24:G:C4	2.74	0.43
2:B:116:ALA:O	2:B:119:VAL:HG12	2.17	0.43
1:A:234:GLU:OE2	1:C:234:GLU:OE1	2.36	0.43
2:B:15:GLU:HG3	2:B:19:LYS:HZ2	1.84	0.43
1:C:166:GLU:N	1:C:166:GLU:OE1	2.51	0.43
1:C:180:PHE:CZ	1:C:184:VAL:HG11	2.54	0.43
1:C:187:ARG:HH21	1:C:215:THR:HG21	1.82	0.43
1:C:364:ALA:O	1:C:367:ARG:HG2	2.19	0.43
1:C:202:GLU:O	1:C:205:ILE:HG23	2.18	0.43
1:A:204:LYS:HA	1:A:204:LYS:HD3	1.80	0.43
2:B:28:ARG:HH11	2:B:92:GLY:CA	2.31	0.43
2:D:52:VAL:HG22	2:D:78:TYR:HB3	2.00	0.43
1:A:254:ASP:O	1:A:258:PRO:HG3	2.18	0.43
1:C:170:LEU:HG	1:C:208:ILE:HG22	1.99	0.43
1:C:187:ARG:HH21	1:C:215:THR:CG2	2.31	0.43
1:A:235:ILE:O	1:A:238:LEU:HB2	2.18	0.43
1:A:350:SER:OG	1:A:352:GLU:HB3	2.18	0.42
3:E:11:A:H2'	3:E:12:A:C8	2.54	0.42
2:D:104:GLU:HA	2:D:105:PRO:HD3	1.70	0.42
2:D:49:ALA:O	2:D:76:ILE:HD13	2.19	0.42
2:D:84:LYS:O	2:D:96:ALA:HB1	2.19	0.42
3:E:12:A:H2'	3:E:13:A:C8	2.54	0.42
1:A:316:TYR:CE1	3:E:25:C:C4	3.07	0.42
2:D:56:GLU:CG	2:D:82:PRO:HA	2.50	0.42
1:A:167:LEU:HD11	1:A:171:LEU:HD12	2.01	0.42
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.78	0.42
1:A:210:GLU:OE2	1:A:211:ALA:N	2.48	0.42
2:D:5:PRO:HB2	2:D:7:TYR:CD2	2.54	0.42
1:C:202:GLU:HA	1:C:205:ILE:CG2	2.50	0.42
3:E:22:G:C2'	3:E:23:A:H5'	2.49	0.42
1:A:230:GLN:HA	1:A:230:GLN:OE1	2.20	0.42
2:B:118:LYS:O	2:B:122:LEU:HD12	2.20	0.42
1:C:211:ALA:HA	1:C:214:LYS:CE	2.50	0.41
1:C:213:GLU:H	1:C:213:GLU:HG2	1.41	0.41
2:B:7:TYR:CE1	2:B:64:VAL:HG23	2.55	0.41
2:B:34:ARG:HG2	2:B:103:ILE:HD11	2.01	0.41
1:C:209:LEU:O	1:C:213:GLU:CD	2.59	0.41
2:B:15:GLU:HG2	2:B:16:LEU:H	1.82	0.41
2:D:60:PRO:HA	4:D:126:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:LYS:C	1:C:373:TYR:CD1	2.93	0.41
2:B:67:LEU:HD23	2:B:67:LEU:HA	1.87	0.41
1:A:342:ILE:HG23	2:B:63:ILE:HG12	2.02	0.41
2:B:53:ILE:CG2	2:B:81:VAL:HG13	2.50	0.41
2:B:13:PRO:HG2	2:B:118:LYS:NZ	2.36	0.41
1:C:208:ILE:HG13	1:C:209:LEU:H	1.83	0.41
1:C:210:GLU:CD	1:C:214:LYS:HE2	2.40	0.41
2:D:100:VAL:HG12	2:D:101:ALA:N	2.35	0.41
1:C:200:LEU:HD11	1:C:205:ILE:HB	2.03	0.41
1:C:196:ARG:O	1:C:199:GLY:N	2.52	0.41
1:A:151:LEU:HD21	1:C:147:LYS:HE2	2.03	0.41
1:A:369:ILE:O	1:A:373:TYR:CD1	2.74	0.41
1:C:170:LEU:C	1:C:171:LEU:HD12	2.41	0.41
1:A:257:ALA:HB1	1:A:260:LEU:HB2	2.03	0.41
1:C:190:ILE:HG12	1:C:212:LYS:HE3	2.03	0.40
1:A:207:LYS:HA	1:A:210:GLU:CD	2.41	0.40
2:D:79:ILE:HG12	2:D:80:TYR:N	2.36	0.40
1:A:236:ASP:O	1:A:237:ARG:C	2.60	0.40
2:B:74:LYS:O	2:B:75:GLU:CD	2.59	0.40
1:A:216:MET:HB2	1:A:216:MET:HE2	1.98	0.40
1:C:159:TRP:HD1	1:C:159:TRP:O	2.03	0.40
1:A:181:VAL:O	1:A:229:ARG:HG2	2.22	0.40
1:A:170:LEU:C	1:A:170:LEU:HD23	2.41	0.40
1:A:186:HIS:CE1	1:A:219:TRP:CZ3	3.09	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	245/379 (65%)	236 (96%)	8 (3%)	1 (0%)	39 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	245/379 (65%)	235 (96%)	10 (4%)	0	100	100
2	B	119/129 (92%)	114 (96%)	5 (4%)	0	100	100
2	D	119/129 (92%)	114 (96%)	5 (4%)	0	100	100
All	All	728/1016 (72%)	699 (96%)	28 (4%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	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	206/324 (64%)	185 (90%)	21 (10%)	9	21
1	C	206/324 (64%)	182 (88%)	24 (12%)	7	15
2	B	98/105 (93%)	86 (88%)	12 (12%)	6	14
2	D	98/105 (93%)	92 (94%)	6 (6%)	23	49
All	All	608/858 (71%)	545 (90%)	63 (10%)	9	20

