



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:36 PM UTC

PDB ID : 3PO3 / pdb_00003po3
Title : Arrested RNA Polymerase II reactivation intermediate
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

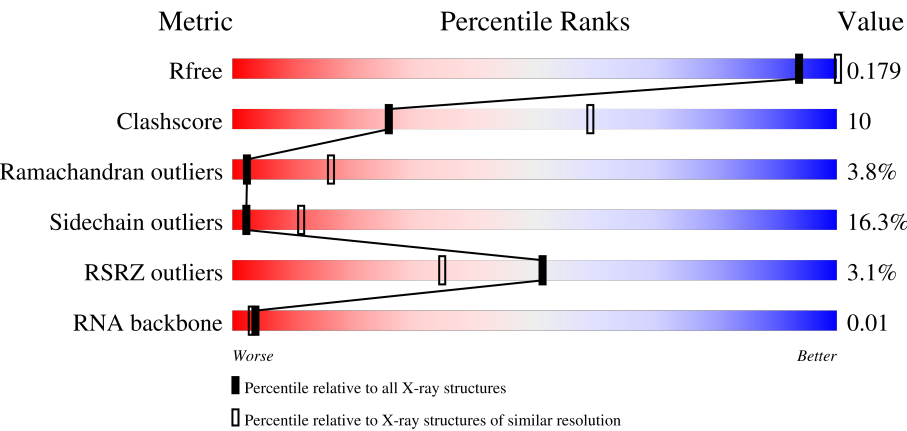
1 Overall quality at a glance i

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.



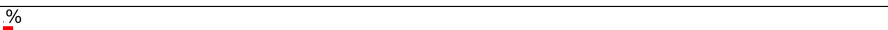
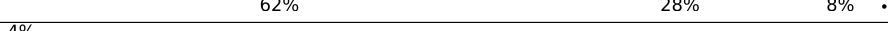
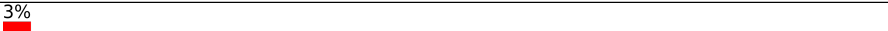
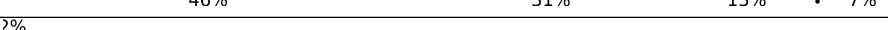
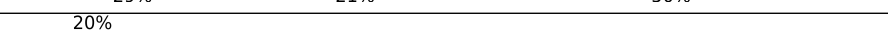
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (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	52%22%7%18% 4%
2	B	1224	61%24%5%9% 4%
3	C	318	49%28%6%16%
4	D	221	48%24%8%20% 5%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	5	
15	S	178	
16	T	27	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 33008 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	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	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	177	Total	C	N	O	S	0	0	0
			1417	876	252	287	2			

- 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	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

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

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit 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	114	Total	C	N	O	S	0	0	0
			919	590	156	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
			364	224	72	64	4			

- Molecule 13 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			144	69	30	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	5	Total	C	N	O	P	0	0	0
			100	45	15	35	5			

- Molecule 15 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	164	Total	C	N	O	S	0	0	0
			1294	809	230	247	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	290	ALA	ASP	engineered mutation	UNP P07273
S	291	ALA	GLU	engineered mutation	UNP P07273

- Molecule 16 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	T	13	Total	Br	C	N	O	P	0	0	0
			266	1	126	44	82	13			

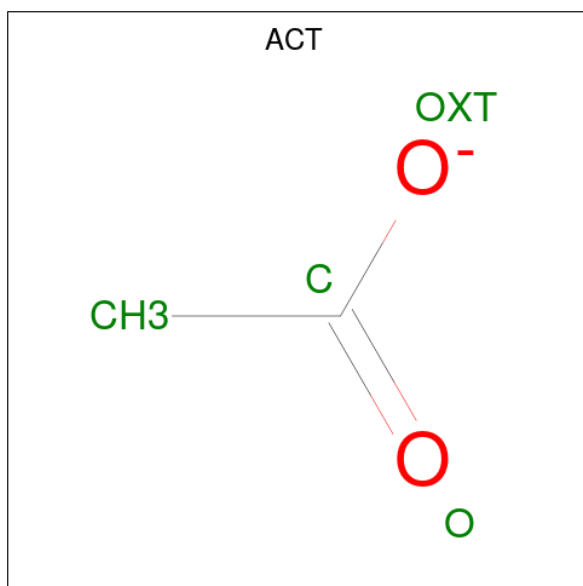
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

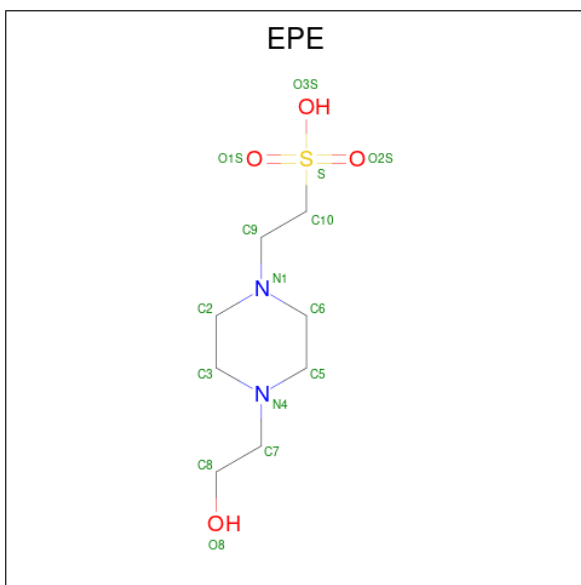
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Mg	0	0
			1	1		

- Molecule 19 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



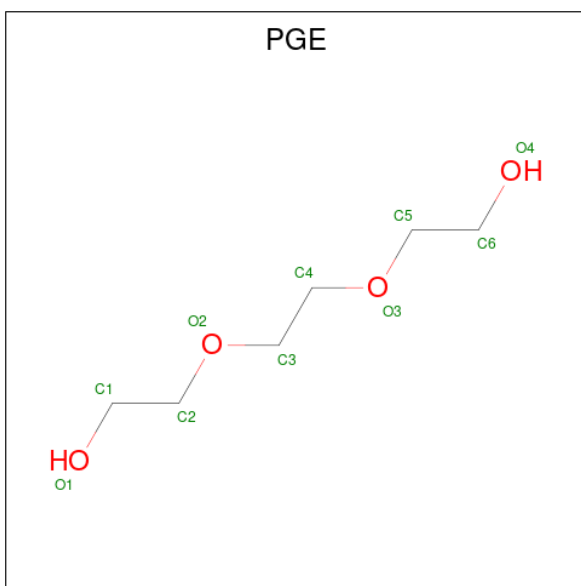
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			4	2	2		
19	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 21 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

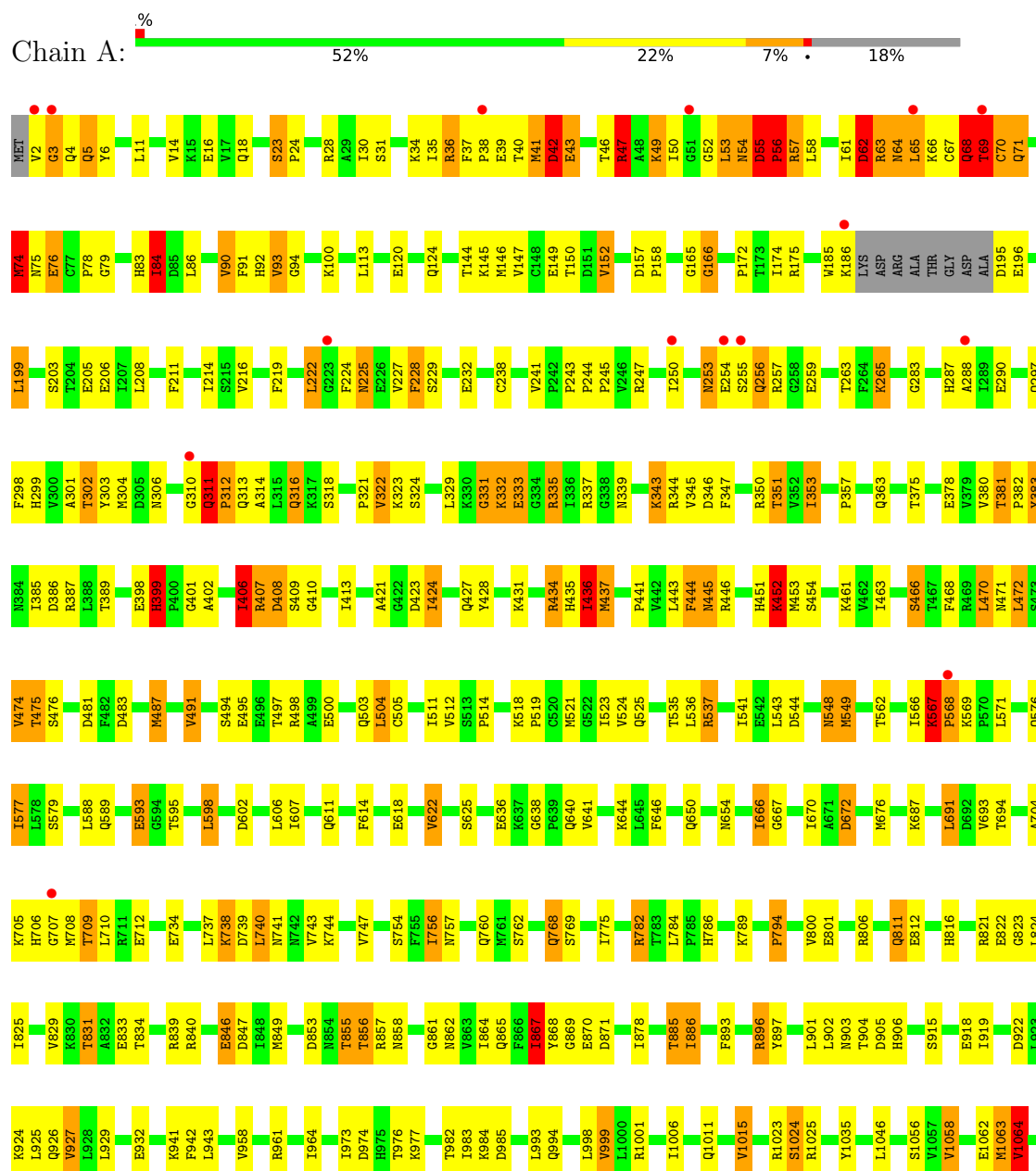


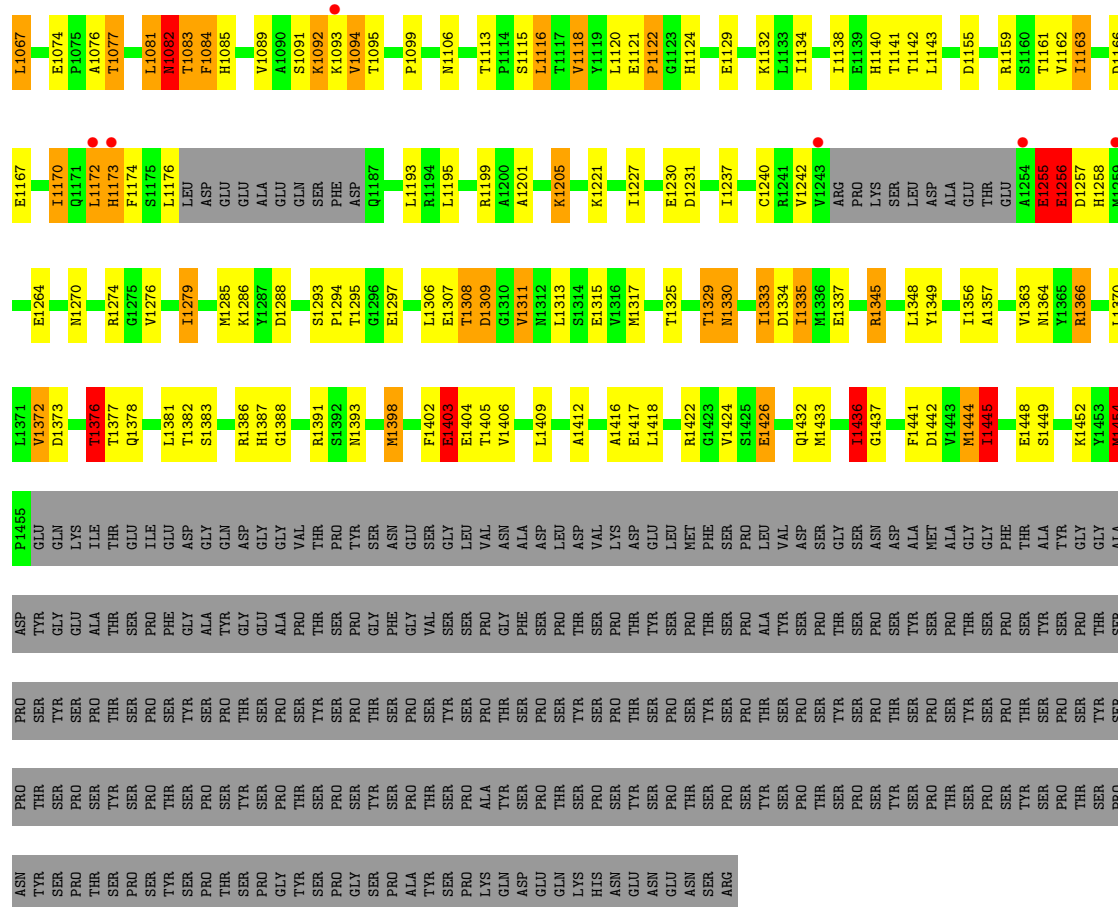
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			10	6	4		

3 Residue-property plots

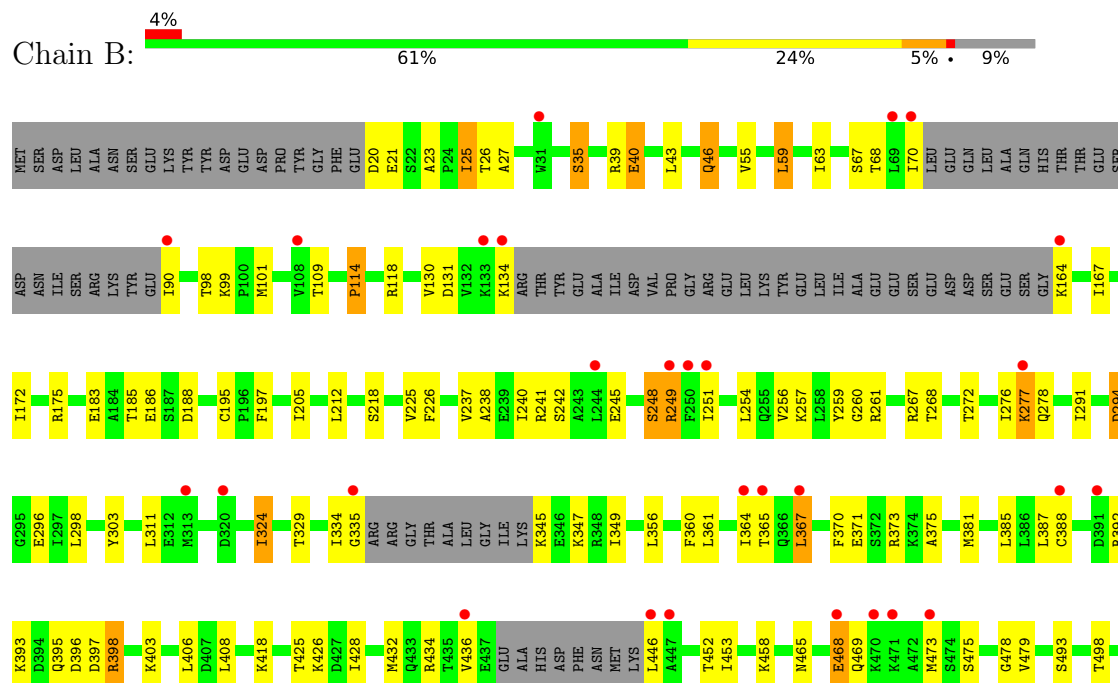
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

