



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:33 PM UTC

PDB ID : 5IP7 / pdb_00005ip7
Title : Structure of RNA Polymerase II-Tfg1 peptide complex
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-09
Resolution : 3.52 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:

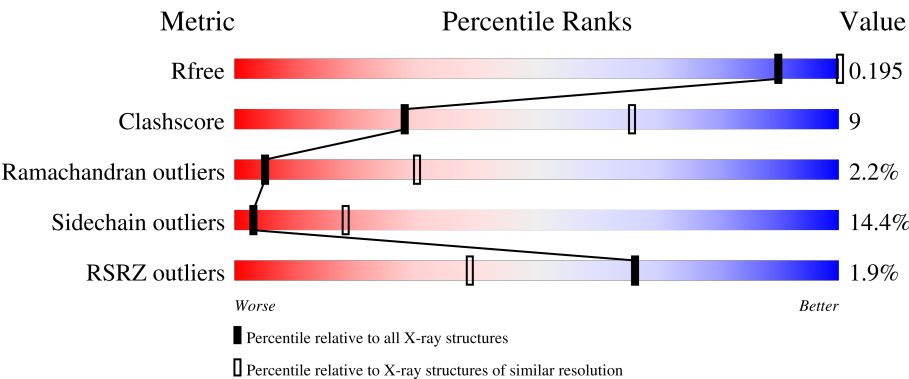
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	54%22%18%
2	B	1223	61%24%5%9% 2%
3	C	266	64%26%9%
4	D	221	52%23%5%19% 5%
5	E	214	79%19%

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Mol	Chain	Length	Quality of chain
6	F	87	% 66%25%9%
7	G	171	% 64%30%5%
8	H	145	3% 60%28%8%
9	I	119	3% 57%34%8%
10	J	65	2% 58%29%11%
11	K	115	2% 70%25%
12	L	46	11% 46%37%17%
13	Q	15	27% 80%20%

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

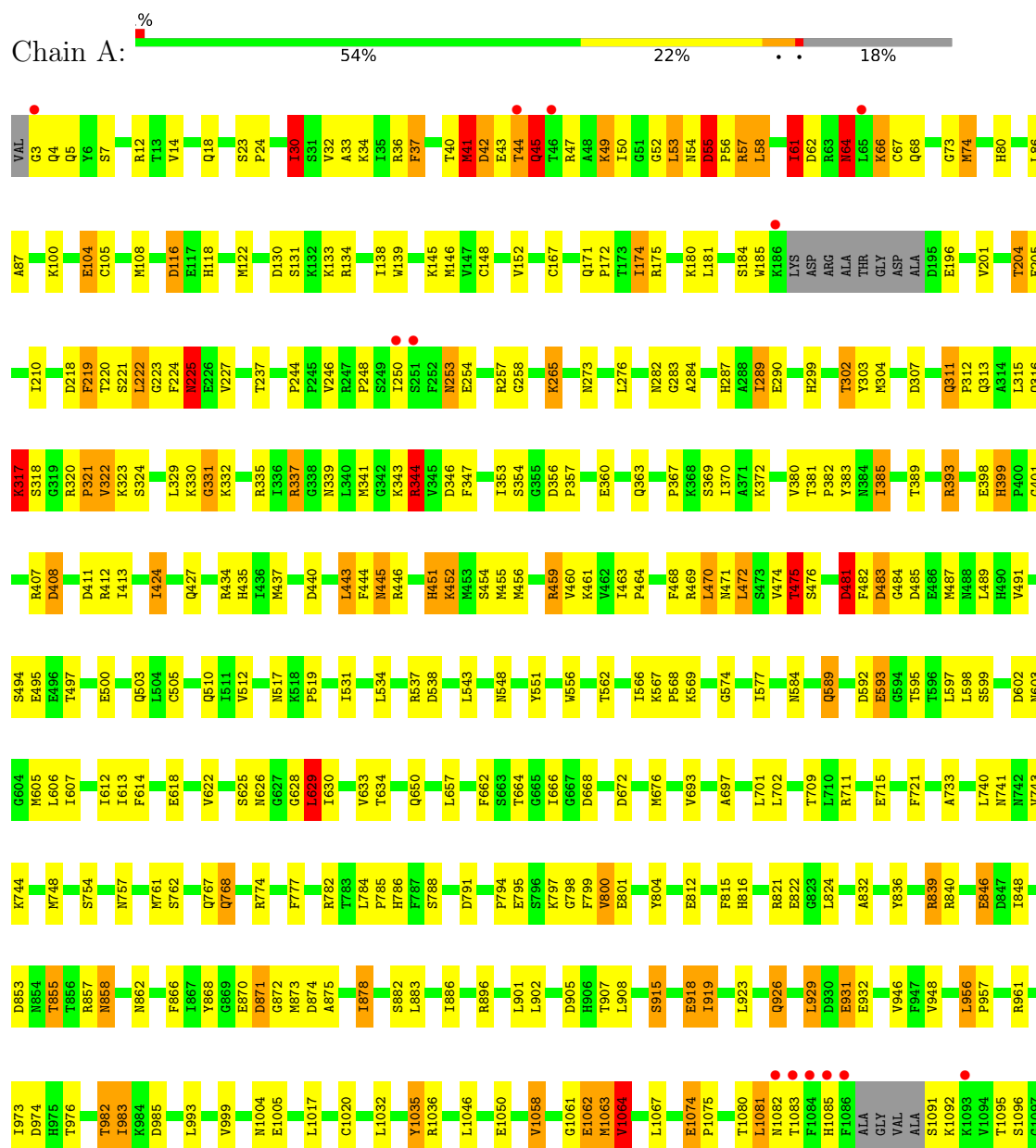
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

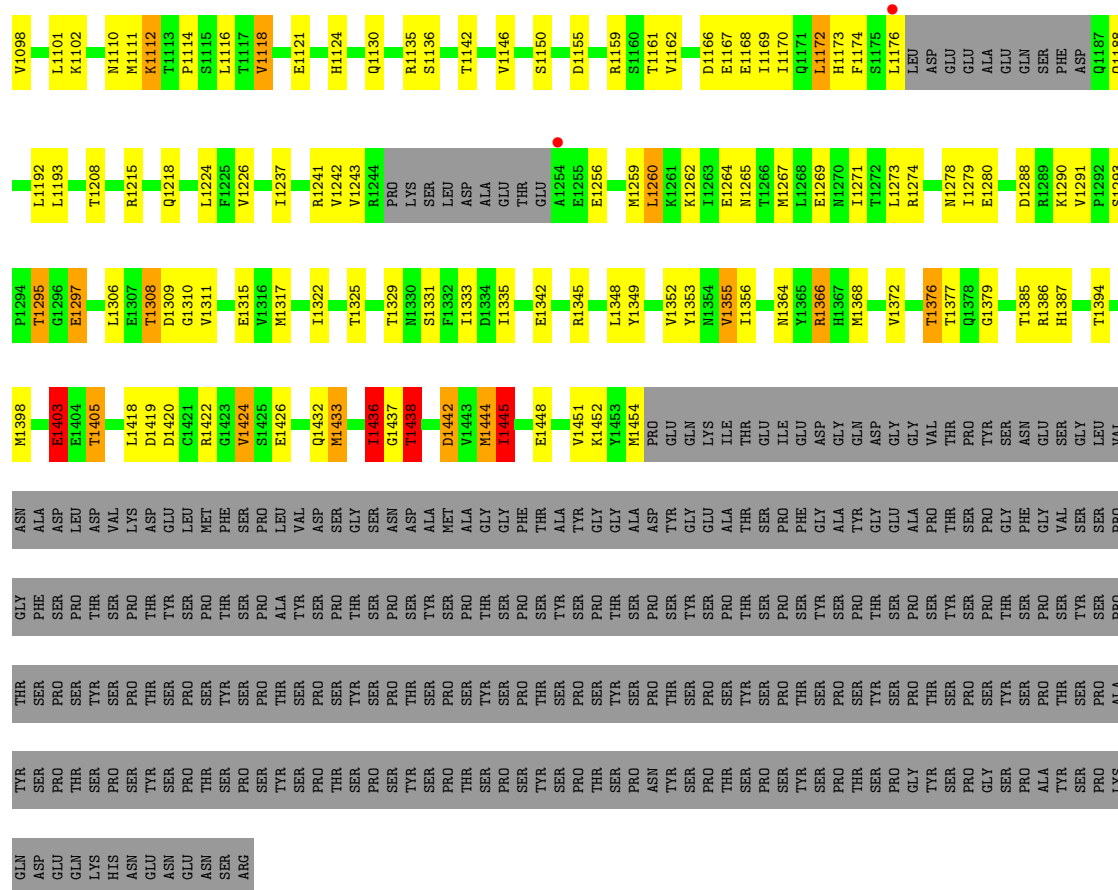
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

3 Residue-property plots

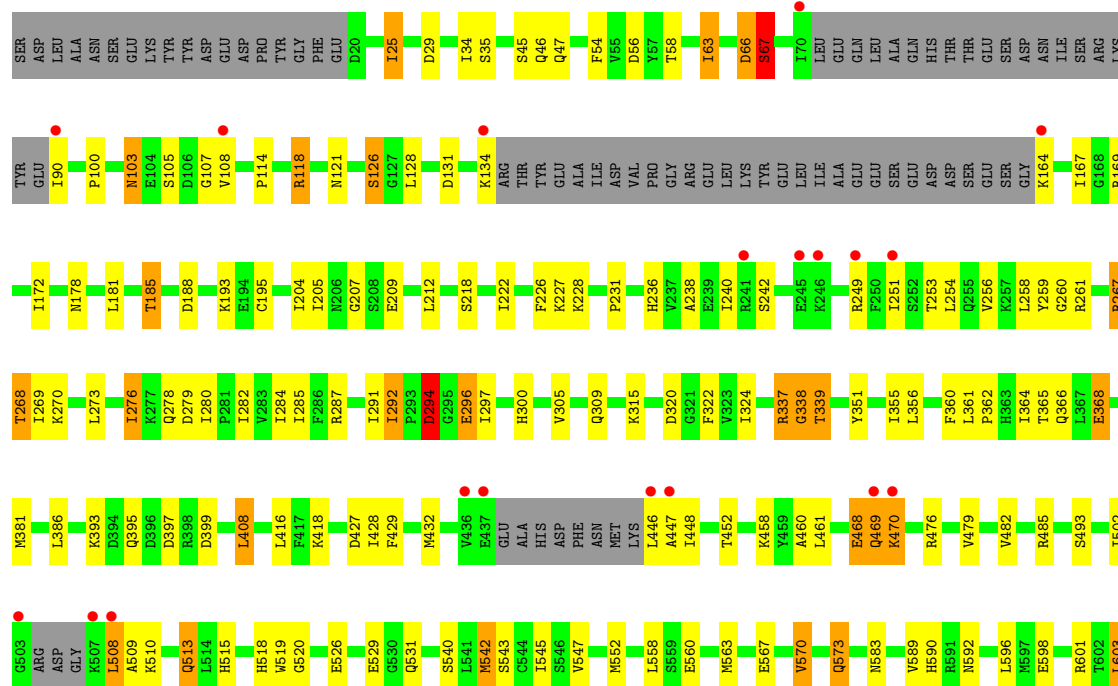
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

