



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 PM UTC

PDB ID : 3PO2 / pdb_00003po2
Title : Arrested RNA Polymerase II elongation complex
Authors : Cheung, A.C.M.; Cramer, P.
Deposited on : 2010-11-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

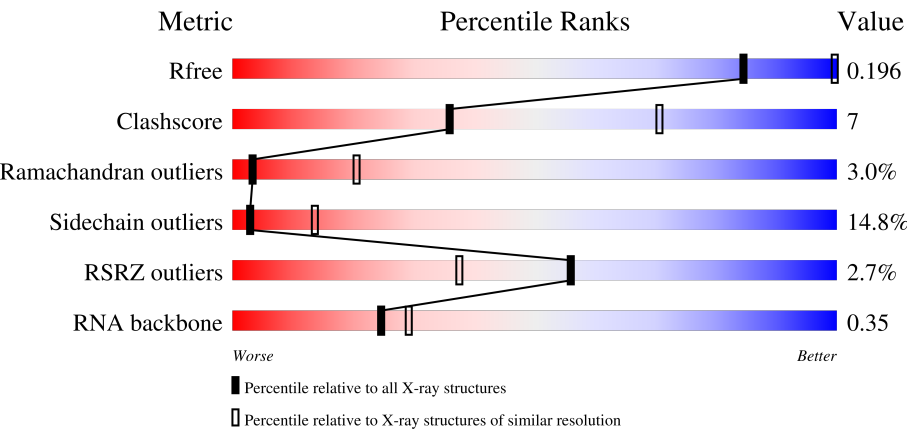
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	55%20%5%18% 4%
2	B	1224	63%23%8% 4%
3	C	318	53%25%5%16%
4	D	221	58%20%19% 5%

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Mol	Chain	Length	Quality of chain
5	E	215	80% 17%
6	F	155	39% 12% 5% 44%
7	G	171	67% 25% 6%
8	H	146	3% 56% 29% 5% 9%
9	I	122	7% 66% 24% 8%
10	J	70	61% 21% 7% 7%
11	K	120	67% 23% 6%
12	L	70	10% 34% 19% 11% 34%
13	N	14	7% 93% 7%
14	P	15	13% 47% 20% 27% 7%
15	T	27	4% 52% 19% 30%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 32287 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	1121	Total	C	N	O	S	0	0	0
			8899	5632	1563	1649	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 DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			288	138	57	80	13			

- Molecule 14 is a RNA chain called RNA product strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	15	Total	C	N	O	P	0	0	0
			300	135	45	105	15			

- Molecule 15 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			389	1	185	66	118	19		

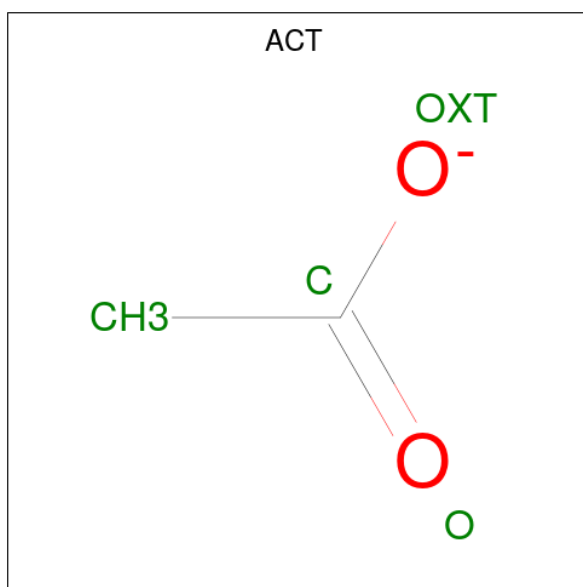
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

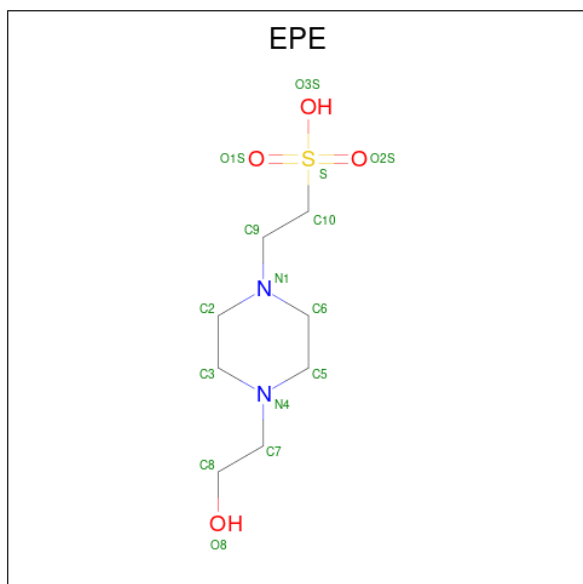
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



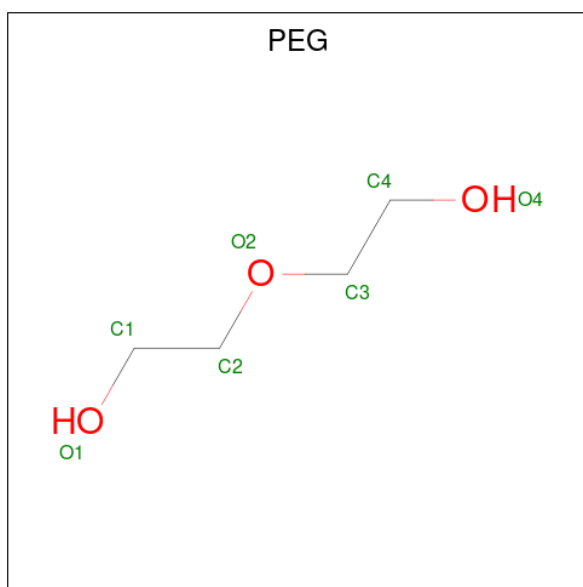
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 20 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

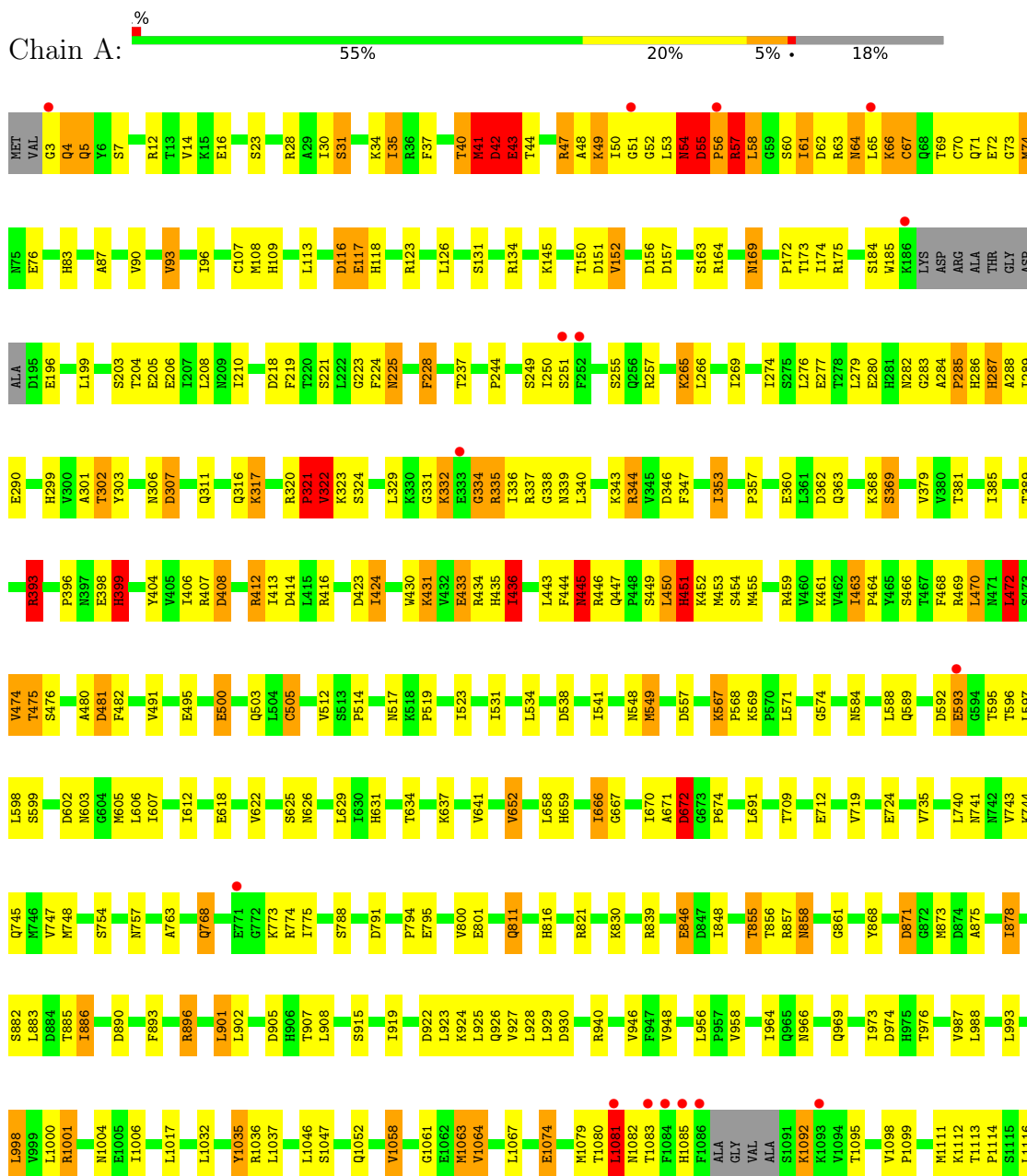


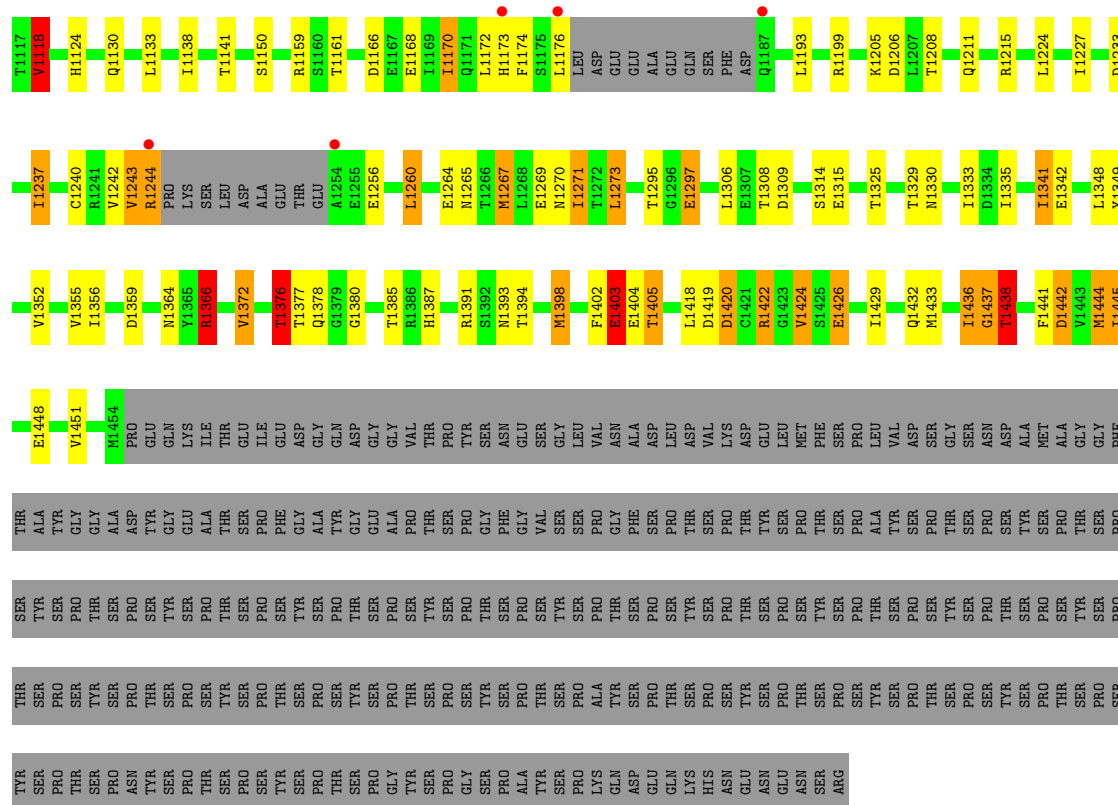
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total	C	O	0	0
			7	4	3		

