



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:46 AM UTC

PDB ID : 5C3E / pdb_00005c3e
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 : 2015-06-17
Resolution : 3.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

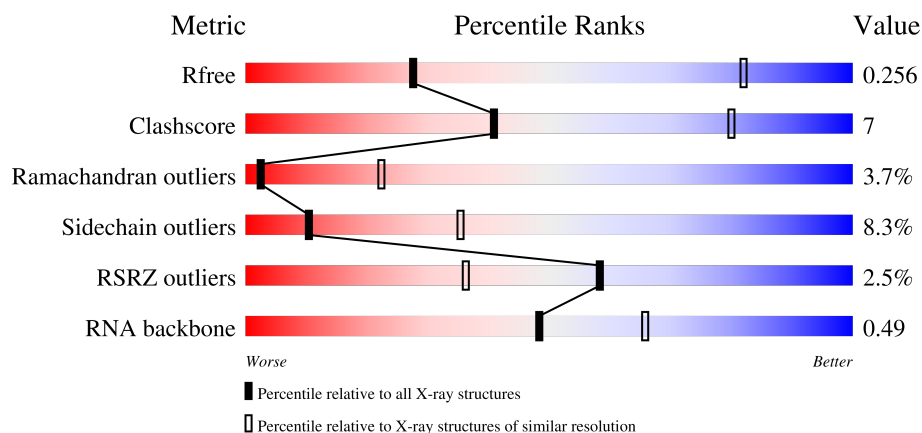
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

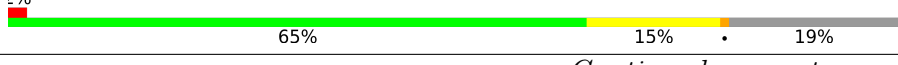
The reported resolution of this entry is 3.70 Å.

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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 2% 82% 14% •
6	F	155	 42% 14% 44%
7	G	179	 % 72% 20% • •
8	H	146	 % 73% 20% 8%
9	I	122	 6% 75% 16% • 7%
10	J	70	 4% 63% 24% 7% 6%
11	K	120	 % 75% 18% • •
12	L	70	 10% 34% 24% • 39%
13	R	9	 11% 78% 22%
14	S	45	 4% 24% 7% 69%
15	U	45	 2% 33% 27% 40%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 32515 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	1430	Total	C	N	O	S	0	0	0
			11227	7069	1962	2134	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0	0
			9130	5767	1599	1708	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
			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	43	Total	C	N	O	S	0	0	0
			344	211	69	60	4			

- Molecule 13 is a RNA chain called Synthetic RNA.

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 Synthetic DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	14	Total	C	N	O	P	0	0	0
			286	137	49	86	14			

- Molecule 15 is a DNA chain called Synthetic DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	27	Total	C	N	O	P	0	0	0
			550	262	101	160	27			

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

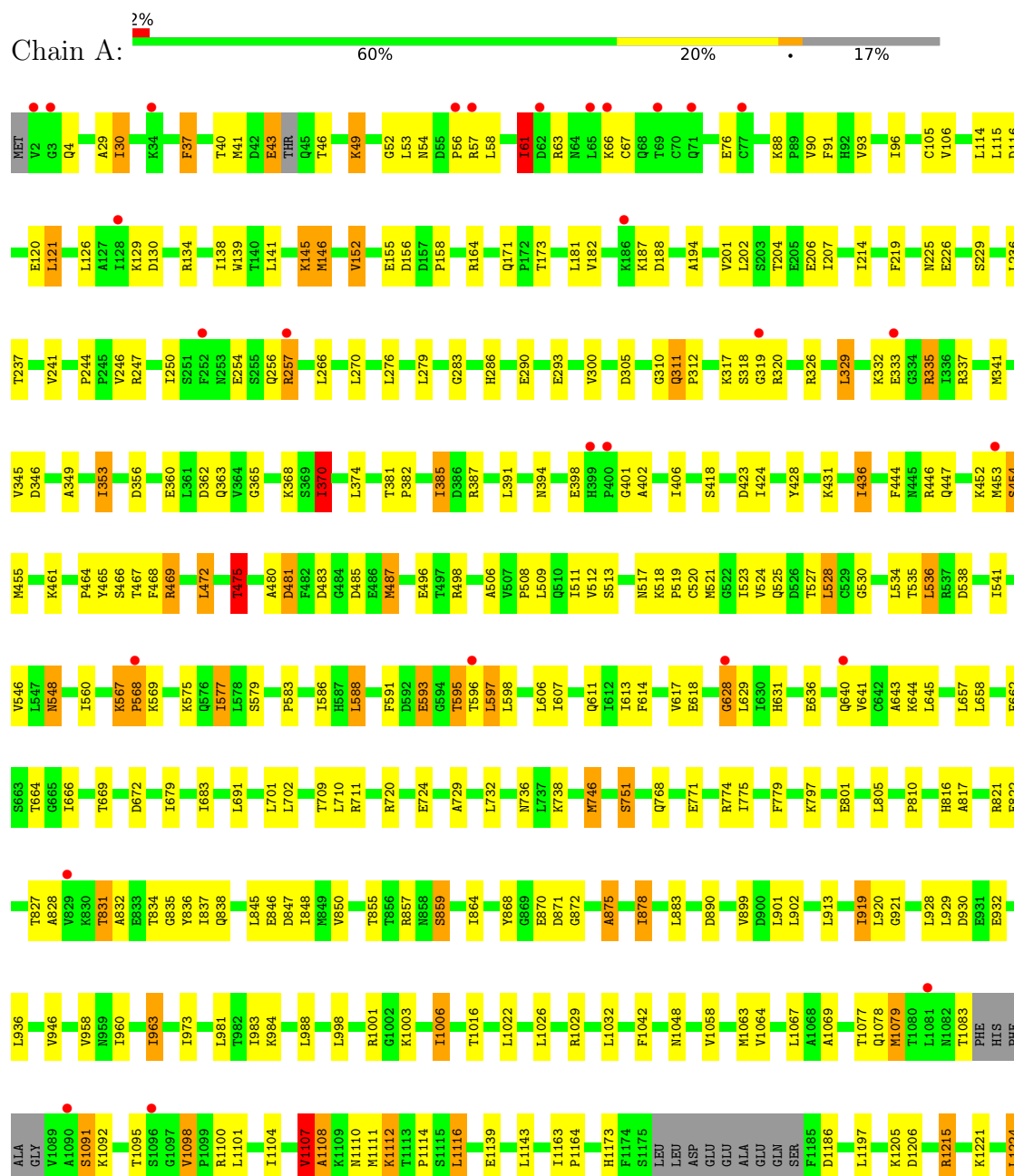
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

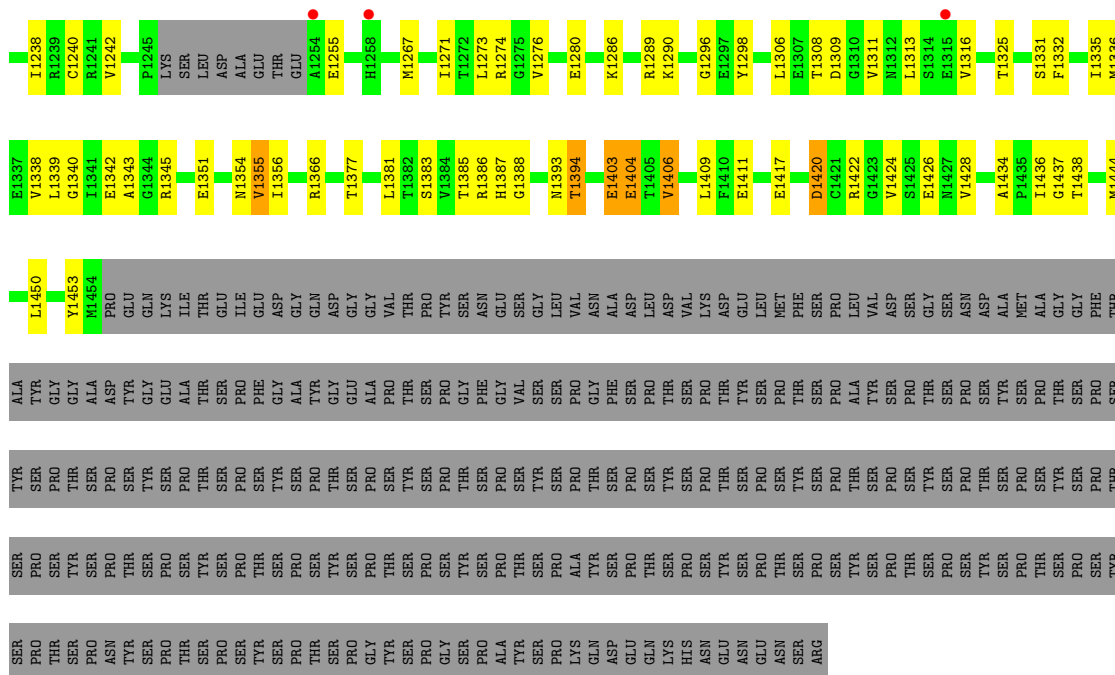
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

