



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:08 PM UTC

PDB ID : 4C2M / pdb_00004c2m
Title : Structure of RNA polymerase I at 2.8 Å resolution
Authors : Engel, C.; Sainsbury, S.; Cheung, A.C.; Kostrewa, D.; Cramer, P.
Deposited on : 2013-08-19
Resolution : 2.80 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

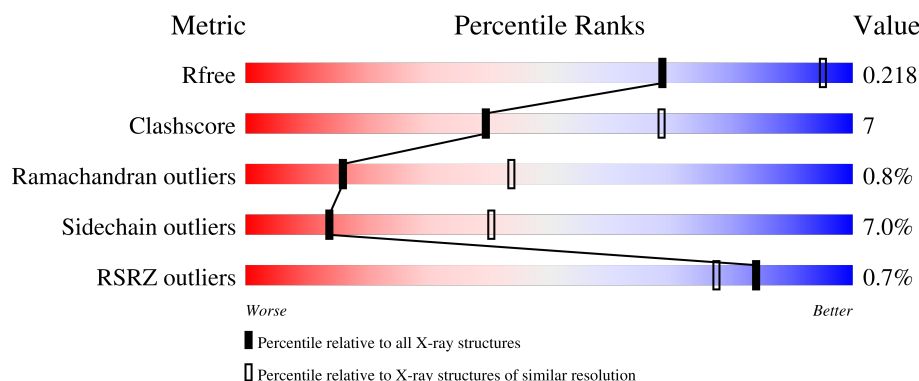
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



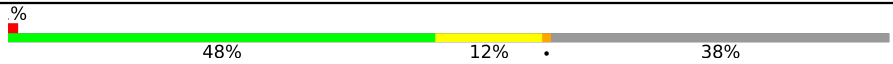
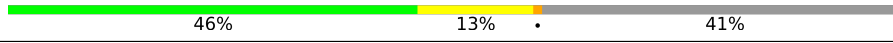
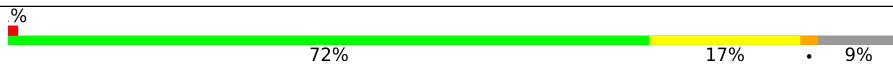
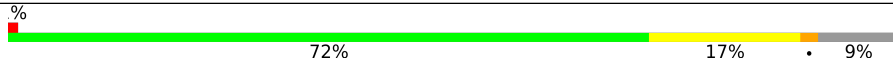
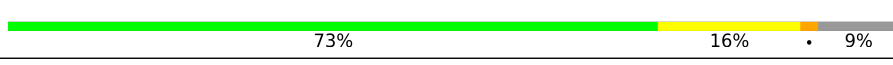
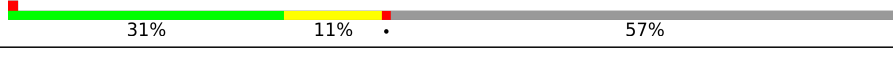
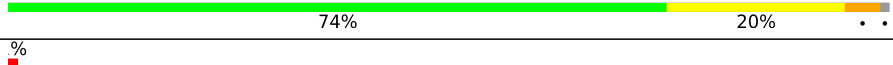
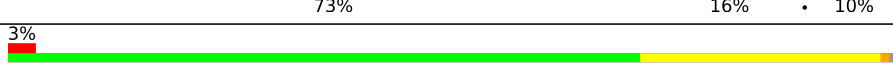
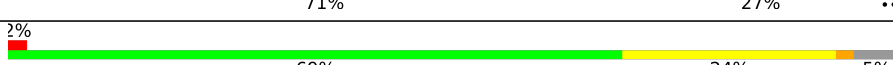
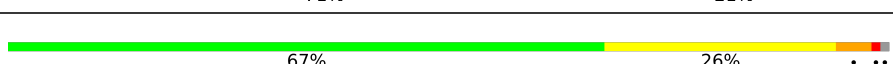
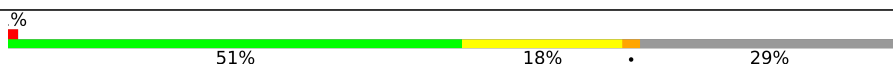
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	1	70	36% 24% • 37%
1	L	70	3% 36% 24% • 37%
2	2	415	19% 5% 75%
2	M	415	19% 7% 74%
3	3	233	% 47% 14% • 38%

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Mol	Chain	Length	Quality of chain
3	N	233	
4	4	326	
4	G	326	
4	O	326	
4	V	326	
5	A	1664	
5	P	1664	
6	B	1203	
6	Q	1203	
7	C	335	
7	R	335	
8	D	137	
8	S	137	
9	E	215	
9	T	215	
10	F	155	
10	U	155	
11	H	146	
11	W	146	
12	I	125	
12	X	125	
13	J	70	
13	Y	70	
14	K	142	
14	Z	142	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 69107 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 POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			
1	L	44	Total	C	N	O	S	0	0	0
			352	217	70	61	4			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	103	Total	C	N	O		0	0	0
			814	517	134	163				
2	M	108	Total	C	N	O		0	0	0
			856	543	142	171				

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	145	Total	C	N	O	S	0	0	0
			1152	735	189	224	4			
3	N	145	Total	C	N	O	S	0	0	0
			1151	735	188	224	4			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	54	Total	C	N	O		0	0	0
			430	262	69	99				
4	G	193	Total	C	N	O	S	0	0	0
			1526	985	262	274	5			
4	O	52	Total	C	N	O		0	0	0
			413	253	64	96				
4	V	197	Total	C	N	O	S	0	0	0
			1557	1001	266	285	5			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	1521	Total	C	N	O	S	0	0	0
			12019	7579	2088	2290	62			
5	P	1518	Total	C	N	O	S	0	0	0
			12000	7567	2085	2286	62			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	1182	Total	C	N	O	S	0	0	0
			9386	5934	1648	1753	51			
6	Q	1164	Total	C	N	O	S	0	0	0
			9261	5862	1623	1725	51			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	305	Total	C	N	O	S	0	0	0
			2423	1539	416	460	8			
7	R	305	Total	C	N	O	S	0	0	0
			2423	1539	416	460	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	D	58	Total	C	N	O	0	0	0
			459	289	78	92			
8	S	59	Total	C	N	O	0	0	0
			467	293	79	95			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	E	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			
9	T	212	Total	C	N	O	S	0	0	0
			1735	1102	306	316	11			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			
10	U	100	Total	C	N	O	S	0	0	0
			823	522	144	154	3			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			
11	W	131	Total	C	N	O	S	0	0	0
			1052	664	176	208	4			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	124	Total	C	N	O	S	0	0	0
			943	584	160	190	9			
12	X	119	Total	C	N	O	S	0	0	0
			900	557	152	182	9			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			
13	Y	69	Total	C	N	O	S	0	0	0
			569	362	101	100	6			

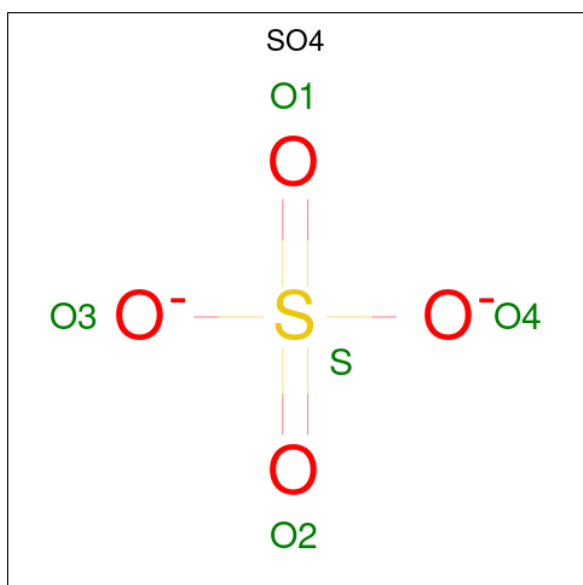
- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	101	Total	C	N	O	S	0	0	0
			793	496	130	162	5			
14	Z	100	Total	C	N	O	S	0	0	0
			786	491	129	161	5			

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	1	1	Total Zn 1 1	0	0
15	A	2	Total Zn 2 2	0	0
15	B	1	Total Zn 1 1	0	0
15	I	2	Total Zn 2 2	0	0
15	J	1	Total Zn 1 1	0	0
15	L	1	Total Zn 1 1	0	0
15	P	2	Total Zn 2 2	0	0
15	Q	1	Total Zn 1 1	0	0
15	X	2	Total Zn 2 2	0	0
15	Y	1	Total Zn 1 1	0	0

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total O S 5 4 1	0	0
16	Q	1	Total O S 5 4 1	0	0

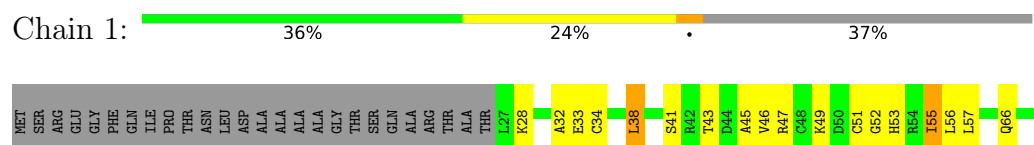
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	3	1	Total O 1 1	0	0
17	A	96	Total O 96 96	0	0
17	B	62	Total O 62 62	0	0
17	C	1	Total O 1 1	0	0
17	D	3	Total O 3 3	0	0
17	E	4	Total O 4 4	0	0
17	F	4	Total O 4 4	0	0
17	G	1	Total O 1 1	0	0
17	H	10	Total O 10 10	0	0
17	I	3	Total O 3 3	0	0
17	N	3	Total O 3 3	0	0
17	O	1	Total O 1 1	0	0
17	P	43	Total O 43 43	0	0
17	Q	15	Total O 15 15	0	0
17	R	1	Total O 1 1	0	0
17	S	1	Total O 1 1	0	0
17	T	4	Total O 4 4	0	0
17	U	4	Total O 4 4	0	0
17	V	2	Total O 2 2	0	0
17	W	1	Total O 1 1	0	0
17	X	2	Total O 2 2	0	0

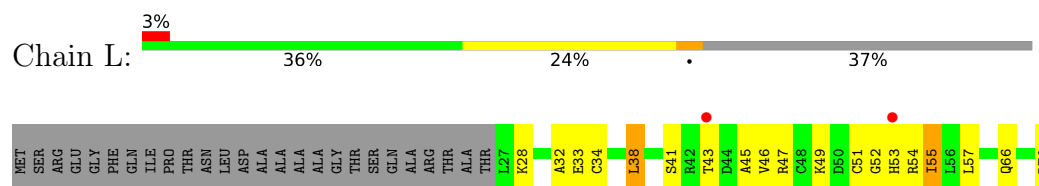
3 Residue-property plots [i](#)

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.

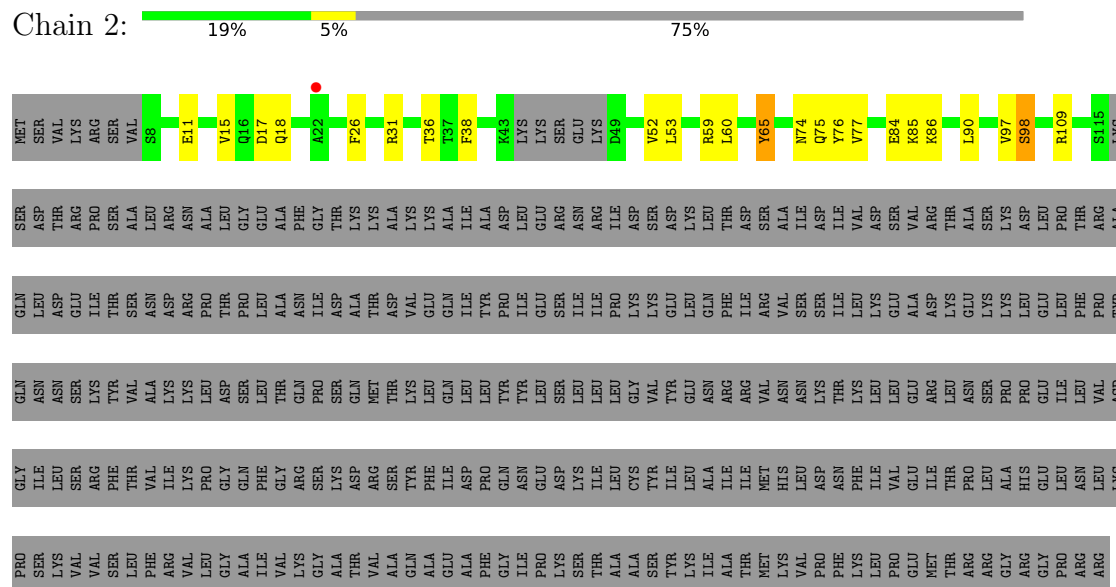
- Molecule 1: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



- Molecule 1: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



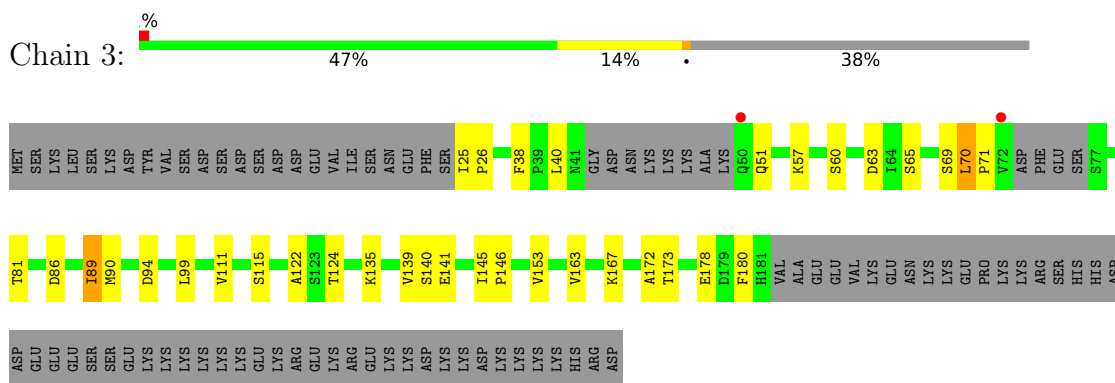
- Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



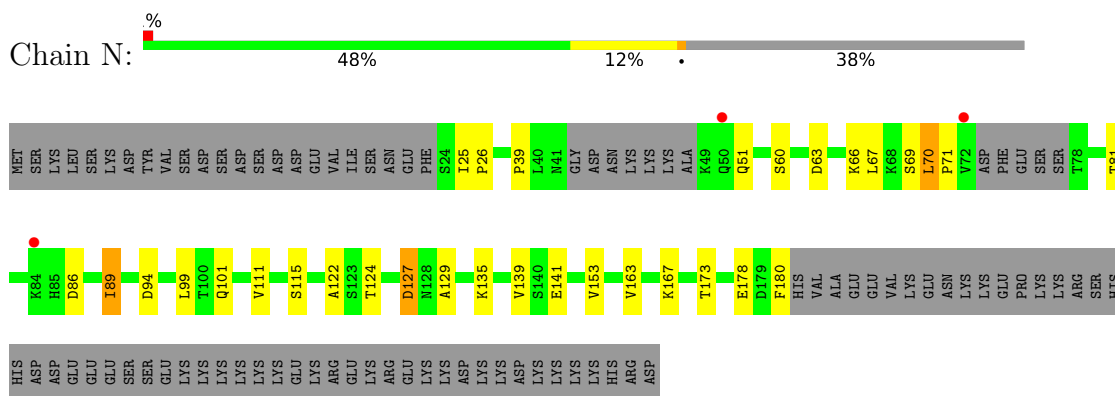
- Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



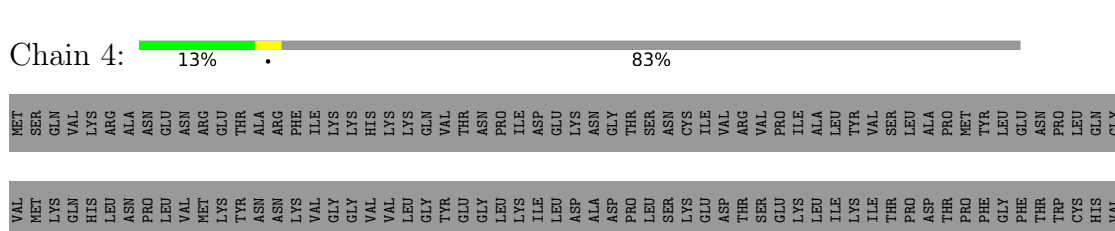
● Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

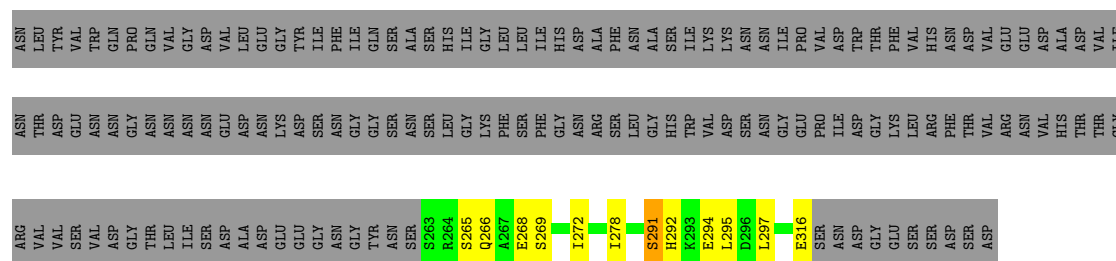


● Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



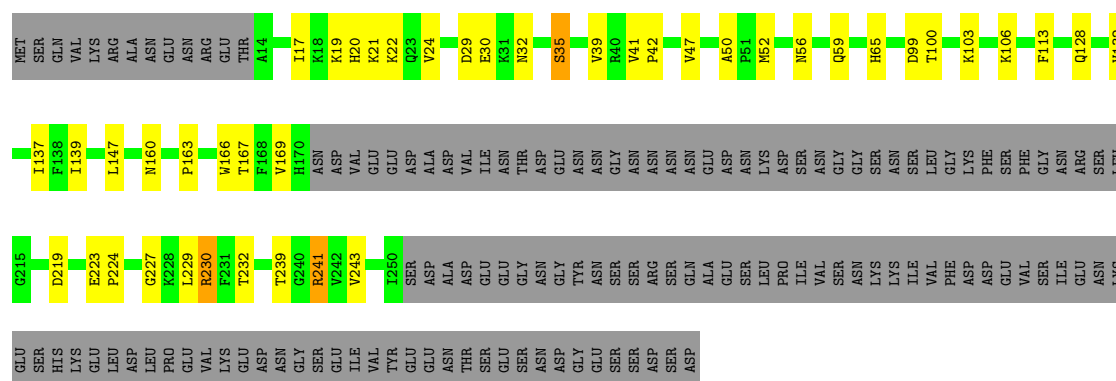
● Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43





