



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:00 am GMT

PDB ID : 5LXY  
Title : Structure of the minimal RBM7 - ZCCHC8 Complex  
Authors : Falk, S.; Finogenova, K.; Benda, C.; Conti, E.  
Deposited on : 2016-09-23  
Resolution : 2.85 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

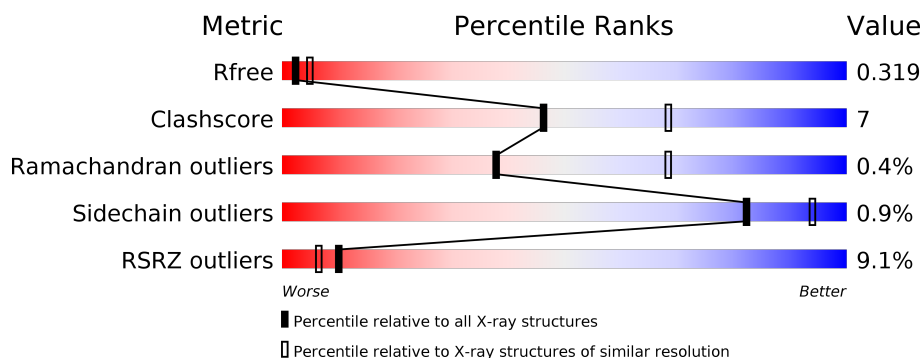
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	90	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>13%</div> </div> </div>
1	B	90	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>18%</div> <div>16%</div> </div> </div>
1	E	90	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>19%</div> </div> </div>
1	G	90	<div> <div>8%</div> <div> <div></div> <div>69%</div> <div>11%</div> <div>20%</div> </div> </div>
1	I	90	<div> <div>12%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>12%</div> </div> </div>
1	K	90	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>•</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	90	
2	C	45	
2	D	45	
2	F	45	
2	H	45	
2	J	45	
2	L	45	
2	N	45	

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
3	BR	J	401	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5491 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 RNA-binding protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			572	380	94	97	1			
1	B	76	Total	C	N	O	S	0	0	0
			555	369	91	94	1			
1	E	73	Total	C	N	O	S	0	0	0
			513	340	86	86	1			
1	G	72	Total	C	N	O	S	0	0	0
			480	312	86	81	1			
1	I	79	Total	C	N	O	S	0	0	0
			541	356	91	93	1			
1	K	71	Total	C	N	O	S	0	0	0
			472	308	81	82	1			
1	M	64	Total	C	N	O	S	0	0	0
			399	253	71	74	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9Y580
A	-2	PRO	-	expression tag	UNP Q9Y580
A	-1	ASP	-	expression tag	UNP Q9Y580
A	0	SER	-	expression tag	UNP Q9Y580
B	-3	GLY	-	expression tag	UNP Q9Y580
B	-2	PRO	-	expression tag	UNP Q9Y580
B	-1	ASP	-	expression tag	UNP Q9Y580
B	0	SER	-	expression tag	UNP Q9Y580
E	-3	GLY	-	expression tag	UNP Q9Y580
E	-2	PRO	-	expression tag	UNP Q9Y580
E	-1	ASP	-	expression tag	UNP Q9Y580
E	0	SER	-	expression tag	UNP Q9Y580
G	-3	GLY	-	expression tag	UNP Q9Y580
G	-2	PRO	-	expression tag	UNP Q9Y580
G	-1	ASP	-	expression tag	UNP Q9Y580

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q9Y580
I	-3	GLY	-	expression tag	UNP Q9Y580
I	-2	PRO	-	expression tag	UNP Q9Y580
I	-1	ASP	-	expression tag	UNP Q9Y580
I	0	SER	-	expression tag	UNP Q9Y580
K	-3	GLY	-	expression tag	UNP Q9Y580
K	-2	PRO	-	expression tag	UNP Q9Y580
K	-1	ASP	-	expression tag	UNP Q9Y580
K	0	SER	-	expression tag	UNP Q9Y580
M	-3	GLY	-	expression tag	UNP Q9Y580
M	-2	PRO	-	expression tag	UNP Q9Y580
M	-1	ASP	-	expression tag	UNP Q9Y580
M	0	SER	-	expression tag	UNP Q9Y580