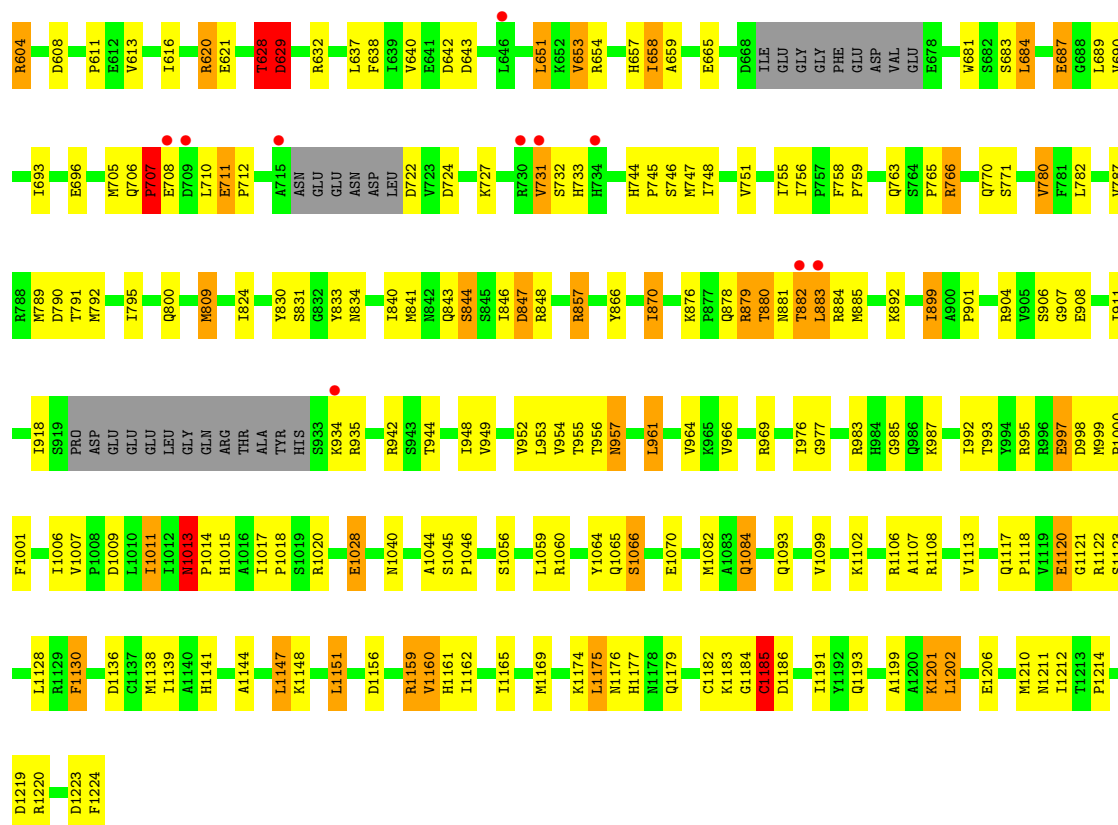
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





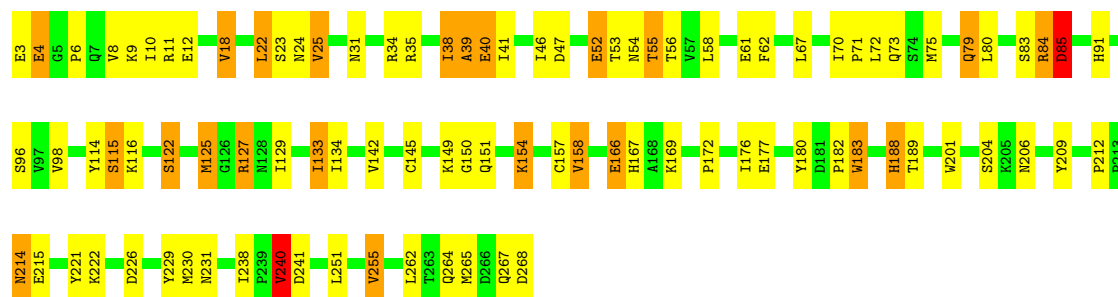
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2





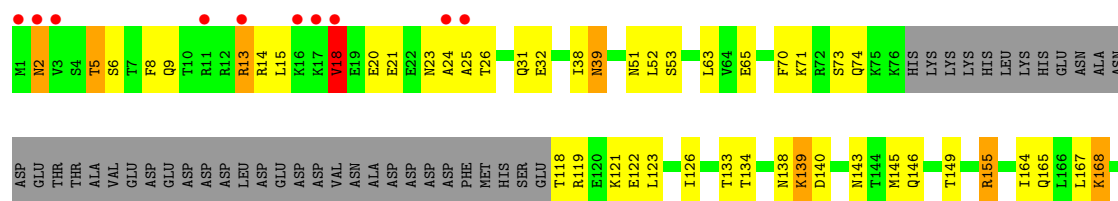
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 64% 26% 9%



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

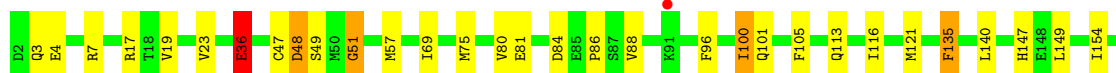
Chain D: 5% 52% 23% 5% 19%





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

Chain E: 79% 19% .



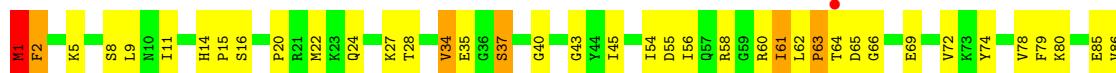
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: % 66% 25% 9%



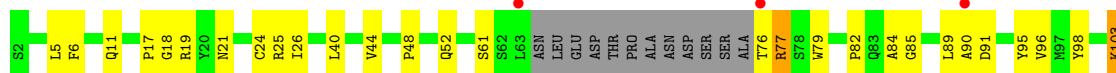
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

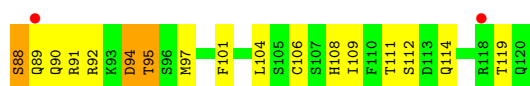
Chain G: % 64% 30% 5% .



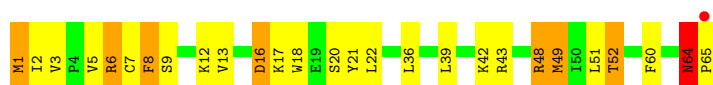
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 3% 60% 28% . . 8%

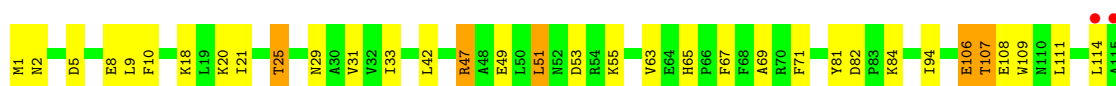




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



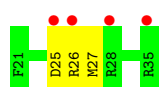
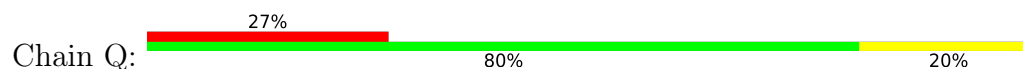
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- 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	221.22Å 392.73Å 282.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 3.52 48.93 – 3.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.93-3.52) 99.9 (48.93-3.52)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.48Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.154 , 0.180 0.172 , 0.195	Depositor DCC
R_{free} test set	2983 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	111.0	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 136.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.007 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.008 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31339	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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	0.93	9/11391 (0.1%)	1.52	123/15402 (0.8%)
2	B	0.86	1/9048 (0.0%)	1.41	71/12200 (0.6%)
3	C	0.85	1/2133 (0.0%)	1.47	21/2891 (0.7%)
4	D	0.91	2/1450 (0.1%)	1.65	31/1945 (1.6%)
5	E	0.80	0/1788	1.42	10/2406 (0.4%)
6	F	1.00	1/717 (0.1%)	1.51	12/967 (1.2%)
7	G	0.86	1/1368 (0.1%)	1.33	9/1844 (0.5%)
8	H	0.82	0/1086	1.31	9/1470 (0.6%)
9	I	0.78	0/989	1.37	7/1331 (0.5%)
10	J	0.94	2/541 (0.4%)	1.60	6/727 (0.8%)
11	K	0.77	0/938	1.31	6/1267 (0.5%)
12	L	0.85	0/365	1.44	5/485 (1.0%)
13	Q	1.28	0/77	1.49	0/105
All	All	0.88	17/31891 (0.1%)	1.46	310/43040 (0.7%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CA-C	10.36	1.66	1.52
4	D	23	ASN	C-N	9.16	1.41	1.33
1	A	57	ARG	CA-CB	7.44	1.66	1.53
1	A	1403	GLU	CA-C	7.19	1.62	1.52
4	D	24	ALA	CA-C	7.12	1.60	1.53
2	B	882	THR	CA-C	6.77	1.61	1.53
1	A	437	MET	SD-CE	6.62	1.96	1.79
3	C	125	MET	SD-CE	6.02	1.94	1.79
1	A	57	ARG	CD-NE	6.00	1.54	1.46
1	A	30	ILE	CG1-CD1	5.97	1.75	1.51
10	J	49	MET	SD-CE	-5.90	1.64	1.79
1	A	456	MET	SD-CE	-5.85	1.65	1.79
1	A	1438	THR	CA-C	5.85	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	MET	C-N	5.74	1.41	1.33
6	F	82	THR	CA-C	-5.54	1.47	1.53
1	A	956	LEU	CA-C	5.47	1.57	1.52
10	J	64	ASN	CA-C	5.22	1.59	1.52

