



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:46 PM GMT

PDB ID : 5C4A
Title : Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors : Barnes, C.O.; Calero, M.; Malik, I.; Saphr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on : 2015-06-17
Resolution : 4.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

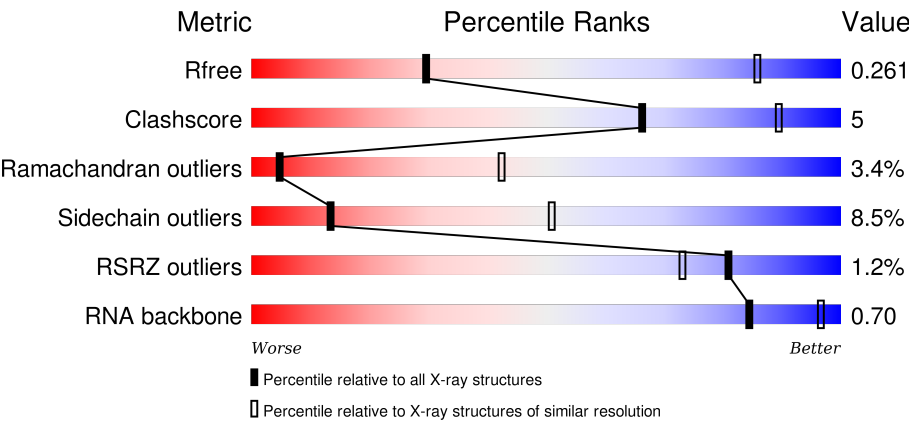
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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.




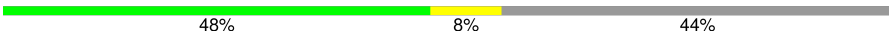








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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 ≥ 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	<div><div></div><div><div></div><div>64%</div><div>16%</div><div>•</div><div>18%</div></div></div>
2	B	1224	<div><div>2%</div><div></div><div><div></div><div>71%</div><div>21%</div><div>•</div><div>5%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>67%</div><div>14%</div><div>•</div><div>17%</div></div></div>
4	D	221	<div><div>3%</div><div></div><div><div></div><div>65%</div><div>11%</div><div>24%</div></div></div>

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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	56	
15	U	56	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 32574 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	1425	Total	C	N	O	S	0	0	0
			11206	7057	1960	2127	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1162	Total	C	N	O	S	0	0	0
			9215	5816	1617	1726	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	168	Total	C	N	O	S	0	0	0
			1331	822	237	270	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	170	Total	C	N	O	S	0	0	0
			1331	857	220	246	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
			927	571	168	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 Scaffold 2 Non-template Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	16	Total	C	N	O	P	0	0	0
			331	158	58	99	16			

- Molecule 15 is a DNA chain called Scaffold 2 Template Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	29	Total	C	N	O	P	0	0	0
			587	280	107	171	29			

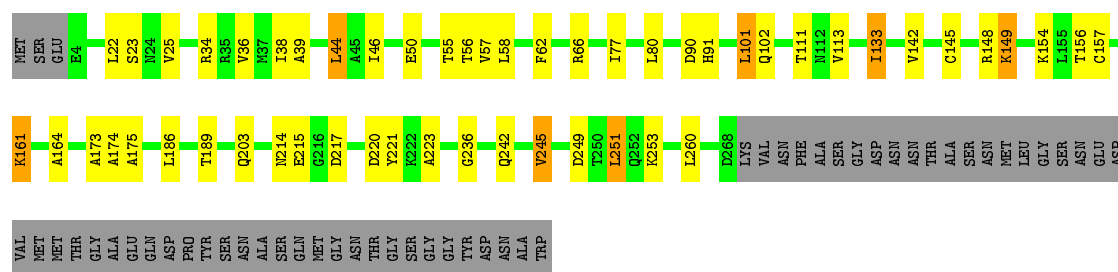
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	1	Total	Zn	0	0
			1	1		
16	A	2	Total	Zn	0	0
			2	2		
16	L	1	Total	Zn	0	0
			1	1		

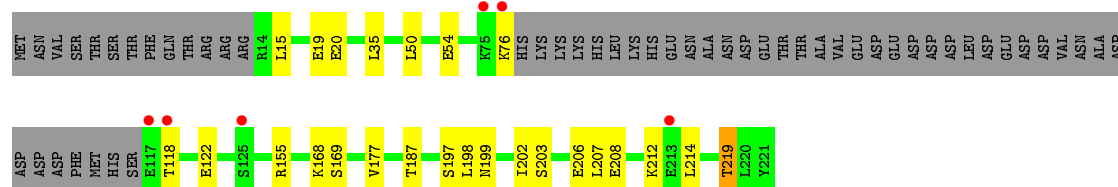
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

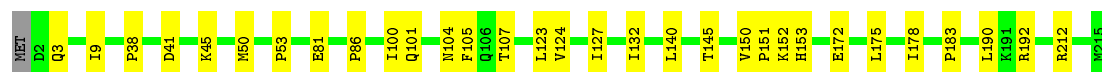
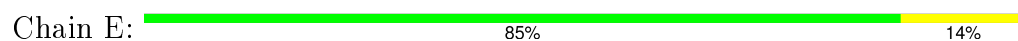




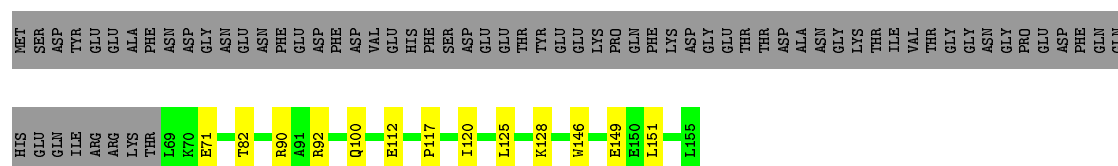
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



