



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:16 am GMT

PDB ID : 5F98  
Title : Crystal structure of RIG-I in complex with Cap-0 RNA  
Authors : Wang, C.; Marcotrigiano, J.; Miller, M.; Jiang, F.  
Deposited on : 2015-12-09  
Resolution : 3.28 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 : 1.7.2 (RC1), CSD as538be (2017)  
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

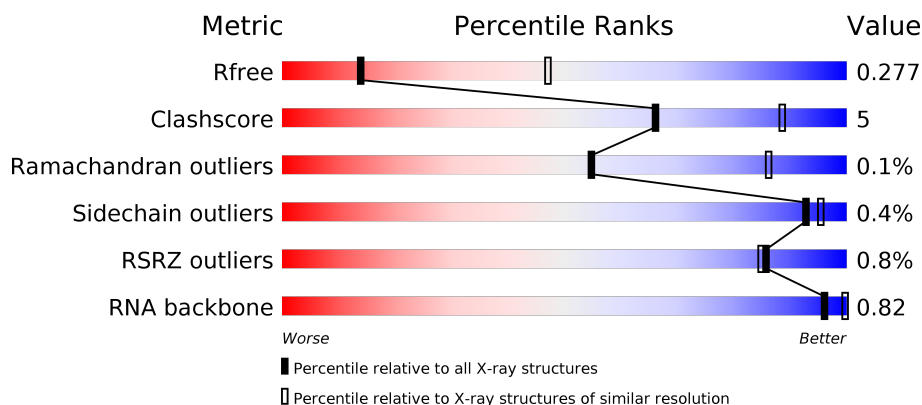
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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	1006 (3.34-3.22)
Clashscore	112137	1070 (3.34-3.22)
Ramachandran outliers	110173	1050 (3.34-3.22)
Sidechain outliers	110143	1049 (3.34-3.22)
RSRZ outliers	101464	1011 (3.34-3.22)
RNA backbone	2435	1089 (3.76-2.80)

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	695	
1	C	695	
1	E	695	
1	G	695	

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Mol	Chain	Length	Quality of chain
1	I	695	 81%12%7%
1	K	695	 85%8%7%
2	B	24	 75%25%
2	D	24	 75%25%
2	F	24	 83%17%
2	H	24	 75%25%
2	J	24	 88%13%
2	L	24	 54%46%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32719 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 Probable ATP-dependent RNA helicase DDX58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5060	3237	855	938	30			
1	C	648	Total	C	N	O	S	0	0	0
			4949	3169	832	917	31			
1	E	641	Total	C	N	O	S	0	0	0
			4832	3087	822	894	29			
1	G	647	Total	C	N	O	S	0	1	0
			4965	3182	836	916	31			
1	I	647	Total	C	N	O	S	0	0	0
			4838	3093	810	906	29			
1	K	644	Total	C	N	O	S	0	0	0
			4859	3115	812	901	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	SER	-	expression tag	UNP O95786
C	231	SER	-	expression tag	UNP O95786
E	231	SER	-	expression tag	UNP O95786
G	231	SER	-	expression tag	UNP O95786
I	231	SER	-	expression tag	UNP O95786
K	231	SER	-	expression tag	UNP O95786

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	D	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	F	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	J	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			
2	L	24	Total	C	N	O	P	0	0	0
			509	229	88	168	24			

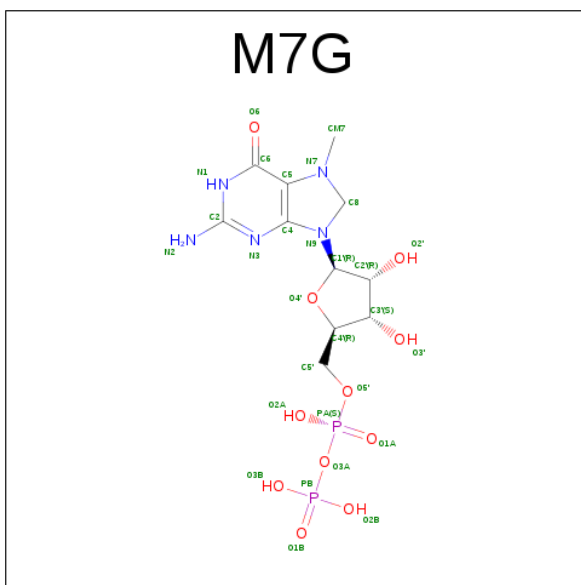
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (three-letter code: M7G) (formula: C<sub>11</sub>H<sub>19</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

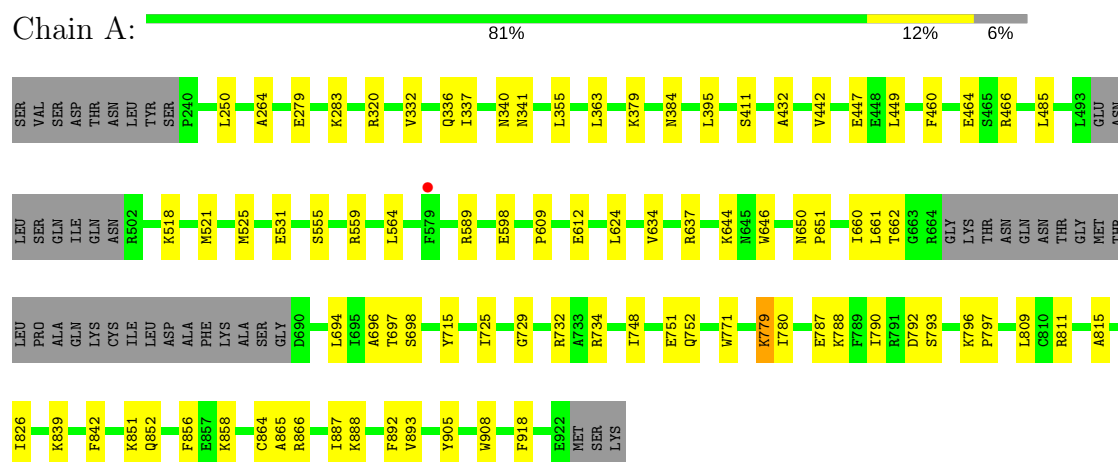


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 29	C 11	N 5	O 11	P 2	0	0
5	D	1	Total 29	C 11	N 5	O 11	P 2	0	0
5	F	1	Total 17	C 5	O 10	P 2		0	0
5	H	1	Total 29	C 11	N 5	O 11	P 2	0	0
5	J	1	Total 29	C 11	N 5	O 11	P 2	0	0
5	L	1	Total 17	C 5	O 10	P 2		0	0

