



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:42 PM UTC

PDB ID : 5IP9 / pdb_00005ip9
Title : Structure of RNA Polymerase II-TFIIF complex
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-09
Resolution : 3.90 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:

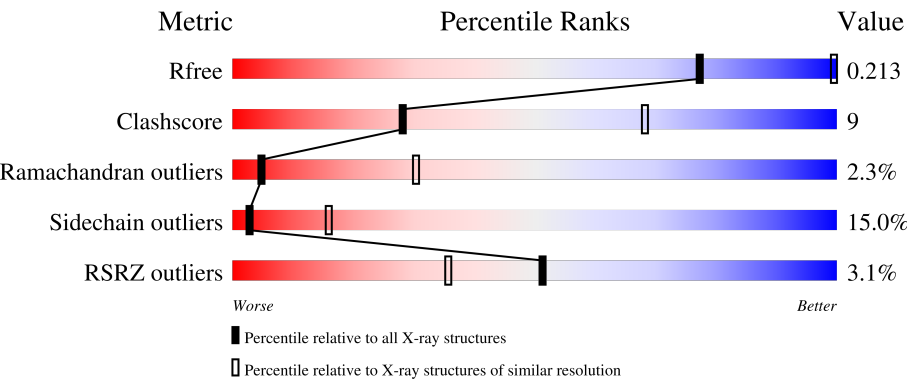
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	1732	2% 52% 24% 5% 18%
2	B	1223	4% 60% 26% 5% 9%
3	C	266	% 66% 28% 6%
4	D	221	4% 56% 18% 8% 19%
5	E	214	76% 22% .

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Mol	Chain	Length	Quality of chain
6	F	87	
7	G	171	
8	H	145	
9	I	119	
10	J	65	
11	K	115	
12	L	46	
13	Q	15	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 31339 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	1421	Total	C	N	O	S	0	0	0
			11190	7052	1957	2119	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1118	Total	C	N	O	S	0	0	0
			8876	5620	1557	1644	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 polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	180	Total	C	N	O	S	0	0	0
			1440	890	256	291	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	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 RPABC5.

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 RPABC4.

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 protein called PHE-ILE-LYS-ARG-ASP-ARG-MET-ARG-ARG-ASN-PHE-LEU-ARG-MET-ARG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	15	Total	C	N	O	S	0	0	0
			78	47	15	15	1			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

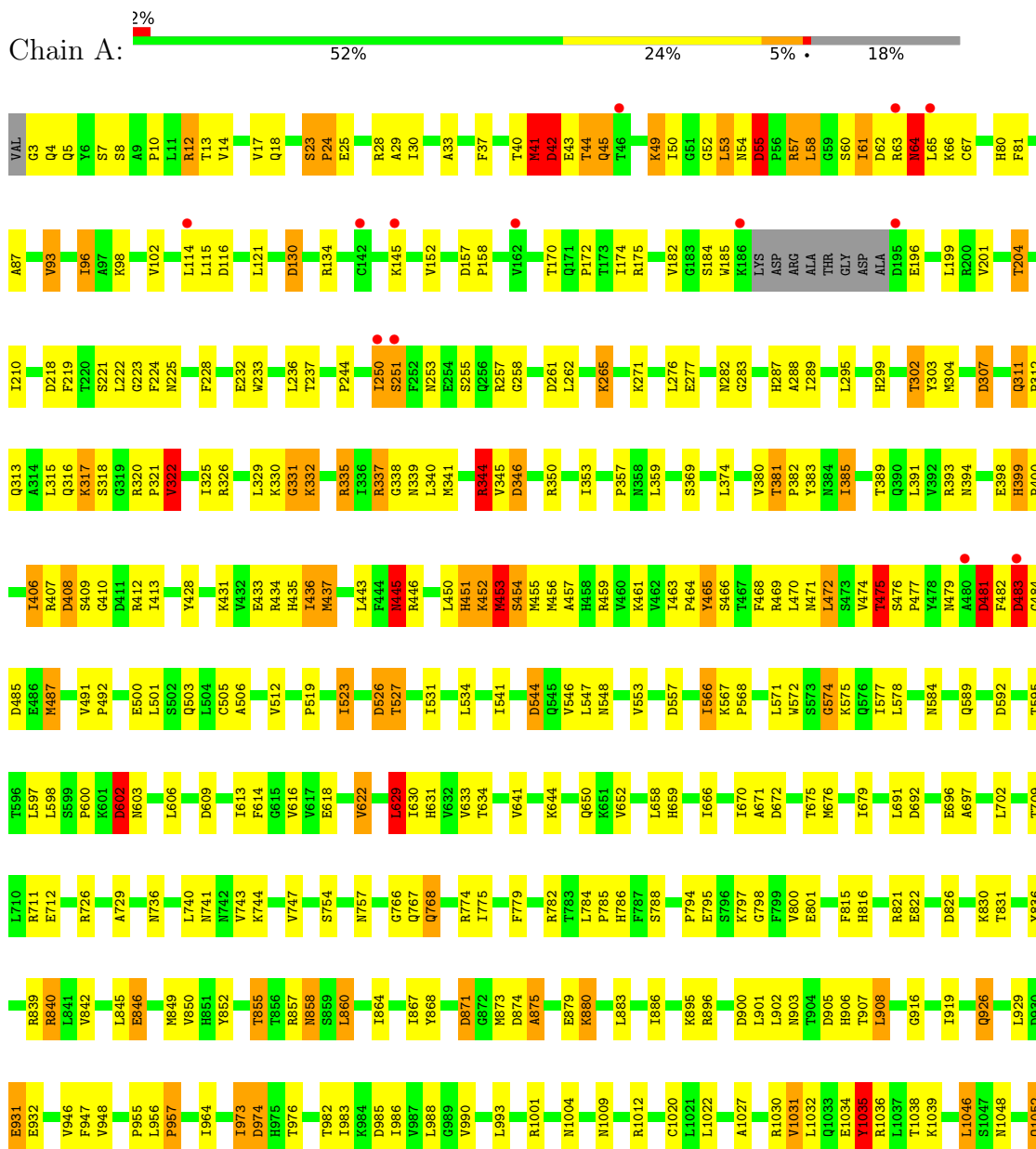
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

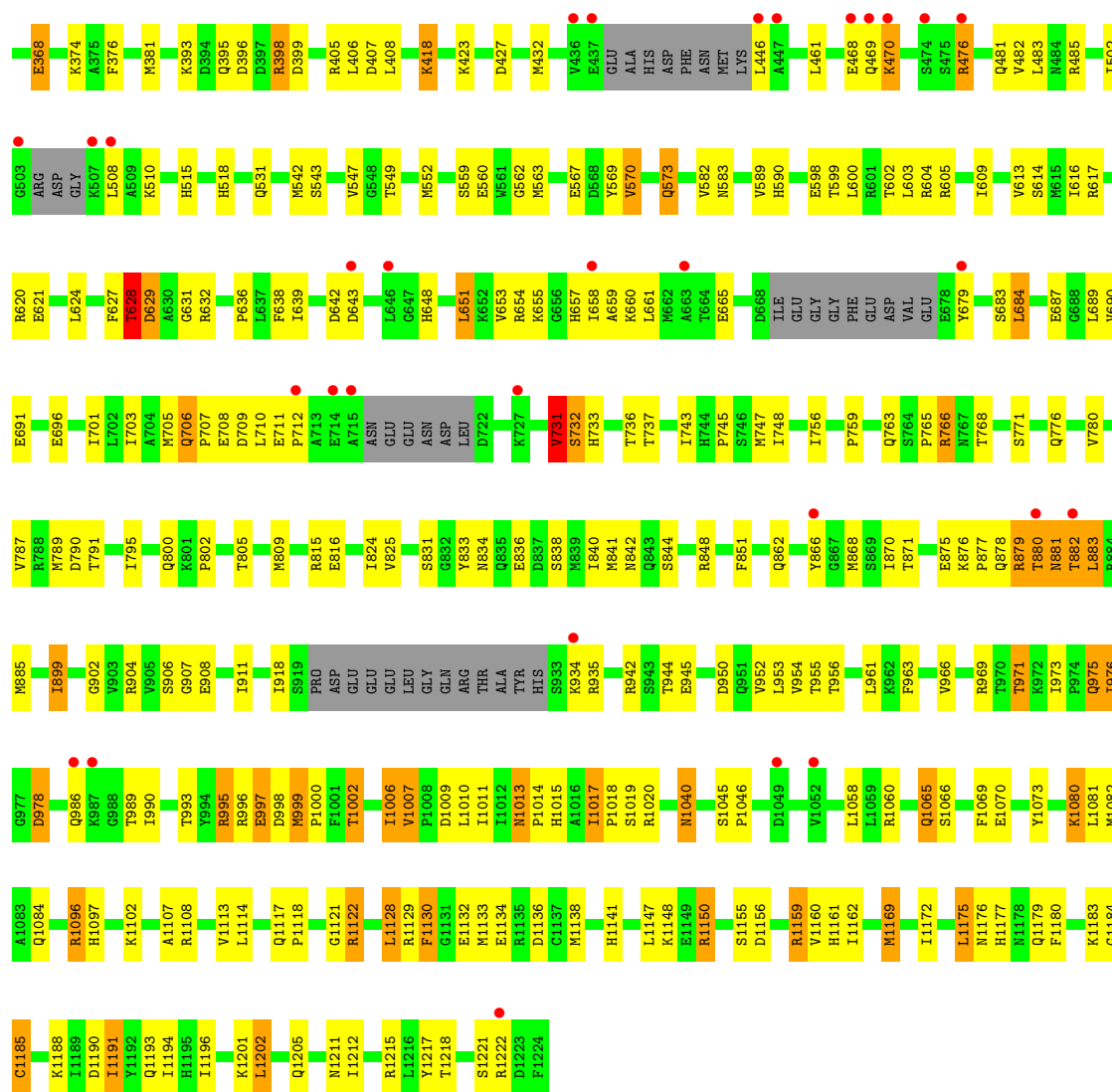
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

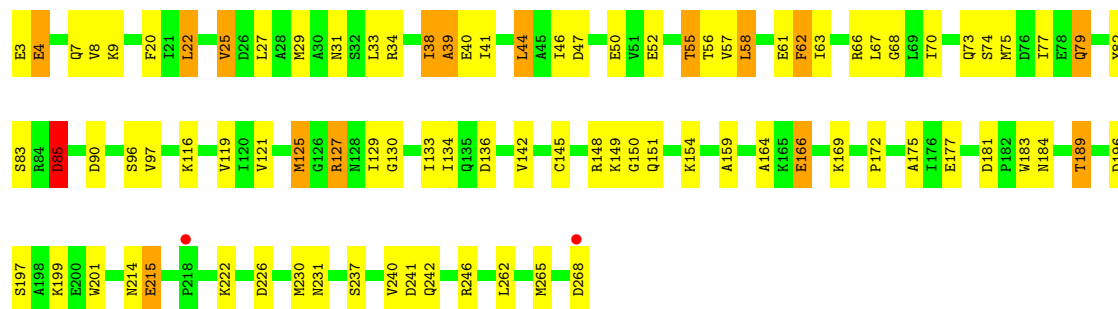
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



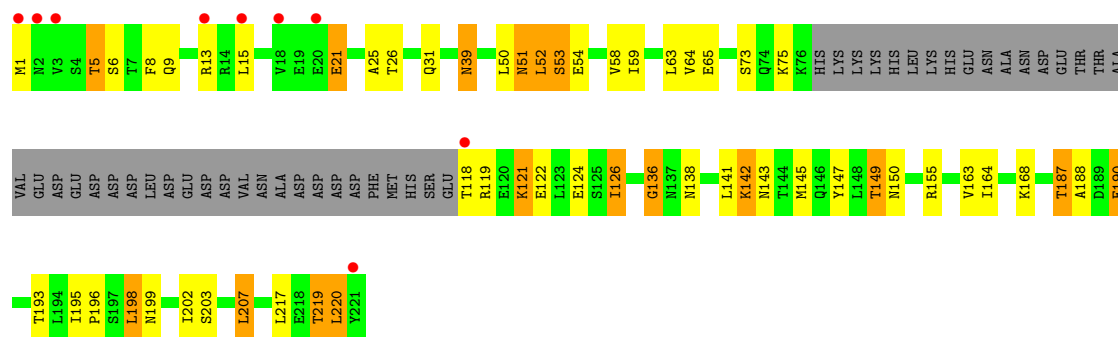


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



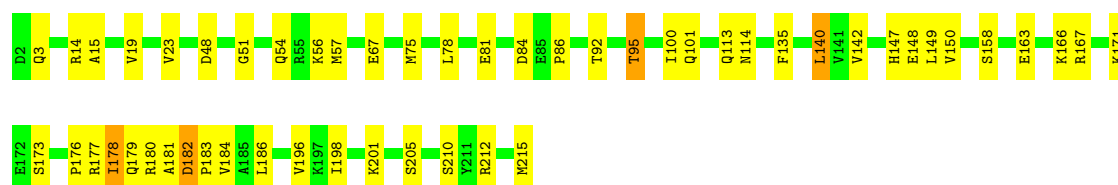
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4





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

Chain E: 76% 22% .