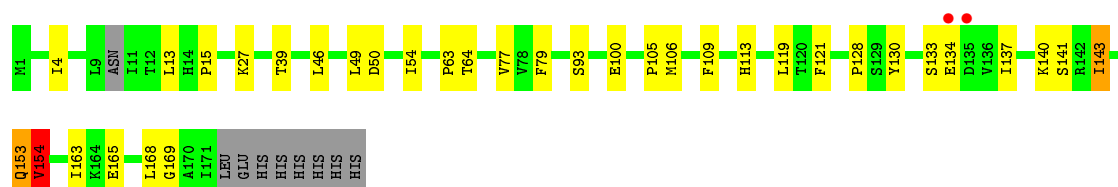
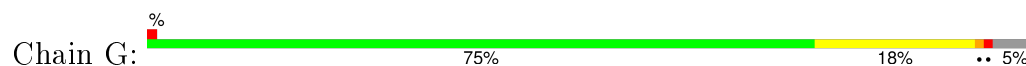
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

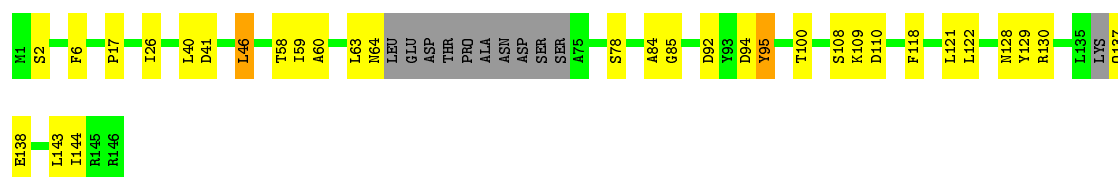


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





- 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')

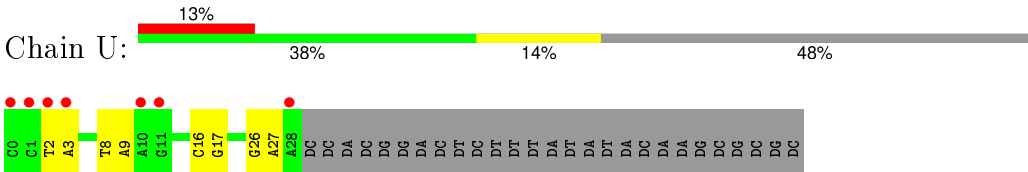


- Molecule 14: Scaffold 2 Non-template Strand



- Molecule 15: Scaffold 2 Template Strand





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	219.83Å 396.71Å 273.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 4.20 39.91 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-4.20) 99.7 (39.91-4.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 4.13Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.224 , 0.242 0.242 , 0.261	Depositor DCC
R_{free} test set	6714 reflections (7.74%)	DCC
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 121.3	EDS
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 86781 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	32574	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.52	0/11407	0.66	0/15428
2	B	0.52	1/9390 (0.0%)	0.67	0/12662
3	C	0.49	0/2124	0.61	0/2879
4	D	0.50	0/1339	0.63	0/1793
5	E	0.51	0/1788	0.60	0/2406
6	F	0.51	0/717	0.64	0/967
7	G	0.50	0/1358	0.66	0/1830
8	H	0.47	0/1097	0.63	0/1484
9	I	0.48	0/945	0.62	0/1273
10	J	0.49	0/549	0.65	0/738
11	K	0.48	0/942	0.60	0/1272
12	L	0.51	0/354	0.65	0/468
13	R	0.78	0/221	0.80	0/343
14	S	0.95	0/370	0.95	0/570
15	U	1.04	0/657	0.95	0/1009
All	All	0.53	1/33258 (0.0%)	0.67	0/45122

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	264	SER	C-N	7.45	1.51	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	265	SER	Mainchain