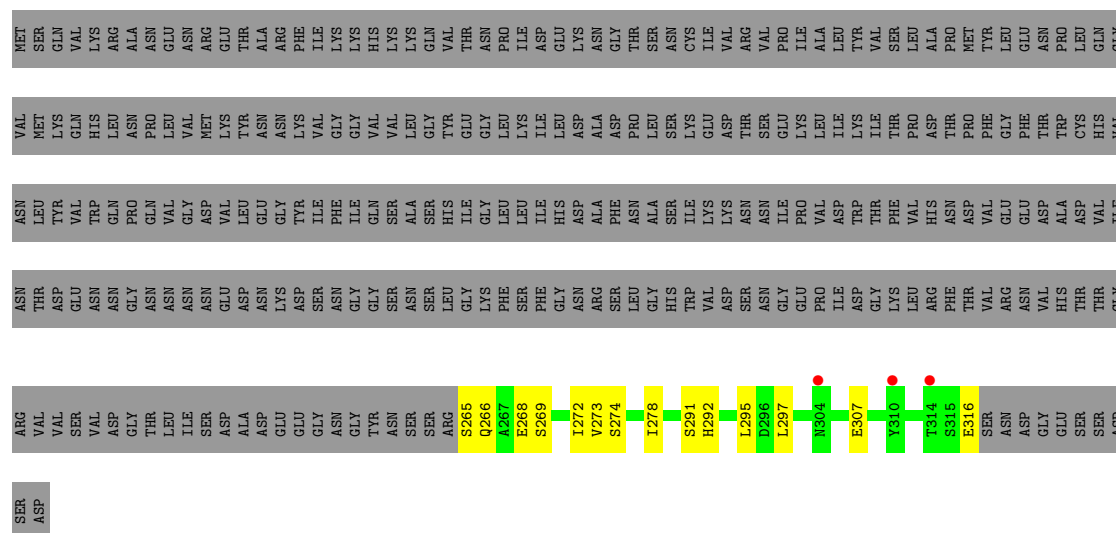
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain G: 46% 13% 41%



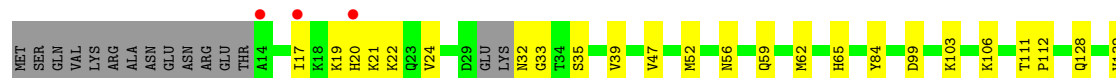
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain O: 12% 84%

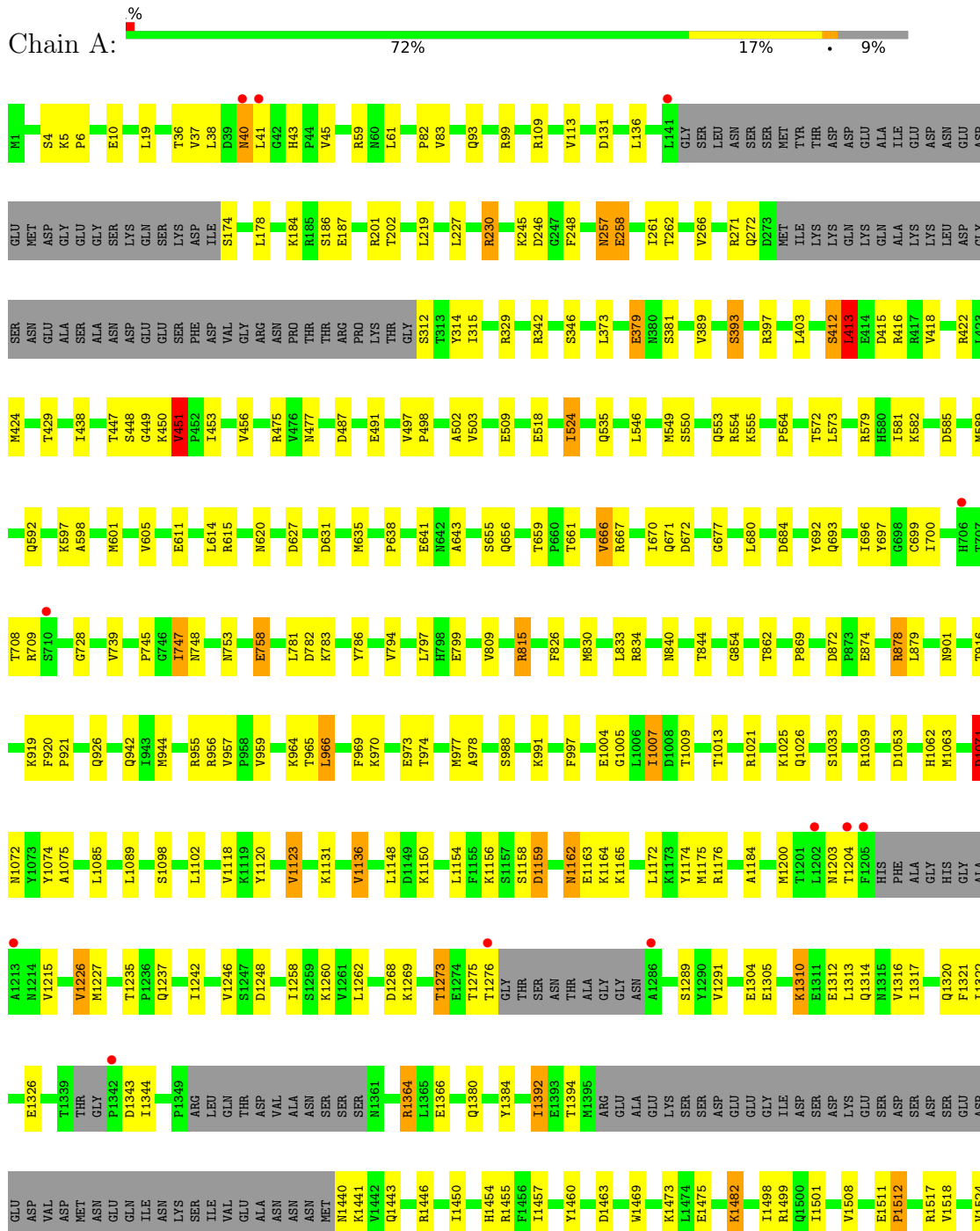


• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

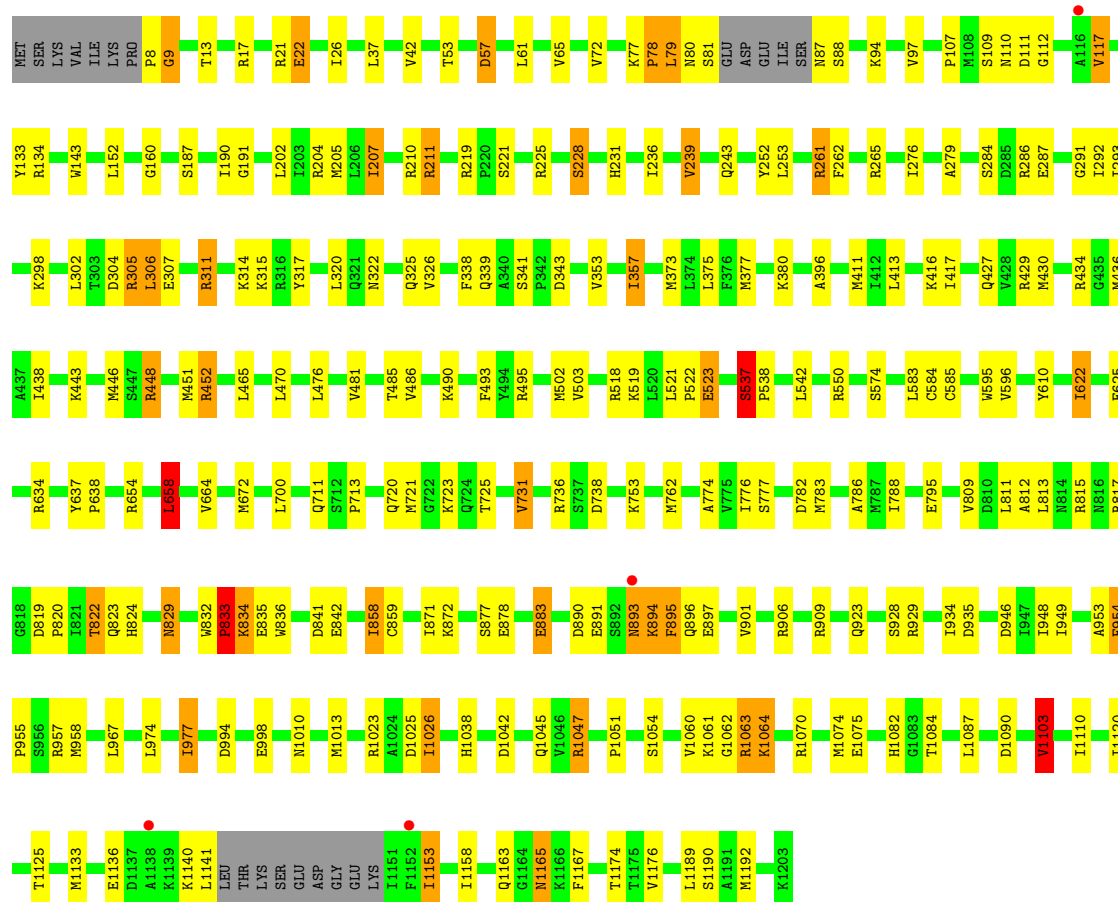
Chain V: 2% 48% 12% 40%



● Molecule 5: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190

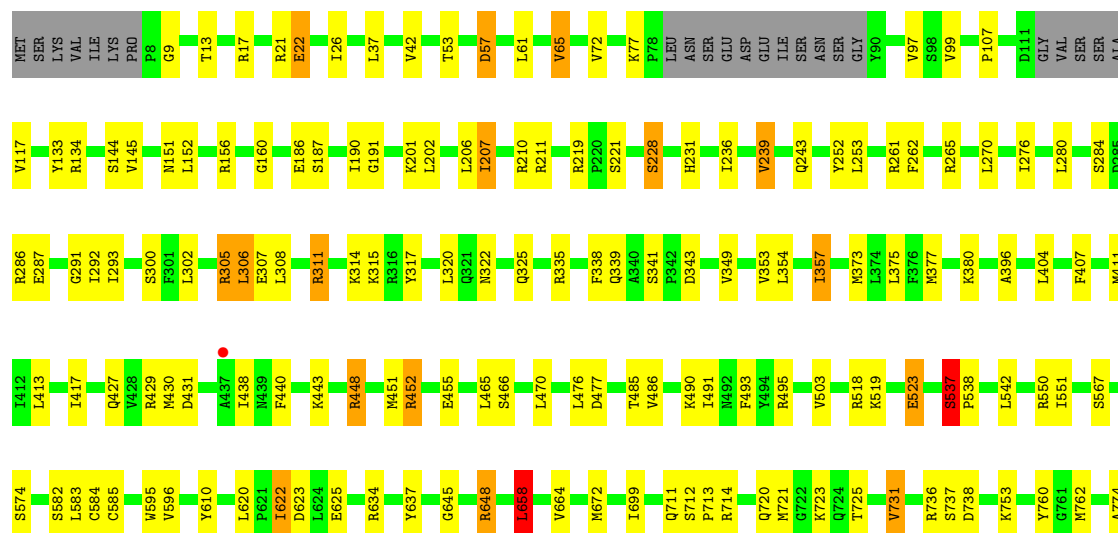


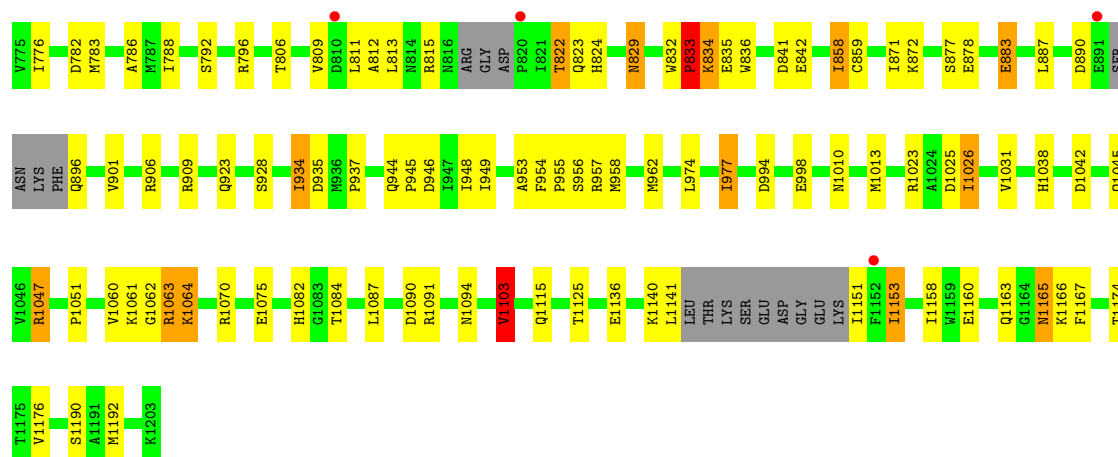
Chain B:  77% 18% . .



• Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

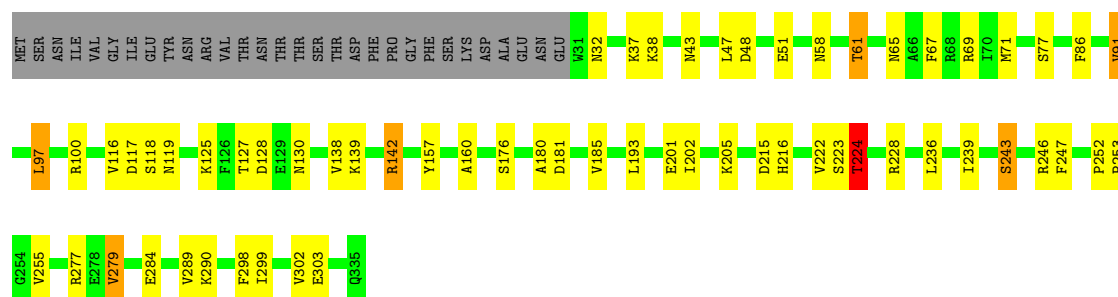
Chain Q:  75% 19% . .





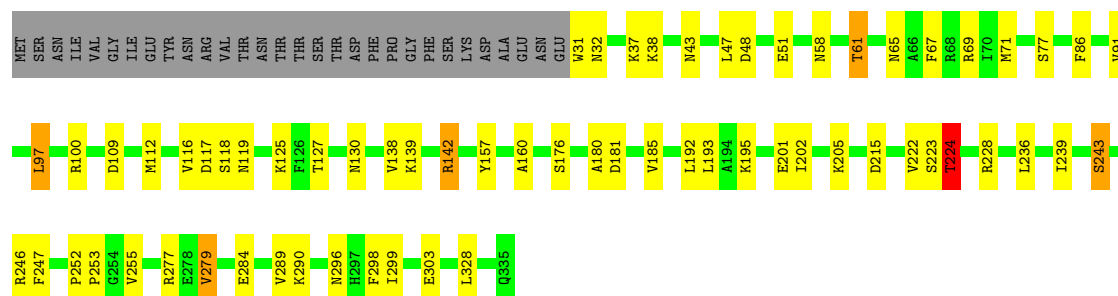
• Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C: 73% 16% 9%



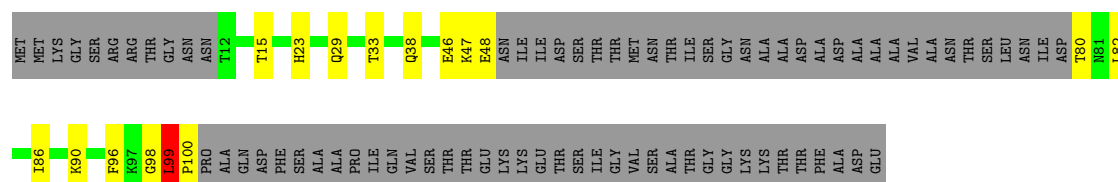
• Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain R: 71% 18% 9%

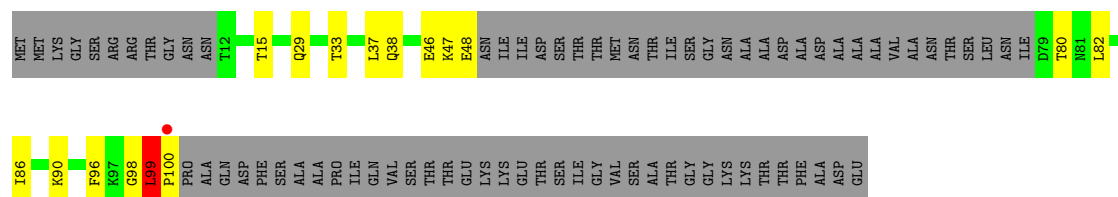
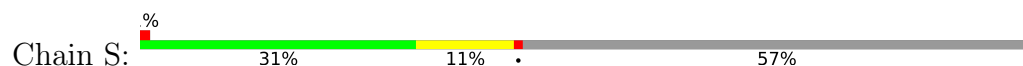


• Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

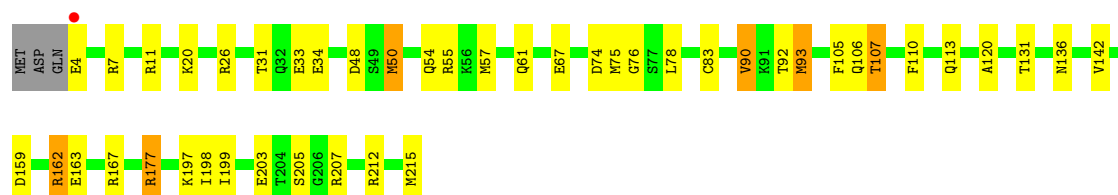
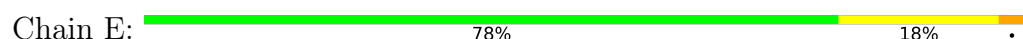
Chain D: 31% 11% 58%