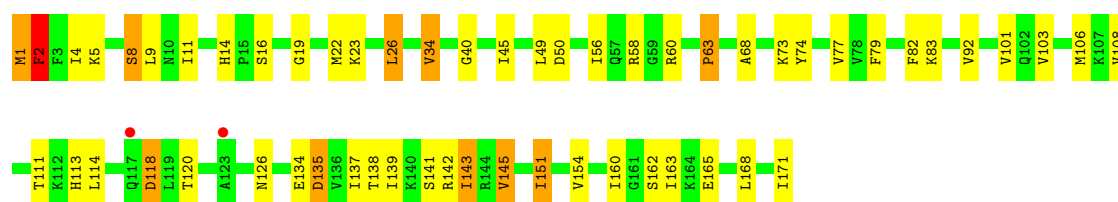
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 69% 26% 5% .



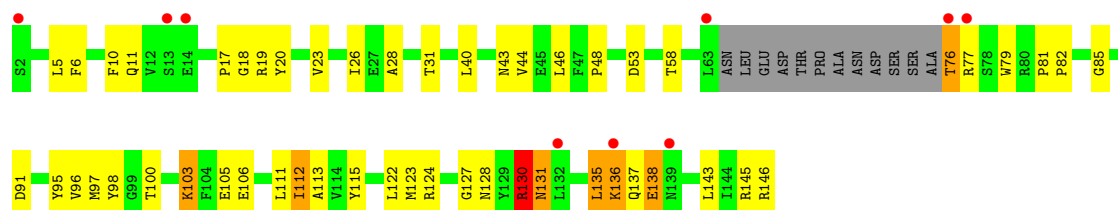
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 67% 27% 6% .

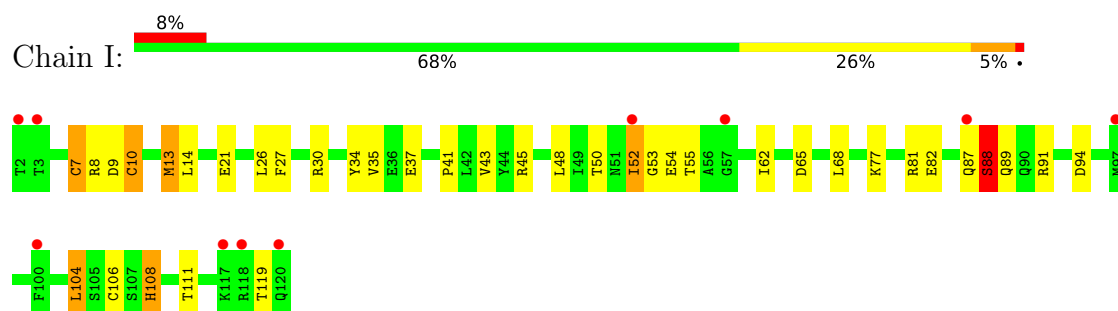


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

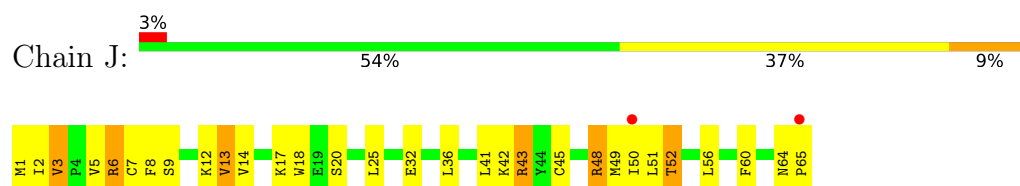
Chain H: 56% 30% 5% 8% .



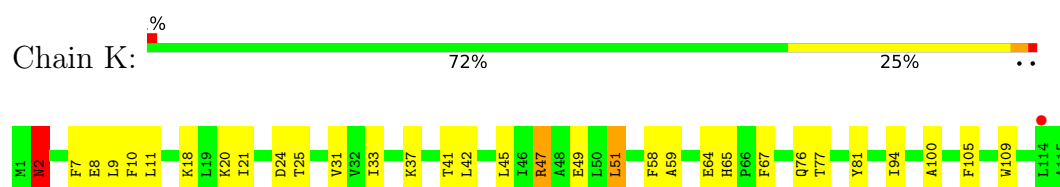
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



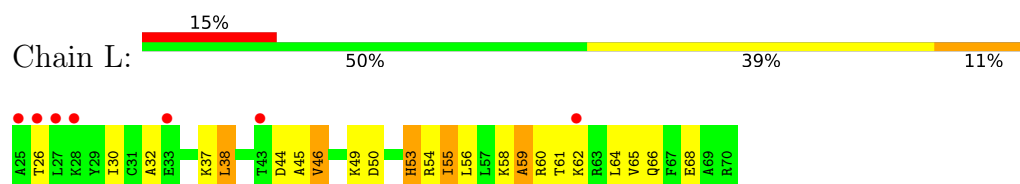
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



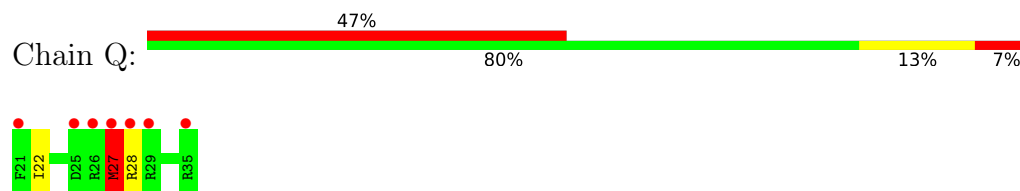
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



- Molecule 13: PHE-ILE-LYS-ARG-ASP-ARG-MET-ARG-ARG-ASN-PHE-LEU-ARG-MET-ARG



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.82Å 392.73Å 283.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.90 48.93 – 3.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-3.90) 99.9 (48.93-3.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.88Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.162 , 0.194 0.182 , 0.213	Depositor DCC
R_{free} test set	2265 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	129.8	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 140.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31339	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.91	9/11391 (0.1%)	1.50	120/15402 (0.8%)
2	B	0.87	2/9048 (0.0%)	1.43	73/12200 (0.6%)
3	C	0.81	0/2133	1.38	14/2891 (0.5%)
4	D	0.86	0/1450	1.64	33/1945 (1.7%)
5	E	0.78	0/1788	1.38	11/2406 (0.5%)
6	F	0.90	0/717	1.47	8/967 (0.8%)
7	G	0.85	0/1368	1.34	10/1844 (0.5%)
8	H	0.77	0/1086	1.31	10/1470 (0.7%)
9	I	0.84	0/989	1.41	6/1331 (0.5%)
10	J	0.87	0/541	1.46	3/727 (0.4%)
11	K	0.75	0/938	1.39	6/1267 (0.5%)
12	L	0.78	0/365	1.38	3/485 (0.6%)
13	Q	3.63	2/77 (2.6%)	2.16	3/105 (2.9%)
All	All	0.88	13/31891 (0.0%)	1.45	300/43040 (0.7%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Q	27	MET	SD-CE	28.20	2.50	1.79
1	A	57	ARG	CA-C	10.60	1.67	1.52
13	Q	27	MET	CG-SD	8.32	2.01	1.80
1	A	57	ARG	CA-CB	6.50	1.64	1.53
2	B	882	THR	CA-C	6.29	1.60	1.52
1	A	437	MET	SD-CE	5.83	1.94	1.79
1	A	487	MET	SD-CE	-5.83	1.65	1.79
1	A	1398	MET	SD-CE	5.67	1.93	1.79
1	A	453	MET	SD-CE	5.59	1.93	1.79
1	A	873	MET	SD-CE	5.58	1.93	1.79
1	A	436	ILE	CG1-CD1	-5.57	1.30	1.51
2	B	1169	MET	SD-CE	-5.47	1.65	1.79
1	A	1433	MET	SD-CE	5.06	1.92	1.79

