



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:07 AM UTC

PDB ID : 4BXX / pdb_00004bxx
Title : Arrested RNA polymerase II-Bye1 complex
Authors : Kinkelin, K.; Wozniak, G.G.; Rothbart, S.B.; Lidschreiber, M.; Strahl, B.D.; Cramer, P.
Deposited on : 2013-07-16
Resolution : 3.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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
Mogul : 2022.3.0, CSD as543be (2022)
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

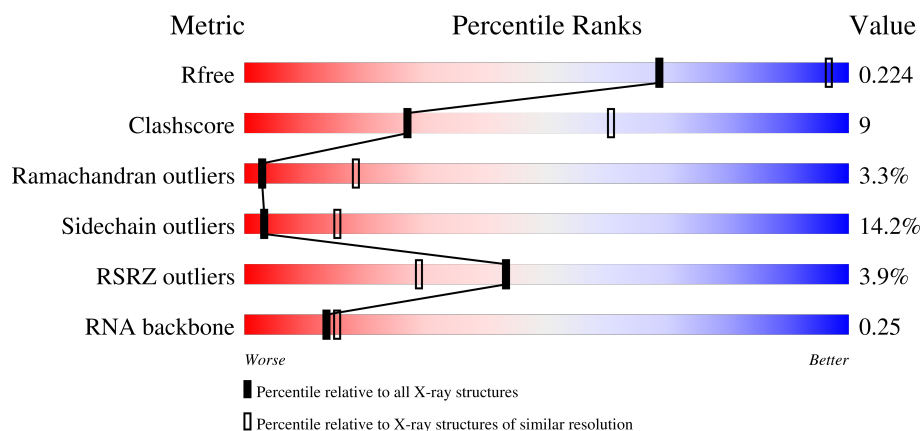
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



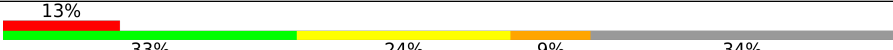
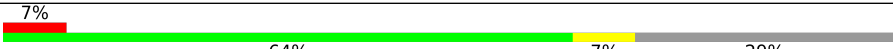
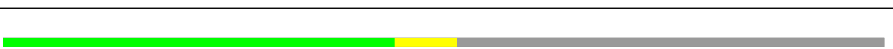
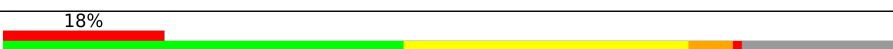
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)
RNA backbone	3983	1020 (3.58-2.98)

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% 53% 23% 5% 18%
2	B	1224	3% 59% 26% 5% 10%
3	C	318	58% 21% 5% 16%
4	D	221	7% 55% 21% • 20%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	27	
16	X	146	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32756 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	1429	Total	C	N	O	S	0	0	0
			11249	7087	1964	2136	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1097	Total	C	N	O	S	0	0	0
			8720	5526	1523	1617	54			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

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 RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	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
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	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	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*GP*AP*GP*GP*TP*AP*AP*GP*CP*TP*AP*

GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	10	Total	C	N	O	P	0	0	0
			209	99	42	58	10			

- Molecule 14 is a RNA chain called 5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	11	Total	C	N	O	P	0	0	0
			220	99	33	77	11			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*AP*CP*CP*TP*GP *GP*TP*GP* BRUP*TP*GP*CP*TP*CP*TP*AP*AP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	14	Total	Br	C	N	O	P	0	0
			287	1	136	49	87	14		

- Molecule 16 is a protein called TRANSCRIPTION FACTOR BYE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	X	120	Total	C	N	O	S	0	0	0
			986	634	164	185	3			

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

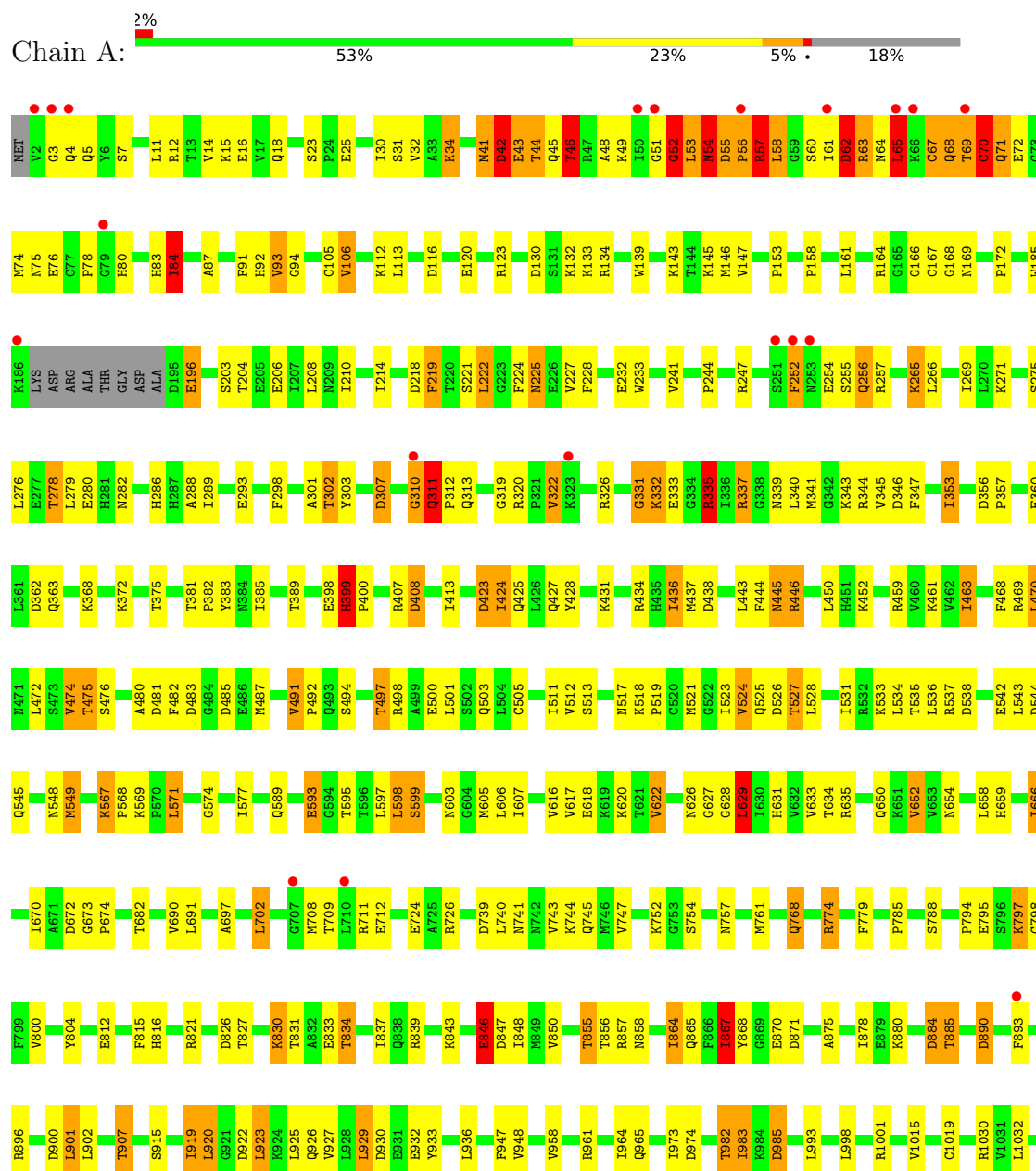
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

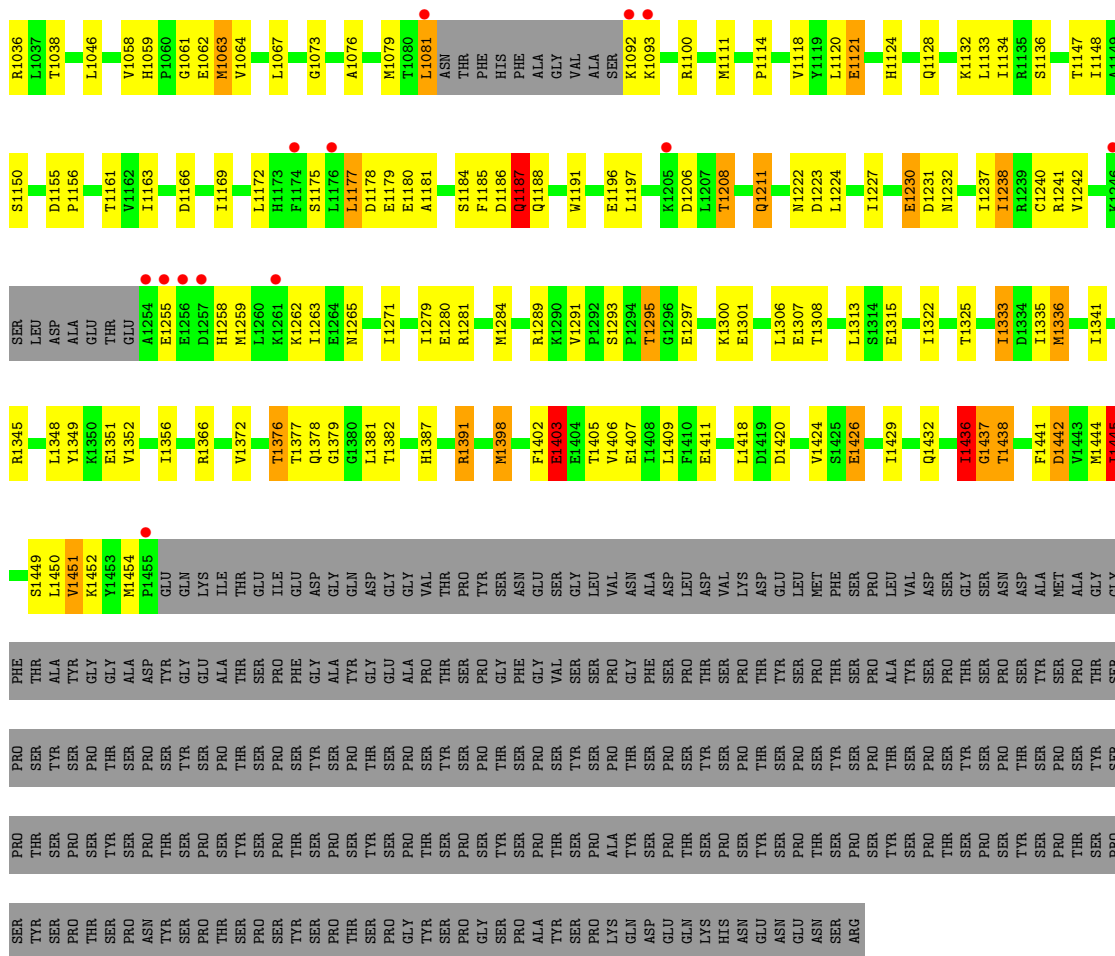
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

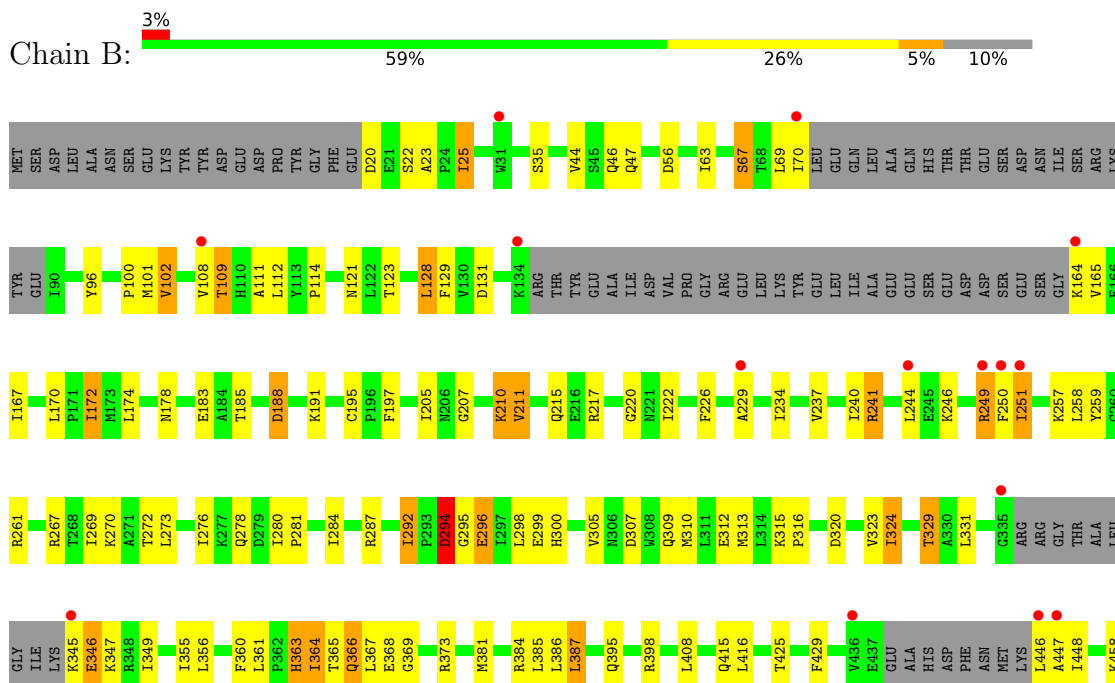
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