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	ASP	CA-CB-CG	13.94	126.54	112.60
1	A	957	PRO	CA-C-N	-11.61	107.66	123.10
1	A	957	PRO	C-N-CA	-11.61	107.66	123.10
4	D	25	ALA	CA-C-N	11.60	140.70	122.49
4	D	25	ALA	C-N-CA	11.60	140.70	122.49
4	D	26	THR	N-CA-C	-11.46	97.51	112.41
6	F	71	GLU	N-CA-C	-10.26	100.77	113.18
3	C	38	ILE	CA-C-N	9.55	132.86	120.44
3	C	38	ILE	C-N-CA	9.55	132.86	120.44
3	C	40	GLU	CA-C-N	-9.55	115.71	122.59
3	C	40	GLU	C-N-CA	-9.55	115.71	122.59
1	A	41	MET	CA-C-N	9.47	139.63	121.54
1	A	41	MET	C-N-CA	9.47	139.63	121.54
3	C	39	ALA	N-CA-C	9.29	121.01	111.07
1	A	1445	ILE	N-CA-CB	8.63	121.35	110.99
1	A	1403	GLU	CA-C-N	-8.54	109.80	122.86
1	A	1403	GLU	C-N-CA	-8.54	109.80	122.86
2	B	296	GLU	N-CA-C	-8.52	100.60	112.45
1	A	452	LYS	N-CA-C	-8.52	101.94	111.14
8	H	138	GLU	N-CA-C	-8.48	101.62	111.03
4	D	31	GLN	N-CA-C	-8.47	101.55	112.23
1	A	629	LEU	N-CA-C	-8.41	102.06	111.82
9	I	9	ASP	CA-CB-CG	8.28	120.88	112.60
10	J	5	VAL	N-CA-C	-8.13	98.10	108.84
7	G	2	PHE	CA-CB-CG	8.04	121.84	113.80
2	B	628	THR	CA-C-N	8.04	136.89	121.54
2	B	628	THR	C-N-CA	8.04	136.89	121.54
1	A	445	ASN	CA-CB-CG	7.99	120.59	112.60
3	C	183	TRP	N-CA-C	-7.94	96.33	108.96
2	B	56	ASP	CA-CB-CG	7.73	120.33	112.60
2	B	1219	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	481	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	57	ARG	CA-CB-CG	7.51	129.12	114.10
1	A	3	GLY	CA-C-N	7.45	135.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	GLY	C-N-CA	7.45	135.76	121.54
4	D	220	LEU	CA-C-N	7.43	135.08	121.70
4	D	220	LEU	C-N-CA	7.43	135.08	121.70
1	A	399	HIS	N-CA-CB	7.36	123.47	110.37
8	H	136	LYS	CA-C-N	7.35	131.19	120.82
8	H	136	LYS	C-N-CA	7.35	131.19	120.82
1	A	61	ILE	N-CA-C	-7.34	104.62	111.45
1	A	44	THR	CA-C-N	7.31	135.51	121.54
1	A	44	THR	C-N-CA	7.31	135.51	121.54
1	A	219	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	1436	ILE	N-CA-CB	-7.21	101.45	111.41
2	B	1136	ASP	CA-CB-CG	7.17	119.77	112.60
2	B	338	GLY	CA-C-N	7.12	135.14	121.54
2	B	338	GLY	C-N-CA	7.12	135.14	121.54
4	D	23	ASN	CA-CB-CG	7.05	119.65	112.60
3	C	62	PHE	CA-C-N	6.92	129.28	120.56
3	C	62	PHE	C-N-CA	6.92	129.28	120.56
2	B	294	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	398	GLU	CA-C-O	-6.83	114.11	121.56
9	I	88	SER	CA-C-N	6.81	134.55	121.54
9	I	88	SER	C-N-CA	6.81	134.55	121.54
2	B	67	SER	CA-C-N	6.72	131.32	121.31
2	B	67	SER	C-N-CA	6.72	131.32	121.31
1	A	495	GLU	CA-C-N	6.68	131.86	120.71
1	A	495	GLU	C-N-CA	6.68	131.86	120.71
2	B	1122	ARG	CA-C-N	6.67	129.11	120.44
2	B	1122	ARG	C-N-CA	6.67	129.11	120.44
1	A	317	LYS	CA-C-N	6.64	130.07	120.38
1	A	317	LYS	C-N-CA	6.64	130.07	120.38
1	A	1064	VAL	N-CA-CB	-6.62	100.30	111.23
1	A	354	SER	CA-C-N	6.54	126.56	120.34
1	A	354	SER	C-N-CA	6.54	126.56	120.34
2	B	479	VAL	N-CA-C	-6.52	104.50	110.82
1	A	794	PRO	CA-C-N	6.49	128.98	120.28
1	A	794	PRO	C-N-CA	6.49	128.98	120.28
3	C	226	ASP	N-CA-C	-6.46	99.59	109.41
1	A	58	LEU	N-CA-C	6.44	120.34	112.23
6	F	77	ASP	N-CA-C	-6.42	100.78	110.28
1	A	346	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	344	ARG	N-CA-C	-6.39	100.10	110.20
1	A	341	MET	CA-C-N	6.38	126.53	121.61
1	A	341	MET	C-N-CA	6.38	126.53	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	VAL	N-CA-C	-6.34	106.11	111.56
1	A	846	GLU	CA-C-N	6.24	132.59	120.99
1	A	846	GLU	C-N-CA	6.24	132.59	120.99
2	B	66	ASP	N-CA-C	-6.24	107.51	114.62
2	B	468	GLU	CA-C-N	6.22	132.89	121.70
2	B	468	GLU	C-N-CA	6.22	132.89	121.70
11	K	53	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	73	GLY	CA-C-N	6.17	133.32	121.54
1	A	73	GLY	C-N-CA	6.17	133.32	121.54
1	A	253	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	1403	GLU	N-CA-C	6.14	123.87	110.80
2	B	642	ASP	CA-C-N	6.14	133.26	121.54
2	B	642	ASP	C-N-CA	6.14	133.26	121.54
4	D	52	LEU	CA-C-N	6.14	128.50	120.28
4	D	52	LEU	C-N-CA	6.14	128.50	120.28
4	D	26	THR	CA-C-N	6.12	131.07	122.08
4	D	26	THR	C-N-CA	6.12	131.07	122.08
1	A	1035	TYR	N-CA-C	-6.11	101.24	110.28
3	C	54	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	1063	MET	CA-C-N	6.08	132.92	121.97
1	A	1063	MET	C-N-CA	6.08	132.92	121.97
3	C	264	GLN	CA-C-N	6.08	128.92	120.29
3	C	264	GLN	C-N-CA	6.08	128.92	120.29
2	B	1184	GLY	CA-C-N	6.06	133.11	121.54
2	B	1184	GLY	C-N-CA	6.06	133.11	121.54
1	A	1385	THR	CA-C-N	6.05	128.67	120.38
1	A	1385	THR	C-N-CA	6.05	128.67	120.38
2	B	1009	ASP	N-CA-C	-6.02	105.01	112.90
12	L	62	LYS	N-CA-C	-6.02	105.42	112.89
1	A	55	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	880	THR	CA-C-N	6.00	132.99	121.54
2	B	880	THR	C-N-CA	6.00	132.99	121.54
1	A	733	ALA	CA-C-N	5.99	128.63	120.54
1	A	733	ALA	C-N-CA	5.99	128.63	120.54
2	B	1013	ASN	N-CA-C	5.98	117.35	109.93
4	D	140	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	629	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	225	ASN	CA-C-N	5.95	128.53	120.38
1	A	225	ASN	C-N-CA	5.95	128.53	120.38
7	G	66	GLY	N-CA-C	5.91	121.31	114.16
3	C	114	TYR	CA-C-N	5.89	128.46	120.38
3	C	114	TYR	C-N-CA	5.89	128.46	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	GLN	CA-C-N	5.89	128.48	120.77
1	A	510	GLN	C-N-CA	5.89	128.48	120.77
3	C	85	ASP	CA-CB-CG	5.87	118.47	112.60
2	B	1040	ASN	CA-CB-CG	5.83	118.43	112.60
1	A	244	PRO	N-CA-C	5.83	117.81	110.70
1	A	331	GLY	N-CA-C	5.83	127.00	113.18
7	G	1	MET	CA-C-N	5.82	132.65	121.54
7	G	1	MET	C-N-CA	5.82	132.65	121.54
1	A	223	GLY	N-CA-C	5.80	121.05	114.67
2	B	1011	ILE	N-CA-CB	5.79	119.51	112.10
1	A	874	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	23	SER	N-CA-C	-5.77	102.32	110.29
1	A	224	PHE	N-CA-C	5.77	117.98	110.53
4	D	70	PHE	CA-CB-CG	5.77	119.57	113.80
2	B	276	ILE	CA-C-N	5.77	132.56	121.54
2	B	276	ILE	C-N-CA	5.77	132.56	121.54
1	A	254	GLU	CB-CG-CD	5.73	122.34	112.60
6	F	148	VAL	N-CA-C	-5.71	104.79	110.62
2	B	103	ASN	CA-CB-CG	5.71	118.31	112.60
2	B	1102	LYS	CA-C-N	5.71	129.03	120.69
2	B	1102	LYS	C-N-CA	5.71	129.03	120.69
5	E	158	SER	CA-C-N	5.71	128.21	120.44
5	E	158	SER	C-N-CA	5.71	128.21	120.44
1	A	1102	LYS	CA-C-N	5.68	128.21	120.54
1	A	1102	LYS	C-N-CA	5.68	128.21	120.54
2	B	1018	PRO	CA-C-N	5.67	127.88	120.28
2	B	1018	PRO	C-N-CA	5.67	127.88	120.28
1	A	791	ASP	CA-CB-CG	5.64	118.24	112.60
2	B	1177	HIS	N-CA-C	-5.63	106.37	113.18
10	J	16	ASP	CA-CB-CG	5.63	118.23	112.60
4	D	2	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	1085	HIS	CA-C-N	5.61	131.79	121.70
1	A	1085	HIS	C-N-CA	5.61	131.79	121.70
2	B	447	ALA	CA-C-N	5.61	130.49	123.14
2	B	447	ALA	C-N-CA	5.61	130.49	123.14
9	I	119	THR	CB-CA-C	5.60	116.39	109.16
2	B	1175	LEU	CA-C-N	5.60	132.23	121.54
2	B	1175	LEU	C-N-CA	5.60	132.23	121.54
1	A	475	THR	CA-C-N	5.53	127.63	120.44
1	A	475	THR	C-N-CA	5.53	127.63	120.44
1	A	537	ARG	CA-C-N	5.52	128.23	120.28
1	A	537	ARG	C-N-CA	5.52	128.23	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	VAL	CA-C-N	5.52	127.67	120.28
1	A	800	VAL	C-N-CA	5.52	127.67	120.28
2	B	780	VAL	N-CA-CB	5.50	117.11	110.95
2	B	880	THR	CB-CA-C	5.49	118.64	110.62
1	A	399	HIS	CA-C-O	-5.49	112.64	120.16
5	E	171	LYS	N-CA-C	-5.49	101.34	110.17
10	J	9	SER	N-CA-C	5.48	116.94	111.07
1	A	62	ASP	CA-CB-CG	5.48	118.08	112.60
4	D	123	LEU	CA-C-N	5.47	127.92	120.54
4	D	123	LEU	C-N-CA	5.47	127.92	120.54
7	G	40	GLY	CA-C-N	5.47	127.55	120.44
7	G	40	GLY	C-N-CA	5.47	127.55	120.44
1	A	408	ASP	CA-C-N	5.46	129.42	120.63
1	A	408	ASP	C-N-CA	5.46	129.42	120.63
6	F	71	GLU	CA-C-N	5.44	127.51	120.44
6	F	71	GLU	C-N-CA	5.44	127.51	120.44
1	A	224	PHE	CA-CB-CG	-5.43	108.37	113.80
8	H	130	ARG	CA-C-N	5.42	128.01	120.63
8	H	130	ARG	C-N-CA	5.42	128.01	120.63
1	A	602	ASP	N-CA-C	-5.42	105.97	112.58
1	A	1061	GLY	N-CA-C	-5.42	108.04	114.48
2	B	732	SER	N-CA-C	5.41	117.07	108.79
4	D	118	THR	CA-C-N	5.41	131.87	121.54
4	D	118	THR	C-N-CA	5.41	131.87	121.54
9	I	53	GLY	CA-C-N	5.39	131.84	121.54
9	I	53	GLY	C-N-CA	5.39	131.84	121.54
1	A	871	ASP	CA-CB-CG	5.38	117.98	112.60
5	E	96	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	1419	ASP	CA-C-N	5.38	128.02	120.28
1	A	1419	ASP	C-N-CA	5.38	128.02	120.28
2	B	1130	PHE	N-CA-C	-5.38	101.48	109.11
1	A	47	ARG	CA-C-N	5.37	131.80	121.54
1	A	47	ARG	C-N-CA	5.37	131.80	121.54
1	A	205	GLU	CA-C-N	5.35	127.40	120.44
1	A	205	GLU	C-N-CA	5.35	127.40	120.44
4	D	14	ARG	CA-C-N	5.35	131.76	121.54
4	D	14	ARG	C-N-CA	5.35	131.76	121.54
1	A	832	ALA	CA-C-N	5.34	127.69	120.38
1	A	832	ALA	C-N-CA	5.34	127.69	120.38
6	F	70	LYS	CA-C-N	5.34	131.99	121.58
6	F	70	LYS	C-N-CA	5.34	131.99	121.58
2	B	427	ASP	CA-CB-CG	5.32	117.92	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	96	SER	N-CA-C	5.32	117.15	109.07
1	A	289	ILE	N-CA-C	-5.29	105.69	110.82
5	E	206	GLY	CA-C-N	5.28	131.28	122.73
5	E	206	GLY	C-N-CA	5.28	131.28	122.73
4	D	168	LYS	CA-C-N	5.27	127.61	120.38
4	D	168	LYS	C-N-CA	5.27	127.61	120.38
1	A	321	PRO	N-CA-C	5.27	123.33	112.47
8	H	90	ALA	N-CA-C	-5.26	102.54	110.70
3	C	267	GLN	N-CA-C	-5.26	106.81	113.43
1	A	222	LEU	N-CA-C	-5.26	101.59	109.79
7	G	55	ASP	CA-CB-CG	5.25	117.85	112.60
12	L	59	ALA	CA-C-N	5.25	131.56	121.54
12	L	59	ALA	C-N-CA	5.25	131.56	121.54
1	A	481	ASP	N-CA-C	-5.25	101.44	109.41
1	A	1035	TYR	CA-C-N	-5.25	111.52	121.54
1	A	1035	TYR	C-N-CA	-5.25	111.52	121.54
2	B	998	ASP	CA-CB-CG	5.25	117.84	112.60
2	B	45	SER	CA-C-N	5.24	127.61	120.54
2	B	45	SER	C-N-CA	5.24	127.61	120.54
1	A	24	PRO	CA-C-N	5.23	127.55	120.38
1	A	24	PRO	C-N-CA	5.23	127.55	120.38
4	D	143	ASN	CA-CB-CG	5.23	117.83	112.60
5	E	135	PHE	CA-CB-CG	5.23	119.03	113.80
2	B	1201	LYS	CA-C-N	5.23	127.56	120.65
2	B	1201	LYS	C-N-CA	5.23	127.56	120.65
2	B	684	LEU	CA-C-N	5.23	127.71	120.29
2	B	684	LEU	C-N-CA	5.23	127.71	120.29
1	A	64	ASN	CA-C-N	5.22	131.52	121.54
1	A	64	ASN	C-N-CA	5.22	131.52	121.54
1	A	411	ASP	CA-C-N	5.22	128.97	121.50
1	A	411	ASP	C-N-CA	5.22	128.97	121.50
1	A	931	GLU	CA-C-N	5.22	127.22	120.44
1	A	931	GLU	C-N-CA	5.22	127.22	120.44
11	K	82	ASP	CA-CB-CG	5.21	117.81	112.60
4	D	39	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	331	GLY	CA-C-N	5.20	131.47	121.54
1	A	331	GLY	C-N-CA	5.20	131.47	121.54
1	A	672	ASP	CA-CB-CG	5.19	117.79	112.60
6	F	154	ASP	CA-C-N	5.19	131.04	121.70
6	F	154	ASP	C-N-CA	5.19	131.04	121.70
10	J	8	PHE	CA-CB-CG	5.18	118.98	113.80
6	F	116	ASP	CA-CB-CG	5.16	117.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	846	ILE	CA-C-N	5.15	127.14	120.44
2	B	846	ILE	C-N-CA	5.15	127.14	120.44
2	B	707	PRO	CA-C-N	5.15	127.49	120.54
2	B	707	PRO	C-N-CA	5.15	127.49	120.54
4	D	167	LEU	CA-C-N	5.15	127.45	120.65
4	D	167	LEU	C-N-CA	5.15	127.45	120.65
2	B	847	ASP	CA-CB-CG	5.15	117.75	112.60
6	F	77	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	451	HIS	CB-CA-C	-5.13	100.59	110.24
2	B	659	ALA	CA-C-N	5.13	127.16	120.28
2	B	659	ALA	C-N-CA	5.13	127.16	120.28
4	D	73	SER	CA-C-N	5.13	127.11	120.44
4	D	73	SER	C-N-CA	5.13	127.11	120.44
3	C	214	ASN	CA-C-N	5.13	127.46	120.54
3	C	214	ASN	C-N-CA	5.13	127.46	120.54
1	A	104	GLU	CB-CG-CD	5.12	121.31	112.60
2	B	469	GLN	CA-C-N	5.11	131.31	121.54
2	B	469	GLN	C-N-CA	5.11	131.31	121.54
4	D	188	ALA	N-CA-C	-5.11	105.71	111.28
2	B	1028	GLU	CA-C-N	5.10	127.07	120.44
2	B	1028	GLU	C-N-CA	5.10	127.07	120.44
1	A	204	THR	CA-C-N	5.10	127.07	120.44
1	A	204	THR	C-N-CA	5.10	127.07	120.44
2	B	1001	PHE	N-CA-C	5.09	116.99	108.99
12	L	49	LYS	CA-C-N	5.09	131.26	121.54
12	L	49	LYS	C-N-CA	5.09	131.26	121.54
1	A	218	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	551	TYR	CA-C-N	5.09	127.61	120.28
1	A	551	TYR	C-N-CA	5.09	127.61	120.28
6	F	79	ARG	N-CA-C	-5.09	100.41	109.06
1	A	287	HIS	CA-C-N	5.09	131.26	121.54
1	A	287	HIS	C-N-CA	5.09	131.26	121.54
1	A	329	LEU	CA-C-N	5.08	128.54	121.02
1	A	329	LEU	C-N-CA	5.08	128.54	121.02
11	K	106	GLU	CA-C-N	5.08	127.40	120.54
11	K	106	GLU	C-N-CA	5.08	127.40	120.54
1	A	1005	GLU	CB-CG-CD	5.07	121.23	112.60
2	B	366	GLN	N-CA-C	-5.07	106.34	112.88
8	H	21	ASN	CA-CB-CG	5.07	117.67	112.60
5	E	48	ASP	CA-CB-CG	5.07	117.67	112.60
4	D	139	LYS	CA-C-N	5.07	127.38	120.54
4	D	139	LYS	C-N-CA	5.07	127.38	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	491	VAL	N-CA-C	5.05	112.87	107.76
3	C	255	VAL	CA-C-N	5.05	127.05	120.28
3	C	255	VAL	C-N-CA	5.05	127.05	120.28
9	I	119	THR	N-CA-C	-5.05	108.39	114.75
1	A	148	CYS	N-CA-C	-5.04	99.57	108.20
7	G	66	GLY	CA-C-N	5.04	128.23	120.82
7	G	66	GLY	C-N-CA	5.04	128.23	120.82
2	B	397	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	320	ASP	CA-CB-CG	5.03	117.63	112.60
10	J	6	ARG	CA-C-N	5.03	128.00	120.87
10	J	6	ARG	C-N-CA	5.03	128.00	120.87
5	E	162	ARG	CA-C-N	5.02	126.97	120.44
5	E	162	ARG	C-N-CA	5.02	126.97	120.44
2	B	126	SER	CA-C-N	5.02	124.74	119.92
2	B	126	SER	C-N-CA	5.02	124.74	119.92
1	A	57	ARG	CG-CD-NE	5.02	123.04	112.00
1	A	1050	GLU	CB-CG-CD	5.01	121.12	112.60
8	H	145	ARG	CA-C-N	5.01	130.72	121.70
8	H	145	ARG	C-N-CA	5.01	130.72	121.70
2	B	231	PRO	CA-C-N	5.01	127.77	120.51
2	B	231	PRO	C-N-CA	5.01	127.77	120.51
11	K	25	THR	CA-C-N	5.01	126.99	120.28
11	K	25	THR	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11190	0	11255	234	0
2	B	8876	0	8919	161	0
3	C	2095	0	2051	51	0
4	D	1440	0	1456	17	0
5	E	1752	0	1776	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	705	0	731	17	0
7	G	1340	0	1357	35	0
8	H	1068	0	1040	21	0
9	I	971	0	927	24	0
10	J	532	0	542	20	0
11	K	920	0	929	25	0
12	L	363	0	386	10	0
13	Q	78	0	36	1	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)
1:A:30:ILE:CD1	1:A:30:ILE:CG1	1.75	1.56
1:A:56:PRO:HB2	1:A:68:GLN:HG3	1.37	1.06
1:A:1081:LEU:HB3	1:A:1082:ASN:HA	1.45	0.98
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.48	0.92
1:A:855:THR:HG21	1:A:857:ARG:HE	1.34	0.92
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.53	0.89
1:A:471:ASN:HD21	1:A:650:GLN:HE22	1.20	0.87
4:D:13:ARG:HH22	4:D:18:VAL:HA	1.44	0.82
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.60	0.82
1:A:369:SER:H	11:K:2:ASN:HD21	1.28	0.81
3:C:98:VAL:H	3:C:122:SER:HB3	1.46	0.80
1:A:56:PRO:HB2	1:A:68:GLN:CG	2.11	0.80
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.80
4:D:155:ARG:HB2	4:D:219:THR:HG21	1.63	0.80
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.63	0.79
2:B:918:ILE:HD11	2:B:935:ARG:HD2	1.62	0.79
7:G:138:THR:HG22	7:G:139:ILE:H	1.49	0.78
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.65	0.77