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	ASP	CA-CB-CG	15.05	127.65	112.60
13	Q	28	ARG	N-CA-C	-13.03	95.66	111.69
1	A	957	PRO	CA-C-N	-11.48	107.83	123.10
1	A	957	PRO	C-N-CA	-11.48	107.83	123.10
1	A	55	ASP	CA-CB-CG	10.64	123.24	112.60
4	D	26	THR	N-CA-C	-10.34	97.29	111.56
4	D	31	GLN	N-CA-C	-9.90	99.92	112.90
4	D	26	THR	CA-C-N	8.72	134.90	122.08
4	D	26	THR	C-N-CA	8.72	134.90	122.08
1	A	452	LYS	N-CA-C	-8.70	101.87	111.36
6	F	71	GLU	N-CA-C	-8.44	102.97	113.18
1	A	445	ASN	CA-CB-CG	8.35	120.95	112.60
3	C	39	ALA	N-CA-C	7.93	119.56	111.07
1	A	592	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	794	PRO	CA-C-N	7.70	130.60	120.28
1	A	794	PRO	C-N-CA	7.70	130.60	120.28
1	A	41	MET	CA-C-N	7.63	136.11	121.54
1	A	41	MET	C-N-CA	7.63	136.11	121.54
1	A	629	LEU	N-CA-C	-7.61	102.96	111.71
2	B	294	ASP	CA-CB-CG	7.60	120.20	112.60
1	A	1072	ILE	N-CA-C	-7.55	105.78	111.90
1	A	452	LYS	CA-C-N	7.39	130.93	120.28
1	A	452	LYS	C-N-CA	7.39	130.93	120.28
4	D	52	LEU	CA-C-N	7.34	129.99	120.44
4	D	52	LEU	C-N-CA	7.34	129.99	120.44
1	A	57	ARG	CA-CB-CG	7.32	128.73	114.10
3	C	38	ILE	CA-C-N	7.26	129.87	120.44
3	C	38	ILE	C-N-CA	7.26	129.87	120.44
1	A	341	MET	CA-C-N	7.25	128.34	121.46
1	A	341	MET	C-N-CA	7.25	128.34	121.46
9	I	9	ASP	CA-CB-CG	7.22	119.82	112.60
2	B	320	ASP	CA-CB-CG	7.18	119.78	112.60
9	I	88	SER	N-CA-C	-7.17	101.06	110.53
2	B	1136	ASP	CA-CB-CG	7.13	119.73	112.60
2	B	296	GLU	N-CA-C	-7.08	102.61	112.45
3	C	183	TRP	N-CA-C	-7.08	98.43	109.25
9	I	53	GLY	CA-C-N	7.04	129.71	120.28
9	I	53	GLY	C-N-CA	7.04	129.71	120.28
2	B	1122	ARG	CA-C-N	7.01	130.01	120.54
2	B	1122	ARG	C-N-CA	7.01	130.01	120.54
1	A	67	CYS	N-CA-C	-7.01	105.27	114.31
10	J	5	VAL	N-CA-C	-6.98	99.62	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	136	LYS	CA-C-N	6.93	130.59	120.82
8	H	136	LYS	C-N-CA	6.93	130.59	120.82
7	G	50	ASP	CA-CB-CG	6.92	119.52	112.60
2	B	282	ILE	CA-C-N	6.89	129.24	120.56
2	B	282	ILE	C-N-CA	6.89	129.24	120.56
1	A	23	SER	N-CA-C	-6.86	101.01	109.65
2	B	1121	GLY	N-CA-C	6.82	121.32	112.18
3	C	85	ASP	CA-CB-CG	6.81	119.41	112.60
2	B	628	THR	CA-C-N	6.78	134.49	121.54
2	B	628	THR	C-N-CA	6.78	134.49	121.54
1	A	223	GLY	N-CA-C	6.71	121.85	114.40
4	D	25	ALA	CA-C-N	6.71	134.71	122.50
4	D	25	ALA	C-N-CA	6.71	134.71	122.50
1	A	399	HIS	N-CA-CB	6.67	122.24	110.37
13	Q	28	ARG	CA-C-N	6.47	129.25	120.44
13	Q	28	ARG	C-N-CA	6.47	129.25	120.44
12	L	59	ALA	CA-C-N	6.46	133.88	121.54
12	L	59	ALA	C-N-CA	6.46	133.88	121.54
1	A	288	ALA	N-CA-C	-6.43	106.65	114.75
1	A	1445	ILE	N-CA-CB	6.43	118.70	110.99
8	H	138	GLU	N-CA-C	-6.42	104.36	111.36
2	B	1040	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	609	ASP	CA-CB-CG	6.40	119.00	112.60
2	B	706	GLN	N-CA-C	-6.40	102.02	110.40
2	B	1175	LEU	CA-C-N	6.39	133.75	121.54
2	B	1175	LEU	C-N-CA	6.39	133.75	121.54
12	L	62	LYS	N-CA-C	-6.39	105.44	113.18
2	B	1222	ARG	N-CA-C	6.36	117.88	111.07
1	A	64	ASN	CA-C-N	6.35	133.66	121.54
1	A	64	ASN	C-N-CA	6.35	133.66	121.54
2	B	338	GLY	CA-C-N	6.35	133.66	121.54
2	B	338	GLY	C-N-CA	6.35	133.66	121.54
7	G	40	GLY	CA-C-N	6.30	129.05	120.54
7	G	40	GLY	C-N-CA	6.30	129.05	120.54
1	A	846	GLU	CA-C-N	6.30	132.71	120.99
1	A	846	GLU	C-N-CA	6.30	132.71	120.99
1	A	481	ASP	CA-CB-CG	6.25	118.85	112.60
2	B	56	ASP	CA-CB-CG	6.23	118.83	112.60
4	D	136	GLY	CA-C-N	6.22	129.24	120.28
4	D	136	GLY	C-N-CA	6.22	129.24	120.28
1	A	800	VAL	CA-C-N	6.19	128.57	120.28
1	A	800	VAL	C-N-CA	6.19	128.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	475	THR	CA-C-N	6.13	128.41	120.44
1	A	475	THR	C-N-CA	6.13	128.41	120.44
4	D	188	ALA	N-CA-C	-6.11	104.73	111.82
1	A	224	PHE	N-CA-C	6.10	118.40	110.53
2	B	45	SER	CA-C-N	6.06	129.22	120.79
2	B	45	SER	C-N-CA	6.06	129.22	120.79
6	F	71	GLU	CA-C-N	6.06	128.40	120.28
6	F	71	GLU	C-N-CA	6.06	128.40	120.28
1	A	1102	LYS	CA-C-N	6.06	128.40	120.28
1	A	1102	LYS	C-N-CA	6.06	128.40	120.28
1	A	399	HIS	CA-CB-CG	-6.05	107.75	113.80
2	B	468	GLU	CA-C-N	6.04	132.58	121.70
2	B	468	GLU	C-N-CA	6.04	132.58	121.70
1	A	381	THR	CB-CA-C	6.04	118.23	108.87
4	D	53	SER	CA-C-N	6.02	128.83	120.29
4	D	53	SER	C-N-CA	6.02	128.83	120.29
11	K	25	THR	CA-C-N	6.00	128.92	120.28
11	K	25	THR	C-N-CA	6.00	128.92	120.28
2	B	628	THR	N-CA-C	-5.99	105.80	113.23
3	C	62	PHE	CA-C-N	5.98	128.09	120.56
3	C	62	PHE	C-N-CA	5.98	128.09	120.56
6	F	77	ASP	N-CA-C	-5.96	101.45	110.28
6	F	77	ASP	CA-CB-CG	5.96	118.56	112.60
4	D	39	ASN	CA-CB-CG	5.93	118.53	112.60
2	B	1009	ASP	CA-CB-CG	5.92	118.52	112.60
6	F	154	ASP	CA-C-N	5.91	132.33	121.70
6	F	154	ASP	C-N-CA	5.91	132.33	121.70
3	C	136	ASP	CA-C-N	5.90	128.51	120.54
3	C	136	ASP	C-N-CA	5.90	128.51	120.54
1	A	317	LYS	CA-C-N	5.88	128.75	120.28
1	A	317	LYS	C-N-CA	5.88	128.75	120.28
4	D	73	SER	CA-C-N	5.84	128.38	120.38
4	D	73	SER	C-N-CA	5.84	128.38	120.38
1	A	1035	TYR	N-CA-C	-5.84	100.31	109.25
5	E	163	GLU	CB-CG-CD	5.84	122.52	112.60
4	D	220	LEU	CA-C-N	5.83	132.20	121.70
4	D	220	LEU	C-N-CA	5.83	132.20	121.70
2	B	222	ILE	CA-C-N	5.82	129.64	122.37
2	B	222	ILE	C-N-CA	5.82	129.64	122.37
1	A	271	LYS	CA-C-N	5.81	128.06	120.28
1	A	271	LYS	C-N-CA	5.81	128.06	120.28
10	J	60	PHE	CA-CB-CG	5.81	119.61	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	822	GLU	CA-C-N	5.79	126.25	119.94
1	A	822	GLU	C-N-CA	5.79	126.25	119.94
1	A	575	LYS	CA-C-N	5.79	128.31	120.44
1	A	575	LYS	C-N-CA	5.79	128.31	120.44
5	E	205	SER	N-CA-C	-5.74	101.69	109.95
1	A	130	ASP	CA-C-N	5.73	128.23	120.38
1	A	130	ASP	C-N-CA	5.73	128.23	120.38
7	G	2	PHE	CA-CB-CG	5.72	119.52	113.80
2	B	40	GLU	CA-C-N	5.72	127.94	120.28
2	B	40	GLU	C-N-CA	5.72	127.94	120.28
1	A	204	THR	CA-C-N	5.70	128.24	120.54
1	A	204	THR	C-N-CA	5.70	128.24	120.54
1	A	526	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	1385	THR	CA-C-N	5.68	128.68	120.38
1	A	1385	THR	C-N-CA	5.68	128.68	120.38
11	K	24	ASP	CA-C-N	5.68	127.82	120.44
11	K	24	ASP	C-N-CA	5.68	127.82	120.44
2	B	736	THR	N-CA-C	-5.67	106.34	113.72
2	B	880	THR	CA-C-N	5.67	132.36	121.54
2	B	880	THR	C-N-CA	5.67	132.36	121.54
2	B	407	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	17	VAL	N-CA-CB	5.63	118.77	111.67
7	G	1	MET	CA-C-N	5.63	132.30	121.54
7	G	1	MET	C-N-CA	5.63	132.30	121.54
1	A	947	PHE	CA-C-N	5.61	129.82	120.62
1	A	947	PHE	C-N-CA	5.61	129.82	120.62
1	A	398	GLU	CA-C-O	-5.60	115.03	121.47
2	B	1156	ASP	CA-CB-CG	5.60	118.20	112.60
9	I	119	THR	N-CA-C	-5.60	108.24	114.62
2	B	1221	SER	CA-C-N	5.59	127.71	120.44
2	B	1221	SER	C-N-CA	5.59	127.71	120.44
4	D	118	THR	CA-C-N	5.59	132.22	121.54
4	D	118	THR	C-N-CA	5.59	132.22	121.54
1	A	400	PRO	CA-C-N	5.59	127.15	122.17
1	A	400	PRO	C-N-CA	5.59	127.15	122.17
7	G	135	ASP	CA-CB-CG	5.58	118.19	112.60
1	A	871	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	481	ASP	N-CA-C	-5.58	101.28	109.81
2	B	1177	HIS	N-CA-C	-5.56	106.50	113.28
1	A	344	ARG	N-CA-C	-5.55	101.42	110.20
2	B	659	ALA	CA-C-N	5.53	127.96	120.38
2	B	659	ALA	C-N-CA	5.53	127.96	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	CA-CB-CG	5.53	118.13	112.60
2	B	684	LEU	CA-C-N	5.52	127.62	120.44
2	B	684	LEU	C-N-CA	5.52	127.62	120.44
1	A	222	LEU	N-CA-C	-5.52	102.73	110.35
5	E	171	LYS	N-CA-C	-5.52	101.28	110.17
2	B	709	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	219	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	24	PRO	CA-C-N	5.49	127.95	120.54
1	A	24	PRO	C-N-CA	5.49	127.95	120.54
1	A	1039	LYS	CA-C-N	5.48	127.88	120.65
1	A	1039	LYS	C-N-CA	5.48	127.88	120.65
1	A	1402	PHE	CA-CB-CG	5.46	119.26	113.80
2	B	642	ASP	CA-C-N	5.46	131.97	121.54
2	B	642	ASP	C-N-CA	5.46	131.97	121.54
4	D	163	VAL	N-CA-C	-5.44	105.42	110.53
4	D	196	PRO	CA-C-N	5.43	127.82	120.38
4	D	196	PRO	C-N-CA	5.43	127.82	120.38
3	C	33	LEU	N-CA-C	-5.43	105.28	111.14
4	D	168	LYS	CA-C-N	5.42	128.29	120.38
4	D	168	LYS	C-N-CA	5.42	128.29	120.38
1	A	1058	VAL	N-CA-CB	5.41	120.99	110.45
1	A	1084	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	346	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	578	LEU	N-CA-C	-5.37	105.51	111.36
4	D	143	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	218	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	39	ARG	N-CA-C	-5.35	105.34	111.07
2	B	469	GLN	CA-C-N	5.35	131.76	121.54
2	B	469	GLN	C-N-CA	5.35	131.76	121.54
2	B	600	LEU	CA-C-N	5.33	127.68	120.38
2	B	600	LEU	C-N-CA	5.33	127.68	120.38
1	A	61	ILE	N-CA-C	-5.32	106.50	111.45
1	A	931	GLU	CA-C-N	5.31	127.34	120.44
1	A	931	GLU	C-N-CA	5.31	127.34	120.44
2	B	998	ASP	CA-C-N	5.30	128.74	120.68
2	B	998	ASP	C-N-CA	5.30	128.74	120.68
3	C	68	GLY	CA-C-N	5.30	127.92	120.28
3	C	68	GLY	C-N-CA	5.30	127.92	120.28
1	A	1336	MET	CA-C-N	5.30	127.91	120.28
1	A	1336	MET	C-N-CA	5.30	127.91	120.28
3	C	181	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	307	ASP	CA-C-N	5.29	128.26	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASP	C-N-CA	5.29	128.26	120.91
1	A	44	THR	CA-C-N	5.29	131.64	121.54
1	A	44	THR	C-N-CA	5.29	131.64	121.54
4	D	124	GLU	CA-C-N	5.26	127.60	120.44
4	D	124	GLU	C-N-CA	5.26	127.60	120.44
5	E	95	THR	CA-C-N	5.26	127.59	120.44
5	E	95	THR	C-N-CA	5.26	127.59	120.44
6	F	111	LEU	N-CA-CB	5.25	118.18	109.88
1	A	58	LEU	N-CA-C	5.24	119.74	112.45
4	D	190	GLU	CB-CG-CD	5.24	121.51	112.60
1	A	557	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	826	ASP	CA-C-N	5.23	127.60	120.54
1	A	826	ASP	C-N-CA	5.23	127.60	120.54
1	A	875	ALA	CA-C-N	5.23	127.82	120.28
1	A	875	ALA	C-N-CA	5.23	127.82	120.28
2	B	842	ASN	CA-C-N	5.22	127.28	120.28
2	B	842	ASN	C-N-CA	5.22	127.28	120.28
7	G	45	ILE	N-CA-C	-5.21	99.60	107.73
8	H	145	ARG	CA-C-N	5.21	131.07	121.70
8	H	145	ARG	C-N-CA	5.21	131.07	121.70
1	A	1271	ILE	CA-C-N	5.20	129.69	122.77
1	A	1271	ILE	C-N-CA	5.20	129.69	122.77
1	A	244	PRO	N-CA-C	5.19	117.04	110.70
11	K	2	ASN	CA-C-N	5.19	127.63	120.67
11	K	2	ASN	C-N-CA	5.19	127.63	120.67
1	A	62	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	602	ASP	N-CA-C	-5.18	104.98	111.92
2	B	902	GLY	CA-C-N	5.17	131.28	121.97
2	B	902	GLY	C-N-CA	5.17	131.28	121.97
1	A	289	ILE	N-CA-C	-5.17	105.50	110.72
1	A	1373	ASP	CA-CB-CG	5.17	117.77	112.60
2	B	67	SER	CA-C-N	5.16	129.00	121.31
2	B	67	SER	C-N-CA	5.16	129.00	121.31
2	B	732	SER	N-CA-C	5.16	116.65	108.96
2	B	41	LYS	N-CA-C	5.16	116.90	111.28
2	B	427	ASP	CA-C-N	5.16	127.06	120.56
2	B	427	ASP	C-N-CA	5.16	127.06	120.56
7	G	118	ASP	CA-CB-CG	5.16	117.76	112.60
2	B	276	ILE	CA-C-N	5.14	131.36	121.54
2	B	276	ILE	C-N-CA	5.14	131.36	121.54
1	A	974	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	1020	CYS	CA-C-N	5.12	127.14	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1020	CYS	C-N-CA	5.12	127.14	120.28
5	E	173	SER	CA-C-N	5.12	128.87	120.63
5	E	173	SER	C-N-CA	5.12	128.87	120.63
2	B	1002	THR	N-CA-C	-5.12	102.91	110.48
1	A	287	HIS	CA-C-N	5.11	130.42	121.52
1	A	287	HIS	C-N-CA	5.11	130.42	121.52
1	A	1039	LYS	N-CA-C	-5.11	105.78	111.36
1	A	900	ASP	CA-CB-CG	5.11	117.71	112.60
7	G	82	PHE	CA-CB-CG	5.11	118.91	113.80
2	B	809	MET	CA-C-N	5.11	127.12	120.28
2	B	809	MET	C-N-CA	5.11	127.12	120.28
5	E	158	SER	CA-C-N	5.09	127.37	120.44
5	E	158	SER	C-N-CA	5.09	127.37	120.44
8	H	130	ARG	CA-C-N	5.09	127.55	120.63
8	H	130	ARG	C-N-CA	5.09	127.55	120.63
4	D	21	GLU	CA-C-N	5.08	128.92	120.94
4	D	21	GLU	C-N-CA	5.08	128.92	120.94
8	H	20	TYR	CA-C-N	5.08	128.03	120.31
8	H	20	TYR	C-N-CA	5.08	128.03	120.31
1	A	544	ASP	CA-C-N	5.08	129.26	120.58
1	A	544	ASP	C-N-CA	5.08	129.26	120.58
1	A	860	LEU	N-CA-C	-5.06	107.49	113.97
1	A	1373	ASP	CA-C-N	5.06	126.93	120.56
1	A	1373	ASP	C-N-CA	5.06	126.93	120.56
5	E	54	GLN	CA-C-N	5.06	127.56	120.28
5	E	54	GLN	C-N-CA	5.06	127.56	120.28
1	A	1055	ARG	CA-C-N	5.06	128.69	120.60
1	A	1055	ARG	C-N-CA	5.06	128.69	120.60
2	B	1121	GLY	CA-C-N	5.05	127.36	120.54
2	B	1121	GLY	C-N-CA	5.05	127.36	120.54
1	A	641	VAL	CA-C-N	5.05	127.04	120.28
1	A	641	VAL	C-N-CA	5.05	127.04	120.28
1	A	1403	GLU	CA-C-N	-5.04	112.78	121.66
1	A	1403	GLU	C-N-CA	-5.04	112.78	121.66
2	B	1130	PHE	CA-CB-CG	-5.04	108.76	113.80
2	B	971	THR	CB-CA-C	5.03	118.34	110.19
4	D	51	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	574	GLY	CA-C-N	5.03	128.36	120.82
1	A	574	GLY	C-N-CA	5.03	128.36	120.82
1	A	331	GLY	CA-C-N	5.02	131.14	121.54
1	A	331	GLY	C-N-CA	5.02	131.14	121.54
2	B	609	ILE	N-CA-CB	5.02	117.49	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	52	ILE	N-CA-CB	5.02	117.78	111.46
2	B	339	THR	CA-C-N	5.01	131.11	121.54
2	B	339	THR	C-N-CA	5.01	131.11	121.54
10	J	9	SER	N-CA-C	5.00	117.13	111.02
4	D	138	ASN	CA-CB-CG	5.00	117.60	112.60
3	C	96	SER	N-CA-C	5.00	116.67	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11190	0	11255	256	0
2	B	8876	0	8919	165	0
3	C	2095	0	2051	44	0
4	D	1440	0	1456	16	0
5	E	1752	0	1776	22	0
6	F	705	0	731	16	0
7	G	1340	0	1357	25	0
8	H	1068	0	1040	25	0
9	I	971	0	927	17	0
10	J	532	0	542	20	0
11	K	920	0	929	22	0
12	L	363	0	386	10	0
13	Q	78	0	36	3	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31339	0	31405	556	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 (556) 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)
13:Q:27:MET:CG	13:Q:27:MET:SD	2.01	1.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.10
1:A:1081:LEU:HB3	1:A:1082:ASN:HA	1.40	1.04
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.24	1.02
13:Q:27:MET:SD	13:Q:27:MET:CE	2.50	0.99
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.53	0.91
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.90
1:A:369:SER:H	11:K:2:ASN:HD21	1.21	0.88
1:A:631:HIS:HE1	1:A:879:GLU:HG2	1.40	0.87
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.19	0.87
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.56	0.87
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.54	0.87
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.57	0.86
1:A:225:ASN:HD22	1:A:228:PHE:H	1.22	0.85
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.23	0.84
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.61	0.83
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.60	0.82
2:B:654:ARG:H	2:B:657:HIS:HD2	1.26	0.81
3:C:125:MET:HB2	3:C:127:ARG:HE	1.44	0.81
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.18	0.79
1:A:1329:THR:HG22	1:A:1331:SER:H	1.48	0.79
10:J:8:PHE:H	10:J:49:MET:HE3	1.51	0.76
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.51	0.76
1:A:1450:LEU:HD21	7:G:19:GLY:O	1.86	0.76
2:B:986:GLN:HE22	2:B:1020:ARG:HD2	1.51	0.76
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.68	0.75
7:G:138:THR:HG22	7:G:139:ILE:H	1.51	0.75
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.67	0.75
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.87	0.74
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.51	0.74
10:J:48:ARG:O	10:J:52:THR:HG22	1.88	0.74
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.50	0.74
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.53	0.73
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.54	0.73
1:A:855:THR:HG21	1:A:857:ARG:HE	1.53	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.72
1:A:53:LEU:HD23	1:A:54:ASN:H	1.55	0.71
1:A:399:HIS:O	1:A:435:HIS:HD2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.71	0.71
1:A:225:ASN:ND2	1:A:228:PHE:H	1.89	0.70
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.70	0.70
1:A:1079:MET:HB3	1:A:1081:LEU:CD2	2.22	0.70
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.57	0.69
1:A:503:GLN:HE21	6:F:90:ARG:HH12	1.39	0.69
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.21	0.69
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.73	0.69
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.75	0.69
10:J:48:ARG:HE	10:J:49:MET:HE2	1.58	0.69
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.75	0.68
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.74	0.68
3:C:20:PHE:HE1	3:C:230:MET:HE3	1.58	0.68
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.76	0.68
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.76	0.68
12:L:38:LEU:HD11	12:L:49:LYS:H	1.59	0.67
2:B:955:THR:HG22	12:L:55:ILE:HA	1.77	0.67
3:C:148:ARG:HB2	3:C:151:GLN:NE2	2.10	0.67
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.77	0.66
3:C:149:LYS:HG3	3:C:150:GLY:H	1.60	0.66
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.75	0.66
3:C:20:PHE:CE1	3:C:230:MET:HE3	2.31	0.66
1:A:1032:LEU:O	1:A:1036:ARG:HD2	1.96	0.65
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.78	0.65
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.78	0.65
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.79	0.65
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.61	0.65
1:A:855:THR:CG2	1:A:857:ARG:HE	2.10	0.65
1:A:1081:LEU:HB3	1:A:1082:ASN:CA	2.23	0.65
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.61	0.65
4:D:155:ARG:CB	4:D:219:THR:HG21	2.28	0.64
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.78	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.80	0.64
2:B:654:ARG:H	2:B:657:HIS:CD2	2.14	0.63
7:G:26:LEU:HB3	7:G:56:ILE:HD11	1.80	0.63
1:A:631:HIS:CE1	1:A:879:GLU:HG2	2.28	0.63
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.79	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.62
1:A:134:ARG:HD2	1:A:221:SER:O	1.99	0.62
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.80	0.62
3:C:55:THR:HB	3:C:151:GLN:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.15	0.62
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.82	0.62
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.81	0.62
2:B:956:THR:HB	12:L:46:VAL:HG21	1.81	0.61
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.82	0.61
2:B:918:ILE:HD11	2:B:935:ARG:HD2	1.82	0.61
7:G:151:ILE:HD11	7:G:160:ILE:HD12	1.82	0.61
2:B:879:ARG:HH11	2:B:885:MET:HE1	1.66	0.61
1:A:353:ILE:HD13	1:A:487:MET:CE	2.31	0.61
2:B:880:THR:H	2:B:883:LEU:HD11	1.65	0.60
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.82	0.60
1:A:53:LEU:HD23	1:A:54:ASN:N	2.16	0.60
2:B:683:SER:O	2:B:687:GLU:HB2	2.01	0.60
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.41	0.60
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.83	0.60
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.83	0.59
2:B:862:GLN:HE21	2:B:961:LEU:HD11	1.67	0.59
8:H:135:LEU:C	8:H:137:GLN:H	2.10	0.59
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.83	0.59
6:F:85:MET:O	6:F:155:LEU:HD11	2.03	0.59
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.66	0.59
1:A:93:VAL:HG12	1:A:304:MET:HE3	1.84	0.59
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.83	0.59
2:B:879:ARG:NH1	2:B:885:MET:HE1	2.17	0.59
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.83	0.59
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.84	0.58
2:B:291:ILE:HD12	2:B:291:ILE:H	1.68	0.58
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.85	0.58
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.39	0.58
2:B:174:LEU:HD11	2:B:204:ILE:HD12	1.86	0.58
1:A:1030:ARG:HA	1:A:1034:GLU:HG3	1.86	0.58
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.22	0.58
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.86	0.57
1:A:49:LYS:HZ2	1:A:61:ILE:H	1.52	0.57
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.85	0.57
1:A:598:LEU:HD13	8:H:124:ARG:HB2	1.85	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.85	0.57
11:K:8:GLU:O	11:K:37:LYS:HD2	2.04	0.57
1:A:1009:ASN:HA	1:A:1012:ARG:HD2	1.87	0.57
1:A:299:HIS:HA	1:A:302:THR:HG22	1.87	0.57
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:H	3:C:151:GLN:HB2	1.70	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.35	0.56
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.40	0.56
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.39	0.56
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.87	0.56
6:F:87:LYS:HA	6:F:155:LEU:HD21	1.87	0.56
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.87	0.56
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.41	0.56
3:C:145:CYS:HA	10:J:2:ILE:HD13	1.87	0.56
11:K:65:HIS:CD2	11:K:67:PHE:H	2.11	0.56
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.88	0.56
4:D:155:ARG:HB3	4:D:219:THR:HG21	1.87	0.56
3:C:46:ILE:HD12	3:C:67:LEU:O	2.05	0.56
2:B:260:GLY:O	2:B:267:ARG:HD3	2.06	0.56
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.08	0.56
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.88	0.56
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.88	0.55
1:A:566:ILE:HD12	8:H:96:VAL:HG12	1.88	0.55
1:A:629:LEU:O	1:A:633:VAL:HG23	2.06	0.55
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.88	0.55
2:B:1215:ARG:HB3	2:B:1217:TYR:CE2	2.41	0.55
2:B:617:ARG:HG3	2:B:624:LEU:HD12	1.87	0.55
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.87	0.55
4:D:187:THR:HB	4:D:190:GLU:H	1.72	0.55
1:A:58:LEU:HD22	1:A:80:HIS:O	2.06	0.55
2:B:706:GLN:H	2:B:710:LEU:HD13	1.72	0.55
3:C:148:ARG:HB2	3:C:151:GLN:HE21	1.71	0.55
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.89	0.55
1:A:883:LEU:O	1:A:886:ILE:HG22	2.07	0.55
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.55	0.55
3:C:184:ASN:HD21	3:C:189:THR:H	1.55	0.54
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.89	0.54
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.89	0.54
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.89	0.54
