



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:33 PM GMT

PDB ID : 5C4X  
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble  
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.  
Deposited on : 2015-06-18  
Resolution : 4.00 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

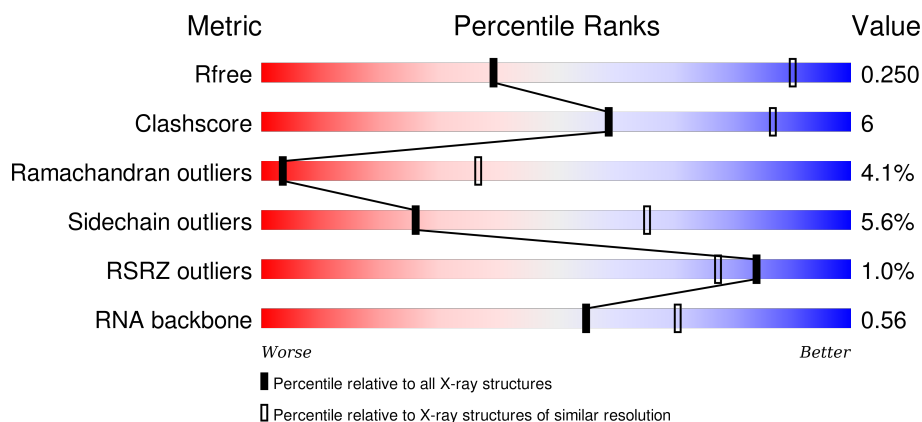
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	179	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	9	
14	S	53	
15	U	53	

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
17	MG	A	1803	-	-	-	X
17	MG	A	1804	-	-	-	X

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33495 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1436	Total	C	N	O	S	0	0	0
			11280	7105	1972	2141	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1172	Total	C	N	O	S	0	0	0
			9293	5866	1630	1741	56			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			2086	1312	347	414	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1417	875	254	286	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1339	861	222	248	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	LEU	-	expression tag	UNP P34087
G	173	GLU	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087
G	178	HIS	-	expression tag	UNP P34087
G	179	HIS	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	135	Total	C	N	O	S	0	0	0
			1080	679	182	214	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	114	Total	C	N	O	S	0	0	0
			921	568	165	178	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	66	Total	C	N	O	S	0	0	0
			540	345	94	95	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 13 is a RNA chain called RNA (5'-R(P\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			197	88	40	60	9			

- Molecule 14 is a DNA chain called NON-TEMPLATE STRAND DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	38	Total	C	N	O	P	0	0	0
			789	373	149	229	38			

- Molecule 15 is a DNA chain called TEMPLATE STRAND DNA (40-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	40	Total	C	N	O	P	0	0	0
			809	384	150	235	40			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	2	Total	Zn	0	0
			2	2		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		



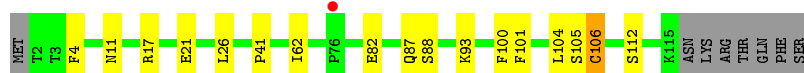
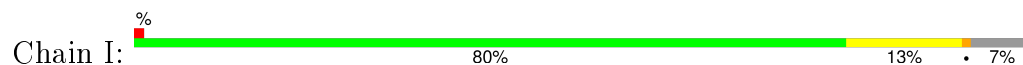








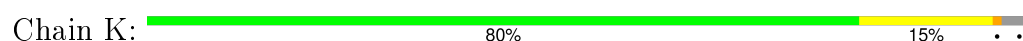
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



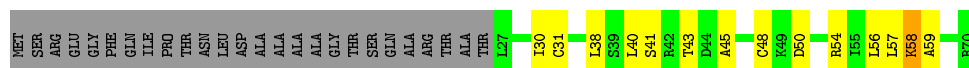
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



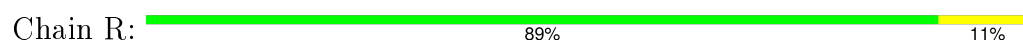
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



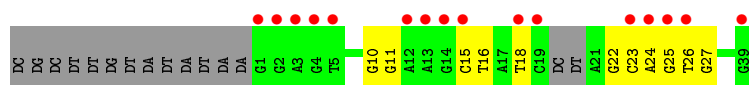
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



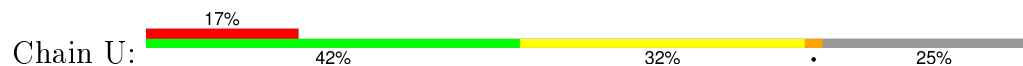
- Molecule 13: RNA (5'-R(P\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3')



- Molecule 14: NON-TEMPLATE STRAND DNA (38-MER)



- Molecule 15: TEMPLATE STRAND DNA (40-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.79 Å   393.36 Å   281.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 4.00 39.65 – 4.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.00-4.00) 96.6 (39.65-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 4.00 Å)	Xtriage
Refinement program	BUSTER	Depositor
R, $R_{free}$	0.210   ,   0.227 0.229   ,   0.250	Depositor DCC
$R_{free}$ test set	2985 reflections (3.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	137.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 155.6	EDS
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 99551 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	33495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.53	0/11485	0.69	1/15536 (0.0%)
2	B	0.51	0/9470	0.68	2/12770 (0.0%)
3	C	0.51	0/2124	0.62	0/2879
4	D	0.53	0/1427	0.64	0/1911
5	E	0.51	0/1788	0.61	0/2406
6	F	0.50	0/717	0.65	0/967
7	G	0.48	0/1367	0.66	0/1844
8	H	0.47	0/1097	0.63	0/1484
9	I	0.47	0/939	0.61	0/1266
10	J	0.53	0/549	0.69	0/738
11	K	0.48	0/942	0.61	0/1272
12	L	0.52	0/354	0.69	0/468
13	R	0.84	0/221	0.82	0/343
14	S	1.16	0/885	1.05	0/1364
15	U	1.15	0/906	1.52	7/1392 (0.5%)
All	All	0.57	0/34271	0.72	10/46640 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	U	35	DA	O5'-P-OP1	-23.98	81.92	110.70
15	U	35	DA	O5'-P-OP2	-22.60	83.58	110.70
15	U	35	DA	OP1-P-OP2	17.52	145.87	119.60
15	U	34	DG	OP1-P-O3'	-11.59	79.69	105.20
15	U	34	DG	OP2-P-O3'	-11.15	80.66	105.20
15	U	34	DG	O3'-P-O5'	7.88	118.97	104.00
1	A	1107	VAL	C-N-CA	5.45	135.31	121.70
2	B	136	THR	C-N-CA	5.23	134.78	121.70
15	U	37	DT	O4'-C1'-N1	5.10	111.57	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	930	ALA	C-N-CA	5.08	134.40	121.70