3 Residue-property plots

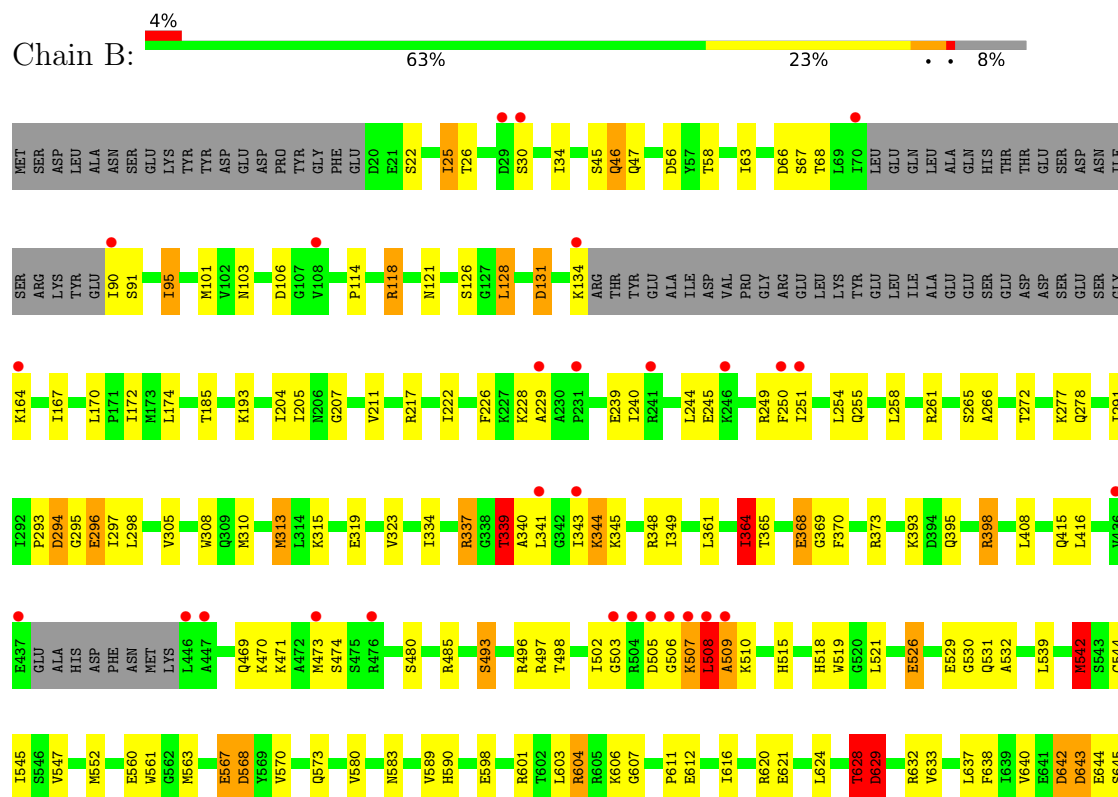
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

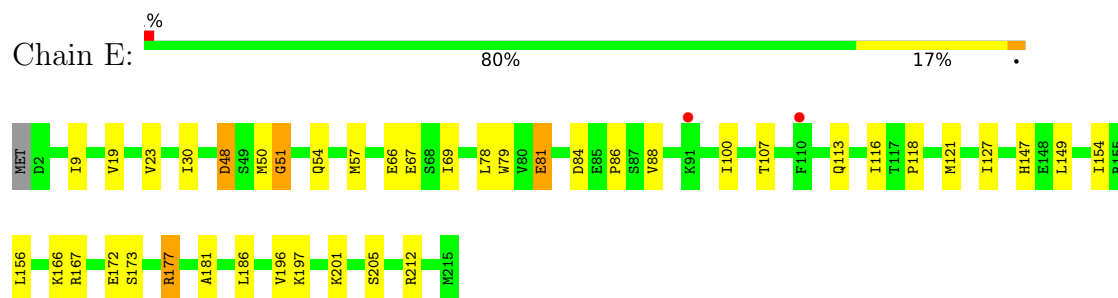




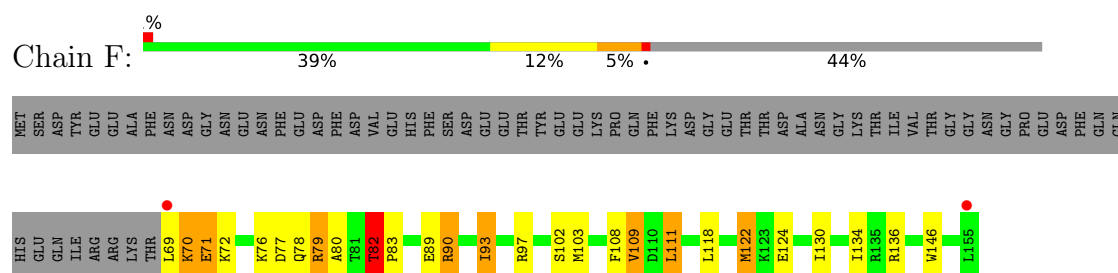
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



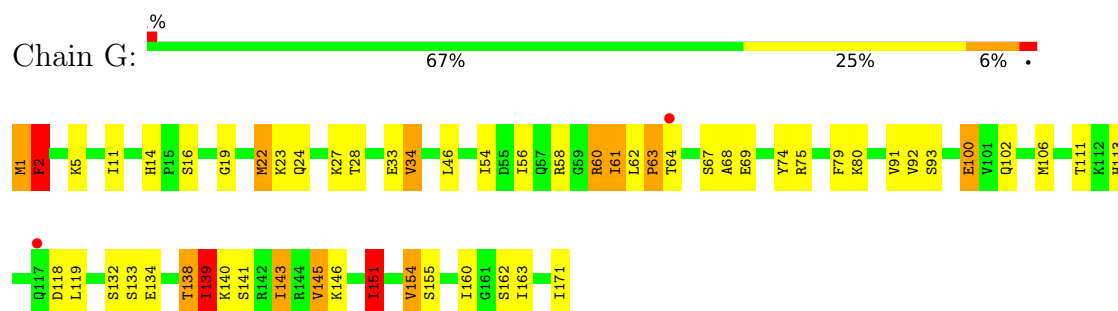
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



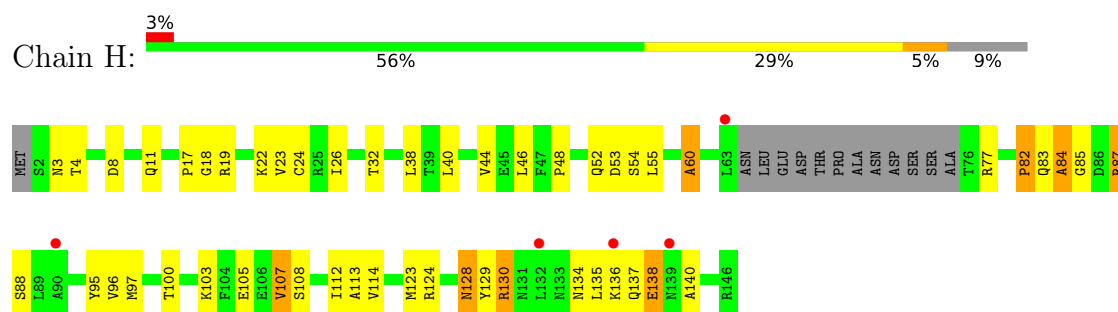
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



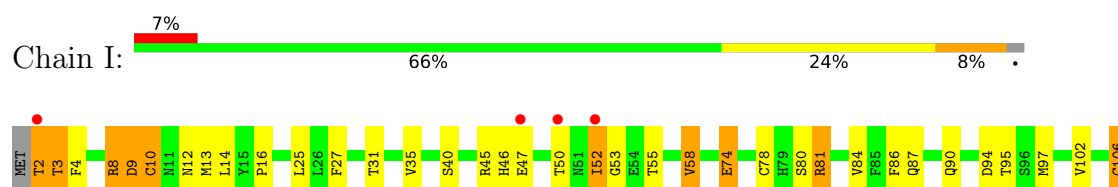
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



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



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

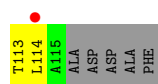




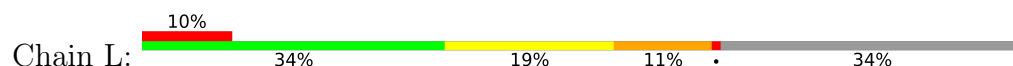
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



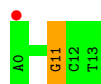
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



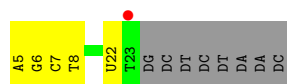
- Molecule 13: DNA non-template strand



- Molecule 14: RNA product strand



- Molecule 15: DNA template strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	224.57Å 394.55Å 282.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.30 48.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.98-3.30) 99.8 (48.98-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.153 , 0.178 0.173 , 0.196	Depositor DCC
R_{free} test set	3690 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	109.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 130.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32287	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, BRU, ZN, ACT, MG, EPE

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	11/11391 (0.1%)	1.54	142/15402 (0.9%)
2	B	0.88	4/9072 (0.0%)	1.47	93/12233 (0.8%)
3	C	0.85	0/2133	1.44	17/2891 (0.6%)
4	D	0.86	1/1450 (0.1%)	1.63	19/1945 (1.0%)
5	E	0.78	0/1788	1.39	7/2406 (0.3%)
6	F	0.96	1/717 (0.1%)	1.45	7/967 (0.7%)
7	G	0.88	2/1368 (0.1%)	1.44	13/1844 (0.7%)
8	H	0.82	0/1086	1.41	11/1470 (0.7%)
9	I	0.79	0/989	1.35	4/1331 (0.3%)
10	J	0.79	0/541	1.51	11/727 (1.5%)
11	K	0.83	0/938	1.36	4/1267 (0.3%)
12	L	1.00	0/365	1.75	11/485 (2.3%)
13	N	0.38	0/324	1.29	2/499 (0.4%)
14	P	1.15	2/329 (0.6%)	1.61	7/506 (1.4%)
15	T	0.47	0/411	1.36	3/630 (0.5%)
All	All	0.87	21/32902 (0.1%)	1.49	351/44603 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	9.92	1.47	1.33
1	A	55	ASP	CA-C	-9.08	1.41	1.52
2	B	882	THR	CA-C	7.61	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	24	ALA	CA-C	7.31	1.62	1.52
6	F	122	MET	SD-CE	6.79	1.96	1.79
7	G	1	MET	C-N	6.67	1.43	1.33
1	A	57	ARG	CA-C	6.36	1.61	1.52
2	B	882	THR	CA-CB	6.12	1.62	1.52
1	A	1398	MET	SD-CE	6.11	1.94	1.79
7	G	151	ILE	CG1-CD1	6.05	1.75	1.51
1	A	1081	LEU	CA-C	6.00	1.60	1.52
14	P	5	C	C1'-N1	5.92	1.57	1.48
1	A	3	GLY	C-N	5.80	1.41	1.33
1	A	474	VAL	CA-C	5.47	1.58	1.52
2	B	542	MET	SD-CE	-5.37	1.66	1.79
1	A	549	MET	SD-CE	-5.36	1.66	1.79
1	A	1438	THR	CA-C	5.33	1.60	1.52
1	A	54	ASN	CA-C	5.28	1.59	1.52
14	P	6	C	C1'-N1	5.22	1.56	1.48
2	B	999	MET	CA-C	5.12	1.58	1.53
1	A	57	ARG	N-CA	5.02	1.52	1.46