1:A:335:ARG:NE	2:B:1202:LEU:HD13	2.23	0.54
2:B:986:GLN:NE2	2:B:1020:ARG:HD2	2.20	0.54
7:G:1:MET:HE1	7:G:79:PHE:CD2	2.42	0.54
1:A:1281:ARG:H	1:A:1309:ASP:HB2	1.72	0.54
2:B:570:VAL:HB	2:B:573:GLN:HB2	1.89	0.54
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG23	9:I:94:ASP:HA	1.90	0.53
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.72	0.53
1:A:671:ALA:HB3	1:A:676:MET:HE2	1.89	0.53
1:A:743:VAL:O	1:A:747:VAL:HG23	2.08	0.53
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.89	0.53
3:C:73:GLN:HE21	3:C:74:SER:H	1.57	0.53
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	1.91	0.53
8:H:95:TYR:HE2	8:H:97:MET:HE2	1.74	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.27	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.89	0.53
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.73	0.53
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.44	0.53
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.90	0.53
8:H:106:GLU:HA	8:H:112:ILE:HG13	1.91	0.53
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.91	0.53
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.74	0.53
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.90	0.53
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.74	0.53
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.24	0.52
1:A:350:ARG:HD2	2:B:1128:LEU:HD21	1.91	0.52
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.89	0.52
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.74	0.52
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.92	0.52
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.09	0.52
8:H:6:PHE:HD2	8:H:130:ARG:HG2	1.74	0.52
1:A:741:ASN:ND2	1:A:744:LYS:H	2.06	0.52
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.75	0.52
1:A:523:ILE:HG23	1:A:527:THR:HB	1.91	0.52
1:A:567:LYS:HE3	8:H:91:ASP:HB2	1.92	0.52
2:B:660:LYS:HB3	2:B:679:TYR:CD2	2.44	0.52
2:B:710:LEU:HA	2:B:733:HIS:CB	2.34	0.52
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	1.91	0.52
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.91	0.52
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.91	0.52
1:A:374:LEU:HB2	1:A:436:ILE:CD1	2.40	0.52
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.92	0.52
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.92	0.52
1:A:399:HIS:O	1:A:435:HIS:CD2	2.60	0.52
12:L:26:THR:O	12:L:37:LYS:HD3	2.09	0.52
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.52
2:B:515:HIS:H	2:B:518:HIS:CD2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.92	0.51
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.90	0.51
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.92	0.51
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.40	0.51
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.53	0.51
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.92	0.51
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.73	0.51
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.91	0.51
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.51
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.45	0.51
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.59	0.51
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.91	0.51
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.11	0.51
2:B:613:VAL:HG22	2:B:628:THR:HA	1.93	0.51
1:A:986:ILE:O	1:A:990:VAL:HG23	2.11	0.51
1:A:1079:MET:HB3	1:A:1081:LEU:HD22	1.92	0.51
8:H:100:THR:HG23	8:H:138:GLU:HA	1.91	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.93	0.51
1:A:316:GLN:HB2	1:A:322:VAL:HG23	1.93	0.51
1:A:451:HIS:HB3	1:A:454:SER:H	1.75	0.51
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	1.93	0.51
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.95	0.50
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.50
3:C:73:GLN:HE21	3:C:75:MET:H	1.59	0.50
1:A:1081:LEU:HG	1:A:1097:GLY:HA3	1.92	0.50
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.93	0.50
7:G:111:THR:HG22	7:G:113:HIS:H	1.77	0.50
1:A:1445:ILE:HD11	7:G:68:ALA:CB	2.41	0.50
1:A:374:LEU:HB2	1:A:436:ILE:HD12	1.94	0.50
1:A:907:THR:HG22	1:A:908:LEU:N	2.27	0.50
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.47	0.50
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.46	0.50
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.26	0.50
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.93	0.50
1:A:709:THR:HB	1:A:712:GLU:H	1.76	0.50
2:B:105:SER:C	2:B:107:GLY:H	2.19	0.50
2:B:999:MET:HE2	2:B:1011:ILE:HD12	1.92	0.50
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.94	0.50
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.77	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50
1:A:335:ARG:HE	2:B:1202:LEU:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.93	0.49
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.93	0.49
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.94	0.49
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.94	0.49
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.51	0.49
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	1.94	0.49
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.94	0.49
1:A:43:GLU:CD	1:A:50:ILE:HG13	2.38	0.49
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.95	0.49
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.47	0.49
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.42	0.49
2:B:308:TRP:CZ3	9:I:45:ARG:HB3	2.47	0.49
1:A:852:TYR:HB3	6:F:81:THR:HG22	1.95	0.49
2:B:308:TRP:HZ3	9:I:45:ARG:HB3	1.78	0.49
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.95	0.49
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.94	0.49
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.94	0.49
2:B:309:GLN:HB2	9:I:52:ILE:HD11	1.94	0.49
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.95	0.49
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.94	0.49
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.94	0.49
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	3.01	0.49
2:B:52:ASN:OD1	2:B:177:LYS:HB2	2.13	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.49
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.42	0.49
7:G:137:ILE:HG12	7:G:143:ILE:HD11	1.95	0.49
2:B:745:PRO:O	2:B:748:ILE:HG12	2.13	0.49
1:A:1048:ASN:O	1:A:1052:GLN:HB2	2.12	0.49
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.94	0.49
7:G:145:VAL:HG13	7:G:163:ILE:HG23	1.94	0.49
2:B:34:ILE:HG12	2:B:542:MET:CE	2.43	0.48
3:C:125:MET:HB2	3:C:127:ARG:NE	2.21	0.48
2:B:944:THR:HB	2:B:1122:ARG:NH2	2.28	0.48
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.95	0.48
6:F:90:ARG:HD3	6:F:155:LEU:HD22	1.95	0.48
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.95	0.48
2:B:276:ILE:HD11	2:B:355:ILE:HD13	1.95	0.48
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.96	0.48
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.95	0.48
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.95	0.48
2:B:883:LEU:HD23	2:B:934:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:VAL:HG13	5:E:78:LEU:HD23	1.96	0.48
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.48	0.48
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.79	0.47
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.94	0.47
1:A:571:LEU:HD12	8:H:46:LEU:HD11	1.96	0.47
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.96	0.47
4:D:52:LEU:HD22	4:D:147:TYR:HE2	1.77	0.47
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.96	0.47
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.95	0.47
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.47
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.49	0.47
6:F:89:GLU:O	6:F:93:ILE:HD12	2.14	0.47
3:C:82:TYR:HB2	3:C:85:ASP:OD2	2.15	0.47
7:G:8:SER:HB3	7:G:73:LYS:HA	1.97	0.47
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.47
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.97	0.47
1:A:98:LYS:O	1:A:102:VAL:HG23	2.14	0.47
1:A:471:ASN:O	1:A:474:VAL:HG12	2.14	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
1:A:332:LYS:H	1:A:337:ARG:CB	2.28	0.47
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.79	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.15	0.47
10:J:6:ARG:HG3	10:J:13:VAL:HG13	1.96	0.47
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.80	0.47
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.80	0.47
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.80	0.47
2:B:766:ARG:HG3	2:B:766:ARG:HH11	1.79	0.47
2:B:1215:ARG:HB3	2:B:1217:TYR:HE2	1.78	0.47
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.79	0.47
4:D:202:ILE:HG21	4:D:207:LEU:HB2	1.96	0.47
2:B:705:MET:H	2:B:710:LEU:HD22	1.79	0.47
3:C:175:ALA:HB3	10:J:43:ARG:HE	1.80	0.47
4:D:145:MET:O	4:D:149:THR:HB	2.15	0.47
1:A:345:VAL:HG12	2:B:1155:SER:HB3	1.96	0.47
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.97	0.47
2:B:997:GLU:CD	2:B:997:GLU:H	2.21	0.47
1:A:406:ILE:HD12	1:A:431:LYS:HB2	1.97	0.46
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.15	0.46
5:E:19:VAL:O	5:E:23:VAL:HG23	2.15	0.46
2:B:95:ILE:HD11	2:B:128:LEU:HG	1.98	0.46
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HA	3:C:159:ALA:HA	1.97	0.46
6:F:147:SER:H	6:F:150:GLU:HG2	1.81	0.46
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.97	0.46
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.97	0.46
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.34	0.46
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.98	0.46
1:A:311:GLN:HE21	1:A:312:PRO:HD2	1.80	0.46
2:B:68:THR:HG23	2:B:91:SER:HB3	1.98	0.46
2:B:336:ARG:HD3	2:B:348:ARG:HD3	1.96	0.46
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.80	0.46
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.98	0.46
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.16	0.46
2:B:1006:ILE:H	2:B:1006:ILE:HG13	1.56	0.46
3:C:77:ILE:HD12	3:C:129:ILE:HD11	1.96	0.46
1:A:313:GLN:HG2	1:A:321:PRO:HB3	1.97	0.46
1:A:880:LYS:HA	1:A:955:PRO:HA	1.97	0.46
5:E:14:ARG:HH12	5:E:142:VAL:HG22	1.81	0.46
1:A:453:MET:O	1:A:456:MET:HE2	2.16	0.46
1:A:786:HIS:H	1:A:786:HIS:CD2	2.34	0.46
1:A:874:ASP:HA	1:A:1058:VAL:HG13	1.98	0.46
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.97	0.46
1:A:344:ARG:HA	2:B:1128:LEU:O	2.16	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.97	0.45
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.27	0.45
1:A:49:LYS:NZ	1:A:61:ILE:H	2.13	0.45
1:A:1329:THR:HG22	1:A:1331:SER:N	2.26	0.45
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.50	0.45
10:J:25:LEU:HD21	10:J:32:GLU:HA	1.98	0.45
1:A:606:LEU:HG	1:A:613:ILE:HD13	1.98	0.45
6:F:118:LEU:O	6:F:122:MET:HG3	2.16	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.15	0.45
1:A:1147:THR:HB	9:I:48:LEU:HD13	1.98	0.45
1:A:446:ARG:NH1	1:A:479:ASN:HB3	2.32	0.45
1:A:1031:VAL:HA	1:A:1035:TYR:CD2	2.52	0.45
2:B:975:GLN:O	2:B:990:ILE:HD12	2.17	0.45
2:B:1040:ASN:HB3	13:Q:22:ILE:CB	2.47	0.45
4:D:54:GLU:O	4:D:58:VAL:HG23	2.17	0.45
1:A:33:ALA:HB2	1:A:57:ARG:HB3	1.99	0.45
1:A:130:ASP:O	1:A:134:ARG:HB2	2.17	0.45
2:B:542:MET:HE2	2:B:747:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:VAL:O	12:L:56:LEU:HB2	2.16	0.45
1:A:1084:PHE:CG	1:A:1085:HIS:N	2.83	0.45
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.98	0.45
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.99	0.45
1:A:265:LYS:HG2	1:A:303:TYR:HA	1.98	0.45
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.99	0.45
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.98	0.45
1:A:903:ASN:HB3	1:A:906:HIS:HB2	1.99	0.45
2:B:766:ARG:HG3	2:B:766:ARG:NH1	2.32	0.45
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.81	0.45
8:H:105:GLU:HB3	8:H:113:ALA:HB3	1.99	0.45
1:A:858:ASN:ND2	1:A:860:LEU:H	2.16	0.44
1:A:864:ILE:HA	1:A:1377:THR:HG21	1.98	0.44
2:B:756:ILE:O	2:B:759:PRO:HD3	2.17	0.44
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.99	0.44
1:A:754:SER:H	1:A:757:ASN:HD22	1.65	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.44
2:B:249:ARG:HH12	2:B:418:LYS:HB3	1.81	0.44
2:B:361:LEU:N	2:B:362:PRO:HD3	2.33	0.44
2:B:848:ARG:HH12	2:B:996:ARG:HD2	1.82	0.44
2:B:1180:PHE:HD1	4:D:1:MET:HG3	1.82	0.44
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.52	0.44
6:F:134:ILE:HG22	6:F:136:ARG:HG3	2.00	0.44
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.98	0.44
1:A:852:TYR:HB3	6:F:81:THR:CG2	2.47	0.44
8:H:76:THR:HG22	8:H:77:ARG:HD2	1.98	0.44
2:B:376:PHE:CE1	2:B:569:TYR:HD2	2.36	0.44
2:B:515:HIS:H	2:B:518:HIS:HD2	1.66	0.44
5:E:179:GLN:O	5:E:182:ASP:HB2	2.18	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD13	2.00	0.44
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.98	0.44
11:K:77:THR:HB	11:K:81:TYR:HD2	1.82	0.44
2:B:731:VAL:HB	2:B:732:SER:H	1.72	0.44
1:A:711:ARG:HH22	9:I:88:SER:HB2	1.82	0.44
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.00	0.44
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.00	0.44
1:A:1276:VAL:HG21	1:A:1316:VAL:HG22	1.99	0.44
1:A:1325:THR:HA	5:E:147:HIS:HA	2.00	0.44
1:A:907:THR:HG22	1:A:908:LEU:H	1.82	0.43
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.53	0.43
3:C:58:LEU:HB3	3:C:63:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:60:ARG:HH22	7:G:63:PRO:HG3	1.82	0.43
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.83	0.43
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.43
3:C:29:MET:HA	11:K:45:LEU:HD13	2.01	0.43
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.99	0.43
2:B:1162:ILE:HG12	2:B:1194:ILE:HG12	2.01	0.43
9:I:82:GLU:HG2	9:I:104:LEU:HD13	1.99	0.43
1:A:768:GLN:CG	1:A:816:HIS:HA	2.37	0.43
1:A:982:THR:H	1:A:985:ASP:HB2	1.82	0.43
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.00	0.43
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.53	0.43
8:H:79:TRP:CH2	8:H:81:PRO:HA	2.54	0.43
1:A:40:THR:HG22	1:A:41:MET:HE3	2.01	0.43
1:A:774:ARG:H	1:A:774:ARG:HG3	1.67	0.43
2:B:866:TYR:O	2:B:870:ILE:HB	2.19	0.43
3:C:148:ARG:HB3	3:C:149:LYS:H	1.65	0.43
8:H:58:THR:HB	8:H:143:LEU:HB2	2.01	0.43
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.01	0.43
1:A:10:PRO:HD2	2:B:1191:ILE:O	2.18	0.43
2:B:242:SER:OG	2:B:362:PRO:HD2	2.19	0.43
2:B:996:ARG:HG2	2:B:1007:VAL:HG11	2.01	0.43
7:G:134:GLU:HG2	7:G:135:ASP:H	1.83	0.43
1:A:262:LEU:HD11	1:A:325:ILE:HG12	2.00	0.43
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.88	0.43
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.83	0.43
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	0.43
2:B:875:GLU:O	2:B:877:PRO:HD3	2.19	0.43
5:E:147:HIS:CD2	5:E:149:LEU:H	2.37	0.43
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.43
1:A:382:PRO:HA	1:A:428:TYR:HE1	1.84	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.62	0.43
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	2.00	0.43
2:B:476:ARG:HB2	2:B:476:ARG:HH21	1.84	0.43
2:B:768:THR:O	2:B:771:SER:HB2	2.19	0.43
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.52	0.42
1:A:374:LEU:HA	2:B:1107:ALA:HB2	2.01	0.42
2:B:398:ARG:HB2	2:B:398:ARG:HH11	1.83	0.42
12:L:32:ALA:HB3	12:L:55:ILE:CG2	2.49	0.42
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.34	0.42
2:B:825:VAL:HG22	2:B:1010:LEU:HB2	2.01	0.42
3:C:125:MET:HG2	3:C:127:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:LYS:HE3	5:E:84:ASP:HB2	2.01	0.42
7:G:14:HIS:HD2	7:G:16:SER:OG	2.02	0.42
1:A:482:PHE:C	1:A:484:GLY:H	2.27	0.42
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.00	0.42
1:A:901:LEU:H	1:A:926:GLN:NE2	2.17	0.42
1:A:1079:MET:HE1	1:A:1356:ILE:HA	2.02	0.42
2:B:125:SER:HA	2:B:171:PRO:HA	2.01	0.42
2:B:1002:THR:HG21	2:B:1070:GLU:OE2	2.20	0.42
2:B:1130:PHE:CG	2:B:1150:ARG:HG3	2.55	0.42
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.01	0.42
8:H:10:PHE:HB3	8:H:28:ALA:HB1	2.02	0.42
9:I:7:CYS:SG	9:I:8:ARG:O	2.78	0.42
1:A:453:MET:HB3	1:A:477:PRO:HB2	1.99	0.42
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.59	0.42
3:C:62:PHE:O	3:C:66:ARG:HG3	2.20	0.42
5:E:15:ALA:O	5:E:19:VAL:HG23	2.18	0.42
10:J:14:VAL:HB	10:J:50:ILE:HD11	2.01	0.42
12:L:53:HIS:ND1	12:L:55:ILE:HG22	2.33	0.42
5:E:178:ILE:HB	5:E:212:ARG:HB3	2.01	0.42
8:H:81:PRO:HA	8:H:82:PRO:HD3	1.90	0.42
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.85	0.42
2:B:614:SER:HB3	2:B:627:PHE:HB2	2.01	0.42
10:J:8:PHE:H	10:J:49:MET:CE	2.26	0.42
1:A:33:ALA:HB2	1:A:57:ARG:CB	2.50	0.42
1:A:1173:HIS:CB	1:A:1227:ILE:HG23	2.50	0.42
1:A:182:VAL:HG22	1:A:201:VAL:HA	2.02	0.42
1:A:692:ASP:O	1:A:696:GLU:HB2	2.20	0.42
2:B:542:MET:HB3	2:B:636:PRO:HD2	2.02	0.42
10:J:7:CYS:HA	10:J:49:MET:HE3	2.02	0.42
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.20	0.42
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.44	0.42
2:B:90:ILE:HG21	2:B:432:MET:SD	2.60	0.42
2:B:121:ASN:HA	2:B:207:GLY:CA	2.50	0.42
10:J:7:CYS:HA	10:J:49:MET:HG2	2.02	0.42
1:A:568:PRO:HG2	8:H:95:TYR:CD1	2.55	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.54	0.41
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.55	0.41
1:A:41:MET:HB2	1:A:42:ASP:H	1.58	0.41
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.50	0.41
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:MET:HB3	1:A:1081:LEU:HD21	2.00	0.41
1:A:1255:GLU:OE2	1:A:1258:HIS:HB3	2.20	0.41
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.20	0.41
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.34	0.41
1:A:956:LEU:HB3	1:A:957:PRO:HD2	2.02	0.41
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.02	0.41
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.50	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.41
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.55	0.41
1:A:867:ILE:HD12	1:A:871:ASP:C	2.45	0.41
1:A:1031:VAL:HA	1:A:1035:TYR:HD2	1.84	0.41
1:A:1081:LEU:CG	1:A:1097:GLY:HA3	2.51	0.41
3:C:242:GLN:O	3:C:246:ARG:HB2	2.20	0.41
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.56	0.41
2:B:309:GLN:HE22	9:I:50:THR:HG23	1.85	0.41
12:L:38:LEU:HD22	12:L:56:LEU:HD21	2.03	0.41
1:A:55:ASP:OD1	1:A:57:ARG:HB2	2.20	0.41
1:A:986:ILE:HD13	1:A:1031:VAL:HB	2.02	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.61	0.41
2:B:126:SER:CB	2:B:172:ILE:HD11	2.50	0.41
2:B:235:SER:HB3	2:B:258:LEU:HD13	2.01	0.41
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.02	0.41
2:B:602:THR:HA	2:B:605:ARG:HB2	2.03	0.41
10:J:45:CYS:O	10:J:48:ARG:HG3	2.21	0.41
1:A:849:MET:HG2	1:A:850:VAL:N	2.35	0.41
1:A:973:ILE:HD11	1:A:1038:THR:HG23	2.02	0.41
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	2.03	0.41
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.21	0.41
1:A:548:ASN:ND2	11:K:47:ARG:HE	2.19	0.41
1:A:675:THR:HG21	1:A:736:ASN:HB2	2.03	0.41
2:B:228:LYS:HD2	2:B:228:LYS:HA	1.91	0.41
2:B:361:LEU:O	2:B:374:LYS:HE2	2.21	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
2:B:978:ASP:O	2:B:989:THR:HA	2.21	0.41
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.03	0.41
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.94	0.41
1:A:622:VAL:HG23	1:A:629:LEU:HD12	2.02	0.41
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	2.03	0.41
1:A:1358:SER:C	1:A:1360:GLY:H	2.29	0.41
7:G:101:VAL:HG12	7:G:103:VAL:HG23	2.03	0.41
8:H:111:LEU:HA	8:H:127:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.99	0.40
1:A:1148:ILE:HD12	1:A:1196:GLU:HG2	2.03	0.40
2:B:210:LYS:HD3	2:B:482:VAL:HG22	2.02	0.40
2:B:212:LEU:HD21	2:B:461:LEU:HD23	2.02	0.40
2:B:318:VAL:HG21	9:I:13:MET:HE3	2.03	0.40
2:B:862:GLN:HG3	2:B:963:PHE:HD1	1.86	0.40
4:D:5:THR:HG21	7:G:74:TYR:OH	2.20	0.40
1:A:1368:MET:HE3	1:A:1368:MET:HB2	1.97	0.40
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	2.03	0.40
7:G:1:MET:SD	7:G:2:PHE:N	2.87	0.40
1:A:23:SER:O	1:A:24:PRO:C	2.62	0.40
1:A:408:ASP:C	1:A:410:GLY:H	2.29	0.40
1:A:472:LEU:HD21	2:B:836:GLU:HG3	2.04	0.40
2:B:234:ILE:HG12	2:B:257:LYS:HB3	2.03	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40
3:C:4:GLU:O	11:K:100:ALA:HB1	2.22	0.40
5:E:182:ASP:O	5:E:186:LEU:HG	2.20	0.40
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.02	0.40
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.57	0.40
1:A:25:GLU:CD	1:A:25:GLU:H	2.30	0.40
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.88	0.40
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.04	0.40
1:A:3:GLY:HA3	2:B:1159:ARG:HB3	2.04	0.40
4:D:121:LYS:H	4:D:121:LYS:HE3	1.86	0.40
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.03	0.40
10:J:8:PHE:N	10:J:49:MET:HE3	2.27	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	1411/1732 (82%)	1237 (88%)	140 (10%)	34 (2%)	4	29
2	B	1102/1223 (90%)	961 (87%)	114 (10%)	27 (2%)	4	29
3	C	264/266 (99%)	240 (91%)	20 (8%)	4 (2%)	8	37
4	D	176/221 (80%)	156 (89%)	15 (8%)	5 (3%)	4	27
5	E	212/214 (99%)	196 (92%)	14 (7%)	2 (1%)	14	47
6	F	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	10	41
8	H	129/145 (89%)	110 (85%)	14 (11%)	5 (4%)	2	21
9	I	117/119 (98%)	100 (86%)	15 (13%)	2 (2%)	7	35
10	J	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	18
11	K	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14	47
12	L	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	0	9
13	Q	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	3898/4419 (88%)	3441 (88%)	368 (9%)	89 (2%)	5	30