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	11280	0	11325	161	0
2	B	9293	0	9282	131	0
3	C	2086	0	2045	42	0
4	D	1417	0	1428	6	0
5	E	1752	0	1776	13	0
6	F	705	0	731	11	0
7	G	1339	0	1357	21	0
8	H	1080	0	1049	12	0
9	I	921	0	870	7	0
10	J	540	0	554	9	0
11	K	924	0	934	9	0
12	L	352	0	378	4	0
13	R	197	0	97	1	0
14	S	789	0	429	8	0
15	U	809	0	447	11	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	2	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	2	0	0	0	0
All	All	33495	0	32702	384	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 6.

All (384) 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:746:MET:HE1	2:B:1015:HIS:HA	1.34	1.06
1:A:697:ALA:HA	1:A:702:LEU:HD11	1.42	1.01
14:S:25:DG:H4'	14:S:26:DT:H5'	1.43	1.00
3:C:148:ARG:NH2	10:J:65:PRO:HD3	1.76	0.99
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.48	0.94
3:C:146:LYS:C	3:C:147:LEU:HD12	1.92	0.90
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.58	0.85
15:U:29:DC:H1'	15:U:30:DC:H5	1.42	0.84
2:B:100:PRO:HG3	2:B:172:ILE:HG21	1.63	0.80
2:B:919:SER:HB2	2:B:920:PRO:HA	1.65	0.79
3:C:77:ILE:HD13	3:C:161:LYS:HE3	1.66	0.78
1:A:105:CYS:SG	1:A:139:TRP:HA	2.24	0.76
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.67	0.75
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.49	0.75
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.70	0.73
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.69	0.73
2:B:145:ARG:HA	2:B:146:GLU:CB	2.18	0.73
2:B:867:GLY:HA3	2:B:868:MET:HB3	1.70	0.73
1:A:746:MET:CE	2:B:1015:HIS:HA	2.17	0.72
1:A:913:LEU:HD11	1:A:982:THR:HA	1.72	0.72
2:B:79:THR:HA	2:B:81:SER:N	2.06	0.71
14:S:25:DG:C4'	14:S:26:DT:H5'	2.19	0.70
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.27	0.69
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.75	0.68
1:A:311:GLN:HG2	1:A:312:PRO:HD3	1.76	0.68
15:U:15:DA:H2''	15:U:16:DC:O5'	1.94	0.67
14:S:15:DC:H2''	14:S:16:DT:H5''	1.76	0.67
11:K:42:LEU:HD23	11:K:46:ILE:HD11	1.76	0.67
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.77	0.67
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.77	0.66
1:A:512:VAL:HA	1:A:519:PRO:HA	1.78	0.66
5:E:124:VAL:HG13	5:E:132:ILE:HG23	1.77	0.66
3:C:147:LEU:N	3:C:147:LEU:HD12	2.10	0.65
3:C:113:VAL:HG23	3:C:147:LEU:HD13	1.78	0.65
2:B:84:ILE:HG22	2:B:140:ILE:HG12	1.79	0.64
1:A:1107:VAL:HG11	1:A:1381:LEU:HD23	1.80	0.64
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.80	0.63
14:S:22:DG:H4'	14:S:24:DA:H2''	1.79	0.63
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.81	0.63
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.80	0.63
2:B:867:GLY:CA	2:B:868:MET:HB3	2.29	0.62
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HD12	2:B:1105:ALA:HB2	1.80	0.62
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.81	0.62
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.82	0.61
15:U:29:DC:H1'	15:U:30:DC:C5	2.32	0.61
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.82	0.61
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.30	0.61
1:A:549:MET:HG2	1:A:577:ILE:HD12	1.83	0.61
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.82	0.61
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.40	0.60
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.82	0.60
15:U:11:DG:H2''	15:U:12:DC:O5'	2.02	0.60
1:A:1081:LEU:HD11	1:A:1085:HIS:HB2	1.83	0.60
1:A:1107:VAL:HA	1:A:1108:ALA:HB3	1.84	0.59
1:A:88:LYS:HD3	1:A:293:GLU:HG3	1.83	0.59
3:C:148:ARG:NH2	10:J:65:PRO:CD	2.60	0.59
1:A:448:PRO:HB3	15:U:19:DT:H1'	1.84	0.59
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.35	0.59
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.38	0.59
2:B:1082:MET:HA	3:C:189:THR:HA	1.84	0.59
1:A:1080:THR:O	1:A:1081:LEU:HB3	2.02	0.59
1:A:40:THR:O	1:A:49:LYS:HG2	2.03	0.59
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.83	0.59
1:A:31:SER:HB2	1:A:83:HIS:HB3	1.85	0.58
2:B:1008:PRO:HB3	2:B:1087:PHE:HE2	1.68	0.58
3:C:148:ARG:O	3:C:149:LYS:C	2.41	0.58
3:C:113:VAL:CG2	3:C:147:LEU:HD13	2.34	0.58
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.84	0.57
3:C:258:ILE:HG13	11:K:19:LEU:HD11	1.85	0.57
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.86	0.57
1:A:519:PRO:HD3	1:A:631:HIS:HD2	1.69	0.57
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.87	0.57
1:A:354:SER:HB2	1:A:469:ARG:HG2	1.87	0.57
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.87	0.56
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.70	0.56
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.88	0.56
2:B:1129:ARG:HG2	15:U:20:DC:H5''	1.86	0.56
1:A:1444:MET:HB3	7:G:58:ARG:HB3	1.88	0.56
2:B:245:GLU:N	2:B:246:LYS:HA	2.20	0.55
3:C:46:ILE:HA	3:C:159:ALA:HA	1.87	0.55
5:E:124:VAL:HG22	5:E:132:ILE:HD13	1.89	0.55
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:CYS:HA	2:B:67:SER:HB2	1.89	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.88	0.55
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.88	0.55
2:B:251:ILE:HB	14:S:18:DT:H5'	1.87	0.55
1:A:382:PRO:HD3	1:A:428:TYR:HE2	1.71	0.55
6:F:146:TRP:HB3	6:F:151:LEU:HD11	1.89	0.55
2:B:161:GLU:HG2	2:B:162:SER:H	1.71	0.55