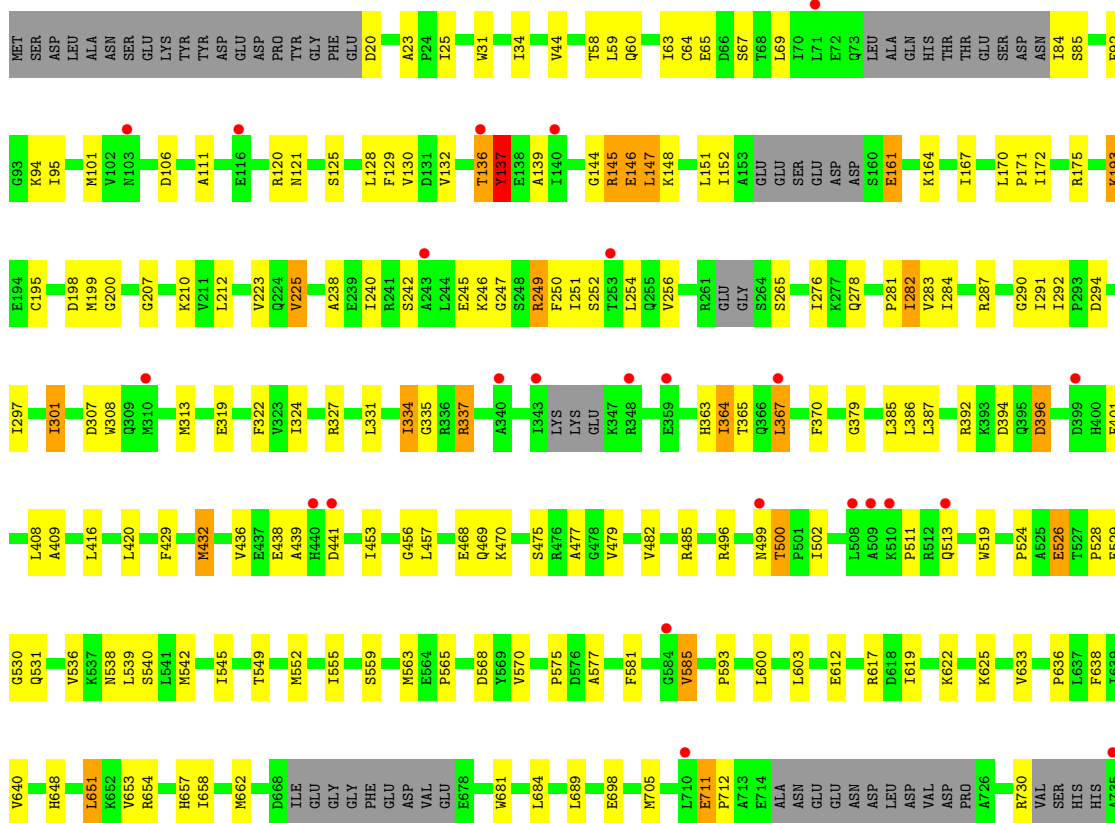
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

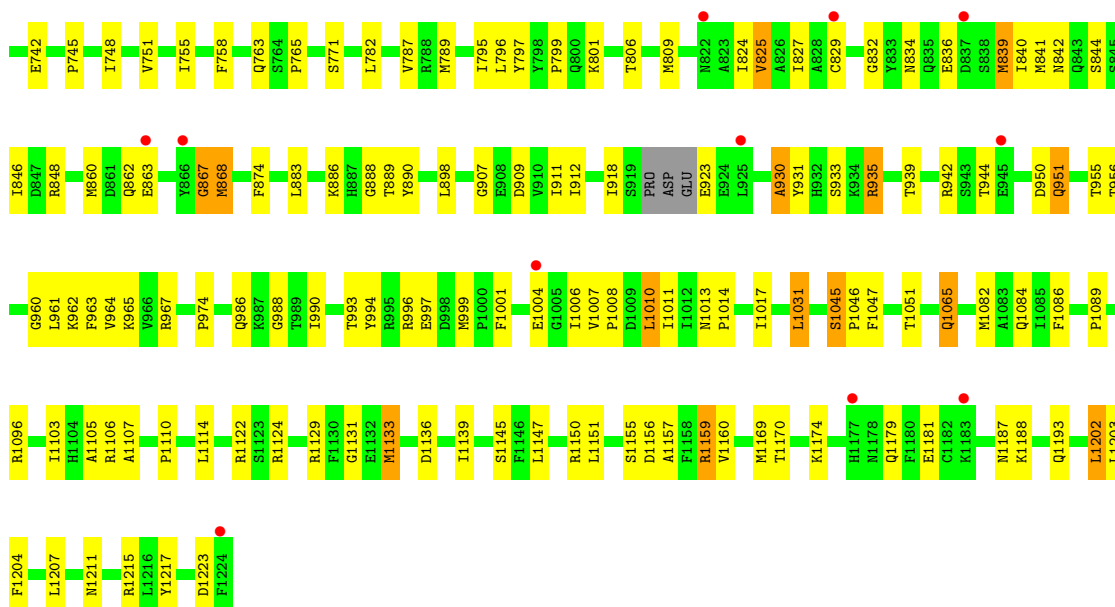
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



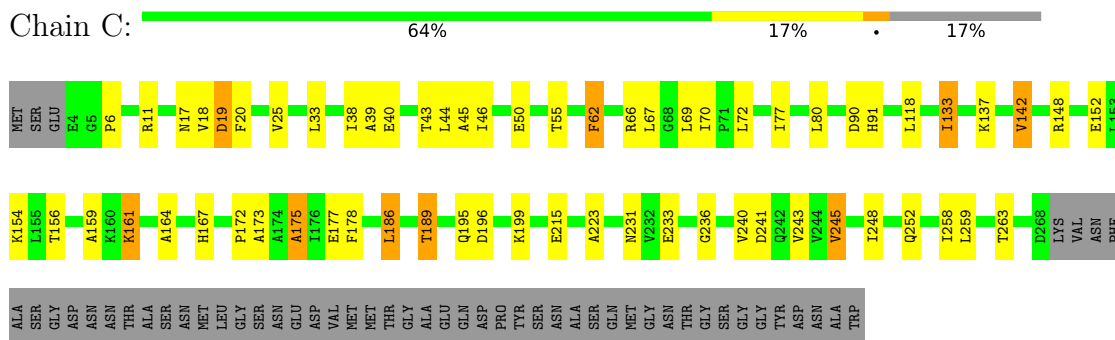


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

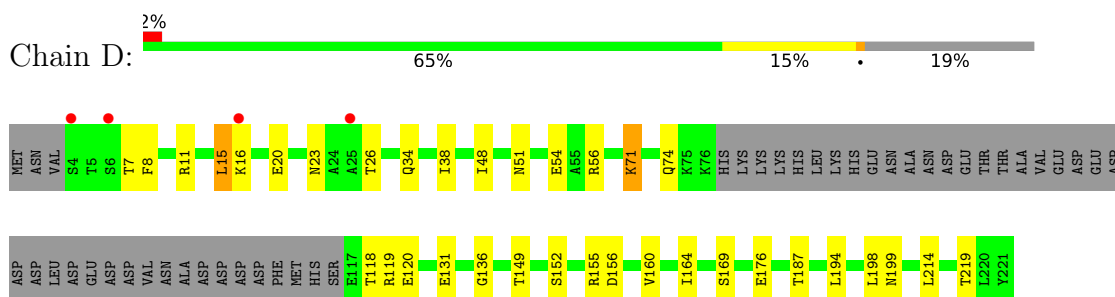




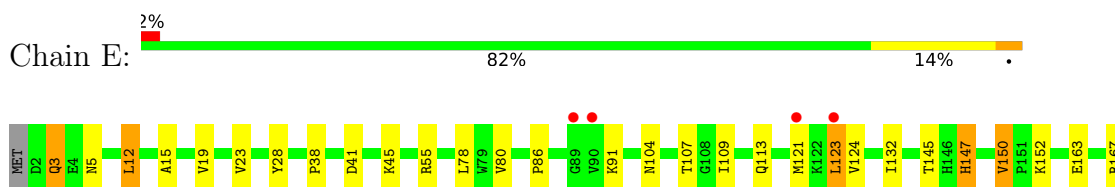
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



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



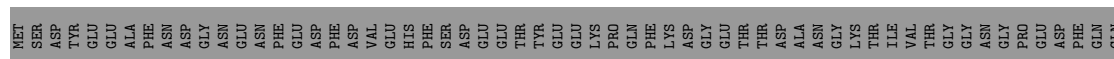
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





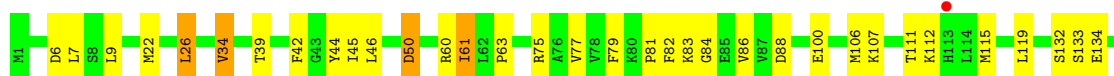
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



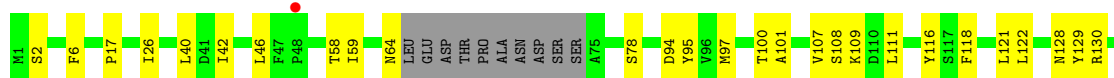
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



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

Chain H:



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

Chain I:

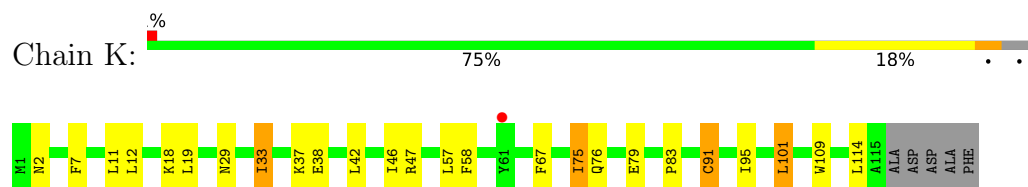


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

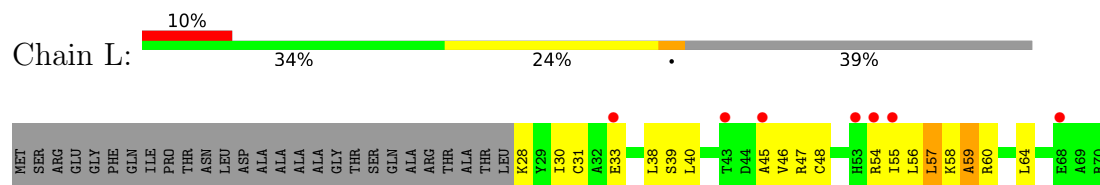
Chain J:



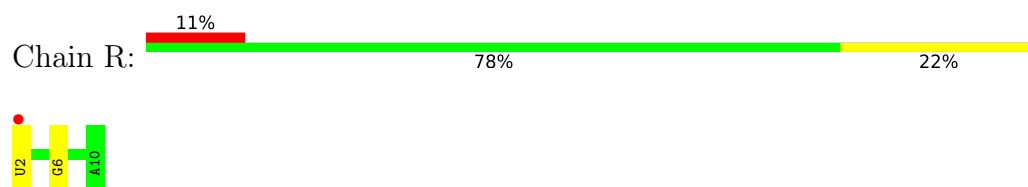
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



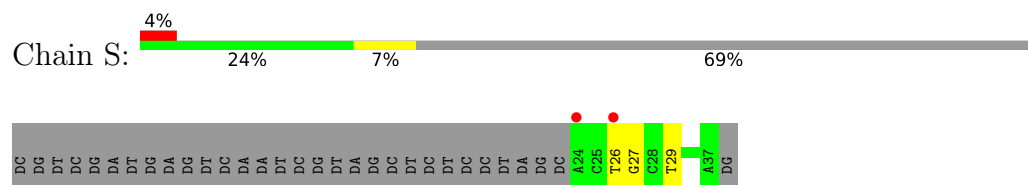
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



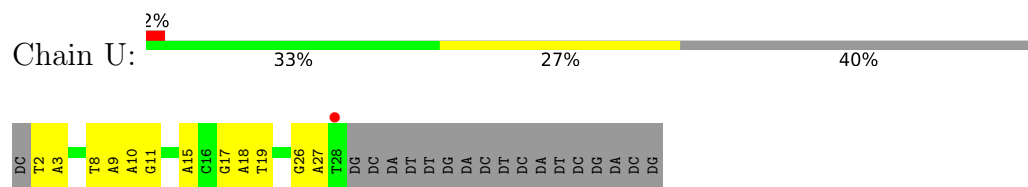
- Molecule 13: Synthetic RNA



- Molecule 14: Synthetic DNA



- Molecule 15: Synthetic DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	219.05Å 390.94Å 278.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 40.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (40.00-3.70) 96.3 (40.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.66Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.2	Depositor
R, R_{free}	0.201 , 0.220 0.233 , 0.256	Depositor DCC
R_{free} test set	3691 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 121.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.108 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.125 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32515	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, 0.333 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: MG, ZN

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	0.74	0/11427	1.37	58/15457 (0.4%)
2	B	0.72	0/9302	1.30	21/12542 (0.2%)
3	C	0.72	0/2124	1.28	3/2879 (0.1%)
4	D	0.70	0/1427	1.39	7/1911 (0.4%)
5	E	0.71	0/1788	1.26	4/2406 (0.2%)
6	F	0.72	0/717	1.29	0/967
7	G	0.73	0/1367	1.23	3/1844 (0.2%)
8	H	0.71	0/1097	1.10	2/1484 (0.1%)
9	I	0.72	0/945	1.25	2/1273 (0.2%)
10	J	0.71	0/549	1.40	2/738 (0.3%)
11	K	0.69	0/942	1.31	2/1272 (0.2%)
12	L	0.75	0/346	1.21	0/457
13	R	0.63	0/221	0.65	0/343
14	S	0.46	0/319	0.61	0/490
15	U	0.55	1/616 (0.2%)	0.62	0/947
All	All	0.72	1/33187 (0.0%)	1.30	104/45010 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	15	DA	O3'-P	-5.35	1.53	1.61

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	123	LEU	CA-C-N	7.45	126.29	120.33
5	E	123	LEU	C-N-CA	7.45	126.29	120.33
2	B	136	THR	CA-C-N	7.36	134.95	121.70
2	B	136	THR	C-N-CA	7.36	134.95	121.70
2	B	436	VAL	N-CA-C	-7.36	105.38	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	506	ALA	CA-C-N	7.23	127.38	120.43
1	A	506	ALA	C-N-CA	7.23	127.38	120.43
2	B	145	ARG	CA-C-N	7.14	134.54	121.70
2	B	145	ARG	C-N-CA	7.14	134.54	121.70
1	A	1098	VAL	N-CA-CB	6.95	114.88	110.50
1	A	831	THR	N-CA-C	-6.87	105.52	114.04
5	E	147	HIS	CA-C-N	6.49	129.27	120.38
5	E	147	HIS	C-N-CA	6.49	129.27	120.38
1	A	219	PHE	CA-CB-CG	6.48	120.28	113.80
1	A	517	ASN	CA-CB-CG	6.42	119.02	112.60
1	A	91	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	1107	VAL	CA-C-N	6.28	133.00	121.70
1	A	1107	VAL	C-N-CA	6.28	133.00	121.70
7	G	88	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	846	GLU	CA-C-N	6.16	129.37	120.38
1	A	846	GLU	C-N-CA	6.16	129.37	120.38
1	A	859	SER	CA-C-N	6.03	128.69	120.54
1	A	859	SER	C-N-CA	6.03	128.69	120.54
4	D	26	THR	N-CA-C	-5.89	106.00	112.72
1	A	244	PRO	N-CA-C	5.82	117.81	110.70
1	A	370	ILE	N-CA-C	-5.81	106.56	111.56
1	A	597	LEU	CA-C-N	5.76	130.36	121.83
1	A	597	LEU	C-N-CA	5.76	130.36	121.83
1	A	37	PHE	CA-CB-CG	5.72	119.52	113.80
2	B	930	ALA	CA-C-N	5.65	131.86	121.70
2	B	930	ALA	C-N-CA	5.65	131.86	121.70
1	A	871	ASP	CA-CB-CG	5.62	118.22	112.60
3	C	172	PRO	CA-C-N	5.61	130.10	121.19
3	C	172	PRO	C-N-CA	5.61	130.10	121.19
3	C	62	PHE	N-CA-C	-5.59	105.10	111.14
1	A	237	THR	N-CA-C	-5.57	107.03	113.88
1	A	1091	SER	CA-C-N	5.55	132.13	121.54
1	A	1091	SER	C-N-CA	5.55	132.13	121.54
1	A	930	ASP	N-CA-C	-5.53	104.89	111.69
11	K	101	LEU	CA-C-N	5.51	127.60	120.44
11	K	101	LEU	C-N-CA	5.51	127.60	120.44
9	I	66	PRO	CA-C-N	5.50	128.42	120.38
9	I	66	PRO	C-N-CA	5.50	128.42	120.38
1	A	1385	THR	CA-C-N	5.49	128.19	120.28
1	A	1385	THR	C-N-CA	5.49	128.19	120.28
2	B	638	PHE	CA-CB-CG	5.49	119.29	113.80
2	B	307	ASP	CA-C-N	5.48	128.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	ASP	C-N-CA	5.48	128.17	120.28
1	A	548	ASN	CA-C-N	5.47	127.55	120.44
1	A	548	ASN	C-N-CA	5.47	127.55	120.44
1	A	29	ALA	CA-C-N	5.44	127.92	120.46
1	A	29	ALA	C-N-CA	5.44	127.92	120.46
1	A	219	PHE	CA-C-N	5.44	128.11	120.28
1	A	219	PHE	C-N-CA	5.44	128.11	120.28
2	B	867	GLY	CA-C-N	5.39	131.41	121.70
2	B	867	GLY	C-N-CA	5.39	131.41	121.70
7	G	50	ASP	CA-CB-CG	5.39	118.00	112.60
1	A	1331	SER	CA-C-N	5.38	129.21	120.60
1	A	1331	SER	C-N-CA	5.38	129.21	120.60
2	B	1065	GLN	CA-C-N	5.35	128.19	120.38
2	B	1065	GLN	C-N-CA	5.35	128.19	120.38
1	A	481	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	1186	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	511	PRO	CA-C-N	5.33	127.68	120.38
2	B	511	PRO	C-N-CA	5.33	127.68	120.38
8	H	128	ASN	CA-C-N	5.32	131.70	121.54
8	H	128	ASN	C-N-CA	5.32	131.70	121.54
2	B	540	SER	CA-C-N	5.30	127.65	120.38
2	B	540	SER	C-N-CA	5.30	127.65	120.38
1	A	1394	THR	CA-C-N	5.30	125.01	119.92
1	A	1394	THR	C-N-CA	5.30	125.01	119.92
1	A	475	THR	CA-C-N	5.29	127.35	120.26
1	A	475	THR	C-N-CA	5.29	127.35	120.26
4	D	156	ASP	CA-C-N	5.27	128.72	120.82
4	D	156	ASP	C-N-CA	5.27	128.72	120.82
1	A	864	ILE	N-CA-C	-5.23	106.70	111.67
7	G	61	ILE	N-CA-CB	5.21	116.78	110.95
10	J	31	ASP	CA-C-N	5.18	127.48	120.38
10	J	31	ASP	C-N-CA	5.18	127.48	120.38
2	B	147	LEU	CA-C-N	5.18	131.44	121.54
2	B	147	LEU	C-N-CA	5.18	131.44	121.54
1	A	206	GLU	CA-C-N	5.15	127.25	120.60
1	A	206	GLU	C-N-CA	5.15	127.25	120.60
1	A	1343	ALA	CA-C-N	5.14	125.68	119.98
1	A	1343	ALA	C-N-CA	5.14	125.68	119.98
1	A	346	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	155	GLU	CA-C-N	5.12	131.31	121.54
1	A	155	GLU	C-N-CA	5.12	131.31	121.54
2	B	500	THR	CB-CA-C	5.12	115.77	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	LYS	CA-C-N	5.09	127.36	120.38
1	A	575	LYS	C-N-CA	5.09	127.36	120.38
1	A	454	SER	CA-C-N	5.08	131.24	121.54
1	A	454	SER	C-N-CA	5.08	131.24	121.54
4	D	176	GLU	CA-C-N	5.08	126.96	120.56
4	D	176	GLU	C-N-CA	5.08	126.96	120.56
1	A	145	LYS	CA-C-N	5.08	131.24	121.54
1	A	145	LYS	C-N-CA	5.08	131.24	121.54
1	A	628	GLY	CA-C-N	5.06	131.21	121.54
1	A	628	GLY	C-N-CA	5.06	131.21	121.54
1	A	1079	MET	CA-C-N	5.05	127.00	120.44
1	A	1079	MET	C-N-CA	5.05	127.00	120.44
1	A	641	VAL	N-CA-C	-5.04	105.62	110.72
4	D	136	GLY	CA-C-N	5.03	127.03	120.28
4	D	136	GLY	C-N-CA	5.03	127.03	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11227	0	11270	172	0
2	B	9130	0	9099	152	0
3	C	2086	0	2045	34	0
4	D	1417	0	1428	7	0
5	E	1752	0	1776	21	0
6	F	705	0	731	12	0
7	G	1339	0	1357	17	0
8	H	1080	0	1049	14	0
9	I	927	0	883	11	0
10	J	540	0	554	16	0
11	K	924	0	934	17	0
12	L	344	0	365	7	0
13	R	197	0	96	1	0
14	S	286	0	160	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	U	550	0	304	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	32515	0	32051	421	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 7.