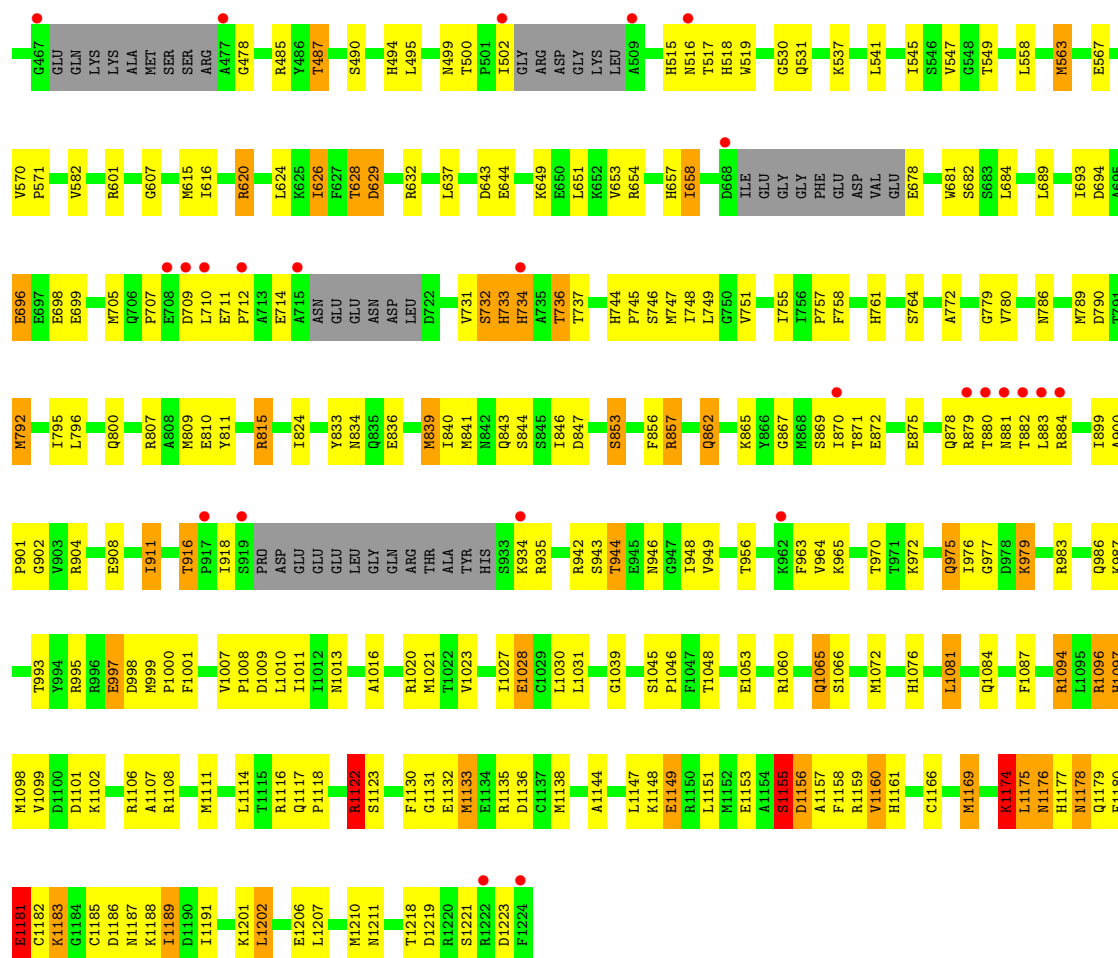
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





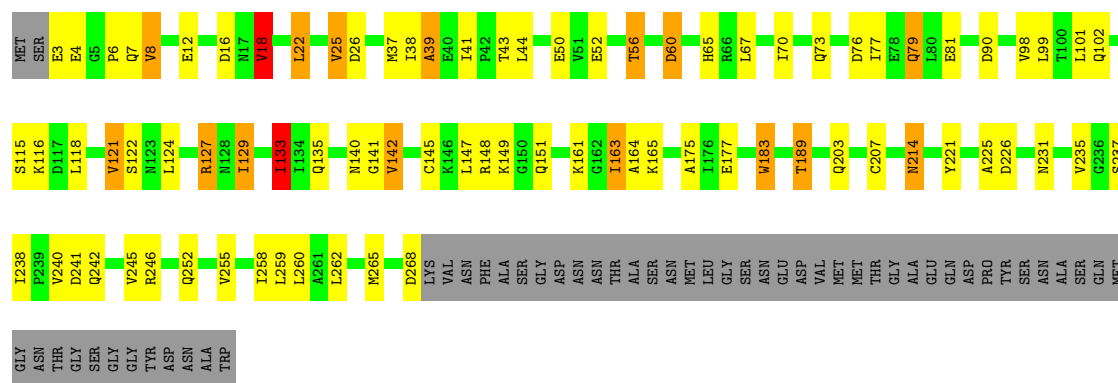
● Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2





• Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

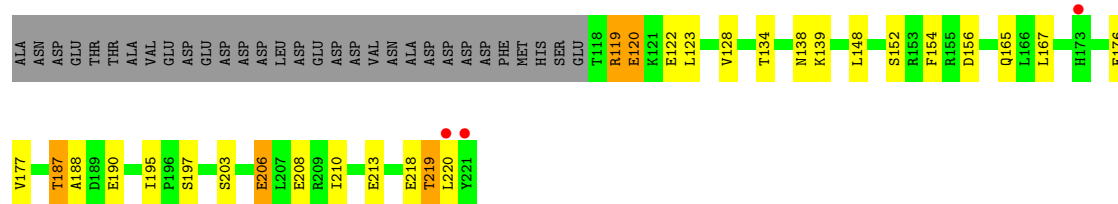
Chain C: 58% 21% 5% 16%



• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

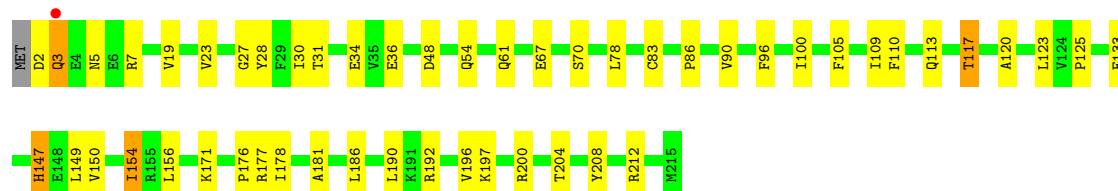
Chain D: 7% 55% 21% 20%





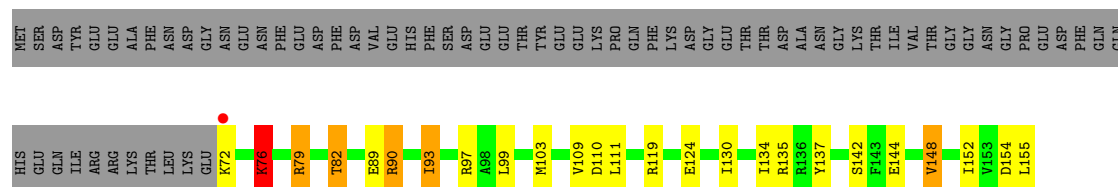
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E: 76% 22%



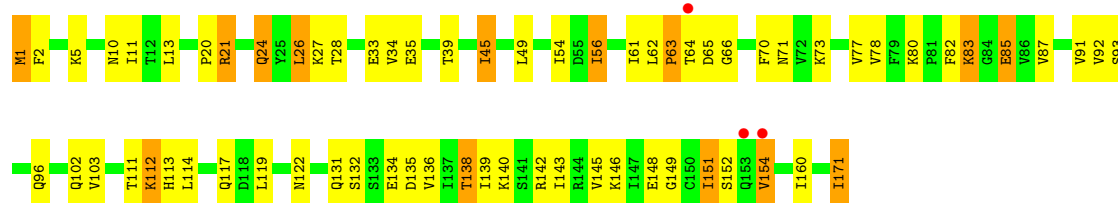
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

Chain F: 38% 12% 46%



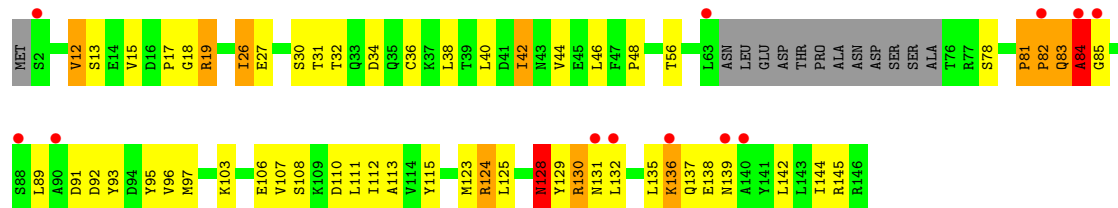
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 2% 60% 32% 8%

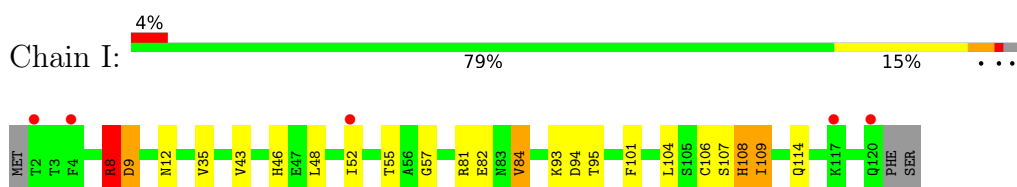


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

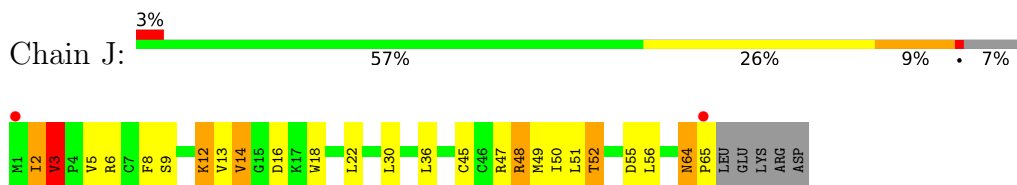
Chain H: 8% 51% 32% 7% 9%



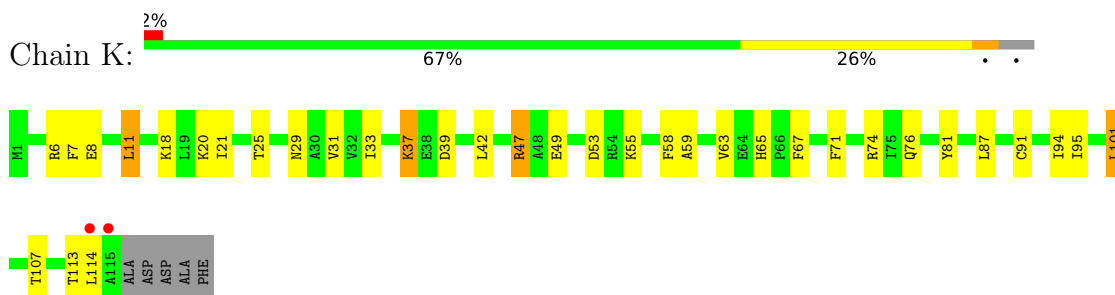
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



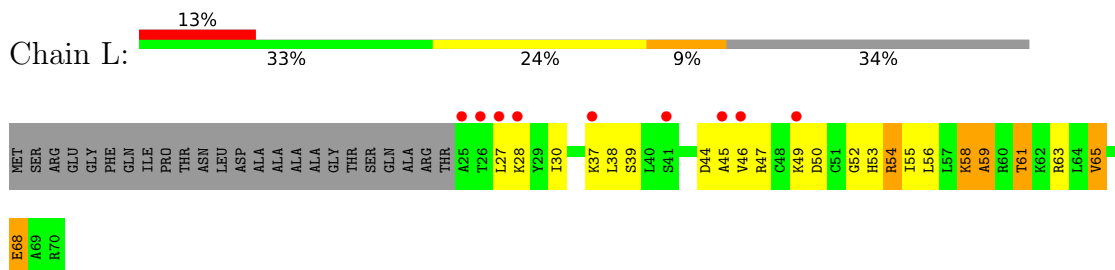
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



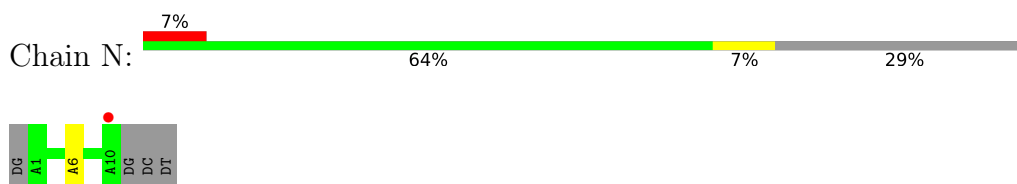
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



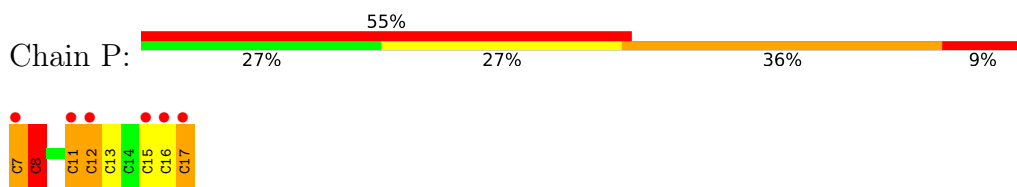
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



- Molecule 13: 5'-D(*GP*AP*GP*GP*TP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'