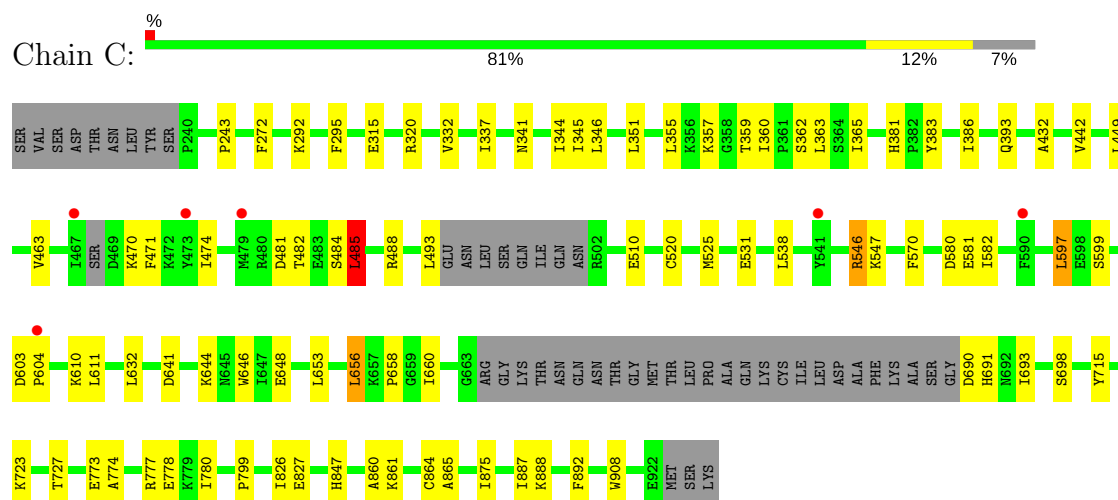
### 3 Residue-property plots

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.

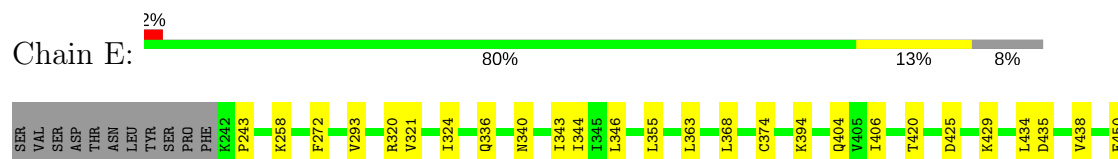
#### • Molecule 1: Probable ATP-dependent RNA helicase DDX58

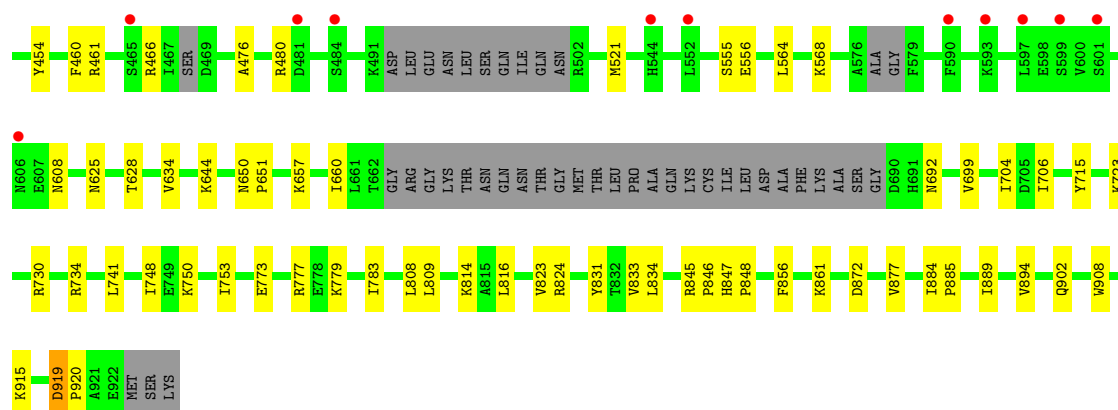


#### • Molecule 1: Probable ATP-dependent RNA helicase DDX58



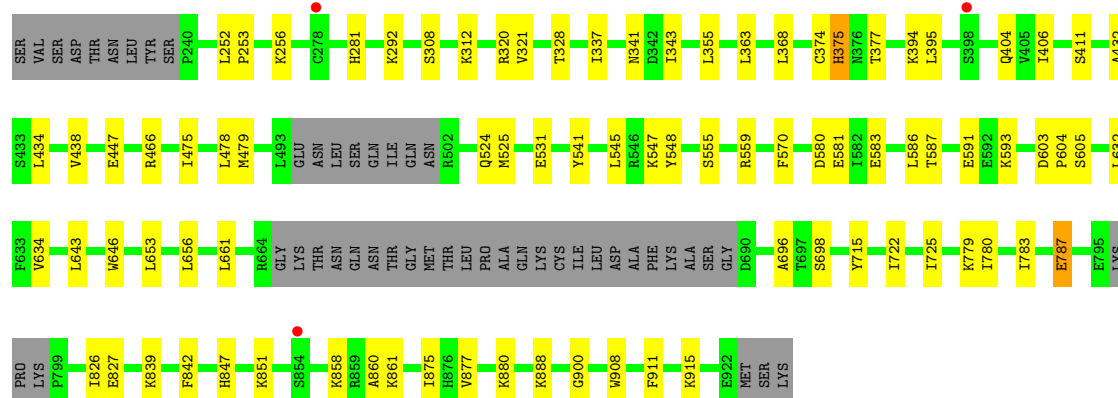
#### • Molecule 1: Probable ATP-dependent RNA helicase DDX58



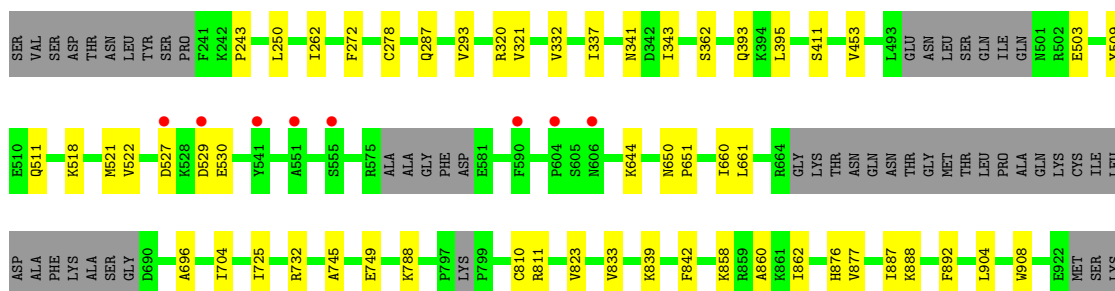


- Molecule 1: Probable ATP-dependent RNA helicase DDX58

Chain G: 81% 12% 7%







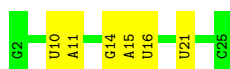
- Molecule 2: RNA (5'-R(P\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*A P\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')

Chain B: 75% 25%



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

Chain D: 75% 25%



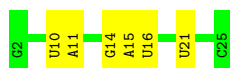
- Molecule 2: RNA (5'-R(P\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*A P\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')

