



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:28 AM UTC

PDB ID : 3S15 / pdb_00003s15
Title : RNA Polymerase II Initiation Complex with a 7-nt RNA
Authors : Liu, X.; Bushnell, D.A.; Silva, D.A.; Huang, X.; Kornberg, R.D.
Deposited on : 2011-05-14
Resolution : 3.30 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

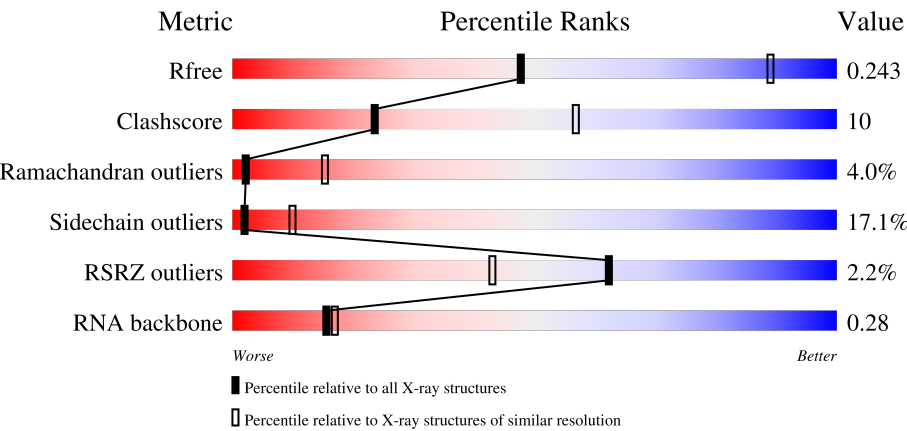
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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% 49% 25% 6% 19% •
2	B	1224	2% 54% 28% 8% 9% •
3	C	318	51% 27% 5% 16% •
4	E	215	66% 29% 5%

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Mol	Chain	Length	Quality of chain
5	F	155	41%14%45%
6	H	146	6% 56%27%7%9%
7	I	122	2% 70%22%6%
8	J	70	40%39%11%7%
9	K	120	% 65%26%5%
10	L	70	4% 31%21%9%34%
11	R	7	100%
12	T	29	3% 31%10%55%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 28717 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	1405	Total	C	N	O	S	0	0	0
			11043	6965	1936	2081	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- 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 polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	7	Total	C	N	O	P	0	0	0
			153	69	33	45	6			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	13	Total	C	N	O	P	0	0	0
			261	125	43	80	13			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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

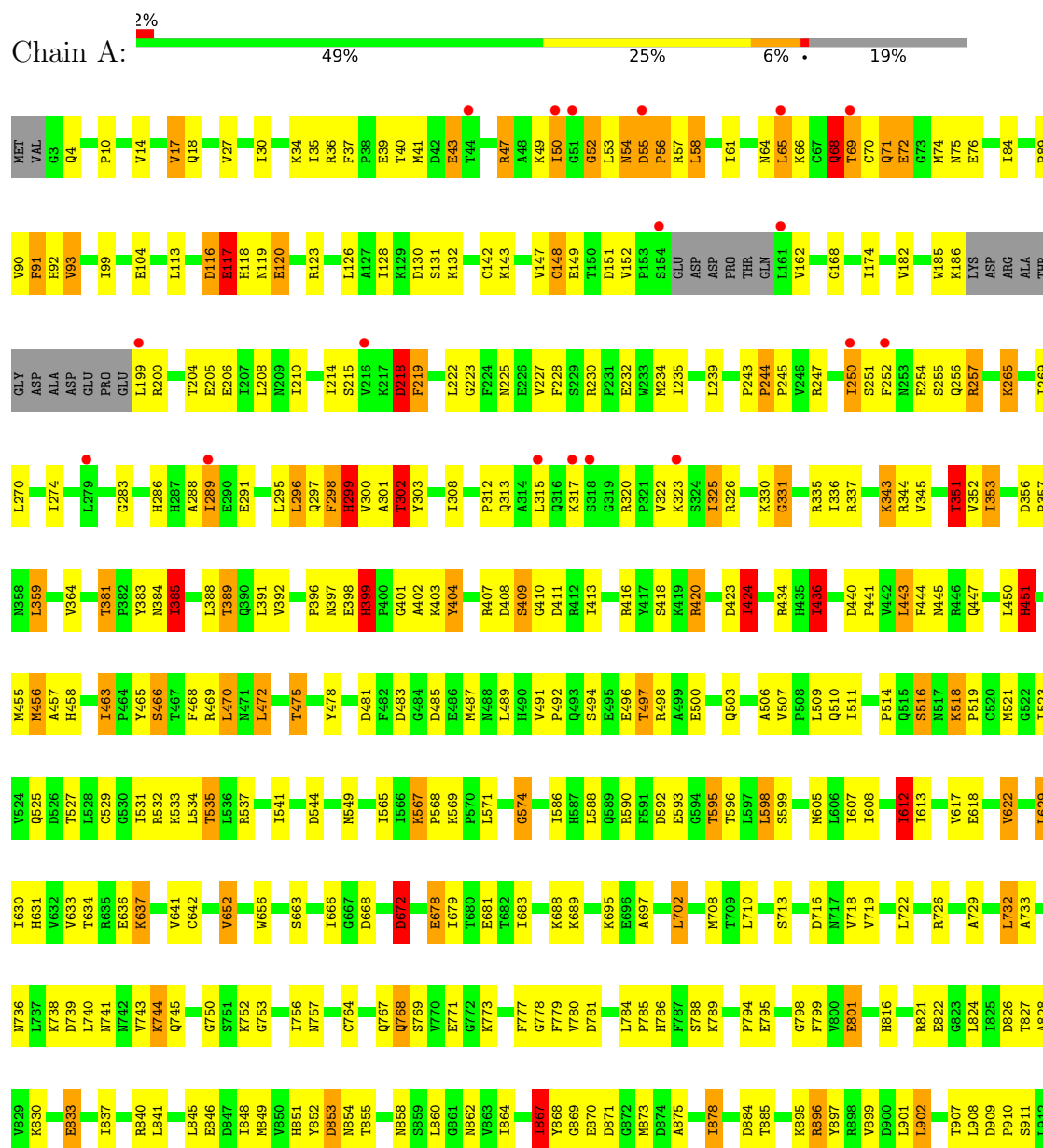
- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

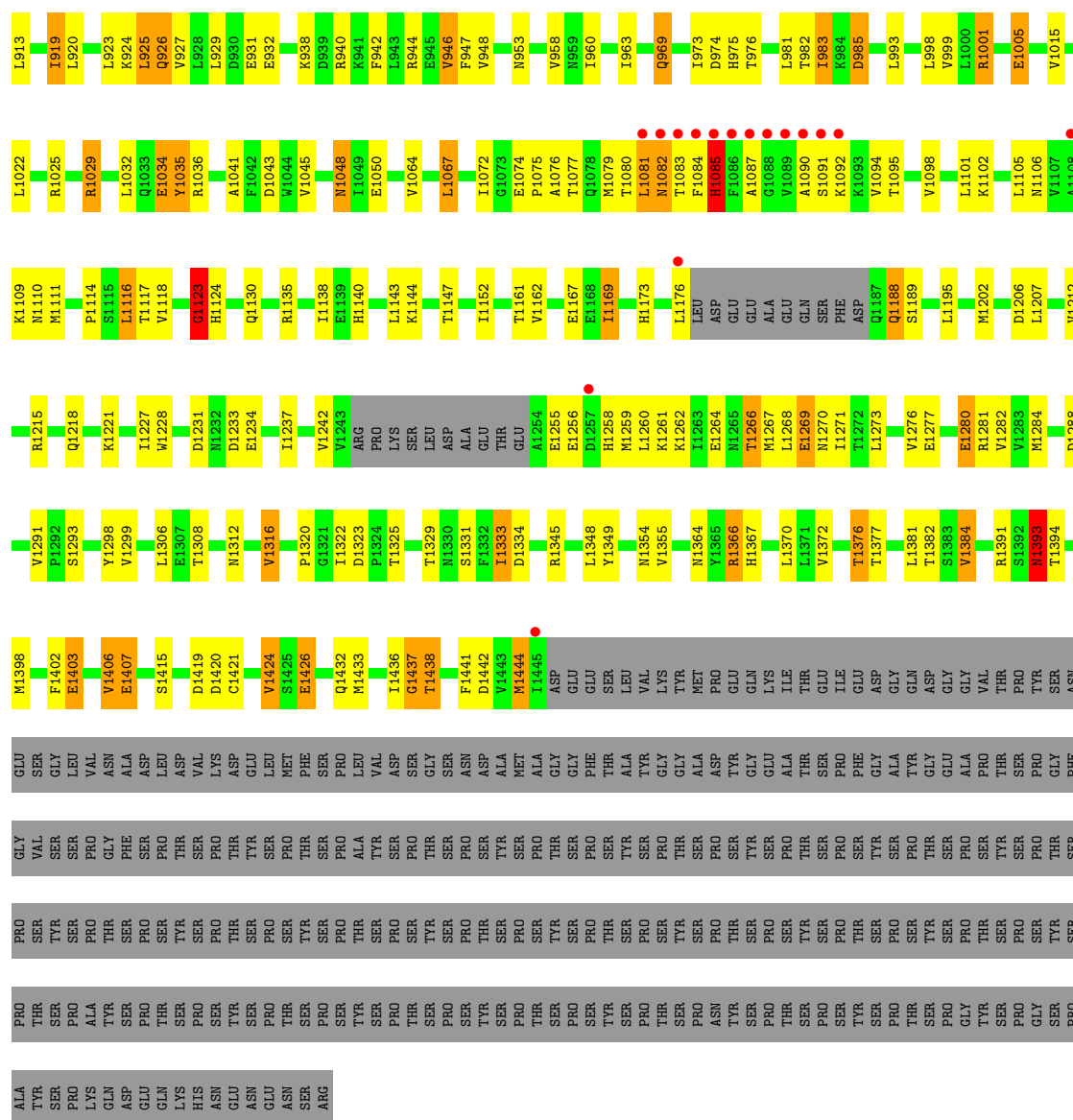
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0
14	B	1	Total 2	Mg 2	0	1

3 Residue-property plots

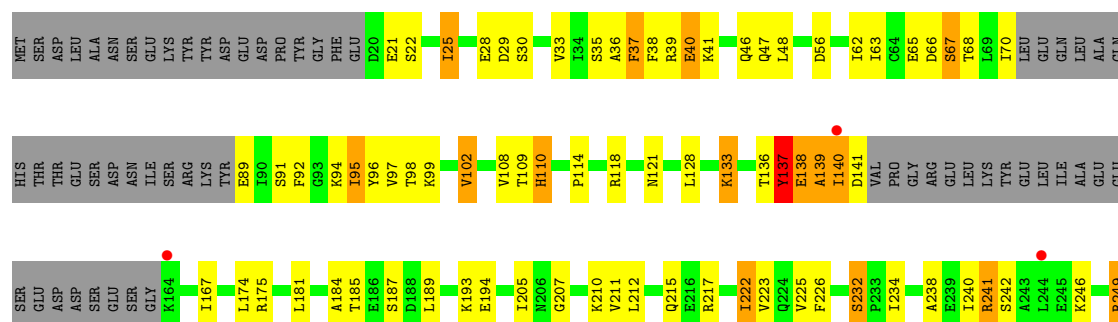
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