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	335	ARG
1	A	775	ILE
2	B	67	SER
2	B	339	THR
2	B	368	GLU
2	B	629	ASP
2	B	731	VAL
2	B	879	ARG
2	B	1046	PRO
4	D	13	ARG
4	D	119	ARG
8	H	17	PRO
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	45	GLN
1	A	65	LEU
1	A	251	SER
1	A	331	GLY

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Mol	Chain	Res	Type
1	A	466	SER
1	A	846	GLU
1	A	1379	GLY
2	B	65	GLU
2	B	364	ILE
2	B	643	ASP
2	B	712	PRO
2	B	907	GLY
2	B	1066	SER
2	B	1096	ARG
2	B	1176	ASN
2	B	1185	CYS
4	D	199	ASN
7	G	2	PHE
8	H	18	GLY
8	H	85	GLY
8	H	128	ASN
10	J	6	ARG
10	J	17	LYS
1	A	41	MET
1	A	114	LEU
1	A	483	ASP
1	A	1403	GLU
2	B	711	GLU
2	B	851	PHE
2	B	881	ASN
3	C	38	ILE
3	C	215	GLU
4	D	75	LYS
4	D	198	LEU
5	E	48	ASP
1	A	49	LYS
1	A	282	ASN
1	A	322	VAL
1	A	1327	ILE
2	B	363	HIS
2	B	470	LYS
2	B	655	LYS
2	B	1017	ILE
3	C	90	ASP
10	J	56	LEU
1	A	196	GLU