Chain F: 83% 17%



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

Chain H: 75% 25%



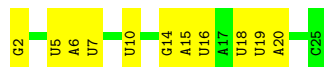
- Molecule 2: RNA (5'-R(P\*GP\*AP\*AP\*UP\*AP\*UP\*AP\*AP\*UP\*AP\*GP\*UP\*GP\*AP\*UP\*A P\*UP\*UP\*AP\*UP\*AP\*UP\*UP\*C)-3')

Chain J: 88% 13%



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

Chain L:  54% 46%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.18Å 174.57Å 309.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.00 – 3.28 84.00 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (84.00-3.28) 92.1 (84.00-3.28)	Depositor EDS
$R_{merge}$	0.56	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, $R_{free}$	0.221 , 0.277 0.222 , 0.277	Depositor DCC
$R_{free}$ test set	2002 reflections (2.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	32719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.51% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M7G, MG

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	0.22	0/5167	0.38	0/7005
1	C	0.22	0/5052	0.41	1/6858 (0.0%)
1	E	0.22	0/4933	0.38	0/6708
1	G	0.22	0/5069	0.37	0/6881
1	I	0.21	0/4942	0.38	0/6730
1	K	0.22	0/4960	0.37	0/6745
2	B	0.13	0/569	0.67	0/883
2	D	0.13	0/569	0.65	0/883
2	F	0.13	0/569	0.66	0/883
2	H	0.13	0/569	0.66	0/883
2	J	0.13	0/569	0.67	0/883
2	L	0.46	1/569 (0.2%)	0.65	0/881
All	All	0.22	1/33537 (0.0%)	0.42	1/46223 (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	I	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	G	OP3-P	-10.66	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	485	LEU	CA-CB-CG	8.52	134.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	477	GLN	Peptide

## 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	5060	0	4907	53	0
1	C	4949	0	4755	49	0
1	E	4832	0	4529	50	0
1	G	4965	0	4768	51	0
1	I	4838	0	4460	51	0
1	K	4859	0	4582	32	0
2	B	509	0	255	3	0
2	D	509	0	255	3	0
2	F	509	0	255	2	0
2	H	509	0	255	3	0
2	J	509	0	255	3	0
2	L	509	0	255	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
5	B	29	0	15	0	0
5	D	29	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	17	0	7	0	0
5	H	29	0	16	0	0
5	J	29	0	15	1	0
5	L	17	0	7	0	0
All	All	32719	0	29607	289	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 5.