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.69	0.74
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.71	0.73
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.19	0.72
1:A:741:ASN:HD22	1:A:744:LYS:H	1.37	0.72
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.71	0.72
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.38	0.71
7:G:34:VAL:O	7:G:37:SER:HB3	1.90	0.71
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.72	0.71
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.09	0.71
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.55	0.71
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.73	0.70
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.07	0.70
1:A:471:ASN:HD21	1:A:650:GLN:NE2	1.89	0.70
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.71	0.70
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.73	0.70
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.73	0.69
1:A:1445:ILE:HG12	7:G:61:ILE:HD11	1.75	0.69
9:I:50:THR:HG22	9:I:52:ILE:H	1.58	0.69
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.39	0.68
7:G:1:MET:HE1	7:G:79:PHE:CE2	2.28	0.68
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.74	0.68
2:B:744:HIS:HD2	2:B:746:SER:H	1.42	0.68
1:A:54:ASN:HD22	1:A:61:ILE:HD11	1.59	0.68
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.59	0.68
7:G:62:LEU:HD21	7:G:69:GLU:HB2	1.75	0.67
10:J:48:ARG:HE	10:J:49:MET:HE2	1.59	0.67
2:B:34:ILE:HG12	2:B:542:MET:CE	2.24	0.67
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.77	0.67
1:A:401:GLY:C	1:A:435:HIS:HD2	2.03	0.67
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.66
2:B:683:SER:O	2:B:687:GLU:HB2	1.95	0.66
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.78	0.66
8:H:135:LEU:C	8:H:137:GLN:H	2.04	0.65
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.97	0.65
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.36	0.65
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.59	0.65
7:G:111:THR:HG22	7:G:113:HIS:H	1.62	0.65
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.78	0.65
2:B:879:ARG:HH11	2:B:885:MET:HE1	1.62	0.65
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:206:ASN:HA	3:C:209:TYR:HD1	1.61	0.64
1:A:1329:THR:HG22	1:A:1331:SER:H	1.63	0.64
2:B:706:GLN:H	2:B:710:LEU:HD13	1.62	0.64
1:A:512:VAL:HA	1:A:519:PRO:HA	1.79	0.64
12:L:68:GLU:CD	12:L:68:GLU:H	2.04	0.64
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.80	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.79	0.64
1:A:49:LYS:HZ2	1:A:61:ILE:H	1.46	0.64
1:A:1081:LEU:CB	1:A:1082:ASN:HA	2.26	0.64
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.80	0.64
7:G:151:ILE:HD11	7:G:160:ILE:HD12	1.79	0.63
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.80	0.63
7:G:1:MET:HE1	7:G:79:PHE:CD2	2.34	0.63
11:K:65:HIS:CD2	11:K:67:PHE:H	2.17	0.62
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.64	0.62
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.81	0.62
1:A:907:THR:HG22	1:A:908:LEU:H	1.63	0.62
9:I:7:CYS:SG	9:I:10:CYS:HB2	2.39	0.62
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.62
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.83	0.61
9:I:74:GLU:HB3	9:I:81:ARG:HD3	1.82	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD12	1.82	0.61
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.82	0.61
1:A:471:ASN:ND2	1:A:650:GLN:HE22	1.96	0.60
1:A:1424:VAL:HG11	2:B:1139:ILE:HG12	1.84	0.60
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.84	0.60
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.66	0.60
1:A:311:GLN:HE21	1:A:312:PRO:HD2	1.66	0.60
4:D:187:THR:HB	4:D:190:GLU:H	1.65	0.60
2:B:883:LEU:HD23	2:B:934:LYS:HB2	1.83	0.60
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.83	0.60
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.84	0.60
5:E:176:PRO:O	5:E:212:ARG:HA	2.02	0.60
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.83	0.60
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.37	0.60
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.83	0.59
6:F:118:LEU:O	6:F:122:MET:HG3	2.02	0.59
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.37	0.59
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.85	0.59
3:C:149:LYS:HG3	3:C:150:GLY:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.68	0.59
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.84	0.59
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.85	0.59
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.03	0.59
1:A:369:SER:H	11:K:2:ASN:ND2	1.97	0.59
11:K:107:THR:O	11:K:111:LEU:HG	2.02	0.59
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.85	0.58
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.28	0.58
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.85	0.58
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.21	0.58
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.85	0.58
1:A:316:GLN:HG3	1:A:317:LYS:H	1.68	0.58
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.85	0.57
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.85	0.57
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.87	0.57
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.40	0.57
1:A:1386:ARG:HB2	1:A:1403:GLU:OE1	2.05	0.57
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.87	0.56
4:D:165:GLN:HA	4:D:168:LYS:HD2	1.87	0.56
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.87	0.56
1:A:225:ASN:HD22	1:A:227:VAL:H	1.52	0.56
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.35	0.56
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.48	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.87	0.56
1:A:464:PRO:HD2	11:K:67:PHE:HD2	1.70	0.56
2:B:126:SER:OG	2:B:172:ILE:HD11	2.06	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.88	0.56
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.88	0.55
2:B:515:HIS:H	2:B:518:HIS:CD2	2.24	0.55
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.86	0.55
12:L:32:ALA:HB3	12:L:55:ILE:HG23	1.88	0.55
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.88	0.55
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.71	0.55
1:A:1074:GLU:HG3	1:A:1075:PRO:HD3	1.88	0.55
2:B:338:GLY:HA3	2:B:351:TYR:HE2	1.71	0.55
1:A:1329:THR:HG22	1:A:1331:SER:N	2.21	0.55
2:B:282:ILE:HA	2:B:285:ILE:HD12	1.89	0.55
2:B:848:ARG:HD2	10:J:8:PHE:O	2.06	0.55
2:B:1165:ILE:HG12	4:D:13:ARG:HE	1.71	0.55
2:B:105:SER:C	2:B:107:GLY:H	2.14	0.55
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HD21	2:B:461:LEU:HD23	1.89	0.55
10:J:8:PHE:H	10:J:49:MET:HE3	1.72	0.55
1:A:1095:THR:HG21	1:A:1112:LYS:HB3	1.88	0.54
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.42	0.54
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.89	0.54
1:A:53:LEU:HD23	1:A:54:ASN:H	1.73	0.54
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.89	0.54
6:F:109:VAL:CG1	6:F:123:LYS:HD3	2.37	0.54
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.90	0.54
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.72	0.54
11:K:65:HIS:HD2	11:K:67:PHE:H	1.53	0.54
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.43	0.54
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.90	0.54
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.73	0.53
1:A:353:ILE:HD13	1:A:487:MET:CE	2.38	0.53
1:A:503:GLN:HE21	6:F:90:ARG:HH12	1.55	0.53
1:A:32:VAL:HG21	1:A:80:HIS:HB2	1.91	0.53
1:A:41:MET:HE1	1:A:61:ILE:HD12	1.90	0.53
1:A:382:PRO:HD3	6:F:104:ASN:HD21	1.73	0.53
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.89	0.53
2:B:955:THR:HG22	12:L:55:ILE:HA	1.89	0.53
1:A:316:GLN:HG3	1:A:317:LYS:HG2	1.91	0.53
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.91	0.53
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.90	0.53
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.91	0.53
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.37	0.53
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.91	0.53
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.91	0.53
9:I:49:ILE:HA	9:I:92:ARG:HH12	1.73	0.52
1:A:472:LEU:O	1:A:475:THR:HB	2.09	0.52
1:A:482:PHE:C	1:A:484:GLY:H	2.17	0.52
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.44	0.52
2:B:901:PRO:O	2:B:949:VAL:O	2.28	0.52
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.91	0.52
2:B:399:ASP:O	2:B:515:HIS:HD2	1.91	0.52
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.91	0.52
1:A:567:LYS:HE3	8:H:91:ASP:HB2	1.92	0.52
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.91	0.52
5:E:17:ARG:HH22	5:E:36:GLU:HG3	1.74	0.52
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.24	0.52
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:VAL:HB	2:B:573:GLN:HB2	1.92	0.52
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.91	0.52
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.91	0.52
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.91	0.52
1:A:1279:ILE:HG13	1:A:1308:THR:HG21	1.92	0.52
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.91	0.51
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.75	0.51
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.90	0.51
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.10	0.51
2:B:654:ARG:H	2:B:657:HIS:CD2	2.18	0.51
2:B:705:MET:H	2:B:710:LEU:HD22	1.76	0.51
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.51
1:A:50:ILE:O	1:A:55:ASP:HB2	2.10	0.51
1:A:858:ASN:ND2	1:A:862:ASN:H	2.08	0.51
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.91	0.51
2:B:47:GLN:NE2	2:B:408:LEU:HD12	2.25	0.51
2:B:429:PHE:HA	2:B:432:MET:HE3	1.93	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
9:I:88:SER:HB3	9:I:91:ARG:HE	1.76	0.51
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.92	0.51
2:B:1160:VAL:HG21	2:B:1169:MET:HE2	1.93	0.51
1:A:709:THR:HG22	1:A:711:ARG:H	1.76	0.51
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.76	0.51
1:A:534:LEU:O	1:A:574:GLY:HA3	2.11	0.51
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.76	0.51
3:C:115:SER:HB2	3:C:142:VAL:H	1.76	0.51
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.92	0.51
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.76	0.51
1:A:146:MET:HA	1:A:171:GLN:HB2	1.93	0.50
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.58	0.50
1:A:568:PRO:HG2	8:H:95:TYR:HD1	1.76	0.50
2:B:1082:MET:HA	3:C:189:THR:HA	1.92	0.50
3:C:55:THR:HB	3:C:151:GLN:HA	1.94	0.50
7:G:14:HIS:CD2	7:G:16:SER:H	2.29	0.50
1:A:1215:ARG:HH21	1:A:1218:GLN:HG3	1.77	0.50
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.93	0.50
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.94	0.50
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.94	0.50
1:A:929:LEU:HD21	1:A:983:ILE:HG12	1.93	0.50
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.92	0.50
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.11	0.50
2:B:744:HIS:CD2	2:B:746:SER:OG	2.64	0.50
2:B:515:HIS:H	2:B:518:HIS:HD2	1.60	0.50
2:B:957:ASN:HD22	2:B:961:LEU:HD11	1.77	0.50
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.93	0.50
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.76	0.50
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.50
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.42	0.50
3:C:180:TYR:OH	3:C:188:HIS:HD2	1.95	0.49
1:A:40:THR:HG22	1:A:41:MET:HE3	1.94	0.49
1:A:36:ARG:NH2	1:A:57:ARG:HH12	2.10	0.49
2:B:291:ILE:HD12	2:B:291:ILE:N	2.27	0.49
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.93	0.49
2:B:315:LYS:HA	9:I:13:MET:HE1	1.93	0.49
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.93	0.49
1:A:401:GLY:C	1:A:435:HIS:CD2	2.87	0.49
1:A:754:SER:N	1:A:757:ASN:HD22	2.10	0.49
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.94	0.49
3:C:73:GLN:HE21	3:C:75:MET:H	1.61	0.49
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.53	0.49
1:A:873:MET:C	1:A:1058:VAL:HG22	2.38	0.49
2:B:756:ILE:O	2:B:759:PRO:HD3	2.12	0.49
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.95	0.49
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.95	0.49
4:D:207:LEU:HA	4:D:210:ILE:HD12	1.95	0.49
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.94	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.48
4:D:13:ARG:NH2	4:D:18:VAL:HA	2.21	0.48
10:J:48:ARG:O	10:J:52:THR:HG22	2.13	0.48
1:A:503:GLN:NE2	6:F:90:ARG:HH22	2.11	0.48
1:A:853:ASP:OD1	1:A:855:THR:HB	2.14	0.48
1:A:901:LEU:HA	1:A:907:THR:HG23	1.95	0.48
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.78	0.48
1:A:452:LYS:HG2	2:B:1141:HIS:CE1	2.48	0.48
2:B:315:LYS:HG2	9:I:13:MET:HE2	1.95	0.48
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.43	0.48
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.95	0.48
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.28	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.96	0.48
9:I:84:VAL:HG23	9:I:104:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.48
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.48	0.48
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.48
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.94	0.48
9:I:59:VAL:HG12	9:I:61:ASP:H	1.79	0.48
1:A:134:ARG:HD2	1:A:221:SER:O	2.13	0.48
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.94	0.48
1:A:464:PRO:HD2	11:K:67:PHE:CD2	2.49	0.48
2:B:1120:GLU:HG3	2:B:1121:GLY:N	2.28	0.48
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.44	0.48
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.95	0.47
1:A:49:LYS:HD3	1:A:61:ILE:HG13	1.96	0.47
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.49	0.47
2:B:901:PRO:HA	2:B:949:VAL:HG12	1.97	0.47
1:A:883:LEU:O	1:A:886:ILE:HG22	2.14	0.47
6:F:87:LYS:HA	6:F:155:LEU:HD21	1.95	0.47
7:G:43:GLY:HA2	7:G:157:ILE:HD11	1.96	0.47
9:I:72:ASP:O	9:I:81:ARG:HD2	2.15	0.47
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.14	0.47
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.79	0.47
2:B:603:LEU:HD22	2:B:608:ASP:HB2	1.96	0.47
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.96	0.47
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.50	0.47
1:A:901:LEU:H	1:A:926:GLN:NE2	2.12	0.47
5:E:147:HIS:CD2	5:E:149:LEU:H	2.32	0.47
1:A:299:HIS:HA	1:A:302:THR:HG22	1.96	0.47
2:B:745:PRO:O	2:B:748:ILE:HG12	2.15	0.47