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	11.89	126.31	111.69
4	D	25	ALA	CA-C-N	10.69	138.67	121.99
4	D	25	ALA	C-N-CA	10.69	138.67	121.99
1	A	288	ALA	N-CA-C	-9.69	102.54	114.75
14	P	5	C	P-O3'-C3'	9.67	134.71	120.20
10	J	5	VAL	N-CA-C	-9.65	96.08	109.21
4	D	26	THR	N-CA-C	-9.62	98.68	113.89
1	A	1403	GLU	CA-C-N	-9.12	108.38	122.60
1	A	1403	GLU	C-N-CA	-9.12	108.38	122.60
2	B	1122	ARG	CA-C-N	9.10	132.47	120.28
2	B	1122	ARG	C-N-CA	9.10	132.47	120.28
1	A	56	PRO	CA-C-N	9.03	138.79	121.54
1	A	56	PRO	C-N-CA	9.03	138.79	121.54
14	P	6	C	N1-C1'-C2'	8.92	125.38	112.00
6	F	71	GLU	N-CA-C	-8.88	102.45	113.38
15	T	8	DT	P-O3'-C3'	8.64	133.16	120.20
1	A	224	PHE	N-CA-C	8.52	120.89	110.41
2	B	645	SER	N-CA-C	-8.44	102.88	113.01
2	B	1174	LYS	N-CA-C	-8.25	99.21	110.68
1	A	61	ILE	N-CA-C	-8.13	104.82	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ASP	CA-CB-CG	8.08	120.68	112.60
2	B	509	ALA	CA-C-N	8.04	131.19	120.58
2	B	509	ALA	C-N-CA	8.04	131.19	120.58
4	D	31	GLN	N-CA-C	-7.98	102.18	112.23
1	A	346	ASP	CA-CB-CG	7.79	120.39	112.60
2	B	508	LEU	N-CA-C	7.72	119.76	110.19
7	G	1	MET	CA-C-N	7.67	136.20	121.54
7	G	1	MET	C-N-CA	7.67	136.20	121.54
7	G	34	VAL	N-CA-C	7.56	118.30	110.36
2	B	1155	SER	CA-C-N	7.50	133.12	121.19
2	B	1155	SER	C-N-CA	7.50	133.12	121.19
1	A	445	ASN	CA-CB-CG	7.49	120.09	112.60
10	J	18	TRP	N-CA-C	7.47	119.21	111.14
1	A	1385	THR	CA-C-N	7.46	130.61	120.38
1	A	1385	THR	C-N-CA	7.46	130.61	120.38
2	B	976	ILE	N-CA-C	7.46	118.23	110.62
1	A	408	ASP	CA-C-N	7.41	131.19	120.38
1	A	408	ASP	C-N-CA	7.41	131.19	120.38
7	G	64	THR	N-CA-C	7.41	120.23	111.71
2	B	628	THR	CA-C-N	7.39	135.66	121.54
2	B	628	THR	C-N-CA	7.39	135.66	121.54
12	L	62	LYS	N-CA-C	-7.33	104.37	113.38
1	A	55	ASP	N-CA-CB	7.30	123.37	110.37
2	B	1130	PHE	N-CA-C	-7.29	98.76	109.11
2	B	1156	ASP	N-CA-C	7.26	123.28	111.37
1	A	331	GLY	N-CA-C	7.25	124.47	112.30
2	B	1223	ASP	CA-CB-CG	7.24	119.84	112.60
3	C	183	TRP	N-CA-C	-7.23	97.91	109.76
2	B	1219	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	399	HIS	N-CA-CB	7.20	123.19	110.37
9	I	9	ASP	CA-CB-CG	7.15	119.75	112.60
7	G	33	GLU	CA-C-N	7.14	129.81	120.60
7	G	33	GLU	C-N-CA	7.14	129.81	120.60
1	A	1403	GLU	N-CA-C	7.12	125.97	110.80
3	C	26	ASP	CA-CB-CG	7.09	119.69	112.60
1	A	219	PHE	CA-CB-CG	7.00	120.80	113.80
14	P	7	C	N1-C1'-C2'	6.96	122.45	112.00
12	L	59	ALA	CA-C-N	6.96	134.84	121.54
12	L	59	ALA	C-N-CA	6.96	134.84	121.54
1	A	1063	MET	CA-C-N	6.82	131.81	120.62
1	A	1063	MET	C-N-CA	6.82	131.81	120.62
12	L	68	GLU	CB-CG-CD	6.80	124.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASN	CA-C-N	6.79	129.68	120.38
1	A	225	ASN	C-N-CA	6.79	129.68	120.38
1	A	1445	ILE	N-CA-CB	6.79	119.93	110.56
1	A	205	GLU	CA-C-N	6.75	129.21	120.44
1	A	205	GLU	C-N-CA	6.75	129.21	120.44
1	A	1271	ILE	N-CA-C	6.73	118.11	109.30
2	B	629	ASP	CA-CB-CG	6.71	119.31	112.60
2	B	95	ILE	N-CA-CB	6.69	118.02	110.72
2	B	1181	GLU	N-CA-C	6.68	125.03	110.80
2	B	1177	HIS	N-CA-C	-6.64	104.40	113.30
4	D	24	ALA	CA-C-N	6.60	131.60	121.83
4	D	24	ALA	C-N-CA	6.60	131.60	121.83
1	A	794	PRO	CA-C-N	6.60	129.13	120.28
1	A	794	PRO	C-N-CA	6.60	129.13	120.28
1	A	218	ASP	CA-CB-CG	6.59	119.19	112.60
6	F	82	THR	CB-CA-C	-6.58	99.09	109.42
2	B	684	LEU	CA-C-N	6.55	128.96	120.44
2	B	684	LEU	C-N-CA	6.55	128.96	120.44
2	B	825	VAL	N-CA-C	6.54	117.28	107.80
2	B	883	LEU	N-CA-C	6.52	119.33	108.96
14	P	5	C	N1-C1'-C2'	6.52	121.78	112.00
1	A	62	ASP	CA-CB-CG	6.51	119.11	112.60
3	C	136	ASP	N-CA-C	6.51	118.42	110.41
1	A	321	PRO	N-CA-C	6.50	125.85	112.47
1	A	466	SER	N-CA-C	6.49	120.80	113.02
1	A	1436	ILE	N-CA-CB	-6.45	102.47	111.25
8	H	87	ARG	N-CA-C	6.45	119.26	110.55
2	B	497	ARG	N-CA-C	6.39	119.94	110.48
2	B	1153	GLU	CB-CG-CD	6.38	123.44	112.60
1	A	63	ARG	CA-C-N	6.38	133.25	121.52
1	A	63	ARG	C-N-CA	6.38	133.25	121.52
6	F	80	ALA	N-CA-C	6.35	120.64	113.02
1	A	436	ILE	CB-CA-C	6.33	120.77	111.33
1	A	58	LEU	N-CA-C	6.32	120.72	112.89
1	A	472	LEU	N-CA-C	6.31	118.97	111.71
4	D	220	LEU	CA-C-N	6.30	133.03	121.70
4	D	220	LEU	C-N-CA	6.30	133.03	121.70
1	A	1173	HIS	CA-C-N	6.28	130.71	120.23
1	A	1173	HIS	C-N-CA	6.28	130.71	120.23
1	A	602	ASP	N-CA-C	-6.27	103.52	111.92
3	C	145	CYS	N-CA-C	6.23	117.76	107.73
1	A	223	GLY	N-CA-C	6.23	121.31	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	880	THR	CA-C-N	6.23	133.44	121.54
2	B	880	THR	C-N-CA	6.23	133.44	121.54
1	A	1035	TYR	CA-C-N	-6.22	111.54	122.62
1	A	1035	TYR	C-N-CA	-6.22	111.54	122.62
1	A	998	LEU	N-CA-C	6.19	118.80	108.96
4	D	136	GLY	CA-C-N	6.19	129.19	120.28
4	D	136	GLY	C-N-CA	6.19	129.19	120.28
1	A	285	PRO	CA-C-N	6.18	133.34	121.54
1	A	285	PRO	C-N-CA	6.18	133.34	121.54
8	H	128	ASN	CA-C-N	6.16	131.11	120.58
8	H	128	ASN	C-N-CA	6.16	131.11	120.58
1	A	54	ASN	CA-C-N	6.15	136.82	121.80
1	A	54	ASN	C-N-CA	6.15	136.82	121.80
2	B	903	VAL	N-CA-C	6.14	118.48	109.63
1	A	408	ASP	CA-CB-CG	6.12	118.72	112.60
8	H	3	ASN	CA-C-N	6.12	129.81	121.05
8	H	3	ASN	C-N-CA	6.12	129.81	121.05
1	A	672	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	54	ASN	CA-CB-CG	6.12	118.72	112.60
1	A	966	ASN	CA-CB-CG	6.11	118.71	112.60
2	B	645	SER	CA-C-N	6.11	131.16	122.24
2	B	645	SER	C-N-CA	6.11	131.16	122.24
7	G	163	ILE	CA-C-N	6.09	128.72	120.44
7	G	163	ILE	C-N-CA	6.09	128.72	120.44
2	B	998	ASP	CA-CB-CG	6.08	118.69	112.60
2	B	1169	MET	CA-C-N	6.07	130.31	120.60
2	B	1169	MET	C-N-CA	6.07	130.31	120.60
2	B	991	GLY	CA-C-N	6.03	128.00	121.97
2	B	991	GLY	C-N-CA	6.03	128.00	121.97
2	B	339	THR	CA-C-N	6.03	132.55	121.70
2	B	339	THR	C-N-CA	6.03	132.55	121.70
1	A	1037	LEU	N-CA-C	6.01	118.72	110.24
2	B	1013	ASN	N-CA-C	6.00	117.22	109.65
14	P	6	C	P-O3'-C3'	6.00	129.21	120.20
2	B	902	GLY	CA-C-N	6.00	128.53	120.50
2	B	902	GLY	C-N-CA	6.00	128.53	120.50
10	J	55	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	228	PHE	N-CA-C	5.96	120.71	112.90
11	K	39	ASP	CA-CB-CG	5.96	118.56	112.60
12	L	68	GLU	N-CA-C	-5.95	100.58	109.15
1	A	474	VAL	CA-C-N	5.92	128.53	120.54
1	A	474	VAL	C-N-CA	5.92	128.53	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	ALA	N-CA-C	5.91	120.00	111.02
2	B	1184	GLY	CA-C-N	5.90	132.81	121.54
2	B	1184	GLY	C-N-CA	5.90	132.81	121.54
1	A	974	ASP	CA-CB-CG	5.88	118.48	112.60
10	J	9	SER	N-CA-C	5.88	117.49	111.14
1	A	398	GLU	CA-C-O	-5.87	114.32	121.36
12	L	64	LEU	CA-C-N	5.84	129.72	121.66
12	L	64	LEU	C-N-CA	5.84	129.72	121.66
1	A	42	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	152	VAL	CB-CA-C	5.82	115.04	109.33
12	L	64	LEU	N-CA-C	5.80	118.66	109.96
3	C	57	VAL	CA-C-N	5.79	130.66	122.09
3	C	57	VAL	C-N-CA	5.79	130.66	122.09
2	B	936	ASP	N-CA-C	5.79	118.84	110.28
7	G	141	SER	N-CA-C	5.79	118.22	110.35
1	A	495	GLU	N-CA-C	-5.78	105.11	111.82
14	P	6	C	P-O5'-C5'	5.77	129.56	120.90
1	A	289	ILE	N-CA-C	-5.75	105.24	110.82
1	A	1138	ILE	N-CA-C	5.75	116.75	111.81
1	A	244	PRO	N-CA-C	5.71	117.67	110.70
10	J	6	ARG	N-CA-C	5.71	122.95	110.80
11	K	63	VAL	N-CA-CB	5.71	117.82	111.89
12	L	63	ARG	N-CA-C	-5.69	100.96	109.15
2	B	1146	PHE	CA-CB-CG	-5.67	108.13	113.80
3	C	38	ILE	CA-C-N	5.65	130.24	120.58
3	C	38	ILE	C-N-CA	5.65	130.24	120.58
4	D	70	PHE	CA-CB-CG	5.65	119.45	113.80
8	H	129	TYR	N-CA-C	5.65	118.64	111.69
1	A	1061	GLY	N-CA-C	-5.64	107.77	114.48
1	A	1404	GLU	N-CA-C	5.64	120.15	112.88
3	C	89	GLU	N-CA-C	-5.63	103.83	111.55
1	A	1269	GLU	N-CA-C	5.61	117.09	110.97
1	A	1237	ILE	N-CA-C	5.60	116.81	108.46
2	B	339	THR	CB-CA-C	5.60	121.56	110.42
8	H	138	GLU	N-CA-C	-5.60	105.18	111.28
2	B	732	SER	N-CA-C	5.59	117.57	109.07
2	B	294	ASP	CA-CB-CG	5.59	118.19	112.60
2	B	106	ASP	CA-C-N	5.58	128.62	120.91
2	B	106	ASP	C-N-CA	5.58	128.62	120.91
2	B	1009	ASP	N-CA-C	-5.58	106.47	113.28
1	A	724	GLU	N-CA-C	-5.57	105.11	111.07
10	J	8	PHE	CA-CB-CG	5.57	119.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	885	MET	N-CA-C	5.56	118.52	110.28
1	A	67	CYS	N-CA-C	-5.56	106.66	113.50
1	A	1081	LEU	CA-C-N	5.56	131.70	121.70
1	A	1081	LEU	C-N-CA	5.56	131.70	121.70
7	G	2	PHE	CA-CB-CG	5.56	119.36	113.80
5	E	48	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	800	VAL	CA-C-N	5.55	127.72	120.28
1	A	800	VAL	C-N-CA	5.55	127.72	120.28
1	A	31	SER	N-CA-C	5.54	118.39	110.24
1	A	886	ILE	N-CA-C	5.54	115.99	110.23
2	B	1009	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	1035	TYR	N-CA-C	-5.54	101.45	110.20
1	A	1424	VAL	N-CA-C	-5.54	105.33	110.53
4	D	29	LEU	N-CA-C	-5.54	101.25	109.94
15	T	5	DA	P-O3'-C3'	5.53	128.50	120.20
2	B	711	GLU	N-CA-C	5.52	122.02	109.81
1	A	1341	ILE	N-CA-C	5.52	116.91	110.62
2	B	902	GLY	N-CA-C	5.51	120.83	114.16
1	A	436	ILE	CA-CB-CG2	5.48	119.81	110.50
1	A	287	HIS	CA-C-N	5.47	131.03	121.52
1	A	287	HIS	C-N-CA	5.47	131.03	121.52
3	C	96	SER	N-CA-C	5.47	117.10	108.96
2	B	934	LYS	N-CA-C	5.46	122.43	110.80
12	L	64	LEU	N-CA-CB	5.46	117.98	109.85
12	L	61	THR	N-CA-C	5.46	117.33	110.24
2	B	901	PRO	N-CA-C	5.45	123.70	112.47
4	D	39	ASN	CA-CB-CG	5.45	118.05	112.60
2	B	758	PHE	CA-C-O	-5.45	116.71	120.47
1	A	73	GLY	CA-C-N	5.45	131.94	121.54
1	A	73	GLY	C-N-CA	5.45	131.94	121.54
1	A	505	CYS	N-CA-C	5.43	119.47	112.41
1	A	1118	VAL	N-CA-C	5.43	115.61	107.51
2	B	296	GLU	N-CA-C	-5.43	104.77	111.40
1	A	451	HIS	N-CA-CB	-5.43	101.44	111.53
2	B	831	SER	CA-CB-OG	-5.42	100.25	111.10
1	A	1085	HIS	CA-C-N	5.41	131.44	121.70
1	A	1085	HIS	C-N-CA	5.41	131.44	121.70
1	A	930	ASP	N-CA-C	-5.41	105.47	111.36
1	A	1335	ILE	CA-C-N	5.40	127.83	120.54
1	A	1335	ILE	C-N-CA	5.40	127.83	120.54
2	B	785	TYR	N-CA-C	5.39	117.85	111.33
6	F	77	ASP	N-CA-C	-5.38	102.92	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	VAL	N-CA-CB	5.37	118.25	110.52
2	B	308	TRP	CA-C-N	5.37	127.42	120.44
2	B	308	TRP	C-N-CA	5.37	127.42	120.44
8	H	87	ARG	CA-C-N	5.36	131.79	121.54
8	H	87	ARG	C-N-CA	5.36	131.79	121.54
1	A	1419	ASP	CA-C-N	5.36	129.18	120.60
1	A	1419	ASP	C-N-CA	5.36	129.18	120.60
10	J	64	ASN	N-CA-C	5.35	121.64	109.81
2	B	415	GLN	CA-C-N	5.34	127.90	120.63
2	B	415	GLN	C-N-CA	5.34	127.90	120.63
8	H	38	LEU	N-CA-C	5.34	117.31	108.13
13	N	11	DG	P-O5'-C5'	5.32	127.98	120.00
1	A	117	GLU	N-CA-C	-5.31	107.10	113.21
1	A	331	GLY	CA-C-N	5.31	131.68	121.54
1	A	331	GLY	C-N-CA	5.31	131.68	121.54
13	N	11	DG	N9-C1'-C2'	5.31	121.46	113.50
1	A	969	GLN	CA-C-N	5.30	127.65	120.38
1	A	969	GLN	C-N-CA	5.30	127.65	120.38
4	D	142	LYS	CA-C-N	5.30	127.38	120.28
4	D	142	LYS	C-N-CA	5.30	127.38	120.28
2	B	568	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	891	ASP	N-CA-C	5.30	119.37	113.01
5	E	172	GLU	CA-C-N	5.30	127.64	120.38
5	E	172	GLU	C-N-CA	5.30	127.64	120.38
7	G	2	PHE	N-CA-C	-5.30	99.52	110.80
1	A	23	SER	N-CA-C	-5.29	102.52	110.24
2	B	882	THR	CB-CA-C	5.29	118.22	111.40
1	A	1170	ILE	N-CA-CB	5.28	116.73	110.55
8	H	55	LEU	N-CA-C	5.28	117.51	108.90
1	A	531	ILE	N-CA-CB	5.28	117.33	110.57
5	E	177	ARG	N-CA-C	5.26	118.39	109.76
1	A	41	MET	CA-C-N	5.25	131.57	121.54
1	A	41	MET	C-N-CA	5.25	131.57	121.54
1	A	237	THR	N-CA-C	-5.25	106.81	113.43
2	B	879	ARG	N-CA-C	5.25	121.98	110.80
3	C	87	PHE	N-CA-C	5.25	119.55	113.20
2	B	1018	PRO	CA-C-N	5.25	127.31	120.28
2	B	1018	PRO	C-N-CA	5.25	127.31	120.28
1	A	846	GLU	CA-C-N	5.25	131.56	121.18
1	A	846	GLU	C-N-CA	5.25	131.56	121.18
10	J	16	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	250	PHE	CA-C-N	5.23	131.38	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	PHE	C-N-CA	5.23	131.38	121.97
2	B	1131	GLY	CA-C-N	5.22	127.59	120.54
2	B	1131	GLY	C-N-CA	5.22	127.59	120.54
10	J	55	ASP	CA-C-N	5.22	128.00	120.38
10	J	55	ASP	C-N-CA	5.22	128.00	120.38
1	A	596	THR	N-CA-C	-5.21	102.48	110.14
3	C	248	ILE	CA-C-N	5.20	127.51	120.38
3	C	248	ILE	C-N-CA	5.20	127.51	120.38
1	A	3	GLY	CA-C-N	5.20	131.47	121.54
1	A	3	GLY	C-N-CA	5.20	131.47	121.54
1	A	332	LYS	N-CA-C	-5.20	99.73	110.80
4	D	25	ALA	N-CA-C	-5.20	101.77	109.83
1	A	896	ARG	N-CA-C	5.19	117.02	111.36
6	F	70	LYS	CA-C-N	5.18	131.23	122.26
6	F	70	LYS	C-N-CA	5.18	131.23	122.26
6	F	108	PHE	CA-CB-CG	-5.18	108.62	113.80
2	B	1224	PHE	CA-CB-CG	5.18	118.98	113.80
2	B	1001	PHE	N-CA-C	5.17	117.25	109.23
14	P	16	C	C4'-C3'-C2'	5.17	107.77	102.60
2	B	986	GLN	N-CA-C	5.17	118.08	107.69
4	D	143	ASN	CA-CB-CG	5.17	117.77	112.60
2	B	687	GLU	N-CA-C	-5.17	106.97	113.28
1	A	791	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	173	THR	CB-CA-C	5.16	120.07	111.30
9	I	52	ILE	N-CA-CB	5.15	118.16	111.67
1	A	224	PHE	CA-CB-CG	-5.14	108.66	113.80
7	G	106	MET	N-CA-C	5.14	117.70	110.14
3	C	110	THR	CB-CA-C	5.14	117.55	109.84
1	A	1366	ARG	N-CA-C	5.14	117.55	111.33
2	B	829	CYS	N-CA-C	-5.13	100.80	108.96
2	B	244	LEU	CA-C-N	5.12	131.33	121.54
2	B	244	LEU	C-N-CA	5.12	131.33	121.54
1	A	381	THR	CB-CA-C	5.12	117.00	109.22
2	B	642	ASP	CA-C-N	5.12	131.31	121.54
2	B	642	ASP	C-N-CA	5.12	131.31	121.54
1	A	368	LYS	CA-C-N	5.11	127.44	120.54
1	A	368	LYS	C-N-CA	5.11	127.44	120.54
3	C	230	MET	N-CA-C	5.11	117.58	109.50
5	E	205	SER	N-CA-C	-5.11	101.93	109.86
1	A	169	ASN	N-CA-C	5.11	121.67	110.80
1	A	329	LEU	CA-C-N	5.11	128.58	121.02
1	A	329	LEU	C-N-CA	5.11	128.58	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	871	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	681	TRP	N-CA-C	-5.10	105.80	111.36
5	E	54	GLN	CA-C-N	5.10	127.12	120.28
5	E	54	GLN	C-N-CA	5.10	127.12	120.28
1	A	1064	VAL	N-CA-CB	-5.10	102.54	110.54
11	K	25	THR	CA-C-N	5.10	127.11	120.28
11	K	25	THR	C-N-CA	5.10	127.11	120.28
2	B	846	ILE	CA-C-N	5.09	127.11	120.28
2	B	846	ILE	C-N-CA	5.09	127.11	120.28
1	A	592	ASP	CA-CB-CG	5.09	117.69	112.60
4	D	26	THR	CA-C-N	5.09	129.78	122.40
4	D	26	THR	C-N-CA	5.09	129.78	122.40
3	C	191	TYR	N-CA-C	5.08	117.53	109.96
1	A	858	ASN	CA-CB-CG	5.08	117.68	112.60
2	B	1162	ILE	CA-CB-CG2	5.08	119.13	110.50
1	A	930	ASP	CA-C-N	5.07	127.03	120.44
1	A	930	ASP	C-N-CA	5.07	127.03	120.44
1	A	1112	LYS	N-CA-C	5.07	116.50	110.97
15	T	6	DG	P-O3'-C3'	5.07	127.81	120.20
10	J	52	THR	CB-CA-C	5.07	119.13	110.56
2	B	694	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	671	ALA	CA-C-N	5.04	128.82	121.31
1	A	671	ALA	C-N-CA	5.04	128.82	121.31
2	B	643	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	393	ARG	CA-C-N	5.04	127.04	120.28
1	A	393	ARG	C-N-CA	5.04	127.04	120.28
1	A	1376	THR	CB-CA-C	5.04	118.66	110.24
1	A	1330	ASN	N-CA-C	-5.04	106.64	112.89
2	B	607	GLY	CA-C-N	5.03	127.72	120.38
2	B	607	GLY	C-N-CA	5.03	127.72	120.38
1	A	307	ASP	CA-C-N	5.03	127.82	120.98
1	A	307	ASP	C-N-CA	5.03	127.82	120.98
2	B	56	ASP	CA-CB-CG	5.03	117.62	112.60
7	G	46	LEU	N-CA-C	5.02	117.52	111.40
9	I	53	GLY	CA-C-N	5.02	126.97	120.44
9	I	53	GLY	C-N-CA	5.02	126.97	120.44
1	A	1270	ASN	N-CA-C	5.00	116.58	111.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Mainchain