All (289) 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:I:477:GLN:HA	1:I:480:ARG:H	1.54	0.72
1:E:644:LYS:HD2	1:E:660:ILE:HD11	1.73	0.71
1:E:258:LYS:HE3	1:E:438:VAL:HG21	1.72	0.71
1:I:443:LYS:NZ	1:I:769:GLN:OE1	2.21	0.69
1:E:831:TYR:OH	1:E:915:LYS:NZ	2.21	0.69
1:A:432:ALA:HA	1:A:780:ILE:HG23	1.76	0.68
1:G:783:ILE:HG22	1:G:787:GLU:OE2	1.94	0.68
1:I:476:ALA:O	1:I:479:MET:HB2	1.94	0.67
1:A:609:PRO:HA	1:A:612:GLU:HG3	1.77	0.67
1:A:466:ARG:NH1	1:A:555:SER:O	2.27	0.67
1:C:432:ALA:HA	1:C:780:ILE:HG23	1.77	0.64
1:K:888:LYS:HA	1:K:908:TRP:HE1	1.62	0.64
1:G:559:ARG:HD3	1:G:646:TRP:HD1	1.63	0.64
1:E:466:ARG:NH2	1:E:555:SER:O	2.31	0.63
1:C:644:LYS:HD3	1:C:660:ILE:HD11	1.81	0.63
1:G:861:LYS:HD2	1:G:875:ILE:HG22	1.81	0.63
1:A:395:LEU:HD12	1:A:788:LYS:HD3	1.81	0.62
1:A:442:VAL:HG21	1:A:449:LEU:HD22	1.81	0.62
1:G:779:LYS:O	1:G:783:ILE:HG13	2.00	0.62
1:A:644:LYS:HD3	1:A:660:ILE:HD11	1.82	0.61
1:A:564:LEU:HD21	1:A:598:GLU:HG2	1.82	0.61
1:A:734:ARG:NH1	1:E:450:GLU:OE2	2.33	0.61
1:G:524:GLN:NE2	1:G:900:GLY:O	2.34	0.61
1:I:559:ARG:HD3	1:I:646:TRP:HD1	1.65	0.61
1:E:425:ASP:O	1:E:429:LYS:HG2	2.01	0.60
1:G:355:LEU:HD11	1:G:363:LEU:HD21	1.83	0.60
1:I:395:LEU:O	1:I:788:LYS:NZ	2.33	0.60
1:K:337:ILE:O	1:K:341:ASN:ND2	2.27	0.60
1:I:861:LYS:HD2	1:I:875:ILE:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:861:LYS:HD2	1:C:875:ILE:HG22	1.83	0.59
1:E:773:GLU:OE2	1:E:777:ARG:NH2	2.36	0.59
1:K:644:LYS:HD2	1:K:660:ILE:HD11	1.84	0.59
1:G:377:THR:HG21	1:G:434:LEU:HG	1.84	0.59
1:G:525:MET:HB2	1:G:531:GLU:HB2	1.84	0.59
1:A:792:ASP:OD1	1:A:793:SER:N	2.36	0.58
2:F:12:G:N2	2:F:15:A:OP2	2.36	0.58
1:I:355:LEU:HD11	1:I:363:LEU:HD21	1.85	0.58
1:G:698:SER:HG	2:H:21:U:HO2'	1.51	0.58
1:C:482:THR:HA	1:C:485:LEU:HD12	1.85	0.58
1:A:559:ARG:HD3	1:A:646:TRP:HD1	1.69	0.58
1:I:858:LYS:HA	1:I:877:VAL:HG12	1.86	0.57
1:G:475:ILE:HG22	1:G:479:MET:HE2	1.85	0.57
1:A:771:TRP:HZ3	1:A:779:LYS:HE3	1.69	0.57
1:G:466:ARG:NH2	1:G:555:SER:O	2.38	0.57
1:E:556:GLU:O	1:E:608:ASN:ND2	2.35	0.57
1:A:355:LEU:HD11	1:A:363:LEU:HD21	1.87	0.56
1:I:295:PHE:HB3	1:I:345:ILE:HG13	1.87	0.56
1:I:521:MET:O	1:I:814:LYS:NZ	2.38	0.56
1:I:377:THR:HG21	1:I:434:LEU:HD21	1.87	0.56
1:C:485:LEU:HA	1:C:488:ARG:CG	2.36	0.55
1:E:699:VAL:O	1:E:723:LYS:NZ	2.37	0.55
1:G:374:CYS:O	1:G:377:THR:HG22	2.07	0.55
1:I:597:LEU:HA	1:I:600:VAL:HG22	1.88	0.55
1:G:826:ILE:HG22	1:G:827:GLU:HG3	1.88	0.55
1:A:337:ILE:O	1:A:341:ASN:ND2	2.32	0.55
1:I:377:THR:HG22	1:I:383:TYR:HB3	1.88	0.55
1:K:860:ALA:HB3	1:K:876:HIS:HB3	1.89	0.55
1:E:814:LYS:NZ	1:E:902:GLN:OE1	2.36	0.55
1:I:337:ILE:O	1:I:341:ASN:ND2	2.34	0.55
1:G:587:THR:O	1:G:591:GLU:HG2	2.08	0.54
1:A:748:ILE:O	1:A:752:GLN:HG2	2.07	0.54
1:C:698:SER:OG	2:D:21:U:O2'	2.25	0.54
1:A:379:LYS:O	1:A:384:ASN:ND2	2.36	0.54
1:I:442:VAL:HG21	1:I:449:LEU:HD22	1.90	0.54
1:G:661:LEU:HB3	1:G:696:ALA:HB2	1.90	0.54
1:I:888:LYS:HG2	1:I:890:GLU:H	1.71	0.54
1:A:279:GLU:O	1:A:283:LYS:HG3	2.08	0.53
1:A:888:LYS:HA	1:A:908:TRP:HE1	1.72	0.53
1:G:632:LEU:HD21	1:G:643:LEU:HD13	1.90	0.53
1:I:580:ASP:OD1	1:I:581:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:292:LYS:NZ	1:I:341:ASN:O	2.41	0.53
1:E:634:VAL:HG12	1:E:715:TYR:HB3	1.90	0.53
1:K:527:ASP:O	1:K:529:ASP:N	2.41	0.53
1:E:324:ILE:HB	1:E:346:LEU:HD23	1.92	0.52
1:G:394:LYS:HG2	1:G:395:LEU:HD12	1.92	0.52
1:G:880:LYS:O	1:K:287:GLN:NE2	2.39	0.52
1:G:580:ASP:OD1	1:G:581:GLU:N	2.42	0.52
1:G:411:SER:HB3	1:G:722:ILE:HG23	1.91	0.52
1:I:477:GLN:HB3	1:I:480:ARG:CB	2.40	0.52
1:C:381:HIS:HD1	1:C:383:TYR:H	1.56	0.52