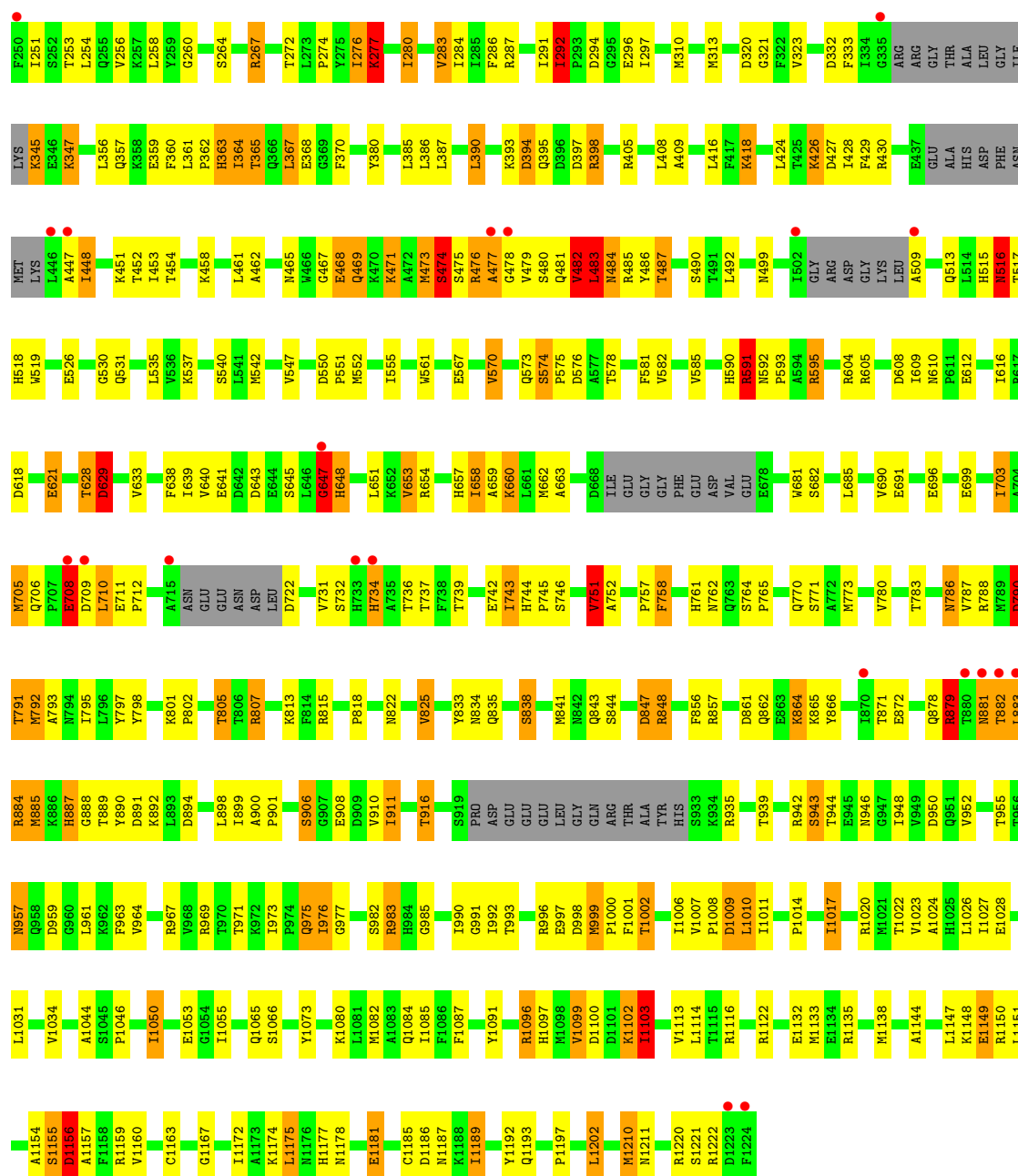
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1





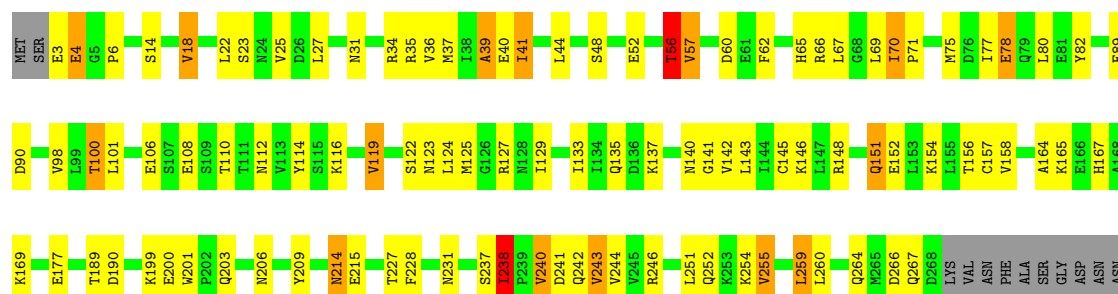
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2





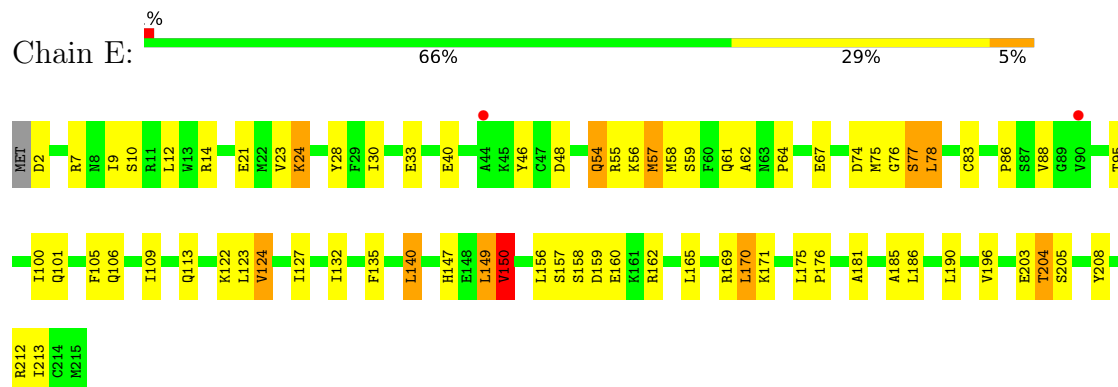
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 51% 27% 5% 16%

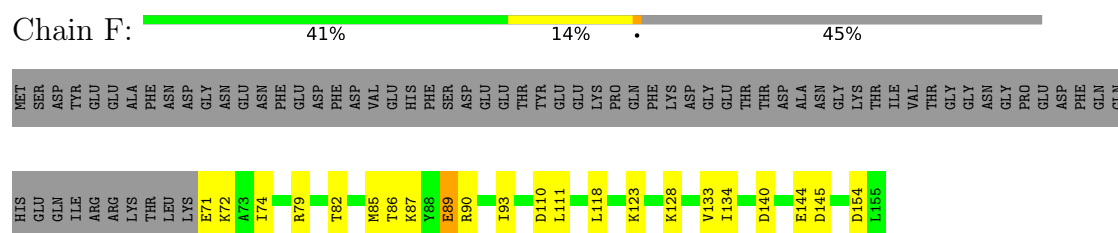


THR
ALA
SER
ASN
MET
LEU
GLY
SER
ASN
GLU
ASP
VAL
MET
MET
THR
GLY
ALA
GLN
ASP
PRO
TYR
SER
ASN
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SER
GLY
GLY
TYR
ASP
ASN
ALA
TRP

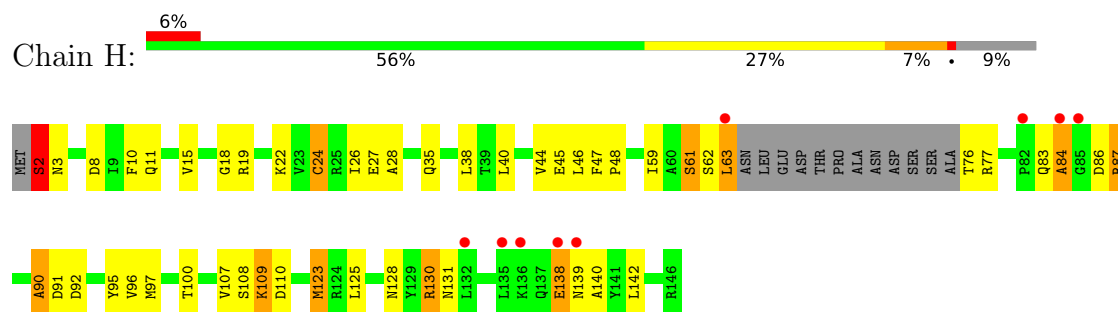
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



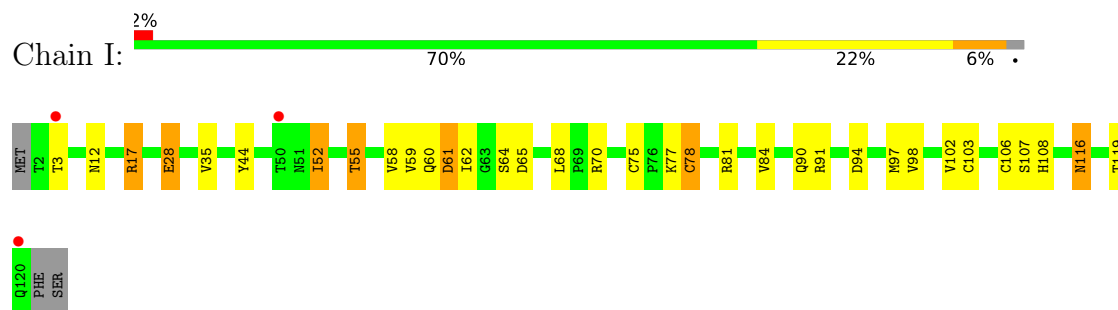
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

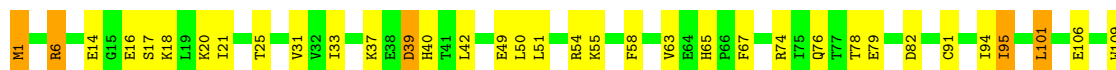


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

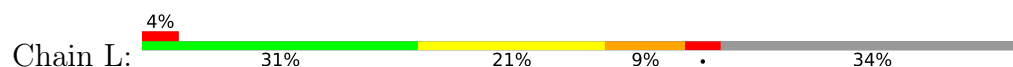




- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

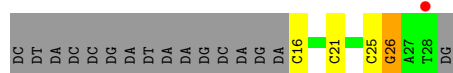
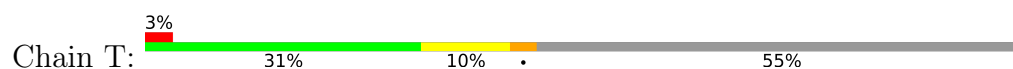


- Molecule 11: RNA (5'-R(*CP*GP*AP*GP*AP*GP*G)-3')



There are no outlier residues recorded for this chain.

- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*GP*AP*TP*AP*AP*GP*CP*AP*GP*AP*CP*GP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.93Å 220.89Å 194.62Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	44.11 – 3.30 44.11 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.11-3.30) 99.9 (44.11-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.32Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.174 , 0.228 0.191 , 0.243	Depositor DCC
R_{free} test set	5242 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 108.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28717	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	3/11241 (0.0%)	1.55	122/15199 (0.8%)
2	B	0.92	6/9033 (0.1%)	1.52	111/12181 (0.9%)
3	C	0.82	1/2133 (0.0%)	1.45	24/2891 (0.8%)
4	E	0.80	0/1788	1.44	16/2406 (0.7%)
5	F	0.86	0/700	1.35	3/945 (0.3%)
6	H	0.79	0/1086	1.34	16/1470 (1.1%)
7	I	0.84	0/989	1.40	4/1331 (0.3%)
8	J	0.91	1/541 (0.2%)	1.63	10/727 (1.4%)
9	K	0.74	0/937	1.38	7/1265 (0.6%)
10	L	0.94	0/365	1.61	8/485 (1.6%)
11	R	0.56	0/172	1.19	0/268
12	T	0.51	0/290	1.55	2/444 (0.5%)
All	All	0.87	11/29275 (0.0%)	1.50	323/39612 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	6.58	1.77	1.51
2	B	881	ASN	C-N	6.00	1.41	1.33
2	B	140	ILE	CA-C	5.77	1.59	1.52
3	C	267	GLN	CA-C	5.67	1.55	1.52
2	B	758	PHE	CA-C	5.66	1.57	1.53
1	A	487	MET	SD-CE	-5.65	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	764	SER	CA-C	5.45	1.58	1.52
2	B	705	MET	SD-CE	-5.34	1.66	1.79
2	B	662	MET	SD-CE	5.33	1.92	1.79
8	J	6	ARG	CA-C	5.19	1.59	1.52
1	A	456	MET	SD-CE	-5.02	1.67	1.79