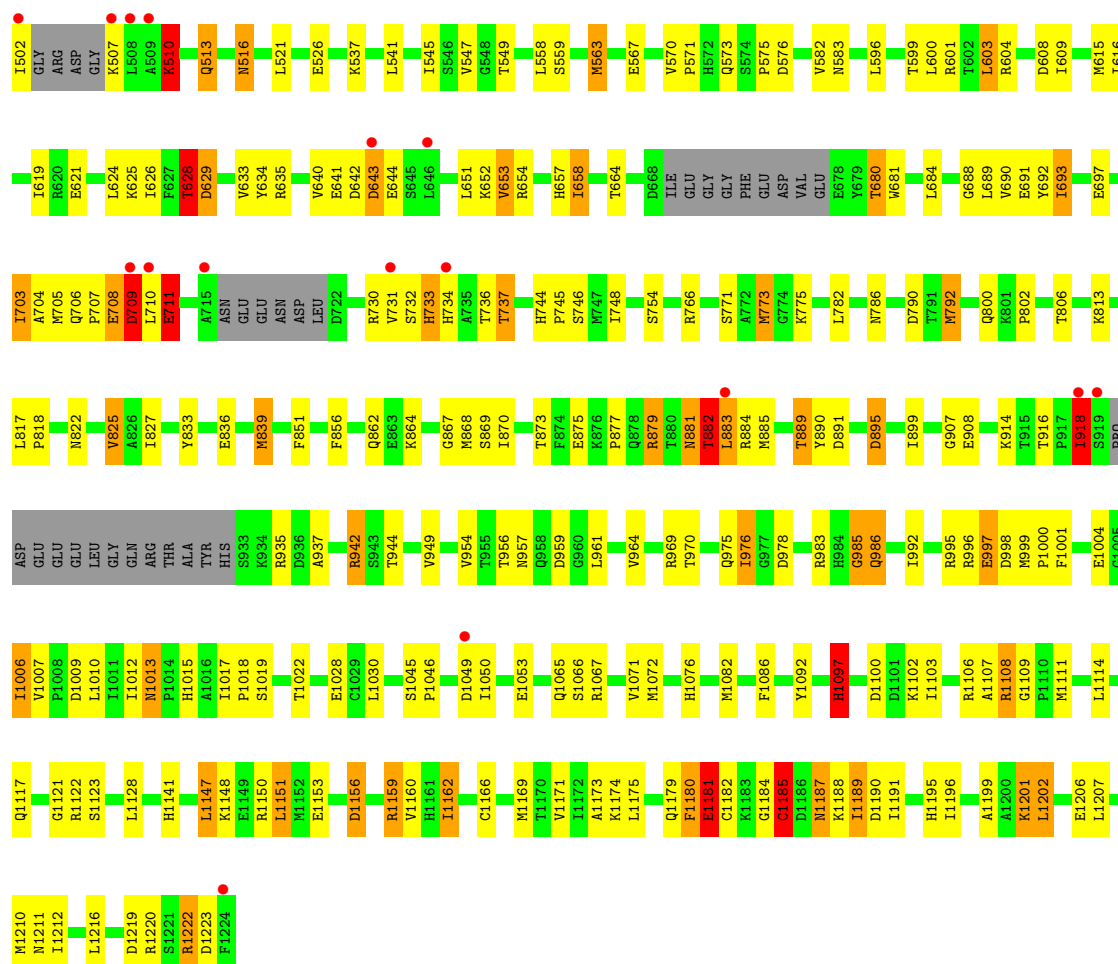
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



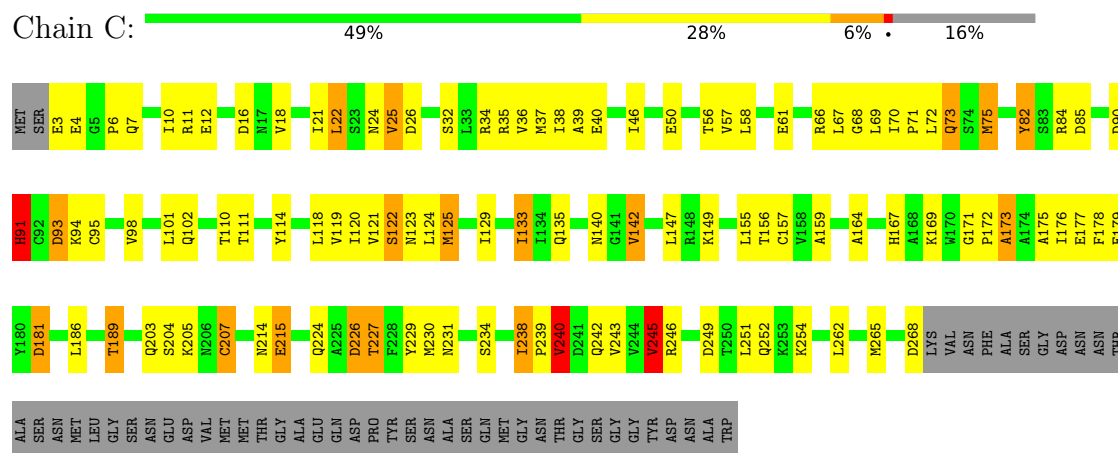


- Molecule 2: DNA-directed RNA polymerase II subunit RPB2



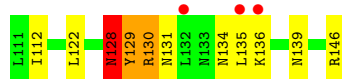


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

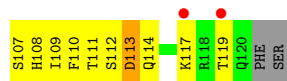
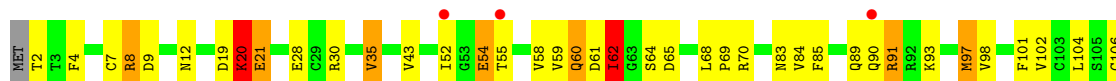


- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

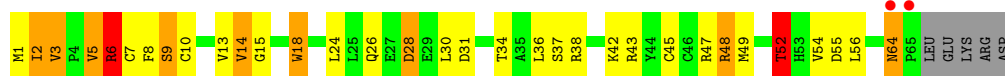




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



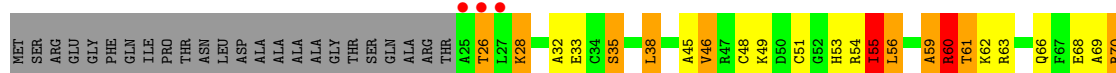
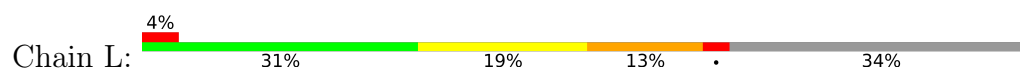
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



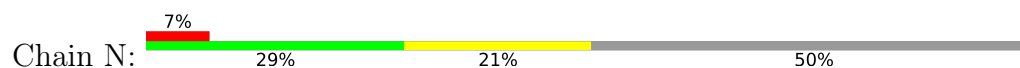
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



- Molecule 13: DNA non-template strand

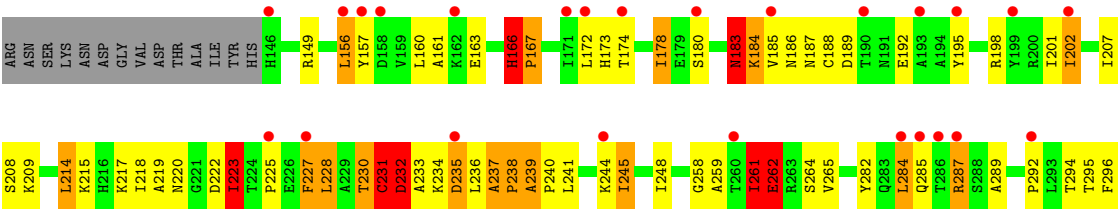


- Molecule 14: RNA product strand





● Molecule 15: Transcription elongation factor S-II



● Molecule 16: 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	220.02Å 395.07Å 280.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.30 49.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.97-3.30) 99.6 (49.97-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.161 , 0.189 0.181 , 0.179	Depositor DCC
R_{free} test set	3598 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	111.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 131.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 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	33008	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 1.93% 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: ACT, MG, ZN, EPE, BRU, PGE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	12/11417 (0.1%)	1.55	139/15442 (0.9%)
2	B	0.87	3/8981 (0.0%)	1.46	87/12108 (0.7%)
3	C	0.87	0/2133	1.42	16/2891 (0.6%)
4	D	0.88	0/1427	1.64	30/1914 (1.6%)
5	E	0.76	0/1788	1.44	9/2406 (0.4%)
6	F	0.90	0/691	1.32	1/933 (0.1%)
7	G	0.93	2/1368 (0.1%)	1.39	6/1844 (0.3%)
8	H	0.79	0/1086	1.35	8/1470 (0.5%)
9	I	0.82	0/989	1.42	12/1331 (0.9%)
10	J	0.89	0/541	1.65	12/727 (1.7%)
11	K	0.85	1/937 (0.1%)	1.35	6/1265 (0.5%)
12	L	0.91	0/366	1.62	8/485 (1.6%)
13	N	0.38	0/162	1.13	0/249
14	P	1.05	0/109	1.78	3/166 (1.8%)
15	S	0.89	0/1317	1.58	15/1778 (0.8%)
16	T	0.46	0/274	1.12	0/421
All	All	0.88	18/33586 (0.1%)	1.49	352/45430 (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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	10.18	1.91	1.51
1	A	56	PRO	C-N	9.19	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	CA-C	-8.54	1.42	1.52
7	G	1	MET	C-N	8.23	1.45	1.33
1	A	69	THR	C-N	7.86	1.44	1.33
1	A	437	MET	SD-CE	7.13	1.97	1.79
1	A	3	GLY	C-N	7.00	1.43	1.33
1	A	56	PRO	CA-C	6.58	1.61	1.52
1	A	1398	MET	SD-CE	6.51	1.95	1.79
1	A	69	THR	CA-C	5.91	1.60	1.52
1	A	453	MET	SD-CE	5.89	1.94	1.79
1	A	436	ILE	CA-CB	5.44	1.60	1.54
2	B	1181	GLU	CA-C	5.23	1.59	1.52
7	G	151	ILE	CG1-CD1	5.21	1.72	1.51
2	B	817	LEU	CA-C	5.16	1.59	1.52
11	K	8	GLU	CA-C	5.08	1.59	1.52
1	A	849	MET	SD-CE	-5.05	1.67	1.79
2	B	1187	ASN	CA-CB	-5.02	1.45	1.53