1:E:808:LEU:HG	1:E:894:VAL:HG22	1.92	0.51
1:K:811:ARG:HD3	1:K:892:PHE:C	2.31	0.51
1:A:634:VAL:HG12	1:A:715:TYR:HB3	1.91	0.51
1:C:337:ILE:O	1:C:341:ASN:ND2	2.33	0.51
1:G:328:THR:HB	1:K:320:ARG:HG2	1.93	0.51
1:A:811:ARG:NH2	1:A:905:TYR:O	2.43	0.51
1:C:580:ASP:OD1	1:C:581:GLU:N	2.44	0.51
1:A:752:GLN:OE1	1:E:460:PHE:HB2	2.11	0.51
1:G:858:LYS:HA	1:G:877:VAL:HG12	1.92	0.51
1:A:729:GLY:O	1:A:732:ARG:NH1	2.44	0.51
1:K:321:VAL:HG22	1:K:343:ILE:HB	1.93	0.51
1:E:657:LYS:H	1:E:692:ASN:HB3	1.76	0.51
1:A:661:LEU:HD22	1:A:694:LEU:HD21	1.92	0.50
1:I:477:GLN:HA	1:I:480:ARG:N	2.23	0.50
1:E:293:VAL:HG22	1:E:368:LEU:HB3	1.92	0.50
1:I:610:LYS:NZ	1:I:716:GLU:OE1	2.37	0.50
1:K:250:LEU:HD22	1:K:262:ILE:HG23	1.94	0.50
1:C:243:PRO:HB3	1:C:272:PHE:CE2	2.47	0.50
1:C:481:ASP:OD1	1:C:484:SER:HB2	2.11	0.49
1:K:362:SER:OG	1:K:393:GLN:OE1	2.30	0.49
1:I:861:LYS:NZ	5:J:101:M7G:O1B	2.45	0.49
1:G:320:ARG:HD2	1:K:332:VAL:HG11	1.94	0.49
2:L:14:G:H2'	2:L:15:A:C8	2.47	0.49
1:G:337:ILE:O	1:G:341:ASN:ND2	2.32	0.49
1:A:336:GLN:O	1:A:340:ASN:ND2	2.45	0.49
1:C:864:CYS:SG	1:C:865:ALA:N	2.86	0.49
1:E:809:LEU:HB3	1:E:816:LEU:HA	1.95	0.49
1:K:661:LEU:HB3	1:K:696:ALA:HB2	1.95	0.49
1:C:690:ASP:OD1	1:C:691:HIS:N	2.39	0.49
1:E:258:LYS:HD2	1:E:773:GLU:OE2	2.13	0.48
1:E:706:ILE:HD11	1:E:730:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:LYS:HD2	1:C:359:THR:HG23	1.95	0.48
1:K:529:ASP:OD1	1:K:530:GLU:N	2.46	0.48
1:E:564:LEU:O	1:E:568:LYS:HG3	2.14	0.48
1:A:336:GLN:HG2	1:A:340:ASN:HD21	1.78	0.48
1:A:864:CYS:SG	1:A:865:ALA:N	2.86	0.48
1:C:355:LEU:HD11	1:C:363:LEU:HD21	1.94	0.48
1:C:888:LYS:HA	1:C:908:TRP:HE1	1.78	0.48
1:G:888:LYS:HA	1:G:908:TRP:HE1	1.77	0.48
1:C:525:MET:HB3	1:C:531:GLU:HB2	1.96	0.48
1:C:774:ALA:O	1:C:778:GLU:HG2	2.12	0.48
1:E:461:ARG:HB2	1:E:741:LEU:HD12	1.95	0.48
1:C:773:GLU:OE2	1:C:777:ARG:NH2	2.47	0.48
1:C:723:LYS:O	1:C:727:THR:OG1	2.24	0.48
1:G:253:PRO:HB3	1:G:438:VAL:HG11	1.95	0.48
1:C:471:PHE:HA	1:C:474:ILE:HD13	1.96	0.47
1:E:521:MET:O	1:E:814:LYS:NZ	2.44	0.47
1:A:787:GLU:HA	1:A:790:ILE:HG22	1.96	0.47
1:I:575:ARG:HA	1:I:579:PHE:CE1	2.49	0.47
1:K:887:ILE:HB	1:K:892:PHE:HE2	1.79	0.47
1:E:919:ASP:HB2	1:E:920:PRO:HD2	1.96	0.47
1:E:394:LYS:NZ	1:E:435:ASP:OD1	2.46	0.46
1:A:809:LEU:HB2	1:A:893:VAL:HG13	1.97	0.46
1:E:823:VAL:HG22	1:E:833:VAL:HG22	1.96	0.46
1:C:295:PHE:HB3	1:C:345:ILE:HG13	1.97	0.46
1:C:362:SER:OG	1:C:393:GLN:OE1	2.32	0.46
1:G:292:LYS:NZ	1:G:341:ASN:O	2.48	0.46
1:I:653:LEU:HB3	1:I:656:LEU:HD12	1.97	0.46
1:C:611:LEU:HD13	1:C:646:TRP:CD1	2.51	0.46
2:H:10:U:H2'	2:H:11:A:C8	2.50	0.46
1:G:404:GLN:HE21	1:G:406:ILE:HD11	1.81	0.46
1:I:814:LYS:NZ	1:I:902:GLN:OE1	2.41	0.46
1:A:411:SER:HB2	1:A:725:ILE:HD12	1.98	0.46
1:I:571:PHE:CD1	1:I:587:THR:HG22	2.51	0.46
2:L:19:U:H2'	2:L:20:A:C8	2.50	0.46
1:I:243:PRO:HB3	1:I:272:PHE:CE2	2.51	0.45
1:I:706:ILE:HG22	1:I:707:ALA:H	1.81	0.45
1:K:810:CYS:SG	1:K:811:ARG:N	2.90	0.45
1:A:332:VAL:HG11	1:C:320:ARG:HD2	1.97	0.45
1:A:624:LEU:HD11	1:E:420:THR:HG21	1.98	0.45
1:A:779:LYS:HE2	1:A:779:LYS:HB3	1.65	0.45
1:G:404:GLN:NE2	1:G:406:ILE:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:5:U:H2'	2:L:6:A:C8	2.52	0.45
1:G:447:GLU:N	1:G:447:GLU:OE1	2.45	0.45
1:E:856:PHE:HD2	1:E:877:VAL:HG21	1.81	0.45
1:I:411:SER:HB2	1:I:725:ILE:HD12	1.98	0.45
1:K:511:GLN:NE2	2:L:10:U:O2'	2.50	0.45
1:C:510:GLU:OE2	1:C:546:ARG:NH1	2.49	0.45
1:C:520:CYS:SG	1:C:538:LEU:HD23	2.57	0.44
1:C:547:LYS:HD2	1:C:570:PHE:CD1	2.53	0.44
1:C:644:LYS:HG2	1:C:648:GLU:OE2	2.17	0.44