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	11206	0	11265	134	0
2	B	9215	0	9210	111	0
3	C	2086	0	2045	23	0
4	D	1331	0	1345	8	0
5	E	1752	0	1776	9	0
6	F	705	0	731	5	0
7	G	1331	0	1350	19	0
8	H	1080	0	1049	10	0
9	I	927	0	883	7	0
10	J	540	0	555	9	0
11	K	924	0	934	3	0
12	L	352	0	377	2	0
13	R	197	0	96	4	0
14	S	331	0	183	2	0
15	U	587	0	326	6	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	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	32574	0	32125	316	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 (316) 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:869:GLY:HA3	1:A:1366:ARG:HG2	1.46	0.98
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.64	0.80
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.64	0.79
1:A:311:GLN:HB2	1:A:312:PRO:HD3	1.67	0.77
1:A:1107:VAL:HA	1:A:1108:ALA:HB3	1.68	0.75
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.70	0.74
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.71	0.70
2:B:145:ARG:HA	2:B:146:GLU:CB	2.22	0.69
3:C:50:GLU:HB2	3:C:156:THR:HB	1.77	0.66
2:B:1138:MET:HB3	2:B:1147:LEU:HD12	1.77	0.66
1:A:394:ASN:HB3	1:A:398:GLU:HB3	1.78	0.65
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.26	0.65
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.79	0.65
2:B:980:PHE:HE2	2:B:990:ILE:HD11	1.61	0.64
15:U:8:DT:H2"	15:U:9:DA:H5"	1.78	0.64
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.78	0.63
1:A:27:VAL:HA	1:A:30:ILE:HG22	1.80	0.63
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.28	0.63
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.81	0.62
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.81	0.62
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.39	0.62
1:A:1107:VAL:CA	1:A:1108:ALA:HB3	2.29	0.62
1:A:105:CYS:SG	1:A:139:TRP:HA	2.39	0.62
2:B:921:ASP:HB3	2:B:928:ARG:HG3	1.81	0.61
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.82	0.61
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.81	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.30	0.61
11:K:42:LEU:HD23	11:K:46:ILE:HD11	1.81	0.61
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.83	0.60
2:B:825:VAL:HG23	2:B:1010:LEU:HD12	1.83	0.60
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.83	0.60
2:B:640:VAL:HA	2:B:651:LEU:HA	1.83	0.60
1:A:842:VAL:HA	1:A:1069:ALA:HB1	1.84	0.60
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.84	0.60
2:B:364:ILE:HD11	2:B:374:LYS:HG3	1.83	0.59
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.82	0.59
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.84	0.58
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.84	0.58
1:A:247:ARG:HD3	1:A:266:LEU:HD13	1.86	0.58
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.86	0.58
1:A:316:GLN:HG2	1:A:322:VAL:HB	1.85	0.58
1:A:512:VAL:HA	1:A:519:PRO:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.03	0.57
2:B:84:ILE:HG22	2:B:138:GLU:HB3	1.85	0.57
1:A:508:PRO:HB2	1:A:639:PRO:O	2.04	0.57
2:B:661:LEU:HD21	2:B:684:LEU:HD11	1.85	0.57
7:G:130:TYR:HB2	7:G:137:ILE:HB	1.87	0.57
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.86	0.57
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.86	0.56
2:B:422:LYS:HG2	2:B:426:LYS:HE2	1.86	0.56
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.87	0.56
3:C:186:LEU:HG	3:C:223:ALA:HB1	1.86	0.56
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.86	0.56
2:B:145:ARG:HA	2:B:146:GLU:HB3	1.87	0.56
2:B:711:GLU:HB3	2:B:712:PRO:HD3	1.88	0.56
1:A:752:LYS:HD2	2:B:1015:HIS:HB3	1.88	0.56
2:B:477:ALA:HB3	13:R:6:G:H5'	1.86	0.55
2:B:80:GLU:O	2:B:81:SER:HB3	2.07	0.55
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.55
2:B:806:THR:HG23	2:B:1045:SER:HA	1.87	0.55
1:A:150:THR:O	1:A:163:SER:HA	2.07	0.55
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	1.88	0.54
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.89	0.54
7:G:143:ILE:HG13	7:G:169:GLY:O	2.07	0.54
3:C:102:GLN:HG3	3:C:154:LYS:HE2	1.88	0.54
2:B:298:LEU:HD12	2:B:311:LEU:HD23	1.90	0.54
1:A:179:LEU:HD22	1:A:297:GLN:HG3	1.90	0.54
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.90	0.54
1:A:1107:VAL:CA	1:A:1108:ALA:CB	2.85	0.54
2:B:346:GLU:O	2:B:347:LYS:HB2	2.08	0.53
1:A:1193:LEU:HD11	1:A:1264:GLU:HB2	1.90	0.53
2:B:79:THR:HG22	2:B:82:ASP:O	2.09	0.53
2:B:980:PHE:CE2	2:B:990:ILE:HD11	2.42	0.53
2:B:213:ILE:HG23	2:B:497:ARG:HB3	1.91	0.53
1:A:1107:VAL:N	1:A:1108:ALA:CB	2.71	0.53
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.91	0.53
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.91	0.53
2:B:1168:LEU:HB2	2:B:1170:THR:HG23	1.91	0.53
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.90	0.52
6:F:128:LYS:HD2	6:F:149:GLU:HA	1.91	0.52
2:B:100:PRO:HG3	2:B:172:ILE:HG21	1.91	0.52
10:J:36:LEU:HD22	10:J:41:LEU:HG	1.92	0.52
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:LEU:HD21	1:A:1029:ARG:HG2	1.92	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CE1	2.45	0.52
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.91	0.52
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.92	0.52
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.91	0.52
1:A:1118:VAL:HG13	1:A:1327:ILE:HD12	1.92	0.52
1:A:842:VAL:HA	1:A:1069:ALA:CB	2.41	0.52
1:A:1290:LYS:HG2	1:A:1298:TYR:HB3	1.91	0.51
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	1.92	0.51
15:U:26:DG:H4'	15:U:27:DA:OP1	2.09	0.51
1:A:1336:MET:HG3	1:A:1381:LEU:HD12	1.92	0.51
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.46	0.51
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.90	0.51
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.92	0.51
2:B:364:ILE:HG23	2:B:585:VAL:HG22	1.92	0.51
1:A:182:VAL:HG12	1:A:201:VAL:HA	1.92	0.51
8:H:58:THR:HB	8:H:143:LEU:HB2	1.91	0.51
3:C:46:ILE:HG12	3:C:157:CYS:HB3	1.92	0.51
1:A:549:MET:HG2	1:A:577:ILE:HD12	1.92	0.51
5:E:9:ILE:HG12	5:E:53:PRO:HG3	1.93	0.51
3:C:148:ARG:HG2	3:C:149:LYS:HG3	1.92	0.50
7:G:93:SER:HB2	7:G:100:GLU:HB2	1.92	0.50
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.92	0.50
5:E:145:THR:HA	5:E:150:VAL:HG11	1.94	0.50
3:C:58:LEU:HD23	3:C:145:CYS:HB2	1.94	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.77	0.50
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.94	0.50
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.93	0.50
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.93	0.50
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.93	0.50
1:A:1107:VAL:N	1:A:1108:ALA:HB2	2.27	0.50
7:G:46:LEU:HD11	7:G:79:PHE:HB2	1.94	0.50
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.45	0.49
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.94	0.49
5:E:38:PRO:HD2	5:E:41:ASP:HB2	1.94	0.49
1:A:317:LYS:HA	1:A:318:SER:C	2.31	0.49
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.94	0.49
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.93	0.49
1:A:1420:ASP:HB2	1:A:1422:ARG:HG2	1.94	0.49
2:B:509:ALA:O	2:B:510:LYS:HB2	2.12	0.49
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:HA	1:A:804:TYR:HB2	1.95	0.49
8:H:110:ASP:HB3	8:H:128:ASN:HD22	1.76	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.13	0.49
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.48	0.49
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.93	0.49
1:A:540:PHE:HB2	1:A:571:LEU:HD23	1.94	0.49
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.95	0.49
7:G:163:ILE:HD12	7:G:169:GLY:HA2	1.95	0.48
1:A:913:LEU:HD11	1:A:982:THR:HA	1.94	0.48
13:R:2:U:O2	13:R:3:C:C2	2.65	0.48
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.95	0.48
15:U:2:DT:H2"	15:U:3:DA:N7	2.29	0.48
2:B:924:GLU:HG2	2:B:925:LEU:H	1.78	0.48
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.94	0.48
1:A:849:MET:HG3	1:A:1063:MET:SD	2.54	0.48
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.95	0.48
7:G:46:LEU:HD21	7:G:105:PRO:HG3	1.95	0.48
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.95	0.48
2:B:373:ARG:HG2	2:B:566:LEU:HB3	1.95	0.48
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.95	0.48
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.94	0.48
1:A:508:PRO:CB	1:A:643:ALA:HB2	2.41	0.48
2:B:509:ALA:C	2:B:511:PRO:HA	2.34	0.48
4:D:155:ARG:HG3	4:D:219:THR:HG21	1.96	0.48
8:H:6:PHE:HB3	8:H:59:ILE:HD12	1.94	0.48
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.49	0.47
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.79	0.47
2:B:499:ASN:HA	2:B:536:VAL:HG22	1.95	0.47
2:B:238:ALA:HB2	2:B:385:LEU:HB2	1.96	0.47