All (352) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	5	VAL	N-CA-C	-11.52	94.90	109.30
14	P	8	C	P-O3'-C3'	10.64	136.16	120.20
4	D	26	THR	N-CA-C	-10.54	96.62	112.54
1	A	56	PRO	CA-C-N	10.46	140.53	121.70
1	A	56	PRO	C-N-CA	10.46	140.53	121.70
1	A	3	GLY	CA-C-N	9.68	140.04	121.54
1	A	3	GLY	C-N-CA	9.68	140.04	121.54
4	D	25	ALA	CA-C-N	9.60	138.92	121.15
4	D	25	ALA	C-N-CA	9.60	138.92	121.15
10	J	18	TRP	N-CA-C	9.31	121.12	110.97
8	H	92	ASP	N-CA-C	-9.19	98.87	111.56
3	C	39	ALA	N-CA-C	9.01	124.55	112.30
5	E	150	VAL	N-CA-C	8.41	115.21	107.56
1	A	491	VAL	N-CA-C	8.25	115.71	107.55
1	A	224	PHE	N-CA-C	8.20	121.35	110.53
1	A	1084	PHE	CA-CB-CG	8.04	121.84	113.80
2	B	773	MET	N-CA-C	7.95	120.02	111.36
1	A	707	GLY	CA-C-N	7.93	136.69	121.54
1	A	707	GLY	C-N-CA	7.93	136.69	121.54
1	A	408	ASP	CA-CB-CG	7.92	120.52	112.60
4	D	31	GLN	N-CA-C	-7.89	102.76	111.36
2	B	296	GLU	N-CA-C	-7.85	101.54	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	54	GLU	N-CA-C	-7.76	102.77	111.07
2	B	1223	ASP	CA-CB-CG	7.70	120.30	112.60
2	B	1190	ASP	CA-CB-CG	7.68	120.28	112.60
2	B	575	PRO	CA-C-N	7.65	130.39	120.44
2	B	575	PRO	C-N-CA	7.65	130.39	120.44
2	B	681	TRP	N-CA-C	-7.57	103.11	111.36
1	A	399	HIS	N-CA-CB	7.48	123.68	110.37
1	A	346	ASP	CA-CB-CG	7.42	120.02	112.60
10	J	26	GLN	N-CA-C	7.39	119.03	110.97
1	A	56	PRO	CB-CA-C	7.34	123.67	111.56
1	A	794	PRO	CA-C-N	7.31	129.94	120.44
1	A	794	PRO	C-N-CA	7.31	129.94	120.44
1	A	288	ALA	N-CA-C	-7.26	104.40	113.55
2	B	709	ASP	CA-CB-CG	7.24	119.84	112.60
15	S	261	ILE	CA-C-N	7.22	130.82	120.79
15	S	261	ILE	C-N-CA	7.22	130.82	120.79
1	A	78	PRO	N-CA-C	-7.17	99.71	111.68
2	B	882	THR	CA-C-N	7.17	135.23	121.54
2	B	882	THR	C-N-CA	7.17	135.23	121.54
1	A	481	ASP	CA-CB-CG	7.09	119.69	112.60
7	G	46	LEU	N-CA-C	7.07	118.63	111.07
12	L	59	ALA	CA-C-N	7.06	135.03	121.54
12	L	59	ALA	C-N-CA	7.06	135.03	121.54
1	A	91	PHE	CA-CB-CG	7.06	120.86	113.80
1	A	1445	ILE	N-CA-CB	7.05	120.30	110.56
9	I	19	ASP	CA-C-N	6.99	129.95	120.38
9	I	19	ASP	C-N-CA	6.99	129.95	120.38
1	A	1076	ALA	CA-C-N	6.97	129.92	120.38
1	A	1076	ALA	C-N-CA	6.97	129.92	120.38
2	B	628	THR	CA-C-N	6.94	134.79	121.54
2	B	628	THR	C-N-CA	6.94	134.79	121.54
2	B	976	ILE	N-CA-C	6.92	117.63	110.36
12	L	62	LYS	N-CA-C	-6.88	103.86	111.36
1	A	408	ASP	N-CA-C	-6.88	103.71	111.07
1	A	244	PRO	N-CA-C	6.87	119.08	110.70
5	E	171	LYS	N-CA-C	-6.84	99.44	110.32
10	J	52	THR	CB-CA-C	6.84	122.13	110.56
1	A	1403	GLU	N-CA-C	6.81	125.31	110.80
2	B	371	GLU	N-CA-C	-6.80	104.86	113.43
4	D	220	LEU	CA-C-N	6.76	133.87	121.70
4	D	220	LEU	C-N-CA	6.76	133.87	121.70
1	A	445	ASN	CA-CB-CG	6.74	119.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	204	THR	CB-CA-C	6.73	122.80	110.88
1	A	1231	ASP	N-CA-C	6.71	121.06	112.34
2	B	1181	GLU	N-CA-C	6.67	125.00	110.80
2	B	1219	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	568	PRO	N-CA-C	6.64	126.15	112.47
8	H	129	TYR	N-CA-C	6.52	119.39	111.82
1	A	55	ASP	N-CA-C	6.50	124.18	109.81
2	B	1189	ILE	N-CA-C	6.47	117.56	111.48
1	A	886	ILE	N-CA-C	6.46	117.99	110.62
9	I	8	ARG	N-CA-C	-6.46	101.43	110.35
2	B	1184	GLY	CA-C-N	6.42	133.80	121.54
2	B	1184	GLY	C-N-CA	6.42	133.80	121.54
11	K	26	LYS	N-CA-C	6.42	120.95	113.18
10	J	55	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	222	LEU	N-CA-C	-6.38	101.93	110.55
4	D	70	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	228	PHE	N-CA-C	6.36	121.23	112.90
1	A	78	PRO	CA-C-N	-6.29	112.07	121.01
1	A	78	PRO	C-N-CA	-6.29	112.07	121.01
2	B	436	VAL	N-CA-C	-6.29	106.60	112.83
4	D	201	LYS	N-CA-C	6.28	118.12	111.28
1	A	205	GLU	CA-C-N	6.26	128.58	120.44
1	A	205	GLU	C-N-CA	6.26	128.58	120.44
1	A	535	THR	N-CA-C	6.26	119.94	112.93
1	A	1095	THR	N-CA-C	-6.26	100.36	110.32
2	B	473	MET	CA-C-N	6.26	132.97	121.70
2	B	473	MET	C-N-CA	6.26	132.97	121.70
1	A	998	LEU	N-CA-C	6.25	118.91	108.96
1	A	1115	SER	N-CA-C	6.24	118.55	108.32
2	B	851	PHE	N-CA-C	6.21	120.44	112.86
4	D	34	GLN	CB-CG-CD	-6.21	102.04	112.60
2	B	1013	ASN	N-CA-C	6.21	117.48	109.72
3	C	91	HIS	N-CA-C	6.18	123.96	110.80
2	B	1156	ASP	N-CA-C	6.14	121.27	111.81
2	B	452	THR	CA-C-N	6.12	128.39	120.56
2	B	452	THR	C-N-CA	6.12	128.39	120.56
1	A	1436	ILE	N-CA-CB	-6.11	100.76	111.39
11	K	39	ASP	CA-CB-CG	6.11	118.71	112.60
5	E	56	LYS	CA-C-N	6.09	128.44	120.28
5	E	56	LYS	C-N-CA	6.09	128.44	120.28
2	B	294	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	672	ASP	CA-CB-CG	6.06	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	55	ILE	N-CA-C	6.05	117.08	111.45
14	P	9	C	P-O3'-C3'	6.03	129.25	120.20
1	A	602	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	188	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	524	VAL	N-CA-C	6.00	116.14	108.82
1	A	398	GLU	CA-C-O	-5.96	114.21	121.36
1	A	1091	SER	CA-C-N	5.96	132.91	121.54
1	A	1091	SER	C-N-CA	5.96	132.91	121.54
2	B	294	ASP	N-CA-C	-5.94	101.49	110.28
1	A	84	ILE	N-CA-CB	5.94	121.20	111.58
15	S	262	GLU	N-CA-C	5.93	118.26	111.02
2	B	703	ILE	N-CA-C	5.92	117.54	108.71
4	D	39	ASN	CA-CB-CG	5.92	118.53	112.60
1	A	344	ARG	N-CA-C	-5.91	100.86	110.20
5	E	48	ASP	CA-CB-CG	5.91	118.51	112.60
9	I	110	PHE	CA-CB-CG	5.91	119.70	113.80
15	S	231	CYS	CA-C-N	5.91	132.82	121.54
15	S	231	CYS	C-N-CA	5.91	132.82	121.54
1	A	47	ARG	CA-C-N	5.89	132.78	121.54
1	A	47	ARG	C-N-CA	5.89	132.78	121.54
1	A	1143	LEU	N-CA-C	-5.86	104.97	111.36
2	B	242	SER	N-CA-C	5.86	118.28	108.73
1	A	1311	VAL	N-CA-C	5.85	116.91	108.48
9	I	93	LYS	N-CA-C	-5.85	104.98	111.36
1	A	1404	GLU	N-CA-C	5.85	121.16	113.20
2	B	711	GLU	N-CA-C	5.85	122.73	109.81
11	K	24	ASP	CA-C-N	5.83	129.57	120.82
11	K	24	ASP	C-N-CA	5.83	129.57	120.82
2	B	1028	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	622	VAL	N-CA-CB	-5.82	104.55	112.28
1	A	301	ALA	CA-C-N	5.81	129.90	120.60
1	A	301	ALA	C-N-CA	5.81	129.90	120.60
12	L	28	LYS	N-CA-C	5.81	120.15	112.72
2	B	883	LEU	N-CA-C	5.80	123.15	110.80
15	S	235	ASP	CA-CB-CG	5.79	118.39	112.60
10	J	6	ARG	CA-C-N	5.77	129.56	121.02
10	J	6	ARG	C-N-CA	5.77	129.56	121.02
1	A	932	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	408	ASP	CA-C-N	5.75	132.52	121.54
1	A	408	ASP	C-N-CA	5.75	132.52	121.54
1	A	451	HIS	CB-CA-C	-5.74	98.93	110.30
1	A	23	SER	N-CA-C	-5.74	102.16	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	172	PRO	CA-C-N	5.73	132.49	121.54
3	C	172	PRO	C-N-CA	5.73	132.49	121.54
1	A	452	LYS	N-CA-C	-5.72	105.12	111.36
10	J	64	ASN	N-CA-C	5.72	122.45	109.81
11	K	2	ASN	N-CA-C	-5.72	104.85	113.89
7	G	2	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	63	ARG	CA-C-N	5.70	130.96	122.86
1	A	63	ARG	C-N-CA	5.70	130.96	122.86
7	G	34	VAL	N-CA-C	5.70	116.75	111.45
10	J	14	VAL	CA-C-N	5.70	126.31	119.98
10	J	14	VAL	C-N-CA	5.70	126.31	119.98
1	A	316	GLN	N-CA-C	-5.69	102.05	110.48
8	H	128	ASN	CA-C-N	5.69	128.96	120.31
8	H	128	ASN	C-N-CA	5.69	128.96	120.31
9	I	62	ILE	N-CA-C	-5.69	105.03	113.39
5	E	205	SER	N-CA-C	-5.68	101.59	110.17
1	A	1330	ASN	N-CA-C	-5.68	105.61	112.54
3	C	181	ASP	CA-CB-CG	5.67	118.27	112.60
4	D	124	GLU	CA-C-N	5.66	128.13	120.38
4	D	124	GLU	C-N-CA	5.66	128.13	120.38
1	A	311	GLN	N-CA-C	5.65	122.29	109.81
2	B	642	ASP	CA-C-N	5.64	132.31	121.54
2	B	642	ASP	C-N-CA	5.64	132.31	121.54
1	A	444	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	474	VAL	CA-C-N	5.58	127.70	120.44
1	A	474	VAL	C-N-CA	5.58	127.70	120.44
1	A	24	PRO	CA-C-N	5.58	127.76	120.28
1	A	24	PRO	C-N-CA	5.58	127.76	120.28
2	B	397	ASP	CA-CB-CG	5.58	118.18	112.60
4	D	24	ALA	CA-C-N	5.57	130.85	122.67
4	D	24	ALA	C-N-CA	5.57	130.85	122.67
2	B	1175	LEU	N-CA-C	5.56	117.02	111.07
1	A	999	VAL	N-CA-C	-5.55	106.39	111.67
2	B	985	GLY	CA-C-N	5.55	130.35	122.24
2	B	985	GLY	C-N-CA	5.55	130.35	122.24
1	A	1416	ALA	CA-C-N	5.55	128.72	120.90
1	A	1416	ALA	C-N-CA	5.55	128.72	120.90
3	C	245	VAL	N-CA-C	5.55	116.94	110.62
1	A	55	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	1201	LYS	N-CA-C	-5.53	104.47	111.11
6	F	154	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	1185	CYS	N-CA-C	-5.52	99.03	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	258	GLY	CA-C-N	5.52	128.69	120.90
15	S	258	GLY	C-N-CA	5.52	128.69	120.90
4	D	23	ASN	CA-CB-CG	5.51	118.11	112.60
2	B	114	PRO	N-CA-C	5.51	121.80	113.81
1	A	331	GLY	CA-C-N	5.51	132.06	121.54
1	A	331	GLY	C-N-CA	5.51	132.06	121.54
15	S	294	THR	CB-CA-C	5.50	117.86	109.34
1	A	1255	GLU	CA-C-N	5.49	132.02	121.54
1	A	1255	GLU	C-N-CA	5.49	132.02	121.54
1	A	1256	GLU	CA-C-N	5.48	128.40	120.79
1	A	1256	GLU	C-N-CA	5.48	128.40	120.79
2	B	681	TRP	CA-C-N	5.47	127.88	120.38
2	B	681	TRP	C-N-CA	5.47	127.88	120.38
2	B	918	ILE	N-CA-CB	5.47	117.31	111.46
1	A	406	ILE	N-CA-CB	5.47	117.61	111.21
4	D	165	GLN	CA-C-N	5.44	127.89	120.54
4	D	165	GLN	C-N-CA	5.44	127.89	120.54
1	A	548	ASN	CA-C-N	5.43	127.50	120.44
1	A	548	ASN	C-N-CA	5.43	127.50	120.44
1	A	1056	SER	N-CA-C	5.43	118.12	111.82
2	B	708	GLU	CA-C-N	5.42	131.89	121.54
2	B	708	GLU	C-N-CA	5.42	131.89	121.54
2	B	1166	CYS	N-CA-C	-5.42	100.86	109.96
2	B	510	LYS	N-CA-C	5.41	121.77	109.81
2	B	818	PRO	N-CA-C	5.41	119.06	111.33
1	A	466	SER	N-CA-C	5.40	118.98	112.93
4	D	169	SER	CA-C-N	5.40	128.27	120.38
4	D	169	SER	C-N-CA	5.40	128.27	120.38
1	A	1230	GLU	CA-C-N	5.40	129.32	120.63
1	A	1230	GLU	C-N-CA	5.40	129.32	120.63
1	A	483	ASP	CA-CB-CG	5.39	117.99	112.60
2	B	1097	HIS	N-CA-CB	5.39	119.60	110.49
9	I	20	LYS	CA-C-N	5.39	127.77	120.38
9	I	20	LYS	C-N-CA	5.39	127.77	120.38
1	A	333	GLU	CB-CG-CD	5.39	121.76	112.60
3	C	93	ASP	N-CA-C	-5.39	107.07	113.97
10	J	9	SER	N-CA-C	5.39	117.01	111.03
1	A	158	PRO	CA-C-N	5.38	127.93	120.29
1	A	158	PRO	C-N-CA	5.38	127.93	120.29
1	A	253	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	229	SER	N-CA-C	5.37	117.43	107.60
7	G	18	PHE	CA-CB-CG	5.37	119.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	TYR	N-CA-C	5.36	118.25	110.42
1	A	42	ASP	CA-CB-CG	5.36	117.96	112.60
2	B	733	HIS	CA-C-N	5.35	131.77	121.54
2	B	733	HIS	C-N-CA	5.35	131.77	121.54
7	G	73	LYS	CG-CD-CE	5.35	123.61	111.30
3	C	226	ASP	N-CA-C	-5.34	99.98	109.06
1	A	1063	MET	CA-C-N	5.33	129.37	120.62
1	A	1063	MET	C-N-CA	5.33	129.37	120.62
2	B	628	THR	N-CA-C	-5.33	105.91	112.90
2	B	1121	GLY	CA-C-N	5.33	127.74	120.54
2	B	1121	GLY	C-N-CA	5.33	127.74	120.54
2	B	825	VAL	N-CA-C	5.33	116.26	108.53
2	B	1173	ALA	N-CA-C	5.33	117.39	108.23
1	A	152	VAL	CB-CA-C	5.33	115.64	109.89
2	B	1180	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	93	VAL	N-CA-CB	5.32	116.41	110.51
2	B	276	ILE	CA-C-N	5.31	131.68	121.54
2	B	276	ILE	C-N-CA	5.31	131.68	121.54
1	A	1122	PRO	N-CA-C	5.30	123.39	112.47
15	S	209	LYS	CA-C-N	5.29	131.23	121.70
15	S	209	LYS	C-N-CA	5.29	131.23	121.70
1	A	38	PRO	CA-C-N	5.29	128.36	120.90
1	A	38	PRO	C-N-CA	5.29	128.36	120.90
9	I	12	ASN	CA-C-N	5.28	128.21	120.71
9	I	12	ASN	C-N-CA	5.28	128.21	120.71
10	J	8	PHE	CA-CB-CG	5.28	119.08	113.80
15	S	183	ASN	CA-CB-CG	5.28	117.88	112.60
9	I	54	GLU	CA-C-N	5.28	131.62	121.54
9	I	54	GLU	C-N-CA	5.28	131.62	121.54
1	A	1313	LEU	CA-C-N	5.26	128.11	120.79
1	A	1313	LEU	C-N-CA	5.26	128.11	120.79
1	A	495	GLU	CA-C-N	5.26	129.50	120.71
1	A	495	GLU	C-N-CA	5.26	129.50	120.71
2	B	1162	ILE	CA-CB-CG2	5.25	119.43	110.50
1	A	1064	VAL	N-CA-CB	-5.25	102.30	110.54
3	C	135	GLN	CA-C-N	5.25	128.67	120.75
3	C	135	GLN	C-N-CA	5.25	128.67	120.75
8	H	110	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	897	TYR	N-CA-C	5.24	120.16	113.55
2	B	1053	GLU	CA-C-N	5.24	125.76	119.94
2	B	1053	GLU	C-N-CA	5.24	125.76	119.94
2	B	890	TYR	CA-C-N	5.23	129.05	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	890	TYR	C-N-CA	5.23	129.05	120.63
1	A	216	VAL	N-CA-CB	5.23	116.67	110.55
2	B	1028	GLU	N-CA-C	-5.22	105.28	110.97
15	S	265	VAL	N-CA-C	5.22	117.06	108.97
3	C	68	GLY	CA-C-N	5.22	128.95	120.60
3	C	68	GLY	C-N-CA	5.22	128.95	120.60
3	C	85	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	1357	ALA	N-CA-C	5.21	117.70	111.71
15	S	161	ALA	N-CA-C	-5.20	107.49	113.88
4	D	200	ASN	CA-C-N	5.18	127.23	120.28
4	D	200	ASN	C-N-CA	5.18	127.23	120.28
3	C	82	TYR	N-CA-C	-5.18	102.61	110.28
1	A	64	ASN	CA-C-N	5.18	131.43	121.54
1	A	64	ASN	C-N-CA	5.18	131.43	121.54
1	A	399	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	1257	ASP	N-CA-C	5.17	117.33	111.02
3	C	224	GLN	N-CA-C	5.17	117.24	109.23
2	B	1122	ARG	CA-C-N	5.17	127.20	120.28
2	B	1122	ARG	C-N-CA	5.17	127.20	120.28
1	A	864	ILE	N-CA-C	-5.17	107.12	111.56
2	B	225	VAL	N-CA-CB	5.16	117.19	110.99
8	H	82	PRO	CA-C-N	5.16	131.40	121.54
8	H	82	PRO	C-N-CA	5.16	131.40	121.54
14	P	7	C	C3'-C2'-C1'	5.16	106.66	101.50
1	A	1201	ALA	CA-C-N	5.15	127.44	120.38
1	A	1201	ALA	C-N-CA	5.15	127.44	120.38
4	D	133	THR	CA-C-N	5.15	129.03	120.94
4	D	133	THR	C-N-CA	5.15	129.03	120.94
7	G	55	ASP	N-CA-C	5.15	116.70	108.41
1	A	495	GLU	N-CA-C	-5.14	106.27	112.54
1	A	1376	THR	CB-CA-C	5.14	118.30	109.15
11	K	85	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	1270	ASN	N-CA-C	5.13	118.94	109.24
1	A	598	LEU	N-CA-C	-5.13	102.48	109.71
4	D	120	GLU	CA-C-N	5.12	127.41	120.44
4	D	120	GLU	C-N-CA	5.12	127.41	120.44
2	B	1017	ILE	N-CA-C	5.12	119.93	108.88
2	B	1071	VAL	CA-C-N	-5.12	114.55	122.59
2	B	1071	VAL	C-N-CA	-5.12	114.55	122.59
1	A	253	ASN	CA-C-N	5.11	131.31	121.54
1	A	253	ASN	C-N-CA	5.11	131.31	121.54
8	H	59	ILE	CB-CA-C	5.11	119.67	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	813	LYS	CA-C-N	5.11	127.63	120.28
2	B	813	LYS	C-N-CA	5.11	127.63	120.28
1	A	1006	ILE	N-CA-CB	5.10	116.52	110.55
2	B	693	ILE	N-CA-C	5.10	115.20	107.75
1	A	345	VAL	N-CA-C	5.10	117.18	108.86
4	D	15	LEU	N-CA-C	-5.10	99.93	110.80
4	D	53	SER	N-CA-C	-5.10	99.94	110.80
12	L	55	ILE	N-CA-CB	5.08	118.45	110.31
1	A	1381	LEU	N-CA-C	5.08	116.93	107.99
1	A	1335	ILE	CA-C-N	5.08	127.34	120.38
1	A	1335	ILE	C-N-CA	5.08	127.34	120.38
3	C	243	VAL	N-CA-C	-5.07	105.45	110.62
4	D	26	THR	CA-C-N	5.07	129.60	122.46
4	D	26	THR	C-N-CA	5.07	129.60	122.46
2	B	371	GLU	CA-C-N	5.07	127.07	120.28
2	B	371	GLU	C-N-CA	5.07	127.07	120.28
2	B	541	LEU	N-CA-C	5.06	117.46	111.33
5	E	126	SER	N-CA-C	5.06	118.95	112.87
12	L	53	HIS	N-CA-C	5.06	117.64	110.10
1	A	1406	VAL	N-CA-C	5.05	115.27	110.42
2	B	978	ASP	N-CA-C	5.05	117.62	110.10
15	S	178	ILE	N-CA-CB	5.05	118.15	110.58
1	A	1454	MET	CB-CA-C	5.05	115.17	110.17
2	B	468	GLU	CA-C-N	5.04	130.78	121.70
2	B	468	GLU	C-N-CA	5.04	130.78	121.70
2	B	1018	PRO	N-CA-C	5.04	120.68	113.47
12	L	56	LEU	N-CA-C	5.04	121.54	110.80
1	A	146	MET	N-CA-C	5.04	118.50	111.30
1	A	831	THR	CB-CA-C	5.03	119.09	110.74
1	A	896	ARG	N-CA-C	5.03	116.76	111.28
1	A	375	THR	N-CA-C	5.03	116.61	108.26
5	E	46	TYR	N-CA-C	5.01	119.67	113.50
2	B	1009	ASP	N-CA-C	-5.01	107.02	113.23
2	B	1153	GLU	CB-CG-CD	5.00	121.11	112.60
1	A	288	ALA	CA-C-N	5.00	127.31	120.46
1	A	288	ALA	C-N-CA	5.00	127.31	120.46