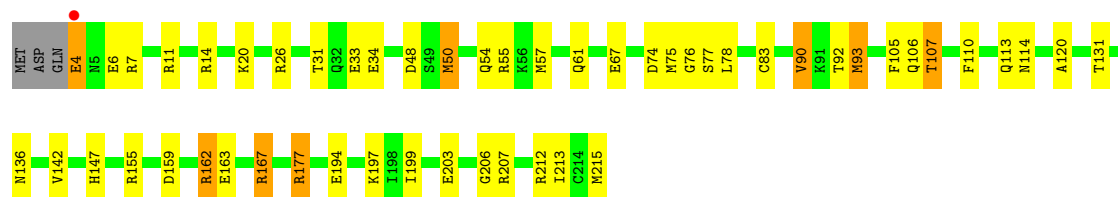
- Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14



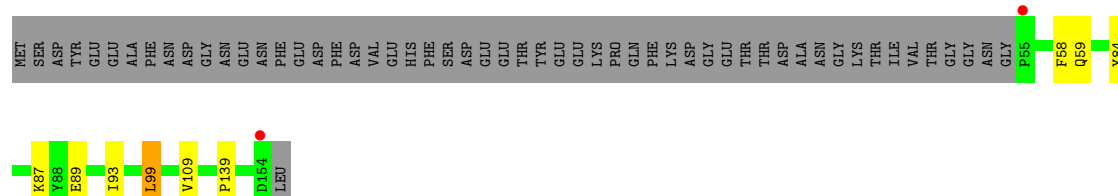
- Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



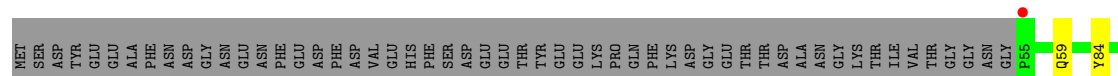
- Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



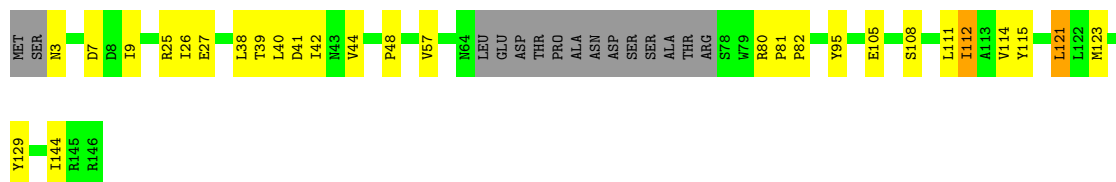
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2





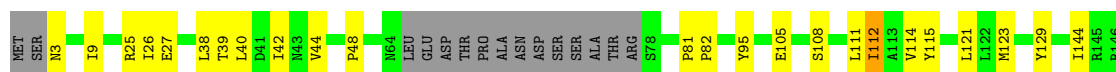
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 71% 18% 10%



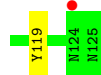
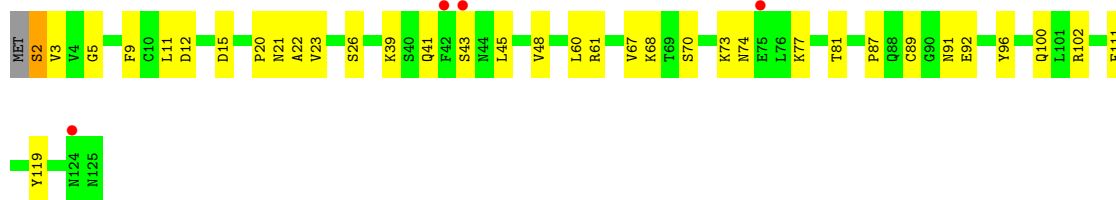
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain W: 73% 16% 10%



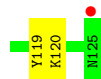
- Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I: 3% 71% 27% 2%



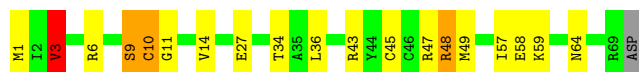
- Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain X: 2% 69% 24% 5%



- Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 71% 21% 2%



- Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



● Molecule 14: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



● Molecule 14: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.74Å 139.02Å 209.55Å 108.06° 95.40° 93.85°	Depositor
Resolution (Å)	39.29 – 2.80 39.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.29-2.80) 99.9 (39.29-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.169 , 0.210 0.181 , 0.218	Depositor DCC
R_{free} test set	6494 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	69107	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	1	0.45	0/354	0.91	2/468 (0.4%)
1	L	0.50	0/354	0.91	2/468 (0.4%)
2	2	0.41	0/829	0.85	0/1114
2	M	0.50	0/872	0.87	0/1170
3	3	0.41	0/1174	0.83	3/1584 (0.2%)
3	N	0.48	0/1172	0.88	1/1580 (0.1%)
4	4	0.50	0/434	1.01	2/584 (0.3%)
4	G	0.50	0/1564	0.84	3/2127 (0.1%)
4	O	0.52	0/417	1.01	3/562 (0.5%)
4	V	0.50	0/1594	0.87	1/2168 (0.0%)
5	A	0.63	0/12236	0.96	38/16523 (0.2%)
5	P	0.59	0/12216	0.94	35/16495 (0.2%)
6	B	0.63	0/9594	0.97	32/12967 (0.2%)
6	Q	0.54	0/9465	0.93	29/12789 (0.2%)
7	C	0.58	2/2475 (0.1%)	0.94	7/3354 (0.2%)
7	R	0.54	2/2475 (0.1%)	0.93	7/3354 (0.2%)
8	D	0.51	0/465	0.81	0/630
8	S	0.54	0/473	0.84	0/641
9	E	0.49	0/1771	0.87	4/2383 (0.2%)
9	T	0.51	0/1771	0.88	3/2383 (0.1%)
10	F	0.58	0/838	0.87	0/1129
10	U	0.57	0/838	0.85	0/1129
11	H	0.52	0/1070	0.88	0/1449
11	W	0.48	0/1070	0.86	1/1449 (0.1%)
12	I	0.54	0/956	0.87	0/1288
12	X	0.51	0/912	0.86	0/1229
13	J	0.59	0/578	0.98	6/775 (0.8%)
13	Y	0.52	0/578	0.98	5/775 (0.6%)
14	K	0.54	0/804	0.93	4/1083 (0.4%)
14	Z	0.52	0/796	0.91	6/1072 (0.6%)
All	All	0.57	4/70145 (0.0%)	0.93	194/94722 (0.2%)

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
5	A	0	2
5	P	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	58	ASN	CG-ND2	-8.39	1.15	1.33
7	R	58	ASN	CG-ND2	-7.77	1.17	1.33
7	R	58	ASN	CG-OD1	-7.51	1.09	1.23
7	C	58	ASN	CG-OD1	-7.28	1.09	1.23

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	223	SER	N-CA-C	-11.20	99.92	112.57
5	P	1071	ASP	N-CA-C	-10.05	97.27	110.53
5	A	1071	ASP	N-CA-C	-9.94	97.41	110.53
7	C	223	SER	N-CA-C	-9.68	101.63	112.57
5	P	1348	VAL	CA-C-N	8.62	130.62	119.84
5	P	1348	VAL	C-N-CA	8.62	130.62	119.84
5	A	956	ARG	CA-C-O	8.58	122.91	117.94
5	A	666	VAL	CB-CA-C	-8.39	102.43	110.65
5	P	666	VAL	CB-CA-C	-7.92	102.89	110.65
6	B	537	SER	CA-C-N	-7.80	111.95	121.00
6	B	537	SER	C-N-CA	-7.80	111.95	121.00
5	A	1344	ILE	N-CA-C	7.78	117.84	110.53
5	P	201	ARG	N-CA-C	7.52	121.56	112.38
7	C	279	VAL	CB-CA-C	-7.40	102.41	111.88
6	B	893	ASN	N-CA-C	7.38	120.24	111.02
6	Q	537	SER	CA-C-N	-7.33	112.50	121.00
6	Q	537	SER	C-N-CA	-7.33	112.50	121.00
5	P	956	ARG	CA-C-O	7.32	122.18	117.94
5	A	413	LEU	N-CA-C	-6.94	104.97	113.50
5	A	201	ARG	N-CA-C	6.90	120.80	112.38
7	R	279	VAL	CB-CA-C	-6.87	103.09	111.88
5	P	413	LEU	N-CA-C	-6.85	105.08	113.50
5	P	258	GLU	N-CA-C	6.82	118.37	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	1103	VAL	CB-CA-C	-6.70	100.51	110.82
6	Q	1023	ARG	NE-CZ-NH2	-6.60	113.26	119.20
6	B	894	LYS	CB-CA-C	-6.57	108.29	117.23
6	B	219	ARG	CA-C-N	6.54	128.01	119.84
6	B	219	ARG	C-N-CA	6.54	128.01	119.84
6	B	1103	VAL	CB-CA-C	-6.53	100.76	110.82
5	A	1123	VAL	CB-CA-C	-6.49	103.54	112.04
7	C	51	GLU	N-CA-C	6.44	119.67	109.50
6	Q	550	ARG	NE-CZ-NH2	-6.44	113.41	119.20
6	B	1023	ARG	NE-CZ-NH2	-6.42	113.43	119.20
5	A	397	ARG	CD-NE-CZ	6.36	133.31	124.40
5	P	1123	VAL	CB-CA-C	-6.35	103.72	112.04
6	B	261	ARG	CD-NE-CZ	6.32	133.24	124.40
13	J	64	ASN	CA-C-N	6.30	126.00	119.82
13	J	64	ASN	C-N-CA	6.30	126.00	119.82
9	E	203	GLU	N-CA-C	-6.25	104.57	111.82
6	Q	219	ARG	CA-C-N	6.25	127.65	119.84
6	Q	219	ARG	C-N-CA	6.25	127.65	119.84
6	B	622	ILE	CB-CA-C	-6.23	102.95	112.05
6	Q	832	TRP	CA-C-N	6.23	127.63	119.84
6	Q	832	TRP	C-N-CA	6.23	127.63	119.84
6	B	452	ARG	NE-CZ-NH2	-6.20	113.62	119.20
6	Q	452	ARG	NE-CZ-NH2	-6.20	113.62	119.20
9	T	167	ARG	CD-NE-CZ	6.15	133.01	124.40
13	Y	3	VAL	CA-C-N	-6.15	113.64	119.85
13	Y	3	VAL	C-N-CA	-6.15	113.64	119.85
6	B	72	VAL	N-CA-C	6.08	117.23	108.48
5	A	59	ARG	CD-NE-CZ	6.06	132.88	124.40
5	P	397	ARG	CD-NE-CZ	6.01	132.81	124.40
6	B	448	ARG	NE-CZ-NH2	-6.00	113.80	119.20
5	P	59	ARG	CD-NE-CZ	5.98	132.77	124.40
5	A	329	ARG	NE-CZ-NH2	-5.96	113.83	119.20
6	B	452	ARG	CD-NE-CZ	5.96	132.75	124.40
6	Q	648	ARG	NE-CZ-NH2	-5.96	113.84	119.20
5	P	1524	VAL	N-CA-C	5.94	116.43	108.11
13	Y	64	ASN	CA-C-N	5.90	125.60	119.82
13	Y	64	ASN	C-N-CA	5.90	125.60	119.82
6	B	658	LEU	N-CA-C	-5.88	100.96	109.31
6	B	832	TRP	CA-C-N	5.88	127.18	119.84
6	B	832	TRP	C-N-CA	5.88	127.18	119.84
5	A	59	ARG	NE-CZ-NH2	-5.87	113.92	119.20
5	A	258	GLU	N-CA-C	5.87	118.15	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	429	ARG	NE-CZ-NH2	-5.86	113.93	119.20
5	P	397	ARG	NE-CZ-NH2	-5.86	113.93	119.20
6	Q	634	ARG	NE-CZ-NH2	-5.85	113.93	119.20
5	A	329	ARG	CD-NE-CZ	5.84	132.58	124.40
4	4	297	LEU	CA-C-N	5.82	127.11	119.84
4	4	297	LEU	C-N-CA	5.82	127.11	119.84
5	P	659	THR	CA-C-N	-5.81	113.76	120.04
5	P	659	THR	C-N-CA	-5.81	113.76	120.04
5	P	329	ARG	CD-NE-CZ	5.80	132.52	124.40
5	A	956	ARG	CB-CA-C	-5.78	108.75	117.07
9	T	167	ARG	NE-CZ-NH2	-5.77	114.00	119.20
5	P	342	ARG	NE-CZ-NH2	-5.77	114.01	119.20
6	B	448	ARG	CD-NE-CZ	5.76	132.47	124.40
9	E	167	ARG	NE-CZ-NH2	-5.75	114.03	119.20
5	P	1544	ASN	CB-CA-C	-5.74	101.87	110.88
5	P	1203	ASN	N-CA-C	5.73	117.78	109.07
9	T	203	GLU	N-CA-C	-5.72	105.18	111.82
7	R	51	GLU	N-CA-C	5.72	118.54	109.50
6	Q	550	ARG	CD-NE-CZ	5.72	132.41	124.40
14	Z	95	HIS	CA-C-N	5.71	126.98	119.84
14	Z	95	HIS	C-N-CA	5.71	126.98	119.84
5	A	416	ARG	NE-CZ-NH2	-5.70	114.07	119.20
6	Q	622	ILE	CB-CA-C	-5.70	103.73	112.05
14	K	44	ARG	CD-NE-CZ	5.69	132.37	124.40
4	O	297	LEU	CA-C-N	5.69	126.95	119.84
4	O	297	LEU	C-N-CA	5.69	126.95	119.84
6	Q	452	ARG	CD-NE-CZ	5.68	132.35	124.40
6	Q	634	ARG	CD-NE-CZ	5.68	132.35	124.40
6	Q	620	LEU	CA-C-N	5.67	126.15	120.14
6	Q	620	LEU	C-N-CA	5.67	126.15	120.14
6	Q	314	LYS	N-CA-C	-5.67	103.01	110.43
5	A	1203	ASN	N-CA-C	5.62	117.62	109.07
5	P	422	ARG	NE-CZ-NH2	-5.62	114.14	119.20
14	K	44	ARG	NE-CZ-NH2	-5.62	114.14	119.20
14	K	95	HIS	CA-C-N	5.61	126.86	119.84
14	K	95	HIS	C-N-CA	5.61	126.86	119.84
5	A	416	ARG	CD-NE-CZ	5.61	132.25	124.40
5	A	1007	ILE	CB-CA-C	-5.60	104.58	112.14
5	P	422	ARG	CD-NE-CZ	5.60	132.24	124.40
6	B	634	ARG	CD-NE-CZ	5.59	132.23	124.40
6	B	634	ARG	NE-CZ-NH2	-5.57	114.19	119.20
5	A	659	THR	CA-C-N	-5.57	114.02	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	659	THR	C-N-CA	-5.57	114.02	119.64
11	W	111	LEU	N-CA-C	5.57	118.63	109.72
5	P	956	ARG	CB-CA-C	-5.56	109.06	117.07
7	R	142	ARG	CD-NE-CZ	5.56	132.18	124.40
6	B	429	ARG	CD-NE-CZ	5.55	132.18	124.40
5	P	59	ARG	NE-CZ-NH2	-5.55	114.20	119.20
5	A	422	ARG	CD-NE-CZ	5.55	132.16	124.40
5	P	397	ARG	NE-CZ-NH1	5.54	127.04	121.50
5	A	498	PRO	CA-C-N	5.54	125.37	119.28
5	A	498	PRO	C-N-CA	5.54	125.37	119.28
6	B	261	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	1	52	GLY	N-CA-C	-5.51	107.66	115.43
5	A	549	MET	N-CA-C	5.50	119.06	110.32
13	J	3	VAL	CA-C-N	-5.49	114.30	119.85
13	J	3	VAL	C-N-CA	-5.49	114.30	119.85
5	P	416	ARG	NE-CZ-NH2	-5.47	114.27	119.20
4	G	241	ARG	CD-NE-CZ	5.46	132.05	124.40
5	A	397	ARG	NE-CZ-NH1	5.46	126.96	121.50
6	B	211	ARG	CB-CA-C	-5.44	100.94	109.70
5	P	416	ARG	CD-NE-CZ	5.42	131.99	124.40
1	L	28	LYS	N-CA-C	5.42	117.94	111.71
7	C	142	ARG	CD-NE-CZ	5.42	131.98	124.40
5	P	1007	ILE	CB-CA-C	-5.41	104.84	112.14
1	L	52	GLY	N-CA-C	-5.40	107.81	115.43
3	N	127	ASP	N-CA-C	-5.39	106.18	114.16
6	Q	1023	ARG	CD-NE-CZ	5.38	131.93	124.40
5	A	245	LYS	N-CA-C	5.37	118.03	109.65
6	Q	658	LEU	N-CA-C	-5.37	101.68	109.31
7	R	142	ARG	NE-CZ-NH2	-5.36	114.38	119.20
5	A	1364	ARG	NE-CZ-NH2	-5.34	114.39	119.20
6	Q	550	ARG	NE-CZ-NH1	5.34	126.84	121.50
5	A	397	ARG	NE-CZ-NH2	-5.34	114.39	119.20
13	Y	11	GLY	N-CA-C	-5.34	107.98	114.92
9	E	167	ARG	CD-NE-CZ	5.33	131.86	124.40
4	V	175	GLU	N-CA-C	5.32	117.26	108.49
6	Q	261	ARG	NE-CZ-NH2	-5.30	114.42	119.20
6	Q	72	VAL	N-CA-C	5.30	116.11	108.48
4	G	219	ASP	N-CA-C	5.29	116.83	109.31
5	A	1482	LYS	N-CA-C	5.28	117.89	110.23
4	O	273	VAL	N-CA-C	5.28	115.91	110.36
5	P	329	ARG	NE-CZ-NH2	-5.28	114.45	119.20
5	A	422	ARG	NE-CZ-NH2	-5.25	114.47	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	744	MET	CA-C-N	5.25	125.19	119.78
5	P	744	MET	C-N-CA	5.25	125.19	119.78
14	Z	44	ARG	CD-NE-CZ	5.25	131.75	124.40
4	G	241	ARG	NE-CZ-NH2	-5.24	114.48	119.20
6	Q	261	ARG	CD-NE-CZ	5.24	131.74	124.40
7	C	185	VAL	CA-C-N	-5.24	114.53	119.76
7	C	185	VAL	C-N-CA	-5.24	114.53	119.76
6	Q	448	ARG	CD-NE-CZ	5.23	131.73	124.40
5	A	1543	SER	CA-C-N	5.23	127.72	120.29
5	A	1543	SER	C-N-CA	5.23	127.72	120.29
3	3	38	PHE	CA-C-N	5.23	126.37	119.84
3	3	38	PHE	C-N-CA	5.23	126.37	119.84
5	A	59	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	1	28	LYS	N-CA-C	5.22	117.71	111.71
6	Q	452	ARG	NE-CZ-NH1	5.21	126.72	121.50
7	R	185	VAL	CA-C-N	-5.21	114.55	119.76
7	R	185	VAL	C-N-CA	-5.21	114.55	119.76
5	A	329	ARG	NE-CZ-NH1	5.20	126.70	121.50
7	C	142	ARG	NE-CZ-NH2	-5.17	114.55	119.20
6	Q	429	ARG	NE-CZ-NH2	-5.17	114.55	119.20
5	A	1364	ARG	CD-NE-CZ	5.16	131.63	124.40
14	Z	93	ILE	CA-C-N	5.16	126.29	119.84
14	Z	93	ILE	C-N-CA	5.16	126.29	119.84
6	B	211	ARG	N-CA-C	5.14	117.49	110.24
13	J	9	SER	CA-C-N	5.12	127.41	120.44
13	J	9	SER	C-N-CA	5.12	127.41	120.44
5	P	230	ARG	NE-CZ-NH2	-5.12	114.59	119.20
6	B	1054	SER	N-CA-C	5.12	117.52	111.33
6	B	88	SER	N-CA-C	5.11	118.14	109.76
5	P	549	MET	N-CA-C	5.11	118.44	110.32
6	B	314	LYS	N-CA-C	-5.10	103.75	110.43
5	A	342	ARG	CD-NE-CZ	5.10	131.54	124.40
5	P	1364	ARG	CD-NE-CZ	5.09	131.53	124.40
5	P	872	ASP	CA-C-N	5.09	126.20	119.84
5	P	872	ASP	C-N-CA	5.09	126.20	119.84
5	A	1524	VAL	N-CA-C	5.08	115.44	108.12
9	E	167	ARG	NE-CZ-NH1	5.07	126.57	121.50
6	Q	448	ARG	NE-CZ-NH2	-5.05	114.66	119.20
6	B	1110	ILE	CB-CA-C	-5.04	105.50	111.65
6	B	261	ARG	NE-CZ-NH1	5.03	126.53	121.50
5	A	342	ARG	NE-CZ-NH2	-5.02	114.68	119.20
3	3	86	ASP	N-CA-C	5.01	117.66	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	521	LEU	CA-C-N	5.00	125.03	119.32
6	B	521	LEU	C-N-CA	5.00	125.03	119.32
14	Z	44	ARG	NE-CZ-NH2	-5.00	114.70	119.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1343	ASP	Peptide
5	A	781	LEU	Peptide
5	P	781	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	352	0	374	9	0
1	L	352	0	374	8	0
2	2	814	0	804	12	0
2	M	856	0	855	14	0
3	3	1152	0	1163	18	0
3	N	1151	0	1169	17	0
4	4	430	0	407	17	0
4	G	1526	0	1540	24	0
4	O	413	0	389	13	0
4	V	1557	0	1555	19	0
5	A	12019	0	12078	175	1
5	P	12000	0	12058	173	1
6	B	9386	0	9279	161	0
6	Q	9261	0	9161	166	0
7	C	2423	0	2412	34	0
7	R	2423	0	2412	39	0
8	D	459	0	462	7	0
8	S	467	0	466	7	0
9	E	1735	0	1764	22	0
9	T	1735	0	1764	25	0
10	F	823	0	841	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	U	823	0	841	8	0
11	H	1052	0	1021	12	0
11	W	1052	0	1021	9	0
12	I	943	0	929	21	0
12	X	900	0	879	23	0
13	J	569	0	585	13	0
13	Y	569	0	585	15	0
14	K	793	0	790	14	0
14	Z	786	0	782	19	0
15	1	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	P	2	0	0	0	0
15	Q	1	0	0	0	0
15	X	2	0	0	0	0
15	Y	1	0	0	0	0
16	B	5	0	0	1	0
16	Q	5	0	0	1	0
17	3	1	0	0	0	0
17	A	96	0	0	5	0
17	B	62	0	0	1	0
17	C	1	0	0	0	0
17	D	3	0	0	0	0
17	E	4	0	0	0	0
17	F	4	0	0	0	0
17	G	1	0	0	0	0
17	H	10	0	0	0	0
17	I	3	0	0	1	0
17	N	3	0	0	0	0
17	O	1	0	0	0	0
17	P	43	0	0	0	0
17	Q	15	0	0	0	0
17	R	1	0	0	0	0
17	S	1	0	0	0	0
17	T	4	0	0	0	0
17	U	4	0	0	0	0
17	V	2	0	0	0	0
17	W	1	0	0	0	0
17	X	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	69107	0	68760	923	1