10:J:3:VAL:HG23	10:J:15:GLY:HA2	1.95	0.47
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.97	0.47
1:A:451:HIS:ND1	1:A:1074:GLU:HG3	2.29	0.47
1:A:709:THR:HG21	9:I:94:ASP:HA	1.95	0.47
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.96	0.47
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.96	0.47
15:U:2:DT:H2"	15:U:3:DA:C8	2.49	0.47
1:A:567:LYS:CB	1:A:568:PRO:CD	2.91	0.46
2:B:64:CYS:HA	2:B:67:SER:HB2	1.96	0.46
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.96	0.46
4:D:168:LYS:HG3	4:D:177:VAL:HG11	1.97	0.46
1:A:883:LEU:HD22	1:A:943:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.98	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.46
8:H:100:THR:HG23	8:H:138:GLU:HB2	1.98	0.46
2:B:84:ILE:CG2	2:B:138:GLU:HB3	2.46	0.46
8:H:110:ASP:HB3	8:H:128:ASN:ND2	2.31	0.46
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.98	0.46
2:B:930:ALA:HA	2:B:931:TYR:C	2.36	0.46
1:A:214:ILE:HG23	1:A:218:ASP:HB2	1.98	0.46
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.97	0.46
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.97	0.46
2:B:63:ILE:HG23	2:B:92:PHE:HB2	1.97	0.46
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.97	0.46
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.51	0.45
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.52	0.45
3:C:57:VAL:HG21	10:J:60:PHE:HB2	1.99	0.45
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.97	0.45
2:B:619:ILE:HD13	9:I:62:ILE:HA	1.99	0.45
2:B:1112:GLN:HG3	13:R:2:U:OP1	2.17	0.45
2:B:1124:ARG:NH2	13:R:2:U:OP2	2.49	0.45
2:B:81:SER:HA	2:B:82:ASP:HA	1.68	0.45
2:B:600:LEU:HA	2:B:603:LEU:HD12	1.97	0.45
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.81	0.45
2:B:85:SER:HB3	2:B:139:ALA:HB3	1.98	0.45
15:U:16:DC:H2"	15:U:17:DG:OP1	2.16	0.45
2:B:327:ARG:HG2	2:B:331:LEU:HD12	1.99	0.45
1:A:1138:ILE:HG22	1:A:1319:VAL:HG21	1.98	0.44
1:A:880:LYS:HA	1:A:955:PRO:HA	1.99	0.44
7:G:49:LEU:HD11	7:G:77:VAL:HG13	1.99	0.44
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.99	0.44
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.99	0.44
1:A:380:VAL:HG21	1:A:426:LEU:HD22	1.99	0.44
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.99	0.44
4:D:203:SER:HB2	4:D:206:GLU:HB2	1.99	0.44
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.33	0.44
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.00	0.44
1:A:523:ILE:HD13	1:A:622:VAL:HG22	2.00	0.44
4:D:202:ILE:HG21	4:D:207:LEU:HD13	2.00	0.43
12:L:47:ARG:HD3	12:L:52:GLY:HA2	2.00	0.43
2:B:230:ALA:HA	2:B:261:ARG:CZ	2.47	0.43
1:A:850:VAL:HG12	1:A:1060:PRO:HA	2.01	0.43
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.18	0.43
14:S:31:DA:H61	15:U:8:DT:H3	1.66	0.43
1:A:344:ARG:CZ	2:B:1120:GLU:HA	2.49	0.43
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.01	0.43
2:B:332:ASP:OD1	2:B:346:GLU:HB3	2.18	0.43
1:A:859:SER:O	1:A:1422:ARG:HD3	2.19	0.43
5:E:101:GLN:HB2	5:E:127:ILE:HD13	1.99	0.43
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.01	0.43
1:A:1394:THR:HB	1:A:1399:ARG:HD3	2.00	0.43
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.83	0.43
9:I:100:PHE:HD1	9:I:111:THR:HG22	1.84	0.43
3:C:220:ASP:HB3	3:C:223:ALA:HB2	2.01	0.43
2:B:80:GLU:O	2:B:81:SER:CB	2.67	0.43
3:C:50:GLU:HB3	12:L:64:LEU:HD21	2.01	0.43
7:G:79:PHE:HE2	7:G:106:MET:HB3	1.83	0.43
2:B:127:GLY:HA2	2:B:169:ARG:HG2	1.99	0.43
3:C:242:GLN:HA	3:C:245:VAL:HG12	2.00	0.43
2:B:205:ILE:HD11	2:B:461:LEU:HD23	2.01	0.43
7:G:121:PHE:HE1	7:G:128:PRO:HB3	1.84	0.43
2:B:63:ILE:HG13	2:B:421:PHE:CZ	2.54	0.43
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.00	0.43
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	2.01	0.42
8:H:2:SER:HB2	8:H:64:ASN:HB2	1.99	0.42
3:C:36:VAL:HG11	3:C:251:LEU:HD12	2.00	0.42
1:A:451:HIS:HD2	1:A:453:MET:HB2	1.84	0.42
1:A:44:THR:N	1:A:45:GLN:HA	2.35	0.42
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.00	0.42
10:J:3:VAL:HG21	10:J:18:TRP:HB2	2.01	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.42
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	2.00	0.42
1:A:919:ILE:HG13	1:A:925:LEU:HD13	2.01	0.42
2:B:338:GLY:HA2	2:B:339:THR:HA	1.72	0.42
2:B:1162:ILE:HG22	2:B:1169:MET:HG3	2.00	0.42
1:A:381:THR:HB	1:A:382:PRO:HD2	2.00	0.42
2:B:526:GLU:HG3	2:B:771:SER:HB2	2.01	0.42
7:G:100:GLU:HG3	7:G:109:PHE:HD1	1.84	0.42
6:F:146:TRP:HB3	6:F:151:LEU:HD11	2.01	0.42
1:A:606:LEU:HD23	1:A:613:ILE:HG13	2.02	0.42
4:D:50:LEU:HB3	4:D:54:GLU:HB3	2.01	0.42
1:A:446:ARG:NE	1:A:480:ALA:HB2	2.34	0.42
1:A:940:ARG:HG2	1:A:941:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.85	0.42
1:A:319:GLY:HA3	2:B:471:LYS:HB2	2.01	0.42
1:A:1409:LEU:HA	1:A:1409:LEU:HD12	1.91	0.42
10:J:6:ARG:HG2	10:J:13:VAL:HA	2.02	0.42
1:A:483:ASP:HA	2:B:988:GLY:HA2	2.01	0.42
7:G:163:ILE:HA	7:G:168:LEU:HD13	2.01	0.42
1:A:212:LYS:HG2	1:A:232:GLU:HG2	2.02	0.42
2:B:1033:LYS:HE3	2:B:1059:LEU:HD11	2.02	0.41
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.02	0.41
1:A:981:LEU:HD13	1:A:986:ILE:HD11	2.01	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.21	0.41
1:A:335:ARG:HA	1:A:339:ASN:HB2	2.02	0.41
1:A:389:THR:O	1:A:393:ARG:HG2	2.21	0.41
3:C:101:LEU:HD21	3:C:113:VAL:HG11	2.01	0.41
2:B:809:MET:HA	2:B:812:LEU:HD12	2.02	0.41
1:A:1383:SER:HB2	1:A:1388:GLY:HA3	2.02	0.41
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.55	0.41
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.01	0.41
2:B:798:TYR:CG	10:J:4:PRO:HG3	2.55	0.41
3:C:221:TYR:HB3	8:H:46:LEU:HD22	2.02	0.41
1:A:1116:LEU:HB2	1:A:1329:THR:HA	2.02	0.41
1:A:1228:TRP:HB3	1:A:1238:ILE:HG23	2.03	0.41
8:H:118:PHE:HB2	8:H:121:LEU:HB2	2.02	0.41
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.02	0.41
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.02	0.41
2:B:868:MET:HG3	2:B:869:SER:N	2.35	0.41
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.02	0.41
2:B:961:LEU:HB3	2:B:962:LYS:H	1.74	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.03	0.41
1:A:354:SER:HB2	1:A:469:ARG:HD3	2.02	0.41
1:A:106:VAL:HG11	1:A:214:ILE:HG12	2.02	0.41
1:A:252:PHE:O	1:A:256:GLN:HB2	2.21	0.41
1:A:1063:MET:O	1:A:1065:GLY:N	2.54	0.41
1:A:469:ARG:HA	1:A:469:ARG:HD3	1.91	0.41
2:B:139:ALA:HB2	2:B:149:TYR:HA	2.02	0.41
7:G:121:PHE:CE1	7:G:128:PRO:HB3	2.56	0.41
1:A:722:LEU:HD23	1:A:767:GLN:HB2	2.03	0.41
1:A:1438:THR:HG22	6:F:92:ARG:HD3	2.03	0.41
1:A:506:ALA:HB3	1:A:509:LEU:HB2	2.01	0.41
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	2.03	0.41
1:A:88:LYS:HD3	1:A:293:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.41
1:A:567:LYS:HE2	1:A:568:PRO:HD3	2.02	0.41
2:B:802:PRO:HG2	2:B:805:THR:HG22	2.01	0.41
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	2.03	0.41
3:C:249:ASP:O	3:C:253:LYS:HG2	2.21	0.41
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.02	0.41
1:A:1345:ARG:HB3	1:A:1376:THR:HG21	2.01	0.41
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.02	0.41
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.02	0.41
2:B:438:GLU:HB2	2:B:439:ALA:HA	2.03	0.41
1:A:1332:PHE:HA	1:A:1335:ILE:HD12	2.03	0.41
2:B:867:GLY:HA3	2:B:868:MET:HG2	2.03	0.41
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.20	0.40
14:S:36:DT:H2''	14:S:37:DA:O4'	2.20	0.40
9:I:58:VAL:HG12	9:I:62:ILE:HD12	2.02	0.40
1:A:1361:SER:HA	1:A:1362:TYR:HA	1.91	0.40
5:E:178:ILE:HB	5:E:212:ARG:HD3	2.04	0.40
4:D:50:LEU:HD11	7:G:4:ILE:CD1	2.51	0.40
1:A:139:TRP:O	1:A:143:LYS:HB2	2.20	0.40
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.40
2:B:756:ILE:O	2:B:759:PRO:HD3	2.20	0.40
2:B:917:PRO:HA	2:B:933:SER:O	2.21	0.40
2:B:220:GLY:HA3	2:B:243:ALA:HB2	2.03	0.40
10:J:20:SER:HB2	10:J:39:LEU:HD21	2.03	0.40
2:B:1006:ILE:HD11	10:J:43:ARG:HB3	2.03	0.40
1:A:1383:SER:HB3	1:A:1385:THR:HG22	2.04	0.40
9:I:53:GLY:HA2	9:I:56:ALA: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	1417/1733 (82%)	1222 (86%)	147 (10%)	48 (3%)	5	42
2	B	1146/1224 (94%)	977 (85%)	124 (11%)	45 (4%)	4	37
3	C	263/318 (83%)	235 (89%)	20 (8%)	8 (3%)	5	45
4	D	164/221 (74%)	150 (92%)	8 (5%)	6 (4%)	4	40
5	E	212/215 (99%)	197 (93%)	9 (4%)	6 (3%)	6	46
6	F	85/155 (55%)	74 (87%)	10 (12%)	1 (1%)	16	62
7	G	166/179 (93%)	147 (89%)	14 (8%)	5 (3%)	5	45
8	H	129/146 (88%)	111 (86%)	10 (8%)	8 (6%)	2	27
9	I	112/122 (92%)	100 (89%)	10 (9%)	2 (2%)	11	55
10	J	64/70 (91%)	57 (89%)	6 (9%)	1 (2%)	12	57
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	42/70 (60%)	31 (74%)	9 (21%)	2 (5%)	3	32
All	All	3913/4573 (86%)	3410 (87%)	371 (10%)	132 (3%)	5	42