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	11214	0	11281	268	0
2	B	8810	0	8847	145	0
3	C	2095	0	2051	60	0
4	D	1417	0	1429	26	0
5	E	1752	0	1776	32	0
6	F	679	0	701	17	0
7	G	1340	0	1357	40	0
8	H	1068	0	1040	19	0
9	I	971	0	927	17	0
10	J	532	0	542	20	0
11	K	919	0	929	24	0
12	L	364	0	386	9	0
13	N	144	0	80	2	0
14	P	100	0	56	1	0
15	S	1294	0	1295	37	0
16	T	266	0	146	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	S	1	0	0	0	0
18	A	1	0	0	0	0
19	A	4	0	3	1	0
19	B	4	0	3	1	0
20	A	15	0	17	2	0
21	L	10	0	14	0	0
All	All	33008	0	32880	628	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.91	1.49
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.41	1.02
1:A:855:THR:HG21	1:A:857:ARG:HE	1.26	0.98
1:A:869:GLY:O	5:E:204:THR:HG21	1.69	0.93
7:G:1:MET:SD	7:G:2:PHE:N	2.44	0.90
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.53	0.90
1:A:567:LYS:HB3	8:H:96:VAL:H	1.36	0.90
3:C:167:HIS:HD2	3:C:169:LYS:H	1.22	0.87
1:A:61:ILE:HG21	1:A:257:ARG:HH12	1.40	0.87
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.56	0.86
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.57	0.86
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.90	0.85
8:H:130:ARG:H	8:H:130:ARG:HD3	1.39	0.85
15:S:239:ALA:H	15:S:240:PRO:HD2	1.41	0.83
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.26	0.83
15:S:230:THR:C	15:S:232:ASP:H	1.87	0.83
1:A:41:MET:HE1	1:A:47:ARG:HG2	1.60	0.81
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.61	0.81
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.46	0.81
2:B:510:LYS:HE3	2:B:510:LYS:HA	1.63	0.80
15:S:214:LEU:HD13	15:S:237:ALA:HB2	1.61	0.80
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.80
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.46	0.79
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.64	0.79
8:H:83:GLN:HG2	11:K:54:ARG:HG2	1.64	0.79
12:L:32:ALA:HB3	12:L:55:ILE:HD13	1.65	0.79
1:A:567:LYS:O	1:A:569:LYS:N	2.14	0.78
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.67	0.77
7:G:111:THR:HG22	7:G:113:HIS:H	1.48	0.75
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.51	0.75
3:C:73:GLN:HE22	3:C:75:MET:H	1.33	0.75
4:D:173:HIS:HD2	4:D:175:PHE:H	1.34	0.74
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.70	0.74
2:B:510:LYS:HB3	2:B:513:GLN:HB2	1.69	0.74
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.34	0.73
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.71	0.73
2:B:707:PRO:O	2:B:711:GLU:HB2	1.88	0.73
3:C:73:GLN:HE22	3:C:75:MET:HB2	1.53	0.73
1:A:399:HIS:O	1:A:435:HIS:HD2	1.72	0.72
1:A:55:ASP:HB2	1:A:58:LEU:HG	1.71	0.72
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.52	0.72
4:D:145:MET:O	4:D:149:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.72	0.70
1:A:57:ARG:HG2	1:A:68:GLN:HB2	1.71	0.70
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.40	0.69
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.40	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.38	0.69
1:A:741:ASN:HD22	1:A:744:LYS:H	1.40	0.69
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.69
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.74	0.68
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.08	0.68
1:A:1159:ARG:HD2	1:A:1174:PHE:CE2	2.28	0.68
2:B:26:THR:HG22	2:B:27:ALA:H	1.58	0.67
3:C:167:HIS:HD2	3:C:169:LYS:N	1.90	0.67
2:B:20:ASP:HB3	2:B:23:ALA:HB2	1.77	0.67
1:A:68:GLN:NE2	1:A:70:CYS:HB3	2.09	0.67
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.75	0.67
3:C:98:VAL:H	3:C:122:SER:HB3	1.58	0.67
1:A:855:THR:CG2	1:A:857:ARG:HE	2.06	0.67
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.35	0.67
15:S:183:ASN:O	15:S:186:ASN:HB3	1.96	0.66
2:B:879:ARG:HG2	2:B:885:MET:HE2	1.77	0.66
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.77	0.66
9:I:7:CYS:SG	9:I:8:ARG:O	2.53	0.66
1:A:67:CYS:SG	1:A:67:CYS:O	2.53	0.66
1:A:68:GLN:O	1:A:70:CYS:N	2.29	0.66
3:C:75:MET:HE2	3:C:239:PRO:HG2	1.79	0.65
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.76	0.65
1:A:646:PHE:O	1:A:650:GLN:HG2	1.96	0.65
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.78	0.65
4:D:173:HIS:CD2	4:D:175:PHE:H	2.15	0.65
3:C:167:HIS:CD2	3:C:169:LYS:H	2.10	0.65
4:D:40:HIS:HB3	7:G:73:LYS:HZ2	1.62	0.65
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.62	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
1:A:55:ASP:OD1	1:A:57:ARG:N	2.30	0.64
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.78	0.64
1:A:55:ASP:HB2	1:A:58:LEU:H	1.62	0.64
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.79	0.64
1:A:67:CYS:O	1:A:68:GLN:O	2.15	0.63
1:A:676:MET:HE1	1:A:762:SER:O	1.98	0.63
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.80	0.63
1:A:304:MET:HE2	2:B:1210:MET:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:SER:HB2	3:C:240:VAL:HG13	1.80	0.63
2:B:570:VAL:HB	2:B:573:GLN:HB2	1.78	0.63
1:A:68:GLN:HE21	1:A:70:CYS:H	1.44	0.62
1:A:61:ILE:HG22	1:A:62:ASP:H	1.63	0.62
1:A:351:THR:HG21	1:A:466:SER:O	1.98	0.62
8:H:89:LEU:C	8:H:91:ASP:H	2.07	0.62
1:A:811:GLN:HE21	1:A:811:GLN:H	1.46	0.62
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.12	0.62
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.00	0.62
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.33	0.62
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.81	0.62
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.82	0.61
1:A:1074:GLU:O	1:A:1077:THR:HB	1.99	0.61
15:S:239:ALA:H	15:S:240:PRO:CD	2.11	0.61
1:A:41:MET:HE2	1:A:257:ARG:HD2	1.82	0.61
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.30	0.61
1:A:50:ILE:HG23	1:A:52:GLY:H	1.65	0.61
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.82	0.61
7:G:62:LEU:O	7:G:65:ASP:O	2.19	0.61
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.83	0.61
2:B:510:LYS:HA	2:B:510:LYS:CE	2.25	0.61
15:S:187:ASN:HD22	15:S:195:TYR:HA	1.66	0.61
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.65	0.61
3:C:66:ARG:NH2	10:J:3:VAL:O	2.33	0.61
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.83	0.61
11:K:65:HIS:HD2	11:K:67:PHE:H	1.47	0.61
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.19	0.60
14:P:11:C:H3'	15:S:287:ARG:CZ	2.31	0.60
1:A:259:GLU:HG2	1:A:263:THR:HG21	1.83	0.60
1:A:61:ILE:HG21	1:A:257:ARG:NH1	2.14	0.60
1:A:709:THR:HB	1:A:712:GLU:HB2	1.83	0.60
1:A:839:ARG:NH2	1:A:1402:PHE:HA	2.17	0.60
3:C:73:GLN:NE2	3:C:75:MET:H	2.00	0.60
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.83	0.59
2:B:167:ILE:O	2:B:453:ILE:HD13	2.02	0.59
1:A:63:ARG:HG3	1:A:74:MET:HE2	1.83	0.59
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.84	0.59
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.83	0.59
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.83	0.59
1:A:823:GLY:HA3	15:S:285:GLN:HB3	1.85	0.59
2:B:792:MET:HA	2:B:856:PHE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:NE	2.08	0.59
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.18	0.58
2:B:704:ALA:HA	2:B:710:LEU:HD12	1.84	0.58
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.03	0.58
9:I:20:LYS:HE2	9:I:21:GLU:H	1.67	0.58
15:S:188:CYS:SG	15:S:192:GLU:HB2	2.43	0.58
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.85	0.58
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.86	0.58
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.58
10:J:48:ARG:HE	10:J:49:MET:HE2	1.67	0.58
15:S:238:PRO:HB2	15:S:240:PRO:HD2	1.84	0.58
1:A:69:THR:O	1:A:71:GLN:HG2	2.04	0.58
1:A:494:SER:O	1:A:498:ARG:HG2	2.04	0.58
1:A:512:VAL:HA	1:A:519:PRO:HA	1.84	0.58
1:A:298:PHE:O	1:A:302:THR:HB	2.03	0.58
1:A:687:LYS:HG3	1:A:794:PRO:HG2	1.86	0.57
7:G:119:LEU:HD12	7:G:130:TYR:HB3	1.86	0.57
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.85	0.57
2:B:654:ARG:H	2:B:657:HIS:CD2	2.16	0.57
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.69	0.57
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.85	0.57
15:S:156:LEU:O	15:S:160:LEU:HB2	2.04	0.57
4:D:8:PHE:HE2	7:G:73:LYS:HD2	1.69	0.57
9:I:59:VAL:C	9:I:61:ASP:H	2.11	0.57
2:B:453:ILE:HD12	2:B:453:ILE:H	1.70	0.57
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.87	0.57
1:A:922:ASP:CG	1:A:925:LEU:HD12	2.29	0.56
1:A:1255:GLU:O	1:A:1256:GLU:HB2	2.05	0.56
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.53	0.56
1:A:53:LEU:CD2	1:A:54:ASN:H	2.18	0.56
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.56
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.86	0.56
2:B:55:VAL:HA	2:B:59:LEU:HD12	1.87	0.56
1:A:79:GLY:HA3	1:A:243:PRO:CB	2.35	0.56
3:C:32:SER:O	3:C:36:VAL:HG23	2.06	0.56
4:D:52:LEU:HB3	4:D:148:LEU:HD23	1.86	0.56
7:G:116:PRO:HG2	7:G:119:LEU:HD23	1.88	0.56
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.88	0.56
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.39	0.56
4:D:118:THR:O	4:D:121:LYS:NZ	2.38	0.56
1:A:924:LYS:O	1:A:927:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ILE:O	4:D:168:LYS:HE3	2.06	0.56
6:F:76:LYS:HA	6:F:79:ARG:CD	2.33	0.56
1:A:68:GLN:HE22	1:A:70:CYS:HB3	1.69	0.56
1:A:332:LYS:O	1:A:333:GLU:HG2	2.06	0.56
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.21	0.56
7:G:14:HIS:CD2	7:G:16:SER:H	2.24	0.56
1:A:299:HIS:HA	1:A:302:THR:HG22	1.87	0.56
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.88	0.55
10:J:1:MET:H1	10:J:56:LEU:H	1.53	0.55
15:S:282:TYR:HE1	15:S:284:LEU:HD12	1.71	0.55
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.71	0.55
10:J:1:MET:HB2	10:J:56:LEU:HD12	1.88	0.55
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.88	0.55
1:A:825:ILE:HG21	2:B:510:LYS:HD2	1.88	0.55
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.88	0.55
3:C:164:ALA:HA	3:C:167:HIS:O	2.05	0.55
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.88	0.55
1:A:92:HIS:HD2	1:A:94:GLY:H	1.53	0.55
1:A:754:SER:H	1:A:757:ASN:HD22	1.55	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.40	0.54
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.89	0.54
2:B:260:GLY:O	2:B:267:ARG:HD3	2.07	0.54
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.40	0.54
1:A:567:LYS:HB3	8:H:96:VAL:N	2.16	0.54
2:B:303:TYR:HD2	2:B:571:PRO:HB3	1.72	0.54
19:B:1225:ACT:H2	4:D:14:ARG:HH21	1.73	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.07	0.54
1:A:511:ILE:HA	1:A:521:MET:HE3	1.89	0.54
1:A:399:HIS:O	1:A:401:GLY:N	2.41	0.54
15:S:185:VAL:HB	15:S:189:ASP:HA	1.90	0.54
1:A:43:GLU:HB2	1:A:46:THR:HB	1.88	0.54
2:B:291:ILE:HD12	2:B:291:ILE:H	1.73	0.54
8:H:5:LEU:HD22	8:H:134:ASN:HA	1.90	0.54
9:I:58:VAL:HG13	9:I:62:ILE:HG21	1.90	0.54
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.90	0.54
1:A:1082:ASN:HD22	1:A:1083:THR:H	1.56	0.54
2:B:516:ASN:H	2:B:516:ASN:HD22	1.55	0.53
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.90	0.53
5:E:14:ARG:HH12	5:E:142:VAL:HG22	1.73	0.53
1:A:640:GLN:HE21	1:A:641:VAL:HG23	1.72	0.53
7:G:112:LYS:O	7:G:115:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:SER:HB3	1:A:497:THR:H	1.74	0.53
1:A:756:ILE:HG22	1:A:760:GLN:HE21	1.72	0.53
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.91	0.53
7:G:34:VAL:O	7:G:37:SER:HB3	2.09	0.53
3:C:84:ARG:HD3	11:K:11:LEU:HD21	1.91	0.53
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.90	0.53
1:A:1418:LEU:HD23	2:B:1222:ARG:HD3	1.91	0.52
1:A:211:PHE:HA	1:A:214:ILE:HD12	1.90	0.52
1:A:737:LEU:HB2	1:A:744:LYS:HD2	1.91	0.52
1:A:175:ARG:HH22	1:A:199:LEU:HD21	1.75	0.52
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.56	0.52
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.91	0.52
1:A:1311:VAL:HG21	1:A:1329:THR:CG2	2.39	0.52
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.36	0.52
4:D:119:ARG:HH21	4:D:120:GLU:HB2	1.74	0.52
1:A:811:GLN:H	1:A:811:GLN:NE2	2.08	0.52
1:A:28:ARG:HD3	1:A:238:CYS:SG	2.49	0.52
1:A:306:ASN:ND2	1:A:321:PRO:O	2.43	0.52
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.91	0.52
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.90	0.52
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.45	0.52
3:C:71:PRO:HB2	3:C:133:ILE:HB	1.91	0.52
1:A:870:GLU:HB2	5:E:204:THR:HG22	1.92	0.52
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.10	0.52
3:C:171:GLY:C	3:C:173:ALA:H	2.17	0.52
15:S:183:ASN:O	15:S:228:LEU:HG	2.10	0.52
15:S:231:CYS:C	15:S:233:ALA:H	2.18	0.52
15:S:238:PRO:CD	15:S:241:LEU:HB3	2.40	0.51
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.91	0.51
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.92	0.51
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	1.92	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
5:E:202:SER:OG	5:E:204:THR:HG22	2.11	0.51
9:I:111:THR:HG22	9:I:113:ASP:H	1.76	0.51
1:A:839:ARG:HH22	1:A:1402:PHE:HA	1.76	0.51
1:A:1454:MET:O	1:A:1454:MET:HG3	2.08	0.51
1:A:537:ARG:HH12	8:H:25:ARG:HH21	1.58	0.51
12:L:38:LEU:HD11	12:L:49:LYS:H	1.74	0.51
15:S:163:GLU:HG2	15:S:215:LYS:HD3	1.93	0.51
7:G:119:LEU:HD22	7:G:132:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:GLN:HG3	1:A:606:LEU:HD13	1.93	0.51
1:A:1199:ARG:HD2	15:S:245:ILE:HD11	1.92	0.51
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.76	0.51
2:B:248:SER:H	2:B:418:LYS:HE2	1.76	0.51
2:B:498:THR:HB	2:B:537:LYS:O	2.10	0.51
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.76	0.50
11:K:65:HIS:CD2	11:K:66:PRO:HD2	2.46	0.50
1:A:256:GLN:HE22	2:B:918:ILE:HD13	1.75	0.50
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.77	0.50
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.08	0.50
4:D:40:HIS:HE1	7:G:75:ARG:HH21	1.57	0.50
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.44	0.50
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.11	0.50
2:B:1019:SER:HB2	15:S:292:PRO:HG3	1.92	0.50
3:C:11:ARG:HD3	3:C:21:ILE:HD11	1.93	0.50
5:E:23:VAL:HG13	5:E:78:LEU:HD22	1.94	0.50
7:G:111:THR:HB	7:G:114:LEU:HB2	1.93	0.50
1:A:47:ARG:HH11	1:A:255:SER:H	1.58	0.50
1:A:500:GLU:O	1:A:504:LEU:HB2	2.12	0.50
1:A:316:GLN:HE21	1:A:322:VAL:H	1.59	0.50
1:A:862:ASN:HA	5:E:174:GLN:HB3	1.93	0.50
1:A:1092:LYS:HD3	15:S:259:ALA:HB3	1.94	0.50
1:A:304:MET:HG2	2:B:1210:MET:HG2	1.92	0.50
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.94	0.50
2:B:641:GLU:HG3	2:B:652:LYS:NZ	2.26	0.50
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.94	0.50
7:G:83:LYS:NZ	7:G:150:CYS:H	2.10	0.50
7:G:138:THR:HG22	7:G:139:ILE:H	1.77	0.50
12:L:68:GLU:C	12:L:70:ARG:H	2.20	0.49
15:S:198:ARG:HA	15:S:201:ILE:HD12	1.94	0.49
3:C:69:LEU:O	10:J:6:ARG:HD2	2.11	0.49
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.93	0.49
2:B:1004:GLU:OE2	2:B:1006:ILE:HD11	2.11	0.49
1:A:56:PRO:HD2	1:A:57:ARG:HB2	1.93	0.49
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.78	0.49
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.95	0.49
9:I:28:GLU:HB3	9:I:35:VAL:HG12	1.93	0.49
1:A:53:LEU:HD22	1:A:54:ASN:H	1.76	0.49
1:A:84:ILE:HD11	1:A:86:LEU:HD23	1.95	0.49
1:A:34:LYS:N	20:A:1735:EPE:H101	2.28	0.49
1:A:1116:LEU:HB2	1:A:1308:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.81	0.49
5:E:22:MET:HE2	5:E:187:TYR:HA	1.95	0.49
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.94	0.49
2:B:40:GLU:HG3	2:B:680:THR:HG22	1.95	0.48
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.94	0.48
2:B:706:GLN:HB2	2:B:709:ASP:HB3	1.94	0.48
3:C:111:THR:HB	3:C:147:LEU:HB2	1.94	0.48
6:F:116:ASP:HB3	6:F:119:ARG:HB2	1.95	0.48
11:K:5:ASP:HB2	11:K:8:GLU:HG3	1.94	0.48
1:A:1372:VAL:O	1:A:1376:THR:HB	2.13	0.48
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.77	0.48
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.48	0.48
12:L:38:LEU:HD11	12:L:49:LYS:HG2	1.95	0.48
2:B:745:PRO:O	2:B:748:ILE:HG12	2.13	0.48
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.95	0.48
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.53	0.48
4:D:23:ASN:HA	4:D:28:GLN:O	2.14	0.48
7:G:83:LYS:CD	7:G:83:LYS:H	2.27	0.48
1:A:31:SER:OG	1:A:83:HIS:HD2	1.97	0.48
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.14	0.48
1:A:903:ASN:HD22	1:A:906:HIS:H	1.61	0.48
1:A:706:HIS:CD2	1:A:706:HIS:H	2.30	0.48