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 (923) 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)
5:A:620:ASN:OD1	5:A:667:ARG:NH2	2.01	0.93
6:B:713:PRO:HG3	12:I:100:GLN:HG3	1.48	0.93
6:Q:26:ILE:HG12	13:Y:58:GLU:HG2	1.51	0.93
5:A:1009:THR:HG21	12:I:102:ARG:H	1.38	0.88
14:Z:66:VAL:HG12	14:Z:67:GLU:HG2	1.55	0.88
6:B:26:ILE:HG12	13:J:58:GLU:HG2	1.56	0.88
6:Q:713:PRO:HG3	12:X:100:GLN:HG3	1.56	0.87
6:B:77:LYS:NZ	6:B:438:ILE:O	2.07	0.86
14:K:66:VAL:HG12	14:K:67:GLU:HG2	1.57	0.85
5:P:620:ASN:OD1	5:P:667:ARG:NH2	2.10	0.85
5:P:1009:THR:HG21	12:X:102:ARG:H	1.39	0.84
7:C:100:ARG:NH2	13:J:3:VAL:O	2.10	0.84
1:I:34:CYS:HB3	1:I:51:CYS:SG	2.18	0.83
6:B:776:ILE:HB	6:B:1026:ILE:HD13	1.60	0.83
7:C:303:GLU:OE1	13:J:43:ARG:NH2	2.11	0.83
6:B:894:LYS:O	6:B:896:GLN:N	2.11	0.82
6:B:396:ALA:HB1	6:B:523:GLU:HG3	1.62	0.81
7:R:100:ARG:NH2	13:Y:3:VAL:O	2.12	0.81
7:R:303:GLU:OE1	13:Y:43:ARG:NH2	2.14	0.81
6:B:152:LEU:HD13	6:B:443:LYS:HG3	1.62	0.80
1:L:34:CYS:HB3	1:L:51:CYS:SG	2.21	0.80
5:A:1316:VAL:HG21	5:A:1498:ILE:HA	1.63	0.79
4:G:22:LYS:HD3	4:G:128:GLN:HG2	1.65	0.79
6:Q:518:ARG:NH2	6:Q:537:SER:O	2.15	0.79
5:P:1242:ILE:HG22	5:P:1536:ILE:HG22	1.64	0.78
6:Q:776:ILE:HB	6:Q:1026:ILE:HD13	1.64	0.78
6:Q:878:GLU:OE2	6:Q:909:ARG:NH1	2.16	0.77
6:B:878:GLU:OE2	6:B:909:ARG:NH1	2.17	0.77
6:Q:77:LYS:NZ	6:Q:438:ILE:O	2.18	0.77
6:B:974:LEU:O	13:J:47:ARG:NH1	2.18	0.76
2:2:60:LEU:HD11	12:X:12:ASP:HB3	1.67	0.76
6:Q:396:ALA:HB1	6:Q:523:GLU:HG3	1.66	0.76
5:P:834:ARG:NH2	6:Q:994:ASP:OD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:974:LEU:O	13:Y:47:ARG:NH1	2.20	0.75
5:P:1316:VAL:HG21	5:P:1498:ILE:HA	1.67	0.74
6:B:518:ARG:NH2	6:B:537:SER:O	2.21	0.74
6:B:211:ARG:NH2	6:B:243:GLN:OE1	2.19	0.74
5:A:497:VAL:HG22	5:A:635:MET:HE1	1.70	0.74
5:P:497:VAL:HG22	5:P:635:MET:HE1	1.69	0.73
6:Q:291:GLY:HA3	6:Q:375:LEU:HD13	1.70	0.73
5:A:38:LEU:HB2	4:O:291:SER:HB3	1.69	0.73
5:P:524:ILE:O	5:P:554:ARG:NH1	2.22	0.72
5:P:641:GLU:HB2	10:U:99:LEU:HD13	1.71	0.72
11:H:40:LEU:HD13	11:H:123:MET:HE3	1.72	0.72
11:W:40:LEU:HD13	11:W:123:MET:HE3	1.72	0.72
5:P:1289:SER:HB3	5:P:1475:GLU:HG2	1.71	0.71
6:Q:711:GLN:HG2	6:Q:713:PRO:HD2	1.71	0.71
5:P:1248:ASP:OD1	5:P:1517:ARG:NH1	2.22	0.71
6:Q:211:ARG:NH2	6:Q:243:GLN:OE1	2.24	0.71
12:I:2:SER:HB2	12:I:11:LEU:HD21	1.72	0.71
2:M:38:PHE:HB3	2:M:53:LEU:HD11	1.73	0.71
5:A:524:ILE:O	5:A:554:ARG:NH1	2.23	0.70
5:A:1007:ILE:HG23	6:B:518:ARG:HD3	1.73	0.70
6:B:1165:ASN:OD1	6:B:1165:ASN:N	2.24	0.70
6:Q:152:LEU:HD13	6:Q:443:LYS:HG3	1.72	0.70
12:X:2:SER:HB2	12:X:11:LEU:HD21	1.72	0.70
5:A:99:ARG:O	5:A:109:ARG:NH2	2.24	0.70
12:I:12:ASP:HB3	2:M:60:LEU:HD11	1.74	0.70
5:A:1366:GLU:CD	6:B:204:ARG:HH22	2.00	0.69
5:A:1246:VAL:O	5:A:1517:ARG:NH2	2.25	0.69
6:Q:623:ASP:O	6:Q:648:ARG:NH2	2.24	0.69
5:A:1120:TYR:O	9:E:207:ARG:NH2	2.22	0.69
5:P:942:GLN:HB2	6:Q:958:MET:HE1	1.75	0.69
6:Q:431:ASP:OD1	6:Q:452:ARG:NH2	2.26	0.69
8:D:99:LEU:HB3	8:D:100:PRO:CD	2.22	0.69
7:R:125:LYS:O	7:R:130:ASN:ND2	2.26	0.68
8:S:99:LEU:HB3	8:S:100:PRO:CD	2.23	0.68
5:A:1184:ALA:HB2	5:A:1649:VAL:HG11	1.75	0.68
6:Q:1165:ASN:OD1	6:Q:1165:ASN:N	2.24	0.68
9:T:76:GLY:HA3	9:T:106:GLN:HB2	1.75	0.68
5:P:1184:ALA:HB2	5:P:1649:VAL:HG11	1.75	0.68
5:A:601:MET:HE2	5:A:656:GLN:HB2	1.75	0.68
6:B:291:GLY:HA3	6:B:375:LEU:HD13	1.74	0.68
6:Q:645:GLY:O	6:Q:648:ARG:HD3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:38:PHE:HB3	2:2:53:LEU:HD11	1.73	0.68
7:R:127:THR:H	7:R:130:ASN:HB2	1.60	0.67
6:B:42:VAL:HG21	6:B:190:ILE:HB	1.76	0.67
7:C:127:THR:H	7:C:130:ASN:HB2	1.59	0.67
5:A:964:LYS:NZ	6:B:672:MET:O	2.27	0.67
5:A:113:VAL:HG21	5:A:178:LEU:HD13	1.77	0.67
5:P:477:ASN:OD1	6:Q:1047:ARG:NH1	2.27	0.67
7:C:125:LYS:O	7:C:130:ASN:ND2	2.27	0.67
6:Q:923:GLN:NE2	6:Q:953:ALA:O	2.28	0.67
9:E:76:GLY:HA3	9:E:106:GLN:HB2	1.76	0.66
6:Q:341:SER:OG	6:Q:343:ASP:OD1	2.12	0.66
6:B:977:ILE:HD11	3:N:163:VAL:HG11	1.77	0.66
6:Q:465:LEU:HA	6:Q:485:THR:HG21	1.76	0.66
3:3:163:VAL:HG11	6:Q:977:ILE:HD11	1.78	0.66
5:P:699:CYS:O	5:P:815:ARG:NH1	2.29	0.65
9:T:55:ARG:NH2	9:T:113:GLN:OE1	2.29	0.65
5:P:99:ARG:O	5:P:109:ARG:NH2	2.29	0.65
5:A:1273:THR:HG23	12:I:48:VAL:HG22	1.79	0.65
5:P:109:ARG:NH1	5:P:230:ARG:O	2.28	0.65
4:V:22:LYS:HD3	4:V:128:GLN:HG2	1.78	0.65
6:B:341:SER:OG	6:B:343:ASP:OD1	2.13	0.65
5:P:131:ASP:HB2	9:T:215:MET:HE1	1.77	0.65
9:T:20:LYS:HE2	9:T:34:GLU:HG2	1.78	0.65
5:A:109:ARG:NH1	5:A:230:ARG:O	2.29	0.65
6:B:711:GLN:HG2	6:B:713:PRO:HD2	1.79	0.65
5:A:1322:ILE:HD12	5:A:1457:ILE:HD11	1.79	0.64
6:B:373:MET:HG3	6:B:377:MET:HE3	1.79	0.64
9:E:197:LYS:HD3	9:E:199:ILE:HD11	1.79	0.64
5:A:799:GLU:HG3	5:A:1062:HIS:ND1	2.11	0.64
5:A:641:GLU:HB2	10:F:99:LEU:HD13	1.79	0.64
5:A:1511:GLU:HG3	12:I:73:LYS:HE3	1.80	0.64
6:B:923:GLN:NE2	6:B:953:ALA:O	2.30	0.64
6:Q:493:PHE:CE2	6:Q:762:MET:HE1	2.33	0.64
8:S:99:LEU:HB3	8:S:100:PRO:HD3	1.80	0.64
5:P:966:LEU:HD22	5:P:997:PHE:CZ	2.33	0.64
5:A:834:ARG:NH2	6:B:994:ASP:OD1	2.31	0.64
11:H:44:VAL:HG22	11:H:48:PRO:HA	1.80	0.64
5:P:1200:MET:HE3	5:P:1575:ILE:HD12	1.80	0.63
8:D:99:LEU:HB3	8:D:100:PRO:HD3	1.78	0.63
12:I:43:SER:N	17:I:2001:HOH:O	2.28	0.63
6:B:493:PHE:HE2	6:B:762:MET:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:373:MET:HG3	6:Q:377:MET:HE3	1.80	0.63
6:B:894:LYS:H	1:L:54:ARG:HH21	1.47	0.63
9:E:20:LYS:HE2	9:E:34:GLU:HG2	1.80	0.63
5:P:1556:GLU:OE2	9:T:212:ARG:NH1	2.32	0.63
5:A:942:GLN:HB2	6:B:958:MET:HE1	1.80	0.63
5:P:964:LYS:NZ	6:Q:672:MET:O	2.31	0.63
11:W:25:ARG:NH1	11:W:27:GLU:OE2	2.32	0.63
5:A:1366:GLU:OE2	6:B:204:ARG:NH2	2.31	0.63
5:A:477:ASN:OD1	6:B:1047:ARG:NH1	2.26	0.62
5:A:942:GLN:HB2	6:B:958:MET:CE	2.30	0.62
11:W:44:VAL:HG22	11:W:48:PRO:HA	1.80	0.62
6:Q:228:SER:HB2	6:Q:253:LEU:HD23	1.81	0.62
5:P:601:MET:HE2	5:P:656:GLN:HB2	1.81	0.61
6:Q:946:ASP:OD2	13:Y:48:ARG:NH2	2.33	0.61
6:B:493:PHE:CE2	6:B:762:MET:HE1	2.35	0.61
9:E:93:MET:HG3	9:E:120:ALA:HB1	1.82	0.61
5:P:67:LEU:HD11	6:Q:1115:GLN:HG3	1.83	0.61
5:P:1005:GLY:O	5:P:1009:THR:HG23	2.01	0.61
6:B:1061:LYS:HD2	4:O:316:GLU:HG3	1.82	0.61
5:P:246:ASP:HB3	5:P:248:PHE:H	1.66	0.61
6:Q:380:LYS:HE3	6:Q:637:TYR:HB3	1.81	0.61
6:Q:493:PHE:HE2	6:Q:762:MET:HE1	1.65	0.61
7:R:86:PHE:HE2	7:R:205:LYS:HG3	1.66	0.61
6:B:923:GLN:NE2	6:B:957:ARG:HD2	2.16	0.61
5:A:246:ASP:HB3	5:A:248:PHE:H	1.66	0.60
5:P:1004:GLU:OE2	6:Q:519:LYS:NZ	2.34	0.60
6:Q:935:ASP:OD1	7:R:69:ARG:NH2	2.34	0.60
7:R:139:LYS:HG2	7:R:201:GLU:HB3	1.83	0.60
5:A:1005:GLY:O	5:A:1009:THR:HG23	2.01	0.60
6:B:465:LEU:HA	6:B:485:THR:HG21	1.83	0.60
5:P:942:GLN:HB2	6:Q:958:MET:CE	2.32	0.60
11:H:25:ARG:NH1	11:H:27:GLU:OE2	2.34	0.60
6:Q:338:PHE:HZ	6:Q:357:ILE:HD12	1.67	0.60
5:A:699:CYS:O	5:A:815:ARG:NH1	2.35	0.60
6:B:538:PRO:HB2	6:B:542:LEU:HG	1.84	0.60
5:P:799:GLU:HG3	5:P:1062:HIS:ND1	2.17	0.59
9:T:93:MET:HG3	9:T:120:ALA:HB1	1.84	0.59
6:B:228:SER:HB2	6:B:253:LEU:HD23	1.84	0.59
3:N:89:ILE:HG12	3:N:139:VAL:HG22	1.85	0.59
6:B:110:ASN:O	6:B:112:GLY:N	2.35	0.59
4:4:316:GLU:HG2	6:Q:1070:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1226:VAL:HG12	5:A:1227:MET:HG2	1.83	0.59
5:A:415:ASP:HA	5:A:418:VAL:HG12	1.84	0.59
5:A:43:HIS:HD2	5:P:61:LEU:HD22	1.68	0.59
5:A:572:THR:HA	4:G:52:MET:HE3	1.85	0.59
6:B:495:ARG:HA	6:B:723:LYS:HG2	1.85	0.58
14:Z:68:GLU:HG2	14:Z:72:LEU:HD23	1.85	0.58
1:1:33:GLU:HG3	1:1:53:HIS:CE1	2.37	0.58
6:B:829:ASN:OD1	6:B:829:ASN:N	2.36	0.58
5:P:415:ASP:HA	5:P:418:VAL:HG12	1.84	0.58
2:2:75:GLN:HB2	3:3:60:SER:HA	1.85	0.58
5:P:113:VAL:HG21	5:P:178:LEU:HD13	1.85	0.58
5:A:598:ALA:HB1	5:A:601:MET:HE3	1.85	0.58
6:B:923:GLN:HG2	6:B:949:ILE:HD11	1.84	0.58
6:Q:1013:MET:SD	6:Q:1026:ILE:HG12	2.43	0.58
14:K:68:GLU:HG2	14:K:72:LEU:HD23	1.86	0.58
9:E:55:ARG:NH2	9:E:113:GLN:OE1	2.36	0.58
6:Q:538:PRO:HB2	6:Q:542:LEU:HG	1.84	0.58
1:1:38:LEU:HD12	1:1:49:LYS:HG3	1.85	0.58
6:B:935:ASP:OD1	7:C:69:ARG:NH2	2.37	0.58
5:A:41:LEU:HD12	5:P:61:LEU:HD21	1.85	0.58
7:R:65:ASN:O	7:R:69:ARG:HG3	2.04	0.58
2:2:11:GLU:N	2:2:86:LYS:O	2.34	0.58
4:G:30:GLU:HA	4:G:32:ASN:N	2.18	0.58
6:Q:210:ARG:NH2	6:Q:625:GLU:OE2	2.37	0.58
2:M:10:ILE:HB	3:N:70:LEU:HB3	1.86	0.57
5:A:1074:TYR:HE2	5:A:1159:ASP:HB3	1.68	0.57
5:A:1556:GLU:OE2	9:E:212:ARG:NH1	2.37	0.57
4:G:56:ASN:HB3	4:G:59:GLN:HB3	1.86	0.57
1:L:33:GLU:HG3	1:L:53:HIS:CE1	2.39	0.57
5:P:4:SER:HB2	5:P:573:LEU:HD22	1.85	0.57
1:L:38:LEU:HD12	1:L:49:LYS:HG3	1.85	0.57
5:P:1322:ILE:HD12	5:P:1457:ILE:HD11	1.85	0.57
6:Q:923:GLN:NE2	6:Q:957:ARG:HD2	2.18	0.57
3:3:69:SER:OG	3:3:70:LEU:N	2.35	0.57
4:4:265:SER:OG	4:4:266:GLN:N	2.38	0.57
4:4:291:SER:HB3	5:P:38:LEU:HB2	1.86	0.57
5:A:1053:ASP:HB3	9:E:205:SER:HB2	1.86	0.57
14:K:49:LEU:HD23	14:K:51:THR:HG23	1.86	0.57
6:B:877:SER:HB3	6:B:1064:LYS:HE3	1.87	0.57
6:Q:322:ASN:HB3	6:Q:325:GLN:H	1.70	0.57
6:Q:762:MET:HE2	6:Q:762:MET:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:159:ASP:OD1	9:T:162:ARG:NH1	2.37	0.57
5:A:4:SER:HB2	5:A:573:LEU:HD22	1.87	0.57
5:A:797:LEU:HD13	5:A:809:VAL:HG21	1.87	0.57
6:Q:21:ARG:NH1	6:Q:22:GLU:OE1	2.38	0.57
5:A:1235:THR:O	5:A:1544:ASN:ND2	2.38	0.57
8:S:48:GLU:OE2	8:S:90:LYS:NZ	2.38	0.57
7:C:86:PHE:HE2	7:C:205:LYS:HG3	1.69	0.56
4:V:56:ASN:HB3	4:V:59:GLN:HB3	1.87	0.56
5:A:1004:GLU:OE2	6:B:519:LYS:NZ	2.37	0.56
6:B:819:ASP:CG	6:B:820:PRO:HD2	2.30	0.56
6:B:894:LYS:N	1:L:54:ARG:HH21	2.03	0.56
6:B:1013:MET:SD	6:B:1026:ILE:HG12	2.45	0.56
9:E:159:ASP:OD1	9:E:162:ARG:NH1	2.39	0.56
5:P:618:TYR:CE1	6:Q:783:MET:HB2	2.41	0.56
5:A:966:LEU:HD22	5:A:997:PHE:CZ	2.41	0.56
6:B:833:PRO:HG2	6:B:836:TRP:CE2	2.40	0.56
2:M:15:VAL:HG22	2:M:90:LEU:HB2	1.88	0.56
5:P:598:ALA:HB1	5:P:601:MET:HE3	1.86	0.56
6:Q:737:SER:HB3	6:Q:806:THR:HG21	1.88	0.56
6:B:243:GLN:O	6:B:411:MET:HE2	2.06	0.56
7:C:253:PRO:HB2	3:N:180:PHE:HD1	1.71	0.56
6:B:859:CYS:HB3	6:B:872:LYS:HB2	1.88	0.56
9:E:90:VAL:HG13	9:E:120:ALA:HA	1.88	0.56
14:Z:49:LEU:HD23	14:Z:51:THR:HG23	1.87	0.56
5:A:449:GLY:O	5:A:451:VAL:N	2.34	0.56
6:B:338:PHE:HZ	6:B:357:ILE:HD12	1.70	0.56
6:B:380:LYS:HE3	6:B:637:TYR:HB3	1.87	0.56
13:J:10:CYS:HB3	13:J:43:ARG:NH1	2.21	0.56
5:A:1162:ASN:HD22	5:A:1165:LYS:HG3	1.71	0.56
7:R:47:LEU:HD23	7:R:48:ASP:H	1.71	0.56
6:Q:317:TYR:HB3	6:Q:320:LEU:HD12	1.88	0.56
3:3:89:ILE:HG12	3:3:139:VAL:HG22	1.88	0.56
6:B:109:SER:OG	6:B:891:GLU:OE2	2.24	0.56
5:P:1273:THR:HG23	12:X:48:VAL:HG22	1.88	0.56
13:Y:10:CYS:HB3	13:Y:43:ARG:NH1	2.21	0.56
6:B:211:ARG:HG2	6:B:239:VAL:CG1	2.36	0.55
5:P:491:GLU:OE2	5:P:815:ARG:NH2	2.39	0.55
2:2:15:VAL:HG22	2:2:90:LEU:HB2	1.88	0.55
5:A:758:GLU:HB3	17:A:2042:HOH:O	2.05	0.55
6:B:946:ASP:OD2	13:J:48:ARG:NH2	2.39	0.55
5:P:19:LEU:HD11	6:Q:1190:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:916:THR:O	5:A:919:LYS:NZ	2.40	0.55
7:C:228:ARG:HD3	3:N:173:THR:OG1	2.06	0.55
6:Q:788:ILE:HB	6:Q:948:ILE:HB	1.89	0.55
4:V:20:HIS:O	4:V:20:HIS:ND1	2.39	0.55
5:A:438:ILE:HG23	6:B:1192:MET:HG2	1.89	0.55
6:Q:829:ASN:OD1	6:Q:829:ASN:N	2.36	0.55
7:C:139:LYS:HG2	7:C:201:GLU:HB3	1.89	0.55
5:P:1120:TYR:O	9:T:207:ARG:NH2	2.32	0.55
9:T:90:VAL:HG13	9:T:120:ALA:HA	1.89	0.55
4:4:292:HIS:ND1	5:P:379:GLU:HB3	2.22	0.55
7:C:65:ASN:O	7:C:69:ARG:HG3	2.07	0.55
4:G:229:LEU:HD12	4:G:230:ARG:H	1.72	0.55
3:N:69:SER:OG	3:N:70:LEU:N	2.37	0.55
6:Q:431:ASP:CG	6:Q:452:ARG:HH22	2.15	0.55
5:A:491:GLU:OE2	5:A:815:ARG:NH2	2.40	0.55
6:B:21:ARG:NH1	6:B:22:GLU:OE1	2.40	0.55
5:P:449:GLY:O	5:P:451:VAL:N	2.34	0.55
6:B:322:ASN:HB3	6:B:325:GLN:H	1.71	0.54
9:T:197:LYS:HD3	9:T:199:ILE:HD11	1.88	0.54
5:A:412:SER:HB3	5:A:415:ASP:H	1.72	0.54
5:A:1162:ASN:HD21	5:A:1164:LYS:HB2	1.71	0.54
5:P:1226:VAL:HG12	5:P:1227:MET:HG2	1.88	0.54
4:V:132:VAL:HG22	4:V:232:THR:HG22	1.89	0.54
6:B:373:MET:O	6:B:377:MET:HG3	2.07	0.54
4:G:20:HIS:O	4:G:20:HIS:ND1	2.38	0.54
4:V:229:LEU:HD12	4:V:230:ARG:H	1.72	0.54
12:X:91:ASN:OD1	12:X:92:GLU:N	2.40	0.54
5:P:325:ASP:HB3	5:P:329:ARG:HH21	1.73	0.54
6:Q:338:PHE:CE1	6:Q:353:VAL:HG22	2.43	0.54
6:B:654:ARG:NH1	17:B:2043:HOH:O	2.38	0.54
4:O:265:SER:OG	4:O:266:GLN:N	2.40	0.54
6:Q:1151:ILE:HG12	4:V:21:LYS:HZ2	1.71	0.54
5:P:412:SER:HB3	5:P:415:ASP:H	1.73	0.54
5:A:379:GLU:HB3	4:O:292:HIS:ND1	2.23	0.54
5:P:1136:VAL:HG22	5:P:1174:TYR:CG	2.43	0.54
6:Q:42:VAL:HG21	6:Q:190:ILE:HB	1.88	0.54
4:4:292:HIS:CE1	5:P:379:GLU:HB3	2.43	0.54
6:B:284:SER:OG	6:B:287:GLU:HG3	2.07	0.54
5:A:1446:ARG:O	5:A:1450:ILE:HG13	2.08	0.53
6:B:700:LEU:N	16:B:2204:SO4:O2	2.30	0.53
12:I:96:TYR:HA	12:I:111:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:12:ILE:HD12	3:N:67:LEU:HB2	1.90	0.53
6:Q:721:MET:HA	6:Q:721:MET:HE2	1.90	0.53
6:B:317:TYR:HB3	6:B:320:LEU:HD12	1.89	0.53
6:B:788:ILE:HB	6:B:948:ILE:HB	1.89	0.53
6:B:929:ARG:HH22	14:K:96:PRO:HB2	1.72	0.53
5:P:745:PRO:HG2	5:P:1075:ALA:HB2	1.91	0.53
6:Q:923:GLN:HG2	6:Q:949:ILE:HD11	1.90	0.53
6:Q:1151:ILE:HG12	4:V:21:LYS:NZ	2.21	0.53
6:B:731:VAL:HG11	13:J:59:LYS:HB3	1.91	0.53
4:G:132:VAL:HG22	4:G:232:THR:HG22	1.90	0.53
5:P:970:LYS:HG2	5:P:973:GLU:HG2	1.90	0.53
5:P:1162:ASN:HD21	5:P:1164:LYS:HB2	1.74	0.53
5:A:671:GLN:HB2	6:B:783:MET:HG2	1.90	0.53
6:Q:833:PRO:HG2	6:Q:836:TRP:CE2	2.44	0.53
5:A:1317:ILE:HA	5:A:1321:PHE:HB3	1.90	0.53
14:K:48:LYS:HE2	14:K:64:GLN:NE2	2.23	0.53
2:M:75:GLN:HB2	3:N:60:SER:HA	1.91	0.53
5:P:1148:LEU:HD22	5:P:1163:GLU:HG3	1.91	0.53
6:Q:858:ILE:HD13	6:Q:872:LYS:O	2.09	0.53
5:A:1136:VAL:HG22	5:A:1174:TYR:CG	2.44	0.53
5:A:1603:MET:HE1	5:A:1621:PHE:CZ	2.44	0.53
6:B:134:ARG:HD2	6:B:160:GLY:HA3	1.91	0.53
6:B:762:MET:HE2	6:B:762:MET:HA	1.91	0.53
5:P:959:VAL:HG22	5:P:965:THR:HG22	1.91	0.53
5:A:1289:SER:HB3	5:A:1475:GLU:HG2	1.91	0.53
4:4:316:GLU:CG	5:P:475:ARG:HH21	2.21	0.53
7:C:215:ASP:CG	1:L:70:ARG:HH22	2.17	0.53
5:A:969:PHE:CE2	5:A:978:ALA:HA	2.44	0.52
5:P:438:ILE:HG23	6:Q:1192:MET:HG2	1.90	0.52
2:M:11:GLU:N	2:M:86:LYS:O	2.36	0.52
5:P:1663:ALA:HB1	4:V:103:LYS:HD2	1.90	0.52
7:C:67:PHE:O	7:C:71:MET:HG3	2.08	0.52
7:C:97:LEU:HD11	7:C:202:ILE:HD13	1.90	0.52
1:1:70:ARG:HH22	7:R:215:ASP:CG	2.17	0.52
6:B:298:LYS:HE3	3:N:101:GLN:OE1	2.10	0.52
14:Z:55:SER:OG	14:Z:57:ASP:OD1	2.26	0.52
13:Y:1:MET:HG2	13:Y:57:ILE:HB	1.91	0.52
5:P:1317:ILE:HA	5:P:1321:PHE:HB3	1.91	0.52
4:G:30:GLU:HA	4:G:32:ASN:H	1.74	0.52
7:R:117:ASP:OD1	7:R:119:ASN:ND2	2.43	0.52
6:B:664:VAL:HG22	6:B:672:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:721:MET:HE2	6:B:721:MET:HA	1.92	0.51
8:D:48:GLU:OE2	8:D:90:LYS:NZ	2.43	0.51
6:Q:284:SER:OG	6:Q:287:GLU:HG3	2.10	0.51
6:Q:293:ILE:HG12	6:Q:306:LEU:HD13	1.92	0.51
6:B:1047:ARG:NH2	6:B:1051:PRO:O	2.43	0.51
5:A:693:GLN:OE1	14:K:88:PHE:HA	2.10	0.51
17:A:2063:HOH:O	6:B:522:PRO:HG3	2.10	0.51
6:B:574:SER:HB2	2:M:97:VAL:HG21	1.92	0.51
5:P:916:THR:O	5:P:919:LYS:NZ	2.44	0.51
6:Q:211:ARG:HG2	6:Q:239:VAL:CG1	2.40	0.51
7:R:47:LEU:HD23	7:R:48:ASP:N	2.24	0.51
5:A:1482:LYS:HE2	6:B:304:ASP:CG	2.36	0.51
5:A:970:LYS:HG2	5:A:973:GLU:HG2	1.92	0.51
6:B:307:GLU:OE2	6:B:311:ARG:NH1	2.43	0.51
5:A:1148:LEU:HD22	5:A:1163:GLU:HG3	1.92	0.51
6:B:22:GLU:O	6:B:26:ILE:HG13	2.10	0.51
5:P:969:PHE:CE2	5:P:978:ALA:HA	2.45	0.51
2:2:97:VAL:HG21	6:Q:574:SER:HB2	1.92	0.51
5:A:799:GLU:HG3	5:A:1062:HIS:CG	2.46	0.51
13:J:1:MET:HG2	13:J:57:ILE:HB	1.93	0.51
5:P:1162:ASN:HD22	5:P:1165:LYS:HG3	1.76	0.51
7:R:157:TYR:HB2	7:R:160:ALA:HB2	1.92	0.51
5:A:40:ASN:N	5:A:40:ASN:OD1	2.44	0.51
5:A:1450:ILE:HD12	5:A:1460:TYR:CD2	2.46	0.51
6:B:833:PRO:O	6:B:834:LYS:HB3	2.10	0.51
6:Q:427:GLN:HA	6:Q:430:MET:HE3	1.92	0.51
4:4:316:GLU:HG3	6:Q:1061:LYS:HD2	1.93	0.51
12:X:96:TYR:HA	12:X:111:PHE:O	2.11	0.51
4:G:224:PRO:HG2	6:Q:430:MET:SD	2.51	0.50
6:Q:833:PRO:O	6:Q:834:LYS:HB3	2.11	0.50
11:W:112:ILE:HD12	11:W:129:TYR:HB2	1.93	0.50
7:C:47:LEU:HD23	7:C:48:ASP:N	2.25	0.50
11:H:38:LEU:HD11	11:H:123:MET:HE2	1.93	0.50
6:Q:338:PHE:CZ	6:Q:357:ILE:HD12	2.46	0.50
5:A:497:VAL:HG21	5:A:605:VAL:HG13	1.92	0.50
5:A:840:ASN:O	5:A:844:THR:HG23	2.11	0.50
6:B:858:ILE:HD13	6:B:872:LYS:O	2.10	0.50
11:H:26:ILE:HD12	11:H:42:ILE:HD12	1.94	0.50
5:A:1175:MET:HE3	10:F:84:TYR:HE2	1.75	0.50
5:P:1571:SER:C	5:P:1573:TYR:H	2.19	0.50
9:T:67:GLU:CD	9:T:67:GLU:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1010:ASN:HB3	6:B:1025:ASP:HB3	1.93	0.50
5:P:952:LEU:HD22	5:P:1004:GLU:HG3	1.94	0.50
5:P:1456:PHE:HB2	5:P:1474:LEU:HD22	1.93	0.50
6:Q:859:CYS:HB3	6:Q:872:LYS:HB2	1.92	0.50
5:P:1482:LYS:HG2	6:Q:308:LEU:HD21	1.94	0.50
14:Z:48:LYS:HE2	14:Z:64:GLN:NE2	2.26	0.50
5:A:747:ILE:HD13	5:A:748:ASN:H	1.77	0.50
5:A:1326:GLU:OE2	5:A:1454:HIS:HB3	2.11	0.50
6:B:338:PHE:CE1	6:B:353:VAL:HG22	2.47	0.50
5:A:1089:LEU:HD11	5:A:1175:MET:HE1	1.92	0.50
5:A:1654:PHE:CZ	10:F:89:GLU:HA	2.47	0.50
12:I:91:ASN:OD1	12:I:92:GLU:N	2.45	0.50
5:P:121:LYS:HE2	5:P:219:LEU:HD11	1.94	0.50
3:3:180:PHE:HD1	7:R:253:PRO:HB2	1.75	0.49
6:B:293:ILE:HG12	6:B:306:LEU:HD13	1.94	0.49
11:H:112:ILE:HD12	11:H:129:TYR:HB2	1.93	0.49
5:P:1019:LEU:HD12	5:P:1227:MET:HG3	1.94	0.49
5:P:1446:ARG:O	5:P:1450:ILE:HG13	2.12	0.49
9:T:54:GLN:HB2	9:T:57:MET:HE2	1.94	0.49
5:A:1647:ASN:O	5:A:1652:GLY:HA3	2.13	0.49
6:Q:610:TYR:HE1	6:Q:658:LEU:HD11	1.77	0.49
6:B:252:TYR:OH	6:B:305:ARG:NH1	2.44	0.49
7:C:157:TYR:HB2	7:C:160:ALA:HB2	1.94	0.49
14:K:55:SER:OG	14:K:57:ASP:OD1	2.28	0.49
6:Q:210:ARG:HH22	6:Q:625:GLU:CD	2.19	0.49
6:B:262:PHE:CD1	6:B:357:ILE:HD13	2.48	0.49
7:C:47:LEU:HD23	7:C:48:ASP:H	1.77	0.49
5:A:643:ALA:HB1	6:B:1087:LEU:HD23	1.93	0.49
11:H:80:ARG:HG3	14:K:108:TYR:CZ	2.47	0.49
5:P:1007:ILE:HG23	6:Q:518:ARG:HD3	1.94	0.49
6:Q:134:ARG:HD2	6:Q:160:GLY:HA3	1.95	0.49
6:B:225:ARG:NH2	6:B:261:ARG:HD3	2.27	0.49
6:Q:307:GLU:OE2	6:Q:311:ARG:NH1	2.46	0.49
7:R:37:LYS:HD2	14:Z:130:VAL:HG22	1.94	0.49
9:T:48:ASP:OD1	9:T:50:MET:HB3	2.12	0.49
4:4:316:GLU:HA	6:Q:1061:LYS:NZ	2.27	0.49
5:A:1039:ARG:CZ	10:F:139:PRO:HG2	2.42	0.49
7:R:67:PHE:O	7:R:71:MET:HG3	2.13	0.49
5:A:93:GLN:HG3	5:A:1627:LEU:CD1	2.42	0.49
4:G:47:VAL:HB	4:G:65:HIS:CD2	2.47	0.49
4:G:137:ILE:HG13	4:G:227:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:747:ILE:HD13	5:P:748:ASN:H	1.78	0.49
5:P:747:ILE:HD13	5:P:748:ASN:N	2.27	0.49
5:P:1312:GLU:O	5:P:1316:VAL:HG23	2.13	0.49
6:Q:883:GLU:HG3	6:Q:906:ARG:HB2	1.95	0.49
7:R:222:VAL:HB	7:R:224:THR:H	1.78	0.49
7:R:239:ILE:HG23	7:R:243:SER:HB3	1.95	0.49
5:A:959:VAL:HG22	5:A:965:THR:HG22	1.95	0.48
5:A:1392:ILE:HD13	5:A:1392:ILE:HA	1.70	0.48
1:L:45:ALA:O	1:L:47:ARG:N	2.46	0.48
6:Q:26:ILE:CG1	13:Y:58:GLU:HG2	2.35	0.48
5:A:697:TYR:CE1	14:K:104:ARG:HB2	2.47	0.48
6:B:210:ARG:NH2	6:B:625:GLU:OE2	2.46	0.48
13:J:6:ARG:HD2	13:J:11:GLY:O	2.13	0.48
6:Q:699:ILE:HB	16:Q:2204:SO4:O3	2.13	0.48
6:B:841:ASP:OD1	6:B:842:GLU:N	2.40	0.48
2:M:65:TYR:CE1	2:M:97:VAL:HB	2.48	0.48
5:P:1603:MET:HE1	5:P:1621:PHE:CZ	2.47	0.48
6:Q:243:GLN:O	6:Q:411:MET:HE2	2.13	0.48
6:Q:877:SER:HB3	6:Q:1064:LYS:HE3	1.95	0.48
7:R:222:VAL:C	7:R:224:THR:H	2.19	0.48
2:2:76:TYR:CE1	3:3:57:LYS:HB2	2.48	0.48
5:A:509:GLU:CG	5:A:579:ARG:HE	2.26	0.48
5:P:412:SER:OG	5:P:413:LEU:N	2.46	0.48
5:P:671:GLN:HB2	6:Q:783:MET:HE3	1.95	0.48
6:B:610:TYR:HE1	6:B:658:LEU:HD11	1.77	0.48
9:E:54:GLN:HB2	9:E:57:MET:HE2	1.96	0.48
5:A:1312:GLU:O	5:A:1316:VAL:HG23	2.13	0.48
6:Q:292:ILE:HB	6:Q:306:LEU:HD11	1.96	0.48
6:Q:585:CYS:HB2	6:Q:595:TRP:CZ3	2.49	0.48
6:Q:1047:ARG:NH2	6:Q:1051:PRO:O	2.46	0.48
5:A:314:TYR:CD2	5:A:424:MET:HG3	2.49	0.48
5:A:475:ARG:HH21	4:O:316:GLU:HG2	1.78	0.48
6:B:584:CYS:HB3	6:B:596:VAL:HG23	1.95	0.48
4:O:265:SER:HB3	4:O:268:GLU:HB2	1.95	0.48
5:P:497:VAL:HG21	5:P:605:VAL:HG13	1.96	0.48
4:V:47:VAL:HB	4:V:65:HIS:CD2	2.48	0.48
4:V:137:ILE:HG13	4:V:227:GLY:O	2.13	0.48
5:P:797:LEU:HD13	5:P:809:VAL:HG21	1.95	0.48
6:Q:731:VAL:HG11	13:Y:59:LYS:HB3	1.94	0.48
6:Q:1010:ASN:HB3	6:Q:1025:ASP:HB3	1.94	0.48
5:A:5:LYS:HB3	5:A:5:LYS:HE2	1.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:869:PRO:HG2	5:A:872:ASP:HB2	1.96	0.48
5:A:1200:MET:HE1	5:A:1569:VAL:HG12	1.95	0.48
9:E:48:ASP:OD1	9:E:50:MET:HB3	2.13	0.48
7:R:252:PRO:HD2	7:R:255:VAL:HG21	1.95	0.48
6:B:434:ARG:HE	4:V:228:LYS:HE3	1.78	0.48
4:G:35:SER:HG	4:G:132:VAL:H	1.62	0.48
5:P:638:PRO:HA	6:Q:1090:ASP:OD2	2.14	0.48
11:W:26:ILE:HD12	11:W:42:ILE:HD12	1.95	0.48
5:A:412:SER:OG	5:A:413:LEU:N	2.47	0.47
6:B:211:ARG:HG2	6:B:239:VAL:HG11	1.96	0.47
5:A:1162:ASN:ND2	5:A:1165:LYS:HG3	2.29	0.47
5:P:592:GLN:HE22	5:P:1380:GLN:HA	1.79	0.47
6:Q:664:VAL:HG22	6:Q:672:MET:HE1	1.95	0.47
5:P:1320:GLN:OE1	5:P:1497:ILE:N	2.47	0.47
2:2:65:TYR:CE1	2:2:97:VAL:HB	2.49	0.47
5:A:901:ASN:OD1	17:A:2057:HOH:O	2.20	0.47
6:B:338:PHE:CZ	6:B:357:ILE:HD12	2.49	0.47
5:P:644:ARG:NH2	10:U:116:ASP:OD1	2.47	0.47