All (132) 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	286	HIS
1	A	385	ILE
1	A	418	SER
1	A	567	LYS
1	A	629	LEU
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1064	VAL
1	A	1108	ALA
1	A	1111	MET
2	B	81	SER
2	B	146	GLU
2	B	248	SER
2	B	252	SER
2	B	334	ILE
2	B	510	LYS
2	B	512	ARG

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Mol	Chain	Res	Type
2	B	712	PRO
2	B	889	THR
2	B	907	GLY
2	B	932	HIS
2	B	1157	ALA
3	C	142	VAL
4	D	20	GLU
7	G	141	SER
7	G	153	GLN
10	J	2	ILE
1	A	43	GLU
1	A	131	SER
1	A	311	GLN
1	A	319	GLY
1	A	335	ARG
1	A	593	GLU
1	A	595	THR
1	A	628	GLY
1	A	701	LEU
1	A	1003	LYS
1	A	1332	PHE
1	A	1437	GLY
2	B	58	THR
2	B	249	ARG
2	B	337	ARG
2	B	345	LYS
2	B	347	LYS
2	B	922	GLU
2	B	923	GLU
2	B	1181	GLU
3	C	214	ASN
4	D	19	GLU
4	D	118	THR
4	D	169	SER
4	D	199	ASN
5	E	3	GLN
5	E	172	GLU
6	F	71	GLU
8	H	109	LYS
8	H	129	TYR
9	I	106	CYS
12	L	45	ALA