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	219	0
2	B	8899	0	8940	126	0
3	C	2095	0	2051	46	0
4	D	1440	0	1456	11	0
5	E	1752	0	1776	14	0
6	F	705	0	731	12	0
7	G	1340	0	1357	24	0
8	H	1068	0	1040	17	0
9	I	971	0	927	21	0
10	J	532	0	542	11	0
11	K	920	0	929	21	0
12	L	363	0	386	6	0
13	N	288	0	159	1	0
14	P	300	0	166	1	0
15	T	389	0	214	1	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	A	4	0	3	0	0
19	D	15	0	17	0	0
20	G	7	0	10	0	0
All	All	32287	0	31959	469	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (469) 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)
7:G:151:ILE:CD1	7:G:151:ILE:CG1	1.75	1.58
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.40	1.02
1:A:53:LEU:HD23	1:A:54:ASN:H	1.24	1.02
1:A:1081:LEU:HB2	1:A:1082:ASN:HA	1.43	0.96
10:J:48:ARG:O	10:J:52:THR:HG22	1.67	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.32	0.92
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.51	0.91
1:A:1081:LEU:HD12	1:A:1082:ASN:HD22	1.38	0.87
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.86
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.56	0.85
1:A:56:PRO:O	1:A:57:ARG:NE	2.10	0.84
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.43	0.82
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.63	0.80
2:B:654:ARG:H	2:B:657:HIS:HD2	1.27	0.79
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.64	0.79
1:A:53:LEU:HD23	1:A:54:ASN:N	1.97	0.78
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.28	0.77
1:A:225:ASN:HD22	1:A:228:PHE:H	1.34	0.75
1:A:55:ASP:N	1:A:56:PRO:HD3	2.01	0.75
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.52	0.75
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.67	0.75
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.68	0.74
2:B:878:GLN:O	2:B:883:LEU:HD21	1.87	0.74
7:G:1:MET:SD	7:G:2:PHE:N	2.61	0.74
1:A:1079:MET:HB3	1:A:1081:LEU:HD23	1.70	0.74
7:G:111:THR:HG22	7:G:113:HIS:H	1.53	0.73
6:F:118:LEU:O	6:F:122:MET:HG3	1.88	0.73
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.70	0.73
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.06	0.73
1:A:855:THR:CG2	1:A:857:ARG:HE	2.01	0.73
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.37	0.73
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.70	0.71
1:A:40:THR:HG22	1:A:41:MET:HG2	1.70	0.71
1:A:472:LEU:O	1:A:475:THR:HB	1.91	0.71
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.56	0.71
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.71	0.71
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.71
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.70
1:A:1079:MET:HB3	1:A:1081:LEU:CD2	2.22	0.69
1:A:1081:LEU:HB2	1:A:1082:ASN:CA	2.19	0.69
9:I:4:PHE:HZ	9:I:13:MET:HE2	1.56	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:LYS:HB2	12:L:39:SER:HA	1.73	0.68
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.76	0.68
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.76	0.68
1:A:316:GLN:HG3	1:A:317:LYS:HG2	1.75	0.67
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.58	0.67
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.76	0.67
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.60	0.67
10:J:48:ARG:HE	10:J:49:MET:HE2	1.60	0.67
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.76	0.67
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.75	0.67
1:A:347:PHE:H	2:B:1107:ALA:HA	1.60	0.67
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.75	0.66
7:G:14:HIS:CD2	7:G:16:SER:H	2.13	0.66
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.77	0.66
2:B:339:THR:HG23	2:B:340:ALA:HB2	1.77	0.66
7:G:1:MET:HE1	7:G:79:PHE:CE1	2.31	0.65
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.78	0.65
3:C:252:GLN:HG2	11:K:95:ILE:HG23	1.77	0.65
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.79	0.65
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.63	0.64
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.78	0.64
1:A:709:THR:HG23	9:I:94:ASP:HA	1.79	0.64
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.62	0.64
1:A:399:HIS:O	1:A:435:HIS:HD2	1.81	0.64
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.78	0.64
14:P:7:C:H2'	14:P:8:C:O4'	1.97	0.64
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.79	0.63
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.31	0.63
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.81	0.63
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.62
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.64	0.62
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.32	0.62
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.81	0.62
2:B:706:GLN:H	2:B:710:LEU:HD13	1.65	0.62
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.80	0.62
2:B:972:LYS:HD2	2:B:1098:MET:HE3	1.82	0.61
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.68	0.61
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.82	0.61
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.82	0.61
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.99	0.61
3:C:98:VAL:H	3:C:122:SER:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:THR:HA	8:H:60:ALA:HB2	1.83	0.61
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.81	0.61
2:B:705:MET:H	2:B:710:LEU:HD22	1.65	0.61
8:H:135:LEU:C	8:H:137:GLN:H	2.09	0.61
3:C:142:VAL:H	10:J:16:ASP:HB3	1.65	0.61
1:A:306:ASN:ND2	1:A:321:PRO:O	2.34	0.61
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.83	0.61
2:B:315:LYS:HA	9:I:13:MET:HE1	1.83	0.61
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.83	0.61
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.81	0.61
1:A:450:LEU:HD23	2:B:1133:MET:HE1	1.83	0.60
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.67	0.60
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.83	0.60
2:B:310:MET:O	2:B:313:MET:HB2	2.00	0.60
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.84	0.60
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.00	0.60
1:A:316:GLN:HG3	1:A:317:LYS:H	1.67	0.59
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.84	0.59
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.34	0.59
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
2:B:883:LEU:HB3	2:B:935:ARG:H	1.68	0.59
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.84	0.59
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.50	0.59
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.36	0.59
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.83	0.59
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.84	0.58
1:A:31:SER:OG	1:A:83:HIS:HD2	1.87	0.58
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.38	0.58
1:A:41:MET:HB3	1:A:49:LYS:HA	1.84	0.58
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.01	0.58
1:A:41:MET:HG3	1:A:42:ASP:H	1.68	0.58
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.86	0.58
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.44	0.58
2:B:1222:ARG:O	2:B:1223:ASP:HB3	2.03	0.58
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.18	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.68	0.57
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.85	0.57
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.86	0.57
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.86	0.57
1:A:134:ARG:HD2	1:A:221:SER:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:OG	1:A:206:GLU:HB2	2.03	0.57
3:C:56:THR:HG22	3:C:58:LEU:H	1.69	0.57
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.27	0.57
1:A:55:ASP:OD1	1:A:57:ARG:HA	2.05	0.57
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.57
1:A:534:LEU:O	1:A:574:GLY:HA3	2.04	0.57
1:A:839:ARG:HH22	1:A:1402:PHE:HA	1.68	0.57
2:B:710:LEU:HA	2:B:733:HIS:CB	2.31	0.57
1:A:225:ASN:ND2	1:A:228:PHE:H	2.01	0.57
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.86	0.56
1:A:299:HIS:HA	1:A:302:THR:HG22	1.88	0.56
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.17	0.56
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.41	0.56
2:B:756:ILE:O	2:B:759:PRO:HD3	2.05	0.56
10:J:6:ARG:HG2	10:J:13:VAL:HG22	1.86	0.56
10:J:48:ARG:HE	10:J:49:MET:CE	2.18	0.56
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.87	0.56
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.88	0.56
1:A:332:LYS:H	1:A:337:ARG:HB2	1.70	0.56
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.87	0.56
12:L:61:THR:HB	12:L:63:ARG:H	1.71	0.56
1:A:568:PRO:HD3	8:H:95:TYR:HA	1.88	0.56
1:A:503:GLN:NE2	6:F:90:ARG:HH22	2.03	0.55
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.87	0.55
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.88	0.55
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.88	0.55
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.88	0.55
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.89	0.55
1:A:593:GLU:HB3	1:A:603:ASN:HD21	1.72	0.55
2:B:507:LYS:HD2	2:B:508:LEU:HD13	1.88	0.55
2:B:901:PRO:O	2:B:949:VAL:O	2.26	0.55
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.89	0.55
6:F:111:LEU:HD12	6:F:111:LEU:H	1.72	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.90	0.54
13:N:11:DG:H1	15:T:7:DC:H42	1.55	0.54
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.89	0.54
7:G:138:THR:HG22	7:G:139:ILE:H	1.72	0.54
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.43	0.54
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.43	0.54
1:A:907:THR:HG22	1:A:908:LEU:H	1.71	0.54
2:B:344:LYS:HG3	2:B:348:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.38	0.53
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.91	0.53
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.90	0.53
3:C:148:ARG:H	3:C:151:GLN:HB2	1.74	0.53
1:A:399:HIS:O	1:A:435:HIS:CD2	2.62	0.53
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.53
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.74	0.53
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.53
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.92	0.52
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.91	0.52
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.91	0.52
1:A:1081:LEU:CB	1:A:1082:ASN:HA	2.30	0.52
1:A:49:LYS:HG2	1:A:61:ILE:HD12	1.91	0.52
2:B:1082:MET:HA	3:C:189:THR:HA	1.91	0.52
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.92	0.52
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.75	0.52
7:G:1:MET:HE1	7:G:79:PHE:CD1	2.45	0.52
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.91	0.52
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.25	0.51
9:I:2:THR:O	9:I:3:THR:HG22	2.10	0.51
1:A:316:GLN:HG3	1:A:317:LYS:N	2.25	0.51
1:A:55:ASP:O	1:A:55:ASP:OD2	2.27	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.45	0.51
1:A:745:GLN:HA	1:A:748:MET:HE3	1.91	0.51
1:A:901:LEU:HA	1:A:907:THR:HG23	1.92	0.51
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.93	0.51
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.44	0.51
1:A:709:THR:HB	1:A:712:GLU:H	1.76	0.51
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.91	0.51
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.76	0.51
2:B:880:THR:O	2:B:883:LEU:HG	2.11	0.51
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.93	0.51
1:A:116:ASP:C	1:A:118:HIS:H	2.19	0.51
1:A:1081:LEU:HD13	1:A:1099:PRO:HD2	1.93	0.51
1:A:1172:LEU:C	1:A:1174:PHE:H	2.19	0.50
12:L:32:ALA:HB3	12:L:55:ILE:HG21	1.93	0.50
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.76	0.50
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.46	0.50
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.94	0.50
9:I:74:GLU:HB3	9:I:81:ARG:HD3	1.93	0.50
1:A:463:ILE:HD12	1:A:464:PRO:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.94	0.50
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.94	0.50
1:A:35:ILE:HA	1:A:52:GLY:O	2.12	0.50
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.44	0.50
3:C:254:LYS:HG2	11:K:42:LEU:HD13	1.92	0.50
5:E:66:GLU:HA	5:E:69:ILE:HD12	1.92	0.50
1:A:335:ARG:HH11	1:A:339:ASN:ND2	2.10	0.50
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.77	0.50
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.10	0.50
7:G:61:ILE:HG13	7:G:68:ALA:HB2	1.94	0.49
8:H:82:PRO:O	8:H:84:ALA:N	2.45	0.49
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.49
1:A:285:PRO:O	1:A:287:HIS:N	2.43	0.49
9:I:50:THR:HG22	9:I:52:ILE:H	1.77	0.49
2:B:955:THR:HB	12:L:54:ARG:O	2.12	0.49
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.95	0.49
4:D:5:THR:HG21	7:G:74:TYR:OH	2.12	0.49
9:I:8:ARG:NE	9:I:9:ASP:OD1	2.45	0.49
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.44	0.49
1:A:855:THR:HG21	1:A:857:ARG:NE	2.15	0.49
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.95	0.48
2:B:278:GLN:HB3	2:B:337:ARG:HG2	1.95	0.48