All (421) 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)
10:J:36:LEU:HD21	10:J:50:ILE:HD11	1.38	1.03
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.49	0.91
1:A:1107:VAL:HA	1:A:1108:ALA:HB2	1.54	0.88
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.61	0.83
2:B:145:ARG:HA	2:B:146:GLU:HB2	1.62	0.81
2:B:136:THR:HA	2:B:137:TYR:HB2	1.63	0.79
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.67	0.77
1:A:374:LEU:HB2	1:A:436:ILE:HD11	1.68	0.75
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.69	0.75
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.67	0.75
2:B:1181:GLU:HB3	2:B:1188:LYS:HG3	1.68	0.74
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.53	0.74
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.53	0.73
1:A:394:ASN:HB3	1:A:398:GLU:HB3	1.71	0.72
1:A:855:THR:HG21	1:A:857:ARG:HE	1.54	0.72
15:U:10:DA:H2''	15:U:11:DG:O5'	1.90	0.72
2:B:145:ARG:HA	2:B:146:GLU:CB	2.21	0.71
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.56	0.70
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.74	0.70
10:J:36:LEU:CD2	10:J:50:ILE:HD11	2.18	0.70
1:A:1107:VAL:HA	1:A:1108:ALA:CB	2.22	0.70
1:A:528:LEU:HD12	1:A:751:SER:H	1.58	0.69
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.76	0.68
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.77	0.67
1:A:1083:THR:HG21	1:A:1095:THR:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:51:ASN:OD1	4:D:54:GLU:HB2	1.96	0.66
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.31	0.66
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.78	0.66
1:A:225:ASN:HB3	1:A:229:SER:H	1.62	0.65
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.77	0.65
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.79	0.65
2:B:559:SER:HA	2:B:563:MET:HB2	1.78	0.63
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.79	0.63
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.63	0.63
2:B:364:ILE:HG22	2:B:585:VAL:HG13	1.81	0.63
15:U:26:DG:H2''	15:U:27:DA:O5'	1.98	0.63
1:A:356:ASP:HB2	1:A:469:ARG:HD2	1.81	0.63
1:A:49:LYS:HD2	1:A:61:ILE:HG12	1.81	0.62
1:A:444:PHE:HE2	1:A:487:MET:SD	2.22	0.62
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.29	0.62
2:B:839:MET:HE3	2:B:1010:LEU:HD13	1.80	0.62
12:L:57:LEU:HD23	12:L:59:ALA:H	1.63	0.62
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	1.80	0.62
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.81	0.61
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.81	0.61
5:E:80:VAL:HG12	5:E:109:ILE:HB	1.82	0.61
2:B:468:GLU:HB3	2:B:470:LYS:HG2	1.82	0.61
2:B:1006:ILE:HD11	10:J:43:ARG:HB3	1.81	0.61
2:B:930:ALA:HA	2:B:931:TYR:C	2.26	0.61
3:C:55:THR:HB	3:C:152:GLU:H	1.65	0.60
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.83	0.60
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.84	0.60
2:B:364:ILE:HG13	2:B:365:THR:H	1.66	0.60
1:A:1116:LEU:HG	1:A:1308:THR:CG2	2.32	0.60
1:A:496:GLU:HB2	6:F:99:LEU:HD12	1.84	0.60
2:B:136:THR:HA	2:B:137:TYR:CB	2.32	0.60
2:B:292:ILE:HD11	2:B:327:ARG:HB2	1.83	0.60
2:B:485:ARG:HH21	2:B:782:LEU:HD11	1.67	0.60
14:S:29:DT:H3	15:U:10:DA:H61	1.50	0.59
1:A:370:ILE:HD13	2:B:1105:ALA:HB2	1.84	0.59
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.83	0.59
2:B:825:VAL:HG23	2:B:1010:LEU:HD12	1.85	0.59
2:B:290:GLY:HA2	2:B:327:ARG:HG3	1.83	0.59
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.84	0.59
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.85	0.59
2:B:956:THR:HG22	2:B:960:GLY:HA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:VAL:CA	1:A:1108:ALA:HB2	2.31	0.58
2:B:363:HIS:HD2	2:B:364:ILE:HG23	1.67	0.58
2:B:367:LEU:HB2	2:B:370:PHE:HE2	1.68	0.58
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.68	0.58
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.85	0.58
3:C:6:PRO:HG2	11:K:101:LEU:HB2	1.85	0.58
2:B:193:LYS:HE3	10:J:64:ASN:HB2	1.85	0.58
1:A:1453:TYR:HB3	6:F:129:LYS:HE2	1.85	0.58
1:A:847:ASP:HB2	1:A:859:SER:H	1.69	0.58
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.86	0.58
1:A:182:VAL:HG12	1:A:201:VAL:HA	1.86	0.58
1:A:1100:ARG:HG3	1:A:1104:ILE:HD11	1.86	0.58
1:A:246:VAL:HA	2:B:1202:LEU:HD21	1.84	0.57
1:A:810:PRO:HB3	2:B:745:PRO:HB3	1.86	0.57
2:B:101:MET:HG2	2:B:111:ALA:HA	1.85	0.57
1:A:834:THR:HG21	1:A:1077:THR:HA	1.86	0.57
2:B:842:ASN:O	2:B:846:ILE:HG12	2.04	0.57
2:B:918:ILE:HB	2:B:935:ARG:HH12	1.69	0.57
1:A:374:LEU:HA	2:B:1107:ALA:HB2	1.87	0.57
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.87	0.57
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.87	0.56
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.40	0.56
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.86	0.56
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.41	0.56
1:A:835:GLY:HA3	15:U:18:DA:H4'	1.88	0.56
1:A:1205:LYS:HB3	1:A:1274:ARG:HH21	1.70	0.56
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.87	0.56
1:A:560:ILE:HD12	8:H:78:SER:HB2	1.88	0.56
1:A:121:LEU:HD22	1:A:141:LEU:HD11	1.87	0.56
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.88	0.56
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.36	0.55
1:A:1215:ARG:HE	1:A:1273:LEU:HA	1.71	0.55
3:C:186:LEU:HD23	3:C:223:ALA:HB1	1.89	0.55
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.88	0.55
8:H:6:PHE:HB3	8:H:59:ILE:HD12	1.89	0.55
1:A:596:THR:C	1:A:598:LEU:H	2.13	0.55
1:A:899:VAL:HB	1:A:1029:ARG:HG3	1.88	0.55
2:B:1133:MET:HG3	15:U:19:DT:H4'	1.88	0.55
1:A:746:MET:HE1	2:B:1014:PRO:HB2	1.88	0.55
7:G:112:LYS:HA	7:G:115:MET:HE3	1.89	0.55
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HG13	2:B:365:THR:N	2.21	0.55
2:B:955:THR:HG22	2:B:956:THR:H	1.72	0.55
3:C:50:GLU:HB2	3:C:156:THR:HB	1.89	0.55
1:A:568:PRO:HD2	1:A:569:LYS:H	1.72	0.54
1:A:662:PHE:HB3	2:B:829:CYS:SG	2.47	0.54
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.54
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.87	0.54
3:C:77:ILE:HG13	3:C:161:LYS:HE3	1.89	0.54
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.73	0.54
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.89	0.54
2:B:225:VAL:H	2:B:396:ASP:HB2	1.73	0.54
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.88	0.54
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.90	0.54
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.89	0.54
2:B:860:MET:HB3	2:B:965:LYS:HG2	1.89	0.54
2:B:1106:ARG:HE	2:B:1110:PRO:HD2	1.73	0.54
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.89	0.54
8:H:58:THR:HB	8:H:143:LEU:HB2	1.90	0.54
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.89	0.53
1:A:311:GLN:HB2	1:A:312:PRO:HD3	1.91	0.53
1:A:444:PHE:CE2	1:A:487:MET:SD	3.01	0.53
1:A:899:VAL:HG11	1:A:929:LEU:HD22	1.90	0.53
2:B:654:ARG:H	2:B:657:HIS:HD2	1.57	0.53
10:J:36:LEU:HD21	10:J:50:ILE:CD1	2.25	0.53
3:C:252:GLN:HB2	11:K:95:ILE:HG23	1.91	0.53
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.53
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.91	0.52
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.91	0.52
2:B:429:PHE:HA	2:B:432:MET:HB2	1.90	0.52
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.92	0.52
1:A:541:ILE:HD13	1:A:577:ILE:HD11	1.91	0.52
1:A:1110:ASN:HB2	14:S:26:DT:OP1	2.08	0.52
1:A:1114:PRO:HB2	1:A:1311:VAL:HB	1.92	0.52
2:B:996:ARG:HH21	3:C:173:ALA:HB1	1.75	0.52
7:G:83:LYS:HE2	7:G:150:CYS:H	1.74	0.52
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.91	0.52
1:A:1332:PHE:HA	1:A:1335:ILE:HD12	1.92	0.52
2:B:144:GLY:HA2	2:B:146:GLU:HB2	1.92	0.52
1:A:567:LYS:HE2	1:A:568:PRO:HD3	1.92	0.52
1:A:567:LYS:HG2	1:A:568:PRO:HD3	1.91	0.52
1:A:1313:LEU:HD23	1:A:1338:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.91	0.52
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.92	0.52
1:A:1006:ILE:HD12	5:E:167:ARG:HB2	1.92	0.51
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.93	0.51
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.92	0.51
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.76	0.51
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.39	0.51
1:A:365:GLY:HA3	1:A:469:ARG:HB3	1.93	0.51
15:U:2:DT:H2''	15:U:3:DA:N7	2.26	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.75	0.51
1:A:382:PRO:HD3	1:A:428:TYR:HE2	1.75	0.51
1:A:832:ALA:HA	15:U:18:DA:H5'	1.91	0.51
5:E:78:LEU:HB3	5:E:107:THR:HB	1.93	0.51
2:B:283:VAL:HG23	2:B:297:ILE:HG21	1.93	0.50
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.93	0.50
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.92	0.50
2:B:210:LYS:HE2	2:B:482:VAL:HG22	1.94	0.50
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.93	0.50
1:A:106:VAL:HG11	1:A:214:ILE:HG12	1.94	0.50
1:A:368:LYS:HB2	11:K:2:ASN:HD21	1.76	0.50
1:A:1280:GLU:HB3	1:A:1309:ASP:HB3	1.93	0.50
2:B:245:GLU:N	2:B:246:LYS:HA	2.26	0.50
4:D:71:LYS:HD3	4:D:74:GLN:HG3	1.94	0.50
1:A:332:LYS:H	1:A:337:ARG:HD3	1.76	0.50
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.93	0.50
5:E:12:LEU:HD11	5:E:55:ARG:HH21	1.76	0.50
2:B:129:PHE:HB3	2:B:164:LYS:HB3	1.93	0.50
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.93	0.50
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.93	0.50
3:C:259:LEU:HD12	11:K:91:CYS:HB3	1.93	0.50
4:D:23:ASN:HB3	7:G:82:PHE:HD1	1.76	0.50
6:F:128:LYS:HD3	6:F:149:GLU:HA	1.94	0.50
2:B:526:GLU:HG3	2:B:771:SER:HB2	1.93	0.50
6:F:109:VAL:HG22	6:F:124:GLU:HG2	1.93	0.50
6:F:130:ILE:HG22	6:F:132:LEU:HB2	1.94	0.50
1:A:381:THR:O	1:A:385:ILE:HG13	2.10	0.49
2:B:195:CYS:O	2:B:198:ASP:HB2	2.12	0.49
2:B:408:LEU:HD13	2:B:545:ILE:HG21	1.93	0.49
2:B:499:ASN:HA	2:B:536:VAL:HG22	1.93	0.49
3:C:46:ILE:HA	3:C:159:ALA:HA	1.94	0.49
4:D:155:ARG:H	4:D:219:THR:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:951:GLN:HG2	12:L:57:LEU:HD11	1.95	0.49
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.92	0.49
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.47	0.49
1:A:317:LYS:HA	1:A:318:SER:C	2.37	0.49
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.94	0.49
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.94	0.49
3:C:50:GLU:HB3	12:L:64:LEU:HD21	1.93	0.49
2:B:565:PRO:HG2	2:B:568:ASP:HB2	1.94	0.49
11:K:75:ILE:HD13	11:K:83:PRO:HB2	1.94	0.49
1:A:512:VAL:HA	1:A:519:PRO:HA	1.95	0.49
2:B:806:THR:HG23	2:B:1045:SER:HA	1.95	0.49
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.95	0.49
2:B:883:LEU:H	2:B:935:ARG:H	1.61	0.49
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.94	0.49
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.95	0.49
1:A:984:LYS:O	1:A:988:LEU:HB2	2.13	0.49
2:B:485:ARG:HE	2:B:782:LEU:HD11	1.77	0.49
2:B:841:MET:SD	2:B:846:ILE:HD11	2.53	0.48
2:B:496:ARG:HB2	2:B:539:LEU:HB2	1.94	0.48
2:B:789:MET:HE1	2:B:967:ARG:HB2	1.95	0.48
1:A:1336:MET:HG3	1:A:1381:LEU:HD13	1.95	0.48