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.96	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.96	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HG2	1.94	0.48
5:E:28:TYR:HA	5:E:64:PRO:HA	1.95	0.48
15:S:244:LYS:O	15:S:248:ILE:HG12	2.14	0.48
2:B:114:PRO:O	2:B:118:ARG:HG3	2.14	0.48
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.96	0.48
1:A:68:GLN:NE2	1:A:70:CYS:H	2.10	0.48
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.96	0.48
2:B:277:LYS:HZ2	2:B:335:GLY:HA2	1.79	0.48
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.95	0.48
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.79	0.48
1:A:768:GLN:CG	1:A:816:HIS:HA	2.44	0.48
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.95	0.48
1:A:421:ALA:HA	1:A:424:ILE:HD11	1.96	0.47
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.96	0.47
3:C:245:VAL:HG12	11:K:102:LYS:HG3	1.96	0.47
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.96	0.47
11:K:65:HIS:CD2	11:K:67:PHE:H	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:HG23	1:A:1024:SER:HB2	1.95	0.47
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.96	0.47
3:C:249:ASP:HA	3:C:252:GLN:HE21	1.79	0.47
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.04	0.47
1:A:824:LEU:HD21	15:S:289:ALA:HB2	1.96	0.47
2:B:996:ARG:NH1	3:C:173:ALA:HB1	2.30	0.47
4:D:56:ARG:HD3	4:D:149:THR:HA	1.96	0.47
15:S:173:HIS:CE1	15:S:219:ALA:HB1	2.50	0.47
15:S:223:ILE:HG22	15:S:225:PRO:HD2	1.97	0.47
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.47
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.50	0.47
1:A:856:THR:HB	1:A:865:GLN:HB2	1.97	0.47
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.97	0.47
3:C:46:ILE:HA	3:C:159:ALA:HA	1.96	0.47
7:G:1:MET:HE1	7:G:79:PHE:CE1	2.50	0.47
8:H:4:THR:HA	8:H:60:ALA:HB2	1.95	0.47
15:S:180:SER:O	15:S:184:LYS:HB2	2.14	0.47
1:A:287:HIS:HA	1:A:290:GLU:CD	2.40	0.47
2:B:238:ALA:HB2	2:B:385:LEU:HB2	1.97	0.47
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.97	0.47
4:D:67:ARG:HH12	4:D:132:GLN:CD	2.22	0.47
15:S:166:HIS:CD2	15:S:167:PRO:HD3	2.49	0.47
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.47
4:D:13:ARG:H	4:D:13:ARG:HE	1.63	0.47
9:I:59:VAL:HG12	9:I:61:ASP:H	1.80	0.47
1:A:382:PRO:HD3	6:F:104:ASN:OD1	2.15	0.47
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.47	0.47
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	1.96	0.47
3:C:181:ASP:OD2	3:C:186:LEU:HB2	2.15	0.47
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.96	0.47
15:S:230:THR:C	15:S:232:ASP:N	2.64	0.47
1:A:435:HIS:O	1:A:437:MET:HG3	2.16	0.46
2:B:599:THR:O	2:B:603:LEU:HB2	2.15	0.46
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.46
10:J:1:MET:N	10:J:54:VAL:O	2.48	0.46
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.45	0.46
1:A:1113:THR:HG22	1:A:1113:THR:O	2.15	0.46
7:G:1:MET:HE1	7:G:79:PHE:CD1	2.51	0.46
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.15	0.46
1:A:452:LYS:HG3	2:B:1141:HIS:CE1	2.50	0.46
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:LYS:O	5:E:47:CYS:HB2	2.16	0.46
1:A:562:THR:O	1:A:576:GLN:NE2	2.48	0.46
5:E:171:LYS:H	5:E:174:GLN:HG3	1.80	0.46
3:C:18:VAL:CG2	11:K:109:TRP:HZ3	2.28	0.46
5:E:176:PRO:O	5:E:212:ARG:HA	2.16	0.46
1:A:2:VAL:HG12	2:B:1195:HIS:CD2	2.51	0.46
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.81	0.46
1:A:942:PHE:CB	19:A:1734:ACT:H1	2.46	0.46
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.16	0.46
6:F:118:LEU:O	6:F:122:MET:HG3	2.16	0.46
1:A:1159:ARG:HD2	1:A:1174:PHE:HE2	1.76	0.46
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.29	0.46
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.98	0.46
3:C:6:PRO:HA	3:C:24:ASN:HB3	1.97	0.46
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.98	0.46
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.51	0.46
1:A:1378:GLN:HG2	5:E:177:ARG:HH12	1.81	0.45
5:E:147:HIS:CD2	5:E:149:LEU:H	2.33	0.45
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.98	0.45
2:B:619:ILE:HG21	9:I:62:ILE:HA	1.99	0.45
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.52	0.45
3:C:142:VAL:HG21	10:J:5:VAL:HG13	1.99	0.45
3:C:169:LYS:HZ3	12:L:70:ARG:HG3	1.80	0.45
1:A:1173:HIS:HB3	1:A:1227:ILE:HD13	1.97	0.45
1:A:1449:SER:HA	1:A:1452:LYS:HD2	1.98	0.45
9:I:59:VAL:C	9:I:61:ASP:N	2.75	0.45
15:S:232:ASP:CG	15:S:235:ASP:HB3	2.41	0.45
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.45
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.57	0.45
1:A:225:ASN:HD22	1:A:227:VAL:H	1.64	0.45
2:B:709:ASP:O	2:B:710:LEU:HD23	2.17	0.45
3:C:18:VAL:HG22	11:K:109:TRP:HZ3	1.81	0.45
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.98	0.45
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.45
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.24	0.45
2:B:558:LEU:HD23	2:B:596:LEU:HD11	1.98	0.45
15:S:157:TYR:CE2	15:S:174:THR:HA	2.51	0.45
1:A:75:ASN:O	1:A:76:GLU:HB2	2.17	0.45
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.99	0.45
8:H:82:PRO:O	8:H:84:ALA:N	2.50	0.45
1:A:982:THR:HG22	1:A:984:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:O	1:A:67:CYS:N	2.50	0.45
1:A:782:ARG:HD3	1:A:789:LYS:HG3	1.99	0.45
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.47	0.45
1:A:1089:VAL:HG21	15:S:261:ILE:HD11	1.98	0.45
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.99	0.45
1:A:56:PRO:HB2	1:A:57:ARG:HB2	1.99	0.45
2:B:345:LYS:O	2:B:347:LYS:HG2	2.16	0.45
2:B:603:LEU:HD22	2:B:608:ASP:HB2	1.98	0.45
2:B:986:GLN:OE1	2:B:1022:THR:HG21	2.17	0.45
3:C:204:SER:O	3:C:207:CYS:HB2	2.17	0.45
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.99	0.45
8:H:6:PHE:HD1	8:H:130:ARG:HG2	1.82	0.45
1:A:549:MET:HB3	1:A:577:ILE:CD1	2.47	0.44
2:B:996:ARG:HH12	3:C:173:ALA:HB1	1.81	0.44
3:C:93:ASP:HB3	3:C:125:MET:HE2	1.99	0.44
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.53	0.44
1:A:41:MET:HB3	1:A:42:ASP:H	1.33	0.44
1:A:421:ALA:HA	1:A:424:ILE:CD1	2.47	0.44
1:A:974:ASP:C	1:A:976:THR:H	2.25	0.44
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.17	0.44
4:D:130:LEU:HD21	4:D:141:LEU:HG	1.99	0.44
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.99	0.44
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.52	0.44
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.99	0.44
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.18	0.44
8:H:79:TRP:CH2	8:H:82:PRO:HD3	2.53	0.44
8:H:129:TYR:CE1	8:H:130:ARG:HG3	2.53	0.44
1:A:69:THR:HB	2:B:1174:LYS:NZ	2.32	0.44
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.99	0.44
12:L:48:CYS:HB3	12:L:51:CYS:O	2.17	0.44
2:B:652:LYS:HD3	2:B:688:GLY:O	2.17	0.44
1:A:55:ASP:HA	1:A:56:PRO:HD3	1.74	0.44
1:A:225:ASN:ND2	1:A:228:PHE:H	2.16	0.44
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.17	0.44
2:B:600:LEU:HB3	2:B:615:MET:SD	2.57	0.44
5:E:67:GLU:CD	5:E:67:GLU:H	2.25	0.44
5:E:111:VAL:HG12	5:E:137:GLU:HG3	1.98	0.44
1:A:36:ARG:NH2	20:A:1735:EPE:O3S	2.51	0.44
1:A:868:TYR:HD2	1:A:1058:VAL:CG2	2.23	0.44
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.81	0.44
1:A:1170:ILE:O	1:A:1174:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.58	0.44
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.52	0.44
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.99	0.44
9:I:84:VAL:HG23	9:I:104:LEU:HD11	1.98	0.44
1:A:203:SER:OG	1:A:206:GLU:HB2	2.17	0.44
1:A:381:THR:HG23	1:A:383:TYR:H	1.81	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.33	0.44
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.18	0.44
1:A:1448:GLU:HG3	1:A:1452:LYS:NZ	2.33	0.44
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.53	0.44
7:G:83:LYS:HD2	7:G:83:LYS:N	2.32	0.44
10:J:7:CYS:HA	10:J:49:MET:HE3	1.98	0.44
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.99	0.43
1:A:402:ALA:HA	1:A:434:ARG:HA	1.99	0.43
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.65	0.43
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.86	0.43
2:B:914:LYS:HE3	2:B:937:ALA:HB1	2.00	0.43
2:B:1114:LEU:HG	2:B:1202:LEU:HD11	2.00	0.43
6:F:74:ILE:HB	6:F:144:GLU:HG2	1.99	0.43
7:G:9:LEU:HD23	7:G:30:LEU:HD12	1.99	0.43
2:B:895:ASP:OD1	2:B:895:ASP:N	2.49	0.43
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.83	0.43
1:A:265:LYS:HG2	1:A:303:TYR:HB2	2.00	0.43
1:A:311:GLN:O	1:A:312:PRO:C	2.62	0.43
1:A:638:GLY:HA3	1:A:640:GLN:HE22	1.82	0.43
1:A:738:LYS:HB2	1:A:740:LEU:HG	2.00	0.43
1:A:1172:LEU:C	1:A:1174:PHE:H	2.25	0.43
3:C:6:PRO:CB	3:C:25:VAL:HG13	2.48	0.43
10:J:28:ASP:HB3	10:J:30:LEU:HD12	2.00	0.43
12:L:60:ARG:HG2	12:L:61:THR:H	1.83	0.43
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.83	0.43
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.83	0.43
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.52	0.43
1:A:256:GLN:HE22	2:B:918:ILE:HG21	1.84	0.43
2:B:705:MET:HE3	2:B:705:MET:HA	1.99	0.43
5:E:170:LEU:HD22	5:E:174:GLN:HB2	2.01	0.43
7:G:62:LEU:O	7:G:63:PRO:C	2.62	0.43
15:S:198:ARG:HH21	15:S:231:CYS:H	1.66	0.43
1:A:55:ASP:CB	1:A:58:LEU:HG	2.44	0.43
1:A:982:THR:HB	1:A:985:ASP:H	1.82	0.43
1:A:1141:THR:OG1	1:A:1205:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:GLN:HE22	7:G:61:ILE:HG12	1.84	0.43
11:K:63:VAL:HG23	11:K:63:VAL:O	2.18	0.43
1:A:55:ASP:HB2	1:A:58:LEU:CG	2.46	0.43
1:A:691:LEU:O	1:A:694:THR:HB	2.18	0.43
1:A:1081:LEU:HD13	1:A:1099:PRO:HD3	2.00	0.43
2:B:641:GLU:HG3	2:B:652:LYS:HZ2	1.82	0.43
1:A:471:ASN:OD1	1:A:650:GLN:NE2	2.51	0.43
2:B:324:ILE:HG13	2:B:329:THR:HG22	2.01	0.43
2:B:706:GLN:HB2	2:B:709:ASP:CB	2.49	0.43
2:B:889:THR:HG22	2:B:891:ASP:OD2	2.18	0.43
10:J:6:ARG:H	10:J:14:VAL:H	1.66	0.43
1:A:598:LEU:HD21	8:H:39:THR:HG21	2.01	0.43
1:A:1062:GLU:HB3	1:A:1064:VAL:HG23	2.01	0.43
13:N:4:DT:H2'	13:N:5:DA:C8	2.53	0.43
1:A:1387:HIS:HA	1:A:1391:ARG:HD3	2.01	0.42
3:C:262:LEU:HB3	11:K:88:LYS:HE2	2.01	0.42
7:G:90:THR:HG23	7:G:142:ARG:HD3	2.01	0.42
8:H:109:LYS:HB3	8:H:110:ASP:H	1.48	0.42
1:A:225:ASN:HD22	1:A:228:PHE:H	1.66	0.42
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.01	0.42
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	2.02	0.42
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.19	0.42
1:A:857:ARG:HD3	1:A:861:GLY:O	2.19	0.42
2:B:918:ILE:HB	2:B:935:ARG:HH21	1.84	0.42
3:C:242:GLN:HB3	3:C:246:ARG:HE	1.84	0.42
4:D:67:ARG:HG3	4:D:68:ARG:N	2.34	0.42
1:A:588:LEU:HB3	1:A:607:ILE:HD12	2.01	0.42
15:S:202:ILE:HD12	15:S:227:PHE:O	2.19	0.42
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.02	0.42
5:E:147:HIS:HB3	5:E:150:VAL:HG23	2.01	0.42
1:A:84:ILE:HG23	1:A:241:VAL:CG2	2.50	0.42
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.49	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.02	0.42
2:B:641:GLU:HB3	2:B:643:ASP:CG	2.44	0.42
2:B:918:ILE:HB	2:B:935:ARG:HE	1.84	0.42
3:C:22:LEU:O	3:C:227:THR:HA	2.19	0.42
12:L:60:ARG:HG2	12:L:61:THR:N	2.35	0.42
1:A:640:GLN:CD	1:A:640:GLN:H	2.26	0.42
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.85	0.42
1:A:1120:LEU:HD11	1:A:1134:ILE:HG13	2.02	0.42
2:B:582:VAL:HG22	2:B:626:ILE:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:PHE:CZ	2:B:398:ARG:HG3	2.54	0.42
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.53	0.42
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.47	0.42
3:C:82:TYR:HB3	3:C:84:ARG:HG2	2.02	0.42
3:C:91:HIS:HA	3:C:95:CYS:SG	2.60	0.42
10:J:24:LEU:HD23	10:J:24:LEU:HA	1.89	0.42
1:A:871:ASP:HB3	5:E:204:THR:HG23	2.01	0.42
1:A:1116:LEU:HB2	1:A:1308:THR:CG2	2.50	0.42
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.02	0.42
2:B:99:LYS:O	2:B:101:MET:HG2	2.20	0.42
2:B:942:ARG:HH11	2:B:942:ARG:HB3	1.84	0.42
3:C:6:PRO:HB3	3:C:25:VAL:HG13	2.02	0.42
7:G:83:LYS:HZ2	7:G:150:CYS:H	1.68	0.42
2:B:291:ILE:HD11	2:B:375:ALA:CB	2.49	0.42
8:H:23:VAL:HG12	8:H:24:CYS:N	2.35	0.42
9:I:69:PRO:HB2	9:I:85:PHE:CZ	2.55	0.42
10:J:43:ARG:O	10:J:47:ARG:HG3	2.19	0.42
15:S:185:VAL:O	15:S:189:ASP:N	2.53	0.42
1:A:62:ASP:O	1:A:63:ARG:C	2.63	0.41
11:K:18:LYS:HE3	11:K:38:GLU:OE2	2.20	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.41
4:D:5:THR:HG21	7:G:74:TYR:OH	2.20	0.41
5:E:7:ARG:O	5:E:11:ARG:HG3	2.20	0.41
5:E:19:VAL:O	5:E:23:VAL:HG23	2.20	0.41
11:K:21:ILE:HG12	11:K:33:ILE:HG12	2.03	0.41
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.18	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.49	0.41
15:S:284:LEU:HB2	15:S:296:PHE:HE1	1.86	0.41
1:A:347:PHE:H	2:B:1107:ALA:HA	1.86	0.41
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.38	0.41
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	2.01	0.41
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.84	0.41
7:G:83:LYS:HG3	7:G:149:GLY:HA2	2.01	0.41
1:A:49:LYS:H	1:A:49:LYS:HG3	1.58	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.70	0.41
3:C:11:ARG:NH1	3:C:229:TYR:HD2	2.18	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.56	0.41
2:B:35:SER:O	2:B:39:ARG:HG3	2.20	0.41
2:B:277:LYS:HG2	2:B:278:GLN:H	1.86	0.41
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.02	0.41
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ILE:HD12	1:A:943:LEU:HB3	2.03	0.41
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.01	0.41
7:G:9:LEU:HD22	7:G:34:VAL:HG23	2.02	0.41
1:A:92:HIS:CD2	1:A:94:GLY:H	2.36	0.41
1:A:847:ASP:HB3	1:A:1398:MET:HE1	2.03	0.41
2:B:558:LEU:HB3	2:B:563:MET:HE3	2.03	0.41
3:C:37:MET:HE3	3:C:176:ILE:HD13	2.03	0.41
4:D:123:LEU:HD11	4:D:150:ASN:HD21	1.85	0.41
1:A:54:ASN:HA	1:A:247:ARG:HH22	1.86	0.41
1:A:70:CYS:HA	2:B:1174:LYS:HG2	2.02	0.41
1:A:514:PRO:HG2	1:A:1067:LEU:HD21	2.02	0.41
1:A:650:GLN:HB2	1:A:654:ASN:ND2	2.36	0.41
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.85	0.41
2:B:1109:GLY:O	2:B:1111:MET:HE2	2.21	0.41
3:C:142:VAL:HG22	10:J:15:GLY:HA3	2.01	0.41
3:C:238:ILE:HG23	3:C:242:GLN:HB2	2.02	0.41
9:I:97:MET:HE3	9:I:97:MET:HB2	1.91	0.41
11:K:109:TRP:O	11:K:112:GLN:HB2	2.21	0.41
15:S:238:PRO:HD2	15:S:241:LEU:HB3	2.02	0.41
1:A:55:ASP:OD1	1:A:56:PRO:C	2.64	0.41
2:B:710:LEU:HD22	2:B:732:SER:O	2.21	0.41
3:C:120:ILE:HD13	3:C:124:LEU:HD11	2.03	0.41
6:F:103:MET:HE1	7:G:66:GLY:H	1.86	0.41
13:N:5:DA:H2"	13:N:6:DA:C8	2.56	0.41
1:A:56:PRO:HG2	1:A:57:ARG:HH21	1.85	0.40
1:A:69:THR:HB	2:B:1174:LYS:HZ1	1.85	0.40
1:A:92:HIS:HE1	2:B:1210:MET:O	2.02	0.40
1:A:470:LEU:HD21	1:A:487:MET:HE3	2.02	0.40
3:C:123:ASN:ND2	3:C:125:MET:H	2.19	0.40
11:K:32:VAL:HG22	11:K:74:ARG:HG3	2.02	0.40
1:A:579:SER:HB3	1:A:611:GLN:HA	2.03	0.40
1:A:961:ARG:HH21	1:A:1025:ARG:HH22	1.69	0.40
1:A:1082:ASN:ND2	1:A:1083:THR:H	2.20	0.40
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.21	0.40
5:E:190:LEU:HD13	5:E:214:CYS:HB2	2.03	0.40
8:H:63:LEU:HB2	8:H:90:ALA:HB2	2.04	0.40
10:J:36:LEU:HD13	10:J:47:ARG:HB3	2.02	0.40
12:L:61:THR:HG21	12:L:63:ARG:HG2	2.04	0.40
1:A:332:LYS:H	1:A:337:ARG:CB	2.35	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG23	2.04	0.40
2:B:277:LYS:H	2:B:277:LYS:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.21	0.40
4:D:130:LEU:O	4:D:134:THR:HB	2.21	0.40
15:S:262:GLU:H	15:S:262:GLU:HG3	1.62	0.40
1:A:743:VAL:O	1:A:747:VAL:HG23	2.21	0.40
1:A:1121:GLU:HB3	1:A:1124:HIS:CD2	2.56	0.40
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.57	0.40
2:B:1117:GLN:NE2	2:B:1199:ALA:HB2	2.37	0.40
2:B:875:GLU:O	2:B:877:PRO:HD3	2.20	0.40
5:E:156:LEU:HD11	5:E:197:LYS:HB2	2.03	0.40
5:E:178:ILE:HB	5:E:212:ARG:HD3	2.04	0.40
6:F:83:PRO:HG2	6:F:84:TYR:CD1	2.57	0.40
8:H:89:LEU:C	8:H:91:ASP:N	2.78	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	1418/1733 (82%)	1255 (88%)	105 (7%)	58 (4%)	2	15
2	B	1090/1224 (89%)	963 (88%)	92 (8%)	35 (3%)	3	19
3	C	264/318 (83%)	238 (90%)	17 (6%)	9 (3%)	3	18
4	D	173/221 (78%)	153 (88%)	14 (8%)	6 (4%)	3	18
5	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	14	43
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	10	37
7	G	169/171 (99%)	154 (91%)	12 (7%)	3 (2%)	6	29
8	H	129/146 (88%)	101 (78%)	18 (14%)	10 (8%)	1	5
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	23
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	8 (18%)	9 (20%)	0	0
15	S	162/178 (91%)	129 (80%)	20 (12%)	13 (8%)	1	5
All	All	4035/4743 (85%)	3558 (88%)	325 (8%)	152 (4%)	2	16