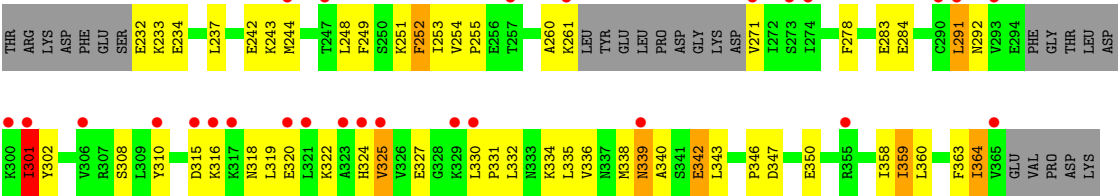
- Molecule 14: 5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP)-3'



- Molecule 15: 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*AP*CP*CP*TP*GP *GP*TP*GP*BRUP*TP*GP*CP*TP*CP*TP*AP*AP*DC)-3'



● Molecule 16: TRANSCRIPTION FACTOR BYE1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.92Å 392.67Å 281.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.28 49.08 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.08-3.28) 99.9 (49.08-3.28)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.180 , 0.208 0.200 , 0.224	Depositor DCC
R_{free} test set	3698 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 131.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32756	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BRU, 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	0.92	12/11450 (0.1%)	1.53	128/15483 (0.8%)
2	B	0.88	4/8889 (0.0%)	1.44	75/11987 (0.6%)
3	C	0.88	2/2133 (0.1%)	1.43	12/2891 (0.4%)
4	D	0.92	1/1365 (0.1%)	1.65	14/1837 (0.8%)
5	E	0.80	0/1788	1.39	14/2406 (0.6%)
6	F	0.97	0/691	1.41	5/933 (0.5%)
7	G	0.91	0/1368	1.36	9/1844 (0.5%)
8	H	0.85	0/1086	1.35	10/1470 (0.7%)
9	I	0.80	0/989	1.28	3/1331 (0.2%)
10	J	0.94	0/541	1.47	3/727 (0.4%)
11	K	0.80	0/938	1.34	2/1267 (0.2%)
12	L	0.96	0/365	1.48	5/485 (1.0%)
13	N	0.42	0/235	0.51	0/361
14	P	1.34	5/241 (2.1%)	0.80	0/370
15	T	0.53	0/298	0.58	0/458
16	X	0.88	0/999	1.61	11/1336 (0.8%)
All	All	0.89	24/33376 (0.1%)	1.45	291/45186 (0.6%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	8.15	1.45	1.33
3	C	4	GLU	CA-C	8.06	1.56	1.52
1	A	867	ILE	CG1-CD1	7.68	1.81	1.51
1	A	3	GLY	C-N	7.09	1.43	1.33
1	A	54	ASN	CA-C	6.77	1.61	1.52
1	A	69	THR	C-N	6.67	1.43	1.33
1	A	437	MET	SD-CE	6.48	1.95	1.79
1	A	57	ARG	CA-C	6.26	1.61	1.52
2	B	881	ASN	C-N	6.24	1.41	1.33
14	P	17	C	C1'-N1	6.13	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	24	ALA	CA-C	5.95	1.60	1.52
1	A	52	GLY	C-N	5.86	1.41	1.33
14	P	15	C	C1'-N1	5.79	1.57	1.48
2	B	1181	GLU	CA-C	5.74	1.60	1.52
1	A	55	ASP	CA-C	-5.69	1.45	1.52
1	A	491	VAL	CA-C	5.54	1.57	1.53
2	B	1189	ILE	CG1-CD1	5.51	1.73	1.51
1	A	67	CYS	CA-C	-5.50	1.48	1.53
2	B	1111	MET	SD-CE	5.46	1.93	1.79
14	P	8	C	C1'-N1	5.36	1.56	1.48
14	P	7	C	C1'-N1	5.36	1.56	1.48
14	P	11	C	C1'-N1	5.13	1.56	1.48
3	C	133	ILE	CG1-CD1	-5.07	1.31	1.51
1	A	69	THR	CA-CB	5.01	1.61	1.53

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	25	ALA	CA-C-N	11.90	141.00	122.08
4	D	25	ALA	C-N-CA	11.90	141.00	122.08
4	D	26	THR	N-CA-C	-10.82	96.89	113.02
1	A	3	GLY	CA-C-N	10.79	142.14	121.54
1	A	3	GLY	C-N-CA	10.79	142.14	121.54
1	A	1403	GLU	CA-C-N	-10.45	107.61	123.17
1	A	1403	GLU	C-N-CA	-10.45	107.61	123.17
2	B	296	GLU	N-CA-C	-10.38	100.35	113.43
2	B	1130	PHE	N-CA-C	-10.35	95.12	109.71
4	D	31	GLN	N-CA-C	-10.03	100.43	111.36
1	A	54	ASN	CA-CB-CG	9.64	122.24	112.60
4	D	54	GLU	N-CA-C	-9.35	101.09	111.28
2	B	975	GLN	CA-C-N	-9.18	113.97	122.97
2	B	975	GLN	C-N-CA	-9.18	113.97	122.97
1	A	56	PRO	CA-C-N	9.18	139.07	121.54
1	A	56	PRO	C-N-CA	9.18	139.07	121.54
1	A	452	LYS	N-CA-C	-8.28	102.21	111.07
1	A	43	GLU	CA-C-N	8.17	137.15	121.54
1	A	43	GLU	C-N-CA	8.17	137.15	121.54
3	C	39	ALA	N-CA-C	8.11	123.73	112.45
2	B	628	THR	CA-C-N	8.07	136.96	121.54
2	B	628	THR	C-N-CA	8.07	136.96	121.54
3	C	183	TRP	N-CA-C	-7.94	96.28	109.46
1	A	1445	ILE	N-CA-CB	7.85	121.39	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	MET	CA-C-N	7.77	128.26	121.58
1	A	341	MET	C-N-CA	7.77	128.26	121.58
1	A	629	LEU	N-CA-C	-7.77	102.81	111.28
8	H	128	ASN	CA-C-N	7.74	131.28	120.29
8	H	128	ASN	C-N-CA	7.74	131.28	120.29
1	A	445	ASN	CA-CB-CG	7.66	120.26	112.60
1	A	143	LYS	CA-C-N	7.62	130.80	120.44
1	A	143	LYS	C-N-CA	7.62	130.80	120.44
1	A	288	ALA	N-CA-C	-7.61	105.16	114.75
1	A	1187	GLN	N-CA-C	-7.50	100.25	110.68
3	C	60	ASP	CA-CB-CG	7.47	120.07	112.60
2	B	294	ASP	N-CA-C	-7.42	100.54	110.55
2	B	736	THR	N-CA-C	-7.23	104.61	113.50
10	J	55	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	399	HIS	N-CA-CB	7.13	123.07	110.37
1	A	219	PHE	CA-CB-CG	7.04	120.84	113.80
2	B	478	GLY	CA-C-N	7.00	130.36	120.42
2	B	478	GLY	C-N-CA	7.00	130.36	120.42
3	C	226	ASP	N-CA-C	-6.87	98.63	109.07
2	B	1155	SER	CA-C-N	6.86	134.65	121.54
2	B	1155	SER	C-N-CA	6.86	134.65	121.54
5	E	171	LYS	N-CA-C	-6.77	99.28	110.17
2	B	1177	HIS	N-CA-C	-6.76	104.24	113.30
2	B	1101	ASP	N-CA-C	-6.74	105.34	113.97
8	H	129	TYR	N-CA-C	6.69	118.66	111.36
1	A	54	ASN	CA-C-N	6.67	138.09	121.80
1	A	54	ASN	C-N-CA	6.67	138.09	121.80
1	A	42	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	346	ASP	CA-CB-CG	6.64	119.24	112.60
10	J	5	VAL	N-CA-C	-6.64	98.72	108.54
1	A	1177	LEU	CA-C-N	6.60	133.57	121.70
1	A	1177	LEU	C-N-CA	6.60	133.57	121.70
12	L	68	GLU	CB-CG-CD	6.55	123.74	112.60
2	B	1122	ARG	CA-C-N	6.49	129.21	120.65
2	B	1122	ARG	C-N-CA	6.49	129.21	120.65
5	E	5	ASN	N-CA-C	-6.48	103.44	112.45
4	D	41	GLN	N-CA-C	-6.45	105.38	113.18
1	A	452	LYS	CA-C-N	6.43	132.95	120.99
1	A	452	LYS	C-N-CA	6.43	132.95	120.99
2	B	1009	ASP	CA-CB-CG	6.41	119.01	112.60
4	D	26	THR	CA-C-N	6.38	131.46	122.08
4	D	26	THR	C-N-CA	6.38	131.46	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1183	LYS	N-CA-C	-6.37	101.69	110.35
2	B	998	ASP	CA-CB-CG	6.36	118.96	112.60
5	E	5	ASN	CA-C-N	6.35	129.07	120.38
5	E	5	ASN	C-N-CA	6.35	129.07	120.38
1	A	224	PHE	N-CA-C	6.34	118.90	110.53
2	B	363	HIS	N-CA-C	-6.34	102.61	110.41
3	C	135	GLN	CA-C-N	6.34	130.14	120.82
3	C	135	GLN	C-N-CA	6.34	130.14	120.82
1	A	84	ILE	N-CA-CB	6.33	120.42	111.82
16	X	278	PHE	CA-CB-CG	6.32	120.12	113.80
2	B	530	GLY	CA-C-N	6.31	129.05	120.54
2	B	530	GLY	C-N-CA	6.31	129.05	120.54
2	B	67	SER	CA-C-N	6.28	130.03	121.05
2	B	67	SER	C-N-CA	6.28	130.03	121.05
2	B	1096	ARG	N-CA-C	-6.27	100.38	109.59
1	A	622	VAL	N-CA-CB	-6.25	102.96	112.15
1	A	537	ARG	CA-C-N	6.25	129.27	120.28
1	A	537	ARG	C-N-CA	6.25	129.27	120.28
2	B	366	GLN	N-CA-C	-6.24	104.03	113.89
2	B	732	SER	N-CA-C	6.21	116.76	108.38
2	B	1186	ASP	CA-C-N	6.20	129.63	120.95
2	B	1186	ASP	C-N-CA	6.20	129.63	120.95
6	F	148	VAL	N-CA-CB	6.19	118.96	110.54
3	C	225	ALA	CA-C-N	6.17	132.43	121.75
3	C	225	ALA	C-N-CA	6.17	132.43	121.75
2	B	1219	ASP	CA-CB-CG	6.12	118.72	112.60
7	G	113	HIS	CA-CB-CG	-6.10	107.70	113.80
2	B	1166	CYS	N-CA-C	-6.08	100.59	110.20
1	A	974	ASP	CA-CB-CG	6.08	118.68	112.60
2	B	1001	PHE	N-CA-C	6.05	119.07	109.50
1	A	1063	MET	CA-C-N	6.04	130.95	120.86
1	A	1063	MET	C-N-CA	6.04	130.95	120.86
1	A	55	ASP	N-CA-CB	6.04	121.12	110.37
8	H	136	LYS	CA-C-N	6.02	130.11	121.50
8	H	136	LYS	C-N-CA	6.02	130.11	121.50
4	D	70	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	1231	ASP	CA-C-N	6.01	129.14	120.79
1	A	1231	ASP	C-N-CA	6.01	129.14	120.79
1	A	724	GLU	N-CA-C	-6.00	104.82	111.36
16	X	233	LYS	CA-C-N	5.99	128.31	120.28
16	X	233	LYS	C-N-CA	5.99	128.31	120.28
1	A	168	GLY	CA-C-N	5.99	132.98	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLY	C-N-CA	5.99	132.98	121.54
9	I	8	ARG	N-CA-C	-5.99	100.79	109.59
2	B	1101	ASP	CA-CB-CG	5.97	118.58	112.60
2	B	1156	ASP	N-CA-C	5.95	123.46	110.80
3	C	121	VAL	CB-CA-C	5.93	117.03	110.62
10	J	8	PHE	CA-CB-CG	5.93	119.73	113.80
2	B	694	ASP	CA-CB-CG	5.89	118.49	112.60
16	X	359	ILE	N-CA-CB	5.88	117.44	110.55
1	A	78	PRO	N-CA-C	-5.88	101.95	111.19
12	L	49	LYS	CA-C-N	5.87	132.75	121.54
12	L	49	LYS	C-N-CA	5.87	132.75	121.54