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.94	0.48
7:G:6:ASP:HA	7:G:75:ARG:HA	1.95	0.48
1:A:105:CYS:SG	1:A:139:TRP:HA	2.54	0.48
1:A:329:LEU:HA	1:A:335:ARG:HB3	1.93	0.48
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.96	0.48
1:A:822:GLU:HB2	2:B:513:GLN:HE22	1.78	0.48
2:B:806:THR:H	2:B:809:MET:HE3	1.79	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.79	0.48
3:C:258:ILE:HG13	11:K:19:LEU:HD11	1.95	0.48
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.96	0.48
10:J:5:VAL:HA	10:J:14:VAL:O	2.13	0.48
7:G:46:LEU:HB2	7:G:77:VAL:HG23	1.94	0.48
7:G:39:THR:HG23	7:G:42:PHE:H	1.79	0.48
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.77	0.48
1:A:446:ARG:HB2	1:A:487:MET:SD	2.54	0.47
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.95	0.47
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.47
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.78	0.47
2:B:1004:GLU:HG3	2:B:1006:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PRO:HD3	1:A:645:LEU:HD13	1.96	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.80	0.47
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.96	0.47
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.97	0.47
6:F:146:TRP:HB3	6:F:151:LEU:HD11	1.96	0.47
15:U:18:DA:H2'	15:U:19:DT:C6	2.49	0.47
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.96	0.47
1:A:855:THR:CG2	1:A:857:ARG:HE	2.25	0.47
1:A:836:TYR:HB2	15:U:17:DG:H4'	1.97	0.47
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.96	0.47
1:A:1420:ASP:HB2	1:A:1422:ARG:HG2	1.97	0.47
3:C:43:THR:HG22	3:C:44:LEU:H	1.80	0.47
1:A:1290:LYS:HG2	1:A:1298:TYR:HB3	1.96	0.47
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.97	0.47
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.96	0.47
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.97	0.47
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.97	0.47
1:A:899:VAL:HG13	1:A:929:LEU:HB3	1.96	0.47
1:A:1386:ARG:HD3	1:A:1403:GLU:HG2	1.96	0.47
2:B:308:TRP:H	2:B:308:TRP:CD1	2.33	0.47
1:A:720:ARG:O	1:A:724:GLU:HB2	2.14	0.46
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.97	0.46
1:A:827:THR:O	1:A:831:THR:HB	2.16	0.46
1:A:360:GLU:HB3	1:A:363:GLN:HB2	1.96	0.46
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.97	0.46
10:J:1:MET:H1	10:J:57:ILE:H	1.62	0.46
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.97	0.46
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.95	0.46
3:C:11:ARG:HB2	3:C:19:ASP:HB3	1.97	0.46
1:A:847:ASP:HB2	1:A:859:SER:N	2.29	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.97	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.30	0.46
1:A:567:LYS:HG3	8:H:94:ASP:O	2.16	0.46
11:K:33:ILE:HD11	11:K:75:ILE:HD11	1.97	0.46
1:A:88:LYS:HD3	1:A:293:GLU:HG3	1.97	0.46
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.31	0.46
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.97	0.46
1:A:1383:SER:HB2	1:A:1388:GLY:HA3	1.97	0.46
2:B:136:THR:CA	2:B:137:TYR:HB2	2.39	0.46
2:B:1179:GLN:HA	2:B:1188:LYS:HE3	1.97	0.46
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:O	10:J:6:ARG:HD2	2.16	0.46
1:A:90:VAL:HA	1:A:204:THR:HG21	1.96	0.45
1:A:114:LEU:HD21	1:A:145:LYS:O	2.15	0.45
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.97	0.45
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.98	0.45
7:G:100:GLU:HB3	7:G:107:LYS:HG2	1.98	0.45
11:K:18:LYS:HE2	11:K:38:GLU:HG2	1.99	0.45
2:B:125:SER:HA	2:B:171:PRO:HA	1.99	0.45
2:B:640:VAL:HA	2:B:651:LEU:HA	1.97	0.45
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.65	0.45
2:B:64:CYS:HA	2:B:67:SER:HB2	1.98	0.45
2:B:848:ARG:HD3	10:J:7:CYS:O	2.17	0.45
4:D:56:ARG:HD2	4:D:149:THR:HA	1.97	0.45
2:B:246:LYS:HE3	2:B:249:ARG:HA	1.99	0.45
2:B:319:GLU:HA	2:B:322:PHE:HB2	1.98	0.45
3:C:67:LEU:HA	3:C:70:ILE:HG12	1.99	0.45
1:A:530:GLY:HA2	1:A:657:LEU:HD13	1.99	0.45
1:A:579:SER:HB3	1:A:611:GLN:HA	1.98	0.45
2:B:85:SER:HB3	2:B:139:ALA:HB3	1.97	0.45
2:B:276:ILE:HG22	2:B:278:GLN:H	1.82	0.45
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.52	0.45
2:B:888:GLY:O	2:B:909:ASP:HA	2.16	0.45
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.98	0.45
15:U:8:DT:H2"	15:U:9:DA:H8	1.82	0.45
1:A:1079:MET:HE1	1:A:1355:VAL:HG12	1.99	0.45
1:A:466:SER:HB2	2:B:1103:ILE:HD13	1.98	0.45
8:H:100:THR:HG23	8:H:138:GLU:HB3	1.99	0.45
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.52	0.45
1:A:134:ARG:O	1:A:138:ILE:HG12	2.17	0.44
2:B:827:ILE:HD13	2:B:1086:PHE:HD2	1.82	0.44
2:B:1204:PHE:HA	2:B:1207:LEU:HD12	1.99	0.44
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.99	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HB3	1.99	0.44
7:G:84:GLY:HA2	7:G:146:LYS:HE2	1.98	0.44
1:A:1022:LEU:HG	1:A:1026:LEU:HD12	2.00	0.44
2:B:886:LYS:O	2:B:890:TYR:HE1	2.00	0.44
1:A:93:VAL:HG11	1:A:305:ASP:HB3	1.99	0.44
1:A:467:THR:HG23	1:A:469:ARG:HH12	1.82	0.44
1:A:536:LEU:HD13	1:A:538:ASP:HB3	2.00	0.44
2:B:846:ILE:HD12	2:B:974:PRO:HG2	1.99	0.44
1:A:335:ARG:HH22	2:B:1114:LEU:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HG2	9:I:97:MET:HE2	2.00	0.44
2:B:44:VAL:HG11	2:B:200:GLY:HA2	2.00	0.44
1:A:669:THR:HG23	1:A:805:LEU:HD13	1.99	0.44
1:A:998:LEU:HD23	1:A:1001:ARG:HD3	1.99	0.44
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.99	0.44
1:A:817:ALA:HB1	2:B:524:PRO:HB2	1.99	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.99	0.44
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.99	0.44
1:A:1116:LEU:HG	1:A:1308:THR:HG22	1.99	0.44
2:B:193:LYS:HB3	2:B:787:VAL:HG11	2.00	0.44
2:B:758:PHE:HZ	2:B:1031:LEU:HD13	1.83	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	1.99	0.44
5:E:178:ILE:HB	5:E:212:ARG:HB3	2.00	0.44
1:A:43:GLU:H	1:A:46:THR:H	1.66	0.44
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.00	0.44
3:C:164:ALA:HA	3:C:167:HIS:O	2.18	0.44
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.99	0.43
2:B:755:ILE:HA	2:B:809:MET:HE2	2.00	0.43
2:B:92:PHE:HD1	2:B:132:VAL:HG22	1.83	0.43
2:B:867:GLY:HA3	2:B:868:MET:HB3	2.00	0.43
2:B:238:ALA:HB2	2:B:385:LEU:HB2	2.00	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HG23	2.00	0.43
1:A:406:ILE:HB	1:A:431:LYS:HB2	2.00	0.43
9:I:50:THR:HB	9:I:52:ILE:HG13	2.00	0.43
12:L:28:LYS:HB2	12:L:39:SER:HA	2.00	0.43
1:A:1377:THR:HB	5:E:176:PRO:HB3	2.00	0.43
1:A:1107:VAL:CA	1:A:1108:ALA:CB	2.95	0.43
2:B:593:PRO:HG2	2:B:617:ARG:HH21	1.83	0.43
3:C:62:PHE:O	3:C:66:ARG:HG3	2.19	0.43
11:K:42:LEU:HD23	11:K:46:ILE:HD11	2.01	0.43
2:B:31:TRP:HA	2:B:34:ILE:HD12	2.00	0.43
2:B:301:ILE:HD13	2:B:379:GLY:HA2	2.00	0.43
2:B:528:PRO:HD2	2:B:536:VAL:O	2.18	0.43
1:A:349:ALA:HB2	1:A:374:LEU:HD11	2.01	0.43
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.01	0.43
1:A:90:VAL:HG21	1:A:300:VAL:HG11	2.00	0.42
10:J:14:VAL:HA	10:J:17:LYS:HD3	2.00	0.42
1:A:606:LEU:HD23	1:A:613:ILE:HG21	2.02	0.42
2:B:600:LEU:HA	2:B:603:LEU:HD12	2.01	0.42
6:F:117:PRO:HA	6:F:120:ILE:HD12	2.01	0.42
9:I:52:ILE:HG13	9:I:52:ILE:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.91	0.42
2:B:392:ARG:HE	9:I:52:ILE:HD13	1.84	0.42
3:C:177:GLU:HB2	3:C:231:ASN:H	1.83	0.42
1:A:588:LEU:HD22	1:A:607:ILE:HD12	2.00	0.42
1:A:709:THR:HG21	9:I:93:LYS:O	2.19	0.42
2:B:883:LEU:HG	2:B:931:TYR:HB3	2.00	0.42
1:A:472:LEU:O	1:A:475:THR:HB	2.19	0.42
1:A:872:GLY:C	1:A:1058:VAL:HG23	2.44	0.42
4:D:56:ARG:HD3	4:D:152:SER:HB2	2.02	0.42
15:U:8:DT:H2''	15:U:9:DA:C8	2.55	0.42
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.85	0.42
2:B:1129:ARG:HE	2:B:1131:GLY:HA2	1.83	0.42
14:S:26:DT:H2''	14:S:27:DG:OP2	2.20	0.42
1:A:513:SER:HB2	1:A:520:CYS:HB3	2.02	0.42
1:A:981:LEU:HD11	1:A:1042:PHE:HB2	2.01	0.42
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.84	0.41
8:H:2:SER:HB2	8:H:64:ASN:HB2	2.02	0.41
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.02	0.41
2:B:394:ASP:HB3	9:I:91:ARG:HD3	2.03	0.41
2:B:801:LYS:HE3	10:J:52:THR:HA	2.02	0.41
2:B:867:GLY:HA3	2:B:868:MET:CB	2.50	0.41
5:E:12:LEU:HD21	5:E:55:ARG:HE	1.85	0.41
1:A:353:ILE:CG2	1:A:487:MET:HB2	2.50	0.41
1:A:709:THR:HG22	1:A:710:LEU:N	2.35	0.41
1:A:1078:GLN:H	1:A:1078:GLN:HG2	1.74	0.41
11:K:29:ASN:HD21	11:K:79:GLU:HA	1.85	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD3	1.99	0.41
2:B:863:GLU:HB2	2:B:962:LYS:HB2	2.02	0.41
7:G:22:MET:HG2	7:G:26:LEU:HD12	2.03	0.41
10:J:20:SER:HB2	10:J:39:LEU:HD21	2.01	0.41
5:E:3:GLN:HG3	5:E:5:ASN:H	1.85	0.41
2:B:438:GLU:HG2	2:B:439:ALA:HA	2.02	0.41
2:B:526:GLU:HB3	2:B:538:ASN:HB2	2.03	0.41
3:C:69:LEU:HD23	10:J:6:ARG:HD3	2.03	0.41
3:C:148:ARG:HH12	10:J:64:ASN:HA	1.85	0.41
10:J:39:LEU:HB3	10:J:41:LEU:HD23	2.02	0.41
1:A:335:ARG:HH12	2:B:1202:LEU:HD13	1.86	0.41
1:A:1111:MET:HG3	1:A:1112:LYS:H	1.85	0.41
2:B:477:ALA:HB3	13:R:6:G:H5'	2.03	0.41
2:B:950:ASP:O	2:B:967:ARG:HB3	2.21	0.41
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:THR:HG22	5:E:184:VAL:HG12	2.02	0.41
9:I:70:ARG:HG2	9:I:84:VAL:HG23	2.01	0.41
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.41
2:B:59:LEU:O	2:B:63:ILE:HG12	2.21	0.41
6:F:86:THR:HG22	6:F:89:GLU:CD	2.46	0.41
7:G:81:PRO:HG3	7:G:106:MET:SD	2.61	0.41
8:H:101:ALA:HA	8:H:116:TYR:HA	2.03	0.40
12:L:31:CYS:HA	12:L:56:LEU:HA	2.02	0.40
1:A:525:GLN:HG3	2:B:836:GLU:HG2	2.04	0.40
1:A:875:ALA:HA	1:A:878:ILE:HD13	2.02	0.40
1:A:1139:GLU:HB3	1:A:1274:ARG:HH12	1.86	0.40
1:A:1325:THR:HA	5:E:147:HIS:HA	2.04	0.40
2:B:334:ILE:HG13	2:B:335:GLY:H	1.84	0.40
2:B:912:ILE:HB	2:B:939:THR:HB	2.03	0.40
8:H:130:ARG:H	8:H:130:ARG:HG3	1.75	0.40
3:C:17:ASN:HA	3:C:233:GLU:HA	2.03	0.40
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.02	0.40
2:B:994:TYR:HB2	2:B:999:MET:HG3	2.03	0.40
2:B:1181:GLU:HA	2:B:1187:ASN:O	2.20	0.40
5:E:15:ALA:O	5:E:19:VAL:HG23	2.20	0.40
7:G:7:LEU:H	7:G:7:LEU:HD23	1.87	0.40
12:L:47:ARG:HA	12:L:54:ARG:HG2	2.02	0.40
1:A:146:MET:O	1:A:171:GLN:HB3	2.21	0.40
1:A:387:ARG:HH12	6:F:115:THR:HB	1.86	0.40
2:B:69:LEU:HD12	2:B:429:PHE:HD1	1.86	0.40
5:E:38:PRO:HD2	5:E:41:ASP:HB2	2.03	0.40
6:F:86:THR:HG23	6:F:89:GLU:H	1.87	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	1420/1733 (82%)	1220 (86%)	141 (10%)	59 (4%)	2	20
2	B	1139/1224 (93%)	973 (85%)	123 (11%)	43 (4%)	2	22
3	C	263/318 (83%)	230 (88%)	26 (10%)	7 (3%)	4	27
4	D	174/221 (79%)	154 (88%)	11 (6%)	9 (5%)	1	17
5	E	212/215 (99%)	194 (92%)	14 (7%)	4 (2%)	6	33
6	F	85/155 (55%)	76 (89%)	6 (7%)	3 (4%)	3	24
7	G	169/179 (94%)	143 (85%)	19 (11%)	7 (4%)	2	20
8	H	129/146 (88%)	105 (81%)	20 (16%)	4 (3%)	3	26
9	I	112/122 (92%)	96 (86%)	13 (12%)	3 (3%)	4	27
10	J	64/70 (91%)	57 (89%)	5 (8%)	2 (3%)	3	26
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	41/70 (59%)	31 (76%)	6 (15%)	4 (10%)	0	6
All	All	3921/4573 (86%)	3388 (86%)	388 (10%)	145 (4%)	2	22