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	65	LEU
1	A	66	LYS
1	A	68	GLN
1	A	69	THR
1	A	74	MET
1	A	254	GLU
1	A	311	GLN
1	A	314	ALA
1	A	410	GLY
1	A	568	PRO
1	A	672	ASP
1	A	708	MET
1	A	709	THR
1	A	1092	LYS
1	A	1122	PRO
1	A	1405	THR
2	B	245	GLU
2	B	249	ARG
2	B	392	ARG
2	B	643	ASP
2	B	731	VAL
2	B	734	HIS
2	B	737	THR
2	B	883	LEU
2	B	1066	SER
2	B	1181	GLU
3	C	90	ASP
3	C	91	HIS
3	C	173	ALA
3	C	215	GLU
4	D	14	ARG

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Mol	Chain	Res	Type
4	D	53	SER
4	D	199	ASN
5	E	104	ASN
7	G	63	PRO
8	H	83	GLN
8	H	139	ASN
9	I	55	THR
9	I	91	ARG
12	L	35	SER
12	L	56	LEU
12	L	59	ALA
12	L	60	ARG
15	S	208	SER
15	S	238	PRO
1	A	43	GLU
1	A	57	ARG
1	A	76	GLU
1	A	166	GLY
1	A	250	ILE
1	A	567	LYS
1	A	593	GLU
1	A	704	ALA
1	A	775	ILE
1	A	1173	HIS
1	A	1256	GLU
2	B	67	SER
2	B	364	ILE
2	B	367	LEU
2	B	629	ASP
2	B	644	GLU
2	B	709	ASP
2	B	867	GLY
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
3	C	149	LYS
3	C	227	THR
4	D	16	LYS
4	D	30	GLY
5	E	3	GLN
8	H	18	GLY
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	45	ALA
15	S	166	HIS
15	S	222	ASP
15	S	223	ILE
15	S	237	ALA
15	S	239	ALA
1	A	54	ASN
1	A	332	LYS
1	A	423	ASP
1	A	525	GLN
1	A	543	LEU
1	A	885	THR
1	A	1403	GLU
2	B	468	GLU
2	B	475	SER
2	B	869	SER
2	B	882	THR
2	B	1185	CYS
2	B	1187	ASN
3	C	110	THR
3	C	214	ASN
7	G	133	SER
7	G	134	GLU
8	H	90	ALA
8	H	128	ASN
8	H	131	ASN
12	L	69	ALA
15	S	207	ILE
1	A	5	GLN
1	A	35	ILE
1	A	56	PRO
1	A	62	ASP
1	A	399	HIS
1	A	1255	GLU
1	A	1437	GLY
2	B	478	GLY
6	F	73	ALA
8	H	17	PRO
8	H	60	ALA
8	H	109	LYS
9	I	60	GLN
10	J	2	ILE