2:B:129:PHE:HB3	2:B:164:LYS:HB3	1.89	0.55
2:B:477:ALA:HB3	13:R:6:G:H5'	1.89	0.54
1:A:679:ILE:HG13	1:A:732:LEU:HD23	1.89	0.54
1:A:266:LEU:HA	1:A:269:ILE:HD12	1.88	0.54
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.89	0.54
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.73	0.54
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.72	0.54
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.89	0.54
2:B:640:VAL:HA	2:B:651:LEU:HA	1.89	0.54
1:A:464:PRO:HB2	11:K:4:PRO:HD3	1.90	0.54
1:A:506:ALA:HB3	1:A:509:LEU:HB2	1.90	0.54
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.90	0.54
2:B:655:LYS:O	2:B:658:ILE:HG22	2.07	0.54
2:B:1122:ARG:HD3	15:U:22:DT:H5''	1.89	0.54
3:C:148:ARG:CZ	10:J:65:PRO:HD3	2.37	0.54
1:A:669:THR:HG23	1:A:805:LEU:HD13	1.90	0.54
1:A:709:THR:HG21	9:I:93:LYS:O	2.07	0.54
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.89	0.53
14:S:23:DC:H2''	14:S:24:DA:OP2	2.09	0.53
15:U:36:DC:H2''	15:U:37:DT:C6	2.43	0.53
1:A:874:ASP:HB3	1:A:877:HIS:CD2	2.42	0.53
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.90	0.53
2:B:860:MET:HB3	2:B:965:LYS:HE3	1.90	0.53
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.89	0.53
1:A:508:PRO:HA	1:A:511:ILE:HG12	1.90	0.53
1:A:4:GLN:O	1:A:5:GLN:HB2	2.08	0.53
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.91	0.53
1:A:908:LEU:HD21	1:A:1029:ARG:HG2	1.89	0.53
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.91	0.52
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.91	0.52
3:C:147:LEU:N	3:C:147:LEU:CD1	2.73	0.52
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.40	0.52
1:A:1091:SER:O	1:A:1092:LYS:HB2	2.09	0.52
2:B:144:GLY:HA2	2:B:146:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD13	1:A:986:ILE:HD11	1.92	0.52
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.90	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52
1:A:821:ARG:HD3	2:B:527:THR:HG21	1.92	0.51
1:A:360:GLU:HB3	1:A:363:GLN:HB2	1.93	0.51
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.92	0.51
2:B:134:LYS:HD3	2:B:159:ASP:HB3	1.93	0.51
1:A:451:HIS:HA	1:A:1070:GLN:HB3	1.93	0.51
1:A:560:ILE:HD12	8:H:78:SER:HB2	1.93	0.51
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.10	0.51
2:B:387:LEU:HD23	2:B:393:LYS:HB2	1.91	0.51
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.92	0.51
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.93	0.51
1:A:316:GLN:O	1:A:318:SER:O	2.27	0.51
1:A:1420:ASP:HB2	1:A:1422:ARG:HG2	1.93	0.51
3:C:70:ILE:HD12	3:C:142:VAL:HG11	1.93	0.51
2:B:1138:MET:HB2	2:B:1147:LEU:HD12	1.93	0.51
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.93	0.51
2:B:867:GLY:HA3	2:B:868:MET:CB	2.38	0.51
2:B:824:ILE:HA	2:B:1089:PRO:HA	1.93	0.51
3:C:113:VAL:CG2	3:C:147:LEU:CD1	2.89	0.51
1:A:317:LYS:HA	1:A:318:SER:C	2.31	0.51
1:A:770:VAL:HG23	1:A:822:GLU:HG3	1.93	0.51
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.93	0.51
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.41	0.50
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.92	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.93	0.50
3:C:113:VAL:HG23	3:C:147:LEU:CD1	2.41	0.50
1:A:353:ILE:CG2	1:A:487:MET:HB2	2.42	0.50
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.46	0.50
2:B:1162:ILE:HG22	2:B:1169:MET:HG3	1.94	0.50
1:A:208:LEU:HD13	1:A:235:ILE:HB	1.93	0.50
3:C:105:GLY:O	3:C:149:LYS:HA	2.12	0.50
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.94	0.50
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.93	0.50
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.47	0.49
1:A:702:LEU:HB2	1:A:710:LEU:HD11	1.93	0.49
2:B:100:PRO:HG3	2:B:172:ILE:CG2	2.39	0.49
3:C:77:ILE:HD11	3:C:161:LYS:HG3	1.94	0.49
8:H:58:THR:HB	8:H:143:LEU:HB2	1.94	0.49
1:A:834:THR:HG21	1:A:1077:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.94	0.49
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.94	0.49
3:C:36:VAL:HG11	3:C:251:LEU:HD12	1.95	0.49
2:B:161:GLU:HG3	2:B:165:VAL:CG1	2.42	0.49
2:B:125:SER:HA	2:B:171:PRO:HA	1.94	0.49
2:B:888:GLY:O	2:B:909:ASP:HA	2.12	0.49
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.95	0.49
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.95	0.49
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.95	0.49
6:F:74:ILE:HB	6:F:144:GLU:HG2	1.93	0.49
11:K:12:LEU:HA	11:K:37:LYS:HD2	1.94	0.49
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.95	0.48
1:A:658:LEU:HD13	2:B:831:SER:HB3	1.94	0.48
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.49	0.48
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.78	0.48
3:C:259:LEU:HA	3:C:262:LEU:HD12	1.96	0.48
1:A:598:LEU:HD11	8:H:124:ARG:HB2	1.95	0.48
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.94	0.48
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.95	0.48
1:A:443:LEU:HD23	1:A:501:LEU:HD21	1.96	0.48
2:B:559:SER:HA	2:B:563:MET:HB2	1.96	0.48
6:F:105:ALA:HA	7:G:16:SER:HA	1.96	0.48
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.96	0.48
1:A:383:TYR:HB3	6:F:115:THR:HA	1.96	0.48
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.95	0.48