- Molecule 2 is a protein called Zinc finger CCHC domain-containing protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	39	Total	C	N	O	S	0	0	0
			288	191	48	48	1			
2	C	39	Total	C	N	O	S	0	0	0
			293	196	48	48	1			
2	F	40	Total	C	N	O	S	0	0	0
			300	198	53	48	1			
2	H	40	Total	C	N	O	S	0	0	0
			296	197	49	49	1			
2	J	38	Total	C	N	O	S	0	0	0
			263	174	46	42	1			
2	L	38	Total	C	N	O	S	0	0	0
			258	172	41	44	1			
2	N	37	Total	C	N	O	S	0	0	0
			249	165	42	41	1			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	280	GLY	-	expression tag	UNP Q6NZY4
D	281	PRO	-	expression tag	UNP Q6NZY4
D	282	ASP	-	expression tag	UNP Q6NZY4
D	283	SER	-	expression tag	UNP Q6NZY4
D	284	MET	-	expression tag	UNP Q6NZY4
C	280	GLY	-	expression tag	UNP Q6NZY4
C	281	PRO	-	expression tag	UNP Q6NZY4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	282	ASP	-	expression tag	UNP Q6NZY4
C	283	SER	-	expression tag	UNP Q6NZY4
C	284	MET	-	expression tag	UNP Q6NZY4
F	280	GLY	-	expression tag	UNP Q6NZY4
F	281	PRO	-	expression tag	UNP Q6NZY4
F	282	ASP	-	expression tag	UNP Q6NZY4
F	283	SER	-	expression tag	UNP Q6NZY4
F	284	MET	-	expression tag	UNP Q6NZY4
H	280	GLY	-	expression tag	UNP Q6NZY4
H	281	PRO	-	expression tag	UNP Q6NZY4
H	282	ASP	-	expression tag	UNP Q6NZY4
H	283	SER	-	expression tag	UNP Q6NZY4
H	284	MET	-	expression tag	UNP Q6NZY4
J	280	GLY	-	expression tag	UNP Q6NZY4
J	281	PRO	-	expression tag	UNP Q6NZY4
J	282	ASP	-	expression tag	UNP Q6NZY4
J	283	SER	-	expression tag	UNP Q6NZY4
J	284	MET	-	expression tag	UNP Q6NZY4
L	280	GLY	-	expression tag	UNP Q6NZY4
L	281	PRO	-	expression tag	UNP Q6NZY4
L	282	ASP	-	expression tag	UNP Q6NZY4
L	283	SER	-	expression tag	UNP Q6NZY4
L	284	MET	-	expression tag	UNP Q6NZY4
N	280	GLY	-	expression tag	UNP Q6NZY4
N	281	PRO	-	expression tag	UNP Q6NZY4
N	282	ASP	-	expression tag	UNP Q6NZY4
N	283	SER	-	expression tag	UNP Q6NZY4
N	284	MET	-	expression tag	UNP Q6NZY4

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Br 1	0	0
3	J	1	Total 1	Br 1	0	0
3	D	1	Total 1	Br 1	0	0
3	H	1	Total 1	Br 1	0	0
3	C	2	Total 2	Br 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	1	Total 1	Br 1	0	0
3	L	1	Total 1	Br 1	0	0
3	F	1	Total 1	Br 1	0	0

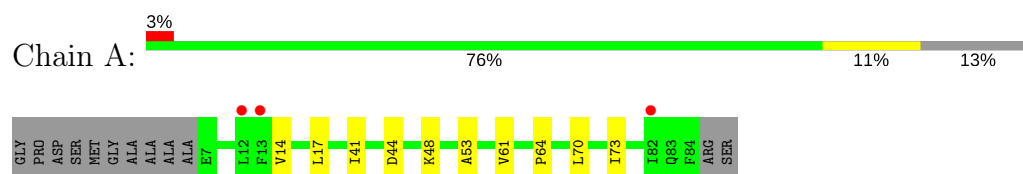
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	O 3	0	0