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.97	0.47
7:G:138:THR:CG2	7:G:139:ILE:H	2.25	0.47
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.95	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.26	0.47
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.15	0.47
1:A:657:LEU:HD11	1:A:662:PHE:HB2	1.97	0.47
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.50	0.47
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.45	0.47
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.79	0.47
3:C:11:ARG:HH21	3:C:229:TYR:HD1	1.62	0.47
1:A:907:THR:HG22	1:A:908:LEU:N	2.29	0.47
2:B:273:LEU:HD12	2:B:280:ILE:HD13	1.97	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.97	0.47
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HH11	1:A:339:ASN:ND2	2.14	0.46
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.46
2:B:789:MET:HE3	2:B:953:LEU:HB2	1.97	0.46
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.46
3:C:31:ASN:O	3:C:34:ARG:HB3	2.15	0.46
4:D:155:ARG:CB	4:D:219:THR:HG21	2.40	0.46
12:L:40:LEU:HD22	12:L:44:ASP:HB3	1.97	0.46
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.39	0.46
3:C:58:LEU:HD22	3:C:145:CYS:HB2	1.96	0.46
1:A:597:LEU:HD13	8:H:103:LYS:HG3	1.98	0.46
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.97	0.46
2:B:428:ILE:HG12	2:B:448:ILE:HG12	1.96	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.15	0.46
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.96	0.46
8:H:103:LYS:HB3	8:H:115:TYR:CD1	2.51	0.46
1:A:369:SER:N	11:K:2:ASN:HD21	2.05	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.46
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.97	0.46
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.97	0.46
1:A:43:GLU:C	1:A:45:GLN:H	2.24	0.46
6:F:90:ARG:HD3	6:F:155:LEU:HD22	1.97	0.46
9:I:7:CYS:SG	9:I:8:ARG:O	2.74	0.46
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.46	0.46
9:I:55:THR:HG21	9:I:109:ILE:HG21	1.97	0.46
1:A:1081:LEU:HD21	1:A:1098:VAL:H	1.81	0.46
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.97	0.46
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.81	0.46
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.98	0.45
2:B:508:LEU:HD13	2:B:508:LEU:H	1.80	0.45
7:G:60:ARG:NH2	7:G:63:PRO:HD3	2.30	0.45
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.97	0.45
1:A:105:CYS:SG	1:A:139:TRP:HA	2.56	0.45
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.99	0.45
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.99	0.45
2:B:296:GLU:O	2:B:300:HIS:HD2	1.99	0.45
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.98	0.45
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.98	0.45
1:A:592:ASP:O	1:A:593:GLU:C	2.60	0.45
1:A:676:MET:HE1	1:A:762:SER:O	2.16	0.45
1:A:1121:GLU:HB3	1:A:1124:HIS:HD2	1.82	0.45
3:C:18:VAL:HG22	3:C:240:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.98	0.45
4:D:63:LEU:O	4:D:133:THR:HG21	2.16	0.45
1:A:1062:GLU:HB3	1:A:1064:VAL:HG23	1.99	0.45
10:J:7:CYS:HA	10:J:49:MET:HG2	1.99	0.45
1:A:122:MET:HE1	1:A:138:ILE:HG12	1.97	0.45
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.64	0.45
2:B:620:ARG:HG3	9:I:57:GLY:HA3	1.99	0.45
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.99	0.45
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.99	0.45
3:C:125:MET:HB2	3:C:127:ARG:NE	2.32	0.45
8:H:106:GLU:HA	8:H:112:ILE:HG13	1.98	0.45
1:A:265:LYS:CG	1:A:303:TYR:HB2	2.46	0.45
1:A:332:LYS:H	1:A:337:ARG:CB	2.30	0.45
2:B:242:SER:OG	2:B:362:PRO:HD2	2.17	0.45
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.64	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.17	0.45
7:G:125:SER:OG	7:G:128:PRO:HA	2.17	0.45
1:A:629:LEU:O	1:A:633:VAL:HG23	2.16	0.45
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.51	0.45
11:K:51:LEU:HD12	11:K:51:LEU:HA	1.88	0.45
1:A:866:PHE:CZ	5:E:211:TYR:HD2	2.35	0.45
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.99	0.45
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.57	0.45
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.31	0.44
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.99	0.44
4:D:8:PHE:HB3	4:D:38:ILE:O	2.17	0.44
4:D:138:ASN:ND2	7:G:35:GLU:HG2	2.32	0.44
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.82	0.44
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.97	0.44
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.98	0.44
1:A:440:ASP:O	1:A:460:VAL:HG23	2.18	0.44
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.99	0.44
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.99	0.44
1:A:1150:SER:HB3	9:I:46:HIS:HB2	1.98	0.44
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.17	0.44
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.84	0.44
1:A:284:ALA:HA	1:A:289:ILE:HD11	2.00	0.44
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.43	0.44
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.99	0.44
3:C:73:GLN:HE21	3:C:75:MET:N	2.15	0.44
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.83	0.44
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.98	0.44
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.48	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.99	0.44
2:B:613:VAL:HG22	2:B:628:THR:HA	2.00	0.44
8:H:89:LEU:HB2	8:H:91:ASP:HB3	2.00	0.44
1:A:67:CYS:SG	1:A:67:CYS:O	2.76	0.43
2:B:291:ILE:HD12	2:B:291:ILE:H	1.83	0.43
2:B:361:LEU:HD11	2:B:381:MET:HE1	2.00	0.43
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.43
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.00	0.43
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.18	0.43
8:H:6:PHE:HD2	8:H:130:ARG:HG2	1.82	0.43
11:K:1:MET:O	11:K:1:MET:HG2	2.18	0.43
1:A:116:ASP:C	1:A:118:HIS:H	2.26	0.43
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.82	0.43
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.33	0.43
2:B:34:ILE:HG12	2:B:542:MET:HE2	1.97	0.43
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.99	0.43
2:B:294:ASP:CG	9:I:12:ASN:HD22	2.25	0.43
1:A:800:VAL:HA	1:A:812:GLU:HG2	2.00	0.43
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	2.00	0.43
2:B:25:ILE:CD1	2:B:658:ILE:HD13	2.47	0.43
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.99	0.43
1:A:668:ASP:HB3	1:A:743:VAL:HG23	2.00	0.43
2:B:542:MET:HG2	2:B:747:MET:HE3	2.01	0.43
3:C:84:ARG:HG3	3:C:85:ASP:N	2.33	0.43
12:L:32:ALA:HB3	12:L:55:ILE:CG2	2.47	0.43
2:B:520:GLY:HA2	2:B:748:ILE:HA	2.00	0.43
3:C:241:ASP:HB3	11:K:109:TRP:CD2	2.53	0.43
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.52	0.43
1:A:363:GLN:HG2	1:A:459:ARG:NH1	2.34	0.43
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.82	0.43
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.83	0.43
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.32	0.43
1:A:1445:ILE:HD12	7:G:22:MET:HE1	2.01	0.43
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.33	0.43
7:G:114:LEU:HD23	7:G:162:SER:HB3	2.01	0.43
13:Q:25:ASP:C	13:Q:27:MET:H	2.27	0.43
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.00	0.43
1:A:1436:ILE:O	1:A:1437:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:MET:O	2:B:993:THR:HA	2.18	0.43
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.19	0.43
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.54	0.43
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.45	0.43
1:A:701:LEU:HD21	9:I:114:GLN:HB3	2.01	0.43
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.19	0.43
1:A:1116:LEU:HD12	1:A:1311:VAL:HG22	2.00	0.43
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.83	0.43
5:E:116:ILE:HB	5:E:121:MET:HE2	2.01	0.43
1:A:100:LYS:HG3	1:A:181:LEU:HD22	2.01	0.42
2:B:770:GLN:HB2	2:B:985:GLY:H	1.84	0.42
7:G:112:LYS:HA	7:G:115:MET:HE3	2.00	0.42
1:A:858:ASN:HD21	1:A:862:ASN:H	1.67	0.42
2:B:309:GLN:HB2	9:I:52:ILE:HD11	2.01	0.42
2:B:892:LYS:HB3	2:B:899:ILE:HD13	2.01	0.42
2:B:899:ILE:HG13	2:B:911:ILE:HA	2.01	0.42
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.01	0.42
3:C:91:HIS:CD2	3:C:158:VAL:HG11	2.54	0.42
8:H:89:LEU:C	8:H:91:ASP:H	2.26	0.42
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.00	0.42
1:A:982:THR:HG23	1:A:985:ASP:OD2	2.19	0.42
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.02	0.42
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.42
2:B:866:TYR:O	2:B:870:ILE:HB	2.19	0.42
10:J:8:PHE:H	10:J:49:MET:CE	2.31	0.42
1:A:393:ARG:HE	1:A:393:ARG:HA	1.84	0.42
1:A:494:SER:HB3	1:A:497:THR:H	1.83	0.42
1:A:1259:MET:HA	1:A:1262:LYS:HD2	2.00	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.85	0.42
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.54	0.42
3:C:182:PRO:HB3	3:C:204:SER:HB3	2.01	0.42
1:A:543:LEU:HD13	8:H:79:TRP:CZ3	2.55	0.42
1:A:697:ALA:HB2	1:A:702:LEU:HD13	2.01	0.42
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.83	0.42
1:A:1172:LEU:C	1:A:1174:PHE:H	2.27	0.42
2:B:338:GLY:O	2:B:339:THR:HG22	2.20	0.42
2:B:468:GLU:HG2	2:B:469:GLN:HB2	2.01	0.42
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.85	0.42
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.55	0.42
1:A:1136:SER:O	1:A:1274:ARG:HD3	2.19	0.42
2:B:707:PRO:O	2:B:711:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:LEU:HG	2:B:1064:TYR:HB2	2.00	0.42
8:H:76:THR:HG22	8:H:77:ARG:HD2	2.01	0.42
1:A:246:VAL:C	1:A:248:PRO:HD3	2.45	0.42
1:A:761:MET:HA	1:A:804:TYR:HB2	2.01	0.42
5:E:19:VAL:O	5:E:23:VAL:HG23	2.20	0.42
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.01	0.42
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.20	0.42
5:E:47:CYS:HB3	5:E:51:GLY:HA2	2.01	0.42
8:H:82:PRO:C	8:H:84:ALA:N	2.78	0.42
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.68	0.42
1:A:180:LYS:HD3	1:A:201:VAL:HG21	2.02	0.42
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.44	0.42
2:B:558:LEU:HD23	2:B:596:LEU:HD11	2.01	0.42
3:C:145:CYS:HA	10:J:2:ILE:HD13	2.02	0.42
7:G:151:ILE:HD11	7:G:160:ILE:HD11	1.97	0.42
8:H:107:VAL:CG2	8:H:111:LEU:HB3	2.50	0.41
1:A:1224:LEU:HD23	1:A:1226:VAL:HG22	2.02	0.41
2:B:209:GLU:O	2:B:482:VAL:HA	2.19	0.41
3:C:206:ASN:HA	3:C:209:TYR:CD1	2.49	0.41
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.03	0.41
2:B:54:PHE:HA	2:B:58:THR:HB	2.02	0.41
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.35	0.41
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.84	0.41
3:C:31:ASN:O	3:C:35:ARG:HG3	2.20	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.85	0.41
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.68	0.41
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.51	0.41
2:B:590:HIS:CD2	2:B:592:ASN:C	2.99	0.41
1:A:353:ILE:HD13	1:A:487:MET:HE2	2.03	0.41
1:A:568:PRO:HD3	8:H:95:TYR:HA	2.03	0.41
12:L:53:HIS:ND1	12:L:55:ILE:HG22	2.36	0.41
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.47	0.41
1:A:1444:MET:HG2	7:G:58:ARG:HB3	2.02	0.41
2:B:131:ASP:HA	2:B:164:LYS:HB3	2.03	0.41
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.03	0.41
3:C:83:SER:O	3:C:84:ARG:C	2.63	0.41
5:E:19:VAL:HG11	5:E:80:VAL:HG11	2.01	0.41
2:B:260:GLY:O	2:B:267:ARG:HD3	2.20	0.41
2:B:705:MET:HE2	2:B:745:PRO:HB3	2.02	0.41
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.03	0.41
3:C:4:GLU:H	3:C:4:GLU:HG2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:HD2	7:G:16:SER:OG	2.04	0.41
11:K:9:LEU:HD23	11:K:69:ALA:HB2	2.02	0.41
1:A:598:LEU:HG	8:H:25:ARG:NH1	2.36	0.41
1:A:598:LEU:HD13	8:H:124:ARG:HB2	2.03	0.41
1:A:872:GLY:O	1:A:1058:VAL:HG23	2.20	0.41
3:C:115:SER:HB2	3:C:142:VAL:N	2.35	0.41
1:A:7:SER:OG	2:B:1161:HIS:HE1	2.04	0.41
2:B:416:LEU:HD11	2:B:460:ALA:HB3	2.03	0.41
2:B:706:GLN:O	2:B:710:LEU:HB2	2.21	0.41
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.56	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.02	0.41
10:J:21:TYR:HA	10:J:39:LEU:HD11	2.02	0.41
11:K:5:ASP:O	11:K:8:GLU:HB2	2.20	0.41
1:A:33:ALA:CB	1:A:57:ARG:HD3	2.51	0.41
1:A:777:PHE:HD2	1:A:782:ARG:HA	1.86	0.41
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.55	0.41
2:B:724:ASP:HB3	2:B:727:LYS:HD2	2.03	0.41
6:F:124:GLU:HB3	6:F:130:ILE:HG13	2.03	0.41
2:B:955:THR:CG2	12:L:55:ILE:HG13	2.51	0.40
4:D:126:ILE:HD13	4:D:145:MET:HE3	2.03	0.40
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.04	0.40
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.85	0.40
1:A:347:PHE:H	2:B:1107:ALA:HA	1.85	0.40
1:A:446:ARG:HB2	1:A:487:MET:SD	2.61	0.40
2:B:121:ASN:ND2	2:B:207:GLY:HA3	2.36	0.40
2:B:540:SER:HB2	2:B:543:SER:HG	1.87	0.40
2:B:844:SER:O	2:B:847:ASP:HB2	2.21	0.40
2:B:880:THR:O	2:B:883:LEU:HG	2.22	0.40
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.56	0.40
6:F:103:MET:HG3	7:G:15:PRO:HG2	2.02	0.40
1:A:104:GLU:HG3	1:A:174:ILE:HD12	2.03	0.40
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.03	0.40
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.02	0.40
1:A:1454:MET:HB2	7:G:20:PRO:HG3	2.02	0.40
3:C:167:HIS:ND1	3:C:169:LYS:HB3	2.37	0.40
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.86	0.40
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.57	0.40
7:G:11:ILE:HD12	7:G:72:VAL:HG21	2.04	0.40
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.86	0.40
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.56	0.40
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PRO:O	1:A:322:VAL:HB	2.21	0.40
1:A:915:SER:O	1:A:918:GLU:HG3	2.21	0.40
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	2.02	0.40
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.90	0.40
3:C:53:THR:HG22	3:C:154:LYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1732 (82%)	1269 (90%)	116 (8%)	26 (2%)	6	34
2	B	1102/1223 (90%)	996 (90%)	79 (7%)	27 (2%)	4	28
3	C	264/266 (99%)	243 (92%)	18 (7%)	3 (1%)	11	44
4	D	176/221 (80%)	155 (88%)	17 (10%)	4 (2%)	5	29
5	E	212/214 (99%)	198 (93%)	10 (5%)	4 (2%)	6	33
6	F	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
7	G	169/171 (99%)	162 (96%)	5 (3%)	2 (1%)	10	42
8	H	129/145 (89%)	105 (81%)	17 (13%)	7 (5%)	1	13
9	I	117/119 (98%)	98 (84%)	17 (14%)	2 (2%)	7	35
10	J	63/65 (97%)	56 (89%)	4 (6%)	3 (5%)	2	16
11	K	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
12	L	44/46 (96%)	33 (75%)	6 (14%)	5 (11%)	0	4
13	Q	13/15 (87%)	11 (85%)	1 (8%)	1 (8%)	1	8
All	All	3898/4419 (88%)	3514 (90%)	300 (8%)	84 (2%)	5	30