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.96	0.48
6:F:76:LYS:HA	6:F:79:ARG:CZ	2.44	0.48
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.95	0.48
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.95	0.47
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.97	0.47
1:A:1116:LEU:HB2	1:A:1329:THR:HA	1.95	0.47
2:B:855:PHE:HB3	2:B:970:THR:HB	1.95	0.47
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.96	0.47
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.96	0.47
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.14	0.47
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.50	0.47
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.96	0.47
2:B:367:LEU:HB2	2:B:370:PHE:HE2	1.80	0.47
6:F:90:ARG:HD2	6:F:155:LEU:HD22	1.97	0.47
2:B:619:ILE:HD13	9:I:62:ILE:HA	1.97	0.47
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG11	1:A:214:ILE:HG12	1.96	0.47
2:B:101:MET:HG2	2:B:111:ALA:HA	1.96	0.47
1:A:1332:PHE:HA	1:A:1335:ILE:HD12	1.97	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.96	0.47
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.95	0.47
1:A:95:PHE:HZ	2:B:1212:ILE:HD11	1.80	0.46
1:A:496:GLU:HB2	6:F:99:LEU:HD12	1.96	0.46
1:A:15:LYS:O	1:A:1421:CYS:HB2	2.15	0.46
2:B:95:ILE:HA	2:B:129:PHE:O	2.15	0.46
2:B:63:ILE:HG23	2:B:92:PHE:HB2	1.97	0.46
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.97	0.46
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.97	0.46
8:H:125:LEU:HG	8:H:130:ARG:HH21	1.79	0.46
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.97	0.46
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.97	0.46
1:A:359:LEU:HD22	1:A:363:GLN:HB3	1.97	0.46
1:A:70:CYS:HB2	2:B:1174:LYS:HG2	1.98	0.46
10:J:14:VAL:HA	10:J:17:LYS:HD3	1.97	0.46
2:B:703:ILE:HA	2:B:740:HIS:O	2.16	0.46
7:G:100:GLU:HB3	7:G:107:LYS:HG2	1.97	0.46
4:D:52:LEU:HD13	4:D:152:SER:HA	1.97	0.46
2:B:130:VAL:O	2:B:165:VAL:HG22	2.16	0.46
2:B:283:VAL:HG23	2:B:297:ILE:HG21	1.98	0.46
14:S:26:DT:H5''	14:S:27:DG:H5'	1.97	0.46
1:A:678:GLU:HB3	1:A:732:LEU:HD21	1.96	0.46
11:K:77:THR:HB	11:K:81:TYR:HD2	1.81	0.46
1:A:102:VAL:HG22	1:A:222:LEU:HD23	1.98	0.46
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.98	0.45
2:B:856:PHE:HB3	2:B:967:ARG:HD2	1.98	0.45
15:U:6:DG:C2'	15:U:7:DA:O5'	2.64	0.45
12:L:31:CYS:HA	12:L:56:LEU:HA	1.97	0.45
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.97	0.45
1:A:859:SER:O	1:A:1422:ARG:HD3	2.16	0.45
2:B:298:LEU:HD12	2:B:311:LEU:HD23	1.98	0.45
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.98	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.51	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.98	0.45
2:B:136:THR:HA	2:B:137:TYR:CB	2.47	0.45
5:E:168:TYR:HB3	5:E:170:LEU:HD12	1.97	0.45
2:B:212:LEU:HD23	2:B:479:VAL:HG12	1.98	0.45
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:ASP:HB2	1:A:858:ASN:HB2	1.99	0.45
1:A:546:VAL:HG23	1:A:577:ILE:HG21	1.99	0.45
1:A:821:ARG:NH1	2:B:534:GLY:HA2	2.32	0.45
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.45
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.32	0.45
3:C:91:HIS:HB2	3:C:96:SER:OG	2.16	0.45
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.99	0.45
2:B:798:TYR:HB3	10:J:4:PRO:HG3	1.99	0.45
2:B:338:GLY:HA2	2:B:339:THR:HA	1.64	0.45
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.99	0.45
1:A:606:LEU:HB3	1:A:613:ILE:HB	1.99	0.45
1:A:746:MET:HE1	2:B:1015:HIS:CA	2.26	0.44
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.99	0.44
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.98	0.44
5:E:178:ILE:HB	5:E:212:ARG:HB3	2.00	0.44
1:A:598:LEU:HD21	8:H:115:TYR:HD1	1.82	0.44
2:B:424:LEU:HD12	2:B:449:ASN:HB3	1.99	0.44
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.00	0.44
5:E:101:GLN:HB2	5:E:127:ILE:HD13	1.99	0.44
4:D:11:ARG:HA	4:D:12:ARG:HA	1.79	0.44
9:I:88:SER:HA	9:I:100:PHE:HE2	1.81	0.44
1:A:326:ARG:NH2	1:A:330:LYS:HE2	2.33	0.44
1:A:818:MET:HG3	2:B:514:LEU:HD23	2.00	0.44
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.99	0.44
2:B:878:GLN:HB2	2:B:881:ASN:HB2	2.00	0.44
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.99	0.44
1:A:1290:LYS:HG2	1:A:1298:TYR:HB3	1.99	0.44
2:B:246:LYS:HE3	2:B:249:ARG:HA	1.99	0.44
7:G:62:LEU:HD12	7:G:67:SER:HB2	1.99	0.44
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.83	0.44
1:A:1288:ASP:HB3	1:A:1300:LYS:HG2	1.99	0.44
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.53	0.44
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.00	0.44
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.00	0.44
2:B:235:SER:HB3	2:B:261:ARG:HG2	2.00	0.43
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.00	0.43
3:C:115:SER:O	3:C:118:LEU:HG	2.18	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.99	0.43
3:C:259:LEU:HD12	11:K:91:CYS:HB3	2.00	0.43
5:E:55:ARG:NH1	5:E:113:GLN:HG3	2.33	0.43
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:930:ALA:HA	2:B:931:TYR:C	2.39	0.43
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.00	0.43
9:I:105:SER:O	9:I:106:CYS:HB3	2.19	0.43
1:A:90:VAL:HA	1:A:204:THR:HG21	1.99	0.43
2:B:130:VAL:HG13	2:B:132:VAL:HG23	2.01	0.43