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	148	VAL
1	A	156	LEU
1	A	206	LYS
1	A	210	GLU
1	A	212	LYS
1	A	213	GLU
1	A	216	MET
1	A	253	MET
1	A	273	ILE

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Mol	Chain	Res	Type
1	A	275	LEU
1	A	297	LYS
1	A	303	LEU
1	A	317	GLN
1	A	323	ARG
1	A	326	TRP
1	A	327	TRP
1	A	328	GLN
1	A	336	LEU
1	A	339	LYS
1	A	360	LYS
2	B	8	VAL
2	B	15	GLU
2	B	35	LYS
2	B	42	LYS
2	B	50	LYS
2	B	52	VAL
2	B	75	GLU
2	B	95	VAL
2	B	110	ASP
2	B	118	LYS
2	B	119	VAL
2	B	122	LEU
1	C	139	ILE
1	C	148	VAL
1	C	151	LEU
1	C	155	ARG
1	C	156	LEU
1	C	170	LEU
1	C	190	ILE
1	C	198	LEU
1	C	203	GLU
1	C	205	ILE
1	C	208	ILE
1	C	209	LEU
1	C	213	GLU
1	C	216	MET
1	C	228	VAL
1	C	231	LEU
1	C	268	LEU
1	C	275	LEU
1	C	297	LYS

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Mol	Chain	Res	Type
1	C	303	LEU
1	C	327	TRP
1	C	336	LEU
1	C	359	LYS
1	C	372	LYS
2	D	26	ILE
2	D	35	LYS
2	D	42	LYS
2	D	50	LYS
2	D	83	SER
2	D	119	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	189	ASN
1	A	302	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	23/24 (95%)	7 (30%)	1 (4%)
3	F	23/24 (95%)	5 (21%)	1 (4%)
All	All	46/48 (95%)	12 (26%)	2 (4%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	4	C
3	E	11	A
3	E	12	A
3	E	16	C
3	E	20	A
3	E	24	G
3	E	25	C
3	F	4	C
3	F	16	C
3	F	20	A
3	F	24	G

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Mol	Chain	Res	Type
3	F	25	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	E	24	G
3	F	24	G

## 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](#)

There are no ligands in this entry.

## 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	247/379 (65%)	0.12	11 (4%) 37 36	59, 80, 123, 159	0
1	C	247/379 (65%)	0.11	7 (2%) 56 57	65, 84, 124, 160	0
2	B	121/129 (93%)	0.20	5 (4%) 41 41	63, 94, 129, 146	0
2	D	121/129 (93%)	0.32	12 (9%) 9 7	69, 100, 139, 149	0
3	E	24/24 (100%)	0.02	1 (4%) 40 39	68, 81, 114, 176	0
3	F	24/24 (100%)	-0.27	1 (4%) 40 39	75, 95, 123, 173	0
All	All	784/1064 (73%)	0.15	37 (4%) 35 34	59, 87, 129, 176	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	SER	7.3
2	D	4	LYS	6.0
1	C	128	SER	5.8
2	B	124	LYS	5.4
1	A	304	ARG	5.2
2	D	6	SER	4.9
2	B	6	SER	4.6
1	C	365	ARG	4.2
3	E	2	C	3.7
1	A	129	GLY	3.5
2	B	38	ASN	3.4
2	B	37	THR	3.3
2	D	38	ASN	3.3
2	D	124	LYS	3.2
2	D	5	PRO	3.1
1	C	373	TYR	2.9
2	B	94	GLU	2.9
1	A	255	ASP	2.8
2	D	41	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	7	TYR	2.7
1	C	127	GLN	2.7
1	C	286	PRO	2.6
3	F	2	C	2.6
2	D	104	GLU	2.4
2	D	37	THR	2.4
1	C	193	GLU	2.4
2	D	25	GLU	2.4
1	A	303	LEU	2.4
1	A	127	GLN	2.4
1	A	341	ALA	2.3
1	C	129	GLY	2.2
1	A	305	THR	2.2
1	A	200	LEU	2.2
2	D	36	GLY	2.1
1	A	356	GLU	2.1
2	D	57	ASP	2.0
1	A	196	ARG	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.