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	45	GLN
1	A	74	MET
1	A	593	GLU
1	A	1403	GLU
1	A	1405	THR
2	B	67	SER
2	B	339	THR
2	B	629	ASP
2	B	731	VAL
2	B	751	VAL
2	B	879	ARG
2	B	1066	SER
2	B	1185	CYS
4	D	13	ARG
4	D	119	ARG
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	331	GLY
1	A	846	GLU
1	A	1379	GLY
2	B	368	GLU
2	B	1046	PRO
2	B	1176	ASN
8	H	17	PRO
8	H	85	GLY
8	H	128	ASN
9	I	89	GLN
10	J	17	LYS
1	A	41	MET
1	A	556	TRP
2	B	364	ILE
2	B	509	ALA
2	B	643	ASP
2	B	707	PRO
2	B	881	ASN
4	D	198	LEU
5	E	36	GLU
5	E	48	ASP
5	E	49	SER
8	H	18	GLY
8	H	52	GLN

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Mol	Chain	Res	Type
12	L	39	SER
1	A	167	CYS
1	A	322	VAL
1	A	599	SER
1	A	870	GLU
2	B	249	ARG
2	B	322	PHE
2	B	470	LYS
2	B	711	GLU
3	C	214	ASN
7	G	63	PRO
10	J	6	ARG
13	Q	26	ARG
1	A	49	LYS
1	A	108	MET
1	A	282	ASN
1	A	399	HIS
1	A	628	GLY
2	B	712	PRO
2	B	907	GLY
2	B	1017	ILE
2	B	1108	ARG
2	B	1223	ASP
4	D	18	VAL
7	G	139	ILE
8	H	132	LEU
8	H	139	ASN
9	I	95	THR
10	J	64	ASN
1	A	55	ASP
1	A	1173	HIS
2	B	108	VAL
12	L	45	ALA
1	A	283	GLY
1	A	1064	VAL
2	B	1214	PRO
1	A	258	GLY
3	C	240	VAL
5	E	51	GLY
1	A	196	GLU
3	C	38	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1519 (82%)	1063 (86%)	181 (14%)	3	18
2	B	967/1060 (91%)	829 (86%)	138 (14%)	3	18
3	C	234/234 (100%)	198 (85%)	36 (15%)	2	16
4	D	160/200 (80%)	130 (81%)	30 (19%)	1	9
5	E	196/196 (100%)	184 (94%)	12 (6%)	17	44
6	F	77/77 (100%)	66 (86%)	11 (14%)	3	18
7	G	152/152 (100%)	130 (86%)	22 (14%)	3	18
8	H	117/127 (92%)	104 (89%)	13 (11%)	6	27
9	I	113/113 (100%)	93 (82%)	20 (18%)	2	10
10	J	60/60 (100%)	50 (83%)	10 (17%)	2	13
11	K	99/99 (100%)	87 (88%)	12 (12%)	5	23
12	L	40/40 (100%)	26 (65%)	14 (35%)	0	2
13	Q	1/15 (7%)	1 (100%)	0	100	100
All	All	3460/3892 (89%)	2961 (86%)	499 (14%)	3	18