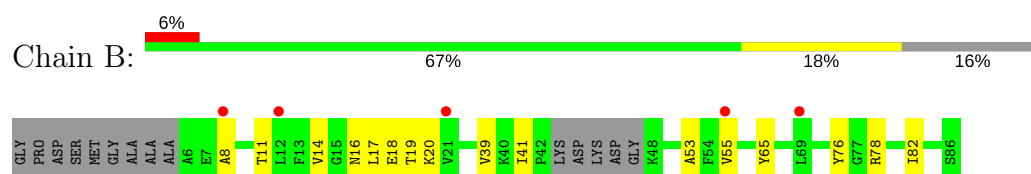
### 3 Residue-property plots [i](#)

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

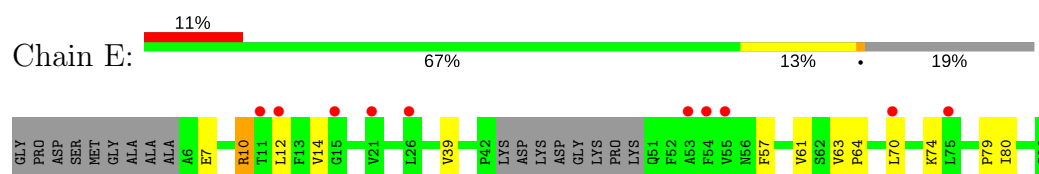
#### • Molecule 1: RNA-binding protein 7



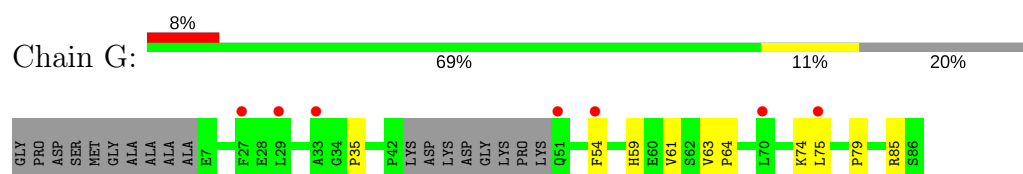
#### • Molecule 1: RNA-binding protein 7



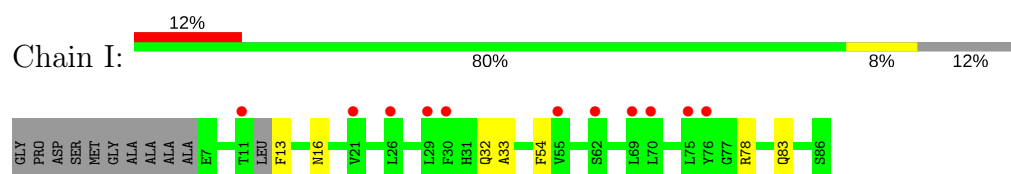
#### • Molecule 1: RNA-binding protein 7



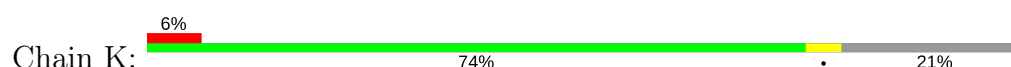
#### • Molecule 1: RNA-binding protein 7



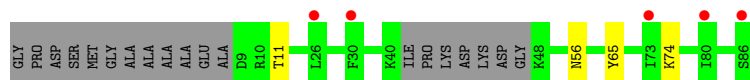
#### • Molecule 1: RNA-binding protein 7



#### • Molecule 1: RNA-binding protein 7







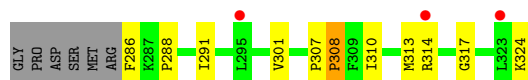
- Molecule 1: RNA-binding protein 7



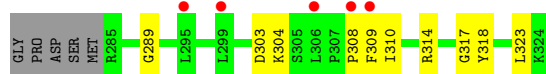
- Molecule 2: Zinc finger CCHC domain-containing protein 8