1:A:874:ASP:HB3	1:A:877:HIS:HD2	1.82	0.43
1:A:562:THR:HG22	8:H:79:TRP:HD1	1.82	0.43
10:J:44:TYR:HA	10:J:47:ARG:HB2	2.01	0.43
2:B:319:GLU:HA	2:B:322:PHE:HB2	2.00	0.43
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.99	0.43
2:B:863:GLU:HB3	2:B:961:LEU:HD22	2.00	0.43
12:L:30:ILE:HG13	12:L:57:LEU:HB2	2.00	0.43
2:B:118:ARG:HG3	2:B:204:ILE:HD13	2.01	0.43
3:C:64:ALA:HA	3:C:67:LEU:HD12	2.00	0.43
1:A:361:LEU:HD21	1:A:511:ILE:HD11	1.99	0.43
3:C:41:ILE:HD11	3:C:247:GLY:HA2	2.01	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.00	0.43
1:A:84:ILE:HA	1:A:84:ILE:HD13	1.85	0.43
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.01	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.43
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.43
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.00	0.43
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.00	0.43
1:A:126:LEU:HD23	1:A:134:ARG:HD2	2.01	0.43
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.59	0.42
1:A:1193:LEU:HD12	1:A:1260:LEU:HG	2.00	0.42
2:B:211:VAL:HG21	2:B:483:LEU:HD13	2.01	0.42
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.42
7:G:108:VAL:HG22	7:G:159:ALA:HB3	2.01	0.42
9:I:82:GLU:HG2	9:I:104:LEU:HD23	2.02	0.42
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	2.01	0.42
2:B:218:SER:HA	2:B:404:LYS:HG2	2.01	0.42
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.00	0.42
3:C:148:ARG:HB3	3:C:151:GLN:OE1	2.19	0.42
3:C:25:VAL:HB	3:C:228:PHE:HE2	1.85	0.42
1:A:834:THR:HG21	1:A:1077:THR:CA	2.49	0.42
1:A:523:ILE:HG23	1:A:527:THR:HB	2.01	0.42
2:B:780:VAL:HG12	2:B:795:ILE:HG13	2.02	0.42
1:A:302:THR:HA	1:A:305:ASP:O	2.20	0.42
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.42
15:U:26:DG:H4'	15:U:27:DA:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:10:DG:H2''	14:S:11:DG:O5'	2.19	0.42
10:J:57:ILE:HG13	10:J:61:LEU:HD23	2.02	0.42
1:A:541:ILE:HG23	1:A:545:GLN:HB3	2.02	0.42
2:B:363:HIS:HD2	2:B:364:ILE:HG13	1.84	0.42
1:A:885:THR:HG22	1:A:940:ARG:HB2	2.02	0.42
7:G:153:GLN:HG2	7:G:154:VAL:HG23	2.02	0.42
2:B:950:ASP:O	2:B:967:ARG:HB3	2.20	0.42
2:B:878:GLN:HB2	2:B:881:ASN:CB	2.49	0.42
2:B:1114:LEU:O	2:B:1198:TYR:HE2	2.03	0.42
2:B:842:ASN:O	2:B:846:ILE:HG12	2.20	0.42
1:A:747:VAL:HG22	1:A:753:GLY:HA3	2.01	0.42
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.55	0.42
1:A:1100:ARG:HG3	1:A:1104:ILE:HD11	2.01	0.42
1:A:1345:ARG:HB3	1:A:1376:THR:HG21	2.01	0.41
2:B:901:PRO:HD3	12:L:58:LYS:HB3	2.02	0.41
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.02	0.41
1:A:726:ARG:HG2	1:A:764:CYS:HB3	2.01	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.00	0.41
2:B:87:LYS:HB2	2:B:137:TYR:HD2	1.85	0.41
1:A:395:GLY:O	1:A:401:GLY:HA3	2.20	0.41
1:A:567:LYS:CB	1:A:568:PRO:CD	2.95	0.41
1:A:182:VAL:HG12	1:A:201:VAL:HA	2.02	0.41
1:A:33:ALA:HB1	1:A:56:PRO:HG2	2.03	0.41
1:A:343:LYS:HD2	2:B:1155:SER:OG	2.20	0.41
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.41
3:C:50:GLU:HB2	3:C:156:THR:HB	2.02	0.41
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.02	0.41
2:B:868:MET:HG3	2:B:869:SER:N	2.35	0.41
1:A:818:MET:HA	2:B:514:LEU:HB3	2.01	0.41
15:U:20:DC:H2'	15:U:21:DC:O4'	2.20	0.41
7:G:144:ARG:HG2	7:G:168:LEU:HD23	2.02	0.41
2:B:778:MET:SD	2:B:794:ASN:HB3	2.61	0.41
3:C:46:ILE:HG12	3:C:157:CYS:HB3	2.02	0.41
1:A:767:GLN:HA	1:A:799:PHE:HA	2.03	0.41
2:B:961:LEU:HB3	2:B:962:LYS:H	1.73	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.50	0.41
7:G:114:LEU:HD23	7:G:161:GLY:O	2.21	0.41
11:K:58:PHE:HE1	11:K:74:ARG:HB3	1.85	0.41
1:A:366:VAL:HG22	1:A:468:PHE:HE1	1.86	0.41
2:B:825:VAL:HG23	2:B:1010:LEU:HG	2.03	0.41
5:E:9:ILE:HG12	5:E:53:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:HA	1:A:462:VAL:CG1	2.51	0.41
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.02	0.41
1:A:1453:TYR:HB3	6:F:129:LYS:HE2	2.03	0.41
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.51	0.40
1:A:845:LEU:HA	1:A:848:ILE:HD12	2.03	0.40
3:C:220:ASP:HB3	3:C:223:ALA:HB2	2.04	0.40
11:K:20:LYS:HB2	11:K:34:THR:HB	2.04	0.40
2:B:420:LEU:HD21	2:B:456:GLY:HA3	2.03	0.40
3:C:177:GLU:O	3:C:230:MET:HB2	2.22	0.40
1:A:722:LEU:HD23	1:A:767:GLN:HB2	2.04	0.40
6:F:100:GLN:HG2	7:G:15:PRO:HB3	2.03	0.40
1:A:1313:LEU:HA	1:A:1316:VAL:HG12	2.03	0.40
2:B:754:SER:HB2	2:B:812:LEU:HD11	2.03	0.40
1:A:645:LEU:O	1:A:649:ILE:HG12	2.22	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	1430/1733 (82%)	1225 (86%)	144 (10%)	61 (4%)	3	35
2	B	1158/1224 (95%)	963 (83%)	142 (12%)	53 (5%)	3	33
3	C	263/318 (83%)	231 (88%)	25 (10%)	7 (3%)	6	47
4	D	174/221 (79%)	149 (86%)	15 (9%)	10 (6%)	2	29
5	E	212/215 (99%)	196 (92%)	9 (4%)	7 (3%)	5	43
6	F	85/155 (55%)	75 (88%)	8 (9%)	2 (2%)	7	50
7	G	169/179 (94%)	142 (84%)	21 (12%)	6 (4%)	4	41
8	H	129/146 (88%)	108 (84%)	13 (10%)	8 (6%)	2	27
9	I	112/122 (92%)	100 (89%)	9 (8%)	3 (3%)	6	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	64/70 (91%)	54 (84%)	9 (14%)	1 (2%)	12	57
11	K	113/120 (94%)	106 (94%)	6 (5%)	1 (1%)	21	66
12	L	42/70 (60%)	30 (71%)	9 (21%)	3 (7%)	1	23
All	All	3951/4573 (86%)	3379 (86%)	410 (10%)	162 (4%)	3	37