5:P:1647:ASN:O	5:P:1652:GLY:HA3	2.14	0.47
6:Q:262:PHE:CD1	6:Q:357:ILE:HD13	2.49	0.47
6:Q:470:LEU:HD21	6:Q:476:LEU:HD12	1.97	0.47
5:A:19:LEU:HD11	6:B:1190:SER:HB2	1.96	0.47
7:C:239:ILE:HG23	7:C:243:SER:HB3	1.96	0.47
6:Q:22:GLU:O	6:Q:26:ILE:HG13	2.14	0.47
5:A:826:PHE:HB3	6:B:777:SER:HB2	1.96	0.47
6:B:736:ARG:HD3	6:B:738:ASP:OD2	2.15	0.47
7:C:117:ASP:OD1	7:C:119:ASN:ND2	2.44	0.47
3:N:111:VAL:HG13	3:N:122:ALA:HB2	1.96	0.47
5:P:1258:ILE:HB	5:P:1501:ILE:HD12	1.96	0.47
6:Q:207:ILE:HG13	6:Q:503:VAL:CG2	2.44	0.47
5:A:258:GLU:HA	5:A:261:ILE:HD12	1.96	0.47
5:A:747:ILE:HD13	5:A:748:ASN:N	2.29	0.47
5:A:1063:MET:HB3	5:A:1063:MET:HE2	1.66	0.47
9:E:61:GLN:HE21	9:E:105:PHE:HE1	1.62	0.47
7:R:61:THR:HA	7:R:298:PHE:CZ	2.49	0.47
7:R:247:PHE:HE1	7:R:289:VAL:HG21	1.79	0.47
8:S:33:THR:HG23	8:S:96:PHE:HD1	1.80	0.47
5:A:1663:ALA:HB1	4:G:103:LYS:HD2	1.97	0.47
5:P:1541:ILE:O	9:T:147:HIS:NE2	2.45	0.47
5:P:1562:ILE:HG21	5:P:1589:MET:HE3	1.96	0.47
4:V:17:ILE:C	4:V:19:LYS:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:38:LEU:HD11	11:W:123:MET:HE2	1.97	0.47
2:2:26:PHE:CE1	2:2:98:SER:HB2	2.50	0.47
5:P:618:TYR:CZ	6:Q:783:MET:HB2	2.50	0.47
3:3:111:VAL:HG13	3:3:122:ALA:HB2	1.97	0.47
5:A:1258:ILE:HB	5:A:1501:ILE:HD12	1.97	0.47
6:B:413:LEU:O	6:B:417:ILE:HG13	2.14	0.47
5:P:700:ILE:HD13	5:P:700:ILE:HA	1.77	0.47
6:Q:280:LEU:HD23	6:Q:354:LEU:HD13	1.97	0.47
9:T:78:LEU:HD13	9:T:107:THR:HB	1.97	0.47
13:Y:6:ARG:HD2	13:Y:11:GLY:O	2.15	0.47
3:3:94:ASP:HB3	3:3:99:LEU:HG	1.97	0.46
6:B:890:ASP:HB3	6:B:896:GLN:OE1	2.16	0.46
7:C:71:MET:HE1	7:C:302:VAL:HG21	1.97	0.46
7:C:222:VAL:HB	7:C:224:THR:H	1.81	0.46
5:P:1654:PHE:CZ	10:U:89:GLU:HA	2.49	0.46
6:Q:812:ALA:HA	6:Q:815:ARG:HD3	1.95	0.46
12:X:77:LYS:HA	12:X:77:LYS:HD3	1.68	0.46
5:A:572:THR:HA	4:G:52:MET:CE	2.45	0.46
6:B:448:ARG:HA	6:B:451:MET:HE3	1.97	0.46
6:B:1103:VAL:HG22	6:B:1176:VAL:HG22	1.97	0.46
7:C:37:LYS:HD2	14:K:130:VAL:HG22	1.97	0.46
8:D:33:THR:HG23	8:D:96:PHE:HD1	1.80	0.46
5:P:1603:MET:HE3	5:P:1603:MET:HB3	1.72	0.46
3:3:173:THR:OG1	7:R:228:ARG:HD3	2.14	0.46
6:B:812:ALA:HA	6:B:815:ARG:HD3	1.95	0.46
4:4:316:GLU:HG3	5:P:475:ARG:HH21	1.80	0.46
5:A:1440:ASN:HA	5:A:1443:GLN:HB2	1.97	0.46
9:E:67:GLU:CD	9:E:67:GLU:H	2.23	0.46
2:M:65:TYR:HE1	2:M:97:VAL:HB	1.81	0.46
5:P:1326:GLU:OE2	5:P:1454:HIS:HB3	2.15	0.46
6:B:774:ALA:HB1	6:B:1026:ILE:HD11	1.97	0.46
6:B:427:GLN:HA	6:B:430:MET:HE3	1.98	0.46
8:D:46:GLU:OE1	8:D:47:LYS:HE2	2.15	0.46
5:P:1089:LEU:HD11	5:P:1175:MET:HE1	1.97	0.46
5:P:1348:VAL:HA	5:P:1349:PRO:HD3	1.68	0.46
5:P:1603:MET:HE2	5:P:1615:TYR:CD2	2.51	0.46
7:R:97:LEU:HD11	7:R:202:ILE:HD13	1.97	0.46
6:B:143:TRP:CE3	6:B:446:MET:HG3	2.50	0.46
6:B:293:ILE:CD1	6:B:302:LEU:HB3	2.46	0.46
6:B:470:LEU:HD21	6:B:476:LEU:HD12	1.97	0.46
6:B:1045:GLN:HB3	6:B:1063:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:23:VAL:O	12:I:39:LYS:NZ	2.49	0.46
6:Q:373:MET:O	6:Q:377:MET:HG3	2.15	0.46
6:Q:1103:VAL:HG22	6:Q:1176:VAL:HG22	1.98	0.46
9:T:61:GLN:HE21	9:T:105:PHE:HE1	1.63	0.46
1:I:45:ALA:O	1:I:47:ARG:N	2.48	0.46
6:B:822:THR:HB	6:B:823:GLN:HG3	1.98	0.46
6:Q:934:ILE:HD12	7:R:69:ARG:CZ	2.46	0.46
5:A:926:GLN:NE2	17:A:2061:HOH:O	2.33	0.46
6:B:265:ARG:NH2	6:B:339:GLN:OE1	2.48	0.46
6:B:934:ILE:HD12	7:C:69:ARG:CZ	2.45	0.46
7:C:228:ARG:HG3	7:C:299:ILE:HB	1.98	0.46
7:C:247:PHE:HE1	7:C:289:VAL:HG21	1.80	0.46
4:G:106:LYS:HB2	4:G:106:LYS:HE3	1.82	0.46
6:Q:190:ILE:HG13	6:Q:191:GLY:N	2.30	0.46
4:4:294:GLU:OE1	6:B:1120:ILE:HD13	2.16	0.46
5:A:93:GLN:HG3	5:A:1627:LEU:HD11	1.98	0.46
6:B:786:ALA:HB1	6:B:928:SER:HB2	1.98	0.46
6:Q:774:ALA:HB1	6:Q:1026:ILE:HD11	1.97	0.46
4:4:316:GLU:CG	6:Q:1070:ARG:HH22	2.28	0.45
14:K:49:LEU:HG	14:K:54:THR:HG21	1.98	0.45
5:A:582:LYS:O	5:A:585:ASP:HB2	2.17	0.45
5:A:638:PRO:HA	6:B:1090:ASP:OD2	2.14	0.45
6:B:795:GLU:HG2	7:C:216:HIS:CD2	2.51	0.45
7:C:176:SER:O	7:C:180:ALA:HB2	2.16	0.45
13:J:36:LEU:HD13	13:J:47:ARG:HB3	1.98	0.45
5:P:840:ASN:O	5:P:844:THR:HG23	2.15	0.45
5:P:1306:TYR:HE2	12:X:60:LEU:HD12	1.81	0.45
6:Q:252:TYR:OH	6:Q:305:ARG:NH1	2.45	0.45
6:Q:792:SER:O	6:Q:796:ARG:HG3	2.15	0.45
9:T:177:ARG:HD3	9:T:215:MET:HB2	1.98	0.45
5:P:258:GLU:HA	5:P:261:ILE:HD12	1.99	0.45
5:P:862:THR:HA	12:X:67:VAL:HG12	1.99	0.45
6:Q:107:PRO:HG2	6:Q:133:TYR:CZ	2.51	0.45
12:I:89:CYS:SG	12:I:91:ASN:HB2	2.56	0.45
6:Q:293:ILE:CD1	6:Q:302:LEU:HB3	2.46	0.45
6:Q:1045:GLN:HB3	6:Q:1063:ARG:HG3	1.98	0.45
5:A:184:LYS:HA	5:A:187:GLU:HG2	1.98	0.45
5:A:598:ALA:CB	5:A:601:MET:HE3	2.47	0.45
5:A:758:GLU:N	17:A:2042:HOH:O	2.36	0.45
5:A:1603:MET:HE2	5:A:1615:TYR:CD2	2.52	0.45
7:C:222:VAL:C	7:C:224:THR:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:49:MET:HE3	13:J:49:MET:HB3	1.79	0.45
5:P:1320:GLN:HE21	5:P:1320:GLN:HB2	1.55	0.45
6:Q:57:ASP:OD1	6:Q:57:ASP:N	2.49	0.45
7:R:296:ASN:OD1	7:R:296:ASN:N	2.48	0.45
13:Y:36:LEU:HD13	13:Y:47:ARG:HB3	1.98	0.45
5:A:589:MET:HE1	5:A:614:LEU:HD13	1.98	0.45
14:K:80:ILE:HD13	14:K:105:ILE:HD11	1.98	0.45
5:P:671:GLN:HB2	6:Q:783:MET:HG2	1.98	0.45
5:P:692:TYR:O	5:P:696:ILE:HG12	2.16	0.45
6:Q:65:VAL:HG13	6:Q:99:VAL:O	2.17	0.45
6:Q:584:CYS:HB3	6:Q:596:VAL:HG23	1.99	0.45
7:R:176:SER:O	7:R:180:ALA:HB2	2.16	0.45
10:U:99:LEU:HB3	4:V:112:PRO:HB3	1.99	0.45
5:A:1237:GLN:H	5:A:1544:ASN:HB2	1.82	0.45
5:P:1162:ASN:ND2	5:P:1165:LYS:HG3	2.31	0.45
7:R:228:ARG:HG3	7:R:299:ILE:HB	1.98	0.45
5:A:1156:LYS:C	5:A:1158:SER:H	2.25	0.45
6:B:26:ILE:CG1	13:J:58:GLU:HG2	2.36	0.45
6:B:292:ILE:HB	6:B:306:LEU:HD11	1.98	0.45
6:B:585:CYS:HB2	6:B:595:TRP:CZ3	2.51	0.45
9:E:7:ARG:O	9:E:11:ARG:HG3	2.17	0.45
5:P:257:ASN:OD1	5:P:258:GLU:N	2.50	0.45
6:Q:207:ILE:HG13	6:Q:503:VAL:HG21	1.99	0.45
6:Q:448:ARG:HA	6:Q:451:MET:HE3	1.97	0.45
7:R:328:LEU:HD11	14:Z:47:ILE:HB	1.98	0.45
1:I:32:ALA:HB3	1:I:55:ILE:HG23	1.99	0.45
5:A:379:GLU:HB3	4:O:292:HIS:CE1	2.52	0.45
5:A:1154:LEU:O	5:A:1158:SER:HB2	2.17	0.45
6:B:190:ILE:HG13	6:B:191:GLY:N	2.32	0.45
6:B:1153:ILE:HA	6:B:1153:ILE:HD13	1.79	0.45
4:G:17:ILE:C	4:G:19:LYS:H	2.25	0.45
2:M:26:PHE:CE1	2:M:98:SER:HB2	2.51	0.45
5:P:89:LEU:HD11	6:Q:1192:MET:SD	2.57	0.45
6:Q:1082:HIS:HB3	6:Q:1084:THR:HG23	1.99	0.45
7:C:91:VAL:HG13	13:J:1:MET:HE1	1.98	0.45
9:E:78:LEU:HD13	9:E:107:THR:HB	1.98	0.45
5:P:1488:ILE:O	5:P:1492:ILE:HD12	2.16	0.45
4:4:316:GLU:CD	6:Q:1070:ARG:HH22	2.25	0.44
6:B:78:PRO:O	6:B:79:LEU:HB3	2.17	0.44
6:B:833:PRO:HG2	6:B:836:TRP:CZ2	2.53	0.44
4:G:163:PRO:HG2	4:G:166:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:201:LYS:NZ	6:Q:466:SER:O	2.50	0.44
5:A:1463:ASP:HB2	5:A:1469:TRP:CE2	2.52	0.44
6:B:205:MET:HE3	6:B:502:MET:O	2.17	0.44
7:C:252:PRO:HD2	7:C:255:VAL:HG21	1.99	0.44
12:I:77:LYS:HA	12:I:77:LYS:HD3	1.68	0.44
5:P:697:TYR:CE1	14:Z:104:ARG:HB2	2.53	0.44
5:P:1511:GLU:HA	5:P:1512:PRO:HD3	1.84	0.44
6:Q:786:ALA:HB1	6:Q:928:SER:HB2	1.98	0.44
7:R:109:ASP:HB3	7:R:112:MET:HE3	2.00	0.44
5:A:671:GLN:HB2	6:B:783:MET:HE3	1.99	0.44
6:B:1158:ILE:HA	6:B:1167:PHE:O	2.17	0.44
9:E:93:MET:CG	9:E:120:ALA:HB1	2.46	0.44
5:P:854:GLY:HA3	5:P:974:THR:O	2.17	0.44
5:P:920:PHE:CD1	5:P:921:PRO:HA	2.53	0.44
6:Q:890:ASP:HB3	6:Q:896:GLN:OE1	2.17	0.44
7:R:192:LEU:HD21	7:R:195:LYS:HE2	1.99	0.44
5:A:1291:VAL:HG22	5:A:1473:LYS:HG3	1.99	0.44
5:P:1555:VAL:HG21	5:P:1593:GLY:HA2	1.99	0.44
6:Q:404:LEU:HD21	6:Q:551:ILE:HG21	1.99	0.44
6:Q:714:ARG:HH22	12:X:100:GLN:NE2	2.16	0.44
9:T:93:MET:CG	9:T:120:ALA:HB1	2.46	0.44
14:Z:49:LEU:HG	14:Z:54:THR:HG21	1.98	0.44
2:2:65:TYR:HE1	2:2:97:VAL:HB	1.82	0.44
5:P:1071:ASP:O	5:P:1072:ASN:HB2	2.17	0.44
6:Q:956:SER:HB3	12:X:107:GLY:HA3	2.00	0.44
6:Q:1158:ILE:HA	6:Q:1167:PHE:O	2.17	0.44
13:Y:10:CYS:HB2	13:Y:12:LYS:H	1.83	0.44
5:A:920:PHE:CD1	5:A:921:PRO:HA	2.52	0.44
6:B:893:ASN:O	6:B:895:PHE:HD1	2.01	0.44
6:Q:411:MET:HB3	6:Q:476:LEU:HD22	2.00	0.44
3:3:172:ALA:HB1	7:R:228:ARG:CZ	2.48	0.44
5:A:257:ASN:OD1	5:A:258:GLU:N	2.51	0.44
5:A:830:MET:HG3	6:B:967:LEU:HD11	1.99	0.44
5:P:413:LEU:HA	5:P:416:ARG:HG2	2.00	0.44
5:P:509:GLU:CG	5:P:579:ARG:HE	2.31	0.44
5:P:693:GLN:OE1	14:Z:88:PHE:HA	2.18	0.44
5:P:1172:LEU:O	5:P:1176:ARG:HG2	2.18	0.44
6:B:411:MET:HB3	6:B:476:LEU:HD22	1.99	0.44
5:P:1574:ALA:HB2	12:X:120:LYS:O	2.18	0.44
7:R:116:VAL:HG11	7:R:125:LYS:HE3	2.00	0.44
5:A:1063:MET:HE1	5:A:1174:TYR:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1313:LEU:O	5:A:1317:ILE:HD12	2.18	0.43
8:D:23:HIS:CD2	10:F:58:PHE:CE1	3.06	0.43
4:G:35:SER:OG	4:G:132:VAL:N	2.46	0.43
5:P:140:THR:HG22	5:P:141:LEU:H	1.83	0.43
5:P:1063:MET:HE1	5:P:1174:TYR:CD2	2.53	0.43
5:P:1129:PRO:O	5:P:1175:MET:HG3	2.17	0.43
12:X:23:VAL:O	12:X:39:LYS:NZ	2.51	0.43
5:A:535:GLN:HA	5:A:546:LEU:HG	1.99	0.43
6:B:94:LYS:HE3	6:B:343:ASP:OD2	2.18	0.43
10:F:93:ILE:HA	10:F:93:ILE:HD13	1.70	0.43
5:A:37:VAL:HG12	5:A:38:LEU:HG	2.00	0.43
5:A:677:GLY:HA3	5:A:786:TYR:OH	2.18	0.43
5:A:862:THR:HA	12:I:67:VAL:HG12	2.00	0.43
6:Q:265:ARG:NH2	6:Q:339:GLN:OE1	2.51	0.43
4:V:163:PRO:HG2	4:V:166:TRP:CD1	2.53	0.43
5:A:1089:LEU:CD1	5:A:1175:MET:HE1	2.48	0.43
6:B:107:PRO:HG2	6:B:133:TYR:CZ	2.52	0.43
5:P:449:GLY:C	5:P:451:VAL:H	2.23	0.43
7:R:86:PHE:CE2	7:R:205:LYS:HG3	2.51	0.43
4:4:316:GLU:HG2	6:Q:1070:ARG:HH22	1.83	0.43
5:A:1175:MET:HE3	10:F:84:TYR:CE2	2.54	0.43
5:A:1499:ARG:HE	5:A:1499:ARG:HB3	1.47	0.43
4:G:41:VAL:HA	4:G:42:PRO:HD3	1.93	0.43
5:P:403:LEU:HD12	5:P:403:LEU:HA	1.71	0.43
5:P:1463:ASP:HB2	5:P:1469:TRP:CE2	2.54	0.43
5:A:833:LEU:C	5:A:944:MET:HE3	2.43	0.43
6:B:322:ASN:ND2	2:M:108:LEU:O	2.52	0.43
6:B:883:GLU:HG3	6:B:906:ARG:HB2	2.01	0.43
12:I:26:SER:O	12:I:39:LYS:HB2	2.19	0.43
5:P:874:GLU:OE2	5:P:878:ARG:HD2	2.17	0.43
6:Q:413:LEU:O	6:Q:417:ILE:HG13	2.19	0.43
6:Q:736:ARG:NH1	6:Q:738:ASP:OD1	2.51	0.43
14:Z:50:LEU:O	14:Z:54:THR:HG23	2.19	0.43
5:A:475:ARG:HE	4:O:316:GLU:HG2	1.84	0.43
5:A:1242:ILE:HG22	5:A:1536:ILE:HG22	2.01	0.43
5:A:1596:LEU:HD22	5:A:1602:GLY:HA2	2.00	0.43
6:B:57:ASP:OD1	6:B:57:ASP:N	2.52	0.43
6:Q:822:THR:HB	6:Q:823:GLN:HG3	2.01	0.43
8:S:37:LEU:HD23	8:S:37:LEU:HA	1.91	0.43
6:B:112:GLY:HA3	6:B:893:ASN:HB3	1.99	0.43
4:G:29:ASP:OD1	4:G:30:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:644:ARG:HH22	10:U:116:ASP:CG	2.27	0.43
5:P:869:PRO:HG2	5:P:872:ASP:HB2	2.00	0.43
5:P:1392:ILE:HD13	5:P:1392:ILE:HA	1.68	0.43
6:B:637:TYR:HA	6:B:638:PRO:HD3	1.87	0.43
6:B:923:GLN:HG2	6:B:949:ILE:CD1	2.47	0.43
6:B:954:PHE:H	6:B:955:PRO:HD2	1.83	0.43
9:E:177:ARG:HD3	9:E:215:MET:HB2	2.00	0.43
3:N:94:ASP:HB3	3:N:99:LEU:HG	2.00	0.43
5:P:273:ASP:OD1	5:P:273:ASP:N	2.50	0.43
8:S:46:GLU:OE1	8:S:47:LYS:HE2	2.18	0.43
5:A:692:TYR:O	5:A:696:ILE:HG12	2.19	0.43
6:B:210:ARG:HH22	6:B:625:GLU:CD	2.27	0.43
2:M:8:SER:O	3:N:71:PRO:HA	2.19	0.43
3:N:25:ILE:HA	3:N:26:PRO:HD3	1.84	0.43
5:P:581:ILE:HD11	5:P:605:VAL:HG21	2.01	0.43
5:P:1317:ILE:O	5:P:1322:ILE:HG12	2.18	0.43
5:P:1596:LEU:HD22	5:P:1602:GLY:HA2	2.01	0.43
11:W:105:GLU:HG2	11:W:115:TYR:HE1	1.83	0.43
4:4:316:GLU:HG2	5:P:475:ARG:HH21	1.84	0.42
5:A:36:THR:HG22	5:A:45:VAL:HG21	2.00	0.42
5:A:449:GLY:C	5:A:451:VAL:H	2.22	0.42
5:A:550:SER:OG	5:A:553:GLN:HG3	2.19	0.42
5:P:40:ASN:OD1	5:P:40:ASN:N	2.50	0.42
5:P:833:LEU:C	5:P:944:MET:HE3	2.44	0.42
5:P:1175:MET:HE3	10:U:84:TYR:HE2	1.84	0.42
2:2:74:ASN:OD1	3:3:57:LYS:HE3	2.19	0.42
5:A:1269:LYS:HB2	5:A:1269:LYS:HE3	1.89	0.42
6:B:1133:MET:HE3	4:G:17:ILE:HD13	2.01	0.42
3:N:81:THR:HG22	3:N:86:ASP:HB3	2.01	0.42
6:Q:144:SER:HA	6:Q:151:ASN:HB3	2.01	0.42
6:Q:206:LEU:HD23	6:Q:206:LEU:HA	1.83	0.42
9:T:114:ASN:OD1	9:T:114:ASN:N	2.52	0.42
2:2:59:ARG:NH2	12:X:12:ASP:OD2	2.51	0.42
5:A:6:PRO:HG3	4:G:113:PHE:CG	2.55	0.42
5:A:964:LYS:HB3	5:A:964:LYS:HE2	1.83	0.42
5:A:1172:LEU:O	5:A:1176:ARG:HG2	2.19	0.42
5:A:1260:LYS:HE2	5:A:1262:LEU:HD21	2.01	0.42
5:P:93:GLN:HG3	5:P:1627:LEU:CD1	2.49	0.42
5:P:905:SER:HB3	12:X:81:THR:HG22	2.01	0.42
5:P:1200:MET:HE1	5:P:1569:VAL:HG12	2.01	0.42
12:X:87:PRO:HG2	12:X:119:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Z:135:PHE:CE2	14:Z:139:ILE:HD11	2.54	0.42
5:A:502:ALA:HA	5:A:581:ILE:CG2	2.49	0.42
4:G:160:ASN:OD1	4:G:160:ASN:N	2.52	0.42
5:P:136:LEU:O	5:P:136:LEU:HG	2.20	0.42
5:P:535:GLN:HA	5:P:546:LEU:HG	2.01	0.42
6:Q:61:LEU:HD23	6:Q:61:LEU:HA	1.72	0.42
14:Z:80:ILE:HD13	14:Z:105:ILE:HD11	2.02	0.42
14:Z:95:HIS:HB3	14:Z:98:GLU:HG2	2.01	0.42
1:1:56:LEU:HB2	6:Q:887:LEU:HB2	2.02	0.42
4:4:265:SER:HB3	4:4:268:GLU:HB2	2.00	0.42
5:A:381:SER:HB2	5:A:453:ILE:CG2	2.50	0.42
5:A:456:VAL:HB	6:B:1192:MET:HE3	2.01	0.42
5:P:572:THR:HA	4:V:52:MET:HE3	2.01	0.42
13:Y:44:TYR:HA	13:Y:47:ARG:HG3	2.01	0.42
5:A:874:GLU:OE2	5:A:878:ARG:HD2	2.20	0.42
5:A:1622:LEU:HD21	6:B:1189:LEU:HD22	2.01	0.42
6:B:207:ILE:HG13	6:B:503:VAL:CG2	2.50	0.42
6:B:470:LEU:HD12	6:B:470:LEU:HA	1.83	0.42
7:C:61:THR:HA	7:C:298:PHE:CZ	2.55	0.42
5:P:5:LYS:HB3	5:P:5:LYS:HE2	1.75	0.42
5:P:456:VAL:HB	6:Q:1192:MET:HE3	2.01	0.42
5:P:498:PRO:HA	5:P:499:PRO:HD3	1.85	0.42
6:Q:211:ARG:HG2	6:Q:239:VAL:HG13	2.02	0.42
7:R:31:TRP:HB3	14:Z:82:LYS:HB3	2.01	0.42
12:X:34:LYS:HA	12:X:34:LYS:HD3	1.85	0.42
3:3:70:LEU:HA	3:3:71:PRO:HD3	1.84	0.42
3:3:145:ILE:HA	3:3:146:PRO:HD3	1.91	0.42
4:4:316:GLU:HA	6:Q:1061:LYS:HZ2	1.82	0.42
6:B:211:ARG:HG2	6:B:239:VAL:HG13	2.01	0.42
1:L:32:ALA:HB3	1:L:55:ILE:HG23	2.01	0.42
5:P:636:HIS:O	5:P:638:PRO:HD3	2.20	0.42
5:P:741:PRO:HA	5:P:742:PRO:HD3	1.69	0.42
5:P:1269:LYS:HB2	5:P:1269:LYS:HE3	1.88	0.42
5:P:1325:LEU:HA	5:P:1492:ILE:HD13	2.01	0.42
6:Q:186:GLU:OE2	6:Q:731:VAL:HB	2.20	0.42
1:1:34:CYS:CB	1:1:51:CYS:SG	2.95	0.42
5:A:592:GLN:HE22	5:A:1380:GLN:HA	1.85	0.42
5:P:574:ASN:OD1	5:P:574:ASN:N	2.53	0.42
6:Q:407:PHE:O	6:Q:411:MET:HG3	2.19	0.42
10:U:94:LEU:HD23	10:U:94:LEU:HA	1.90	0.42
5:A:219:LEU:HA	5:A:219:LEU:HD23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:50:LEU:O	14:K:54:THR:HG23	2.20	0.42
6:Q:262:PHE:CE1	6:Q:357:ILE:HD13	2.54	0.42
6:Q:1087:LEU:HD23	6:Q:1087:LEU:HA	1.94	0.42
7:R:236:LEU:HD11	7:R:290:LYS:HG3	2.02	0.42
9:T:83:CYS:HB2	9:T:110:PHE:CZ	2.55	0.42
10:U:93:ILE:HD13	10:U:93:ILE:HA	1.68	0.42
5:A:1005:GLY:HA3	12:I:100:GLN:O	2.20	0.42
6:B:416:LYS:HA	6:B:416:LYS:HD3	1.87	0.42
7:C:116:VAL:HG11	7:C:125:LYS:HE3	2.01	0.42
11:H:41:ASP:HB2	11:H:121:LEU:HB3	2.02	0.42
11:H:81:PRO:HA	11:H:82:PRO:HD2	1.76	0.42
5:P:799:GLU:HG3	5:P:1062:HIS:CG	2.55	0.42
5:P:1053:ASP:HA	5:P:1124:LEU:HD13	2.01	0.42
6:Q:1160:GLU:HG2	6:Q:1166:LYS:HG2	2.02	0.42
5:A:1268:ASP:OD1	12:I:61:ARG:NH2	2.52	0.41
6:B:1070:ARG:HH22	4:O:316:GLU:CG	2.33	0.41
6:Q:736:ARG:HD3	6:Q:738:ASP:OD2	2.20	0.41
12:X:2:SER:HA	12:X:9:PHE:O	2.20	0.41
12:X:89:CYS:SG	12:X:91:ASN:HB2	2.60	0.41
1:1:33:GLU:HG3	1:1:53:HIS:ND1	2.35	0.41
5:A:680:LEU:O	5:A:728:GLY:HA3	2.20	0.41
6:B:8:PRO:HB2	6:B:9:GLY:H	1.74	0.41
5:P:631:ASP:OD1	5:P:631:ASP:N	2.51	0.41
5:P:986:PHE:CD2	6:Q:958:MET:HE2	2.56	0.41
5:P:1460:TYR:CD1	5:P:1460:TYR:C	2.98	0.41
6:B:465:LEU:HA	6:B:465:LEU:HD23	1.92	0.41
6:B:809:VAL:HG13	6:B:901:VAL:HB	2.01	0.41
7:C:236:LEU:HD11	7:C:290:LYS:HG3	2.02	0.41
6:Q:335:ARG:HA	6:Q:349:VAL:HG11	2.03	0.41
14:Z:93:ILE:HA	14:Z:94:PRO:HD2	1.73	0.41
6:B:262:PHE:CE1	6:B:357:ILE:HD13	2.56	0.41
5:P:502:ALA:HA	5:P:581:ILE:CG2	2.50	0.41
5:P:681:THR:O	5:P:729:LYS:NZ	2.52	0.41
5:P:1113:HIS:HA	5:P:1116:GLN:HG2	2.03	0.41
5:P:1613:MET:HG2	5:P:1618:THR:HG23	2.01	0.41
8:S:82:LEU:O	8:S:86:ILE:HG23	2.21	0.41
4:V:62:MET:HE2	4:V:84:TYR:HE1	1.85	0.41
5:A:487:ASP:HB2	5:A:615:ARG:HB3	2.02	0.41
5:A:672:ASP:HB2	6:B:783:MET:SD	2.61	0.41
5:A:854:GLY:HA3	5:A:974:THR:O	2.21	0.41
5:P:451:VAL:HA	5:P:452:PRO:HD3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:1025:LYS:HD2	5:P:1025:LYS:HA	1.84	0.41
6:Q:809:VAL:HG13	6:Q:901:VAL:HB	2.03	0.41
9:T:26:ARG:O	9:T:75:MET:HE1	2.21	0.41
5:A:82:PRO:HD3	5:A:393:SER:OG	2.20	0.41
5:A:1025:LYS:HG2	5:A:1615:TYR:HD1	1.85	0.41
5:A:1071:ASP:O	5:A:1072:ASN:HB2	2.21	0.41
5:A:1248:ASP:OD1	5:A:1517:ARG:NH1	2.49	0.41
6:B:427:GLN:OE1	6:B:452:ARG:NH1	2.54	0.41
11:H:105:GLU:HG2	11:H:115:TYR:HE1	1.84	0.41
6:Q:954:PHE:H	6:Q:955:PRO:HD2	1.86	0.41
7:R:37:LYS:HA	14:Z:130:VAL:HG11	2.02	0.41
9:T:155:ARG:HD2	9:T:194:GLU:OE2	2.21	0.41
13:Y:49:MET:HE3	13:Y:49:MET:HB3	1.77	0.41
5:A:227:LEU:HD23	5:A:227:LEU:HA	1.84	0.41
5:A:977:MET:HE1	5:A:991:LYS:HD2	2.01	0.41
6:B:977:ILE:HG21	6:B:977:ILE:HD13	1.72	0.41
4:G:50:ALA:HA	4:G:113:PHE:CD2	2.56	0.41
5:P:582:LYS:O	5:P:585:ASP:HB2	2.20	0.41
5:P:1348:VAL:HG11	6:Q:270:LEU:CD1	2.51	0.41
9:T:7:ARG:O	9:T:11:ARG:HG3	2.20	0.41
6:Q:495:ARG:HA	6:Q:723:LYS:HG2	2.03	0.41
6:Q:833:PRO:HG2	6:Q:836:TRP:CZ2	2.56	0.41
6:Q:841:ASP:OD1	6:Q:842:GLU:N	2.44	0.41
11:W:81:PRO:HA	11:W:82:PRO:HD2	1.78	0.41
12:X:20:PRO:C	12:X:22:ALA:H	2.28	0.41
12:X:99:LEU:HD23	12:X:99:LEU:HA	1.89	0.41
3:3:25:ILE:HA	3:3:26:PRO:HD3	1.88	0.41
3:3:63:ASP:OD1	3:3:65:SER:OG	2.36	0.41
3:3:90:MET:HE3	3:3:90:MET:HB2	1.87	0.41
3:3:140:SER:HB3	6:Q:567:SER:O	2.20	0.41
4:4:292:HIS:HD2	4:4:295:LEU:HD22	1.86	0.41
5:A:745:PRO:HG2	5:A:1075:ALA:HB2	2.02	0.41
5:A:753:ASN:HB2	5:A:782:ASP:OD2	2.21	0.41
6:B:279:ALA:HB2	6:B:326:VAL:HG12	2.03	0.41
12:I:68:LYS:HE2	12:I:68:LYS:HB3	1.95	0.41
3:N:63:ASP:OD2	3:N:66:LYS:NZ	2.35	0.41
3:N:127:ASP:OD2	3:N:129:ALA:HB2	2.21	0.41
5:P:184:LYS:HA	5:P:187:GLU:HG2	2.02	0.41
5:P:643:ALA:HB1	6:Q:1087:LEU:HD23	2.03	0.41
5:P:1235:THR:O	5:P:1544:ASN:ND2	2.54	0.41
5:P:1314:GLN:HG3	5:P:1315:ASN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:211:ARG:HG2	6:Q:239:VAL:HG11	2.02	0.41
6:Q:286:ARG:HA	6:Q:286:ARG:HD2	1.86	0.41
6:Q:491:ILE:HB	6:Q:495:ARG:HD2	2.03	0.41
6:Q:923:GLN:HG2	6:Q:949:ILE:CD1	2.50	0.41
6:Q:1153:ILE:HA	6:Q:1153:ILE:HD13	1.72	0.41
4:V:106:LYS:HB2	4:V:106:LYS:HE3	1.85	0.41
5:A:379:GLU:HB3	4:O:292:HIS:HD1	1.86	0.41
5:A:879:LEU:HD23	5:A:879:LEU:HA	1.97	0.41
6:B:286:ARG:HA	6:B:286:ARG:HD2	1.88	0.41
6:B:1051:PRO:HA	4:O:307:GLU:O	2.21	0.41
12:I:20:PRO:C	12:I:22:ALA:H	2.29	0.41
4:O:295:LEU:HD12	4:O:295:LEU:HA	1.87	0.41
5:P:389:VAL:O	5:P:393:SER:HB2	2.20	0.41
5:P:847:LEU:HD23	5:P:847:LEU:HA	1.91	0.41
6:Q:937:PRO:HB2	6:Q:1013:MET:HE2	2.03	0.41
5:A:429:THR:HG21	4:O:274:SER:CB	2.51	0.40
5:A:597:LYS:HB2	6:B:1082:HIS:CE1	2.56	0.40
5:A:1305:GLU:HG3	12:I:60:LEU:HG	2.03	0.40
5:A:1317:ILE:O	5:A:1322:ILE:HG12	2.21	0.40
6:B:736:ARG:NH1	6:B:738:ASP:OD1	2.54	0.40
12:I:2:SER:HA	12:I:9:PHE:O	2.21	0.40
5:P:598:ALA:CB	5:P:601:MET:HE3	2.50	0.40
11:W:95:TYR:HD2	11:W:144:ILE:HD12	1.85	0.40
14:Z:54:THR:HG22	14:Z:62:SER:H	1.86	0.40
5:A:131:ASP:HB2	9:E:215:MET:HE1	2.03	0.40
5:A:389:VAL:O	5:A:393:SER:HB2	2.22	0.40
5:A:403:LEU:HD12	5:A:403:LEU:HA	1.71	0.40
5:A:1511:GLU:HA	5:A:1512:PRO:HD3	1.96	0.40
5:A:1603:MET:HE3	5:A:1603:MET:HB3	1.79	0.40
6:B:1082:HIS:HB3	6:B:1084:THR:HG23	2.01	0.40
9:E:83:CYS:HB2	9:E:110:PHE:CZ	2.56	0.40
12:I:87:PRO:HG2	12:I:119:TYR:CE2	2.56	0.40
5:P:256:LEU:HA	5:P:256:LEU:HD23	1.85	0.40
6:Q:338:PHE:HZ	6:Q:357:ILE:CD1	2.33	0.40
6:Q:760:TYR:O	6:Q:762:MET:HE3	2.21	0.40
6:Q:1090:ASP:HA	6:Q:1094:ASN:HB2	2.02	0.40
5:A:631:ASP:OD1	5:A:631:ASP:N	2.55	0.40
6:B:436:MET:HE1	6:B:448:ARG:HD3	2.02	0.40
6:B:550:ARG:HD3	6:B:550:ARG:HA	1.81	0.40
7:C:128:ASP:OD1	7:C:128:ASP:N	2.54	0.40
11:H:7:ASP:HA	11:H:57:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:11:GLU:O	2:M:87:SER:HA	2.22	0.40
5:P:1365:LEU:HD23	5:P:1365:LEU:HA	1.79	0.40
6:Q:145:VAL:HG22	6:Q:440:PHE:HB3	2.04	0.40
6:Q:156:ARG:NE	6:Q:455:GLU:OE2	2.50	0.40
6:Q:962:MET:HE3	6:Q:1031:VAL:HG11	2.03	0.40
7:R:31:TRP:HB2	14:Z:82:LYS:HD2	2.04	0.40
3:3:40:LEU:HD12	3:3:40:LEU:HA	1.82	0.40
6:B:61:LEU:HA	6:B:61:LEU:HD23	1.75	0.40
9:E:26:ARG:O	9:E:75:MET:HE1	2.20	0.40
14:K:54:THR:HG22	14:K:62:SER:H	1.86	0.40
5:P:439:ASP:OD1	5:P:441:THR:HB	2.21	0.40
5:P:487:ASP:HB2	5:P:615:ARG:HB3	2.04	0.40
6:Q:944:GLN:HA	6:Q:945:PRO:HD3	1.96	0.40
7:R:246:ARG:HD2	7:R:284:GLU:OE2	2.22	0.40
4:V:32:ASN:CG	4:V:33:GLY:H	2.29	0.40
4:V:111:THR:HB	4:V:112:PRO:HD2	2.04	0.40
12:X:2:SER:HB3	12:X:3:VAL:H	1.70	0.40
13:Y:58:GLU:HA	13:Y:61:LEU:HD12	2.03	0.40
5:A:1384:TYR:CE2	6:B:1074:MET:HG2	2.57	0.40
5:A:1613:MET:HG2	5:A:1618:THR:HG23	2.03	0.40
7:C:246:ARG:HD2	7:C:284:GLU:OE2	2.21	0.40
8:D:82:LEU:O	8:D:86:ILE:HG23	2.20	0.40
9:E:198:ILE:CD1	9:E:212:ARG:HG3	2.51	0.40
11:H:95:TYR:HD2	11:H:144:ILE:HD12	1.86	0.40
3:N:70:LEU:HA	3:N:71:PRO:HD3	1.84	0.40
5:P:18:ILE:HD12	5:P:354:SER:HB3	2.03	0.40
5:P:1533:GLU:OE2	9:T:14:ARG:NH2	2.54	0.40
6:Q:712:SER:N	6:Q:713:PRO:HD2	2.36	0.40
9:T:4:GLU:C	9:T:6:GLU:H	2.28	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1310:LYS:NZ	5:P:838:GLU:OE2[1_556]	2.07	0.13