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	647	GLY	CA-C-N	12.19	143.64	121.70
2	B	647	GLY	C-N-CA	12.19	143.64	121.70
10	L	58	LYS	N-CA-C	10.74	126.18	113.18
1	A	1162	VAL	N-CA-C	-10.30	103.44	113.53
1	A	218	ASP	CA-C-N	10.20	140.07	121.70
1	A	218	ASP	C-N-CA	10.20	140.07	121.70
2	B	37	PHE	N-CA-C	-9.77	98.07	110.19
3	C	56	THR	CA-C-N	9.38	132.70	120.60
3	C	56	THR	C-N-CA	9.38	132.70	120.60
8	J	5	VAL	N-CA-C	-9.37	97.50	109.58
12	T	16	DC	P-O3'-C3'	9.05	133.77	120.20
4	E	150	VAL	N-CA-C	8.47	115.27	107.56
1	A	298	PHE	CA-C-N	8.38	136.78	121.70
1	A	298	PHE	C-N-CA	8.38	136.78	121.70
6	H	2	SER	CA-C-N	8.31	136.66	121.70
6	H	2	SER	C-N-CA	8.31	136.66	121.70
1	A	999	VAL	N-CA-C	-8.18	105.25	112.12
2	B	1103	ILE	N-CA-CB	8.16	120.82	110.05
1	A	117	GLU	CA-C-N	7.94	136.00	121.70
1	A	117	GLU	C-N-CA	7.94	136.00	121.70
2	B	629	ASP	CA-CB-CG	7.94	120.54	112.60
2	B	628	THR	CA-C-N	7.91	136.65	121.54
2	B	628	THR	C-N-CA	7.91	136.65	121.54
2	B	345	LYS	CA-C-N	7.65	135.47	121.70
2	B	345	LYS	C-N-CA	7.65	135.47	121.70
1	A	794	PRO	CA-C-N	7.58	130.77	120.54
1	A	794	PRO	C-N-CA	7.58	130.77	120.54
2	B	575	PRO	CA-C-N	7.57	130.43	120.28
2	B	575	PRO	C-N-CA	7.57	130.43	120.28
3	C	40	GLU	N-CA-C	7.56	122.14	113.15
1	A	288	ALA	N-CA-C	-7.53	103.89	113.23
2	B	1156	ASP	N-CA-C	7.51	126.80	110.80
3	C	39	ALA	N-CA-C	7.50	122.91	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	ILE	N-CA-C	-7.48	103.23	110.42
2	B	648	HIS	N-CA-CB	7.47	123.20	110.50
1	A	351	THR	CA-C-N	7.42	130.44	120.50
1	A	351	THR	C-N-CA	7.42	130.44	120.50
2	B	479	VAL	N-CA-C	-7.42	98.92	108.93
2	B	140	ILE	CA-C-N	7.38	134.99	121.70
2	B	140	ILE	C-N-CA	7.38	134.99	121.70
2	B	109	THR	CB-CA-C	7.36	121.89	109.75
2	B	1155	SER	CA-C-N	7.35	135.57	121.54
2	B	1155	SER	C-N-CA	7.35	135.57	121.54
12	T	26	DG	P-O3'-C3'	7.28	131.12	120.20
6	H	61	SER	CA-C-N	7.19	135.28	121.54
6	H	61	SER	C-N-CA	7.19	135.28	121.54
2	B	66	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	466	SER	N-CA-C	7.15	121.60	113.02
1	A	1269	GLU	N-CA-C	7.13	118.84	111.14
1	A	1123	GLY	CA-C-N	7.09	134.47	121.70
1	A	1123	GLY	C-N-CA	7.09	134.47	121.70
2	B	1189	ILE	N-CA-C	7.01	117.58	111.90
2	B	535	LEU	N-CA-C	-6.94	104.45	113.12
2	B	881	ASN	CA-C-N	6.91	132.18	121.19
2	B	881	ASN	C-N-CA	6.91	132.18	121.19
6	H	92	ASP	N-CA-C	-6.89	103.27	113.61
1	A	116	ASP	CA-C-N	6.83	133.99	121.70
1	A	116	ASP	C-N-CA	6.83	133.99	121.70
2	B	474	SER	CA-C-N	6.82	131.61	120.63
2	B	474	SER	C-N-CA	6.82	131.61	120.63
2	B	447	ALA	CA-C-N	6.78	132.03	123.14
2	B	447	ALA	C-N-CA	6.78	132.03	123.14
1	A	69	THR	CA-C-N	6.69	129.55	120.38
1	A	69	THR	C-N-CA	6.69	129.55	120.38
2	B	910	VAL	CA-C-N	6.67	129.10	120.56
2	B	910	VAL	C-N-CA	6.67	129.10	120.56
2	B	140	ILE	N-CA-C	6.65	117.34	110.36
2	B	581	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	544	ASP	CA-C-N	6.57	129.38	120.44
1	A	544	ASP	C-N-CA	6.57	129.38	120.44
1	A	244	PRO	N-CA-C	6.56	118.70	110.70
1	A	397	ASN	N-CA-C	6.51	121.35	113.41
1	A	1098	VAL	N-CA-CB	6.51	114.88	110.52
3	C	57	VAL	N-CA-CB	-6.50	103.30	110.51
3	C	200	GLU	N-CA-C	6.49	119.35	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	48	ASP	CA-CB-CG	6.49	119.09	112.60
2	B	320	ASP	CA-CB-CG	6.46	119.06	112.60
8	J	9	SER	N-CA-C	6.45	118.00	110.97
2	B	739	THR	N-CA-C	-6.44	106.05	114.04
2	B	99	LYS	N-CA-C	-6.42	101.43	110.29
2	B	66	ASP	N-CA-C	-6.41	104.51	112.90
1	A	481	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	136	THR	CA-C-N	6.40	133.77	121.54
2	B	136	THR	C-N-CA	6.40	133.77	121.54
10	L	40	LEU	N-CA-C	6.38	119.41	109.52
2	B	427	ASP	CA-CB-CG	6.36	118.96	112.60
3	C	82	TYR	N-CA-C	-6.34	100.17	110.20
3	C	108	GLU	N-CA-C	-6.34	104.45	111.36
1	A	1207	LEU	N-CA-C	6.33	119.82	109.24
1	A	485	ASP	CA-CB-CG	6.33	118.93	112.60
3	C	60	ASP	CA-CB-CG	6.32	118.92	112.60
2	B	1066	SER	N-CA-C	6.31	119.83	111.75
1	A	1280	GLU	N-CA-C	6.28	117.92	111.14
1	A	596	THR	N-CA-C	-6.27	100.22	109.81
1	A	424	ILE	N-CA-C	6.26	122.36	109.34
4	E	203	GLU	CA-C-N	6.25	131.00	120.88
4	E	203	GLU	C-N-CA	6.25	131.00	120.88
1	A	932	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	1407	GLU	CB-CG-CD	6.20	123.14	112.60
2	B	397	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	1085	HIS	CA-C-N	6.16	129.15	120.28
1	A	1085	HIS	C-N-CA	6.16	129.15	120.28
1	A	652	VAL	N-CA-CB	6.15	117.60	110.65
2	B	280	ILE	N-CA-C	6.13	115.29	108.05
1	A	947	PHE	CA-C-N	6.13	129.18	120.53
1	A	947	PHE	C-N-CA	6.13	129.18	120.53
1	A	1256	GLU	N-CA-C	6.13	119.59	111.75
1	A	445	ASN	CA-CB-CG	6.11	118.71	112.60
3	C	62	PHE	N-CA-C	-6.11	104.53	111.07
3	C	238	ILE	N-CA-CB	-6.08	105.13	111.64
1	A	1419	ASP	CA-C-N	6.08	128.42	120.28
1	A	1419	ASP	C-N-CA	6.08	128.42	120.28
1	A	451	HIS	CB-CA-C	-6.06	99.07	110.16
4	E	56	LYS	CA-C-N	6.03	128.36	120.28
4	E	56	LYS	C-N-CA	6.03	128.36	120.28
2	B	825	VAL	N-CA-C	6.02	116.97	108.36
10	L	50	ASP	CA-C-N	6.01	133.03	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	50	ASP	C-N-CA	6.01	133.03	121.54
2	B	276	ILE	CA-C-N	6.01	133.02	121.54
2	B	276	ILE	C-N-CA	6.01	133.02	121.54
2	B	1009	ASP	N-CA-C	-6.00	105.03	112.90
3	C	135	GLN	CA-C-N	6.00	129.63	121.05
3	C	135	GLN	C-N-CA	6.00	129.63	121.05
3	C	243	VAL	N-CA-CB	6.00	117.17	110.51
2	B	516	ASN	CA-C-N	5.97	129.10	120.38
2	B	516	ASN	C-N-CA	5.97	129.10	120.38
2	B	609	ILE	N-CA-C	-5.94	99.79	108.11
1	A	1228	TRP	N-CA-C	5.91	118.06	109.07
2	B	976	ILE	N-CA-C	5.87	121.56	109.34
1	A	864	ILE	N-CA-C	-5.87	106.09	111.67
9	K	106	GLU	CA-C-N	5.86	128.06	120.44
9	K	106	GLU	C-N-CA	5.86	128.06	120.44
1	A	985	ASP	CA-CB-CG	5.86	118.46	112.60
4	E	170	LEU	CA-C-N	5.86	131.76	122.62
4	E	170	LEU	C-N-CA	5.86	131.76	122.62
1	A	853	ASP	CA-CB-CG	5.84	118.44	112.60
2	B	722	ASP	CA-C-N	5.82	128.30	120.50
2	B	722	ASP	C-N-CA	5.82	128.30	120.50
2	B	471	LYS	CA-C-N	5.81	128.38	120.54
2	B	471	LYS	C-N-CA	5.81	128.38	120.54
2	B	847	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	1288	ASP	CA-CB-CG	5.80	118.40	112.60
2	B	476	ARG	CA-C-N	5.80	132.61	121.54
2	B	476	ARG	C-N-CA	5.80	132.61	121.54
10	L	68	GLU	N-CA-C	-5.80	99.84	109.46
2	B	971	THR	CB-CA-C	5.80	119.31	109.80
1	A	946	VAL	N-CA-C	-5.78	105.48	110.74
1	A	483	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	289	ILE	CA-C-N	5.77	128.02	120.28
1	A	289	ILE	C-N-CA	5.77	128.02	120.28
2	B	882	THR	N-CA-C	5.76	120.83	111.37
1	A	336	ILE	N-CA-C	5.76	115.84	110.42
1	A	884	ASP	N-CA-C	5.76	118.33	111.71
1	A	1001	ARG	N-CA-C	5.76	120.68	113.43
9	K	82	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	1377	THR	N-CA-C	5.73	119.79	112.34
1	A	399	HIS	N-CA-CB	5.72	120.55	110.37
7	I	78	CYS	CA-C-N	-5.71	113.59	123.25
7	I	78	CYS	C-N-CA	-5.71	113.59	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	87	LYS	CA-C-N	5.70	128.38	120.29
5	F	87	LYS	C-N-CA	5.70	128.38	120.29
2	B	834	ASN	CA-CB-CG	5.70	118.30	112.60
4	E	160	GLU	CA-C-N	5.69	127.84	120.44
4	E	160	GLU	C-N-CA	5.69	127.84	120.44
1	A	436	ILE	CB-CA-C	5.69	118.95	111.33
2	B	648	HIS	CA-CB-CG	-5.69	108.11	113.80
2	B	110	HIS	N-CA-CB	-5.68	102.10	110.85
6	H	138	GLU	N-CA-C	-5.67	105.62	112.54
1	A	718	VAL	CA-C-N	5.65	127.89	120.60
1	A	718	VAL	C-N-CA	5.65	127.89	120.60
9	K	21	ILE	N-CA-C	5.65	115.47	106.88
1	A	204	THR	CA-C-N	5.65	127.85	120.28
1	A	204	THR	C-N-CA	5.65	127.85	120.28
2	B	139	ALA	CA-C-N	5.65	127.88	120.60
2	B	139	ALA	C-N-CA	5.65	127.88	120.60
6	H	91	ASP	CA-C-N	5.65	131.10	122.29
6	H	91	ASP	C-N-CA	5.65	131.10	122.29
2	B	1154	ALA	N-CA-C	-5.64	100.62	109.25
1	A	71	GLN	CA-C-N	5.63	132.29	121.54
1	A	71	GLN	C-N-CA	5.63	132.29	121.54
1	A	27	VAL	CA-C-N	5.60	127.72	120.44
1	A	27	VAL	C-N-CA	5.60	127.72	120.44
8	J	1	MET	CA-C-N	5.58	132.02	121.97
8	J	1	MET	C-N-CA	5.58	132.02	121.97
1	A	827	THR	N-CA-C	-5.57	104.60	111.40
2	B	591	ARG	N-CA-C	-5.57	101.39	110.20
2	B	452	THR	CA-C-N	5.57	127.67	120.88
2	B	452	THR	C-N-CA	5.57	127.67	120.88
2	B	659	ALA	CA-C-N	5.57	128.00	120.38
2	B	659	ALA	C-N-CA	5.57	128.00	120.38
1	A	750	GLY	CA-C-N	5.56	128.19	120.29
1	A	750	GLY	C-N-CA	5.56	128.19	120.29
2	B	790	ASP	CA-CB-CG	5.56	118.16	112.60
8	J	53	HIS	CA-C-N	5.55	130.65	123.11
8	J	53	HIS	C-N-CA	5.55	130.65	123.11
8	J	18	TRP	N-CA-C	5.54	117.18	111.03
2	B	47	GLN	CA-C-N	5.54	127.64	120.44
2	B	47	GLN	C-N-CA	5.54	127.64	120.44
2	B	1186	ASP	CA-C-N	5.54	128.63	120.82
2	B	1186	ASP	C-N-CA	5.54	128.63	120.82
3	C	34	ARG	CA-C-N	5.51	127.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	34	ARG	C-N-CA	5.51	127.60	120.44
1	A	529	CYS	CA-C-N	5.48	126.02	119.94
1	A	529	CYS	C-N-CA	5.48	126.02	119.94
2	B	363	HIS	N-CA-C	-5.47	101.23	109.60
3	C	78	GLU	CB-CG-CD	5.46	121.89	112.60
2	B	222	ILE	CB-CA-C	5.46	118.26	110.84
2	B	736	THR	CA-C-N	5.46	131.97	121.54
2	B	736	THR	C-N-CA	5.46	131.97	121.54
1	A	463	ILE	N-CA-C	5.45	115.16	109.01
2	B	660	LYS	CA-C-N	5.44	127.83	120.44
2	B	660	LYS	C-N-CA	5.44	127.83	120.44
2	B	276	ILE	N-CA-C	5.42	115.90	107.99
1	A	1255	GLU	CA-C-N	5.42	128.29	120.38
1	A	1255	GLU	C-N-CA	5.42	128.29	120.38
2	B	394	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	537	ARG	CA-C-N	5.39	127.51	120.28
1	A	537	ARG	C-N-CA	5.39	127.51	120.28
1	A	1092	LYS	CA-C-N	5.39	128.42	120.82
1	A	1092	LYS	C-N-CA	5.39	128.42	120.82
2	B	593	PRO	CA-C-N	5.38	127.48	120.28
2	B	593	PRO	C-N-CA	5.38	127.48	120.28
2	B	628	THR	N-CA-C	-5.38	106.89	113.50
1	A	1035	TYR	N-CA-C	-5.36	101.73	110.20
9	K	78	THR	CA-C-N	5.35	128.45	120.90
9	K	78	THR	C-N-CA	5.35	128.45	120.90
1	A	592	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	451	HIS	N-CA-CB	-5.33	102.06	111.39
1	A	1169	ILE	CA-C-N	5.33	127.99	120.42
1	A	1169	ILE	C-N-CA	5.33	127.99	120.42
2	B	184	ALA	N-CA-C	5.30	117.92	110.23
3	C	255	VAL	N-CA-C	-5.30	105.22	111.00
2	B	861	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	703	ILE	N-CA-C	5.30	116.61	108.71
4	E	48	ASP	CA-C-N	5.29	127.62	120.38
4	E	48	ASP	C-N-CA	5.29	127.62	120.38
1	A	798	GLY	N-CA-C	5.28	123.35	115.64
2	B	731	VAL	CA-C-N	5.28	128.58	120.82
2	B	731	VAL	C-N-CA	5.28	128.58	120.82
6	H	130	ARG	CA-C-N	5.28	131.62	121.54
6	H	130	ARG	C-N-CA	5.28	131.62	121.54
3	C	119	VAL	N-CA-C	5.28	115.58	107.77
1	A	1384	VAL	CA-C-N	5.27	130.99	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1384	VAL	C-N-CA	5.27	130.99	122.29
1	A	408	ASP	N-CA-C	-5.27	102.25	110.10
2	B	786	ASN	CA-CB-CG	5.27	117.87	112.60
6	H	91	ASP	N-CA-C	5.27	117.76	108.75
6	H	92	ASP	CA-C-N	5.26	130.55	120.97
6	H	92	ASP	C-N-CA	5.26	130.55	120.97
6	H	139	ASN	CA-C-N	5.26	131.58	121.54
6	H	139	ASN	C-N-CA	5.26	131.58	121.54
10	L	62	LYS	CA-C-N	5.25	127.58	120.38
10	L	62	LYS	C-N-CA	5.25	127.58	120.38
10	L	62	LYS	N-CA-C	-5.25	106.65	113.16
6	H	139	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	1072	ILE	N-CA-C	-5.23	106.58	111.45
1	A	726	ARG	CA-C-N	5.22	127.22	120.44
1	A	726	ARG	C-N-CA	5.22	127.22	120.44
2	B	140	ILE	CA-C-O	-5.22	115.84	121.27
2	B	807	ARG	CA-C-N	5.22	127.27	120.28
2	B	807	ARG	C-N-CA	5.22	127.27	120.28
1	A	1005	GLU	CA-C-N	5.20	127.12	120.56
1	A	1005	GLU	C-N-CA	5.20	127.12	120.56
5	F	140	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	791	THR	CB-CA-C	-5.19	101.59	109.89
2	B	363	HIS	CA-C-O	-5.19	116.12	121.98
8	J	57	ILE	CA-C-N	5.18	127.17	120.44
8	J	57	ILE	C-N-CA	5.18	127.17	120.44
2	B	292	ILE	N-CA-C	5.17	120.04	108.88
3	C	259	LEU	CA-C-N	5.16	127.20	120.28
3	C	259	LEU	C-N-CA	5.16	127.20	120.28
2	B	215	GLN	N-CA-C	5.15	117.00	108.20
1	A	302	THR	CB-CA-C	5.14	119.33	110.79
1	A	478	TYR	CA-C-N	5.14	129.44	122.19
1	A	478	TYR	C-N-CA	5.14	129.44	122.19
9	K	39	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	331	GLY	CA-C-N	5.14	131.36	121.54
1	A	331	GLY	C-N-CA	5.14	131.36	121.54
1	A	612	ILE	N-CA-CB	5.14	117.63	111.31
1	A	907	THR	N-CA-C	-5.13	103.91	110.53
1	A	777	PHE	CA-CB-CG	5.13	118.93	113.80
3	C	237	SER	CA-C-N	5.13	128.91	121.68
3	C	237	SER	C-N-CA	5.13	128.91	121.68
1	A	948	VAL	CA-C-N	5.13	127.15	120.28
1	A	948	VAL	C-N-CA	5.13	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	N-CA-C	5.11	116.84	109.07
8	J	55	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	250	ILE	N-CA-CB	5.11	119.66	111.23
2	B	805	THR	N-CA-C	5.11	117.43	109.52
2	B	916	THR	CB-CA-C	5.10	116.97	110.13
1	A	1043	ASP	CA-C-N	5.10	127.07	120.44
1	A	1043	ASP	C-N-CA	5.10	127.07	120.44
1	A	1271	ILE	N-CA-C	5.10	114.95	108.12
2	B	232	SER	N-CA-C	5.09	117.39	110.01
2	B	884	ARG	CA-C-N	5.08	128.42	120.75
2	B	884	ARG	C-N-CA	5.08	128.42	120.75
2	B	982	SER	N-CA-C	-5.08	103.98	110.53
1	A	142	CYS	N-CA-C	5.07	118.50	112.72
1	A	296	LEU	N-CA-C	-5.07	105.40	112.45
1	A	1090	ALA	N-CA-C	5.07	118.93	112.34
7	I	81	ARG	N-CA-C	-5.06	107.61	112.97
2	B	56	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	786	ASN	CA-C-N	5.06	127.87	121.85
2	B	786	ASN	C-N-CA	5.06	127.87	121.85
1	A	733	ALA	CA-C-N	5.05	128.40	120.82
1	A	733	ALA	C-N-CA	5.05	128.40	120.82
1	A	708	MET	N-CA-C	5.05	117.06	109.23
3	C	110	THR	CB-CA-C	5.05	117.07	110.06
1	A	58	LEU	N-CA-C	5.03	118.68	112.54
1	A	17	VAL	N-CA-CB	5.03	118.24	111.90
2	B	894	ASP	CA-C-N	5.03	127.27	120.38
2	B	894	ASP	C-N-CA	5.03	127.27	120.38
7	I	116	ASN	N-CA-C	5.03	118.31	110.32
1	A	574	GLY	CA-C-N	5.02	127.32	120.54
1	A	574	GLY	C-N-CA	5.02	127.32	120.54
4	E	21	GLU	CA-C-N	5.01	126.96	120.44
4	E	21	GLU	C-N-CA	5.01	126.96	120.44
1	A	345	VAL	N-CA-C	5.01	117.02	108.86
2	B	663	ALA	N-CA-C	-5.01	105.82	111.28
1	A	795	GLU	CB-CG-CD	5.00	121.11	112.60
1	A	1138	ILE	N-CA-C	5.00	115.95	111.90
4	E	54	GLN	CA-C-N	5.00	127.40	120.29
4	E	54	GLN	C-N-CA	5.00	127.40	120.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	647	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11043	0	11133	253	0
2	B	8861	0	8884	225	0
3	C	2095	0	2051	49	0
4	E	1752	0	1776	31	0
5	F	688	0	707	9	0
6	H	1068	0	1040	28	0
7	I	971	0	927	10	0
8	J	532	0	542	27	0
9	K	919	0	929	17	0
10	L	363	0	386	13	0
11	R	153	0	78	0	0
12	T	261	0	148	5	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
All	All	28717	0	28601	587	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 10.