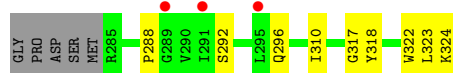
- Molecule 2: Zinc finger CCHC domain-containing protein 8



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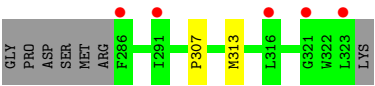


- Molecule 2: Zinc finger CCHC domain-containing protein 8

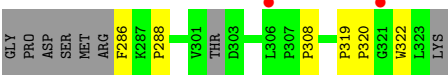


- Molecule 2: Zinc finger CCHC domain-containing protein 8





● Molecule 2: Zinc finger CCHC domain-containing protein 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.77Å 66.58Å 111.91Å 90.00° 126.57° 90.00°	Depositor
Resolution (Å)	71.79 – 2.85 71.79 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.79-2.85) 99.8 (71.79-2.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.262 , 0.300 0.291 , 0.319	Depositor DCC
$R_{free}$ test set	1244 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.1	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 97.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h-2*1,-k,l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: BR

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	0.30	0/586	0.47	0/800
1	B	0.29	0/568	0.48	0/777
1	E	0.27	0/525	0.45	0/720
1	G	0.26	0/488	0.42	0/669
1	I	0.26	0/551	0.43	0/751
1	K	0.26	0/483	0.40	0/662
1	M	0.25	0/402	0.42	0/547
2	C	0.33	0/303	0.63	0/414
2	D	0.33	0/298	0.52	0/409
2	F	0.33	0/310	0.60	0/423
2	H	0.29	0/306	0.54	0/420
2	J	0.31	0/271	0.55	0/371
2	L	0.30	0/267	0.54	0/370
2	N	0.30	0/258	0.48	0/354
All	All	0.29	0/5616	0.49	0/7687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	572	0	547	6	0
1	B	555	0	524	10	1
1	E	513	0	461	7	0
1	G	480	0	408	7	0
1	I	541	0	469	5	0
1	K	472	0	372	4	0
1	M	399	0	292	6	0
2	C	293	0	280	9	0
2	D	288	0	267	3	0
2	F	300	0	281	10	0
2	H	296	0	278	7	0
2	J	263	0	232	8	0
2	L	258	0	222	2	0
2	N	249	0	194	3	0
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	F	1	0	0	1	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
3	J	1	0	0	2	0
3	L	1	0	0	0	0
3	N	1	0	0	0	0
4	B	3	0	0	0	0
All	All	5491	0	4827	74	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 (74) 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:B:14:VAL:HG12	1:B:17:LEU:HD21	1.73	0.69
1:B:18:GLU:HG3	1:B:20:LYS:H	1.58	0.69
1:I:32:GLN:NE2	2:J:288:PRO:O	2.18	0.67
2:J:312:ARG:HG3	3:J:401:BR:BR	2.53	0.63
2:F:309:PHE:HA	3:F:401:BR:BR	2.54	0.62
1:M:17:LEU:O	1:M:19:THR:N	2.33	0.62
1:E:7:GLU:HA	1:E:10:ARG:HD3	1.82	0.61
2:C:291:ILE:HD13	2:C:308:PRO:HG3	1.83	0.59
1:B:16:ASN:OD1	1:B:78:ARG:NH2	2.31	0.59
1:E:74:LYS:HA	1:E:79:PRO:HA	1.85	0.59
2:C:286:PHE:CE2	2:C:288:PRO:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:THR:HA	1:K:56:ASN:HA	1.85	0.58
2:N:319:PRO:HB2	2:N:322:TRP:HD1	1.68	0.58