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	1	42/70 (60%)	37 (88%)	3 (7%)	2 (5%)	2	6
1	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2	6
2	2	99/415 (24%)	93 (94%)	4 (4%)	2 (2%)	6	21
2	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	6	22
3	3	139/233 (60%)	122 (88%)	15 (11%)	2 (1%)	9	30
3	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	5	19
4	4	52/326 (16%)	49 (94%)	3 (6%)	0	100	100
4	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	11	36
4	O	50/326 (15%)	46 (92%)	4 (8%)	0	100	100
4	V	191/326 (59%)	175 (92%)	15 (8%)	1 (0%)	24	55
5	A	1505/1664 (90%)	1434 (95%)	62 (4%)	9 (1%)	21	51
5	P	1502/1664 (90%)	1433 (95%)	59 (4%)	10 (1%)	18	47
6	B	1176/1203 (98%)	1116 (95%)	47 (4%)	13 (1%)	11	36
6	Q	1152/1203 (96%)	1104 (96%)	42 (4%)	6 (0%)	24	55
7	C	303/335 (90%)	288 (95%)	13 (4%)	2 (1%)	18	47
7	R	303/335 (90%)	289 (95%)	12 (4%)	2 (1%)	18	47
8	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	9
8	S	55/137 (40%)	51 (93%)	2 (4%)	2 (4%)	2	10
9	E	210/215 (98%)	198 (94%)	11 (5%)	1 (0%)	24	55
9	T	210/215 (98%)	199 (95%)	9 (4%)	2 (1%)	12	38
10	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
10	U	98/155 (63%)	98 (100%)	0	0	100	100
11	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
11	W	127/146 (87%)	119 (94%)	8 (6%)	0	100	100
12	I	122/125 (98%)	107 (88%)	12 (10%)	3 (2%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	X	115/125 (92%)	102 (89%)	10 (9%)	3 (3%)	4	15
13	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
13	Y	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
14	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
14	Z	98/142 (69%)	92 (94%)	6 (6%)	0	100	100
All	All	8537/11124 (77%)	8066 (94%)	400 (5%)	71 (1%)	16	44