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.48
1:A:396:PRO:HG2	1:A:416:ARG:HB3	1.94	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.48	0.48
2:B:955:THR:OG1	2:B:956:THR:N	2.45	0.48
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.95	0.48
8:H:95:TYR:HE2	8:H:97:MET:HE2	1.78	0.48
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.95	0.48
1:A:55:ASP:H	1:A:56:PRO:HD3	1.77	0.48
1:A:56:PRO:CD	1:A:58:LEU:HG	2.43	0.48
1:A:343:LYS:HE3	2:B:1156:ASP:OD2	2.13	0.48
1:A:369:SER:H	11:K:2:ASN:HD21	1.62	0.48
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.28	0.48
2:B:126:SER:OG	2:B:172:ILE:HD11	2.14	0.48
4:D:185:CYS:HB3	4:D:190:GLU:HB3	1.96	0.48
1:A:1387:HIS:HA	1:A:1391:ARG:HH11	1.77	0.48
11:K:107:THR:O	11:K:111:LEU:HG	2.14	0.48
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.60	0.48
1:A:393:ARG:HH22	1:A:424:ILE:H	1.62	0.48
3:C:22:LEU:O	3:C:227:THR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:VAL:HG23	3:C:58:LEU:HD13	1.96	0.48
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.94	0.48
7:G:62:LEU:HD21	7:G:69:GLU:HB2	1.95	0.48
2:B:34:ILE:HG12	2:B:542:MET:CE	2.44	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.48
1:A:334:GLY:H	1:A:338:GLY:HA3	1.79	0.47
2:B:644:GLU:C	2:B:646:LEU:H	2.16	0.47
1:A:362:ASP:OD1	1:A:459:ARG:NH1	2.43	0.47
3:C:91:HIS:HA	3:C:95:CYS:SG	2.54	0.47
2:B:561:TRP:O	2:B:590:HIS:HE1	1.98	0.47
1:A:49:LYS:NZ	1:A:55:ASP:HB3	2.30	0.47
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.96	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.14	0.47
4:D:13:ARG:HH22	4:D:18:VAL:HA	1.80	0.47
1:A:255:SER:H	2:B:918:ILE:HD13	1.78	0.47
1:A:922:ASP:CG	1:A:925:LEU:HD12	2.39	0.47
4:D:13:ARG:HH12	4:D:18:VAL:HB	1.77	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.96	0.47
2:B:644:GLU:C	2:B:646:LEU:N	2.72	0.47
2:B:1106:ARG:HG2	2:B:1127:GLY:HA2	1.97	0.47
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.15	0.47
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.45	0.47
9:I:4:PHE:CZ	9:I:13:MET:HE2	2.44	0.47
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.46
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.97	0.46
2:B:1179:GLN:HA	4:D:1:MET:HE3	1.97	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.80	0.46
5:E:79:TRP:HE1	5:E:81:GLU:HG3	1.79	0.46
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.97	0.46
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.97	0.46
8:H:100:THR:HG23	8:H:138:GLU:HA	1.96	0.46
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.98	0.46
2:B:530:GLY:O	2:B:532:ALA:N	2.45	0.46
4:D:165:GLN:HA	4:D:168:LYS:HD2	1.97	0.46
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.97	0.46
1:A:1150:SER:HB3	9:I:46:HIS:CB	2.46	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.98	0.46
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.15	0.46
3:C:180:TYR:OH	3:C:188:HIS:HD2	1.98	0.46
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:LEU:HD22	12:L:56:LEU:HD21	1.98	0.46
1:A:1418:LEU:HD23	2:B:1222:ARG:HE	1.81	0.45
3:C:56:THR:HG22	3:C:57:VAL:N	2.31	0.45
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.80	0.45
1:A:754:SER:H	1:A:757:ASN:HD22	1.64	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.97	0.45
1:A:43:GLU:OE2	1:A:48:ALA:HB3	2.16	0.45
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.98	0.45
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.80	0.45
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.32	0.45
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.99	0.45
1:A:12:ARG:HD3	2:B:1218:THR:HB	1.98	0.45
1:A:53:LEU:CD2	1:A:54:ASN:H	2.12	0.45
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.97	0.45
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.99	0.45
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.98	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.82	0.45
1:A:883:LEU:O	1:A:886:ILE:HG22	2.17	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.98	0.45
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.98	0.45
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.99	0.45
1:A:404:TYR:CD2	1:A:412:ARG:HG2	2.51	0.45
3:C:37:MET:HA	3:C:41:ILE:HD12	1.98	0.45
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.99	0.45
4:D:66:ARG:HD2	4:D:133:THR:HB	1.97	0.45
1:A:379:VAL:HG22	1:A:431:LYS:HD3	1.99	0.45
1:A:67:CYS:H	1:A:71:GLN:HA	1.82	0.45
1:A:538:ASP:HB3	8:H:22:LYS:HG3	1.98	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	1.99	0.44
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.12	0.44
5:E:147:HIS:CD2	5:E:149:LEU:H	2.35	0.44
1:A:41:MET:HA	1:A:50:ILE:HB	1.99	0.44
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.16	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.44
2:B:912:ILE:HB	2:B:939:THR:HB	1.97	0.44
5:E:50:MET:SD	5:E:51:GLY:N	2.90	0.44
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.53	0.44
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.00	0.44
2:B:294:ASP:H	9:I:12:ASN:HD22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.99	0.44
1:A:672:ASP:HB3	1:A:674:PRO:HD2	1.99	0.44
9:I:16:PRO:HB3	9:I:25:LEU:HD11	2.00	0.44
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.23	0.44
2:B:345:LYS:HA	2:B:349:ILE:HD13	1.99	0.44
2:B:1177:HIS:HB3	2:B:1179:GLN:NE2	2.32	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.44
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.83	0.44
2:B:844:SER:O	2:B:847:ASP:HB2	2.17	0.44
2:B:889:THR:HG22	2:B:891:ASP:H	1.83	0.44
9:I:78:CYS:SG	9:I:80:SER:HB3	2.58	0.44
1:A:1243:VAL:HG22	1:A:1244:ARG:H	1.83	0.44
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.83	0.44
1:A:123:ARG:HA	1:A:126:LEU:HD12	2.00	0.43
2:B:765:PRO:O	2:B:769:TYR:HD1	2.00	0.43
7:G:60:ARG:NH2	7:G:63:PRO:HD3	2.33	0.43
9:I:45:ARG:NH1	9:I:47:GLU:OE1	2.51	0.43
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.53	0.43
2:B:833:TYR:HB3	2:B:992:ILE:CG2	2.48	0.43
4:D:54:GLU:CD	4:D:164:ILE:HD11	2.43	0.43
7:G:93:SER:OG	7:G:100:GLU:HB2	2.18	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.01	0.43
2:B:361:LEU:HB3	2:B:364:ILE:HD12	2.00	0.43
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.98	0.43
3:C:89:GLU:O	3:C:90:ASP:HB3	2.18	0.43
3:C:184:ASN:ND2	3:C:189:THR:O	2.51	0.43
1:A:107:CYS:C	1:A:109:HIS:H	2.27	0.43
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.84	0.43
1:A:744:LYS:HG2	1:A:748:MET:HE2	2.00	0.43
1:A:795:GLU:HG2	2:B:731:VAL:HG11	2.00	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HD12	2.01	0.43
1:A:67:CYS:C	1:A:69:THR:H	2.27	0.43
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.43
1:A:626:ASN:O	1:A:631:HIS:ND1	2.51	0.43
1:A:811:GLN:H	1:A:811:GLN:NE2	2.17	0.43
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.53	0.43
9:I:87:GLN:HE22	9:I:97:MET:HG2	1.84	0.43
1:A:41:MET:HB3	1:A:41:MET:HE2	1.88	0.43
2:B:493:SER:HB3	2:B:775:LYS:HE2	2.00	0.43
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.84	0.43
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:LYS:HE3	11:K:38:GLU:HG2	2.01	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.52	0.42
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.42
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.00	0.42
1:A:55:ASP:OD1	1:A:57:ARG:CA	2.67	0.42
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.00	0.42
5:E:118:PRO:HA	5:E:121:MET:HB2	2.00	0.42
1:A:923:LEU:O	1:A:927:VAL:HG23	2.19	0.42
2:B:46:GLN:H	2:B:46:GLN:HG3	1.62	0.42
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.83	0.42
7:G:19:GLY:O	7:G:22:MET:HB2	2.19	0.42
1:A:51:GLY:O	1:A:56:PRO:HB3	2.19	0.42
1:A:93:VAL:HG13	1:A:301:ALA:CB	2.50	0.42
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.02	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.02	0.42
1:A:70:CYS:SG	1:A:72:GLU:HB2	2.59	0.42
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.52	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.59	0.42
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.47	0.42
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.01	0.42
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.01	0.42
1:A:768:GLN:HG2	1:A:816:HIS:HA	2.01	0.42
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.01	0.42
3:C:99:LEU:HA	3:C:119:VAL:O	2.20	0.42
11:K:49:GLU:HG3	11:K:94:ILE:HG13	2.01	0.42
1:A:1081:LEU:HD12	1:A:1082:ASN:ND2	2.20	0.42
1:A:1095:THR:HG23	1:A:1113:THR:HG23	2.02	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
7:G:91:VAL:HG23	7:G:143:ILE:HD13	2.02	0.42
7:G:154:VAL:HG23	7:G:155:SER:H	1.83	0.42
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.34	0.41
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.20	0.41
1:A:517:ASN:HD22	1:A:1364:ASN:ND2	2.18	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
1:A:42:ASP:O	1:A:44:THR:N	2.53	0.41
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.20	0.41
1:A:472:LEU:HD21	2:B:835:GLN:HB3	2.01	0.41
1:A:768:GLN:CG	1:A:816:HIS:HA	2.50	0.41
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.50	0.41
2:B:506:GLY:HA3	2:B:507:LYS:HA	1.80	0.41
2:B:745:PRO:O	2:B:748:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:OE1	4:D:14:ARG:NH2	2.53	0.41
1:A:571:LEU:HD12	8:H:46:LEU:HD11	2.02	0.41
1:A:1081:LEU:HD21	1:A:1098:VAL:HG23	2.02	0.41
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.34	0.41
1:A:151:ASP:HA	1:A:163:SER:HA	2.02	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.51	0.41
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	2.02	0.41
2:B:567:GLU:H	2:B:567:GLU:CD	2.27	0.41
3:C:6:PRO:HB2	11:K:101:LEU:HD13	2.01	0.41
1:A:37:PHE:CD1	1:A:52:GLY:CA	3.03	0.41
1:A:353:ILE:HD12	1:A:482:PHE:HD2	1.86	0.41
1:A:998:LEU:HD23	1:A:1001:ARG:HG3	2.01	0.41
1:A:1150:SER:HB3	9:I:46:HIS:HB3	2.02	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:1098:MET:HE2	2:B:1098:MET:HB2	1.82	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	2.02	0.41
6:F:109:VAL:HG21	6:F:124:GLU:HA	2.02	0.41
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.86	0.41
11:K:49:GLU:HG3	11:K:94:ILE:HG12	2.02	0.41
1:A:282:ASN:O	1:A:284:ALA:N	2.52	0.41
1:A:598:LEU:HD13	8:H:124:ARG:HB2	2.03	0.41
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.54	0.41
2:B:30:SER:O	2:B:34:ILE:HG13	2.20	0.41
2:B:1175:LEU:HG	2:B:1175:LEU:O	2.21	0.41
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.02	0.41
1:A:453:MET:HE1	1:A:514:PRO:HD2	2.03	0.41
2:B:68:THR:HG23	2:B:91:SER:HB3	2.03	0.41
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.51	0.41
2:B:1097:HIS:CD2	2:B:1097:HIS:N	2.88	0.41
8:H:114:VAL:HG21	8:H:134:ASN:HD22	1.85	0.41
8:H:130:ARG:H	8:H:130:ARG:HG3	1.54	0.41
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.86	0.41
1:A:774:ARG:H	1:A:774:ARG:HG2	1.60	0.41
1:A:1436:ILE:O	1:A:1437:GLY:C	2.63	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.55	0.41
5:E:156:LEU:HD21	5:E:197:LYS:HB2	2.03	0.41
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.28	0.40
2:B:398:ARG:HH11	2:B:398:ARG:HB2	1.86	0.40
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.40
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.35	0.40
3:C:46:ILE:HA	3:C:159:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.21	0.40
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.54	0.40
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.19	0.40
1:A:1116:LEU:H	1:A:1308:THR:HB	1.85	0.40
2:B:473:MET:HA	2:B:474:SER:HA	1.71	0.40
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.03	0.40
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.50	0.40
11:K:21:ILE:HD13	11:K:84:LYS:HG2	2.03	0.40
1:A:857:ARG:HD3	1:A:861:GLY:O	2.22	0.40
1:A:1243:VAL:HG13	1:A:1244:ARG:H	1.85	0.40
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.91	0.40
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.46	0.40
2:B:343:ILE:HA	2:B:344:LYS:HA	1.91	0.40
2:B:662:MET:HA	2:B:665:GLU:HB2	2.03	0.40
2:B:1138:MET:HB3	2:B:1147:LEU:HG	2.04	0.40
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.57	0.40
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1411/1733 (81%)	1279 (91%)	94 (7%)	38 (3%)	4	22
2	B	1107/1224 (90%)	997 (90%)	74 (7%)	36 (3%)	3	19
3	C	264/318 (83%)	235 (89%)	23 (9%)	6 (2%)	5	25
4	D	176/221 (80%)	157 (89%)	15 (8%)	4 (2%)	5	25
5	E	212/215 (99%)	201 (95%)	9 (4%)	2 (1%)	14	43
6	F	85/155 (55%)	78 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	157 (93%)	7 (4%)	5 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	129/146 (88%)	105 (81%)	10 (8%)	14 (11%)	0	2
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	23
10	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	3	19
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0	0
All	All	3890/4565 (85%)	3501 (90%)	271 (7%)	118 (3%)	3	20