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Mol	Chain	Res	Type
12	L	33	GLU
15	S	227	PHE
15	S	295	THR
1	A	71	GLN
1	A	253	ASN
1	A	322	VAL
1	A	331	GLY
1	A	424	ILE
1	A	846	GLU
1	A	1082	ASN
2	B	792	MET
2	B	907	GLY
2	B	1097	HIS
4	D	119	ARG
8	H	35	GLN
10	J	64	ASN
12	L	26	THR
12	L	46	VAL
15	S	167	PRO
15	S	232	ASP
1	A	705	LYS
1	A	958	VAL
2	B	248	SER
2	B	711	GLU
2	B	1108	ARG
15	S	261	ILE
1	A	3	GLY
1	A	283	GLY
2	B	1171	VAL
1	A	55	ASP
2	B	870	ILE
1	A	165	GLY
1	A	310	GLY
3	C	240	VAL
1	A	312	PRO

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	1246/1520 (82%)	1045 (84%)	201 (16%)	2	12
2	B	962/1061 (91%)	814 (85%)	148 (15%)	2	12
3	C	234/274 (85%)	193 (82%)	41 (18%)	2	9
4	D	157/200 (78%)	120 (76%)	37 (24%)	1	4
5	E	196/197 (100%)	176 (90%)	20 (10%)	7	26
6	F	74/137 (54%)	67 (90%)	7 (10%)	8	29
7	G	152/152 (100%)	122 (80%)	30 (20%)	1	6
8	H	117/128 (91%)	103 (88%)	14 (12%)	5	20
9	I	113/116 (97%)	89 (79%)	24 (21%)	1	5
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	7
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	11
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	2
15	S	141/153 (92%)	117 (83%)	24 (17%)	2	10
All	All	3591/4162 (86%)	3007 (84%)	584 (16%)	2	11

All (584) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	23	SER
1	A	30	ILE
1	A	36	ARG
1	A	39	GLU
1	A	40	THR
1	A	41	MET
1	A	47	ARG
1	A	49	LYS
1	A	53	LEU
1	A	55	ASP
1	A	62	ASP
1	A	64	ASN
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	74	MET
1	A	84	ILE

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Mol	Chain	Res	Type
1	A	90	VAL
1	A	93	VAL
1	A	100	LYS
1	A	113	LEU
1	A	120	GLU
1	A	124	GLN
1	A	144	THR
1	A	145	LYS
1	A	147	VAL
1	A	149	GLU
1	A	152	VAL
1	A	157	ASP
1	A	174	ILE
1	A	186	LYS
1	A	195	ASP
1	A	196	GLU
1	A	199	LEU
1	A	208	LEU
1	A	225	ASN
1	A	232	GLU
1	A	256	GLN
1	A	265	LYS
1	A	302	THR
1	A	313	GLN
1	A	318	SER
1	A	323	LYS
1	A	324	SER
1	A	329	LEU
1	A	335	ARG
1	A	343	LYS
1	A	351	THR
1	A	353	ILE
1	A	363	GLN
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	409	SER

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Mol	Chain	Res	Type
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
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	487	MET
1	A	504	LEU
1	A	505	CYS
1	A	518	LYS
1	A	523	ILE
1	A	536	LEU
1	A	537	ARG
1	A	541	ILE
1	A	544	ASP
1	A	549	MET
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	593	GLU
1	A	595	THR
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	636	GLU
1	A	644	LYS
1	A	666	ILE
1	A	691	LEU
1	A	693	VAL
1	A	710	LEU
1	A	734	GLU
1	A	738	LYS
1	A	739	ASP

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Mol	Chain	Res	Type
1	A	740	LEU
1	A	756	ILE
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	801	GLU
1	A	806	ARG
1	A	811	GLN
1	A	821	ARG
1	A	822	GLU
1	A	829	VAL
1	A	831	THR
1	A	833	GLU
1	A	834	THR
1	A	846	GLU
1	A	855	THR
1	A	856	THR
1	A	867	ILE
1	A	878	ILE
1	A	896	ARG
1	A	904	THR
1	A	905	ASP
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	927	VAL
1	A	929	LEU
1	A	941	LYS
1	A	964	ILE
1	A	973	ILE
1	A	977	LYS
1	A	983	ILE
1	A	999	VAL
1	A	1001	ARG
1	A	1015	VAL
1	A	1024	SER
1	A	1058	VAL
1	A	1064	VAL
1	A	1067	LEU
1	A	1077	THR
1	A	1081	LEU
1	A	1082	ASN

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Mol	Chain	Res	Type
1	A	1083	THR
1	A	1084	PHE
1	A	1085	HIS
1	A	1093	LYS
1	A	1094	VAL
1	A	1116	LEU
1	A	1118	VAL
1	A	1129	GLU
1	A	1132	LYS
1	A	1142	THR
1	A	1163	ILE
1	A	1167	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1195	LEU
1	A	1205	LYS
1	A	1221	LYS
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1264	GLU
1	A	1274	ARG
1	A	1279	ILE
1	A	1286	LYS
1	A	1288	ASP
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	1325	THR
1	A	1329	THR
1	A	1330	ASN
1	A	1333	ILE
1	A	1334	ASP
1	A	1335	ILE
1	A	1345	ARG
1	A	1366	ARG
1	A	1370	LEU

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Mol	Chain	Res	Type
1	A	1372	VAL
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1393	ASN
1	A	1403	GLU
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1436	ILE
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1454	MET
2	B	21	GLU
2	B	25	ILE
2	B	35	SER
2	B	40	GLU
2	B	43	LEU
2	B	46	GLN
2	B	59	LEU
2	B	63	ILE
2	B	68	THR
2	B	70	ILE
2	B	90	ILE
2	B	98	THR
2	B	109	THR
2	B	130	VAL
2	B	134	LYS
2	B	172	ILE
2	B	175	ARG
2	B	183	GLU
2	B	185	THR
2	B	186	GLU
2	B	205	ILE
2	B	212	LEU
2	B	218	SER
2	B	240	ILE
2	B	241	ARG
2	B	249	ARG
2	B	251	ILE
2	B	261	ARG

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Mol	Chain	Res	Type
2	B	272	THR
2	B	277	LYS
2	B	294	ASP
2	B	298	LEU
2	B	324	ILE
2	B	334	ILE
2	B	349	ILE
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	387	LEU
2	B	388	CYS
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	403	LYS
2	B	406	LEU
2	B	425	THR
2	B	426	LYS
2	B	434	ARG
2	B	446	LEU
2	B	458	LYS
2	B	465	ASN
2	B	469	GLN
2	B	479	VAL
2	B	493	SER
2	B	502	ILE
2	B	507	LYS
2	B	510	LYS
2	B	513	GLN
2	B	516	ASN
2	B	547	VAL
2	B	549	THR
2	B	559	SER
2	B	563	MET
2	B	567	GLU
2	B	576	ASP
2	B	601	ARG
2	B	603	LEU
2	B	604	ARG
2	B	609	ILE
2	B	616	ILE

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Mol	Chain	Res	Type
2	B	621	GLU
2	B	624	LEU
2	B	625	LYS
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	653	VAL
2	B	658	ILE
2	B	664	THR
2	B	680	THR
2	B	690	VAL
2	B	691	GLU
2	B	703	ILE
2	B	708	GLU
2	B	730	ARG
2	B	733	HIS
2	B	736	THR
2	B	737	THR
2	B	754	SER
2	B	766	ARG
2	B	775	LYS
2	B	786	ASN
2	B	790	ASP
2	B	806	THR
2	B	836	GLU
2	B	839	MET
2	B	862	GLN
2	B	864	LYS
2	B	868	MET
2	B	873	THR
2	B	881	ASN
2	B	882	THR
2	B	884	ARG
2	B	889	THR
2	B	895	ASP
2	B	908	GLU
2	B	916	THR
2	B	918	ILE
2	B	942	ARG
2	B	944	THR
2	B	954	VAL
2	B	956	THR

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Mol	Chain	Res	Type
2	B	959	ASP
2	B	964	VAL
2	B	970	THR
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1045	SER
2	B	1049	ASP
2	B	1050	ILE
2	B	1065	GLN
2	B	1072	MET
2	B	1076	HIS
2	B	1097	HIS
2	B	1102	LYS
2	B	1106	ARG
2	B	1123	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1179	GLN
2	B	1189	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1212	ILE
2	B	1216	LEU
2	B	1220	ARG
2	B	1222	ARG
3	C	3	GLU
3	C	4	GLU
3	C	7	GLN
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU

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Mol	Chain	Res	Type
3	C	25	VAL
3	C	26	ASP
3	C	34	ARG
3	C	40	GLU
3	C	50	GLU
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	73	GLN
3	C	75	MET
3	C	94	LYS
3	C	102	GLN
3	C	119	VAL
3	C	121	VAL
3	C	122	SER
3	C	125	MET
3	C	129	ILE
3	C	133	ILE
3	C	142	VAL
3	C	155	LEU
3	C	156	THR
3	C	179	GLU
3	C	189	THR
3	C	203	GLN
3	C	205	LYS
3	C	207	CYS
3	C	215	GLU
3	C	226	ASP
3	C	230	MET
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	254	LYS
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	8	PHE
4	D	9	GLN
4	D	13	ARG
4	D	14	ARG
4	D	21	GLU
4	D	22	GLU

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Mol	Chain	Res	Type
4	D	23	ASN
4	D	28	GLN
4	D	31	GLN
4	D	32	GLU
4	D	38	ILE
4	D	39	ASN
4	D	45	GLU
4	D	46	GLU
4	D	47	LEU
4	D	52	LEU
4	D	53	SER
4	D	60	LYS
4	D	65	GLU
4	D	67	ARG
4	D	74	GLN
4	D	121	LYS
4	D	123	LEU
4	D	126	ILE
4	D	130	LEU
4	D	137	ASN
4	D	139	LYS
4	D	149	THR
4	D	156	ASP
4	D	164	ILE
4	D	168	LYS
4	D	197	SER
4	D	211	LEU
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	6	GLU
5	E	8	ASN
5	E	31	THR
5	E	40	GLU
5	E	70	SER
5	E	78	LEU
5	E	91	LYS
5	E	94	LYS
5	E	104	ASN
5	E	106	GLN
5	E	107	THR