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	76	GLU
1	A	194	ALA
1	A	319	GLY
1	A	385	ILE
1	A	418	SER
1	A	567	LYS
1	A	629	LEU
1	A	640	GLN
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1064	VAL
1	A	1092	LYS
1	A	1108	ALA
2	B	58	THR
2	B	80	GLU
2	B	137	TYR
2	B	146	GLU
2	B	148	LYS
2	B	161	GLU
2	B	221	ASN
2	B	282	ILE
2	B	334	ILE
2	B	345	LYS
2	B	440	HIS
2	B	507	LYS
2	B	712	PRO
2	B	907	GLY
2	B	921	ASP
2	B	1157	ALA
3	C	142	VAL

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Mol	Chain	Res	Type
3	C	161	LYS
4	D	19	GLU
4	D	20	GLU
4	D	199	ASN
5	E	115	ASN
5	E	172	GLU
6	F	73	ALA
7	G	141	SER
7	G	153	GLN
10	J	2	ILE
1	A	5	GLN
1	A	59	GLY
1	A	131	SER
1	A	156	ASP
1	A	286	HIS
1	A	628	GLY
1	A	1085	HIS
1	A	1112	LYS
1	A	1221	LYS
1	A	1403	GLU
1	A	1437	GLY
2	B	81	SER
2	B	199	MET
2	B	247	GLY
2	B	252	SER
2	B	470	LYS
2	B	511	PRO
2	B	575	PRO
2	B	648	HIS
2	B	926	GLY
2	B	931	TYR
2	B	933	SER
2	B	935	ARG
2	B	943	SER
3	C	91	HIS
3	C	215	GLU
4	D	15	LEU
4	D	169	SER
5	E	45	LYS
8	H	109	LYS
8	H	129	TYR
9	I	106	CYS