1:E:404:GLN:HE21	1:E:406:ILE:HD11	1.83	0.44
1:G:432:ALA:HA	1:G:780:ILE:HG23	1.98	0.44
1:I:326:GLY:N	2:J:25:C:OP1	2.49	0.44
1:E:454:TYR:OH	1:E:734:ARG:NH2	2.50	0.44
1:E:884:ILE:HG13	1:E:885:PRO:HD2	1.99	0.44
1:E:750:LYS:HD2	1:E:753:ILE:HD11	2.00	0.44
1:G:281:HIS:CE1	1:G:368:LEU:HB2	2.52	0.44
1:E:344:ILE:HG22	1:E:346:LEU:HG	2.00	0.44
1:G:308:SER:O	1:G:312:LYS:HG2	2.17	0.44
1:G:321:VAL:HG22	1:G:343:ILE:HB	1.99	0.44
1:C:641:ASP:OD1	1:C:641:ASP:N	2.50	0.44
1:I:728:ARG:NH2	1:I:758:GLU:OE1	2.50	0.44
2:F:19:U:H2'	2:F:20:A:C8	2.53	0.44
1:I:587:THR:O	1:I:590:PHE:N	2.50	0.44
1:A:464:GLU:O	1:A:609:PRO:HG2	2.17	0.44
1:I:889:ILE:HB	1:I:908:TRP:CE2	2.52	0.44
1:E:320:ARG:HG2	1:I:328:THR:HB	1.98	0.44
1:E:336:GLN:HG2	1:E:340:ASN:HD21	1.83	0.44
1:I:299:GLN:HB3	1:I:301:PRO:HD2	1.98	0.43
1:C:826:ILE:HG22	1:C:827:GLU:HG3	2.00	0.43
2:L:6:A:H2'	2:L:7:U:C6	2.53	0.43
1:C:292:LYS:NZ	1:C:341:ASN:O	2.48	0.43
1:C:351:LEU:HD23	1:C:386:ILE:HD13	1.99	0.43
1:E:650:ASN:HA	1:E:651:PRO:HD3	1.86	0.43
1:C:485:LEU:HA	1:C:488:ARG:HG3	1.99	0.43
2:D:10:U:H2'	2:D:11:A:C8	2.54	0.43
1:G:653:LEU:HB3	1:G:656:LEU:HD12	1.99	0.43
1:I:527:ASP:O	1:I:529:ASP:N	2.44	0.43
1:K:503:GLU:O	1:K:509:TYR:HB2	2.18	0.43
1:A:852:GLN:HG3	1:A:856:PHE:O	2.17	0.43
1:C:653:LEU:HD23	1:C:656:LEU:HD22	2.00	0.43
1:E:321:VAL:HG22	1:E:343:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:278:CYS:SG	1:K:293:VAL:HG11	2.59	0.43
1:K:704:ILE:H	1:K:704:ILE:HG13	1.52	0.43
1:A:661:LEU:HB3	1:A:696:ALA:HB2	2.01	0.43
1:C:485:LEU:HA	1:C:488:ARG:HG2	2.01	0.43
1:C:632:LEU:HD11	1:C:715:TYR:HB2	2.00	0.43
1:I:806:LYS:HD2	1:I:911:PHE:HZ	1.84	0.43
1:A:250:LEU:HD21	1:A:264:ALA:HB2	2.00	0.43
1:G:541:TYR:HD1	1:G:586:LEU:HD11	1.84	0.43
2:L:19:U:H2'	2:L:20:A:H8	1.82	0.43
1:G:368:LEU:HD11	1:G:406:ILE:HG12	2.01	0.43
1:G:545:LEU:HA	1:G:548:TYR:HD2	1.84	0.43
1:I:243:PRO:HB3	1:I:272:PHE:HE2	1.83	0.43
1:I:658:PRO:HA	1:I:693:ILE:HG23	2.01	0.43
1:A:826:ILE:HG12	1:A:918:PHE:HB2	2.01	0.42
1:G:478:LEU:HD21	1:G:593:LYS:HG3	2.01	0.42
1:K:858:LYS:HA	1:K:877:VAL:HG12	2.01	0.42
1:E:429:LYS:HG2	1:E:429:LYS:H	1.65	0.42
1:G:547:LYS:HG3	1:G:570:PHE:CE1	2.54	0.42
1:K:411:SER:HB2	1:K:725:ILE:HD12	2.00	0.42
1:E:460:PHE:HB3	1:E:748:ILE:HD12	2.00	0.42
2:H:14:G:H2'	2:H:15:A:C8	2.54	0.42
1:I:348:PRO:HB2	1:I:382:PRO:HB2	2.00	0.42
1:A:518:LYS:HA	1:A:521:MET:HE2	2.02	0.42
1:C:847:HIS:H	1:C:860:ALA:HA	1.85	0.42
1:K:243:PRO:HB3	1:K:272:PHE:CE2	2.55	0.42
1:A:796:LYS:N	1:A:797:PRO:HD3	2.34	0.42
2:B:24:U:H2'	2:B:25:C:C6	2.54	0.42
1:G:847:HIS:H	1:G:860:ALA:HA	1.83	0.42
1:A:815:ALA:HB2	1:A:866:ARG:HD2	2.02	0.42
1:E:847:HIS:HA	1:E:848:PRO:HD3	1.92	0.42
1:G:252:LEU:O	1:G:256:LYS:HG3	2.19	0.42
1:G:634:VAL:HG12	1:G:715:TYR:HB3	2.00	0.42
1:K:745:ALA:O	1:K:749:GLU:HG3	2.19	0.42
1:A:662:THR:HG22	1:A:697:THR:HG23	2.02	0.42
1:I:852:GLN:HG3	1:I:856:PHE:O	2.20	0.42
1:C:603:ASP:HA	1:C:604:PRO:HD3	1.92	0.42
1:E:476:ALA:O	1:E:480:ARG:HG3	2.20	0.42
1:G:911:PHE:O	1:G:915:LYS:NZ	2.46	0.42
1:I:698:SER:OG	2:J:21:U:O2'	2.20	0.42
1:K:842:PHE:CD1	1:K:862:ILE:HG23	2.55	0.42
1:A:525:MET:HB2	1:A:531:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:541:TYR:HD1	1:I:586:LEU:HD11	1.85	0.42
1:A:336:GLN:HG2	1:A:340:ASN:ND2	2.35	0.41
1:I:916:ILE:H	1:I:916:ILE:HG13	1.63	0.41
1:K:650:ASN:HA	1:K:651:PRO:HD3	1.91	0.41
1:E:845:ARG:HA	1:E:846:PRO:HD3	1.96	0.41
1:A:320:ARG:HD2	1:C:332:VAL:HG11	2.02	0.41
1:E:355:LEU:HD11	1:E:363:LEU:HD21	2.02	0.41
1:E:861:LYS:NZ	1:E:872:ASP:OD2	2.47	0.41
1:G:583:GLU:O	1:G:587:THR:OG1	2.29	0.41