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	67	CYS
1	A	76	GLU
1	A	158	PRO
1	A	310	GLY
1	A	385	ILE
1	A	401	GLY
1	A	567	LYS
1	A	595	THR
1	A	629	LEU
1	A	751	SER
1	A	775	ILE
1	A	1016	THR
1	A	1092	LYS
1	A	1108	ALA
2	B	58	THR
2	B	137	TYR
2	B	146	GLU
2	B	148	LYS
2	B	151	LEU
2	B	152	ILE

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Mol	Chain	Res	Type
2	B	575	PRO
2	B	907	GLY
2	B	933	SER
2	B	1156	ASP
2	B	1157	ALA
3	C	142	VAL
3	C	161	LYS
4	D	15	LEU
7	G	141	SER
7	G	153	GLN
9	I	98	VAL
9	I	106	CYS
1	A	146	MET
1	A	152	VAL
1	A	156	ASP
1	A	188	ASP
1	A	194	ALA
1	A	250	ILE
1	A	257	ARG
1	A	283	GLY
1	A	286	HIS
1	A	319	GLY
1	A	423	ASP
1	A	875	ALA
1	A	1091	SER
1	A	1437	GLY
2	B	247	GLY
2	B	252	SER
2	B	282	ILE
2	B	337	ARG
2	B	367	LEU
2	B	712	PRO
2	B	751	VAL
2	B	889	THR
2	B	1046	PRO
3	C	175	ALA
3	C	215	GLU
4	D	20	GLU
4	D	118	THR
4	D	198	LEU
6	F	71	GLU
6	F	72	LYS