All (587) 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	1.77	1.60
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.42	1.01
1:A:494:SER:HB3	1:A:497:THR:HB	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.97	0.97
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.46	0.94
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.15	0.93
1:A:535:THR:HG21	1:A:617:VAL:H	1.32	0.92
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.54	0.88
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.03	0.86
1:A:1123:GLY:HA3	1:A:1124:HIS:HB2	1.58	0.86
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.59	0.84
2:B:706:GLN:O	2:B:710:LEU:HB2	1.78	0.84
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.60	0.84
2:B:654:ARG:H	2:B:657:HIS:HD2	1.25	0.83
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.61	0.82
1:A:131:SER:HB3	1:A:223:GLY:HA2	1.61	0.81
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.62	0.81
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.46	0.80
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.64	0.79
3:C:167:HIS:HD2	3:C:169:LYS:H	1.28	0.79
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.47	0.78
1:A:869:GLY:O	4:E:204:THR:HG21	1.84	0.77
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.68	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.49	0.75
2:B:1050:ILE:HG23	2:B:1055:ILE:HD11	1.67	0.75
4:E:77:SER:HB3	4:E:105:PHE:HA	1.68	0.75
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.67	0.74
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.53	0.74
8:J:1:MET:N	8:J:57:ILE:H	1.85	0.74
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.52	0.74
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.53	0.74
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.17	0.74
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.69	0.73
1:A:535:THR:HG21	1:A:617:VAL:N	2.04	0.73
2:B:906:SER:HA	2:B:946:ASN:HB3	1.70	0.73
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.71	0.73
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.69	0.72
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.72	0.72
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.37	0.72
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.70	0.72
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.23	0.71
1:A:535:THR:CG2	1:A:617:VAL:H	2.03	0.71
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.73	0.71
1:A:565:ILE:CG2	1:A:567:LYS:HE3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.19	0.70
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.73	0.70
2:B:744:HIS:HD2	2:B:746:SER:H	1.40	0.70
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.56	0.70
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.57	0.70
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.57	0.69
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.27	0.69
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.73	0.69
1:A:43:GLU:HG3	1:A:50:ILE:HG12	1.75	0.69
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.73	0.69
1:A:924:LYS:O	1:A:927:VAL:HG12	1.93	0.68
2:B:211:VAL:CG2	2:B:483:LEU:HD13	2.24	0.68
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.76	0.67
2:B:705:MET:HE3	2:B:742:GLU:HG3	1.76	0.67
2:B:428:ILE:HD11	2:B:448:ILE:HA	1.76	0.67
3:C:56:THR:HG21	3:C:145:CYS:SG	2.34	0.66
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.23	0.66
2:B:843:GLN:HB2	2:B:993:THR:HB	1.78	0.65
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.77	0.65
1:A:1091:SER:HB2	1:A:1281:ARG:HH12	1.61	0.65
1:A:567:LYS:HB3	6:H:96:VAL:H	1.60	0.65
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.10	0.64
2:B:345:LYS:HA	2:B:347:LYS:H	1.62	0.64
3:C:167:HIS:CD2	3:C:169:LYS:H	2.14	0.64
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.80	0.64
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.30	0.64
2:B:91:SER:HB3	2:B:133:LYS:HB2	1.80	0.64
1:A:741:ASN:HD22	1:A:744:LYS:H	1.44	0.64
1:A:219:PHE:HZ	1:A:230:ARG:HG2	1.63	0.63
2:B:542:MET:HE1	2:B:743:ILE:HG13	1.80	0.63
2:B:864:LYS:HB3	2:B:872:GLU:H	1.62	0.63
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.28	0.63
2:B:900:ALA:HA	10:L:58:LYS:HD3	1.81	0.63
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.92	0.63
6:H:100:THR:HG23	6:H:138:GLU:HA	1.79	0.63
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.93	0.63
2:B:40:GLU:HG2	2:B:681:TRP:HB3	1.81	0.63
9:K:91:CYS:O	9:K:95:ILE:HG12	1.99	0.63
2:B:516:ASN:H	2:B:516:ASN:HD22	1.48	0.62
2:B:618:ASP:OD2	2:B:621:GLU:HB2	1.99	0.62
3:C:22:LEU:HD21	9:K:101:LEU:HD21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:ARG:O	2:B:478:GLY:N	2.31	0.62
6:H:24:CYS:HB2	6:H:44:VAL:HG21	1.80	0.62
2:B:137:TYR:H	2:B:137:TYR:HD2	1.47	0.62
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.81	0.62
2:B:906:SER:HA	2:B:946:ASN:CB	2.29	0.61
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.33	0.61
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.82	0.61
6:H:2:SER:N	6:H:61:SER:HG	1.98	0.61
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.00	0.61
8:J:44:TYR:HA	8:J:47:ARG:HG3	1.83	0.61
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.82	0.60
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.83	0.60
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.82	0.60
3:C:98:VAL:H	3:C:122:SER:HB2	1.65	0.60
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.82	0.60
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.83	0.60
1:A:41:MET:HB2	1:A:49:LYS:HA	1.82	0.60
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.61	0.60
2:B:801:LYS:O	8:J:52:THR:CG2	2.49	0.60
3:C:98:VAL:HG22	3:C:158:VAL:HG22	1.83	0.60
1:A:518:LYS:HA	1:A:631:HIS:CD2	2.36	0.60
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.84	0.60
3:C:165:LYS:O	9:K:6:ARG:NH1	2.34	0.60
8:J:1:MET:H2	8:J:57:ILE:H	1.47	0.60
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.83	0.60
2:B:241:ARG:HG3	2:B:253:THR:HG22	1.82	0.60
1:A:152:VAL:HG23	1:A:162:VAL:HB	1.84	0.60
1:A:117:GLU:H	1:A:118:HIS:CB	2.15	0.59
2:B:249:ARG:HH11	2:B:251:ILE:HD11	1.66	0.59
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.66	0.59
1:A:666:ILE:HD13	2:B:1026:LEU:HB2	1.84	0.59
1:A:913:LEU:HD11	1:A:981:LEU:O	2.02	0.59
1:A:34:LYS:HD3	1:A:36:ARG:HH21	1.67	0.59
1:A:225:ASN:HD22	1:A:228:PHE:H	1.49	0.59
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.68	0.59
1:A:860:LEU:HD21	1:A:1394:THR:HA	1.85	0.58
2:B:515:HIS:HD2	2:B:517:THR:H	1.51	0.58
2:B:879:ARG:O	2:B:882:THR:HG22	2.03	0.58
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.84	0.58
1:A:55:ASP:O	1:A:57:ARG:N	2.37	0.58
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG21	1:A:466:SER:O	2.03	0.58
2:B:515:HIS:CD2	2:B:517:THR:H	2.22	0.58
7:I:65:ASP:HB3	7:I:68:LEU:HD12	1.85	0.58
2:B:835:GLN:O	2:B:838:SER:HB2	2.04	0.58
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.69	0.58
1:A:511:ILE:HA	1:A:521:MET:HE3	1.86	0.57
1:A:218:ASP:H	1:A:219:PHE:HB3	1.69	0.57
2:B:482:VAL:HG11	12:T:26:DG:H5"	1.86	0.57
4:E:62:ALA:HB3	4:E:78:LEU:HB3	1.85	0.57
1:A:299:HIS:O	1:A:301:ALA:N	2.37	0.57
1:A:567:LYS:HB3	6:H:96:VAL:N	2.19	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.70	0.57
2:B:38:PHE:H	2:B:41:LYS:HB2	1.69	0.57
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.57
3:C:123:ASN:ND2	3:C:125:MET:HG3	2.19	0.57
2:B:901:PRO:HD3	10:L:58:LYS:HB3	1.87	0.56
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.56
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.40	0.56
7:I:17:ARG:HB2	7:I:28:GLU:HG2	1.86	0.56
1:A:982:THR:HB	1:A:985:ASP:H	1.70	0.56
2:B:211:VAL:O	2:B:480:SER:HA	2.04	0.56
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.87	0.56
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.85	0.56
1:A:356:ASP:HB3	1:A:359:LEU:HB2	1.88	0.56
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.37	0.56
1:A:75:ASN:HA	2:B:1116:ARG:NH1	2.21	0.56
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.69	0.56
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.88	0.55
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.86	0.55
1:A:503:GLN:HE21	5:F:90:ARG:HH12	1.53	0.55
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.36	0.55
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.55
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.35	0.55
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.89	0.55
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.87	0.55
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.88	0.55
10:L:31:CYS:HA	10:L:56:LEU:HD23	1.88	0.55
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.87	0.55
3:C:37:MET:HA	3:C:41:ILE:HD11	1.89	0.55
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.87	0.55
2:B:35:SER:O	2:B:39:ARG:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:CD	2.82	0.55
2:B:706:GLN:H	2:B:710:LEU:HG	1.72	0.55
4:E:64:PRO:HD3	4:E:76:GLY:HA2	1.89	0.55
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	1.89	0.54
2:B:140:ILE:HB	2:B:141:ASP:HB2	1.89	0.54
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.41	0.54
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.07	0.54
3:C:167:HIS:HD2	3:C:169:LYS:N	2.03	0.54
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.42	0.54
1:A:516:SER:HB3	1:A:518:LYS:HG2	1.89	0.54
1:A:523:ILE:HG23	1:A:527:THR:HG22	1.90	0.54
2:B:879:ARG:HA	2:B:879:ARG:CZ	2.38	0.54
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.89	0.54
3:C:14:SER:HA	9:K:114:LEU:HD23	1.89	0.54
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.89	0.54
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.89	0.54
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.89	0.54
8:J:32:GLU:CD	8:J:32:GLU:H	2.14	0.54
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.73	0.54
1:A:519:PRO:HD3	1:A:631:HIS:HD2	1.72	0.54
4:E:64:PRO:HB3	4:E:75:MET:HE2	1.91	0.53
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.90	0.53
2:B:94:LYS:HG2	2:B:96:TYR:CZ	2.43	0.53
4:E:165:LEU:HD13	4:E:170:LEU:HB2	1.91	0.53
10:L:32:ALA:HB3	10:L:55:ILE:HB	1.90	0.53
2:B:486:TYR:OH	2:B:1096:ARG:HB3	2.09	0.53
1:A:982:THR:H	1:A:985:ASP:HB2	1.73	0.53
2:B:313:MET:HE2	2:B:390:LEU:HG	1.91	0.53
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.91	0.53
2:B:1082:MET:HE3	3:C:190:ASP:HB2	1.90	0.53
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.90	0.53
5:F:85:MET:HG3	5:F:89:GLU:HB3	1.91	0.53
2:B:1009:ASP:OD2	8:J:48:ARG:NH2	2.42	0.53
1:A:64:ASN:HB3	1:A:66:LYS:HZ3	1.74	0.53
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.43	0.53
2:B:999:MET:HE3	2:B:999:MET:HA	1.91	0.53
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.38	0.52
1:A:456:MET:HE2	1:A:510:GLN:CB	2.39	0.52
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.91	0.52
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.90	0.52
4:E:124:VAL:HG13	4:E:132:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	6:H:96:VAL:H	2.23	0.52
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.25	0.52
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.92	0.52
1:A:117:GLU:H	1:A:118:HIS:HB2	1.75	0.52
2:B:97:VAL:HG22	2:B:128:LEU:HD23	1.91	0.52
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.91	0.52
1:A:567:LYS:HG2	6:H:96:VAL:H	1.74	0.51
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.91	0.51
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.91	0.51
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.57	0.51
1:A:1393:ASN:H	1:A:1393:ASN:HD22	1.58	0.51
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.93	0.51
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.51
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.26	0.51
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.50	0.51
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.92	0.51
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.92	0.51
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.92	0.51
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.91	0.51
2:B:975:GLN:O	2:B:990:ILE:HD12	2.11	0.51
2:B:957:ASN:HD21	2:B:959:ASP:HB2	1.75	0.51
8:J:1:MET:H1	8:J:57:ILE:H	1.58	0.51
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.40	0.51
3:C:31:ASN:O	3:C:35:ARG:HG3	2.09	0.51
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.93	0.51
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.93	0.51
3:C:57:VAL:HG11	8:J:57:ILE:HD12	1.93	0.51
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.93	0.51
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.76	0.51
2:B:605:ARG:HH21	2:B:639:ILE:HG12	1.76	0.51
1:A:605:MET:HE2	1:A:607:ILE:HG12	1.93	0.50
2:B:451:LYS:HA	2:B:454:THR:HB	1.92	0.50
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.44	0.50
2:B:610:ASN:OD1	2:B:612:GLU:HG2	2.11	0.50
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.94	0.50
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.58	0.50
2:B:286:PHE:HB3	2:B:297:ILE:HG12	1.92	0.50
2:B:526:GLU:CD	2:B:752:ALA:HB3	2.37	0.50
2:B:574:SER:HB3	2:B:591:ARG:HH22	1.77	0.50
2:B:744:HIS:CD2	2:B:746:SER:OG	2.65	0.50
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:185:ALA:HA	4:E:190:LEU:HD12	1.94	0.50
2:B:310:MET:O	2:B:313:MET:HB2	2.11	0.50
2:B:473:MET:C	2:B:475:SER:H	2.19	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.50
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.41	0.50
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.93	0.50
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.94	0.50
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.42	0.50
1:A:469:ARG:NH2	2:B:991:GLY:O	2.45	0.49
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.49
2:B:211:VAL:CG2	2:B:483:LEU:HA	2.42	0.49
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.94	0.49
1:A:47:ARG:NH1	1:A:47:ARG:HA	2.26	0.49
1:A:531:ILE:O	1:A:535:THR:HB	2.12	0.49
1:A:833:GLU:O	1:A:837:ILE:HG12	2.13	0.49
1:A:1215:ARG:HH21	1:A:1218:GLN:HG3	1.76	0.49
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.53	0.49
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.49
1:A:567:LYS:CG	6:H:96:VAL:H	2.25	0.49
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.49
2:B:167:ILE:HD12	2:B:424:LEU:HD21	1.94	0.49
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.94	0.49
1:A:974:ASP:C	1:A:976:THR:H	2.21	0.49
2:B:889:THR:HG22	2:B:891:ASP:HB2	1.94	0.49
1:A:456:MET:HE2	1:A:510:GLN:HB3	1.95	0.49
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.94	0.49
2:B:818:PRO:HG3	8:J:54:VAL:HG21	1.93	0.49
2:B:862:GLN:HG2	2:B:963:PHE:HB2	1.93	0.49
1:A:10:PRO:HD2	2:B:1192:TYR:HA	1.95	0.49
1:A:120:GLU:HA	1:A:123:ARG:HD3	1.94	0.49
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.95	0.49
2:B:398:ARG:HD2	2:B:509:ALA:HB2	1.95	0.49
2:B:550:ASP:OD1	2:B:552:MET:HB2	2.13	0.49
2:B:1175:LEU:C	2:B:1177:HIS:H	2.21	0.49
5:F:110:ASP:O	5:F:123:LYS:HE2	2.13	0.49
8:J:1:MET:HB2	8:J:56:LEU:HB2	1.95	0.49
1:A:99:ILE:HD13	1:A:234:MET:HE3	1.95	0.48
2:B:210:LYS:HE2	2:B:462:ALA:O	2.13	0.48
2:B:696:GLU:O	2:B:699:GLU:HB2	2.13	0.48
1:A:399:HIS:O	1:A:401:GLY:N	2.45	0.48