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG
1	A	74	MET
1	A	169	ASN
1	A	286	HIS
1	A	593	GLU
1	A	1243	VAL
1	A	1403	GLU
1	A	1405	THR
2	B	245	GLU
2	B	368	GLU
2	B	509	ALA
2	B	531	GLN
2	B	643	ASP
2	B	879	ARG
2	B	1046	PRO
2	B	1066	SER
2	B	1176	ASN
3	C	91	HIS
4	D	13	ARG
4	D	119	ARG
7	G	139	ILE
7	G	154	VAL
8	H	83	GLN
8	H	84	ALA
8	H	88	SER
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	38	LEU
12	L	39	SER
12	L	50	ASP
12	L	56	LEU
12	L	59	ALA
12	L	60	ARG
1	A	76	GLU
1	A	251	SER
1	A	257	ARG
1	A	283	GLY
1	A	335	ARG
1	A	775	ILE
1	A	1081	LEU
2	B	67	SER
2	B	229	ALA
2	B	277	LYS
2	B	364	ILE
2	B	629	ASP
2	B	712	PRO
2	B	731	VAL
2	B	907	GLY
2	B	958	GLN
2	B	1157	ALA
2	B	1181	GLU
2	B	1223	ASP
3	C	141	GLY
4	D	199	ASN
7	G	63	PRO
8	H	17	PRO
8	H	18	GLY
8	H	85	GLY
8	H	128	ASN
8	H	136	LYS
12	L	45	ALA
1	A	5	GLN
1	A	108	MET
1	A	156	ASP
1	A	321	PRO
1	A	399	HIS
1	A	846	GLU
1	A	1092	LYS
1	A	1377	THR