2:C:307:PRO:HG2	2:F:317:GLY:HA2	1.86	0.58
2:D:310:ILE:O	2:D:314:ARG:HG3	2.04	0.57
2:J:302:THR:O	2:J:304:LYS:N	2.36	0.57
1:A:70:LEU:HA	1:A:73:ILE:HD12	1.87	0.55
1:B:18:GLU:HG2	1:B:76:TYR:HB2	1.88	0.55
2:C:310:ILE:O	2:C:314:ARG:HG3	2.06	0.55
1:M:30:PHE:HD2	1:M:57:PHE:HZ	1.55	0.55
1:G:74:LYS:HA	1:G:79:PRO:HA	1.89	0.54
1:M:74:LYS:HE2	1:M:79:PRO:HG3	1.88	0.54
1:M:36:VAL:HA	1:M:57:PHE:HA	1.90	0.54
1:B:41:ILE:HG12	1:B:53:ALA:HB2	1.90	0.54
2:N:286:PHE:CE2	2:N:288:PRO:HG3	2.43	0.53
2:C:301:VAL:HG13	2:F:318:TYR:CE1	2.43	0.53
1:E:12:LEU:HD12	1:E:57:PHE:HE2	1.74	0.52
1:G:54:PHE:CE1	1:G:85:ARG:HD2	2.44	0.51
1:B:18:GLU:HG2	1:B:76:TYR:CB	2.39	0.51
1:G:35:PRO:HD3	2:H:322:TRP:CD2	2.44	0.51
2:H:324:LYS:HA	1:K:74:LYS:H	1.76	0.50
1:I:33:ALA:O	2:J:319:PRO:HB3	2.12	0.50
1:B:14:VAL:HG22	1:B:82:ILE:HG12	1.94	0.49
2:F:310:ILE:O	2:F:314:ARG:HG3	2.12	0.49
1:G:61:VAL:O	1:G:64:PRO:HD2	2.12	0.49
1:A:41:ILE:HG12	1:A:53:ALA:HB2	1.94	0.48
1:E:10:ARG:HA	1:E:63:VAL:HG21	1.95	0.48
2:J:309:PHE:HA	3:J:401:BR:BR	2.69	0.47
1:I:16:ASN:O	1:I:78:ARG:HD3	2.15	0.47
1:B:39:VAL:HG22	1:B:55:VAL:HG22	1.97	0.47
1:G:59:HIS:HB3	3:G:101:BR:BR	2.70	0.47
1:A:14:VAL:HG22	1:A:17:LEU:HD21	1.96	0.47
2:J:310:ILE:O	2:J:314:ARG:HG3	2.14	0.47
1:M:37:ILE:N	1:M:56:ASN:O	2.43	0.46
1:K:65:TYR:OH	2:L:313:MET:HG3	2.16	0.46
1:E:61:VAL:O	1:E:64:PRO:HD2	2.16	0.45
2:H:318:TYR:CD1	2:H:323:LEU:HG	2.51	0.45
2:D:307:PRO:HD2	2:C:317:GLY:HA2	1.97	0.45
1:A:73:ILE:HA	2:C:324:LYS:HB3	1.97	0.45
2:D:289:GLY:O	2:D:308:PRO:HD2	2.16	0.45
2:F:303:ASP:OD1	2:F:304:LYS:N	2.51	0.44
1:I:13:PHE:HD1	1:I:54:PHE:CE1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:VAL:HB	1:E:64:PRO:HD3	1.99	0.44
2:F:289:GLY:O	2:F:308:PRO:HD2	2.17	0.44
1:G:75:LEU:HA	1:G:75:LEU:HD23	1.87	0.44
2:H:292:SER:O	2:H:296:GLN:HB2	2.18	0.44
2:J:310:ILE:HD13	2:J:310:ILE:HA	1.85	0.43
2:F:323:LEU:HD23	2:F:323:LEU:HA	1.80	0.43
2:H:317:GLY:HA2	2:L:307:PRO:HD2	2.01	0.43
1:A:44:ASP:N	1:A:48:LYS:O	2.51	0.42
1:M:39:VAL:HG22	1:M:55:VAL:HG22	2.01	0.42
2:H:288:PRO:HB2	2:H:310:ILE:HD11	2.01	0.42
1:E:70:LEU:O	1:E:80:ILE:HD11	2.19	0.42
1:B:8:ALA:HA	1:B:11:THR:HG22	2.01	0.42
1:A:61:VAL:O	1:A:64:PRO:HD2	2.19	0.41
1:B:65:TYR:OH	2:C:313:MET:HG3	2.20	0.41
2:F:310:ILE:HD13	2:F:310:ILE:HA	1.94	0.41
2:C:308:PRO:HA	2:F:318:TYR:HB3	2.01	0.41
2:N:319:PRO:HA	2:N:320:PRO:HD3	1.92	0.41
3:C:401:BR:BR	2:F:323:LEU:HD12	2.75	0.41
2:H:324:LYS:HA	1:K:74:LYS:N	2.36	0.41
1:I:13:PHE:HB3	1:I:83:GLN:O	2.20	0.41
1:G:63:VAL:HB	1:G:64:PRO:HD3	2.02	0.40
2:J:319:PRO:HB2	2:J:322:TRP:HD1	1.86	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:B:19:THR:OG1	1:B:19:THR:OG1[2_556]	2.09	0.11