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1606	SER
6	B	111	ASP
6	B	895	PHE
7	C	224	THR
8	D	99	LEU
12	I	41	GLN
5	P	1533	GLU
7	R	224	THR
8	S	99	LEU
12	X	41	GLN
5	A	412	SER
5	A	448	SER
5	A	1394	THR
5	A	1533	GLU
6	B	817	ARG
6	B	1140	LYS
8	D	98	GLY
9	E	50	MET
12	I	5	GLY
5	P	412	SER
5	P	448	SER
5	P	1348	VAL
5	P	1394	THR
5	P	1606	SER
9	T	50	MET
12	X	5	GLY
1	1	46	VAL
2	2	85	LYS
5	A	450	LYS
6	B	78	PRO

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Mol	Chain	Res	Type
4	G	99	ASP
12	I	21	ASN
1	L	46	VAL
2	M	85	LYS
5	P	450	LYS
8	S	98	GLY
4	V	99	ASP
12	X	21	ASN
1	1	43	THR
3	3	115	SER
6	B	834	LYS
4	G	100	THR
1	L	43	THR
2	M	36	THR
3	N	115	SER
5	P	564	PRO
5	P	1572	ARG
6	Q	834	LYS
6	Q	1140	LYS
2	2	36	THR
5	A	451	VAL
5	A	564	PRO
6	B	80	ASN
6	B	117	VAL
6	B	1062	GLY
6	B	1063	ARG
7	C	32	ASN
5	P	451	VAL
6	Q	1062	GLY
6	Q	1063	ARG
7	R	32	ASN
3	3	70	LEU
5	A	1512	PRO
6	Q	9	GLY
6	B	9	GLY
3	N	70	LEU
3	N	39	PRO
6	Q	833	PRO
9	T	206	GLY
6	B	833	PRO
6	B	954	PHE