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Mol	Chain	Res	Type
7	G	50	ASP
10	J	2	ILE
12	L	45	ALA
1	A	130	ASP
1	A	256	GLN
1	A	402	ALA
1	A	418	SER
1	A	452	LYS
1	A	568	PRO
1	A	593	GLU
1	A	640	GLN
1	A	779	PHE
1	A	1112	LYS
1	A	1404	GLU
2	B	249	ARG
2	B	250	PHE
2	B	265	SER
2	B	441	ASP
2	B	502	ILE
2	B	711	GLU
2	B	935	ARG
2	B	1223	ASP
3	C	40	GLU
3	C	90	ASP
5	E	3	GLN
5	E	91	LYS
5	E	104	ASN
6	F	78	GLN
7	G	63	PRO
8	H	109	LYS
12	L	59	ALA
1	A	4	GLN
1	A	54	ASN
1	A	57	ARG
1	A	63	ARG
1	A	335	ARG
1	A	453	MET
1	A	465	TYR
1	A	1003	LYS
1	A	1221	LYS
2	B	475	SER
2	B	531	GLN

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Mol	Chain	Res	Type
2	B	577	ALA
2	B	648	HIS
2	B	951	GLN
2	B	1045	SER
4	D	8	PHE
4	D	16	LYS
4	D	169	SER
4	D	199	ASN
7	G	132	SER
7	G	154	VAL
8	H	17	PRO
8	H	108	SER
9	I	11	ASN
10	J	6	ARG
1	A	424	ILE
1	A	958	VAL
1	A	1206	ASP
1	A	1403	GLU
2	B	147	LEU
2	B	161	GLU
2	B	199	MET
2	B	961	LEU
2	B	1215	ARG
4	D	119	ARG
8	H	129	TYR
12	L	60	ARG
1	A	591	PHE
1	A	628	GLY
1	A	870	GLU
2	B	1017	ILE
2	B	1169	MET
3	C	243	VAL
5	E	45	LYS
7	G	133	SER
1	A	61	ILE
1	A	1107	VAL
12	L	55	ILE
2	B	301	ILE
2	B	832	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	1245/1520 (82%)	1119 (90%)	126 (10%)	7	29
2	B	986/1061 (93%)	902 (92%)	84 (8%)	10	35
3	C	233/274 (85%)	217 (93%)	16 (7%)	14	41
4	D	156/200 (78%)	143 (92%)	13 (8%)	10	35
5	E	196/197 (100%)	189 (96%)	7 (4%)	31	54
6	F	77/137 (56%)	75 (97%)	2 (3%)	40	60
7	G	152/160 (95%)	143 (94%)	9 (6%)	18	44
8	H	118/128 (92%)	114 (97%)	4 (3%)	32	55
9	I	108/116 (93%)	100 (93%)	8 (7%)	13	39
10	J	61/65 (94%)	53 (87%)	8 (13%)	4	20
11	K	99/102 (97%)	94 (95%)	5 (5%)	21	47
12	L	38/57 (67%)	32 (84%)	6 (16%)	2	15
All	All	3469/4017 (86%)	3181 (92%)	288 (8%)	10	35

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	40	THR
1	A	41	MET
1	A	43	GLU
1	A	53	LEU
1	A	61	ILE
1	A	96	ILE
1	A	115	LEU
1	A	116	ASP
1	A	120	GLU
1	A	121	LEU
1	A	126	LEU
1	A	129	LYS
1	A	152	VAL

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	173	THR
1	A	181	LEU
1	A	187	LYS
1	A	226	GLU
1	A	236	LEU
1	A	241	VAL
1	A	247	ARG
1	A	257	ARG
1	A	266	LEU
1	A	270	LEU
1	A	276	LEU
1	A	279	LEU
1	A	290	GLU
1	A	311	GLN
1	A	320	ARG
1	A	329	LEU
1	A	333	GLU
1	A	341	MET
1	A	353	ILE
1	A	370	ILE
1	A	391	LEU
1	A	436	ILE
1	A	447	GLN
1	A	454	SER
1	A	455	MET
1	A	461	LYS
1	A	469	ARG
1	A	472	LEU
1	A	475	THR
1	A	481	ASP
1	A	485	ASP
1	A	487	MET
1	A	498	ARG
1	A	509	LEU
1	A	511	ILE
1	A	518	LYS
1	A	521	MET
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	528	LEU

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Mol	Chain	Res	Type
1	A	534	LEU
1	A	536	LEU
1	A	546	VAL
1	A	577	ILE
1	A	586	ILE
1	A	588	LEU
1	A	593	GLU
1	A	595	THR
1	A	597	LEU
1	A	618	GLU
1	A	636	GLU
1	A	644	LYS
1	A	658	LEU
1	A	664	THR
1	A	666	ILE
1	A	691	LEU
1	A	701	LEU
1	A	702	LEU
1	A	732	LEU
1	A	738	LYS
1	A	746	MET
1	A	771	GLU
1	A	821	ARG
1	A	837	ILE
1	A	838	GLN
1	A	848	ILE
1	A	878	ILE
1	A	883	LEU
1	A	913	LEU
1	A	919	ILE
1	A	920	LEU
1	A	928	LEU
1	A	932	GLU
1	A	936	LEU
1	A	963	ILE
1	A	973	ILE
1	A	983	ILE
1	A	1006	ILE
1	A	1032	LEU
1	A	1067	LEU
1	A	1098	VAL
1	A	1101	LEU

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Mol	Chain	Res	Type
1	A	1116	LEU
1	A	1143	LEU
1	A	1173	HIS
1	A	1215	ARG
1	A	1224	LEU
1	A	1242	VAL
1	A	1255	GLU
1	A	1276	VAL
1	A	1286	LYS
1	A	1289	ARG
1	A	1306	LEU
1	A	1316	VAL
1	A	1345	ARG
1	A	1354	ASN
1	A	1355	VAL
1	A	1356	ILE
1	A	1366	ARG
1	A	1387	HIS
1	A	1393	ASN
1	A	1394	THR
1	A	1404	GLU
1	A	1406	VAL
1	A	1409	LEU
1	A	1411	GLU
1	A	1417	GLU
1	A	1420	ASP
1	A	1426	GLU
1	A	1450	LEU
2	B	25	ILE
2	B	65	GLU
2	B	84	ILE
2	B	106	ASP
2	B	130	VAL
2	B	137	TYR
2	B	161	GLU
2	B	167	ILE
2	B	170	LEU
2	B	172	ILE
2	B	175	ARG
2	B	193	LYS
2	B	223	VAL
2	B	225	VAL

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Mol	Chain	Res	Type
2	B	240	ILE
2	B	242	SER
2	B	251	ILE
2	B	254	LEU
2	B	282	ILE
2	B	324	ILE
2	B	331	LEU
2	B	334	ILE
2	B	337	ARG
2	B	364	ILE
2	B	387	LEU
2	B	396	ASP
2	B	401	PHE
2	B	432	MET
2	B	453	ILE
2	B	469	GLN
2	B	479	VAL
2	B	500	THR
2	B	526	GLU
2	B	529	GLU
2	B	549	THR
2	B	552	MET
2	B	555	ILE
2	B	570	VAL
2	B	585	VAL
2	B	612	GLU
2	B	619	ILE
2	B	633	VAL
2	B	651	LEU
2	B	658	ILE
2	B	662	MET
2	B	698	GLU
2	B	711	GLU
2	B	730	ARG
2	B	748	ILE
2	B	795	ILE
2	B	797	TYR
2	B	825	VAL
2	B	839	MET
2	B	844	SER
2	B	868	MET
2	B	874	PHE