## 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	76/90 (84%)	76 (100%)	0	0	100	100
1	B	72/90 (80%)	72 (100%)	0	0	100	100
1	E	69/90 (77%)	68 (99%)	1 (1%)	0	100	100
1	G	68/90 (76%)	67 (98%)	1 (2%)	0	100	100
1	I	75/90 (83%)	74 (99%)	1 (1%)	0	100	100
1	K	67/90 (74%)	66 (98%)	1 (2%)	0	100	100
1	M	54/90 (60%)	53 (98%)	1 (2%)	0	100	100
2	C	37/45 (82%)	36 (97%)	0	1 (3%)	6	20
2	D	37/45 (82%)	35 (95%)	2 (5%)	0	100	100
2	F	38/45 (84%)	36 (95%)	2 (5%)	0	100	100
2	H	38/45 (84%)	37 (97%)	1 (3%)	0	100	100
2	J	36/45 (80%)	34 (94%)	1 (3%)	1 (3%)	6	19
2	L	36/45 (80%)	35 (97%)	1 (3%)	0	100	100
2	N	33/45 (73%)	32 (97%)	0	1 (3%)	5	18
All	All	736/945 (78%)	721 (98%)	12 (2%)	3 (0%)	38	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	303	ASP
2	C	308	PRO
2	N	308	PRO

### 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	54/75 (72%)	54 (100%)	0	100	100
1	B	52/75 (69%)	52 (100%)	0	100	100
1	E	44/75 (59%)	41 (93%)	3 (7%)	18	43
1	G	36/75 (48%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	42/75 (56%)	42 (100%)	0	100	100
1	K	33/75 (44%)	33 (100%)	0	100	100
1	M	24/75 (32%)	24 (100%)	0	100	100
2	C	28/39 (72%)	28 (100%)	0	100	100
2	D	27/39 (69%)	26 (96%)	1 (4%)	39	71
2	F	27/39 (69%)	27 (100%)	0	100	100
2	H	28/39 (72%)	28 (100%)	0	100	100
2	J	21/39 (54%)	21 (100%)	0	100	100
2	L	21/39 (54%)	21 (100%)	0	100	100
2	N	17/39 (44%)	17 (100%)	0	100	100
All	All	454/798 (57%)	450 (99%)	4 (1%)	82	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	302	THR
1	E	10	ARG
1	E	14	VAL
1	E	39	VAL