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:848:ARG:HD3	8:J:11:GLY:HA2	1.95	0.48
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.29	0.48
3:C:148:ARG:HB3	3:C:151:GLN:HG3	1.96	0.48
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.95	0.48
7:I:103:CYS:O	7:I:107:SER:HA	2.13	0.48
8:J:6:ARG:HA	8:J:12:LYS:O	2.12	0.48
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.48
4:E:46:TYR:HD2	4:E:57:MET:HB3	1.78	0.48
1:A:34:LYS:HD2	1:A:57:ARG:HH22	1.78	0.48
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.96	0.48
1:A:91:PHE:H	1:A:297:GLN:HE22	1.61	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.96	0.48
5:F:79:ARG:NH1	5:F:145:ASP:O	2.46	0.48
8:J:64:ASN:N	8:J:65:PRO:HD2	2.29	0.48
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.95	0.47
1:A:206:GLU:O	1:A:210:ILE:HG12	2.13	0.47
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.96	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.95	0.47
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.68	0.47
2:B:892:LYS:HA	10:L:63:ARG:HH22	1.80	0.47
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.29	0.47
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.95	0.47
9:K:65:HIS:CD2	9:K:67:PHE:H	2.32	0.47
1:A:1144:LYS:HG3	1:A:1268:LEU:HB3	1.95	0.47
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.12	0.47
2:B:879:ARG:O	2:B:882:THR:CG2	2.63	0.47
3:C:251:LEU:O	3:C:255:VAL:HG23	2.15	0.47
6:H:130:ARG:H	6:H:130:ARG:HD2	1.79	0.47
1:A:447:GLN:NE2	12:T:21:DC:H4'	2.30	0.47
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.50	0.47
3:C:22:LEU:CD2	9:K:101:LEU:HD21	2.44	0.47
4:E:78:LEU:HD21	4:E:109:ILE:HG12	1.97	0.47
10:L:61:THR:HB	10:L:63:ARG:H	1.80	0.47
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.96	0.47
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.79	0.47
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.96	0.47
9:K:79:GLU:CD	9:K:79:GLU:H	2.23	0.47
1:A:739:ASP:OD2	6:H:19:ARG:HD3	2.15	0.47
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.97	0.47
2:B:857:ARG:NH2	12:T:25:DC:OP1	2.48	0.47
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:7:CYS:HA	8:J:49:MET:HG2	1.97	0.47
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.50	0.46
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.50	0.46
1:A:104:GLU:HG3	1:A:174:ILE:HD12	1.95	0.46
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.96	0.46
1:A:826:ASP:HB2	1:A:1082:ASN:CB	2.45	0.46
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.51	0.46
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.97	0.46
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.97	0.46
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.97	0.46
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.55	0.46
8:J:36:LEU:HD13	8:J:47:ARG:HB3	1.97	0.46
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.98	0.46
2:B:639:ILE:CD1	2:B:691:GLU:HB2	2.42	0.46
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.96	0.46
1:A:420:ARG:HE	1:A:420:ARG:HB3	1.53	0.46
7:I:75:CYS:O	7:I:78:CYS:O	2.33	0.46
1:A:299:HIS:HA	1:A:302:THR:HB	1.96	0.46
1:A:826:ASP:HB2	1:A:1082:ASN:HB3	1.96	0.46
2:B:363:HIS:O	2:B:364:ILE:HB	2.15	0.46
4:E:147:HIS:CD2	4:E:149:LEU:H	2.33	0.46
1:A:58:LEU:HD12	1:A:243:PRO:HA	1.98	0.46
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.98	0.46
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.97	0.46
1:A:533:LYS:HE2	1:A:745:GLN:HE22	1.81	0.46
1:A:858:ASN:HD21	1:A:862:ASN:HB2	1.80	0.46
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.46	0.46
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.98	0.46
1:A:1323:ASP:OD1	1:A:1325:THR:CG2	2.64	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.17	0.45
1:A:942:PHE:O	1:A:946:VAL:HG23	2.16	0.45
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.97	0.45
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.82	0.45
2:B:1156:ASP:HB3	2:B:1197:PRO:CB	2.46	0.45
4:E:159:ASP:HA	4:E:162:ARG:HH11	1.81	0.45
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.82	0.45
3:C:148:ARG:H	3:C:151:GLN:HG3	1.80	0.45
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.52	0.45
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.99	0.45
2:B:792:MET:CE	12:T:25:DC:H5'	2.47	0.45
6:H:95:TYR:HE2	6:H:97:MET:CG	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:CYS:HB3	1:A:168:GLY:H	1.82	0.45
1:A:1067:LEU:HD22	1:A:1367:HIS:CE1	2.52	0.45
1:A:1123:GLY:HA3	1:A:1124:HIS:CB	2.39	0.45
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.52	0.45
2:B:847:ASP:O	3:C:65:HIS:HE1	2.00	0.45
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.98	0.45
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.97	0.45
1:A:1080:THR:HG23	1:A:1085:HIS:HE1	1.81	0.45
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.52	0.45
1:A:436:ILE:CD1	1:A:491:VAL:HG11	2.38	0.45
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.98	0.45
2:B:976:ILE:O	2:B:990:ILE:HB	2.16	0.45
2:B:1185:CYS:C	2:B:1187:ASN:H	2.25	0.45
3:C:69:LEU:O	8:J:6:ARG:NH1	2.50	0.45
1:A:56:PRO:HB2	1:A:57:ARG:HH21	1.82	0.45
2:B:30:SER:HB2	2:B:743:ILE:O	2.17	0.45
3:C:6:PRO:HB2	9:K:101:LEU:HG	1.98	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.17	0.45
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.51	0.45
2:B:801:LYS:O	8:J:52:THR:HG22	2.15	0.45
2:B:887:HIS:HA	2:B:888:GLY:O	2.17	0.45
3:C:124:LEU:O	3:C:127:ARG:HG2	2.17	0.45
1:A:265:LYS:HE3	1:A:299:HIS:HB3	1.99	0.45
2:B:592:ASN:HD21	2:B:595:ARG:HD3	1.81	0.45
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.82	0.44
1:A:525:GLN:HE21	2:B:835:GLN:HG2	1.82	0.44
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.47	0.44
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.99	0.44
6:H:28:ALA:HB3	6:H:38:LEU:HB3	1.99	0.44
1:A:343:LYS:CE	2:B:1156:ASP:HB2	2.48	0.44
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.47	0.44
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.44
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.45	0.44
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.83	0.44
1:A:404:TYR:HA	1:A:413:ILE:O	2.18	0.44
1:A:518:LYS:HA	1:A:631:HIS:HD2	1.81	0.44
1:A:944:ARG:HG2	1:A:1298:TYR:OH	2.17	0.44
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.98	0.44
1:A:1188:GLN:HB3	1:A:1189:SER:H	1.60	0.44
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.98	0.44
4:E:55:ARG:HA	4:E:58:MET:HE2	2.00	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.44
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.37	0.44
2:B:223:VAL:HG11	2:B:380:TYR:HE2	1.83	0.44
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.99	0.44
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.48	0.44
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.18	0.44
9:K:95:ILE:HG12	9:K:95:ILE:H	1.60	0.44
1:A:75:ASN:H	2:B:1116:ARG:HH22	1.65	0.44
1:A:265:LYS:HD2	1:A:322:VAL:HG21	1.99	0.44
2:B:68:THR:HG22	2:B:91:SER:HA	2.00	0.44
2:B:883:LEU:C	2:B:885:MET:H	2.26	0.44
2:B:1082:MET:HA	3:C:189:THR:HA	2.00	0.44
1:A:351:THR:HG22	1:A:352:VAL:H	1.83	0.43
1:A:388:LEU:O	1:A:392:VAL:HG23	2.18	0.43
2:B:62:ILE:HG23	2:B:418:LYS:HG2	2.00	0.43
1:A:919:ILE:HD11	1:A:925:LEU:HG	2.00	0.43
1:A:1152:ILE:HB	7:I:44:TYR:HB3	2.00	0.43
2:B:638:PHE:CD2	2:B:653:VAL:HG21	2.53	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.19	0.43
4:E:204:THR:HG22	4:E:205:SER:N	2.33	0.43
1:A:503:GLN:HE21	5:F:90:ARG:NH1	2.16	0.43
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	2.00	0.43
2:B:473:MET:H	2:B:473:MET:HG3	1.48	0.43
2:B:516:ASN:H	2:B:516:ASN:ND2	2.14	0.43
2:B:762:ASN:ND2	2:B:1024:ALA:HB3	2.33	0.43
2:B:770:GLN:HG2	2:B:983:ARG:O	2.18	0.43
2:B:1100:ASP:OD2	9:K:1:MET:HB3	2.18	0.43
4:E:77:SER:HB2	4:E:106:GLN:H	1.83	0.43
10:L:46:VAL:HG12	10:L:56:LEU:HD12	1.99	0.43
1:A:92:HIS:HE1	2:B:1210:MET:O	2.01	0.43
1:A:729:ALA:O	1:A:732:LEU:HB2	2.19	0.43
2:B:212:LEU:HD13	2:B:409:ALA:HA	2.01	0.43
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.99	0.43
1:A:568:PRO:HG2	6:H:46:LEU:HB3	2.00	0.43
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	2.01	0.43
4:E:24:LYS:HB2	4:E:30:ILE:HB	2.00	0.43
10:L:42:ARG:HD2	10:L:43:THR:H	1.84	0.43
1:A:117:GLU:N	1:A:118:HIS:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLN:HA	1:A:799:PHE:HA	2.00	0.43
2:B:277:LYS:H	2:B:277:LYS:HG3	1.37	0.43
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.43
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.01	0.43
1:A:629:LEU:O	1:A:633:VAL:HG23	2.19	0.43
1:A:663:SER:HA	2:B:1014:PRO:HG3	2.00	0.43
2:B:526:GLU:HG3	2:B:771:SER:HB3	2.01	0.43
2:B:561:TRP:O	2:B:590:HIS:HE1	2.01	0.43
2:B:792:MET:HA	2:B:856:PHE:O	2.19	0.43
2:B:887:HIS:H	2:B:890:TYR:HE1	1.67	0.43
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.18	0.43
2:B:260:GLY:O	2:B:267:ARG:HD3	2.18	0.43
2:B:908:GLU:HG2	2:B:943:SER:HA	2.01	0.43
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	2.00	0.43
1:A:1143:LEU:HD23	1:A:1267:MET:HB3	2.01	0.42
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.91	0.42
2:B:574:SER:HB3	2:B:591:ARG:HH12	1.84	0.42
2:B:848:ARG:HD2	8:J:8:PHE:O	2.18	0.42
2:B:942:ARG:HH22	12:T:25:DC:P	2.42	0.42
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.01	0.42
6:H:123:MET:HE2	6:H:142:LEU:HD22	2.01	0.42
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	2.01	0.42
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.01	0.42
2:B:976:ILE:HG23	2:B:977:GLY:N	2.34	0.42
8:J:7:CYS:O	8:J:8:PHE:C	2.61	0.42
10:L:27:LEU:HB3	10:L:37:LYS:HE2	2.01	0.42
1:A:57:ARG:CB	1:A:68:GLN:HG2	2.49	0.42
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.00	0.42
1:A:785:PRO:HG2	2:B:703:ILE:HD12	2.01	0.42
1:A:1320:PRO:HG3	4:E:7:ARG:HH12	1.84	0.42
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.42
2:B:1017:ILE:HD12	2:B:1026:LEU:HD21	2.02	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.42
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.01	0.42
2:B:33:VAL:O	2:B:36:ALA:HB3	2.20	0.42
2:B:483:LEU:O	2:B:484:ASN:HB2	2.19	0.42
1:A:70:CYS:O	1:A:72:GLU:HG2	2.20	0.42
1:A:780:VAL:HG13	1:A:789:LYS:HE2	2.01	0.42
2:B:95:ILE:HD11	2:B:128:LEU:HB3	2.02	0.42
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.01	0.42
1:A:68:GLN:O	1:A:70:CYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ARG:HH22	1:A:440:ASP:CG	2.27	0.42
1:A:1116:LEU:H	1:A:1308:THR:HB	1.84	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.63	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.50	0.42
2:B:405:ARG:NE	2:B:629:ASP:OD1	2.45	0.42
3:C:3:GLU:HG3	3:C:4:GLU:HG3	2.01	0.42
4:E:10:SER:O	4:E:14:ARG:HG3	2.20	0.42
1:A:55:ASP:N	1:A:56:PRO:HD2	2.35	0.42
1:A:230:ARG:HB3	1:A:232:GLU:HG2	2.02	0.42
1:A:298:PHE:HA	1:A:299:HIS:O	2.20	0.42
1:A:385:ILE:O	1:A:389:THR:OG1	2.38	0.42
1:A:456:MET:HE1	1:A:521:MET:HE2	2.02	0.42
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.44	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.37	0.42
1:A:47:ARG:HA	1:A:47:ARG:CZ	2.50	0.42
1:A:396:PRO:HG2	1:A:416:ARG:HB3	2.02	0.42
1:A:457:ALA:O	1:A:507:VAL:HG23	2.20	0.42
1:A:822:GLU:HG3	2:B:513:GLN:NE2	2.34	0.42
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.54	0.42
3:C:167:HIS:HE1	10:L:70:ARG:O	2.03	0.42
4:E:46:TYR:CE2	4:E:58:MET:HA	2.55	0.42
1:A:443:LEU:HD13	1:A:455:MET:HE2	2.02	0.41
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.84	0.41
1:A:851:HIS:C	1:A:853:ASP:H	2.28	0.41
2:B:899:ILE:HD12	2:B:911:ILE:HA	2.02	0.41
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.02	0.41
1:A:472:LEU:O	1:A:475:THR:HB	2.20	0.41
1:A:753:GLY:HA2	1:A:757:ASN:HD22	1.84	0.41
1:A:885:THR:O	1:A:940:ARG:HD2	2.20	0.41
4:E:64:PRO:CD	4:E:76:GLY:HA2	2.49	0.41
5:F:71:GLU:HA	5:F:72:LYS:C	2.44	0.41
1:A:58:LEU:HD12	1:A:244:PRO:HD3	2.02	0.41
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.02	0.41
2:B:487:THR:HG22	2:B:490:SER:H	1.84	0.41
2:B:643:ASP:C	2:B:645:SER:H	2.28	0.41
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.55	0.41
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.01	0.41
1:A:381:THR:HG22	1:A:384:ASN:CG	2.45	0.41
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.19	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
1:A:909:ASP:C	1:A:911:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:PRO:C	2:B:363:HIS:O	2.62	0.41
1:A:409:SER:O	1:A:411:ASP:N	2.54	0.41
2:B:492:LEU:HB3	2:B:751:VAL:HG21	2.02	0.41
5:F:79:ARG:HG2	5:F:144:GLU:HG2	2.03	0.41
1:A:523:ILE:CG2	1:A:527:THR:HG22	2.49	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.64	0.41
1:A:929:LEU:HD11	1:A:983:ILE:HD12	2.03	0.41
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.01	0.41
2:B:364:ILE:HD13	2:B:585:VAL:HG13	2.03	0.41
2:B:708:GLU:O	2:B:710:LEU:N	2.54	0.41
2:B:807:ARG:HA	2:B:807:ARG:HD2	1.93	0.41
9:K:39:ASP:HB2	9:K:40:HIS:H	1.74	0.41
2:B:36:ALA:C	2:B:37:PHE:O	2.60	0.41
2:B:477:ALA:HB1	2:B:499:ASN:HD21	1.85	0.41
2:B:482:VAL:O	2:B:483:LEU:C	2.62	0.41
3:C:52:GLU:HB3	3:C:154:LYS:HB3	2.02	0.41
4:E:55:ARG:HH12	4:E:113:GLN:CD	2.28	0.41
7:I:62:ILE:HG21	7:I:102:VAL:HG11	2.02	0.41
1:A:326:ARG:HA	1:A:1406:VAL:HG21	2.03	0.41
1:A:497:THR:HG21	2:B:1149:GLU:CD	2.46	0.41
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	2.03	0.41
2:B:95:ILE:HG13	2:B:96:TYR:N	2.36	0.41
4:E:175:LEU:HD23	4:E:213:ILE:HB	2.03	0.41
1:A:55:ASP:H	1:A:56:PRO:HD2	1.86	0.41
1:A:265:LYS:HE3	1:A:299:HIS:CD2	2.56	0.41
2:B:426:LYS:HE2	2:B:430:ARG:HH22	1.85	0.41
2:B:797:TYR:O	8:J:1:MET:HG3	2.20	0.41
1:A:313:GLN:HB3	1:A:322:VAL:H	1.86	0.40
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.56	0.40
1:A:1266:THR:HA	1:A:1270:ASN:HD22	1.86	0.40
1:A:1333:ILE:HG12	1:A:1381:LEU:HD12	2.02	0.40
7:I:61:ASP:OD2	7:I:61:ASP:N	2.53	0.40
1:A:1135:ARG:HG2	1:A:1282:VAL:HB	2.03	0.40
2:B:283:VAL:HG22	2:B:321:GLY:HA3	2.03	0.40
2:B:367:LEU:HB3	2:B:368:GLU:H	1.73	0.40
2:B:864:LYS:N	2:B:872:GLU:HB2	2.36	0.40
2:B:898:LEU:HD11	2:B:964:VAL:HG11	2.03	0.40
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.40
2:B:1163:CYS:O	2:B:1167:GLY:HA2	2.21	0.40
3:C:18:VAL:O	3:C:231:ASN:HA	2.21	0.40
1:A:117:GLU:H	1:A:118:HIS:CG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.55	0.40
2:B:274:PRO:HG3	2:B:359:GLU:O	2.22	0.40
2:B:386:LEU:O	2:B:390:LEU:HD12	2.22	0.40
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.85	0.40
2:B:551:PRO:HA	2:B:628:THR:HG21	2.04	0.40
1:A:89:PRO:HG2	1:A:205:GLU:HA	2.03	0.40
1:A:325:ILE:HB	2:B:1210:MET:SD	2.62	0.40
2:B:225:VAL:HG11	2:B:385:LEU:HA	2.04	0.40
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.36	0.40
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1395/1733 (80%)	1210 (87%)	126 (9%)	59 (4%)	2	14
2	B	1096/1224 (90%)	948 (86%)	102 (9%)	46 (4%)	2	14
3	C	264/318 (83%)	237 (90%)	21 (8%)	6 (2%)	5	25
4	E	212/215 (99%)	197 (93%)	11 (5%)	4 (2%)	6	28
5	F	83/155 (54%)	76 (92%)	6 (7%)	1 (1%)	10	37
6	H	129/146 (88%)	109 (84%)	9 (7%)	11 (8%)	0	4
7	I	117/122 (96%)	95 (81%)	18 (15%)	4 (3%)	3	18
8	J	63/70 (90%)	56 (89%)	5 (8%)	2 (3%)	3	19
9	K	112/120 (93%)	104 (93%)	6 (5%)	2 (2%)	6	29
10	L	44/70 (63%)	29 (66%)	9 (20%)	6 (14%)	0	1
All	All	3515/4173 (84%)	3061 (87%)	313 (9%)	141 (4%)	2	15