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Mol	Chain	Res	Type
1	A	409	SER
1	A	465	TYR
1	A	600	PRO
1	A	1122	PRO
1	A	1365	TYR
1	A	1405	THR
2	B	340	ALA
2	B	648	HIS
2	B	707	PRO
3	C	214	ASN
7	G	63	PRO
8	H	136	LYS
9	I	89	GLN
9	I	91	ARG
11	K	64	GLU
12	L	45	ALA
1	A	55	ASP
1	A	250	ILE
1	A	283	GLY
1	A	332	LYS
1	A	1081	LEU
2	B	58	THR
5	E	51	GLY
1	A	258	GLY
1	A	916	GLY
1	A	93	VAL
1	A	1437	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1519 (82%)	1047 (84%)	197 (16%)	2	15
2	B	967/1060 (91%)	822 (85%)	145 (15%)	3	16
3	C	234/234 (100%)	196 (84%)	38 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	160/200 (80%)	134 (84%)	26 (16%)	2	14
5	E	196/196 (100%)	176 (90%)	20 (10%)	7	26
6	F	77/77 (100%)	67 (87%)	10 (13%)	4	19
7	G	152/152 (100%)	131 (86%)	21 (14%)	3	18
8	H	117/127 (92%)	104 (89%)	13 (11%)	6	23
9	I	113/113 (100%)	96 (85%)	17 (15%)	3	16
10	J	60/60 (100%)	51 (85%)	9 (15%)	3	16
11	K	99/99 (100%)	90 (91%)	9 (9%)	9	31
12	L	40/40 (100%)	28 (70%)	12 (30%)	0	2
13	Q	1/15 (7%)	0	1 (100%)	0	0
All	All	3460/3892 (89%)	2942 (85%)	518 (15%)	3	16