2	B	1136	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	491	VAL	N-CA-C	5.84	112.88	107.56
1	A	672	ASP	CA-CB-CG	5.83	118.43	112.60
2	B	56	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	1407	GLU	CB-CG-CD	5.77	122.41	112.60
6	F	76	LYS	CA-C-N	5.74	128.55	120.28
6	F	76	LYS	C-N-CA	5.74	128.55	120.28
1	A	331	GLY	N-CA-C	5.74	126.79	113.18
2	B	346	GLU	CA-C-N	5.73	128.43	120.29
2	B	346	GLU	C-N-CA	5.73	128.43	120.29
9	I	93	LYS	CA-C-N	5.73	128.23	120.38
9	I	93	LYS	C-N-CA	5.73	128.23	120.38
8	H	110	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	524	VAL	N-CA-CB	-5.72	101.79	111.23
2	B	809	MET	CA-C-N	5.71	127.87	120.44
2	B	809	MET	C-N-CA	5.71	127.87	120.44
2	B	1011	ILE	N-CA-CB	5.70	119.40	112.10
1	A	1211	GLN	CA-C-N	5.69	127.94	120.60
1	A	1211	GLN	C-N-CA	5.69	127.94	120.60
1	A	827	THR	N-CA-C	-5.68	102.87	111.56
5	E	54	GLN	CA-C-N	5.68	127.89	120.28
5	E	54	GLN	C-N-CA	5.68	127.89	120.28
1	A	222	LEU	N-CA-C	-5.66	103.23	110.53
4	D	14	ARG	CA-C-N	5.66	132.34	121.54
4	D	14	ARG	C-N-CA	5.66	132.34	121.54
1	A	1436	ILE	N-CA-CB	-5.63	103.59	111.25
12	L	59	ALA	CA-C-N	5.63	129.69	121.31
12	L	59	ALA	C-N-CA	5.63	129.69	121.31
1	A	900	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	1335	ILE	CA-C-N	5.61	127.73	120.44
1	A	1335	ILE	C-N-CA	5.61	127.73	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1181	GLU	N-CA-C	5.61	122.74	110.80
5	E	96	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	947	PHE	CA-C-N	5.56	128.37	120.53
1	A	947	PHE	C-N-CA	5.56	128.37	120.53
1	A	408	ASP	CA-C-N	5.54	127.64	120.44
1	A	408	ASP	C-N-CA	5.54	127.64	120.44
11	K	39	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	1180	PHE	CA-CB-CG	-5.52	108.28	113.80
7	G	63	PRO	CA-C-O	-5.52	117.23	121.31
1	A	408	ASP	CA-CB-CG	5.49	118.09	112.60
7	G	154	VAL	CA-C-N	5.49	134.36	121.52
7	G	154	VAL	C-N-CA	5.49	134.36	121.52
1	A	398	GLU	CA-C-O	-5.49	114.78	121.36
7	G	33	GLU	CA-C-N	5.49	127.58	120.56
7	G	33	GLU	C-N-CA	5.49	127.58	120.56
1	A	517	ASN	CA-CB-CG	5.48	118.08	112.60
2	B	628	THR	N-CA-C	-5.48	105.72	112.90
1	A	483	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	307	ASP	N-CA-C	-5.46	103.79	110.61
1	A	1403	GLU	N-CA-C	5.45	122.41	110.80
2	B	1174	LYS	N-CA-C	-5.45	103.97	111.81
2	B	320	ASP	CA-CB-CG	5.45	118.05	112.60
2	B	607	GLY	CA-C-N	5.44	127.84	120.38
2	B	607	GLY	C-N-CA	5.44	127.84	120.38
1	A	544	ASP	CA-C-N	5.44	127.84	120.44
1	A	544	ASP	C-N-CA	5.44	127.84	120.44
2	B	188	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	1181	ALA	CA-C-N	5.44	131.49	121.70
1	A	1181	ALA	C-N-CA	5.44	131.49	121.70
1	A	53	LEU	N-CA-CB	5.43	120.07	111.43
1	A	846	GLU	CA-C-N	5.42	131.90	121.54
1	A	846	GLU	C-N-CA	5.42	131.90	121.54
1	A	335	ARG	CA-C-N	5.41	127.32	120.72
1	A	335	ARG	C-N-CA	5.41	127.32	120.72
1	A	256	GLN	CA-C-N	5.41	131.86	121.54
1	A	256	GLN	C-N-CA	5.41	131.86	121.54
1	A	91	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	310	GLY	CA-C-N	5.40	134.97	121.80
1	A	310	GLY	C-N-CA	5.40	134.97	121.80
1	A	598	LEU	N-CA-C	-5.38	104.62	113.50
2	B	1131	GLY	CA-C-N	5.38	127.80	120.54
2	B	1131	GLY	C-N-CA	5.38	127.80	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PRO	N-CA-C	5.38	117.26	110.70
1	A	794	PRO	CA-C-N	5.38	127.43	120.44
1	A	794	PRO	C-N-CA	5.38	127.43	120.44
1	A	833	GLU	CA-C-N	5.37	127.47	120.28
1	A	833	GLU	C-N-CA	5.37	127.47	120.28
2	B	44	VAL	CA-C-N	5.37	127.73	120.38
2	B	44	VAL	C-N-CA	5.37	127.73	120.38
1	A	1232	ASN	CA-C-N	5.36	129.30	121.31
1	A	1232	ASN	C-N-CA	5.36	129.30	121.31
2	B	250	PHE	CA-CB-CG	5.35	119.15	113.80
11	K	53	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	654	ASN	CA-CB-CG	5.34	117.94	112.60
2	B	1009	ASP	N-CA-C	-5.33	106.62	113.23
1	A	526	ASP	CA-CB-CG	5.33	117.92	112.60
2	B	1133	MET	CA-C-N	5.33	127.42	120.28
2	B	1133	MET	C-N-CA	5.33	127.42	120.28
1	A	399	HIS	CA-C-O	-5.32	112.88	120.16
5	E	125	PRO	CA-C-N	5.30	128.12	120.38
5	E	125	PRO	C-N-CA	5.30	128.12	120.38
1	A	333	GLU	CB-CG-CD	5.29	121.59	112.60
1	A	307	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	123	ARG	CA-C-N	5.29	127.31	120.44
1	A	123	ARG	C-N-CA	5.29	127.31	120.44
1	A	542	GLU	CA-C-N	5.28	131.63	121.54
1	A	542	GLU	C-N-CA	5.28	131.63	121.54
1	A	804	TYR	CA-C-N	5.28	127.31	120.44
1	A	804	TYR	C-N-CA	5.28	127.31	120.44
5	E	27	GLY	CA-C-N	5.28	128.72	120.75
5	E	27	GLY	C-N-CA	5.28	128.72	120.75
2	B	1186	ASP	CA-CB-CG	5.27	117.87	112.60
6	F	82	THR	CB-CA-C	-5.26	101.16	109.42
7	G	34	VAL	N-CA-C	5.26	115.47	110.53
1	A	485	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	1221	SER	N-CA-C	-5.25	108.63	114.62
16	X	291	LEU	CA-C-N	5.25	128.31	120.95
16	X	291	LEU	C-N-CA	5.25	128.31	120.95
1	A	1437	GLY	CA-C-N	5.25	128.04	120.38
1	A	1437	GLY	C-N-CA	5.25	128.04	120.38
16	X	338	MET	CA-C-N	5.24	131.56	121.54
16	X	338	MET	C-N-CA	5.24	131.56	121.54
8	H	92	ASP	CA-C-N	5.23	130.93	122.29
8	H	92	ASP	C-N-CA	5.23	130.93	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1061	GLY	N-CA-C	-5.23	108.25	114.48
2	B	1081	LEU	CA-C-N	5.23	127.81	120.28
2	B	1081	LEU	C-N-CA	5.23	127.81	120.28
5	E	48	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	1013	ASN	N-CA-C	5.23	116.24	109.65
1	A	864	ILE	N-CA-C	-5.22	107.32	111.81
1	A	438	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	749	LEU	CA-C-N	5.21	125.77	122.18
2	B	749	LEU	C-N-CA	5.21	125.77	122.18
2	B	815	ARG	CA-C-N	5.21	127.68	120.29
2	B	815	ARG	C-N-CA	5.21	127.68	120.29
1	A	985	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	218	ASP	CA-CB-CG	5.20	117.80	112.60
3	C	18	VAL	N-CA-CB	5.20	118.75	112.10
1	A	319	GLY	CA-C-N	5.18	127.59	120.39
1	A	319	GLY	C-N-CA	5.18	127.59	120.39
2	B	733	HIS	CA-C-N	5.18	127.47	120.38
2	B	733	HIS	C-N-CA	5.18	127.47	120.38
1	A	1313	LEU	CA-C-N	5.17	128.58	120.82
1	A	1313	LEU	C-N-CA	5.17	128.58	120.82
1	A	890	ASP	CA-C-N	5.17	127.16	120.44
1	A	890	ASP	C-N-CA	5.17	127.16	120.44
1	A	627	GLY	CA-C-N	5.17	131.53	121.41
1	A	627	GLY	C-N-CA	5.17	131.53	121.41
2	B	684	LEU	CA-C-N	5.16	127.46	120.44
2	B	684	LEU	C-N-CA	5.16	127.46	120.44
3	C	214	ASN	CA-C-N	5.15	128.55	120.82
3	C	214	ASN	C-N-CA	5.15	128.55	120.82
7	G	65	ASP	N-CA-C	-5.15	100.51	108.90
1	A	69	THR	CA-C-N	5.12	131.32	121.54
1	A	69	THR	C-N-CA	5.12	131.32	121.54
1	A	307	ASP	CA-C-N	5.12	128.22	120.75
1	A	307	ASP	C-N-CA	5.12	128.22	120.75
5	E	147	HIS	CA-C-N	5.11	127.90	120.79
5	E	147	HIS	C-N-CA	5.11	127.90	120.79
4	D	23	ASN	CA-C-O	-5.11	114.84	120.36
1	A	474	VAL	CA-C-N	5.10	127.43	120.54
1	A	474	VAL	C-N-CA	5.10	127.43	120.54
7	G	2	PHE	CA-CB-CG	5.09	118.89	113.80
8	H	84	ALA	CA-C-N	5.09	125.73	120.03
8	H	84	ALA	C-N-CA	5.09	125.73	120.03
1	A	271	LYS	CA-C-N	5.08	127.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	LYS	C-N-CA	5.08	127.09	120.28
6	F	154	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	1420	ASP	CA-CB-CG	5.06	117.66	112.60
16	X	301	ILE	CA-C-N	5.06	131.20	121.54
16	X	301	ILE	C-N-CA	5.06	131.20	121.54
1	A	930	ASP	N-CA-C	-5.06	105.68	111.14
1	A	932	GLU	CB-CG-CD	5.05	121.19	112.60
2	B	1065	GLN	CA-C-N	5.05	131.19	121.54
2	B	1065	GLN	C-N-CA	5.05	131.19	121.54
2	B	681	TRP	N-CA-C	-5.04	105.70	111.14
4	D	120	GLU	N-CA-C	-5.03	105.88	111.36
2	B	1130	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	481	ASP	CA-CB-CG	5.02	117.62	112.60
4	D	23	ASN	CA-CB-CG	5.02	117.62	112.60
16	X	363	PHE	CA-CB-CG	5.00	118.80	113.80