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Mol	Chain	Res	Type
1	A	63	ARG
1	A	117	GLU
1	A	152	VAL
1	A	188	ASP
1	A	423	ASP
1	A	1115	SER
1	A	1221	LYS
1	A	1403	GLU
2	B	75	ALA
2	B	76	GLN
2	B	78	THR
2	B	164	LYS
2	B	199	MET
2	B	531	GLN
2	B	575	PRO
2	B	648	HIS
2	B	711	GLU
2	B	884	ARG
3	C	91	HIS
3	C	174	ALA
4	D	198	LEU
5	E	45	LYS
7	G	50	ASP
7	G	63	PRO
7	G	154	VAL
8	H	17	PRO
8	H	84	ALA
8	H	85	GLY
8	H	108	SER
9	I	47	GLU
1	A	67	CYS
1	A	158	PRO
1	A	314	ALA
1	A	424	ILE
1	A	568	PRO
1	A	779	PHE
1	A	958	VAL
1	A	1112	LYS
2	B	935	ARG
2	B	951	GLN
2	B	1017	ILE
2	B	1046	PRO

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Mol	Chain	Res	Type
2	B	1156	ASP
3	C	90	ASP
5	E	104	ASN
12	L	59	ALA
1	A	4	GLN
1	A	54	ASN
1	A	426	LEU
1	A	591	PHE
2	B	147	LEU
2	B	198	ASP
2	B	250	PHE
2	B	440	HIS
3	C	161	LYS
3	C	215	GLU
5	E	50	MET
8	H	60	ALA
8	H	78	SER
1	A	48	ALA
2	B	80	GLU
2	B	143	PRO
2	B	282	ILE
2	B	919	SER
3	C	149	LYS
2	B	1045	SER
5	E	86	PRO
2	B	343	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	1244/1520 (82%)	1128 (91%)	116 (9%)	11	46
2	B	1002/1061 (94%)	900 (90%)	102 (10%)	9	41
3	C	233/274 (85%)	219 (94%)	14 (6%)	24	63
4	D	146/200 (73%)	138 (94%)	8 (6%)	27	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	188 (96%)	8 (4%)	37	73
6	F	77/137 (56%)	73 (95%)	4 (5%)	29	68
7	G	151/160 (94%)	141 (93%)	10 (7%)	21	60
8	H	118/128 (92%)	108 (92%)	10 (8%)	13	51
9	I	108/116 (93%)	103 (95%)	5 (5%)	33	70
10	J	61/65 (94%)	57 (93%)	4 (7%)	21	60
11	K	99/102 (97%)	92 (93%)	7 (7%)	18	58
12	L	39/57 (68%)	33 (85%)	6 (15%)	3	24
All	All	3474/4017 (86%)	3180 (92%)	294 (8%)	13	51