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Mol	Chain	Res	Type
1	A	1437	GLY
2	B	341	LEU
2	B	369	GLY
2	B	707	PRO
2	B	880	THR
2	B	1185	CYS
2	B	1222	ARG
7	G	2	PHE
8	H	52	GLN
8	H	60	ALA
9	I	10	CYS
9	I	95	THR
1	A	35	ILE
1	A	41	MET
1	A	47	ARG
1	A	1378	GLN
2	B	711	GLU
3	C	142	VAL
4	D	15	LEU
7	G	67	SER
8	H	108	SER
8	H	140	ALA
9	I	3	THR
12	L	26	THR
1	A	322	VAL
1	A	958	VAL
2	B	266	ALA
2	B	339	THR
2	B	526	GLU
2	B	1108	ARG
3	C	90	ASP
5	E	48	ASP
5	E	51	GLY
8	H	107	VAL
10	J	17	LYS
1	A	196	GLU
1	A	334	GLY
3	C	214	ASN
2	B	295	GLY
8	H	82	PRO
1	A	567	LYS
1	A	599	SER

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Mol	Chain	Res	Type
2	B	503	GLY
2	B	1017	ILE
2	B	751	VAL
3	C	240	VAL

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	1244/1520 (82%)	1060 (85%)	184 (15%)	3	13
2	B	969/1061 (91%)	812 (84%)	157 (16%)	2	11
3	C	234/274 (85%)	201 (86%)	33 (14%)	3	14
4	D	160/200 (80%)	132 (82%)	28 (18%)	2	9
5	E	196/197 (100%)	181 (92%)	15 (8%)	12	37
6	F	77/137 (56%)	64 (83%)	13 (17%)	2	10
7	G	152/152 (100%)	127 (84%)	25 (16%)	2	11
8	H	117/128 (91%)	104 (89%)	13 (11%)	6	22
9	I	113/116 (97%)	100 (88%)	13 (12%)	5	21
10	J	60/65 (92%)	51 (85%)	9 (15%)	3	13
11	K	99/102 (97%)	85 (86%)	14 (14%)	3	14
12	L	40/57 (70%)	31 (78%)	9 (22%)	1	5
All	All	3461/4009 (86%)	2948 (85%)	513 (15%)	3	13

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	28	ARG
1	A	30	ILE
1	A	34	LYS
1	A	40	THR
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	49	LYS
1	A	60	SER
1	A	64	ASN
1	A	65	LEU
1	A	66	LYS
1	A	74	MET
1	A	90	VAL
1	A	93	VAL
1	A	113	LEU
1	A	116	ASP
1	A	117	GLU
1	A	131	SER
1	A	145	LYS
1	A	150	THR
1	A	152	VAL
1	A	157	ASP
1	A	164	ARG
1	A	174	ILE
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	210	ILE
1	A	249	SER
1	A	250	ILE
1	A	265	LYS
1	A	274	ILE
1	A	277	GLU
1	A	279	LEU
1	A	280	GLU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	317	LYS
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	324	SER
1	A	336	ILE
1	A	344	ARG
1	A	353	ILE
1	A	369	SER

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Mol	Chain	Res	Type
1	A	385	ILE
1	A	389	THR
1	A	393	ARG
1	A	406	ILE
1	A	408	ASP
1	A	412	ARG
1	A	423	ASP
1	A	424	ILE
1	A	431	LYS
1	A	433	GLU
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	500	GLU
1	A	505	CYS
1	A	523	ILE
1	A	541	ILE
1	A	549	MET
1	A	557	ASP
1	A	584	ASN
1	A	588	LEU
1	A	595	THR
1	A	597	LEU
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	629	LEU

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Mol	Chain	Res	Type
1	A	634	THR
1	A	652	VAL
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	719	VAL
1	A	735	VAL
1	A	740	LEU
1	A	768	GLN
1	A	773	LYS
1	A	788	SER
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	830	LYS
1	A	848	ILE
1	A	855	THR
1	A	856	THR
1	A	858	ASN
1	A	878	ILE
1	A	882	SER
1	A	896	ARG
1	A	901	LEU
1	A	905	ASP
1	A	915	SER
1	A	919	ILE
1	A	924	LYS
1	A	929	LEU
1	A	948	VAL
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	987	VAL
1	A	988	LEU
1	A	1000	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1035	TYR
1	A	1047	SER
1	A	1052	GLN
1	A	1058	VAL
1	A	1064	VAL

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Mol	Chain	Res	Type
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	1118	VAL
1	A	1133	LEU
1	A	1159	ARG
1	A	1168	GLU
1	A	1170	ILE
1	A	1176	LEU
1	A	1206	ASP
1	A	1208	THR
1	A	1211	GLN
1	A	1227	ILE
1	A	1237	ILE
1	A	1242	VAL
1	A	1244	ARG
1	A	1256	GLU
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1267	MET
1	A	1273	LEU
1	A	1295	THR
1	A	1297	GLU
1	A	1314	SER
1	A	1315	GLU
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1355	VAL
1	A	1356	ILE
1	A	1359	ASP
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1420	ASP
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1448	GLU
1	A	1451	VAL
2	B	22	SER
2	B	25	ILE
2	B	26	THR
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	66	ASP
2	B	90	ILE
2	B	95	ILE
2	B	101	MET
2	B	103	ASN
2	B	118	ARG
2	B	128	LEU
2	B	131	ASP
2	B	134	LYS
2	B	167	ILE
2	B	185	THR
2	B	205	ILE
2	B	211	VAL
2	B	217	ARG
2	B	222	ILE
2	B	228	LYS
2	B	240	ILE
2	B	249	ARG
2	B	251	ILE
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	265	SER
2	B	272	THR
2	B	298	LEU

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Mol	Chain	Res	Type
2	B	305	VAL
2	B	313	MET
2	B	319	GLU
2	B	323	VAL
2	B	334	ILE
2	B	337	ARG
2	B	339	THR
2	B	344	LYS
2	B	364	ILE
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	398	ARG
2	B	416	LEU
2	B	469	GLN
2	B	470	LYS
2	B	471	LYS
2	B	480	SER
2	B	485	ARG
2	B	493	SER
2	B	498	THR
2	B	502	ILE
2	B	505	ASP
2	B	507	LYS
2	B	508	LEU
2	B	510	LYS
2	B	529	GLU
2	B	542	MET
2	B	544	CYS
2	B	547	VAL
2	B	552	MET
2	B	560	GLU
2	B	563	MET
2	B	567	GLU
2	B	568	ASP
2	B	570	VAL
2	B	573	GLN
2	B	580	VAL
2	B	589	VAL
2	B	598	GLU
2	B	601	ARG
2	B	603	LEU

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Mol	Chain	Res	Type
2	B	604	ARG
2	B	606	LYS
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	624	LEU
2	B	628	THR
2	B	642	ASP
2	B	653	VAL
2	B	658	ILE
2	B	665	GLU
2	B	678	GLU
2	B	680	THR
2	B	682	SER
2	B	687	GLU
2	B	690	VAL
2	B	699	GLU
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	737	THR
2	B	780	VAL
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	795	ILE
2	B	831	SER
2	B	870	ILE
2	B	871	THR
2	B	876	LYS
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	899	ILE
2	B	904	ARG
2	B	908	GLU
2	B	914	LYS
2	B	915	THR

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Mol	Chain	Res	Type
2	B	942	ARG
2	B	948	ILE
2	B	955	THR
2	B	958	GLN
2	B	961	LEU
2	B	964	VAL
2	B	970	THR
2	B	976	ILE
2	B	979	LYS
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1041	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1070	GLU
2	B	1076	HIS
2	B	1098	MET
2	B	1106	ARG
2	B	1123	SER
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1175	LEU
2	B	1183	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1224	PHE
3	C	3	GLU

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Mol	Chain	Res	Type
3	C	7	GLN
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	40	GLU
3	C	52	GLU
3	C	79	GLN
3	C	83	SER
3	C	90	ASP
3	C	100	THR
3	C	115	SER
3	C	116	LYS
3	C	121	VAL
3	C	122	SER
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	149	LYS
3	C	154	LYS
3	C	155	LEU
3	C	156	THR
3	C	188	HIS
3	C	215	GLU
3	C	222	LYS
3	C	226	ASP
3	C	238	ILE
3	C	240	VAL
3	C	260	LEU
3	C	262	LEU
3	C	265	MET
3	C	268	ASP
4	D	1	MET
4	D	5	THR
4	D	6	SER
4	D	8	PHE
4	D	9	GLN
4	D	12	ARG
4	D	14	ARG
4	D	15	LEU
4	D	21	GLU
4	D	32	GLU

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Mol	Chain	Res	Type
4	D	39	ASN
4	D	47	LEU
4	D	53	SER
4	D	60	LYS
4	D	65	GLU
4	D	74	GLN
4	D	121	LYS
4	D	123	LEU
4	D	134	THR
4	D	150	ASN
4	D	153	ARG
4	D	158	GLU
4	D	164	ILE
4	D	197	SER
4	D	203	SER
4	D	206	GLU
4	D	213	GLU
4	D	221	TYR
5	E	9	ILE
5	E	30	ILE
5	E	57	MET
5	E	67	GLU
5	E	78	LEU
5	E	81	GLU
5	E	84	ASP
5	E	100	ILE
5	E	107	THR
5	E	127	ILE
5	E	154	ILE
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	196	VAL
6	F	69	LEU
6	F	70	LYS
6	F	71	GLU
6	F	72	LYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	90	ARG
6	F	93	ILE