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Mol	Chain	Res	Type
2	B	911	ILE
2	B	923	GLU
2	B	942	ARG
2	B	944	THR
2	B	986	GLN
2	B	990	ILE
2	B	993	THR
2	B	997	GLU
2	B	1010	LEU
2	B	1011	ILE
2	B	1013	ASN
2	B	1031	LEU
2	B	1051	THR
2	B	1065	GLN
2	B	1084	GLN
2	B	1096	ARG
2	B	1122	ARG
2	B	1124	ARG
2	B	1133	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1202	LEU
2	B	1203	LEU
2	B	1211	ASN
2	B	1217	TYR
3	C	19	ASP
3	C	25	VAL
3	C	33	LEU
3	C	80	LEU
3	C	91	HIS
3	C	118	LEU
3	C	133	ILE
3	C	137	LYS
3	C	142	VAL
3	C	154	LYS
3	C	186	LEU
3	C	189	THR
3	C	195	GLN
3	C	240	VAL

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Mol	Chain	Res	Type
3	C	245	VAL
3	C	263	THR
4	D	7	THR
4	D	11	ARG
4	D	15	LEU
4	D	34	GLN
4	D	38	ILE
4	D	48	ILE
4	D	71	LYS
4	D	120	GLU
4	D	131	GLU
4	D	160	VAL
4	D	164	ILE
4	D	187	THR
4	D	214	LEU
5	E	12	LEU
5	E	121	MET
5	E	123	LEU
5	E	150	VAL
5	E	152	LYS
5	E	175	LEU
5	E	198	ILE
6	F	79	ARG
6	F	111	LEU
7	G	26	LEU
7	G	34	VAL
7	G	61	ILE
7	G	111	THR
7	G	119	LEU
7	G	134	GLU
7	G	154	VAL
7	G	160	ILE
7	G	165	GLU
8	H	26	ILE
8	H	46	LEU
8	H	107	VAL
8	H	111	LEU
9	I	7	CYS
9	I	17	ARG
9	I	21	GLU
9	I	26	LEU
9	I	52	ILE

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Mol	Chain	Res	Type
9	I	59	VAL
9	I	93	LYS
9	I	104	LEU
10	J	2	ILE
10	J	3	VAL
10	J	24	LEU
10	J	30	LEU
10	J	39	LEU
10	J	46	CYS
10	J	57	ILE
10	J	64	ASN
11	K	33	ILE
11	K	57	LEU
11	K	75	ILE
11	K	91	CYS
11	K	114	LEU
12	L	30	ILE
12	L	33	GLU
12	L	40	LEU
12	L	46	VAL
12	L	57	LEU
12	L	58	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	18	GLN
1	A	169	ASN
1	A	282	ASN
1	A	458	HIS
1	A	479	ASN
1	A	510	GLN
1	A	515	GLN
1	A	548	ASN
1	A	706	HIS
1	A	717	ASN
1	A	767	GLN
1	A	838	GLN
1	A	851	HIS
1	A	854	ASN
1	A	1048	ASN

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Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1211	GLN
1	A	1218	GLN
1	A	1222	ASN
1	A	1258	HIS
1	A	1265	ASN
1	A	1270	ASN
1	A	1312	ASN
1	A	1387	HIS
2	B	73	GLN
2	B	121	ASN
2	B	206	ASN
2	B	433	GLN
2	B	469	GLN
2	B	481	GLN
2	B	592	ASN
2	B	763	GLN
2	B	767	ASN
2	B	794	ASN
2	B	800	GLN
2	B	862	GLN
2	B	887	HIS
2	B	986	GLN
2	B	1013	ASN
2	B	1093	GLN
2	B	1193	GLN
2	B	1205	GLN
2	B	1211	ASN
3	C	7	GLN
3	C	24	ASN
3	C	54	ASN
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
4	D	9	GLN
4	D	41	GLN
4	D	138	ASN
5	E	5	ASN
5	E	61	GLN
5	E	63	ASN
5	E	99	HIS
5	E	113	GLN

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Mol	Chain	Res	Type
6	F	100	GLN
6	F	104	ASN
7	G	10	ASN
7	G	71	ASN
7	G	96	GLN
8	H	21	ASN
9	I	22	ASN
9	I	83	ASN
9	I	90	GLN
11	K	104	ASN
12	L	66	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	0	1 (12%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	1430/1733 (82%)	0.11	31 (2%) 62 39	47, 113, 205, 298	0
2	B	1157/1224 (94%)	0.30	35 (3%) 52 32	47, 128, 231, 294	0
3	C	265/318 (83%)	0.06	0 100 100	57, 113, 177, 299	0
4	D	178/221 (80%)	0.06	4 (2%) 62 39	60, 118, 193, 250	0
5	E	214/215 (99%)	0.30	5 (2%) 61 38	63, 159, 239, 274	0
6	F	87/155 (56%)	-0.26	0 100 100	46, 78, 133, 162	0
7	G	171/179 (95%)	-0.00	2 (1%) 76 51	59, 98, 151, 229	0
8	H	135/146 (92%)	0.34	2 (1%) 72 46	99, 162, 231, 247	0
9	I	114/122 (93%)	0.48	7 (6%) 27 18	70, 160, 237, 280	0
10	J	66/70 (94%)	0.02	3 (4%) 38 24	53, 103, 177, 216	0
11	K	115/120 (95%)	-0.20	1 (0%) 81 58	56, 105, 158, 176	0
12	L	43/70 (61%)	0.75	7 (16%) 4 6	75, 141, 215, 234	0
13	R	9/9 (100%)	1.11	1 (11%) 10 11	143, 199, 257, 275	0
14	S	14/45 (31%)	1.57	2 (14%) 6 8	261, 296, 300, 300	0
15	U	27/45 (60%)	1.06	1 (3%) 45 28	136, 253, 300, 300	0
All	All	4025/4672 (86%)	0.19	101 (2%) 58 36	46, 121, 222, 300	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	113	HIS	4.6
1	A	56	PRO	4.3
2	B	925	LEU	4.3
2	B	508	LEU	4.3
1	A	69	THR	4.2
10	J	66	LEU	3.9
2	B	584	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	140	ILE	3.6
13	R	2	U	3.6
1	A	3	GLY	3.6
1	A	1096	SER	3.6
1	A	319	GLY	3.6
1	A	2	VAL	3.4
2	B	863	GLU	3.4
2	B	513	GLN	3.4
4	D	25	ALA	3.3
15	U	28	DT	3.3
1	A	1090	ALA	3.2
4	D	4	SER	3.2
2	B	866	TYR	3.1
2	B	945	GLU	3.1
1	A	71	GLN	3.0
5	E	121	MET	3.0
14	S	26	DT	3.0
2	B	837	ASP	3.0
9	I	11	ASN	3.0
2	B	71	LEU	2.9
1	A	596	THR	2.6
2	B	1183	LYS	2.6
2	B	440	HIS	2.6
5	E	123	LEU	2.6
12	L	55	ILE	2.6
10	J	16	ASP	2.5
8	H	135	LEU	2.5
1	A	62	ASP	2.5
2	B	1224	PHE	2.5
1	A	399	HIS	2.5
1	A	257	ARG	2.5
4	D	6	SER	2.5
1	A	453	MET	2.5
14	S	24	DA	2.5
2	B	103	ASN	2.5
12	L	33	GLU	2.5
1	A	186	LYS	2.5
1	A	568	PRO	2.5
1	A	77	CYS	2.5
1	A	66	LYS	2.4
1	A	1081	LEU	2.4
9	I	98	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
11	K	61	TYR	2.4
1	A	128	ILE	2.4
2	B	359	GLU	2.4
1	A	829	VAL	2.4
2	B	735	ALA	2.4
2	B	829	CYS	2.3
5	E	89	GLY	2.3
12	L	54	ARG	2.3
5	E	171	LYS	2.3
1	A	333	GLU	2.3
2	B	116	GLU	2.3
2	B	1177	HIS	2.3
1	A	34	LYS	2.3
4	D	16	LYS	2.3
9	I	97	MET	2.3
2	B	822	ASN	2.3
1	A	252	PHE	2.3
10	J	65	PRO	2.3
9	I	13	MET	2.3
12	L	43	THR	2.3
1	A	400	PRO	2.3
5	E	90	VAL	2.3
2	B	343	ILE	2.2
2	B	509	ALA	2.2
2	B	348	ARG	2.2
9	I	63	GLY	2.2
1	A	65	LEU	2.2
12	L	53	HIS	2.2
12	L	45	ALA	2.2
1	A	640	GLN	2.2
1	A	57	ARG	2.2
2	B	710	LEU	2.2
2	B	367	LEU	2.2
7	G	158	HIS	2.1
1	A	628	GLY	2.1
12	L	68	GLU	2.1
2	B	340	ALA	2.1
2	B	399	ASP	2.1
2	B	253	THR	2.1
1	A	1258	HIS	2.1
2	B	441	ASP	2.1
8	H	48	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1004	GLU	2.1
2	B	243	ALA	2.1
9	I	87	GLN	2.1
9	I	100	PHE	2.1
2	B	499	ASN	2.1
1	A	1315	GLU	2.0
2	B	510	LYS	2.0
2	B	136	THR	2.0
2	B	310	MET	2.0
1	A	1254	ALA	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	C	401	1/1	0.90	0.23	193,193,193,193	0
17	MG	A	1804	1/1	0.95	0.13	63,63,63,63	0
16	ZN	A	1802	1/1	0.98	0.09	67,67,67,67	0
16	ZN	A	1801	1/1	0.99	0.04	90,90,90,90	0
16	ZN	I	202	1/1	0.99	0.09	183,183,183,183	0
17	MG	A	1803	1/1	0.99	0.07	82,82,82,82	0
16	ZN	B	1301	1/1	0.99	0.05	72,72,72,72	0
16	ZN	J	101	1/1	1.00	0.02	93,93,93,93	0
16	ZN	L	101	1/1	1.00	0.02	93,93,93,93	0
16	ZN	I	201	1/1	1.00	0.02	113,113,113,113	0
16	ZN	C	402	1/1	1.00	0.03	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.