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	11249	0	11312	272	0
2	B	8720	0	8744	163	0
3	C	2095	0	2051	40	0
4	D	1356	0	1319	19	0
5	E	1752	0	1776	21	0
6	F	679	0	701	20	0
7	G	1340	0	1357	39	0
8	H	1068	0	1040	35	0
9	I	971	0	927	13	0
10	J	532	0	542	15	0
11	K	920	0	929	20	0
12	L	363	0	386	10	0
13	N	209	0	113	1	0
14	P	220	0	122	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	T	287	0	157	1	0
16	X	986	0	1009	18	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32756	0	32485	602	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 9.

All (602) 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:867:ILE:CG1	1:A:867:ILE:CD1	1.81	1.55
1:A:53:LEU:HD23	1:A:54:ASN:H	1.06	1.10
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.03
1:A:855:THR:HG21	1:A:857:ARG:HE	1.22	1.02
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.39	1.01
4:D:53:SER:HB3	4:D:152:SER:HB2	1.45	0.95
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.47	0.94
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.15	0.92
2:B:705:MET:H	2:B:710:LEU:HD12	1.35	0.90
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.53	0.89
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.56	0.88
7:G:1:MET:HE1	7:G:80:LYS:O	1.74	0.87
1:A:53:LEU:HD23	1:A:54:ASN:N	1.89	0.86
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.40	0.86
1:A:567:LYS:HB3	8:H:96:VAL:N	1.92	0.84
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.59	0.83
2:B:972:LYS:HD2	2:B:1098:MET:HE3	1.61	0.82
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.44	0.82
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.61	0.81
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.60	0.81
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.63	0.81
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.63	0.80
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.62	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:H	2:B:657:HIS:HD2	1.30	0.78
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.65	0.78
1:A:62:ASP:HB3	1:A:64:ASN:HD22	1.47	0.77
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.65	0.77
3:C:142:VAL:H	10:J:16:ASP:HB3	1.50	0.76
16:X:248:LEU:O	16:X:252:PHE:HB3	1.85	0.76
16:X:316:LYS:HG2	16:X:320:GLU:HB3	1.68	0.76
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.68	0.75
1:A:53:LEU:CD2	1:A:54:ASN:H	1.96	0.75
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.67	0.75
1:A:1444:MET:HE3	6:F:135:ARG:HB2	1.67	0.75
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.69	0.75
4:D:53:SER:HB3	4:D:152:SER:CB	2.18	0.73
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.71	0.72
1:A:43:GLU:HB2	1:A:46:THR:HB	1.69	0.72
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.72	0.72
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.71	0.72
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.72	0.72
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.71	0.72
1:A:61:ILE:HG22	1:A:62:ASP:H	1.53	0.71
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.72	0.71
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.25	0.71
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.71	0.71
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.26	0.71
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.71	0.71
6:F:103:MET:HE2	7:G:66:GLY:H	1.56	0.70
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.70
2:B:744:HIS:HD2	2:B:746:SER:H	1.36	0.70
10:J:48:ARG:O	10:J:52:THR:HG22	1.91	0.69
10:J:48:ARG:HE	10:J:49:MET:HE2	1.57	0.69
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.74	0.69
1:A:34:LYS:HZ1	1:A:57:ARG:HH12	1.40	0.69
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.28	0.69
1:A:754:SER:H	1:A:757:ASN:HD22	1.41	0.68
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.23	0.68
1:A:626:ASN:O	1:A:631:HIS:HD2	1.76	0.68
1:A:41:MET:HB2	1:A:49:LYS:HA	1.74	0.68
1:A:535:THR:HG21	1:A:617:VAL:H	1.58	0.68
7:G:1:MET:CE	7:G:80:LYS:O	2.40	0.68
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.68
1:A:255:SER:H	2:B:935:ARG:HH22	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.68
1:A:907:THR:HG21	1:A:920:LEU:HD12	1.76	0.67
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.75	0.67
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.77	0.67
1:A:52:GLY:H	1:A:56:PRO:HB3	1.59	0.67
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.77	0.66
1:A:626:ASN:O	1:A:631:HIS:CD2	2.49	0.66
2:B:872:GLU:HG2	2:B:916:THR:HG23	1.78	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.97	0.65
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.79	0.64
1:A:42:ASP:C	1:A:44:THR:H	2.05	0.64
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.77	0.64
2:B:853:SER:HB3	2:B:1094:ARG:HH11	1.63	0.64
1:A:527:THR:HG21	1:A:650:GLN:HA	1.80	0.64
6:F:76:LYS:HA	6:F:79:ARG:CD	2.28	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.94	0.63
1:A:203:SER:OG	1:A:206:GLU:HB2	1.98	0.63
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.62	0.63
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.63	0.63
16:X:322:LYS:HD2	16:X:346:PRO:HD3	1.80	0.63
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.63	0.63
8:H:91:ASP:C	8:H:93:TYR:H	2.05	0.63
12:L:61:THR:HB	12:L:63:ARG:HG3	1.81	0.63
7:G:138:THR:HG22	7:G:139:ILE:H	1.63	0.62
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.97	0.62
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.81	0.62
7:G:21:ARG:NH1	7:G:24:GLN:H	1.98	0.62
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.82	0.62
6:F:99:LEU:O	6:F:103:MET:HG2	2.00	0.62
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.81	0.62
1:A:52:GLY:N	1:A:56:PRO:HB3	2.14	0.61
1:A:1185:PHE:C	1:A:1187:GLN:H	2.07	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.82	0.61
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.63	0.61
1:A:1451:VAL:O	1:A:1454:MET:HG3	2.00	0.61
16:X:339:ASN:HA	16:X:343:LEU:HD11	1.83	0.61
4:D:187:THR:HB	4:D:190:GLU:H	1.65	0.61
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.35	0.61
1:A:1184:SER:C	1:A:1186:ASP:H	2.08	0.60
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.60
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.47	0.60
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.66	0.60
1:A:901:LEU:HA	1:A:907:THR:HG23	1.83	0.60
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.83	0.60
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.82	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.84	0.60
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.02	0.60
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.32	0.60
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.68	0.59
1:A:1128:GLN:HE21	1:A:1132:LYS:HE2	1.67	0.59
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.65	0.59
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.17	0.59
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.85	0.59
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.84	0.59
5:E:147:HIS:CD2	5:E:149:LEU:H	2.20	0.59
7:G:112:LYS:HE2	7:G:112:LYS:O	2.02	0.59
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.02	0.59
1:A:57:ARG:O	1:A:68:GLN:HG2	2.02	0.59
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.84	0.59
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.83	0.59
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.84	0.59
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.84	0.59
1:A:1336:MET:HE2	1:A:1381:LEU:HD12	1.83	0.59
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.59
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.67	0.58
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.86	0.58
2:B:902:GLY:O	12:L:65:VAL:HG11	2.04	0.58
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.67	0.58
1:A:55:ASP:HA	1:A:58:LEU:H	1.68	0.58
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.68	0.58
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.58
2:B:862:GLN:HG3	2:B:963:PHE:HD1	1.68	0.58
12:L:28:LYS:HB2	12:L:39:SER:HA	1.84	0.58
7:G:83:LYS:HD2	7:G:149:GLY:HA2	1.86	0.58
1:A:1230:GLU:OE1	16:X:308:SER:HA	2.04	0.57
1:A:933:TYR:HA	1:A:936:LEU:HD12	1.85	0.57
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.86	0.57
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.85	0.57
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.87	0.57
1:A:709:THR:HG23	9:I:94:ASP:HA	1.87	0.57
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.86	0.57
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.40	0.57
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.51	0.57
2:B:20:ASP:HB2	2:B:23:ALA:HB2	1.87	0.56
1:A:92:HIS:HD2	1:A:94:GLY:H	1.52	0.56
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	2.02	0.56
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.51	0.56
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.87	0.56
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.86	0.56
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.36	0.56
1:A:535:THR:HG21	1:A:616:VAL:HA	1.86	0.56
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.85	0.56
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.87	0.56
1:A:55:ASP:N	1:A:56:PRO:HD3	2.21	0.56
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.88	0.56
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.88	0.56
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.87	0.56
7:G:10:ASN:ND2	7:G:71:ASN:HD22	2.03	0.56
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.26	0.56
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.86	0.56
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.05	0.55
1:A:1177:LEU:HD21	16:X:237:LEU:HA	1.88	0.55
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.06	0.55
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.88	0.55
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.70	0.55
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.41	0.55
2:B:244:LEU:HD21	2:B:366:GLN:HE22	1.71	0.55
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.89	0.55
1:A:567:LYS:CB	8:H:96:VAL:H	2.06	0.55
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.89	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.35	0.55
1:A:855:THR:CG2	1:A:857:ARG:HE	2.08	0.55
3:C:98:VAL:H	3:C:122:SER:HB3	1.71	0.55
1:A:885:THR:HG22	1:A:893:PHE:HE2	1.71	0.54
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.90	0.54
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.89	0.54
2:B:323:VAL:HG23	2:B:324:ILE:HD12	1.89	0.54
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.89	0.54
1:A:65:LEU:HD23	1:A:71:GLN:HB2	1.89	0.54
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.90	0.54
8:H:89:LEU:C	8:H:91:ASP:H	2.16	0.54
8:H:135:LEU:C	8:H:137:GLN:H	2.14	0.54
1:A:41:MET:O	1:A:42:ASP:C	2.50	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.14	0.54
1:A:743:VAL:O	1:A:747:VAL:HG23	2.08	0.54
1:A:709:THR:HB	1:A:712:GLU:H	1.73	0.54
3:C:252:GLN:HG2	11:K:95:ILE:HG23	1.90	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.89	0.54
1:A:252:PHE:HD2	1:A:256:GLN:HB3	1.73	0.54
1:A:708:MET:HG2	1:A:712:GLU:HB3	1.89	0.54
2:B:1158:PHE:CE2	2:B:1160:VAL:HG13	2.42	0.54
12:L:47:ARG:HG3	12:L:54:ARG:HG3	1.89	0.54
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.07	0.53
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.53
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.89	0.53
2:B:654:ARG:H	2:B:657:HIS:CD2	2.19	0.53
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.44	0.53
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.90	0.53
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.91	0.53
8:H:82:PRO:C	8:H:84:ALA:H	2.15	0.53
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.90	0.53
1:A:494:SER:H	1:A:497:THR:HG22	1.73	0.53
2:B:35:SER:HA	2:B:811:TYR:HE1	1.73	0.53
2:B:882:THR:HG22	2:B:884:ARG:H	1.74	0.53
1:A:298:PHE:O	1:A:302:THR:HB	2.08	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.74	0.53
4:D:52:LEU:HB3	4:D:148:LEU:CD2	2.39	0.53
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.35	0.53
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.89	0.53
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.91	0.53
4:D:32:GLU:O	7:G:5:LYS:HE2	2.08	0.53
1:A:43:GLU:CD	1:A:48:ALA:HB3	2.34	0.53
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.90	0.53
16:X:234:GLU:HA	16:X:237:LEU:HD12	1.91	0.52
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.90	0.52
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.90	0.52
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.52
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.90	0.52
1:A:134:ARG:HD2	1:A:221:SER:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:H	2:B:710:LEU:CD1	2.16	0.52
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.90	0.52
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.91	0.52
1:A:856:THR:HB	1:A:865:GLN:HB2	1.92	0.52
12:L:27:LEU:HB3	12:L:37:LYS:HD3	1.90	0.52
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.95	0.52
1:A:535:THR:CG2	1:A:616:VAL:HA	2.40	0.52
2:B:234:ILE:HG12	2:B:257:LYS:HB3	1.91	0.52
1:A:55:ASP:O	1:A:55:ASP:OD2	2.28	0.51
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.91	0.51
1:A:923:LEU:O	1:A:927:VAL:HG23	2.11	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.75	0.51
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.76	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.55	0.51
2:B:373:ARG:HH21	2:B:567:GLU:HG2	1.75	0.51
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.76	0.51
2:B:882:THR:HB	2:B:934:LYS:C	2.36	0.51
7:G:1:MET:SD	7:G:1:MET:C	2.94	0.51
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.92	0.51
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.76	0.51
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.93	0.51
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.91	0.51
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.51	0.51
3:C:76:ASP:O	3:C:79:GLN:HG2	2.11	0.51
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.92	0.50
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.46	0.50
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.92	0.50
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.52	0.50
5:E:109:ILE:HG12	5:E:133:GLU:HB2	1.92	0.50
7:G:21:ARG:HD3	7:G:24:GLN:HB2	1.92	0.50
2:B:582:VAL:HG22	2:B:626:ILE:HD12	1.94	0.50
5:E:117:THR:HB	5:E:120:ALA:H	1.75	0.50
11:K:65:HIS:CD2	11:K:67:PHE:H	2.29	0.50
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.93	0.50
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.46	0.50
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.23	0.50
3:C:18:VAL:O	3:C:231:ASN:HA	2.11	0.50
5:E:19:VAL:O	5:E:23:VAL:HG23	2.12	0.50
1:A:450:LEU:HD23	2:B:1133:MET:HE1	1.94	0.50
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.60	0.50
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:THR:HB	1:A:985:ASP:H	1.77	0.50
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.93	0.50
4:D:219:THR:HG23	4:D:220:LEU:H	1.76	0.50
1:A:1208:THR:HB	1:A:1211:GLN:H	1.77	0.50
1:A:41:MET:CB	1:A:49:LYS:HA	2.42	0.49
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.12	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.94	0.49
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.28	0.49
2:B:1188:LYS:H	2:B:1189:ILE:HD12	1.77	0.49
1:A:225:ASN:ND2	1:A:228:PHE:H	2.10	0.49
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.49
1:A:816:HIS:HE2	2:B:764:SER:H	1.59	0.49
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.47	0.49
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.94	0.49
7:G:91:VAL:CG2	7:G:143:ILE:HD12	2.43	0.49
16:X:360:LEU:O	16:X:364:ILE:HB	2.13	0.49
1:A:55:ASP:C	1:A:57:ARG:H	2.18	0.49
1:A:1079:MET:HB3	1:A:1081:LEU:HD21	1.93	0.49
2:B:295:GLY:H	2:B:298:LEU:HB2	1.78	0.49
2:B:487:THR:HG22	2:B:490:SER:H	1.77	0.49
2:B:1096:ARG:O	2:B:1097:HIS:CG	2.66	0.49
2:B:515:HIS:H	2:B:518:HIS:CD2	2.31	0.49