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	55	ASP
1	A	56	PRO
1	A	69	THR
1	A	72	GLU
1	A	117	GLU
1	A	215	SER
1	A	219	PHE
1	A	257	ARG
1	A	299	HIS
1	A	315	LEU
1	A	404	TYR
1	A	410	GLY
1	A	424	ILE
1	A	567	LYS
1	A	672	ASP
1	A	923	LEU
1	A	1087	ALA
1	A	1123	GLY
1	A	1167	GLU
2	B	67	SER
2	B	137	TYR
2	B	138	GLU
2	B	465	ASN
2	B	477	ALA
2	B	482	VAL
2	B	484	ASN
2	B	709	ASP
2	B	734	HIS
2	B	737	THR
2	B	751	VAL
2	B	883	LEU
2	B	1156	ASP
2	B	1221	SER
3	C	227	THR
4	E	86	PRO
6	H	62	SER
6	H	131	ASN
6	H	140	ALA
8	J	2	ILE
10	L	51	CYS
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	283	GLY
1	A	300	VAL
1	A	312	PRO
1	A	399	HIS
1	A	418	SER
1	A	423	ASP
1	A	969	GLN
1	A	975	HIS
1	A	1437	GLY
2	B	277	LYS
2	B	364	ILE
2	B	468	GLU
2	B	469	GLN
2	B	474	SER
2	B	483	LEU
2	B	531	GLN
2	B	648	HIS
2	B	708	GLU
2	B	712	PRO
2	B	792	MET
2	B	879	ARG
2	B	1046	PRO
2	B	1155	SER
3	C	48	SER
3	C	141	GLY
4	E	77	SER
6	H	18	GLY
6	H	90	ALA
6	H	108	SER
6	H	110	ASP
7	I	52	ILE
7	I	60	GLN
8	J	6	ARG
9	K	16	GLU
10	L	46	VAL
10	L	55	ILE
10	L	59	ALA
1	A	65	LEU
1	A	68	GLN
1	A	71	GLN
1	A	91	PHE