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	22	PHE
1	A	40	THR
1	A	43	GLU
1	A	44	THR
1	A	53	LEU
1	A	57	ARG
1	A	58	LEU
1	A	70	CYS
1	A	93	VAL
1	A	114	LEU
1	A	121	LEU
1	A	152	VAL
1	A	173	THR
1	A	204	THR
1	A	236	LEU
1	A	247	ARG
1	A	257	ARG
1	A	266	LEU
1	A	307	ASP
1	A	315	LEU
1	A	320	ARG
1	A	383	TYR
1	A	459	ARG
1	A	467	THR
1	A	469	ARG

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Mol	Chain	Res	Type
1	A	470	LEU
1	A	485	ASP
1	A	498	ARG
1	A	509	LEU
1	A	515	GLN
1	A	517	ASN
1	A	521	MET
1	A	527	THR
1	A	536	LEU
1	A	546	VAL
1	A	567	LYS
1	A	595	THR
1	A	597	LEU
1	A	618	GLU
1	A	622	VAL
1	A	630	ILE
1	A	635	ARG
1	A	640	GLN
1	A	644	LYS
1	A	657	LEU
1	A	666	ILE
1	A	672	ASP
1	A	701	LEU
1	A	702	LEU
1	A	710	LEU
1	A	732	LEU
1	A	738	LYS
1	A	746	MET
1	A	771	GLU
1	A	774	ARG
1	A	782	ARG
1	A	791	ASP
1	A	811	GLN
1	A	826	ASP
1	A	830	LYS
1	A	838	GLN
1	A	841	LEU
1	A	849	MET
1	A	860	LEU
1	A	880	LYS
1	A	895	LYS
1	A	899	VAL

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Mol	Chain	Res	Type
1	A	913	LEU
1	A	919	ILE
1	A	920	LEU
1	A	932	GLU
1	A	936	LEU
1	A	938	LYS
1	A	961	ARG
1	A	963	ILE
1	A	980	ASP
1	A	981	LEU
1	A	988	LEU
1	A	998	LEU
1	A	1003	LYS
1	A	1009	ASN
1	A	1015	VAL
1	A	1016	THR
1	A	1045	VAL
1	A	1058	VAL
1	A	1067	LEU
1	A	1096	SER
1	A	1100	ARG
1	A	1104	ILE
1	A	1109	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1135	ARG
1	A	1143	LEU
1	A	1155	ASP
1	A	1166	ASP
1	A	1186	ASP
1	A	1224	LEU
1	A	1238	ILE
1	A	1297	GLU
1	A	1299	VAL
1	A	1303	GLU
1	A	1316	VAL
1	A	1354	ASN
1	A	1362	TYR
1	A	1371	LEU
1	A	1381	LEU
1	A	1387	HIS
1	A	1409	LEU

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Mol	Chain	Res	Type
1	A	1418	LEU
1	A	1420	ASP
1	A	1422	ARG
1	A	1433	MET
1	A	1443	VAL
1	A	1450	LEU
2	B	21	GLU
2	B	22	SER
2	B	61	ASP
2	B	69	LEU
2	B	73	GLN
2	B	95	ILE
2	B	106	ASP
2	B	129	PHE
2	B	130	VAL
2	B	147	LEU
2	B	164	LYS
2	B	170	LEU
2	B	242	SER
2	B	244	LEU
2	B	251	ILE
2	B	254	LEU
2	B	310	MET
2	B	324	ILE
2	B	334	ILE
2	B	341	LEU
2	B	344	LYS
2	B	384	ARG
2	B	396	ASP
2	B	401	PHE
2	B	435	THR
2	B	466	TRP
2	B	469	GLN
2	B	473	MET
2	B	485	ARG
2	B	512	ARG
2	B	535	LEU
2	B	552	MET
2	B	555	ILE
2	B	563	MET
2	B	570	VAL
2	B	585	VAL

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Mol	Chain	Res	Type
2	B	602	THR
2	B	629	ASP
2	B	639	ILE
2	B	651	LEU
2	B	658	ILE
2	B	662	MET
2	B	667	GLN
2	B	678	GLU
2	B	682	SER
2	B	694	ASP
2	B	748	ILE
2	B	778	MET
2	B	786	ASN
2	B	791	THR
2	B	797	TYR
2	B	801	LYS
2	B	825	VAL
2	B	829	CYS
2	B	837	ASP
2	B	865	LYS
2	B	868	MET
2	B	873	THR
2	B	874	PHE
2	B	875	GLU
2	B	878	GLN
2	B	883	LEU
2	B	904	ARG
2	B	919	SER
2	B	924	GLU
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	950	ASP
2	B	953	LEU
2	B	955	THR
2	B	956	THR
2	B	957	ASN
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	979	LYS
2	B	986	GLN

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Mol	Chain	Res	Type
2	B	990	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1031	LEU
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1103	ILE
2	B	1106	ARG
2	B	1112	GLN
2	B	1114	LEU
2	B	1122	ARG
2	B	1123	SER
2	B	1124	ARG
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1182	CYS
2	B	1194	ILE
2	B	1201	LYS
2	B	1203	LEU
3	C	23	SER
3	C	34	ARG
3	C	44	LEU
3	C	55	THR
3	C	56	THR
3	C	80	LEU
3	C	101	LEU
3	C	111	THR
3	C	133	ILE
3	C	203	GLN
3	C	217	ASP
3	C	245	VAL
3	C	251	LEU
3	C	260	LEU
4	D	15	LEU
4	D	35	LEU
4	D	76	LYS
4	D	122	GLU