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	28	ARG
1	A	30	ILE
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	53	LEU
1	A	55	ASP
1	A	60	SER
1	A	63	ARG
1	A	64	ASN
1	A	96	ILE
1	A	115	LEU
1	A	116	ASP
1	A	121	LEU
1	A	145	LYS
1	A	152	VAL
1	A	170	THR

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Mol	Chain	Res	Type
1	A	174	ILE
1	A	199	LEU
1	A	204	THR
1	A	210	ILE
1	A	232	GLU
1	A	236	LEU
1	A	237	THR
1	A	250	ILE
1	A	251	SER
1	A	253	ASN
1	A	255	SER
1	A	257	ARG
1	A	261	ASP
1	A	265	LYS
1	A	277	GLU
1	A	295	LEU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	317	LYS
1	A	318	SER
1	A	320	ARG
1	A	322	VAL
1	A	329	LEU
1	A	330	LYS
1	A	337	ARG
1	A	344	ARG
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	406	ILE
1	A	408	ASP
1	A	412	ARG
1	A	433	GLU
1	A	434	ARG
1	A	437	MET
1	A	443	LEU
1	A	445	ASN

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Mol	Chain	Res	Type
1	A	450	LEU
1	A	451	HIS
1	A	453	MET
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	500	GLU
1	A	505	CYS
1	A	523	ILE
1	A	526	ASP
1	A	527	THR
1	A	541	ILE
1	A	544	ASP
1	A	566	ILE
1	A	577	ILE
1	A	584	ASN
1	A	597	LEU
1	A	602	ASP
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	644	LYS
1	A	666	ILE
1	A	670	ILE
1	A	691	LEU
1	A	740	LEU
1	A	768	GLN
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG
1	A	830	LYS

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Mol	Chain	Res	Type
1	A	831	THR
1	A	839	ARG
1	A	840	ARG
1	A	842	VAL
1	A	855	THR
1	A	858	ASN
1	A	880	LYS
1	A	895	LYS
1	A	896	ARG
1	A	905	ASP
1	A	908	LEU
1	A	919	ILE
1	A	926	GLN
1	A	929	LEU
1	A	931	GLU
1	A	932	GLU
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	983	ILE
1	A	988	LEU
1	A	1001	ARG
1	A	1031	VAL
1	A	1035	TYR
1	A	1046	LEU
1	A	1052	GLN
1	A	1058	VAL
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1074	GLU
1	A	1080	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1092	LYS
1	A	1110	ASN
1	A	1112	LYS
1	A	1116	LEU
1	A	1120	LEU
1	A	1132	LYS

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Mol	Chain	Res	Type
1	A	1133	LEU
1	A	1135	ARG
1	A	1146	VAL
1	A	1147	THR
1	A	1159	ARG
1	A	1167	GLU
1	A	1168	GLU
1	A	1170	ILE
1	A	1176	LEU
1	A	1187	GLN
1	A	1188	GLN
1	A	1208	THR
1	A	1227	ILE
1	A	1237	ILE
1	A	1242	VAL
1	A	1256	GLU
1	A	1265	ASN
1	A	1266	THR
1	A	1269	GLU
1	A	1277	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1317	MET
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1356	ILE
1	A	1361	SER
1	A	1366	ARG
1	A	1371	LEU
1	A	1376	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1404	GLU
1	A	1405	THR
1	A	1406	VAL
1	A	1426	GLU

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Mol	Chain	Res	Type
1	A	1428	VAL
1	A	1438	THR
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1452	LYS
2	B	25	ILE
2	B	26	THR
2	B	35	SER
2	B	44	VAL
2	B	46	GLN
2	B	63	ILE
2	B	68	THR
2	B	90	ILE
2	B	103	ASN
2	B	122	LEU
2	B	128	LEU
2	B	167	ILE
2	B	169	ARG
2	B	172	ILE
2	B	178	ASN
2	B	205	ILE
2	B	211	VAL
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	240	ILE
2	B	251	ILE
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	267	ARG
2	B	284	ILE
2	B	313	MET
2	B	324	ILE
2	B	336	ARG
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	357	GLN
2	B	365	THR
2	B	368	GLU

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Mol	Chain	Res	Type
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	399	ASP
2	B	408	LEU
2	B	418	LYS
2	B	423	LYS
2	B	446	LEU
2	B	470	LYS
2	B	476	ARG
2	B	481	GLN
2	B	483	LEU
2	B	485	ARG
2	B	502	ILE
2	B	508	LEU
2	B	510	LYS
2	B	531	GLN
2	B	543	SER
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	559	SER
2	B	560	GLU
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	573	GLN
2	B	582	VAL
2	B	589	VAL
2	B	598	GLU
2	B	599	THR
2	B	603	LEU
2	B	604	ARG
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	628	THR
2	B	651	LEU
2	B	658	ILE
2	B	665	GLU
2	B	690	VAL
2	B	696	GLU

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Mol	Chain	Res	Type
2	B	708	GLU
2	B	731	VAL
2	B	737	THR
2	B	743	ILE
2	B	766	ARG
2	B	780	VAL
2	B	789	MET
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	815	ARG
2	B	816	GLU
2	B	831	SER
2	B	844	SER
2	B	868	MET
2	B	871	THR
2	B	876	LYS
2	B	878	GLN
2	B	881	ASN
2	B	882	THR
2	B	883	LEU
2	B	899	ILE
2	B	904	ARG
2	B	906	SER
2	B	908	GLU
2	B	942	ARG
2	B	945	GLU
2	B	953	LEU
2	B	971	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	978	ASP
2	B	995	ARG
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1013	ASN
2	B	1019	SER
2	B	1045	SER
2	B	1058	LEU