1:C:360:ILE:HG23	1:C:365:ILE:HD12	2.01	0.41
1:I:525:MET:HA	1:I:526:PRO:HD3	1.94	0.41
2:D:14:G:H2'	2:D:15:A:C8	2.56	0.41
1:E:824:ARG:HD2	1:E:834:LEU:HD12	2.02	0.41
1:E:889:ILE:HB	1:E:908:TRP:CE2	2.56	0.41
1:G:374:CYS:SG	1:G:375:HIS:N	2.93	0.41
1:G:851:LYS:H	1:G:858:LYS:HB2	1.86	0.41
1:A:485:LEU:HD11	1:A:589:ARG:CZ	2.51	0.41
1:A:650:ASN:HA	1:A:651:PRO:HD3	1.88	0.41
1:E:884:ILE:HD12	1:E:884:ILE:HA	1.96	0.41
1:A:698:SER:HG	2:B:21:U:HO2'	1.54	0.41
1:A:851:LYS:H	1:A:858:LYS:HB2	1.86	0.41
1:A:637:ARG:NH2	2:B:22:A:OP2	2.51	0.41
1:C:344:ILE:HG22	1:C:346:LEU:HG	2.03	0.41
1:C:597:LEU:O	1:C:599:SER:N	2.44	0.41
1:E:625:ASN:O	1:E:628:THR:OG1	2.38	0.41
1:G:603:ASP:HA	1:G:604:PRO:HD3	1.86	0.41
1:K:521:MET:HB2	1:K:904:LEU:HD21	2.02	0.41
1:K:823:VAL:HG22	1:K:833:VAL:HG22	2.01	0.41
1:A:447:GLU:H	1:A:447:GLU:HG2	1.61	0.41
1:C:887:ILE:HB	1:C:892:PHE:HE2	1.86	0.41
1:C:463:VAL:HG21	1:C:610:LYS:HG2	2.02	0.41
1:C:470:LYS:O	1:C:471:PHE:HD1	2.03	0.41
1:I:550:ASP:N	1:I:550:ASP:OD1	2.52	0.41
1:G:603:ASP:OD2	1:G:605:SER:OG	2.27	0.41
1:I:559:ARG:NH2	1:I:562:ASP:OD1	2.42	0.41
1:I:661:LEU:HB3	1:I:696:ALA:HB2	2.03	0.41
1:K:839:LYS:HA	1:K:842:PHE:CE2	2.56	0.41
1:K:518:LYS:HE3	2:L:18:U:H5''	2.03	0.41
1:C:442:VAL:HG21	1:C:449:LEU:HD22	2.02	0.40
1:G:411:SER:HB2	1:G:725:ILE:HD12	2.03	0.40
1:A:839:LYS:HA	1:A:842:PHE:CE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:ILE:H	1:C:582:ILE:HD12	1.87	0.40
1:E:779:LYS:O	1:E:783:ILE:HG13	2.21	0.40
1:I:559:ARG:HD3	1:I:646:TRP:CD1	2.50	0.40
1:I:514:VAL:HG11	2:J:18:U:H4'	2.02	0.40
1:K:453:VAL:HG13	1:K:732:ARG:HB2	2.03	0.40
1:E:374:CYS:HB2	1:E:434:LEU:HD11	2.04	0.40
1:A:521:MET:SD	1:A:811:ARG:HB3	2.61	0.40
1:C:658:PRO:HA	1:C:693:ILE:HG23	2.04	0.40
1:E:243:PRO:HB3	1:E:272:PHE:CE2	2.56	0.40
1:K:395:LEU:HD12	1:K:788:LYS:HD2	2.03	0.40
1:A:460:PHE:HE2	1:A:751:GLU:HG2	1.87	0.40
1:A:887:ILE:HB	1:A:892:PHE:HE2	1.86	0.40
1:G:839:LYS:HA	1:G:842:PHE:CE2	2.57	0.40
1:I:525:MET:HB3	1:I:531:GLU:HB2	2.04	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	644/695 (93%)	602 (94%)	42 (6%)	0	100	100
1	C	640/695 (92%)	595 (93%)	44 (7%)	1 (0%)	51	82
1	E	631/695 (91%)	588 (93%)	42 (7%)	1 (0%)	51	82
1	G	640/695 (92%)	596 (93%)	43 (7%)	1 (0%)	51	82
1	I	639/695 (92%)	588 (92%)	51 (8%)	0	100	100
1	K	634/695 (91%)	596 (94%)	38 (6%)	0	100	100
All	All	3828/4170 (92%)	3565 (93%)	260 (7%)	3 (0%)	55	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	799	PRO
1	G	375	HIS
1	E	704	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	537/623 (86%)	536 (100%)	1 (0%)	94	97
1	C	516/623 (83%)	510 (99%)	6 (1%)	75	86
1	E	487/623 (78%)	486 (100%)	1 (0%)	94	97
1	G	517/623 (83%)	516 (100%)	1 (0%)	94	97
1	I	480/623 (77%)	477 (99%)	3 (1%)	89	93
1	K	495/623 (80%)	494 (100%)	1 (0%)	94	97
All	All	3032/3738 (81%)	3019 (100%)	13 (0%)	93	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	779	LYS
1	C	315	GLU
1	C	485	LEU
1	C	493	LEU
1	C	546	ARG
1	C	597	LEU
1	C	656	LEU
1	E	919	ASP
1	G	787	GLU
1	I	399	SER
1	I	477	GLN
1	I	813	CYS
1	K	522	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	340	ASN
1	C	298	ASN
1	C	507	GLN
1	E	289	GLN
1	E	305	GLN
1	E	340	ASN
1	G	619	GLN
1	G	708	GLN
1	I	340	ASN
1	I	708	GLN
1	K	511	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	23/24 (95%)	2 (8%)	0
2	D	23/24 (95%)	1 (4%)	0
2	F	23/24 (95%)	0	0
2	H	23/24 (95%)	1 (4%)	0
2	J	23/24 (95%)	0	0
2	L	23/24 (95%)	1 (4%)	0
All	All	138/144 (95%)	5 (3%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	11	A
2	B	16	U
2	D	16	U
2	H	16	U
2	L	16	U