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Mol	Chain	Res	Type
12	L	45	ALA
1	A	4	GLN
1	A	146	MET
1	A	465	TYR
1	A	593	GLU
1	A	1081	LEU
1	A	1206	ASP
1	A	1270	ASN
1	A	1404	GLU
2	B	78	THR
2	B	249	ARG
2	B	250	PHE
2	B	347	LYS
2	B	441	ASP
2	B	531	GLN
2	B	711	GLU
2	B	869	SER
2	B	889	THR
4	D	8	PHE
4	D	16	LYS
4	D	118	THR
4	D	198	LEU
5	E	3	GLN
5	E	50	MET
7	G	50	ASP
8	H	17	PRO
8	H	60	ALA
8	H	108	SER
9	I	11	ASN
12	L	59	ALA
1	A	42	ASP
1	A	67	CYS
1	A	595	THR
1	A	1107	VAL
2	B	465	ASN
2	B	831	SER
2	B	832	GLY
2	B	884	ARG
2	B	951	GLN
2	B	1041	GLU
2	B	1181	GLU
3	C	90	ASP

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Mol	Chain	Res	Type
3	C	174	ALA
6	F	72	LYS
7	G	132	SER
7	G	154	VAL
8	H	78	SER
11	K	70	ARG
12	L	41	SER
1	A	54	ASN
1	A	152	VAL
1	A	158	PRO
1	A	188	ASP
1	A	399	HIS
1	A	423	ASP
1	A	424	ILE
1	A	453	MET
1	A	626	ASN
1	A	779	PHE
1	A	958	VAL
1	A	1086	PHE
1	A	1094	VAL
1	A	1111	MET
1	A	1120	LEU
1	A	1314	SER
2	B	608	ASP
2	B	922	GLU
2	B	961	LEU
2	B	1046	PRO
5	E	104	ASN
7	G	63	PRO
8	H	128	ASN
9	I	21	GLU
1	A	568	PRO
1	A	1115	SER
2	B	751	VAL
2	B	1045	SER
3	C	175	ALA
4	D	11	ARG
1	A	61	ILE
1	A	410	GLY
1	A	147	VAL
1	A	308	ILE
5	E	127	ILE

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Mol	Chain	Res	Type
2	B	143	PRO
2	B	343	ILE
8	H	85	GLY

### 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	1250/1520 (82%)	1167 (93%)	83 (7%)	21	60
2	B	1009/1061 (95%)	956 (95%)	53 (5%)	28	67
3	C	233/274 (85%)	221 (95%)	12 (5%)	29	68
4	D	156/200 (78%)	150 (96%)	6 (4%)	40	74
5	E	196/197 (100%)	191 (97%)	5 (3%)	54	81
6	F	77/137 (56%)	72 (94%)	5 (6%)	21	61
7	G	152/160 (95%)	144 (95%)	8 (5%)	28	67
8	H	118/128 (92%)	114 (97%)	4 (3%)	44	77
9	I	107/116 (92%)	103 (96%)	4 (4%)	41	75
10	J	61/65 (94%)	54 (88%)	7 (12%)	7	36
11	K	99/102 (97%)	94 (95%)	5 (5%)	29	68
12	L	39/57 (68%)	34 (87%)	5 (13%)	5	31
All	All	3497/4017 (87%)	3300 (94%)	197 (6%)	26	65

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	22	PHE
1	A	43	GLU
1	A	44	THR
1	A	70	CYS
1	A	77	CYS
1	A	84	ILE

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Mol	Chain	Res	Type
1	A	90	VAL
1	A	93	VAL
1	A	117	GLU
1	A	141	LEU
1	A	151	ASP
1	A	176	LYS
1	A	204	THR
1	A	226	GLU
1	A	247	ARG
1	A	270	LEU
1	A	303	TYR
1	A	311	GLN
1	A	329	LEU
1	A	337	ARG
1	A	356	ASP
1	A	363	GLN
1	A	375	THR
1	A	411	ASP
1	A	419	LYS
1	A	447	GLN
1	A	468	PHE
1	A	470	LEU
1	A	475	THR
1	A	509	LEU
1	A	511	ILE
1	A	513	SER
1	A	524	VAL
1	A	527	THR
1	A	567	LYS
1	A	595	THR
1	A	597	LEU
1	A	636	GLU
1	A	666	ILE
1	A	672	ASP
1	A	701	LEU
1	A	771	GLU
1	A	774	ARG
1	A	785	PRO
1	A	821	ARG
1	A	838	GLN
1	A	854	ASN
1	A	860	LEU

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Mol	Chain	Res	Type
1	A	895	LYS
1	A	919	ILE
1	A	932	GLU
1	A	938	LYS
1	A	981	LEU
1	A	983	ILE
1	A	1003	LYS
1	A	1016	THR
1	A	1022	LEU
1	A	1037	LEU
1	A	1077	THR
1	A	1079	MET
1	A	1081	LEU
1	A	1086	PHE
1	A	1101	LEU
1	A	1107	VAL
1	A	1110	ASN
1	A	1116	LEU
1	A	1120	LEU
1	A	1135	ARG
1	A	1215	ARG
1	A	1234	GLU
1	A	1286	LYS
1	A	1289	ARG
1	A	1306	LEU
1	A	1315	GLU
1	A	1316	VAL
1	A	1345	ARG
1	A	1366	ARG
1	A	1371	LEU
1	A	1394	THR
1	A	1404	GLU
1	A	1409	LEU
1	A	1447	GLU
2	B	28	GLU
2	B	63	ILE
2	B	66	ASP
2	B	69	LEU
2	B	84	ILE
2	B	217	ARG
2	B	282	ILE
2	B	294	ASP

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Mol	Chain	Res	Type
2	B	333	PHE
2	B	341	LEU
2	B	401	PHE
2	B	424	LEU
2	B	429	PHE
2	B	431	TYR
2	B	466	TRP
2	B	505	ASP
2	B	529	GLU
2	B	555	ILE
2	B	570	VAL
2	B	601	ARG
2	B	612	GLU
2	B	658	ILE
2	B	678	GLU
2	B	783	THR
2	B	797	TYR
2	B	825	VAL
2	B	829	CYS
2	B	836	GLU
2	B	837	ASP
2	B	865	LYS
2	B	874	PHE
2	B	921	ASP
2	B	944	THR
2	B	945	GLU
2	B	953	LEU
2	B	972	LYS
2	B	979	LYS
2	B	986	GLN
2	B	987	LYS
2	B	1065	GLN
2	B	1072	MET
2	B	1093	GLN
2	B	1106	ARG
2	B	1108	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1150	ARG
2	B	1166	CYS
2	B	1194	ILE
2	B	1201	LYS