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	78/90 (86%)	0.39	3 (3%) 41 35	45, 76, 134, 148	0
1	B	76/90 (84%)	0.40	5 (6%) 19 14	55, 90, 130, 145	0
1	E	73/90 (81%)	0.56	10 (13%) 3 2	71, 112, 148, 159	0
1	G	72/90 (80%)	0.39	7 (9%) 8 5	82, 120, 153, 165	0
1	I	79/90 (87%)	0.69	11 (13%) 3 2	92, 132, 197, 234	0
1	K	71/90 (78%)	0.32	5 (7%) 17 12	84, 125, 165, 196	0
1	M	64/90 (71%)	0.55	7 (10%) 6 4	94, 130, 154, 167	0
2	C	39/45 (86%)	0.48	3 (7%) 14 10	59, 77, 101, 116	0
2	D	39/45 (86%)	0.32	1 (2%) 56 52	58, 77, 98, 106	0
2	F	40/45 (88%)	0.51	5 (12%) 4 3	61, 89, 157, 172	0
2	H	40/45 (88%)	0.59	3 (7%) 15 11	73, 109, 151, 156	0
2	J	38/45 (84%)	0.51	4 (10%) 7 4	75, 119, 152, 182	0
2	L	38/45 (84%)	0.60	5 (13%) 4 2	85, 126, 148, 164	0
2	N	37/45 (82%)	0.35	2 (5%) 26 22	92, 124, 173, 206	0
All	All	784/945 (82%)	0.47	71 (9%) 10 6	45, 110, 156, 234	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	33	ALA	5.7
1	M	36	VAL	5.0
1	I	55	VAL	4.9
1	M	25	LEU	4.7
1	I	11	THR	4.4
1	M	57	PHE	4.4
2	H	289	GLY	4.3
1	I	21	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	L	291	ILE	4.1
1	K	73	ILE	4.1
1	G	75	LEU	4.0
1	M	73	ILE	4.0
1	E	26	LEU	3.7
1	E	54	PHE	3.5
1	G	70	LEU	3.5
2	N	306	LEU	3.4
1	E	12	LEU	3.2
1	I	29	LEU	3.2
2	L	323	LEU	3.2
1	I	76	TYR	3.1
2	H	295	LEU	3.1
1	A	12	LEU	3.1
1	E	70	LEU	3.1
1	G	51	GLN	3.0
1	E	11	THR	2.9
1	E	53	ALA	2.9
1	K	80	ILE	2.9
1	B	12	LEU	2.9
1	I	70	LEU	2.9
1	E	55	VAL	2.9
2	F	308	PRO	2.8
2	L	316	LEU	2.7
1	I	26	LEU	2.7
1	B	69	LEU	2.7
2	C	323	LEU	2.7
1	I	62	SER	2.7
1	I	30	PHE	2.6
1	K	30	PHE	2.6
1	G	29	LEU	2.6
1	A	82	ILE	2.5
2	J	323	LEU	2.5
2	N	321	GLY	2.5
2	F	299	LEU	2.5
1	B	55	VAL	2.5
1	M	23	GLU	2.5
1	E	75	LEU	2.5
2	F	295	LEU	2.5
2	L	321	GLY	2.5
2	F	306	LEU	2.4
1	E	21	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	291	ILE	2.4
2	L	286	PHE	2.4
2	J	295	LEU	2.4
2	F	309	PHE	2.3
1	A	13	PHE	2.3
2	D	299	LEU	2.3
1	K	26	LEU	2.3
1	E	15	GLY	2.2
1	B	8	ALA	2.2
1	I	69	LEU	2.2
2	H	291	ILE	2.2
1	G	27	PHE	2.1
1	M	75	LEU	2.1
1	I	75	LEU	2.1
1	G	54	PHE	2.1
2	J	317	GLY	2.1
1	K	86	SER	2.1
1	M	30	PHE	2.0
2	C	314	ARG	2.0
1	B	21	VAL	2.0
2	C	295	LEU	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(Å <sup>2</sup> )	Q<0.9
3	BR	H	401	1/1	0.91	0.25	-0.16	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BR	C	402	1/1	0.52	0.15	-0.99	230,230,230,230	0
3	BR	L	401	1/1	0.88	0.12	-1.48	128,128,128,128	0
3	BR	N	401	1/1	0.91	0.08	-1.92	165,165,165,165	0
3	BR	F	401	1/1	0.89	0.12	-2.34	157,157,157,157	0
3	BR	J	401	1/1	0.89	0.07	-2.56	130,130,130,130	0
3	BR	C	401	1/1	0.99	0.10	-3.14	86,86,86,86	0
3	BR	D	401	1/1	0.87	0.07	-3.14	106,106,106,106	0
3	BR	G	101	1/1	0.69	0.12	-	232,232,232,232	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.