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.94	0.49
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.60	0.49
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.95	0.49
1:A:535:THR:HG21	1:A:617:VAL:N	2.27	0.48
2:B:792:MET:HA	2:B:856:PHE:O	2.13	0.48
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.78	0.48
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.39	0.48
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.53	0.48
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.97	0.48
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.95	0.48
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.96	0.48
2:B:345:LYS:C	2:B:347:LYS:H	2.21	0.48
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.96	0.48
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.96	0.48
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.95	0.48
5:E:83:CYS:HB2	5:E:110:PHE:CZ	2.49	0.48
16:X:249:PHE:HA	16:X:252:PHE:HD1	1.79	0.48
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.95	0.48
2:B:515:HIS:CD2	2:B:517:THR:H	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:12:C:HS'	14:P:13:C:HS'	1.96	0.48
1:A:549:MET:HG2	1:A:652:VAL:HG22	1.96	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.96	0.48
16:X:255:PRO:HG3	16:X:316:LYS:HD3	1.96	0.48
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.78	0.48
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.96	0.48
1:A:67:CYS:C	1:A:68:GLN:HG3	2.38	0.47
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.96	0.47
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.47
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.79	0.47
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.96	0.47
16:X:242:GLU:HB2	16:X:283:GLU:HG3	1.95	0.47
1:A:92:HIS:HE1	2:B:1210:MET:O	1.97	0.47
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.95	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.97	0.47
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.50	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.97	0.47
2:B:558:LEU:HB3	2:B:563:MET:HE3	1.97	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.47
2:B:847:ASP:O	3:C:65:HIS:HE1	1.97	0.47
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.96	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.09	0.47
1:A:225:ASN:HD22	1:A:227:VAL:H	1.62	0.47
1:A:1150:SER:H	9:I:46:HIS:HB3	1.79	0.47
2:B:1185:CYS:C	2:B:1187:ASN:H	2.22	0.47
4:D:40:HIS:CG	7:G:73:LYS:HZ1	2.33	0.47
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.97	0.47
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.97	0.47
7:G:112:LYS:HE3	7:G:119:LEU:O	2.15	0.47
10:J:12:LYS:HZ2	10:J:13:VAL:H	1.63	0.47
2:B:516:ASN:H	2:B:516:ASN:HD22	1.63	0.47
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.47
1:A:225:ASN:ND2	1:A:227:VAL:H	2.13	0.47
1:A:492:PRO:CB	1:A:497:THR:HG23	2.45	0.47
7:G:132:SER:HB3	7:G:135:ASP:H	1.79	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.28	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.96	0.46
2:B:841:MET:O	2:B:993:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.41	0.46
1:A:1454:MET:HG2	7:G:20:PRO:HB3	1.97	0.46
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.78	0.46
5:E:31:THR:HG23	5:E:34:GLU:H	1.80	0.46
1:A:925:LEU:HD22	1:A:983:ILE:HB	1.96	0.46
1:A:1449:SER:HA	1:A:1452:LYS:HG2	1.96	0.46
1:A:658:LEU:HD21	2:B:1076:HIS:CD2	2.50	0.46
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.80	0.46
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.51	0.46
7:G:82:PHE:O	7:G:85:GLU:HB2	2.14	0.46
7:G:91:VAL:HG23	7:G:143:ILE:HD12	1.97	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.98	0.46
4:D:23:ASN:HA	4:D:28:GLN:O	2.16	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.48	0.46
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.42	0.46
1:A:42:ASP:C	1:A:44:THR:N	2.72	0.46
16:X:325:VAL:HG12	16:X:330:LEU:HB2	1.97	0.46
4:D:219:THR:HG23	4:D:220:LEU:N	2.31	0.45
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.98	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.45
3:C:37:MET:HA	3:C:41:ILE:HD12	1.98	0.45
3:C:133:ILE:HD13	3:C:237:SER:HA	1.98	0.45
3:C:258:ILE:N	3:C:258:ILE:HD12	2.32	0.45
8:H:42:ILE:HG23	8:H:95:TYR:CE2	2.51	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.98	0.45
2:B:101:MET:HG2	2:B:111:ALA:HA	1.99	0.45
2:B:259:TYR:HE2	2:B:270:LYS:HB2	1.80	0.45
2:B:745:PRO:O	2:B:748:ILE:HG12	2.16	0.45
1:A:839:ARG:HH21	1:A:843:LYS:HE2	1.81	0.45
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.46	0.45
2:B:1176:ASN:H	2:B:1178:ASN:H	1.62	0.45
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.98	0.45
4:D:54:GLU:O	4:D:58:VAL:HG23	2.16	0.45
1:A:961:ARG:O	1:A:965:GLN:HG3	2.16	0.45
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.99	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.17	0.45
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.97	0.45
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.97	0.45
7:G:122:ASN:HD22	7:G:131:GLN:HE22	1.64	0.45
1:A:25:GLU:CD	1:A:25:GLU:H	2.25	0.45
1:A:423:ASP:HB3	1:A:424:ILE:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.51	0.45
16:X:331:PRO:HB2	16:X:334:LYS:HB2	1.99	0.45
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.45
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.99	0.45
3:C:79:GLN:HG3	3:C:127:ARG:HD2	1.99	0.45
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.99	0.45
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.98	0.45
8:H:95:TYR:HE1	8:H:97:MET:CG	2.20	0.45
1:A:56:PRO:CD	1:A:58:LEU:HG	2.47	0.44
1:A:275:SER:O	1:A:279:LEU:HG	2.17	0.44
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.00	0.44
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.99	0.44
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.17	0.44
3:C:115:SER:HB3	3:C:142:VAL:HB	1.99	0.44
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.44
5:E:61:GLN:HG3	5:E:105:PHE:CE1	2.52	0.44
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.83	0.44
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.98	0.44
2:B:188:ASP:HA	2:B:191:LYS:HD2	2.00	0.44
2:B:246:LYS:HA	2:B:249:ARG:HH21	1.81	0.44
2:B:779:GLY:HA2	2:B:796:LEU:HB2	1.99	0.44
4:D:154:PHE:HA	4:D:219:THR:HB	1.97	0.44
16:X:249:PHE:HA	16:X:252:PHE:CD1	2.53	0.44
1:A:62:ASP:O	1:A:63:ARG:C	2.61	0.44
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.99	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.99	0.44
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.83	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.44
2:B:901:PRO:HD3	12:L:58:LYS:HB3	2.00	0.44
2:B:979:LYS:HE3	2:B:987:LYS:HD2	1.99	0.44
3:C:6:PRO:HB3	3:C:25:VAL:HG13	2.00	0.44
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.99	0.44
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.99	0.44
1:A:55:ASP:O	1:A:55:ASP:CG	2.60	0.44
1:A:982:THR:H	1:A:985:ASP:HB2	1.83	0.44
2:B:237:VAL:HG22	2:B:257:LYS:HG2	2.00	0.44
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.98	0.44
9:I:8:ARG:O	9:I:9:ASP:CB	2.66	0.44
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.18	0.44
1:A:311:GLN:O	1:A:312:PRO:C	2.60	0.44
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.47	0.44
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.58	0.44
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.99	0.44
3:C:43:THR:HG22	3:C:44:LEU:H	1.82	0.44
6:F:89:GLU:O	6:F:93:ILE:HD12	2.18	0.44
2:B:865:LYS:HE2	2:B:869:SER:HA	1.99	0.44
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.00	0.44
4:D:40:HIS:CG	7:G:73:LYS:NZ	2.86	0.44
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.99	0.44
1:A:567:LYS:CB	8:H:95:TYR:HA	2.46	0.43
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.18	0.43
5:E:154:ILE:O	5:E:196:VAL:HA	2.18	0.43
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.99	0.43
1:A:153:PRO:HA	1:A:161:LEU:HA	2.00	0.43
2:B:234:ILE:CG2	2:B:237:VAL:HG23	2.47	0.43
7:G:10:ASN:HD21	7:G:71:ASN:HD22	1.65	0.43
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.32	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.99	0.43
2:B:649:LYS:HD3	2:B:736:THR:O	2.18	0.43
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.48	0.43
2:B:220:GLY:HA2	2:B:241:ARG:HB3	2.00	0.43
2:B:294:ASP:H	9:I:12:ASN:HD22	1.66	0.43
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.18	0.43
13:N:6:DA:H61	15:T:12:DT:H3	1.66	0.43
1:A:332:LYS:H	1:A:337:ARG:HB2	1.82	0.43
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.18	0.43
1:A:922:ASP:CG	1:A:925:LEU:HD12	2.43	0.43
5:E:61:GLN:HG3	5:E:105:PHE:HE1	1.84	0.43
6:F:103:MET:HE2	7:G:66:GLY:N	2.29	0.43
11:K:65:HIS:HD2	11:K:67:PHE:H	1.66	0.43
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.53	0.43
7:G:92:VAL:CG2	7:G:102:GLN:HB2	2.49	0.43
8:H:125:LEU:HG	8:H:130:ARG:NH2	2.34	0.43
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.84	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.19	0.43
1:A:49:LYS:NZ	1:A:60:SER:HA	2.34	0.43
2:B:309:GLN:HG3	9:I:52:ILE:HD11	2.00	0.43
3:C:258:ILE:CD1	11:K:42:LEU:HD21	2.49	0.43
1:A:1059:HIS:HE1	6:F:155:LEU:HD21	1.84	0.43
10:J:14:VAL:HG13	10:J:50:ILE:HD11	2.01	0.43
16:X:347:ASP:O	16:X:350:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.00	0.43
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.83	0.43
2:B:211:VAL:HG21	2:B:494:HIS:CE1	2.53	0.43
3:C:163:ILE:HD12	3:C:165:LYS:HB2	2.00	0.43
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.34	0.42
8:H:113:ALA:HA	8:H:125:LEU:O	2.19	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.54	0.42
1:A:362:ASP:CG	1:A:459:ARG:HH11	2.27	0.42
1:A:774:ARG:HG3	1:A:797:LYS:HD3	2.01	0.42
2:B:69:LEU:HD21	2:B:425:THR:HG22	2.02	0.42
2:B:757:PRO:HG2	2:B:1028:GLU:HG3	2.02	0.42
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.34	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.01	0.42
10:J:48:ARG:HE	10:J:49:MET:CE	2.30	0.42
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.55	0.42
2:B:101:MET:HB3	2:B:109:THR:HG22	2.02	0.42
2:B:999:MET:HG3	2:B:1000:PRO:HD2	2.00	0.42
8:H:30:SER:HB3	8:H:36:CYS:HB3	2.00	0.42
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.67	0.42
1:A:512:VAL:HA	1:A:519:PRO:HA	2.01	0.42
2:B:515:HIS:CD2	2:B:516:ASN:N	2.88	0.42
7:G:146:LYS:HD3	7:G:148:GLU:OE2	2.19	0.42
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.51	0.42
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.02	0.42
1:A:1092:LYS:HD3	1:A:1093:LYS:HE3	2.01	0.42
1:A:382:PRO:HA	1:A:428:TYR:CE1	2.55	0.42
1:A:739:ASP:H	8:H:19:ARG:NH1	2.17	0.42
2:B:47:GLN:NE2	2:B:408:LEU:HD12	2.34	0.42
2:B:315:LYS:N	2:B:316:PRO:HD2	2.34	0.42
2:B:882:THR:C	2:B:884:ARG:H	2.26	0.42
2:B:100:PRO:HG3	2:B:172:ILE:HD13	2.02	0.42
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.90	0.42
1:A:741:ASN:ND2	1:A:743:VAL:HB	2.34	0.42
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.02	0.42
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.42
8:H:123:MET:HE1	8:H:142:LEU:HD11	2.01	0.42
2:B:515:HIS:HD2	2:B:517:THR:H	1.67	0.42
2:B:1181:GLU:HG3	2:B:1182:CYS:N	2.34	0.42
8:H:44:VAL:HG13	8:H:48:PRO:HA	2.01	0.42
12:L:28:LYS:H	12:L:39:SER:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:X:244:MET:HG2	16:X:310:TYR:CE2	2.55	0.42
1:A:830:LYS:O	1:A:834:THR:HB	2.20	0.42
2:B:296:GLU:O	2:B:300:HIS:CD2	2.73	0.42
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.50	0.42
3:C:56:THR:HG23	3:C:147:LEU:HD23	2.02	0.42
9:I:8:ARG:O	9:I:9:ASP:HB2	2.20	0.42
1:A:463:ILE:HD13	1:A:469:ARG:HD2	2.02	0.41
1:A:511:ILE:HA	1:A:521:MET:HE3	2.01	0.41
1:A:673:GLY:N	1:A:674:PRO:HD2	2.35	0.41
1:A:1147:THR:HB	9:I:48:LEU:HD22	2.02	0.41
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.20	0.41
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.02	0.41
16:X:318:ASN:HB3	16:X:346:PRO:HD2	2.02	0.41
1:A:31:SER:OG	1:A:83:HIS:HD2	2.03	0.41
1:A:32:VAL:HG21	1:A:80:HIS:HB2	2.01	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.56	0.41
1:A:595:THR:HG23	1:A:599:SER:HB3	2.01	0.41
2:B:123:THR:HG23	2:B:205:ILE:HA	2.02	0.41
2:B:1081:LEU:O	3:C:189:THR:HG23	2.20	0.41
7:G:21:ARG:HH11	7:G:24:GLN:H	1.68	0.41
1:A:280:GLU:C	1:A:282:ASN:H	2.29	0.41
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.86	0.41
2:B:165:VAL:HG11	2:B:448:ILE:HD13	2.02	0.41
2:B:294:ASP:H	9:I:12:ASN:ND2	2.17	0.41
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.89	0.41
1:A:92:HIS:HD2	1:A:94:GLY:N	2.18	0.41
1:A:254:GLU:HB3	2:B:935:ARG:NH2	2.35	0.41
1:A:1284:MET:HA	1:A:1306:LEU:HD23	2.02	0.41
9:I:84:VAL:HB	9:I:104:LEU:HD21	2.03	0.41
11:K:8:GLU:O	11:K:37:LYS:HD3	2.19	0.41
14:P:7:C:H2'	14:P:8:C:C6	2.55	0.41
1:A:67:CYS:O	1:A:68:GLN:C	2.62	0.41
1:A:105:CYS:SG	1:A:139:TRP:HA	2.61	0.41
7:G:62:LEU:HA	7:G:63:PRO:HD3	1.84	0.41
9:I:101:PHE:O	9:I:109:ILE:HA	2.21	0.41
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.03	0.41
1:A:278:THR:O	1:A:282:ASN:HB2	2.20	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.02	0.41
4:D:27:LEU:HD11	4:D:176:GLU:OE2	2.20	0.41
1:A:42:ASP:HB3	1:A:45:GLN:H	1.86	0.41
2:B:696:GLU:O	2:B:699:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.03	0.41
3:C:241:ASP:O	3:C:245:VAL:HG23	2.21	0.41
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.21	0.41
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	2.02	0.41
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.01	0.41
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.02	0.41
7:G:143:ILE:HG22	7:G:145:VAL:HG23	2.03	0.41
8:H:83:GLN:C	8:H:85:GLY:H	2.29	0.41
1:A:494:SER:HB3	1:A:497:THR:HB	2.03	0.41
1:A:535:THR:HB	1:A:616:VAL:HG13	2.03	0.41
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.03	0.41
1:A:1352:VAL:O	1:A:1356:ILE:HD12	2.20	0.41
2:B:35:SER:HA	2:B:811:TYR:CE1	2.54	0.41
2:B:310:MET:HE1	2:B:387:LEU:HD12	2.02	0.41
10:J:36:LEU:HD13	10:J:47:ARG:HB3	2.02	0.41
11:K:59:ALA:HA	11:K:74:ARG:O	2.20	0.41
1:A:92:HIS:CD2	1:A:94:GLY:H	2.37	0.41
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.03	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.55	0.41
1:A:1445:ILE:CD1	7:G:70:PHE:CZ	3.04	0.41
2:B:210:LYS:HA	2:B:210:LYS:HD2	1.94	0.41
2:B:324:ILE:HG23	2:B:329:THR:HB	2.03	0.41
3:C:8:VAL:HG13	3:C:22:LEU:HD12	2.02	0.41
2:B:346:GLU:H	2:B:349:ILE:HD12	1.86	0.40
2:B:734:HIS:CD2	2:B:734:HIS:H	2.39	0.40
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.86	0.40
2:B:944:THR:HB	2:B:1122:ARG:HH21	1.86	0.40
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.56	0.40
1:A:884:ASP:CG	1:A:1030:ARG:HH12	2.29	0.40
1:A:1402:PHE:CD2	1:A:1403:GLU:HG3	2.54	0.40
2:B:541:LEU:HB2	2:B:747:MET:HE3	2.03	0.40
2:B:810:GLU:HG3	2:B:815:ARG:HH12	1.86	0.40
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.37	0.40
5:E:86:PRO:HA	5:E:113:GLN:HB2	2.02	0.40
6:F:72:LYS:HD2	6:F:142:SER:HB3	2.03	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40
16:X:342:GLU:H	16:X:342:GLU:HG3	1.61	0.40
3:C:73:GLN:O	3:C:129:ILE:HA	2.21	0.40
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.57	0.40
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.20	0.40
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:HG2	1:A:606:LEU:HD13	2.03	0.40
1:A:1121:GLU:HB3	1:A:1124:HIS:HD2	1.86	0.40
1:A:1258:HIS:O	1:A:1262:LYS:HG3	2.22	0.40
7:G:92:VAL:HG21	7:G:102:GLN:HB2	2.03	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	1419/1733 (82%)	1259 (89%)	111 (8%)	49 (4%)	3	17
2	B	1075/1224 (88%)	962 (90%)	78 (7%)	35 (3%)	3	18
3	C	264/318 (83%)	242 (92%)	15 (6%)	7 (3%)	4	21
4	D	173/221 (78%)	151 (87%)	17 (10%)	5 (3%)	3	20
5	E	212/215 (99%)	201 (95%)	9 (4%)	2 (1%)	14	43
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	153 (90%)	15 (9%)	1 (1%)	21	51
8	H	129/146 (88%)	100 (78%)	16 (12%)	13 (10%)	0	3
9	I	117/122 (96%)	99 (85%)	16 (14%)	2 (2%)	7	30
10	J	63/70 (90%)	54 (86%)	5 (8%)	4 (6%)	1	7
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	11 (25%)	6 (14%)	0	1
16	X	114/146 (78%)	99 (87%)	9 (8%)	6 (5%)	1	10
All	All	3974/4711 (84%)	3530 (89%)	314 (8%)	130 (3%)	3	18