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	317	LYS
1	A	331	GLY
1	A	595	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1393	ASN
2	B	139	ALA
2	B	629	ASP
2	B	943	SER
2	B	1017	ILE
2	B	1157	ALA
3	C	214	ASN
4	E	59	SER
5	F	154	ASP
10	L	56	LEU
10	L	64	LEU
1	A	214	ILE
1	A	254	GLU
1	A	569	LYS
1	A	852	TYR
1	A	1034	GLU
2	B	467	GLY
2	B	881	ASN
2	B	884	ARG
2	B	887	HIS
2	B	1181	GLU
2	B	1211	ASN
3	C	90	ASP
3	C	142	VAL
6	H	84	ALA
6	H	128	ASN
7	I	3	THR
1	A	35	ILE
1	A	52	GLY
1	A	119	ASN
1	A	251	SER
1	A	255	SER
1	A	910	PRO
1	A	958	VAL
2	B	367	LEU
2	B	608	ASP

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Mol	Chain	Res	Type
2	B	711	GLU
2	B	864	LYS
4	E	124	VAL
6	H	3	ASN
6	H	109	LYS
7	I	77	LYS
9	K	37	LYS
1	A	149	GLU
1	A	286	HIS
1	A	409	SER
1	A	593	GLU
2	B	647	GLY
2	B	108	VAL
2	B	1099	VAL
1	A	385	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1520 (81%)	1009 (82%)	216 (18%)	2	9
2	B	967/1061 (91%)	804 (83%)	163 (17%)	2	10
3	C	234/274 (85%)	199 (85%)	35 (15%)	3	13
4	E	196/197 (100%)	167 (85%)	29 (15%)	3	13
5	F	75/137 (55%)	67 (89%)	8 (11%)	6	24
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	10
7	I	113/116 (97%)	96 (85%)	17 (15%)	3	13
8	J	60/65 (92%)	44 (73%)	16 (27%)	0	2
9	K	99/102 (97%)	82 (83%)	17 (17%)	2	10
10	L	40/57 (70%)	28 (70%)	12 (30%)	0	1
All	All	3126/3657 (86%)	2593 (83%)	533 (17%)	2	10

All (533) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	30	ILE
1	A	39	GLU
1	A	43	GLU
1	A	47	ARG
1	A	50	ILE
1	A	53	LEU
1	A	54	ASN
1	A	61	ILE
1	A	65	LEU
1	A	68	GLN
1	A	74	MET
1	A	90	VAL
1	A	93	VAL
1	A	113	LEU
1	A	116	ASP
1	A	117	GLU
1	A	120	GLU
1	A	126	LEU
1	A	128	ILE
1	A	132	LYS
1	A	143	LYS
1	A	147	VAL
1	A	148	CYS
1	A	182	VAL
1	A	186	LYS
1	A	199	LEU
1	A	208	LEU
1	A	218	ASP
1	A	222	LEU
1	A	227	VAL
1	A	235	ILE
1	A	252	PHE
1	A	256	GLN
1	A	257	ARG
1	A	265	LYS
1	A	269	ILE
1	A	270	LEU
1	A	274	ILE
1	A	289	ILE
1	A	291	GLU
1	A	295	LEU
1	A	296	LEU

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Mol	Chain	Res	Type
1	A	299	HIS
1	A	302	THR
1	A	308	ILE
1	A	320	ARG
1	A	323	LYS
1	A	325	ILE
1	A	330	LYS
1	A	335	ARG
1	A	337	ARG
1	A	343	LYS
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	389	THR
1	A	391	LEU
1	A	398	GLU
1	A	403	LYS
1	A	407	ARG
1	A	420	ARG
1	A	424	ILE
1	A	436	ILE
1	A	443	LEU
1	A	450	LEU
1	A	451	HIS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	489	LEU
1	A	496	GLU
1	A	497	THR
1	A	500	GLU
1	A	516	SER
1	A	518	LYS
1	A	532	ARG
1	A	535	THR
1	A	541	ILE
1	A	571	LEU

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Mol	Chain	Res	Type
1	A	588	LEU
1	A	590	ARG
1	A	595	THR
1	A	598	LEU
1	A	612	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	636	GLU
1	A	637	LYS
1	A	652	VAL
1	A	672	ASP
1	A	678	GLU
1	A	688	LYS
1	A	689	LYS
1	A	695	LYS
1	A	702	LEU
1	A	710	LEU
1	A	713	SER
1	A	716	ASP
1	A	719	VAL
1	A	722	LEU
1	A	732	LEU
1	A	738	LYS
1	A	740	LEU
1	A	744	LYS
1	A	752	LYS
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	771	GLU
1	A	773	LYS
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	830	LYS
1	A	833	GLU
1	A	841	LEU
1	A	845	LEU
1	A	846	GLU

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Mol	Chain	Res	Type
1	A	849	MET
1	A	854	ASN
1	A	867	ILE
1	A	878	ILE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	908	LEU
1	A	919	ILE
1	A	920	LEU
1	A	925	LEU
1	A	926	GLN
1	A	931	GLU
1	A	938	LYS
1	A	953	ASN
1	A	960	ILE
1	A	969	GLN
1	A	973	ILE
1	A	998	LEU
1	A	1001	ARG
1	A	1005	GLU
1	A	1015	VAL
1	A	1025	ARG
1	A	1029	ARG
1	A	1034	GLU
1	A	1035	TYR
1	A	1048	ASN
1	A	1050	GLU
1	A	1067	LEU
1	A	1077	THR
1	A	1081	LEU
1	A	1082	ASN
1	A	1084	PHE
1	A	1085	HIS
1	A	1094	VAL
1	A	1095	THR
1	A	1109	LYS
1	A	1110	ASN
1	A	1116	LEU
1	A	1117	THR
1	A	1130	GLN
1	A	1147	THR

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Mol	Chain	Res	Type
1	A	1161	THR
1	A	1169	ILE
1	A	1173	HIS
1	A	1176	LEU
1	A	1188	GLN
1	A	1206	ASP
1	A	1221	LYS
1	A	1227	ILE
1	A	1231	ASP
1	A	1233	ASP
1	A	1234	GLU
1	A	1237	ILE
1	A	1242	VAL
1	A	1258	HIS
1	A	1259	MET
1	A	1261	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1266	THR
1	A	1269	GLU
1	A	1273	LEU
1	A	1277	GLU
1	A	1280	GLU
1	A	1284	MET
1	A	1291	VAL
1	A	1316	VAL
1	A	1322	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1354	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1398	MET
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1415	SER
1	A	1420	ASP
1	A	1424	VAL