All (499) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	12	ARG
1	A	30	ILE
1	A	34	LYS
1	A	37	PHE
1	A	42	ASP
1	A	44	THR
1	A	45	GLN
1	A	53	LEU
1	A	55	ASP
1	A	58	LEU
1	A	61	ILE

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Mol	Chain	Res	Type
1	A	64	ASN
1	A	66	LYS
1	A	74	MET
1	A	116	ASP
1	A	131	SER
1	A	145	LYS
1	A	152	VAL
1	A	174	ILE
1	A	204	THR
1	A	210	ILE
1	A	220	THR
1	A	225	ASN
1	A	237	THR
1	A	250	ILE
1	A	253	ASN
1	A	257	ARG
1	A	265	LYS
1	A	290	GLU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	313	GLN
1	A	315	LEU
1	A	317	LYS
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	324	SER
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	393	ARG
1	A	408	ASP
1	A	412	ARG
1	A	424	ILE
1	A	427	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN

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Mol	Chain	Res	Type
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	489	LEU
1	A	500	GLU
1	A	505	CYS
1	A	538	ASP
1	A	562	THR
1	A	577	ILE
1	A	584	ASN
1	A	589	GLN
1	A	613	ILE
1	A	618	GLU
1	A	625	SER
1	A	626	ASN
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	740	LEU
1	A	768	GLN
1	A	788	SER
1	A	795	GLU
1	A	801	GLU
1	A	821	ARG
1	A	824	LEU
1	A	839	ARG
1	A	848	ILE
1	A	855	THR
1	A	858	ASN
1	A	878	ILE
1	A	882	SER
1	A	896	ARG
1	A	905	ASP

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Mol	Chain	Res	Type
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	923	LEU
1	A	926	GLN
1	A	929	LEU
1	A	931	GLU
1	A	932	GLU
1	A	948	VAL
1	A	961	ARG
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	982	THR
1	A	983	ILE
1	A	1035	TYR
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	1091	SER
1	A	1092	LYS
1	A	1096	SER
1	A	1110	ASN
1	A	1112	LYS
1	A	1118	VAL
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1159	ARG
1	A	1167	GLU
1	A	1168	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1188	GLN
1	A	1192	LEU
1	A	1208	THR

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Mol	Chain	Res	Type
1	A	1237	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1256	GLU
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1269	GLU
1	A	1280	GLU
1	A	1288	ASP
1	A	1290	LYS
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1355	VAL
1	A	1356	ILE
1	A	1366	ARG
1	A	1376	THR
1	A	1387	HIS
1	A	1394	THR
1	A	1398	MET
1	A	1405	THR
1	A	1420	ASP
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1436	ILE
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1448	GLU
1	A	1451	VAL

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Mol	Chain	Res	Type
1	A	1452	LYS
2	B	25	ILE
2	B	35	SER
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	90	ILE
2	B	103	ASN
2	B	118	ARG
2	B	128	LEU
2	B	134	LYS
2	B	167	ILE
2	B	169	ARG
2	B	185	THR
2	B	205	ILE
2	B	218	SER
2	B	222	ILE
2	B	228	LYS
2	B	240	ILE
2	B	251	ILE
2	B	253	THR
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	267	ARG
2	B	268	THR
2	B	284	ILE
2	B	292	ILE
2	B	294	ASP
2	B	305	VAL
2	B	324	ILE
2	B	337	ARG
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	408	LEU
2	B	418	LYS
2	B	446	LEU
2	B	452	THR
2	B	458	LYS
2	B	470	LYS
2	B	476	ARG

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Mol	Chain	Res	Type
2	B	485	ARG
2	B	493	SER
2	B	502	ILE
2	B	508	LEU
2	B	510	LYS
2	B	513	GLN
2	B	529	GLU
2	B	531	GLN
2	B	542	MET
2	B	547	VAL
2	B	552	MET
2	B	560	GLU
2	B	563	MET
2	B	567	GLU
2	B	570	VAL
2	B	573	GLN
2	B	589	VAL
2	B	598	GLU
2	B	601	ARG
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	653	VAL
2	B	658	ILE
2	B	665	GLU
2	B	687	GLU
2	B	690	VAL
2	B	696	GLU
2	B	708	GLU
2	B	722	ASP
2	B	731	VAL
2	B	766	ARG
2	B	780	VAL
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	809	MET
2	B	831	SER