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Mol	Chain	Res	Type
4	D	187	THR
4	D	197	SER
4	D	214	LEU
4	D	219	THR
5	E	81	GLU
5	E	107	THR
5	E	123	LEU
5	E	140	LEU
5	E	152	LYS
5	E	175	LEU
5	E	190	LEU
5	E	192	ARG
6	F	82	THR
6	F	90	ARG
6	F	112	GLU
6	F	125	LEU
7	G	13	LEU
7	G	39	THR
7	G	64	THR
7	G	113	HIS
7	G	119	LEU
7	G	133	SER
7	G	134	GLU
7	G	140	LYS
7	G	143	ILE
7	G	154	VAL
8	H	26	ILE
8	H	40	LEU
8	H	41	ASP
8	H	46	LEU
8	H	63	LEU
8	H	92	ASP
8	H	94	ASP
8	H	95	TYR
8	H	130	ARG
8	H	137	GLN
9	I	5	ARG
9	I	17	ARG
9	I	26	LEU
9	I	44	TYR
9	I	59	VAL
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	3	VAL
10	J	23	ASN
10	J	24	LEU
11	K	42	LEU
11	K	61	TYR
11	K	73	LEU
11	K	75	ILE
11	K	79	GLU
11	K	92	ASN
11	K	114	LEU
12	L	27	LEU
12	L	37	LYS
12	L	43	THR
12	L	57	LEU
12	L	58	LYS
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	611	GLN
1	A	1078	GLN
4	D	41	GLN
8	H	131	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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 [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, 95th 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 ²)	Q<0.9
1	A	1425/1733 (82%)	-0.34	4 (0%) 94 92	50, 116, 208, 300	0
2	B	1162/1224 (94%)	-0.20	22 (1%) 70 60	50, 131, 241, 300	0
3	C	265/318 (83%)	-0.30	0 100 100	50, 121, 191, 240	0
4	D	168/221 (76%)	0.02	6 (3%) 46 36	78, 178, 284, 300	0
5	E	214/215 (99%)	-0.33	0 100 100	65, 148, 226, 282	0
6	F	87/155 (56%)	-0.46	0 100 100	51, 94, 173, 238	0
7	G	170/179 (94%)	-0.21	2 (1%) 81 73	57, 128, 270, 300	0
8	H	135/146 (92%)	-0.08	0 100 100	99, 164, 236, 292	0
9	I	114/122 (93%)	-0.05	1 (0%) 85 80	78, 155, 214, 280	0
10	J	66/70 (94%)	-0.45	0 100 100	67, 121, 194, 218	0
11	K	115/120 (95%)	-0.36	0 100 100	50, 116, 179, 237	0
12	L	44/70 (62%)	-0.34	0 100 100	82, 157, 207, 241	0
13	R	9/9 (100%)	0.64	0 100 100	158, 185, 278, 293	0
14	S	16/56 (28%)	2.14	6 (37%) 0 1	111, 278, 300, 300	0
15	U	29/56 (51%)	1.21	7 (24%) 1 2	111, 262, 300, 300	0
All	All	4019/4694 (85%)	-0.24	48 (1%) 81 73	50, 129, 238, 300	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	134	GLU	5.0
14	S	38	DG	4.8
15	U	28	DA	4.0
14	S	39	DG	4.0
4	D	125	SER	3.8
2	B	932	HIS	3.8
14	S	24	DT	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	346	GLU	3.4
2	B	921	ASP	3.3
15	U	3	DA	3.3
2	B	923	GLU	3.3
1	A	251	SER	3.1
15	U	10	DA	3.1
15	U	11	DG	3.1
9	I	101	PHE	3.0
2	B	339	THR	2.9
2	B	337	ARG	2.8
4	D	117	GLU	2.8
2	B	161	GLU	2.7
2	B	920	PRO	2.7
15	U	0	DC	2.7
14	S	32	DT	2.6
2	B	160	SER	2.6
2	B	933	SER	2.6
15	U	2	DT	2.6
14	S	37	DA	2.6
4	D	76	LYS	2.5
2	B	340	ALA	2.5
4	D	75	LYS	2.5
1	A	255	SER	2.4
2	B	926	GLY	2.4
2	B	338	GLY	2.4
2	B	76	GLN	2.4
1	A	44	THR	2.4
15	U	1	DC	2.3
4	D	118	THR	2.3
14	S	34	DG	2.3
4	D	213	GLU	2.3
1	A	1185	PHE	2.3
2	B	108	VAL	2.2
2	B	882	THR	2.1
2	B	150	GLU	2.1
7	G	135	ASP	2.1
2	B	468	GLU	2.1
2	B	929	THR	2.0
2	B	336	ARG	2.0
2	B	922	GLU	2.0
2	B	136	THR	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, 95th 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(\AA^2)	Q<0.9
17	MG	A	1804	1/1	0.72	0.30	0.75	71,71,71,71	0
16	ZN	J	101	1/1	0.97	0.19	-1.29	90,90,90,90	0
16	ZN	B	1301	1/1	0.98	0.09	-1.40	60,60,60,60	0
16	ZN	A	1802	1/1	0.98	0.08	-1.59	68,68,68,68	0
16	ZN	I	201	1/1	0.99	0.06	-1.66	115,115,115,115	0
16	ZN	C	401	1/1	0.99	0.05	-1.68	82,82,82,82	0
16	ZN	L	101	1/1	0.99	0.05	-1.89	91,91,91,91	0
16	ZN	A	1801	1/1	0.98	0.06	-2.97	101,101,101,101	0
16	ZN	I	202	1/1	0.90	0.06	-3.17	155,155,155,155	0
17	MG	A	1803	1/1	0.88	0.12	-7.06	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.