There are no RNA pucker outliers to report.

## 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 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
5	M7G	B	101	2	27,31,31	3.99	12 (44%)	29,49,49	1.56	6 (20%)
5	M7G	D	101	2	27,31,31	4.00	12 (44%)	29,49,49	1.64	8 (27%)
5	M7G	F	101	2	16,17,31	3.67	5 (31%)	16,26,49	0.85	1 (6%)
5	M7G	H	101	2	27,31,31	4.00	12 (44%)	29,49,49	1.74	9 (31%)
5	M7G	J	101	2	27,31,31	3.99	12 (44%)	29,49,49	1.58	6 (20%)
5	M7G	L	101	2	16,17,31	3.67	5 (31%)	16,26,49	0.84	1 (6%)

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
5	M7G	B	101	2	-	0/16/44/44	0/3/3/3
5	M7G	D	101	2	-	0/16/44/44	0/3/3/3
5	M7G	F	101	2	-	0/12/25/44	0/1/1/3
5	M7G	H	101	2	-	0/16/44/44	0/3/3/3
5	M7G	J	101	2	-	0/16/44/44	0/3/3/3
5	M7G	L	101	2	-	0/12/25/44	0/1/1/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	M7G	C3'-C4'	-8.52	1.30	1.53
5	D	101	M7G	C3'-C4'	-8.42	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	101	M7G	C3'-C4'	-8.38	1.31	1.53
5	B	101	M7G	C3'-C4'	-8.37	1.31	1.53
5	H	101	M7G	C3'-C4'	-8.36	1.31	1.53
5	J	101	M7G	C3'-C4'	-8.32	1.31	1.53
5	F	101	M7G	O4'-C1'	-6.06	1.29	1.43
5	L	101	M7G	O4'-C1'	-6.05	1.30	1.43
5	J	101	M7G	O4'-C1'	-4.97	1.30	1.42
5	B	101	M7G	O4'-C1'	-4.95	1.30	1.42
5	D	101	M7G	O4'-C1'	-4.87	1.30	1.42
5	H	101	M7G	O4'-C1'	-4.85	1.30	1.42
5	L	101	M7G	O2'-C2'	-2.96	1.36	1.43
5	F	101	M7G	O2'-C2'	-2.95	1.36	1.43
5	J	101	M7G	O2'-C2'	-2.68	1.36	1.43
5	B	101	M7G	O2'-C2'	-2.67	1.36	1.43
5	H	101	M7G	O2'-C2'	-2.63	1.36	1.43
5	D	101	M7G	O2'-C2'	-2.59	1.37	1.43
5	J	101	M7G	C8-N9	3.03	1.49	1.45
5	J	101	M7G	O3'-C3'	3.03	1.49	1.43
5	F	101	M7G	O3'-C3'	3.05	1.50	1.43
5	D	101	M7G	C8-N9	3.07	1.49	1.45
5	D	101	M7G	O3'-C3'	3.07	1.50	1.43
5	H	101	M7G	O3'-C3'	3.08	1.50	1.43
5	H	101	M7G	C8-N9	3.08	1.49	1.45
5	B	101	M7G	O3'-C3'	3.09	1.50	1.43
5	L	101	M7G	O3'-C3'	3.10	1.50	1.43
5	B	101	M7G	C8-N9	3.10	1.49	1.45
5	H	101	M7G	C2-N2	4.52	1.43	1.34
5	J	101	M7G	C2-N2	4.56	1.43	1.34
5	D	101	M7G	C2-N2	4.57	1.43	1.34
5	B	101	M7G	C2-N2	4.59	1.43	1.34
5	H	101	M7G	C2-N1	5.00	1.44	1.35
5	J	101	M7G	C2-N1	5.06	1.44	1.35
5	B	101	M7G	C2-N1	5.09	1.44	1.35
5	D	101	M7G	C2-N1	5.11	1.44	1.35
5	H	101	M7G	C6-N1	5.73	1.43	1.33
5	D	101	M7G	C6-N1	5.77	1.43	1.33
5	B	101	M7G	C2-N3	5.80	1.45	1.35
5	B	101	M7G	C6-N1	5.80	1.43	1.33
5	J	101	M7G	C6-N1	5.82	1.43	1.33
5	H	101	M7G	C2-N3	5.83	1.46	1.35
5	J	101	M7G	C2-N3	5.83	1.46	1.35
5	D	101	M7G	C2-N3	5.86	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	101	M7G	O4'-C4'	6.71	1.60	1.45
5	B	101	M7G	O4'-C4'	6.77	1.60	1.45
5	J	101	M7G	O4'-C4'	6.78	1.60	1.45
5	D	101	M7G	O4'-C4'	6.78	1.60	1.45
5	B	101	M7G	C6-C5	8.19	1.51	1.41
5	D	101	M7G	C6-C5	8.23	1.51	1.41
5	J	101	M7G	C6-C5	8.26	1.51	1.41
5	H	101	M7G	C6-C5	8.33	1.51	1.41
5	J	101	M7G	C4-N3	8.53	1.45	1.34
5	B	101	M7G	C4-N3	8.58	1.45	1.34
5	D	101	M7G	C4-N3	8.58	1.45	1.34
5	H	101	M7G	C4-N3	8.84	1.45	1.34
5	F	101	M7G	O4'-C4'	9.21	1.59	1.44
5	L	101	M7G	O4'-C4'	9.28	1.60	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	101	M7G	C5-C4-N3	-4.31	119.28	126.47
5	D	101	M7G	C5-C4-N3	-3.72	120.26	126.47
5	J	101	M7G	C5-C4-N3	-3.61	120.45	126.47
5	B	101	M7G	C5-C4-N3	-3.56	120.53	126.47
5	H	101	M7G	N1-C2-N3	-3.33	120.05	125.45
5	J	101	M7G	N1-C2-N3	-3.24	120.20	125.45
5	B	101	M7G	N1-C2-N3	-3.23	120.22	125.45
5	D	101	M7G	N1-C2-N3	-3.22	120.22	125.45
5	D	101	M7G	C5-C6-N1	-2.36	119.67	123.37
5	J	101	M7G	C5-C6-N1	-2.34	119.70	123.37
5	B	101	M7G	C5-C6-N1	-2.32	119.73	123.37
5	H	101	M7G	C5-C6-N1	-2.15	120.00	123.37
5	B	101	M7G	C2-N3-C4	2.22	120.17	113.95
5	J	101	M7G	C2-N3-C4	2.25	120.26	113.95
5	D	101	M7G	C2-N3-C4	2.26	120.30	113.95
5	H	101	M7G	C3'-C2'-C1'	2.28	105.80	101.43
5	L	101	M7G	C1'-C2'-C3'	2.39	105.35	101.67
5	H	101	M7G	C2'-C3'-C4'	2.40	107.29	102.62
5	D	101	M7G	C2'-C3'-C4'	2.41	107.31	102.62
5	D	101	M7G	C3'-C2'-C1'	2.43	106.10	101.43
5	H	101	M7G	C2-N3-C4	2.55	121.12	113.95
5	F	101	M7G	C1'-C2'-C3'	2.59	105.65	101.67
5	H	101	M7G	C6-N1-C2	2.67	119.90	116.06
5	H	101	M7G	C5-C4-N9	2.72	110.26	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	101	M7G	N3-C4-N9	2.72	130.45	126.98
5	J	101	M7G	C5-C4-N9	2.80	110.39	106.31
5	D	101	M7G	C6-N1-C2	2.82	120.12	116.06
5	B	101	M7G	C6-N1-C2	2.83	120.13	116.06
5	J	101	M7G	C6-N1-C2	2.84	120.14	116.06
5	B	101	M7G	C5-C4-N9	2.85	110.45	106.31
5	D	101	M7G	C5-C4-N9	2.91	110.54	106.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	101	M7G	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	650/695 (93%)	-0.12	1 (0%) 94 95	16, 52, 88, 122	0
1	C	648/695 (93%)	-0.03	6 (0%) 84 83	16, 53, 97, 135	0
1	E	641/695 (92%)	0.09	11 (1%) 70 67	20, 60, 97, 108	0
1	G	647/695 (93%)	-0.00	3 (0%) 90 89	22, 53, 87, 106	0
1	I	647/695 (93%)	-0.07	3 (0%) 90 89	19, 57, 96, 121	0
1	K	644/695 (92%)	0.03	8 (1%) 79 76	21, 57, 97, 123	0
2	B	24/24 (100%)	-0.18	0 100 100	32, 43, 122, 140	0
2	D	24/24 (100%)	-0.30	0 100 100	20, 39, 117, 133	0
2	F	24/24 (100%)	-0.24	0 100 100	34, 51, 111, 118	0
2	H	24/24 (100%)	-0.22	0 100 100	30, 43, 121, 124	0
2	J	24/24 (100%)	-0.28	0 100 100	29, 42, 118, 131	0
2	L	24/24 (100%)	-0.20	0 100 100	33, 45, 114, 132	0
All	All	4021/4314 (93%)	-0.02	32 (0%) 86 85	16, 55, 96, 140	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	473	TYR	4.9
1	E	606	ASN	4.4
1	E	590	PHE	4.0
1	E	599	SER	3.6
1	I	476	ALA	3.4
1	C	479	MET	3.1
1	C	467	ILE	2.9
1	K	529	ASP	2.8
1	E	484	SER	2.8
1	K	606	ASN	2.7
1	E	481	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	579	PHE	2.6
1	K	555	SER	2.5
1	E	544	HIS	2.5
1	K	604	PRO	2.5
1	I	578	GLY	2.5
1	E	597	LEU	2.4
1	E	593	LYS	2.3
1	K	527	ASP	2.3
1	E	552	LEU	2.3
1	E	465	SER	2.3
1	K	590	PHE	2.2
1	G	854	SER	2.2
1	I	548	TYR	2.2
1	K	541	TYR	2.2
1	K	551	ALA	2.1
1	C	541	TYR	2.1
1	C	604	PRO	2.1
1	G	398	SER	2.1
1	E	601	SER	2.1
1	C	590	PHE	2.0
1	G	278	CYS	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
4	MG	I	1002	1/1	0.69	0.36	1.74	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	E	1002	1/1	0.83	0.19	1.24	46,46,46,46	0
5	M7G	J	101	29/29	0.92	0.24	0.11	43,107,137,143	0
5	M7G	B	101	29/29	0.94	0.23	0.09	48,112,135,137	0
3	ZN	G	1001	1/1	0.99	0.23	0.06	96,96,96,96	0
5	M7G	D	101	29/29	0.93	0.20	0.03	42,99,123,127	0
5	M7G	H	101	29/29	0.90	0.21	-0.37	46,93,124,131	0
4	MG	G	1002	1/1	0.90	0.20	-0.47	27,27,27,27	0
4	MG	K	1002	1/1	0.91	0.19	-0.52	18,18,18,18	0
5	M7G	L	101	17/29	0.94	0.16	-0.99	39,67,94,100	0
3	ZN	I	1001	1/1	0.98	0.13	-1.11	44,44,44,44	0
4	MG	C	1002	1/1	0.95	0.13	-1.48	21,21,21,21	0
3	ZN	K	1001	1/1	0.96	0.11	-1.50	69,69,69,69	0
3	ZN	A	1001	1/1	0.98	0.13	-1.56	46,46,46,46	0
3	ZN	C	1001	1/1	0.92	0.11	-1.70	50,50,50,50	0
3	ZN	E	1001	1/1	0.96	0.10	-1.74	73,73,73,73	0
4	MG	A	1002	1/1	0.92	0.10	-1.98	28,28,28,28	0
5	M7G	F	101	17/29	0.95	0.13	-2.72	64,88,103,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.