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Mol	Chain	Res	Type
2	B	843	GLN
2	B	844	SER
2	B	857	ARG
2	B	870	ILE
2	B	876	LYS
2	B	878	GLN
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	899	ILE
2	B	906	SER
2	B	908	GLU
2	B	942	ARG
2	B	944	THR
2	B	954	VAL
2	B	956	THR
2	B	957	ASN
2	B	961	LEU
2	B	964	VAL
2	B	976	ILE
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1013	ASN
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1070	GLU
2	B	1084	GLN
2	B	1106	ARG
2	B	1113	VAL
2	B	1120	GLU
2	B	1123	SER
2	B	1128	LEU
2	B	1147	LEU
2	B	1148	LYS
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL

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Mol	Chain	Res	Type
2	B	1162	ILE
2	B	1174	LYS
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1185	CYS
2	B	1186	ASP
2	B	1191	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1220	ARG
2	B	1224	PHE
3	C	3	GLU
3	C	4	GLU
3	C	8	VAL
3	C	9	LYS
3	C	12	GLU
3	C	18	VAL
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	40	GLU
3	C	52	GLU
3	C	55	THR
3	C	56	THR
3	C	79	GLN
3	C	80	LEU
3	C	84	ARG
3	C	85	ASP
3	C	115	SER
3	C	116	LYS
3	C	122	SER
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	134	ILE
3	C	154	LYS
3	C	158	VAL
3	C	166	GLU
3	C	176	ILE
3	C	188	HIS

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Mol	Chain	Res	Type
3	C	215	GLU
3	C	222	LYS
3	C	238	ILE
3	C	240	VAL
3	C	262	LEU
3	C	265	MET
3	C	268	ASP
4	D	2	ASN
4	D	5	THR
4	D	6	SER
4	D	9	GLN
4	D	15	LEU
4	D	18	VAL
4	D	20	GLU
4	D	21	GLU
4	D	32	GLU
4	D	39	ASN
4	D	51	ASN
4	D	53	SER
4	D	65	GLU
4	D	71	LYS
4	D	74	GLN
4	D	121	LYS
4	D	122	GLU
4	D	134	THR
4	D	139	LYS
4	D	146	GLN
4	D	149	THR
4	D	155	ARG
4	D	164	ILE
4	D	187	THR
4	D	193	THR
4	D	213	GLU
4	D	215	SER
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	3	GLN
5	E	36	GLU
5	E	57	MET
5	E	69	ILE
5	E	75	MET

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Mol	Chain	Res	Type
5	E	81	GLU
5	E	84	ASP
5	E	100	ILE
5	E	101	GLN
5	E	154	ILE
5	E	177	ARG
5	E	196	VAL
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	93	ILE
6	F	97	ARG
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
7	G	1	MET
7	G	5	LYS
7	G	8	SER
7	G	24	GLN
7	G	28	THR
7	G	34	VAL
7	G	37	SER
7	G	56	ILE
7	G	61	ILE
7	G	64	THR
7	G	65	ASP
7	G	80	LYS
7	G	90	THR
7	G	92	VAL
7	G	106	MET
7	G	143	ILE
7	G	145	VAL
7	G	151	ILE
7	G	152	SER
7	G	163	ILE
7	G	165	GLU
7	G	171	ILE
8	H	5	LEU
8	H	11	GLN

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Mol	Chain	Res	Type
8	H	19	ARG
8	H	26	ILE
8	H	61	SER
8	H	77	ARG
8	H	103	LYS
8	H	110	ASP
8	H	112	ILE
8	H	130	ARG
8	H	135	LEU
8	H	137	GLN
8	H	146	ARG
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	18	GLU
9	I	21	GLU
9	I	31	THR
9	I	35	VAL
9	I	40	SER
9	I	43	VAL
9	I	49	ILE
9	I	50	THR
9	I	55	THR
9	I	77	LYS
9	I	81	ARG
9	I	87	GLN
9	I	90	GLN
9	I	94	ASP
9	I	95	THR
9	I	97	MET
9	I	111	THR
10	J	1	MET
10	J	12	LYS
10	J	13	VAL
10	J	16	ASP
10	J	20	SER
10	J	22	LEU
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	18	LYS

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Mol	Chain	Res	Type
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	84	LYS
11	K	106	GLU
11	K	107	THR
11	K	114	LEU
12	L	27	LEU
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	62	LYS
12	L	64	LEU
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU
12	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	18	GLN
1	A	83	HIS
1	A	118	HIS
1	A	209	ASN
1	A	225	ASN
1	A	299	HIS
1	A	311	GLN
1	A	339	ASN
1	A	399	HIS
1	A	427	GLN
1	A	435	HIS
1	A	451	HIS

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Mol	Chain	Res	Type
1	A	490	HIS
1	A	503	GLN
1	A	517	ASN
1	A	650	GLN
1	A	700	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	858	ASN
1	A	881	GLN
1	A	926	GLN
1	A	935	GLN
1	A	959	ASN
1	A	1033	GLN
1	A	1124	HIS
1	A	1128	GLN
1	A	1211	GLN
1	A	1265	ASN
1	A	1354	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	47	GLN
2	B	53	GLN
2	B	110	HIS
2	B	115	GLN
2	B	121	ASN
2	B	178	ASN
2	B	278	GLN
2	B	300	HIS
2	B	309	GLN
2	B	325	GLN
2	B	433	GLN
2	B	484	ASN
2	B	513	GLN
2	B	518	HIS
2	B	531	GLN
2	B	573	GLN
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	740	HIS
2	B	744	HIS

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Mol	Chain	Res	Type
2	B	770	GLN
2	B	776	GLN
2	B	842	ASN
2	B	843	GLN
2	B	862	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1097	HIS
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1179	GLN
2	B	1195	HIS
2	B	1211	ASN
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	131	HIS
3	C	184	ASN
3	C	188	HIS
3	C	203	GLN
4	D	23	ASN
4	D	41	GLN
4	D	137	ASN
4	D	143	ASN
4	D	165	GLN
4	D	179	GLN
5	E	5	ASN
5	E	8	ASN
5	E	63	ASN
5	E	147	HIS
6	F	104	ASN
7	G	14	HIS
7	G	122	ASN
7	G	126	ASN
7	G	158	HIS

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Mol	Chain	Res	Type
8	H	11	GLN
8	H	21	ASN
8	H	35	GLN
8	H	134	ASN
8	H	137	GLN
9	I	11	ASN
9	I	12	ASN
9	I	23	ASN
9	I	46	HIS
9	I	51	ASN
9	I	116	ASN
11	K	2	ASN
11	K	29	ASN
11	K	65	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 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

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	1421/1732 (82%)	-0.29	15 (1%) 78 52	64, 112, 182, 240	0
2	B	1118/1223 (91%)	-0.11	29 (2%) 57 32	68, 126, 195, 228	0
3	C	266/266 (100%)	-0.36	0 100 100	80, 116, 160, 192	0
4	D	180/221 (81%)	-0.02	10 (5%) 30 17	97, 131, 188, 211	0
5	E	214/214 (100%)	-0.19	1 (0%) 87 67	91, 157, 206, 216	0
6	F	87/87 (100%)	-0.51	1 (1%) 78 52	69, 92, 124, 138	0
7	G	171/171 (100%)	-0.33	1 (0%) 85 64	83, 112, 149, 185	0
8	H	133/145 (91%)	0.10	5 (3%) 44 24	118, 160, 196, 204	0
9	I	119/119 (100%)	0.07	3 (2%) 58 33	123, 153, 195, 219	0
10	J	65/65 (100%)	-0.29	1 (1%) 72 44	89, 113, 155, 173	0
11	K	115/115 (100%)	-0.54	2 (1%) 69 41	79, 112, 160, 181	0
12	L	46/46 (100%)	0.52	5 (10%) 10 7	97, 155, 190, 204	0
13	Q	15/15 (100%)	1.46	4 (26%) 1 2	132, 200, 214, 222	0
All	All	3950/4419 (89%)	-0.20	77 (1%) 66 39	64, 122, 191, 240	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	7.8
10	J	65	PRO	6.5
4	D	3	VAL	6.3
1	A	65	LEU	5.8
12	L	27	LEU	5.6
2	B	882	THR	5.1
4	D	2	ASN	4.8
8	H	136	LYS	4.7
2	B	70	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
8	H	63	LEU	4.1
2	B	446	LEU	4.1
1	A	1254	ALA	4.0
4	D	24	ALA	4.0
1	A	44	THR	3.6
6	F	69	LEU	3.5
4	D	1	MET	3.5
1	A	1083	THR	3.5
1	A	186	LYS	3.5
1	A	1084	PHE	3.4
11	K	114	LEU	3.3
2	B	245	GLU	3.3
2	B	447	ALA	3.2
2	B	507	LYS	3.2
2	B	436	VAL	3.2
2	B	134	LYS	3.1
1	A	46	THR	3.1
4	D	18	VAL	3.1
2	B	508	LEU	3.1
12	L	25	ALA	3.0
1	A	1176	LEU	3.0
13	Q	35	ARG	3.0
1	A	251	SER	3.0
1	A	1085	HIS	2.9
4	D	13	ARG	2.9
2	B	708	GLU	2.9
8	H	139	ASN	2.9
1	A	1093	LYS	2.9
2	B	883	LEU	2.9
13	Q	25	ASP	2.8
4	D	25	ALA	2.8
12	L	26	THR	2.8
2	B	469	GLN	2.7
2	B	251	ILE	2.7
2	B	934	LYS	2.7
2	B	709	ASP	2.6
7	G	64	THR	2.5
2	B	503	GLY	2.5
2	B	731	VAL	2.5
9	I	89	GLN	2.5
12	L	28	LYS	2.5
13	Q	28	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	90	ILE	2.5
2	B	646	LEU	2.5
2	B	164	LYS	2.4
2	B	241	ARG	2.4
2	B	108	VAL	2.4
13	Q	26	ARG	2.4
2	B	437	GLU	2.4
2	B	715	ALA	2.3
4	D	17	LYS	2.3
2	B	734	HIS	2.2
1	A	1082	ASN	2.2
8	H	90	ALA	2.2
9	I	118	ARG	2.2
2	B	730	ARG	2.1
2	B	246	LYS	2.1
1	A	250	ILE	2.1
2	B	249	ARG	2.1
9	I	52	ILE	2.1
4	D	16	LYS	2.1
8	H	76	THR	2.1
2	B	470	LYS	2.1
5	E	91	LYS	2.1
1	A	3	GLY	2.0
4	D	11	ARG	2.0
12	L	66	GLN	2.0
11	K	115	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
15	MG	A	1803	1/1	0.84	0.26	62,62,62,62	0
14	ZN	L	101	1/1	0.99	0.03	151,151,151,151	0
14	ZN	I	202	1/1	0.99	0.04	209,209,209,209	0
14	ZN	C	301	1/1	1.00	0.01	94,94,94,94	0
14	ZN	I	201	1/1	1.00	0.01	125,125,125,125	0
14	ZN	A	1801	1/1	1.00	0.02	164,164,164,164	0
14	ZN	J	101	1/1	1.00	0.03	110,110,110,110	0
14	ZN	A	1802	1/1	1.00	0.03	97,97,97,97	0
14	ZN	B	1301	1/1	1.00	0.05	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.