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Mol	Chain	Res	Type
2	B	1060	ARG
2	B	1065	GLN
2	B	1080	LYS
2	B	1081	LEU
2	B	1113	VAL
2	B	1128	LEU
2	B	1133	MET
2	B	1134	GLU
2	B	1138	MET
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1188	LYS
2	B	1190	ASP
2	B	1191	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
3	C	3	GLU
3	C	4	GLU
3	C	7	GLN
3	C	9	LYS
3	C	22	LEU
3	C	25	VAL
3	C	27	LEU
3	C	40	GLU
3	C	44	LEU
3	C	50	GLU
3	C	52	GLU
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	79	GLN
3	C	83	SER

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Mol	Chain	Res	Type
3	C	85	ASP
3	C	116	LYS
3	C	119	VAL
3	C	121	VAL
3	C	125	MET
3	C	127	ARG
3	C	133	ILE
3	C	134	ILE
3	C	142	VAL
3	C	154	LYS
3	C	166	GLU
3	C	189	THR
3	C	197	SER
3	C	215	GLU
3	C	222	LYS
3	C	226	ASP
3	C	237	SER
3	C	240	VAL
3	C	262	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	6	SER
4	D	8	PHE
4	D	9	GLN
4	D	15	LEU
4	D	21	GLU
4	D	39	ASN
4	D	51	ASN
4	D	53	SER
4	D	63	LEU
4	D	64	VAL
4	D	65	GLU
4	D	121	LYS
4	D	122	GLU
4	D	126	ILE
4	D	142	LYS
4	D	149	THR
4	D	150	ASN
4	D	164	ILE
4	D	187	THR
4	D	193	THR

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Mol	Chain	Res	Type
4	D	203	SER
4	D	207	LEU
4	D	217	LEU
4	D	219	THR
4	D	220	LEU
5	E	3	GLN
5	E	57	MET
5	E	67	GLU
5	E	75	MET
5	E	81	GLU
5	E	92	THR
5	E	95	THR
5	E	100	ILE
5	E	101	GLN
5	E	114	ASN
5	E	140	LEU
5	E	148	GLU
5	E	166	LYS
5	E	177	ARG
5	E	178	ILE
5	E	182	ASP
5	E	184	VAL
5	E	196	VAL
5	E	198	ILE
5	E	210	SER
6	F	69	LEU
6	F	70	LYS
6	F	71	GLU
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	96	THR
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
7	G	5	LYS
7	G	8	SER
7	G	11	ILE
7	G	22	MET
7	G	23	LYS
7	G	26	LEU
7	G	34	VAL

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Mol	Chain	Res	Type
7	G	83	LYS
7	G	92	VAL
7	G	106	MET
7	G	108	VAL
7	G	118	ASP
7	G	120	THR
7	G	126	ASN
7	G	141	SER
7	G	142	ARG
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	154	VAL
7	G	171	ILE
8	H	5	LEU
8	H	11	GLN
8	H	19	ARG
8	H	26	ILE
8	H	31	THR
8	H	53	ASP
8	H	76	THR
8	H	103	LYS
8	H	112	ILE
8	H	130	ARG
8	H	131	ASN
8	H	135	LEU
8	H	146	ARG
9	I	7	CYS
9	I	10	CYS
9	I	13	MET
9	I	21	GLU
9	I	30	ARG
9	I	35	VAL
9	I	43	VAL
9	I	54	GLU
9	I	55	THR
9	I	62	ILE
9	I	77	LYS
9	I	81	ARG
9	I	87	GLN
9	I	88	SER
9	I	104	LEU

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Mol	Chain	Res	Type
9	I	108	HIS
9	I	111	THR
10	J	1	MET
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	20	SER
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	2	ASN
11	K	9	LEU
11	K	18	LYS
11	K	20	LYS
11	K	31	VAL
11	K	41	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
12	L	30	ILE
12	L	38	LEU
12	L	44	ASP
12	L	46	VAL
12	L	53	HIS
12	L	54	ARG
12	L	55	ILE
12	L	61	THR
12	L	64	LEU
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU
13	Q	27	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	68	GLN
1	A	209	ASN
1	A	225	ASN
1	A	299	HIS

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	339	ASN
1	A	435	HIS
1	A	451	HIS
1	A	490	HIS
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	548	ASN
1	A	576	GLN
1	A	603	ASN
1	A	631	HIS
1	A	650	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	926	GLN
1	A	935	GLN
1	A	968	GLN
1	A	972	HIS
1	A	975	HIS
1	A	1070	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1130	GLN
1	A	1211	GLN
1	A	1265	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	178	ASN
2	B	300	HIS
2	B	309	GLN
2	B	415	GLN
2	B	433	GLN
2	B	484	ASN

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Mol	Chain	Res	Type
2	B	518	HIS
2	B	538	ASN
2	B	740	HIS
2	B	744	HIS
2	B	767	ASN
2	B	843	GLN
2	B	862	GLN
2	B	878	GLN
2	B	958	GLN
2	B	986	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1112	GLN
2	B	1117	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1195	HIS
2	B	1211	ASN
3	C	54	ASN
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	128	ASN
3	C	151	GLN
3	C	184	ASN
3	C	231	ASN
4	D	28	GLN
4	D	41	GLN
4	D	132	GLN
4	D	143	ASN
4	D	165	GLN
4	D	179	GLN
5	E	5	ASN
5	E	8	ASN
5	E	147	HIS
6	F	104	ASN
7	G	14	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	22	ASN
9	I	51	ASN

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Mol	Chain	Res	Type
9	I	79	HIS
9	I	116	ASN
11	K	2	ASN
11	K	65	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1421/1732 (82%)	-0.06	27 (1%) 66 46	55, 112, 198, 278	0
2	B	1118/1223 (91%)	0.11	43 (3%) 44 32	59, 127, 216, 300	0
3	C	266/266 (100%)	-0.12	2 (0%) 82 64	76, 117, 173, 219	0
4	D	180/221 (81%)	0.13	9 (5%) 34 26	92, 131, 203, 241	0
5	E	214/214 (100%)	0.08	0 100 100	86, 162, 233, 254	0
6	F	87/87 (100%)	-0.21	2 (2%) 61 43	59, 89, 131, 142	0
7	G	171/171 (100%)	-0.15	2 (1%) 76 55	79, 111, 158, 224	0
8	H	133/145 (91%)	0.21	9 (6%) 23 21	104, 166, 223, 237	0
9	I	119/119 (100%)	0.38	10 (8%) 17 18	128, 157, 227, 246	0
10	J	65/65 (100%)	0.07	2 (3%) 51 36	85, 111, 162, 184	0
11	K	115/115 (100%)	-0.26	1 (0%) 81 62	66, 113, 165, 200	0
12	L	46/46 (100%)	0.68	7 (15%) 5 8	98, 169, 211, 238	0
13	Q	15/15 (100%)	2.04	7 (46%) 0 1	108, 188, 212, 222	0
All	All	3950/4419 (89%)	0.03	121 (3%) 51 36	55, 122, 210, 300	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	9.3
4	D	3	VAL	6.0
1	A	65	LEU	5.4
2	B	446	LEU	5.1
12	L	27	LEU	5.0
2	B	436	VAL	4.6
13	Q	28	ARG	4.4
2	B	658	ILE	4.4
2	B	715	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
13	Q	27	MET	4.0
1	A	1254	ALA	3.9
2	B	447	ALA	3.9
1	A	186	LYS	3.9
1	A	1083	THR	3.8
13	Q	21	PHE	3.8
4	D	18	VAL	3.8
2	B	341	LEU	3.8
1	A	1084	PHE	3.8
9	I	97	MET	3.7
8	H	63	LEU	3.7
2	B	70	ILE	3.6
12	L	62	LYS	3.6
10	J	65	PRO	3.5
2	B	246	LYS	3.5
2	B	882	THR	3.5
11	K	114	LEU	3.5
2	B	437	GLU	3.4
1	A	1126	ALA	3.4
2	B	727	LYS	3.3
2	B	164	LYS	3.3
1	A	1085	HIS	3.2
9	I	3	THR	3.2
1	A	251	SER	3.2
8	H	136	LYS	3.1
2	B	108	VAL	3.1
2	B	340	ALA	3.1
1	A	1176	LEU	3.1
4	D	15	LEU	3.1
2	B	474	SER	3.0
2	B	468	GLU	3.0
2	B	508	LEU	2.9
9	I	2	THR	2.9
12	L	25	ALA	2.9
1	A	114	LEU	2.9
8	H	14	GLU	2.9
12	L	33	GLU	2.9
4	D	1	MET	2.8
6	F	69	LEU	2.8
1	A	480	ALA	2.8
8	H	132	LEU	2.8
1	A	1187	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
13	Q	29	ARG	2.8
2	B	134	LYS	2.8
2	B	469	GLN	2.8
3	C	218	PRO	2.7
1	A	142	CYS	2.7
4	D	221	TYR	2.7
8	H	2	SER	2.7
9	I	52	ILE	2.7
1	A	145	LYS	2.7
1	A	1080	THR	2.7
9	I	100	PHE	2.6
1	A	1092	LYS	2.6
2	B	503	GLY	2.6
1	A	483	ASP	2.6
6	F	72	LYS	2.6
3	C	268	ASP	2.6
2	B	470	LYS	2.6
8	H	13	SER	2.5
4	D	20	GLU	2.5
1	A	195	ASP	2.5
4	D	13	ARG	2.5
2	B	880	THR	2.5
8	H	77	ARG	2.5
2	B	1049	ASP	2.4
2	B	714	GLU	2.4
9	I	57	GLY	2.4
1	A	1173	HIS	2.4
2	B	712	PRO	2.4
2	B	507	LYS	2.4
12	L	26	THR	2.4
13	Q	25	ASP	2.4
13	Q	26	ARG	2.4
8	H	139	ASN	2.4
12	L	28	LYS	2.4
9	I	87	GLN	2.4
8	H	76	THR	2.4
2	B	866	TYR	2.4
2	B	934	LYS	2.4
1	A	1244	ARG	2.3
1	A	1093	LYS	2.3
2	B	266	ALA	2.3
2	B	1222	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	117	LYS	2.3
10	J	50	ILE	2.3
2	B	643	ASP	2.3
2	B	262	GLU	2.2
2	B	476	ARG	2.2
1	A	250	ILE	2.2
9	I	118	ARG	2.2
2	B	250	PHE	2.2
1	A	63	ARG	2.2
13	Q	35	ARG	2.1
2	B	339	THR	2.1
7	G	117	GLN	2.1
4	D	118	THR	2.1
12	L	43	THR	2.1
7	G	123	ALA	2.1
4	D	2	ASN	2.1
9	I	120	GLN	2.1
2	B	679	TYR	2.1
2	B	344	LYS	2.1
2	B	663	ALA	2.1
2	B	986	GLN	2.1
2	B	987	LYS	2.1
2	B	646	LEU	2.0
1	A	46	THR	2.0
1	A	1125	ALA	2.0
2	B	245	GLU	2.0
1	A	162	VAL	2.0
2	B	1052	VAL	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(Å ²)	Q<0.9
15	MG	A	1803	1/1	0.72	0.38	50,50,50,50	0
14	ZN	L	101	1/1	0.99	0.03	149,149,149,149	0
14	ZN	I	202	1/1	0.99	0.04	211,211,211,211	0
14	ZN	C	301	1/1	1.00	0.03	94,94,94,94	0
14	ZN	I	201	1/1	1.00	0.03	127,127,127,127	0
14	ZN	A	1801	1/1	1.00	0.02	163,163,163,163	0
14	ZN	J	101	1/1	1.00	0.05	111,111,111,111	0
14	ZN	A	1802	1/1	1.00	0.04	97,97,97,97	0
14	ZN	B	1301	1/1	1.00	0.07	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.