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Mol	Chain	Res	Type
6	F	102	SER
6	F	103	MET
6	F	109	VAL
6	F	111	LEU
7	G	2	PHE
7	G	5	LYS
7	G	11	ILE
7	G	22	MET
7	G	23	LYS
7	G	24	GLN
7	G	28	THR
7	G	34	VAL
7	G	56	ILE
7	G	60	ARG
7	G	61	ILE
7	G	75	ARG
7	G	80	LYS
7	G	100	GLU
7	G	118	ASP
7	G	133	SER
7	G	134	GLU
7	G	138	THR
7	G	139	ILE
7	G	143	ILE
7	G	145	VAL
7	G	146	LYS
7	G	151	ILE
7	G	162	SER
7	G	171	ILE
8	H	8	ASP
8	H	11	GLN
8	H	19	ARG
8	H	23	VAL
8	H	26	ILE
8	H	32	THR
8	H	53	ASP
8	H	54	SER
8	H	77	ARG
8	H	103	LYS
8	H	107	VAL
8	H	112	ILE
8	H	130	ARG

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Mol	Chain	Res	Type
9	I	2	THR
9	I	8	ARG
9	I	10	CYS
9	I	31	THR
9	I	35	VAL
9	I	40	SER
9	I	58	VAL
9	I	74	GLU
9	I	81	ARG
9	I	84	VAL
9	I	90	GLN
9	I	106	CYS
9	I	117	LYS
10	J	1	MET
10	J	3	VAL
10	J	12	LYS
10	J	20	SER
10	J	38	ARG
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	1	MET
11	K	6	ARG
11	K	18	LYS
11	K	25	THR
11	K	31	VAL
11	K	33	ILE
11	K	34	THR
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	63	VAL
11	K	103	THR
11	K	113	THR
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	53	HIS
12	L	54	ARG
12	L	64	LEU
12	L	65	VAL

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Mol	Chain	Res	Type
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 (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	5	GLN
1	A	18	GLN
1	A	64	ASN
1	A	83	HIS
1	A	118	HIS
1	A	225	ASN
1	A	253	ASN
1	A	311	GLN
1	A	339	ASN
1	A	425	GLN
1	A	427	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	490	HIS
1	A	503	GLN
1	A	517	ASN
1	A	548	ASN
1	A	611	GLN
1	A	626	ASN
1	A	631	HIS
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	757	ASN
1	A	768	GLN
1	A	811	GLN
1	A	858	ASN
1	A	926	GLN
1	A	975	HIS
1	A	994	GLN
1	A	1082	ASN
1	A	1128	GLN
1	A	1140	HIS

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Mol	Chain	Res	Type
1	A	1354	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	53	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	325	GLN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	499	ASN
2	B	518	HIS
2	B	590	HIS
2	B	657	HIS
2	B	686	ASN
2	B	744	HIS
2	B	767	ASN
2	B	776	GLN
2	B	786	ASN
2	B	1013	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1084	GLN
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1176	ASN
2	B	1177	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	79	GLN
3	C	102	GLN
3	C	112	ASN
3	C	131	HIS
3	C	188	HIS
3	C	267	GLN
4	D	28	GLN
4	D	37	GLN
4	D	41	GLN

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Mol	Chain	Res	Type
4	D	150	ASN
4	D	179	GLN
4	D	216	ASN
5	E	32	GLN
5	E	115	ASN
5	E	147	HIS
6	F	104	ASN
7	G	10	ASN
7	G	14	HIS
7	G	57	GLN
7	G	97	HIS
7	G	122	ASN
7	G	153	GLN
8	H	11	GLN
8	H	33	GLN
8	H	35	GLN
8	H	137	GLN
9	I	12	ASN
9	I	114	GLN
11	K	2	ASN
11	K	29	ASN
11	K	65	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	15/15 (100%)	7 (46%)	2 (13%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	6	C
14	P	7	C
14	P	8	C
14	P	16	C
14	P	17	C
14	P	18	C
14	P	19	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	5	C
14	P	16	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	15,14	18,21,22	0.77	0	25,30,33	2.22	7 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	15,14	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	5.24	119.37	113.34
15	T	22	BRU	C4-N3-C2	-5.13	120.61	127.34
15	T	22	BRU	O4-C4-C5	-4.42	120.16	125.80
15	T	22	BRU	N3-C2-N1	4.33	120.53	114.89
15	T	22	BRU	BR-C5-C4	2.96	121.43	118.02
15	T	22	BRU	O4'-C1'-N1	2.13	111.65	107.86
15	T	22	BRU	C6-C5-C4	-2.06	118.58	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	PEG	G	172	-	6,6,6	0.50	0	5,5,5	0.31	0
18	ACT	A	1734	-	3,3,3	0.80	0	3,3,3	1.33	0
19	EPE	D	222	-	15,15,15	0.65	0	19,20,20	1.90	7 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PEG	G	172	-	-	2/4/4/4	-
19	EPE	D	222	-	-	3/9/19/19	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	222	EPE	C5-N4-C3	4.53	118.60	108.84
19	D	222	EPE	C7-N4-C5	2.86	118.87	111.24
19	D	222	EPE	O2S-S-C10	2.63	110.69	106.73
19	D	222	EPE	C7-N4-C3	2.50	117.89	111.24
19	D	222	EPE	C6-C5-N4	2.30	115.29	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	222	EPE	C9-N1-C6	-2.27	105.18	111.24
19	D	222	EPE	C2-C3-N4	2.10	114.88	110.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	222	EPE	C10-C9-N1-C2
19	D	222	EPE	C10-C9-N1-C6
19	D	222	EPE	C8-C7-N4-C5
20	G	172	PEG	C4-C3-O2-C2
20	G	172	PEG	O1-C1-C2-O2

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	1421/1733 (81%)	-0.27	21 (1%) 72 53	66, 108, 173, 229	0
2	B	1121/1224 (91%)	-0.07	43 (3%) 44 30	68, 119, 185, 221	0
3	C	266/318 (83%)	-0.43	0 100 100	81, 108, 153, 188	0
4	D	180/221 (81%)	-0.01	11 (6%) 27 18	90, 120, 172, 195	0
5	E	214/215 (99%)	-0.25	2 (0%) 81 65	87, 146, 197, 206	0
6	F	87/155 (56%)	-0.44	2 (2%) 61 42	71, 90, 127, 136	0
7	G	171/171 (100%)	-0.30	2 (1%) 76 58	83, 107, 150, 175	0
8	H	133/146 (91%)	0.21	5 (3%) 44 30	111, 154, 193, 214	0
9	I	119/122 (97%)	0.15	8 (6%) 24 16	118, 148, 190, 209	0
10	J	65/70 (92%)	-0.50	1 (1%) 72 53	90, 107, 150, 161	0
11	K	115/120 (95%)	-0.55	1 (0%) 81 65	75, 108, 144, 161	0
12	L	46/70 (65%)	1.07	7 (15%) 5 5	89, 181, 199, 204	0
13	N	14/14 (100%)	0.44	1 (7%) 22 15	203, 228, 278, 279	0
14	P	15/15 (100%)	0.33	2 (13%) 7 6	151, 172, 214, 227	0
15	T	18/27 (66%)	0.43	1 (5%) 30 20	133, 199, 284, 287	0
All	All	3985/4621 (86%)	-0.18	107 (2%) 56 37	66, 115, 186, 287	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1086	PHE	10.3
12	L	25	ALA	8.1
2	B	508	LEU	7.5
12	L	27	LEU	7.3
2	B	882	THR	6.6
2	B	446	LEU	6.0
4	D	24	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
8	H	63	LEU	5.6
2	B	708	GLU	5.5
1	A	65	LEU	5.3
1	A	186	LYS	5.2
12	L	26	THR	5.1
4	D	3	VAL	5.0
2	B	70	ILE	5.0
1	A	1176	LEU	4.7
4	D	1	MET	4.6
4	D	2	ASN	4.6
2	B	251	ILE	4.4
2	B	509	ALA	4.4
1	A	1093	LYS	4.4
2	B	709	ASP	4.3
15	T	23	DT	4.2
6	F	69	LEU	4.0
1	A	1084	PHE	4.0
8	H	90	ALA	3.9
8	H	132	LEU	3.9
4	D	76	LYS	3.8
9	I	50	THR	3.7
2	B	134	LYS	3.6
1	A	1254	ALA	3.6
2	B	715	ALA	3.6
11	K	114	LEU	3.5
2	B	934	LYS	3.5
12	L	46	VAL	3.4
2	B	507	LYS	3.4
1	A	1083	THR	3.4
2	B	436	VAL	3.3
2	B	164	LYS	3.3
13	N	0	DA	3.3
4	D	25	ALA	3.2
1	A	1187	GLN	3.2
10	J	65	PRO	3.1
1	A	251	SER	3.1
8	H	139	ASN	3.1
2	B	919	SER	3.0
2	B	29	ASP	3.0
1	A	1085	HIS	3.0
12	L	28	LYS	3.0
4	D	8	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
9	I	118	ARG	3.0
5	E	91	LYS	2.9
8	H	136	LYS	2.9
4	D	18	VAL	2.9
9	I	52	ILE	2.9
9	I	120	GLN	2.9
2	B	506	GLY	2.9
2	B	473	MET	2.9
1	A	252	PHE	2.8
2	B	710	LEU	2.7
1	A	56	PRO	2.7
1	A	51	GLY	2.6
1	A	333	GLU	2.6
12	L	49	LYS	2.6
9	I	47	GLU	2.6
2	B	246	LYS	2.6
9	I	117	LYS	2.5
1	A	1173	HIS	2.5
2	B	250	PHE	2.5
9	I	2	THR	2.5
2	B	504	ARG	2.5
2	B	476	ARG	2.4
2	B	712	PRO	2.4
2	B	108	VAL	2.4
2	B	918	ILE	2.4
7	G	64	THR	2.4
2	B	503	GLY	2.4
2	B	881	ASN	2.4
2	B	878	GLN	2.4
2	B	887	HIS	2.3
1	A	1081	LEU	2.3
1	A	1244	ARG	2.3
4	D	221	TYR	2.3
7	G	117	GLN	2.3
9	I	119	THR	2.3
1	A	771	GLU	2.3
2	B	229	ALA	2.3
2	B	341	LEU	2.3
2	B	884	ARG	2.3
5	E	110	PHE	2.2
2	B	343	ILE	2.2
2	B	437	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	2.2
4	D	118	THR	2.2
12	L	37	LYS	2.2
2	B	447	ALA	2.2
4	D	10	THR	2.1
6	F	155	LEU	2.1
14	P	5	C	2.1
2	B	1222	ARG	2.1
2	B	231	PRO	2.1
2	B	883	LEU	2.1
1	A	593	GLU	2.1
2	B	90	ILE	2.0
2	B	241	ARG	2.0
14	P	16	C	2.0
2	B	30	SER	2.0
2	B	505	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	BRU	T	22	20/21	0.92	0.09	110,169,284,288	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	ACT	A	1734	4/4	0.93	0.20	67,89,129,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	PEG	G	172	7/7	0.96	0.15	74,118,300,300	0
19	EPE	D	222	15/15	0.97	0.07	53,72,130,170	0
16	ZN	L	1071	1/1	0.98	0.06	225,225,225,225	0
16	ZN	I	1121	1/1	1.00	0.01	124,124,124,124	0
16	ZN	I	1122	1/1	1.00	0.02	199,199,199,199	0
16	ZN	J	1066	1/1	1.00	0.02	105,105,105,105	0
16	ZN	A	2456	1/1	1.00	0.02	156,156,156,156	0
17	MG	A	2458	1/1	1.00	0.04	78,78,78,78	0
16	ZN	A	2457	1/1	1.00	0.01	94,94,94,94	0
16	ZN	B	2225	1/1	1.00	0.03	99,99,99,99	0
16	ZN	C	1269	1/1	1.00	0.01	93,93,93,93	0

6.5 Other polymers

There are no such residues in this entry.