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	44	THR
1	A	54	ASN
1	A	57	ARG
1	A	70	CYS
1	A	74	MET
1	A	76	GLU
1	A	169	ASN
1	A	257	ARG
1	A	536	LEU
1	A	567	LYS
1	A	597	LEU
1	A	628	GLY
1	A	1175	SER
1	A	1403	GLU
2	B	367	LEU
2	B	629	ASP
2	B	731	VAL
2	B	751	VAL
2	B	772	ALA
2	B	879	ARG
2	B	1046	PRO
2	B	1097	HIS
2	B	1176	ASN
2	B	1181	GLU
2	B	1223	ASP
3	C	161	LYS
4	D	15	LEU
8	H	78	SER
8	H	139	ASN
16	X	315	ASP
16	X	339	ASN
1	A	58	LEU
1	A	65	LEU
1	A	166	GLY
1	A	525	GLN
1	A	846	GLU
1	A	1180	GLU
1	A	1271	ILE
1	A	1405	THR
1	A	1437	GLY
2	B	108	VAL
2	B	447	ALA

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Mol	Chain	Res	Type
2	B	867	GLY
2	B	880	THR
2	B	1066	SER
2	B	1175	LEU
3	C	141	GLY
4	D	13	ARG
4	D	18	VAL
4	D	53	SER
8	H	18	GLY
8	H	81	PRO
8	H	82	PRO
9	I	9	ASP
10	J	6	ARG
12	L	50	ASP
12	L	53	HIS
12	L	56	LEU
16	X	260	ALA
16	X	340	ALA
1	A	42	ASP
1	A	167	CYS
1	A	286	HIS
1	A	311	GLN
1	A	399	HIS
1	A	423	ASP
1	A	543	LEU
1	A	593	GLU
1	A	1255	GLU
2	B	67	SER
2	B	229	ALA
2	B	364	ILE
2	B	643	ASP
2	B	711	GLU
2	B	712	PRO
2	B	1157	ALA
7	G	154	VAL
8	H	83	GLN
8	H	108	SER
9	I	95	THR
12	L	45	ALA
1	A	62	ASP
1	A	332	LYS
1	A	1206	ASP

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Mol	Chain	Res	Type
2	B	307	ASP
2	B	792	MET
2	B	943	SER
3	C	90	ASP
3	C	142	VAL
3	C	149	LYS
4	D	19	GLU
5	E	36	GLU
8	H	84	ALA
8	H	128	ASN
10	J	64	ASN
12	L	59	ALA
1	A	46	THR
1	A	310	GLY
1	A	322	VAL
1	A	424	ILE
1	A	599	SER
1	A	958	VAL
1	A	1188	GLN
2	B	251	ILE
2	B	305	VAL
2	B	368	GLU
2	B	883	LEU
3	C	175	ALA
5	E	3	GLN
8	H	17	PRO
10	J	2	ILE
1	A	5	GLN
2	B	707	PRO
2	B	1108	ARG
2	B	1155	SER
3	C	214	ASN
8	H	19	ARG
8	H	131	ASN
8	H	136	LYS
10	J	3	VAL
16	X	302	TYR
1	A	52	GLY
12	L	52	GLY
1	A	331	GLY
1	A	1156	PRO
2	B	369	GLY

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Mol	Chain	Res	Type
16	X	301	ILE
1	A	158	PRO
1	A	196	GLU

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	1251/1520 (82%)	1064 (85%)	187 (15%)	3	14
2	B	952/1061 (90%)	824 (87%)	128 (13%)	4	17
3	C	234/274 (85%)	203 (87%)	31 (13%)	4	18
4	D	140/200 (70%)	116 (83%)	24 (17%)	2	10
5	E	196/197 (100%)	181 (92%)	15 (8%)	12	37
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	20
7	G	152/152 (100%)	126 (83%)	26 (17%)	2	10
8	H	117/128 (91%)	99 (85%)	18 (15%)	2	13
9	I	113/116 (97%)	103 (91%)	10 (9%)	9	32
10	J	60/65 (92%)	51 (85%)	9 (15%)	3	14
11	K	99/102 (97%)	86 (87%)	13 (13%)	4	18
12	L	40/57 (70%)	30 (75%)	10 (25%)	0	2
16	X	110/136 (81%)	87 (79%)	23 (21%)	1	5
All	All	3538/4145 (85%)	3035 (86%)	503 (14%)	3	15

All (503) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	LYS
1	A	18	GLN
1	A	30	ILE
1	A	34	LYS

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Mol	Chain	Res	Type
1	A	41	MET
1	A	46	THR
1	A	62	ASP
1	A	63	ARG
1	A	65	LEU
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	71	GLN
1	A	84	ILE
1	A	93	VAL
1	A	106	VAL
1	A	112	LYS
1	A	113	LEU
1	A	120	GLU
1	A	132	LYS
1	A	145	LYS
1	A	146	MET
1	A	147	VAL
1	A	196	GLU
1	A	204	THR
1	A	208	LEU
1	A	210	ILE
1	A	225	ASN
1	A	232	GLU
1	A	252	PHE
1	A	265	LYS
1	A	278	THR
1	A	289	ILE
1	A	293	GLU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	313	GLN
1	A	320	ARG
1	A	322	VAL
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	353	ILE
1	A	372	LYS
1	A	375	THR

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Mol	Chain	Res	Type
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	389	THR
1	A	408	ASP
1	A	425	GLN
1	A	427	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	497	THR
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	538	ASP
1	A	545	GLN
1	A	549	MET
1	A	571	LEU
1	A	577	ILE
1	A	593	GLU
1	A	598	LEU
1	A	618	GLU
1	A	620	LYS
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	652	VAL

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Mol	Chain	Res	Type
1	A	666	ILE
1	A	670	ILE
1	A	682	THR
1	A	690	VAL
1	A	691	LEU
1	A	702	LEU
1	A	726	ARG
1	A	740	LEU
1	A	752	LYS
1	A	768	GLN
1	A	774	ARG
1	A	788	SER
1	A	795	GLU
1	A	797	LYS
1	A	821	ARG
1	A	826	ASP
1	A	830	LYS
1	A	831	THR
1	A	834	THR
1	A	837	ILE
1	A	848	ILE
1	A	855	THR
1	A	858	ASN
1	A	864	ILE
1	A	867	ILE
1	A	878	ILE
1	A	880	LYS
1	A	884	ASP
1	A	885	THR
1	A	890	ASP
1	A	896	ARG
1	A	901	LEU
1	A	907	THR
1	A	919	ILE
1	A	920	LEU
1	A	923	LEU
1	A	929	LEU
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	982	THR
1	A	983	ILE

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Mol	Chain	Res	Type
1	A	998	LEU
1	A	1001	ARG
1	A	1038	THR
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1120	LEU
1	A	1121	GLU
1	A	1133	LEU
1	A	1134	ILE
1	A	1136	SER
1	A	1172	LEU
1	A	1178	ASP
1	A	1179	GLU
1	A	1187	GLN
1	A	1208	THR
1	A	1222	ASN
1	A	1223	ASP
1	A	1227	ILE
1	A	1230	GLU
1	A	1237	ILE
1	A	1238	ILE
1	A	1242	VAL
1	A	1263	ILE
1	A	1265	ASN
1	A	1280	GLU
1	A	1281	ARG
1	A	1289	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1300	LYS
1	A	1301	GLU
1	A	1307	GLU
1	A	1315	GLU
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1376	THR

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Mol	Chain	Res	Type
1	A	1378	GLN
1	A	1382	THR
1	A	1391	ARG
1	A	1398	MET
1	A	1403	GLU
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1445	ILE
1	A	1450	LEU
1	A	1451	VAL
2	B	22	SER
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	102	VAL
2	B	109	THR
2	B	128	LEU
2	B	167	ILE
2	B	172	ILE
2	B	178	ASN
2	B	183	GLU
2	B	185	THR
2	B	210	LYS
2	B	211	VAL
2	B	217	ARG
2	B	222	ILE
2	B	240	ILE
2	B	241	ARG
2	B	249	ARG
2	B	251	ILE
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	278	GLN
2	B	292	ILE
2	B	294	ASP
2	B	312	GLU
2	B	324	ILE

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Mol	Chain	Res	Type
2	B	329	THR
2	B	331	LEU
2	B	361	LEU
2	B	365	THR
2	B	381	MET
2	B	384	ARG
2	B	387	LEU
2	B	398	ARG
2	B	415	GLN
2	B	416	LEU
2	B	446	LEU
2	B	458	LYS
2	B	485	ARG
2	B	487	THR
2	B	495	LEU
2	B	500	THR
2	B	502	ILE
2	B	531	GLN
2	B	537	LYS
2	B	547	VAL
2	B	549	THR
2	B	563	MET
2	B	570	VAL
2	B	601	ARG
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	624	LEU
2	B	626	ILE
2	B	628	THR
2	B	644	GLU
2	B	651	LEU
2	B	658	ILE
2	B	678	GLU
2	B	682	SER
2	B	696	GLU
2	B	709	ASP
2	B	714	GLU
2	B	734	HIS
2	B	737	THR
2	B	755	ILE
2	B	780	VAL

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Mol	Chain	Res	Type
2	B	786	ASN
2	B	790	ASP
2	B	795	ILE
2	B	839	MET
2	B	844	SER
2	B	853	SER
2	B	857	ARG
2	B	862	GLN
2	B	870	ILE
2	B	871	THR
2	B	875	GLU
2	B	878	GLN
2	B	908	GLU
2	B	911	ILE
2	B	916	THR
2	B	918	ILE
2	B	942	ARG
2	B	944	THR
2	B	946	ASN
2	B	956	THR
2	B	964	VAL
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	979	LYS
2	B	986	GLN
2	B	997	GLU
2	B	1007	VAL
2	B	1028	GLU
2	B	1048	THR
2	B	1053	GLU
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1094	ARG
2	B	1102	LYS
2	B	1106	ARG
2	B	1122	ARG
2	B	1123	SER
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS

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Mol	Chain	Res	Type
2	B	1149	GLU
2	B	1151	LEU
2	B	1153	GLU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1169	MET
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1179	GLN
2	B	1181	GLU
2	B	1183	LYS
2	B	1191	ILE
2	B	1202	LEU
2	B	1211	ASN
3	C	3	GLU
3	C	7	GLN
3	C	8	VAL
3	C	12	GLU
3	C	16	ASP
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	38	ILE
3	C	50	GLU
3	C	52	GLU
3	C	56	THR
3	C	60	ASP
3	C	79	GLN
3	C	81	GLU
3	C	102	GLN
3	C	121	VAL
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	163	ILE
3	C	189	THR
3	C	203	GLN
3	C	235	VAL

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Mol	Chain	Res	Type
3	C	238	ILE
3	C	240	VAL
3	C	260	LEU
3	C	265	MET
3	C	268	ASP
4	D	23	ASN
4	D	34	GLN
4	D	35	LEU
4	D	44	GLU
4	D	47	LEU
4	D	52	LEU
4	D	60	LYS
4	D	65	GLU
4	D	119	ARG
4	D	122	GLU
4	D	123	LEU
4	D	128	VAL
4	D	134	THR
4	D	139	LYS
4	D	156	ASP
4	D	165	GLN
4	D	187	THR
4	D	195	ILE
4	D	197	SER
4	D	206	GLU
4	D	210	ILE
4	D	213	GLU
4	D	218	GLU
4	D	219	THR
5	E	2	ASP
5	E	3	GLN
5	E	7	ARG
5	E	30	ILE
5	E	67	GLU
5	E	70	SER
5	E	78	LEU
5	E	117	THR
5	E	123	LEU
5	E	154	ILE
5	E	178	ILE
5	E	190	LEU
5	E	192	ARG