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Mol	Chain	Res	Type
2	B	1202	LEU
2	B	1217	TYR
2	B	1220	ARG
3	C	11	ARG
3	C	55	THR
3	C	75	MET
3	C	77	ILE
3	C	100	THR
3	C	101	LEU
3	C	186	LEU
3	C	197	SER
3	C	203	GLN
3	C	238	ILE
3	C	245	VAL
3	C	251	LEU
4	D	50	LEU
4	D	51	ASN
4	D	52	LEU
4	D	144	THR
4	D	152	SER
4	D	214	LEU
5	E	81	GLU
5	E	96	PHE
5	E	170	LEU
5	E	175	LEU
5	E	207	ARG
6	F	72	LYS
6	F	77	ASP
6	F	112	GLU
6	F	123	LYS
6	F	125	LEU
7	G	6	ASP
7	G	13	LEU
7	G	31	LEU
7	G	39	THR
7	G	55	ASP
7	G	112	LYS
7	G	115	MET
7	G	133	SER
8	H	26	ILE
8	H	40	LEU
8	H	63	LEU

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Mol	Chain	Res	Type
8	H	95	TYR
9	I	4	PHE
9	I	17	ARG
9	I	26	LEU
9	I	87	GLN
10	J	2	ILE
10	J	3	VAL
10	J	9	SER
10	J	24	LEU
10	J	38	ARG
10	J	42	LYS
10	J	46	CYS
11	K	42	LEU
11	K	61	TYR
11	K	73	LEU
11	K	75	ILE
11	K	102	LYS
12	L	40	LEU
12	L	43	THR
12	L	50	ASP
12	L	54	ARG
12	L	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	118	HIS
1	A	517	ASN
1	A	736	ASN
1	A	877	HIS
1	A	1390	ASN
2	B	224	GLN
2	B	494	HIS
2	B	572	HIS
2	B	800	GLN
2	B	1084	GLN
2	B	1195	HIS
3	C	140	ASN
9	I	46	HIS
9	I	108	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/9 (77%)	0	0

There are no RNA backbone outliers to report.

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 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	1436/1733 (82%)	-0.31	0 100 100	62, 176, 266, 296	0
2	B	1172/1224 (95%)	-0.17	12 (1%) 84 77	73, 189, 282, 300	0
3	C	265/318 (83%)	-0.28	0 100 100	95, 184, 251, 288	0
4	D	178/221 (80%)	-0.25	1 (0%) 90 86	128, 206, 266, 293	0
5	E	214/215 (99%)	-0.26	0 100 100	105, 228, 280, 291	0
6	F	87/155 (56%)	-0.33	0 100 100	86, 151, 218, 234	0
7	G	171/179 (95%)	-0.28	0 100 100	120, 178, 253, 300	0
8	H	135/146 (92%)	-0.24	0 100 100	158, 232, 286, 294	0
9	I	114/122 (93%)	0.01	1 (0%) 85 80	137, 224, 283, 293	0
10	J	66/70 (94%)	-0.19	0 100 100	93, 186, 243, 270	0
11	K	115/120 (95%)	-0.20	0 100 100	92, 175, 245, 284	0
12	L	44/70 (62%)	-0.12	0 100 100	142, 237, 271, 297	0
13	R	9/9 (100%)	-0.21	0 100 100	201, 226, 298, 299	0
14	S	38/53 (71%)	1.74	16 (42%) 0 1	300, 300, 300, 300	0
15	U	40/53 (75%)	1.23	9 (22%) 1 2	183, 300, 300, 300	0
All	All	4084/4688 (87%)	-0.21	39 (0%) 84 77	62, 189, 282, 300	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	U	38	DC	4.3
15	U	39	DC	4.2
14	S	3	DA	4.2
15	U	37	DT	4.1
15	U	34	DG	3.5
14	S	1	DG	3.4
15	U	35	DA	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	13	ARG	3.3
14	S	23	DC	3.3
2	B	508	LEU	3.2
14	S	24	DA	3.2
2	B	150	GLU	3.1
14	S	19	DC	3.0
14	S	2	DG	3.0
15	U	31	DA	3.0
15	U	36	DC	2.9
15	U	33	DG	2.8
15	U	32	DC	2.8
2	B	509	ALA	2.7
9	I	76	PRO	2.7
14	S	25	DG	2.6
14	S	39	DG	2.6
14	S	14	DG	2.5
14	S	15	DC	2.5
2	B	148	LYS	2.5
14	S	26	DT	2.4
14	S	13	DA	2.4
14	S	12	DA	2.4
2	B	136	THR	2.3
14	S	18	DT	2.3
2	B	714	GLU	2.3
14	S	4	DG	2.2
2	B	344	LYS	2.2
2	B	503	GLY	2.2
2	B	919	SER	2.2
2	B	655	LYS	2.1
2	B	656	GLY	2.1
2	B	507	LYS	2.1
14	S	5	DT	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

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
17	MG	A	1804	1/1	0.49	1.42	18.97	166,166,166,166	0
17	MG	A	1803	1/1	0.53	0.60	15.83	171,171,171,171	0
16	ZN	I	201	1/1	0.99	0.15	-0.03	173,173,173,173	0
16	ZN	B	1301	1/1	0.98	0.16	-0.11	166,166,166,166	0
16	ZN	J	101	1/1	0.99	0.28	-1.15	172,172,172,172	0
16	ZN	C	402	1/1	1.00	0.09	-1.22	148,148,148,148	0
16	ZN	L	101	1/1	0.95	0.10	-1.83	188,188,188,188	0
16	ZN	A	1802	1/1	0.98	0.09	-2.30	166,166,166,166	0
16	ZN	A	1801	1/1	0.98	0.04	-2.64	153,153,153,153	0
16	ZN	I	202	1/1	0.96	0.03	-3.13	216,216,216,216	0
16	ZN	C	401	1/1	0.86	0.35	-	174,174,174,174	0

## 6.5 Other polymers

There are no such residues in this entry.