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Mol	Chain	Res	Type
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
2	B	21	GLU
2	B	22	SER
2	B	25	ILE
2	B	28	GLU
2	B	40	GLU
2	B	46	GLN
2	B	48	LEU
2	B	63	ILE
2	B	65	GLU
2	B	70	ILE
2	B	89	GLU
2	B	95	ILE
2	B	98	THR
2	B	102	VAL
2	B	133	LYS
2	B	137	TYR
2	B	138	GLU
2	B	174	LEU
2	B	175	ARG
2	B	185	THR
2	B	187	SER
2	B	189	LEU
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	232	SER
2	B	234	ILE
2	B	240	ILE
2	B	241	ARG
2	B	242	SER
2	B	246	LYS
2	B	249	ARG
2	B	254	LEU
2	B	264	SER
2	B	267	ARG
2	B	272	THR
2	B	276	ILE

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Mol	Chain	Res	Type
2	B	277	LYS
2	B	280	ILE
2	B	283	VAL
2	B	292	ILE
2	B	296	GLU
2	B	323	VAL
2	B	332	ASP
2	B	347	LYS
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	387	LEU
2	B	390	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	408	LEU
2	B	416	LEU
2	B	418	LYS
2	B	426	LYS
2	B	429	PHE
2	B	448	ILE
2	B	453	ILE
2	B	458	LYS
2	B	468	GLU
2	B	469	GLN
2	B	471	LYS
2	B	473	MET
2	B	474	SER
2	B	481	GLN
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	487	THR
2	B	516	ASN
2	B	537	LYS
2	B	540	SER
2	B	547	VAL
2	B	555	ILE
2	B	567	GLU
2	B	570	VAL
2	B	574	SER

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Mol	Chain	Res	Type
2	B	576	ASP
2	B	578	THR
2	B	582	VAL
2	B	591	ARG
2	B	595	ARG
2	B	604	ARG
2	B	616	ILE
2	B	621	GLU
2	B	633	VAL
2	B	641	GLU
2	B	653	VAL
2	B	658	ILE
2	B	660	LYS
2	B	682	SER
2	B	685	LEU
2	B	690	VAL
2	B	708	GLU
2	B	710	LEU
2	B	732	SER
2	B	734	HIS
2	B	743	ILE
2	B	751	VAL
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	813	LYS
2	B	815	ARG
2	B	838	SER
2	B	841	MET
2	B	844	SER
2	B	848	ARG
2	B	865	LYS
2	B	866	TYR
2	B	878	GLN
2	B	879	ARG
2	B	885	MET
2	B	906	SER
2	B	911	ILE
2	B	939	THR
2	B	944	THR

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Mol	Chain	Res	Type
2	B	948	ILE
2	B	955	THR
2	B	957	ASN
2	B	973	ILE
2	B	975	GLN
2	B	983	ARG
2	B	992	ILE
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1028	GLU
2	B	1034	VAL
2	B	1050	ILE
2	B	1053	GLU
2	B	1065	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1102	LYS
2	B	1103	ILE
2	B	1113	VAL
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1149	GLU
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1160	VAL
2	B	1172	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU
2	B	1189	ILE
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1222	ARG

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Mol	Chain	Res	Type
3	C	4	GLU
3	C	18	VAL
3	C	23	SER
3	C	25	VAL
3	C	36	VAL
3	C	41	ILE
3	C	56	THR
3	C	70	ILE
3	C	75	MET
3	C	78	GLU
3	C	80	LEU
3	C	89	GLU
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	129	ILE
3	C	137	LYS
3	C	151	GLN
3	C	152	GLU
3	C	156	THR
3	C	157	CYS
3	C	199	LYS
3	C	203	GLN
3	C	214	ASN
3	C	215	GLU
3	C	238	ILE
3	C	240	VAL
3	C	243	VAL
3	C	244	VAL
3	C	252	GLN
3	C	254	LYS
3	C	259	LEU
3	C	260	LEU
3	C	264	GLN
3	C	266	ASP
4	E	2	ASP
4	E	9	ILE
4	E	24	LYS
4	E	33	GLU
4	E	40	GLU
4	E	54	GLN
4	E	57	MET

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Mol	Chain	Res	Type
4	E	61	GLN
4	E	67	GLU
4	E	74	ASP
4	E	78	LEU
4	E	83	CYS
4	E	88	VAL
4	E	95	THR
4	E	100	ILE
4	E	101	GLN
4	E	122	LYS
4	E	123	LEU
4	E	127	ILE
4	E	140	LEU
4	E	149	LEU
4	E	150	VAL
4	E	156	LEU
4	E	157	SER
4	E	158	SER
4	E	169	ARG
4	E	171	LYS
4	E	196	VAL
4	E	204	THR
5	F	74	ILE
5	F	82	THR
5	F	86	THR
5	F	89	GLU
5	F	111	LEU
5	F	118	LEU
5	F	128	LYS
5	F	133	VAL
6	H	2	SER
6	H	8	ASP
6	H	11	GLN
6	H	15	VAL
6	H	22	LYS
6	H	24	CYS
6	H	26	ILE
6	H	27	GLU
6	H	35	GLN
6	H	45	GLU
6	H	59	ILE
6	H	63	LEU

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Mol	Chain	Res	Type
6	H	76	THR
6	H	77	ARG
6	H	83	GLN
6	H	86	ASP
6	H	87	ARG
6	H	107	VAL
6	H	109	LYS
6	H	123	MET
7	I	17	ARG
7	I	28	GLU
7	I	35	VAL
7	I	52	ILE
7	I	55	THR
7	I	59	VAL
7	I	61	ASP
7	I	64	SER
7	I	70	ARG
7	I	84	VAL
7	I	90	GLN
7	I	91	ARG
7	I	94	ASP
7	I	97	MET
7	I	98	VAL
7	I	116	ASN
7	I	119	THR
8	J	2	ILE
8	J	3	VAL
8	J	9	SER
8	J	13	VAL
8	J	19	GLU
8	J	22	LEU
8	J	23	ASN
8	J	26	GLN
8	J	27	GLU
8	J	31	ASP
8	J	48	ARG
8	J	52	THR
8	J	57	ILE
8	J	59	LYS
8	J	62	ARG
8	J	64	ASN
9	K	1	MET

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Mol	Chain	Res	Type
9	K	6	ARG
9	K	14	GLU
9	K	17	SER
9	K	18	LYS
9	K	20	LYS
9	K	25	THR
9	K	31	VAL
9	K	33	ILE
9	K	42	LEU
9	K	50	LEU
9	K	51	LEU
9	K	54	ARG
9	K	55	LYS
9	K	63	VAL
9	K	95	ILE
9	K	101	LEU
10	L	27	LEU
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	50	ASP
10	L	54	ARG
10	L	55	ILE
10	L	58	LYS
10	L	61	THR
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	64	ASN
1	A	68	GLN
1	A	92	HIS
1	A	118	HIS
1	A	225	ASN
1	A	297	GLN
1	A	306	ASN

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Mol	Chain	Res	Type
1	A	339	ASN
1	A	390	GLN
1	A	394	ASN
1	A	445	ASN
1	A	451	HIS
1	A	503	GLN
1	A	525	GLN
1	A	584	ASN
1	A	631	HIS
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	854	ASN
1	A	877	HIS
1	A	935	GLN
1	A	966	ASN
1	A	1085	HIS
1	A	1124	HIS
1	A	1130	GLN
1	A	1140	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1270	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	255	GLN
2	B	325	GLN
2	B	395	GLN
2	B	465	ASN
2	B	469	GLN
2	B	481	GLN
2	B	484	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	592	ASN

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Mol	Chain	Res	Type
2	B	657	HIS
2	B	667	GLN
2	B	686	ASN
2	B	744	HIS
2	B	762	ASN
2	B	763	GLN
2	B	767	ASN
2	B	822	ASN
2	B	843	GLN
2	B	951	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1161	HIS
2	B	1195	HIS
3	C	17	ASN
3	C	65	HIS
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	151	GLN
3	C	167	HIS
3	C	231	ASN
3	C	242	GLN
3	C	267	GLN
4	E	32	GLN
4	E	63	ASN
6	H	83	GLN
6	H	133	ASN
7	I	12	ASN
7	I	90	GLN
7	I	120	GLN
8	J	23	ASN
9	K	29	ASN
9	K	52	ASN
9	K	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	6/7 (85%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1405/1733 (81%)	0.02	34 (2%) 59 40	48, 92, 168, 202	0
2	B	1114/1224 (91%)	-0.06	24 (2%) 62 43	43, 79, 139, 202	0
3	C	266/318 (83%)	-0.24	0 100 100	52, 80, 117, 169	0
4	E	214/215 (99%)	0.09	2 (0%) 81 65	69, 130, 190, 204	0
5	F	85/155 (54%)	-0.17	0 100 100	66, 97, 133, 162	0
6	H	133/146 (91%)	0.32	9 (6%) 23 16	86, 127, 158, 170	0
7	I	119/122 (97%)	0.06	3 (2%) 58 39	59, 97, 131, 150	0
8	J	65/70 (92%)	-0.47	0 100 100	47, 70, 100, 127	0
9	K	114/120 (95%)	-0.22	1 (0%) 81 65	60, 87, 112, 127	0
10	L	46/70 (65%)	0.54	3 (6%) 25 17	65, 109, 149, 161	0
11	R	7/7 (100%)	-0.37	0 100 100	89, 97, 131, 139	0
12	T	13/29 (44%)	0.62	1 (7%) 19 14	110, 124, 160, 169	0
All	All	3581/4209 (85%)	-0.02	77 (2%) 62 43	43, 90, 161, 204	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	7.6
1	A	1089	VAL	6.9
1	A	1087	ALA	5.9
1	A	1082	ASN	5.6
2	B	715	ALA	5.5
1	A	1083	THR	4.5
6	H	63	LEU	4.3
1	A	1090	ALA	4.3
2	B	709	ASP	4.2
10	L	27	LEU	4.0
1	A	1088	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	477	ALA	3.9
2	B	882	THR	3.8
6	H	132	LEU	3.6
1	A	154	SER	3.5
1	A	51	GLY	3.5
2	B	446	LEU	3.4
1	A	65	LEU	3.4
1	A	1085	HIS	3.2
2	B	509	ALA	3.2
1	A	323	LYS	3.2
1	A	1108	ALA	3.2
2	B	883	LEU	3.2
1	A	69	THR	3.1
9	K	114	LEU	3.1
6	H	85	GLY	3.1
1	A	252	PHE	3.1
1	A	1176	LEU	3.1
2	B	478	GLY	3.0
1	A	161	LEU	3.0
1	A	1092	LYS	2.9
1	A	1091	SER	2.9
1	A	318	SER	2.9
2	B	708	GLU	2.8
2	B	502	ILE	2.8
2	B	335	GLY	2.7
2	B	881	ASN	2.7
1	A	1081	LEU	2.7
2	B	1224	PHE	2.7
6	H	82	PRO	2.7
1	A	199	LEU	2.7
1	A	250	ILE	2.6
2	B	447	ALA	2.6
2	B	250	PHE	2.6
10	L	55	ILE	2.5
1	A	317	LYS	2.5
2	B	880	THR	2.4
2	B	870	ILE	2.4
1	A	55	ASP	2.4
7	I	120	GLN	2.4
6	H	135	LEU	2.4
1	A	289	ILE	2.4
1	A	1257	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	50	ILE	2.3
1	A	44	THR	2.3
2	B	733	HIS	2.3
1	A	1084	PHE	2.3
2	B	140	ILE	2.3
4	E	90	VAL	2.3
2	B	164	LYS	2.3
6	H	139	ASN	2.3
7	I	50	THR	2.2
2	B	647	GLY	2.2
10	L	25	ALA	2.2
2	B	244	LEU	2.2
7	I	3	THR	2.2
1	A	1445	ILE	2.2
4	E	44	ALA	2.2
2	B	734	HIS	2.2
1	A	216	VAL	2.1
12	T	28	DT	2.1
6	H	138	GLU	2.1
1	A	279	LEU	2.1
1	A	315	LEU	2.1
2	B	1223	ASP	2.1
6	H	136	LYS	2.0
6	H	84	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
14	MG	B	2002[A]	1/1	0.89	0.21	41,41,41,41	1
14	MG	B	2002[B]	1/1	0.89	0.21	3,3,3,3	1
13	ZN	A	1734	1/1	0.95	0.06	236,236,236,236	0
14	MG	A	2001	1/1	0.99	0.02	68,68,68,68	0
13	ZN	A	1735	1/1	0.99	0.04	112,112,112,112	0
13	ZN	B	1307	1/1	0.99	0.04	147,147,147,147	0
13	ZN	J	101	1/1	1.00	0.02	75,75,75,75	0
13	ZN	L	105	1/1	1.00	0.02	112,112,112,112	0
13	ZN	C	319	1/1	1.00	0.01	78,78,78,78	0
13	ZN	I	203	1/1	1.00	0.04	98,98,98,98	0
13	ZN	I	204	1/1	1.00	0.02	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.