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Mol	Chain	Res	Type
5	E	200	ARG
5	E	204	THR
6	F	76	LYS
6	F	79	ARG
6	F	82	THR
6	F	90	ARG
6	F	93	ILE
6	F	110	ASP
6	F	111	LEU
6	F	119	ARG
6	F	152	ILE
7	G	1	MET
7	G	11	ILE
7	G	13	LEU
7	G	21	ARG
7	G	24	GLN
7	G	26	LEU
7	G	28	THR
7	G	39	THR
7	G	45	ILE
7	G	56	ILE
7	G	61	ILE
7	G	64	THR
7	G	83	LYS
7	G	85	GLU
7	G	93	SER
7	G	96	GLN
7	G	111	THR
7	G	112	LYS
7	G	114	LEU
7	G	117	GLN
7	G	134	GLU
7	G	138	THR
7	G	140	LYS
7	G	151	ILE
7	G	152	SER
7	G	171	ILE
8	H	12	VAL
8	H	13	SER
8	H	26	ILE
8	H	27	GLU
8	H	31	THR

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Mol	Chain	Res	Type
8	H	32	THR
8	H	34	ASP
8	H	42	ILE
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL
8	H	111	LEU
8	H	112	ILE
8	H	124	ARG
8	H	128	ASN
8	H	130	ARG
8	H	132	LEU
8	H	138	GLU
9	I	8	ARG
9	I	35	VAL
9	I	55	THR
9	I	81	ARG
9	I	82	GLU
9	I	84	VAL
9	I	107	SER
9	I	108	HIS
9	I	109	ILE
9	I	114	GLN
10	J	2	ILE
10	J	3	VAL
10	J	12	LYS
10	J	14	VAL
10	J	22	LEU
10	J	30	LEU
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	6	ARG
11	K	11	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS
11	K	47	ARG
11	K	101	LEU

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Mol	Chain	Res	Type
11	K	107	THR
11	K	113	THR
11	K	114	LEU
12	L	30	ILE
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	65	VAL
12	L	68	GLU
16	X	232	GLU
16	X	243	LYS
16	X	251	LYS
16	X	252	PHE
16	X	253	ILE
16	X	254	VAL
16	X	261	LYS
16	X	271	VAL
16	X	284	GLU
16	X	291	LEU
16	X	292	ASN
16	X	301	ILE
16	X	319	LEU
16	X	324	HIS
16	X	325	VAL
16	X	327	GLU
16	X	332	LEU
16	X	335	LEU
16	X	336	VAL
16	X	342	GLU
16	X	358	ILE
16	X	359	ILE
16	X	364	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	124	GLN
1	A	171	GLN
1	A	209	ASN
1	A	225	ASN
1	A	287	HIS
1	A	299	HIS
1	A	316	GLN
1	A	339	ASN
1	A	358	ASN
1	A	425	GLN
1	A	435	HIS
1	A	503	GLN
1	A	515	GLN
1	A	545	GLN
1	A	548	ASN
1	A	611	GLN
1	A	631	HIS
1	A	640	GLN
1	A	660	ASN
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1070	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1140	HIS
1	A	1187	GLN
1	A	1188	GLN
1	A	1218	GLN
1	A	1258	HIS

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Mol	Chain	Res	Type
1	A	1387	HIS
1	A	1432	GLN
2	B	46	GLN
2	B	47	GLN
2	B	121	ASN
2	B	255	GLN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	363	HIS
2	B	366	GLN
2	B	383	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	657	HIS
2	B	734	HIS
2	B	740	HIS
2	B	744	HIS
2	B	767	ASN
2	B	786	ASN
2	B	794	ASN
2	B	842	ASN
2	B	843	GLN
2	B	957	ASN
2	B	1015	HIS
2	B	1065	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	65	HIS
3	C	73	GLN
3	C	123	ASN
3	C	135	GLN
3	C	242	GLN
4	D	23	ASN
4	D	28	GLN
4	D	37	GLN

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Mol	Chain	Res	Type
4	D	39	ASN
4	D	132	GLN
4	D	137	ASN
4	D	143	ASN
4	D	179	GLN
5	E	115	ASN
5	E	147	HIS
7	G	10	ASN
7	G	14	HIS
7	G	24	GLN
7	G	71	ASN
7	G	117	GLN
7	G	122	ASN
8	H	128	ASN
8	H	133	ASN
9	I	11	ASN
9	I	12	ASN
9	I	83	ASN
9	I	89	GLN
9	I	114	GLN
10	J	53	HIS
11	K	44	ASN
11	K	65	HIS
12	L	53	HIS
12	L	66	GLN
16	X	281	ASN
16	X	318	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/11 (90%)	5 (50%)	2 (20%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	C
14	P	11	C
14	P	12	C
14	P	16	C
14	P	17	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	11	C
14	P	16	C

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	15	18,21,22	1.63	4 (22%)	25,30,33	2.32	9 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15	-	2/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C2-N1	3.78	1.44	1.38
15	T	22	BRU	C6-C5	3.23	1.40	1.34
15	T	22	BRU	C4-C5	2.82	1.50	1.45
15	T	22	BRU	C4-N3	-2.19	1.34	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	5.17	119.28	113.34
15	T	22	BRU	N3-C2-N1	5.03	121.44	114.89
15	T	22	BRU	C4-N3-C2	-4.44	121.52	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	BR-C5-C4	3.74	122.33	118.02
15	T	22	BRU	O4-C4-C5	-3.43	121.43	125.80
15	T	22	BRU	C6-C5-C4	-3.34	117.28	120.67
15	T	22	BRU	O2-C2-N3	-2.57	116.74	121.49
15	T	22	BRU	O4'-C1'-N1	2.45	112.21	107.86
15	T	22	BRU	C6-N1-C2	-2.24	119.07	121.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	22	BRU	O4'-C4'-C5'-O5'
15	T	22	BRU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	4.65
1	A	1173:HIS	C	1174:PHE	N	3.16

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	1429/1733 (82%)	-0.08	33 (2%) 61 41	59, 101, 164, 229	0
2	B	1097/1224 (89%)	0.12	40 (3%) 46 31	59, 114, 175, 208	0
3	C	266/318 (83%)	-0.30	0 100 100	77, 101, 141, 173	0
4	D	177/221 (80%)	0.16	15 (8%) 16 13	80, 111, 165, 179	0
5	E	214/215 (99%)	-0.05	1 (0%) 87 75	76, 135, 181, 211	0
6	F	84/155 (54%)	-0.53	1 (1%) 76 58	63, 83, 110, 134	0
7	G	171/171 (100%)	-0.15	3 (1%) 67 49	73, 100, 139, 166	0
8	H	133/146 (91%)	0.55	12 (9%) 15 12	112, 148, 183, 209	0
9	I	119/122 (97%)	0.35	5 (4%) 40 26	116, 148, 186, 203	0
10	J	65/70 (92%)	-0.25	2 (3%) 51 34	82, 101, 138, 146	0
11	K	115/120 (95%)	-0.33	2 (1%) 69 50	70, 103, 141, 155	0
12	L	46/70 (65%)	1.07	9 (19%) 3 3	86, 180, 196, 201	0
13	N	10/14 (71%)	1.16	1 (10%) 12 10	239, 248, 270, 275	0
14	P	11/11 (100%)	1.82	6 (54%) 0 0	204, 214, 222, 224	0
15	T	13/27 (48%)	0.77	0 100 100	165, 186, 260, 263	0
16	X	120/146 (82%)	1.35	27 (22%) 2 2	172, 203, 219, 229	0
All	All	4070/4763 (85%)	0.05	157 (3%) 43 29	59, 110, 188, 275	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.1
1	A	1081	LEU	7.3
2	B	502	ILE	6.7
2	B	467	GLY	6.6
1	A	2	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
2	B	1224	PHE	6.0
1	A	1176	LEU	6.0
2	B	509	ALA	5.9
2	B	446	LEU	5.8
8	H	132	LEU	5.8
16	X	291	LEU	5.7
2	B	709	ASP	5.4
8	H	136	LYS	5.3
4	D	24	ALA	5.2
2	B	882	THR	5.2
11	K	114	LEU	5.1
2	B	883	LEU	5.0
12	L	25	ALA	4.8
16	X	300	LYS	4.7
8	H	63	LEU	4.7
1	A	65	LEU	4.6
12	L	26	THR	4.6
2	B	249	ARG	4.6
2	B	335	GLY	4.4
1	A	186	LYS	4.3
12	L	27	LEU	4.3
2	B	881	ASN	4.3
8	H	139	ASN	4.3
16	X	274	ILE	4.3
16	X	301	ILE	4.3
16	X	257	THR	4.2
16	X	324	HIS	4.1
1	A	3	GLY	4.1
16	X	244	MET	3.9
16	X	323	ALA	3.9
8	H	90	ALA	3.8
11	K	115	ALA	3.7
16	X	320	GLU	3.7
2	B	70	ILE	3.6
2	B	251	ILE	3.6
4	D	25	ALA	3.5
2	B	715	ALA	3.5
1	A	50	ILE	3.5
16	X	261	LYS	3.4
1	A	251	SER	3.4
4	D	15	LEU	3.4
16	X	271	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
16	X	290	CYS	3.4
16	X	365	VAL	3.3
2	B	734	HIS	3.3
1	A	253	ASN	3.3
2	B	134	LYS	3.3
12	L	37	LYS	3.3
1	A	1254	ALA	3.3
2	B	934	LYS	3.2
6	F	72	LYS	3.2
2	B	108	VAL	3.2
9	I	52	ILE	3.2
2	B	477	ALA	3.2
16	X	339	ASN	3.2
2	B	250	PHE	3.2
10	J	65	PRO	3.2
4	D	31	GLN	3.1
16	X	273	SER	3.1
2	B	164	LYS	3.1
4	D	76	LYS	3.1
4	D	14	ARG	3.1
1	A	1174	PHE	3.1
14	P	12	C	3.0
16	X	330	LEU	3.0
8	H	82	PRO	3.0
1	A	1092	LYS	3.0
9	I	117	LYS	3.0
4	D	173	HIS	2.9
16	X	325	VAL	2.9
16	X	315	ASP	2.9
9	I	4	PHE	2.9
16	X	293	VAL	2.9
1	A	1093	LYS	2.8
16	X	310	TYR	2.8
1	A	56	PRO	2.8
1	A	1256	GLU	2.8
2	B	447	ALA	2.8
2	B	712	PRO	2.8
2	B	710	LEU	2.8
1	A	1455	PRO	2.7
4	D	221	TYR	2.7
13	N	10	DA	2.7
8	H	88	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	310	GLY	2.7
2	B	962	LYS	2.6
16	X	317	LYS	2.6
2	B	1222	ARG	2.6
12	L	28	LYS	2.6
1	A	707	GLY	2.6
9	I	2	THR	2.6
1	A	252	PHE	2.6
4	D	9	GLN	2.6
1	A	1255	GLU	2.6
4	D	19	GLU	2.6
1	A	79	GLY	2.5
8	H	140	ALA	2.5
2	B	884	ARG	2.5
8	H	131	ASN	2.5
10	J	1	MET	2.5
16	X	355	ARG	2.5
7	G	153	GLN	2.5
9	I	120	GLN	2.5
4	D	220	LEU	2.5
4	D	22	GLU	2.4
2	B	917	PRO	2.4
2	B	870	ILE	2.4
14	P	17	C	2.4
4	D	13	ARG	2.4
12	L	49	LYS	2.4
14	P	16	C	2.4
8	H	2	SER	2.4
5	E	3	GLN	2.3
2	B	879	ARG	2.3
12	L	45	ALA	2.3
14	P	7	C	2.3
7	G	64	THR	2.3
4	D	21	GLU	2.3
1	A	51	GLY	2.3
16	X	247	THR	2.3
1	A	1205	LYS	2.3
2	B	436	VAL	2.3
2	B	244	LEU	2.2
1	A	66	LYS	2.2
1	A	1246	LYS	2.2
4	D	12	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	668	ASP	2.2
7	G	154	VAL	2.2
12	L	41	SER	2.2
1	A	61	ILE	2.2
1	A	1257	ASP	2.2
12	L	46	VAL	2.2
8	H	85	GLY	2.2
16	X	321	LEU	2.1
2	B	919	SER	2.1
16	X	316	LYS	2.1
8	H	84	ALA	2.1
2	B	880	THR	2.1
2	B	229	ALA	2.1
1	A	893	PHE	2.1
2	B	31	TRP	2.1
1	A	323	LYS	2.1
2	B	345	LYS	2.1
2	B	708	GLU	2.1
1	A	1261	LYS	2.1
2	B	516	ASN	2.1
14	P	11	C	2.1
1	A	4	GLN	2.1
16	X	306	VAL	2.0
16	X	329	LYS	2.0
14	P	15	C	2.0
1	A	710	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.71	0.18	191,208,212,215	0

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
17	ZN	L	1071	1/1	0.97	0.06	207,207,207,207	0
18	MG	A	2458	1/1	0.98	0.06	77,77,77,77	0
17	ZN	I	1122	1/1	0.99	0.03	196,196,196,196	0
17	ZN	C	1269	1/1	1.00	0.02	81,81,81,81	0
17	ZN	I	1121	1/1	1.00	0.04	124,124,124,124	0
17	ZN	A	2456	1/1	1.00	0.02	141,141,141,141	0
17	ZN	J	1066	1/1	1.00	0.03	90,90,90,90	0
17	ZN	A	2457	1/1	1.00	0.04	79,79,79,79	0
17	ZN	B	2225	1/1	1.00	0.05	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.