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Mol	Chain	Res	Type
5	E	152	LYS
5	E	154	ILE
5	E	156	LEU
5	E	161	LYS
5	E	165	LEU
5	E	173	SER
5	E	174	GLN
5	E	204	THR
6	F	72	LYS
6	F	103	MET
6	F	109	VAL
6	F	111	LEU
6	F	115	THR
6	F	134	ILE
6	F	148	VAL
7	G	2	PHE
7	G	8	SER
7	G	21	ARG
7	G	22	MET
7	G	34	VAL
7	G	37	SER
7	G	39	THR
7	G	45	ILE
7	G	49	LEU
7	G	61	ILE
7	G	65	ASP
7	G	73	LYS
7	G	83	LYS
7	G	90	THR
7	G	92	VAL
7	G	96	GLN
7	G	107	LYS
7	G	114	LEU
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	152	SER
7	G	153	GLN
7	G	154	VAL

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Mol	Chain	Res	Type
7	G	164	LYS
7	G	165	GLU
7	G	171	ILE
8	H	8	ASP
8	H	9	ILE
8	H	11	GLN
8	H	26	ILE
8	H	38	LEU
8	H	89	LEU
8	H	109	LYS
8	H	110	ASP
8	H	112	ILE
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	136	LYS
8	H	146	ARG
9	I	2	THR
9	I	9	ASP
9	I	20	LYS
9	I	21	GLU
9	I	30	ARG
9	I	35	VAL
9	I	43	VAL
9	I	52	ILE
9	I	54	GLU
9	I	60	GLN
9	I	62	ILE
9	I	64	SER
9	I	70	ARG
9	I	83	ASN
9	I	89	GLN
9	I	90	GLN
9	I	91	ARG
9	I	97	MET
9	I	98	VAL
9	I	107	SER
9	I	113	ASP
9	I	114	GLN
9	I	117	LYS
9	I	119	THR
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	3	VAL
10	J	13	VAL
10	J	28	ASP
10	J	31	ASP
10	J	34	THR
10	J	37	SER
10	J	38	ARG
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	11	LEU
11	K	12	LEU
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	26	LYS
11	K	29	ASN
11	K	31	VAL
11	K	33	ILE
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	64	GLU
11	K	101	LEU
11	K	103	THR
12	L	26	THR
12	L	28	LYS
12	L	35	SER
12	L	38	LEU
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	60	ARG
12	L	61	THR
12	L	66	GLN
12	L	70	ARG
15	S	149	ARG
15	S	156	LEU
15	S	166	HIS
15	S	172	LEU
15	S	178	ILE

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Mol	Chain	Res	Type
15	S	183	ASN
15	S	184	LYS
15	S	202	ILE
15	S	214	LEU
15	S	217	LYS
15	S	218	ILE
15	S	220	ASN
15	S	223	ILE
15	S	228	LEU
15	S	230	THR
15	S	231	CYS
15	S	232	ASP
15	S	234	LYS
15	S	236	LEU
15	S	245	ILE
15	S	262	GLU
15	S	264	SER
15	S	284	LEU
15	S	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	75	ASN
1	A	83	HIS
1	A	92	HIS
1	A	124	GLN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS
1	A	311	GLN
1	A	316	GLN
1	A	339	ASN
1	A	358	ASN
1	A	390	GLN
1	A	427	GLN
1	A	435	HIS
1	A	445	ASN

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Mol	Chain	Res	Type
1	A	471	ASN
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	548	ASN
1	A	631	HIS
1	A	640	GLN
1	A	650	GLN
1	A	698	GLN
1	A	741	ASN
1	A	742	ASN
1	A	757	ASN
1	A	760	GLN
1	A	768	GLN
1	A	811	GLN
1	A	903	ASN
1	A	906	HIS
1	A	926	GLN
1	A	966	ASN
1	A	994	GLN
1	A	1085	HIS
1	A	1128	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1188	GLN
1	A	1211	GLN
1	A	1232	ASN
1	A	1265	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1387	HIS
1	A	1432	GLN
2	B	53	GLN
2	B	178	ASN
2	B	300	HIS
2	B	309	GLN
2	B	350	GLN
2	B	357	GLN
2	B	383	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN

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Mol	Chain	Res	Type
2	B	518	HIS
2	B	587	HIS
2	B	657	HIS
2	B	744	HIS
2	B	767	ASN
2	B	776	GLN
2	B	842	ASN
2	B	862	GLN
2	B	881	ASN
2	B	958	GLN
2	B	975	GLN
2	B	1013	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1097	HIS
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1195	HIS
2	B	1211	ASN
3	C	7	GLN
3	C	17	ASN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	128	ASN
3	C	151	GLN
3	C	167	HIS
3	C	252	GLN
4	D	9	GLN
4	D	37	GLN
4	D	40	HIS
4	D	41	GLN
4	D	150	ASN
4	D	173	HIS
4	D	179	GLN
5	E	5	ASN
5	E	32	GLN
5	E	63	ASN
5	E	115	ASN

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Mol	Chain	Res	Type
5	E	147	HIS
7	G	10	ASN
7	G	14	HIS
7	G	24	GLN
7	G	53	ASN
7	G	57	GLN
7	G	96	GLN
7	G	122	ASN
8	H	134	ASN
9	I	23	ASN
9	I	89	GLN
10	J	26	GLN
11	K	65	HIS
11	K	96	ASN
15	S	169	GLN
15	S	173	HIS
15	S	187	ASN
15	S	252	ASN
15	S	255	ASN
15	S	257	GLN
15	S	283	GLN
15	S	285	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/5 (100%)	3 (60%)	2 (40%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	C
14	P	9	C
14	P	10	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	7	C
14	P	8	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	$\# Z > 2$
16	BRU	T	22	14,16	18,21,22	0.70	0	25,30,33	2.18	9 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BRU	T	22	14,16	-	2/7/21/22	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	22	BRU	C5-C4-N3	4.86	118.93	113.34
16	T	22	BRU	N3-C2-N1	4.69	120.99	114.89
16	T	22	BRU	C4-N3-C2	-4.63	121.27	127.34
16	T	22	BRU	O4-C4-C5	-3.46	121.39	125.80
16	T	22	BRU	O4'-C1'-N1	3.18	113.51	107.86
16	T	22	BRU	BR-C5-C4	2.81	121.26	118.02
16	T	22	BRU	O2-C2-N3	-2.28	117.27	121.49
16	T	22	BRU	C6-C5-C4	-2.21	118.43	120.67
16	T	22	BRU	C6-N1-C2	-2.08	119.23	121.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\# Z > 2$
21	PGE	L	71	-	9,9,9	0.48	0	8,8,8	0.32	0
20	EPE	A	1735	-	15,15,15	0.59	0	19,20,20	2.04	6 (31%)
19	ACT	A	1734	-	3,3,3	0.74	0	3,3,3	1.20	0
19	ACT	B	1225	-	3,3,3	0.94	0	3,3,3	1.79	1 (33%)

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
21	PGE	L	71	-	-	3/7/7/7	-
20	EPE	A	1735	-	-	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(°)
20	A	1735	EPE	C5-N4-C3	4.97	119.54	108.84
20	A	1735	EPE	C7-N4-C3	3.53	120.64	111.24
20	A	1735	EPE	C7-N4-C5	3.17	119.68	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1735	EPE	C9-N1-C2	-2.72	103.99	111.24
19	B	1225	ACT	OXT-C-CH3	2.35	124.90	115.05
20	A	1735	EPE	C3-C2-N1	2.33	115.35	110.65
20	A	1735	EPE	C5-C6-N1	-2.24	106.14	110.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	L	71	PGE	O2-C3-C4-O3
21	L	71	PGE	O3-C5-C6-O4
21	L	71	PGE	O1-C1-C2-O2
20	A	1735	EPE	C10-C9-N1-C2
20	A	1735	EPE	C10-C9-N1-C6
20	A	1735	EPE	C8-C7-N4-C5

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1735	EPE	2	0
19	A	1734	ACT	1	0
19	B	1225	ACT	1	0

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	1426/1733 (82%)	-0.25	21 (1%) 72 53	67, 109, 163, 215	0
2	B	1108/1224 (90%)	-0.04	44 (3%) 42 28	69, 126, 191, 217	0
3	C	266/318 (83%)	-0.40	0 100 100	86, 116, 160, 193	0
4	D	177/221 (80%)	-0.02	11 (6%) 26 18	81, 118, 183, 202	0
5	E	214/215 (99%)	-0.30	1 (0%) 87 76	88, 141, 188, 203	0
6	F	84/155 (54%)	-0.56	2 (2%) 59 40	70, 90, 122, 136	0
7	G	171/171 (100%)	-0.30	1 (0%) 85 73	82, 105, 148, 171	0
8	H	133/146 (91%)	0.15	6 (4%) 38 25	121, 158, 197, 205	0
9	I	119/122 (97%)	0.02	5 (4%) 40 26	123, 156, 197, 216	0
10	J	65/70 (92%)	-0.36	2 (3%) 51 35	95, 117, 159, 177	0
11	K	114/120 (95%)	-0.42	2 (1%) 67 49	85, 112, 157, 173	0
12	L	46/70 (65%)	0.43	3 (6%) 25 17	93, 158, 183, 202	0
13	N	7/14 (50%)	0.83	1 (14%) 6 5	217, 222, 231, 234	0
14	P	5/5 (100%)	1.36	1 (20%) 3 2	238, 239, 244, 247	0
15	S	164/178 (92%)	0.83	26 (15%) 5 4	116, 181, 240, 254	0
16	T	12/27 (44%)	0.25	0 100 100	162, 195, 247, 252	0
All	All	4111/4789 (85%)	-0.13	126 (3%) 51 35	67, 119, 191, 254	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	THR	8.0
2	B	509	ALA	7.0
2	B	70	ILE	6.8
12	L	27	LEU	6.8
2	B	335	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
15	S	171	ILE	5.4
4	D	24	ALA	5.1
2	B	507	LYS	4.9
2	B	446	LEU	4.9
1	A	568	PRO	4.8
1	A	2	VAL	4.8
15	S	157	TYR	4.6
2	B	90	ILE	4.4
8	H	63	LEU	4.4
15	S	286	THR	4.4
4	D	18	VAL	4.3
1	A	3	GLY	4.2
1	A	1254	ALA	4.1
15	S	156	LEU	4.0
2	B	710	LEU	4.0
10	J	65	PRO	4.0
1	A	51	GLY	4.0
4	D	25	ALA	4.0
2	B	134	LYS	4.0
8	H	132	LEU	3.7
2	B	508	LEU	3.6
1	A	254	GLU	3.6
15	S	309	SER	3.6
1	A	186	LYS	3.5
15	S	202	ILE	3.5
2	B	388	CYS	3.5
6	F	155	LEU	3.5
11	K	114	LEU	3.4
2	B	471	LYS	3.4
2	B	391	ASP	3.4
1	A	310	GLY	3.4
12	L	26	THR	3.4
15	S	180	SER	3.3
15	S	227	PHE	3.3
1	A	65	LEU	3.2
14	P	11	C	3.1
4	D	76	LYS	3.1
2	B	249	ARG	3.1
2	B	646	LEU	3.1
4	D	4	SER	3.1
12	L	25	ALA	3.1
2	B	731	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	709	ASP	3.0
2	B	715	ALA	3.0
2	B	883	LEU	3.0
2	B	447	ALA	3.0
1	A	1172	LEU	3.0
1	A	288	ALA	3.0
15	S	199	TYR	2.9
2	B	244	LEU	2.9
15	S	172	LEU	2.9
4	D	221	TYR	2.9
2	B	470	LYS	2.9
4	D	15	LEU	2.8
2	B	473	MET	2.8
8	H	90	ALA	2.8
1	A	255	SER	2.8
15	S	285	GLN	2.8
9	I	119	THR	2.8
1	A	1173	HIS	2.7
8	H	135	LEU	2.7
15	S	158	ASP	2.7
2	B	502	ILE	2.7
2	B	1224	PHE	2.7
13	N	2	DG	2.6
15	S	190	THR	2.6
2	B	919	SER	2.6
2	B	69	LEU	2.6
2	B	108	VAL	2.6
6	F	72	LYS	2.6
15	S	195	TYR	2.6
2	B	250	PHE	2.5
1	A	1243	VAL	2.5
15	S	225	PRO	2.5
2	B	918	ILE	2.5
15	S	162	LYS	2.5
1	A	250	ILE	2.4
2	B	367	LEU	2.4
15	S	284	LEU	2.4
2	B	251	ILE	2.4
15	S	193	ALA	2.4
2	B	164	LYS	2.4
10	J	64	ASN	2.4
2	B	734	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	436	VAL	2.4
1	A	38	PRO	2.3
15	S	292	PRO	2.3
2	B	365	THR	2.3
9	I	55	THR	2.3
15	S	146	HIS	2.3
2	B	277	LYS	2.3
2	B	364	ILE	2.3
2	B	643	ASP	2.3
9	I	90	GLN	2.3
8	H	76	THR	2.3
8	H	136	LYS	2.3
15	S	244	LYS	2.3
2	B	313	MET	2.2
15	S	185	VAL	2.2
15	S	235	ASP	2.2
2	B	31	TRP	2.2
4	D	16	LYS	2.2
4	D	10	THR	2.2
4	D	13	ARG	2.1
2	B	1049	ASP	2.1
15	S	174	THR	2.1
9	I	52	ILE	2.1
1	A	1259	MET	2.1
1	A	223	GLY	2.1
2	B	320	ASP	2.1
11	K	113	THR	2.1
15	S	260	THR	2.1
1	A	1093	LYS	2.1
9	I	117	LYS	2.1
4	D	8	PHE	2.1
5	E	152	LYS	2.1
15	S	287	ARG	2.1
7	G	64	THR	2.1
2	B	468	GLU	2.1
2	B	133	LYS	2.0
1	A	707	GLY	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	BRU	T	22	20/21	0.71	0.16	138,213,293,294	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(Å ²)	Q<0.9
21	PGE	L	71	10/10	0.87	0.22	116,149,279,292	0
19	ACT	B	1225	4/4	0.95	0.16	46,51,87,298	0
19	ACT	A	1734	4/4	0.97	0.11	72,95,126,151	0
20	EPE	A	1735	15/15	0.98	0.08	25,77,245,245	0
17	ZN	L	1071	1/1	0.99	0.02	158,158,158,158	0
17	ZN	S	999	1/1	0.99	0.02	215,215,215,215	0
17	ZN	I	1122	1/1	0.99	0.03	186,186,186,186	0
17	ZN	A	2457	1/1	1.00	0.03	87,87,87,87	0
17	ZN	B	2225	1/1	1.00	0.03	94,94,94,94	0
18	MG	A	2458	1/1	1.00	0.02	83,83,83,83	0
17	ZN	C	1269	1/1	1.00	0.01	94,94,94,94	0
17	ZN	I	1121	1/1	1.00	0.01	130,130,130,130	0
17	ZN	A	2456	1/1	1.00	0.02	145,145,145,145	0
17	ZN	J	1066	1/1	1.00	0.02	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.