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	1	39/57 (68%)	34 (87%)	5 (13%)	4	15
1	L	39/57 (68%)	34 (87%)	5 (13%)	4	15
2	2	93/371 (25%)	84 (90%)	9 (10%)	8	25
2	M	98/371 (26%)	86 (88%)	12 (12%)	5	16
3	3	135/220 (61%)	126 (93%)	9 (7%)	15	42
3	N	135/220 (61%)	127 (94%)	8 (6%)	18	48
4	4	52/291 (18%)	48 (92%)	4 (8%)	12	36
4	G	171/291 (59%)	158 (92%)	13 (8%)	12	36
4	O	50/291 (17%)	47 (94%)	3 (6%)	17	47
4	V	175/291 (60%)	163 (93%)	12 (7%)	14	41
5	A	1345/1465 (92%)	1254 (93%)	91 (7%)	14	42
5	P	1343/1465 (92%)	1247 (93%)	96 (7%)	13	39
6	B	1033/1053 (98%)	966 (94%)	67 (6%)	15	43
6	Q	1019/1053 (97%)	952 (93%)	67 (7%)	15	43
7	C	269/296 (91%)	254 (94%)	15 (6%)	19	50
7	R	269/296 (91%)	254 (94%)	15 (6%)	19	50
8	D	55/116 (47%)	50 (91%)	5 (9%)	9	28
8	S	56/116 (48%)	51 (91%)	5 (9%)	9	29
9	E	194/197 (98%)	180 (93%)	14 (7%)	13	39
9	T	194/197 (98%)	177 (91%)	17 (9%)	9	29
10	F	90/137 (66%)	86 (96%)	4 (4%)	25	59
10	U	90/137 (66%)	86 (96%)	4 (4%)	25	59
11	H	115/128 (90%)	107 (93%)	8 (7%)	14	40
11	W	115/128 (90%)	108 (94%)	7 (6%)	17	46
12	I	109/110 (99%)	102 (94%)	7 (6%)	16	44
12	X	104/110 (94%)	98 (94%)	6 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	J	64/65 (98%)	56 (88%)	8 (12%)	4	15
13	Y	64/65 (98%)	56 (88%)	8 (12%)	4	15
14	K	91/130 (70%)	82 (90%)	9 (10%)	7	24
14	Z	90/130 (69%)	82 (91%)	8 (9%)	9	29
All	All	7696/9854 (78%)	7155 (93%)	541 (7%)	14	40

All (541) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	38	LEU
1	1	41	SER
1	1	55	ILE
1	1	57	LEU
1	1	66	GLN
2	2	17	ASP
2	2	18	GLN
2	2	31	ARG
2	2	52	VAL
2	2	65	TYR
2	2	77	VAL
2	2	84	GLU
2	2	98	SER
2	2	109	ARG
3	3	51	GLN
3	3	81	THR
3	3	89	ILE
3	3	124	THR
3	3	135	LYS
3	3	141	GLU
3	3	153	VAL
3	3	167	LYS
3	3	178	GLU
4	4	269	SER
4	4	272	ILE
4	4	278	ILE
4	4	291	SER
5	A	10	GLU
5	A	40	ASN
5	A	61	LEU
5	A	83	VAL
5	A	136	LEU

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Mol	Chain	Res	Type
5	A	174	SER
5	A	186	SER
5	A	202	THR
5	A	230	ARG
5	A	257	ASN
5	A	262	THR
5	A	266	VAL
5	A	271	ARG
5	A	272	GLN
5	A	312	SER
5	A	315	ILE
5	A	346	SER
5	A	373	LEU
5	A	379	GLU
5	A	393	SER
5	A	413	LEU
5	A	447	THR
5	A	451	VAL
5	A	503	VAL
5	A	518	GLU
5	A	524	ILE
5	A	555	LYS
5	A	611	GLU
5	A	627	ASP
5	A	655	SER
5	A	661	THR
5	A	666	VAL
5	A	670	ILE
5	A	684	ASP
5	A	700	ILE
5	A	708	THR
5	A	709	ARG
5	A	739	VAL
5	A	747	ILE
5	A	758	GLU
5	A	783	LYS
5	A	794	VAL
5	A	815	ARG
5	A	878	ARG
5	A	955	ARG
5	A	957	VAL
5	A	966	LEU

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Mol	Chain	Res	Type
5	A	988	SER
5	A	1013	THR
5	A	1021	ARG
5	A	1026	GLN
5	A	1033	SER
5	A	1071	ASP
5	A	1085	LEU
5	A	1098	SER
5	A	1102	LEU
5	A	1118	VAL
5	A	1123	VAL
5	A	1131	LYS
5	A	1136	VAL
5	A	1150	LYS
5	A	1159	ASP
5	A	1162	ASN
5	A	1204	THR
5	A	1215	VAL
5	A	1226	VAL
5	A	1273	THR
5	A	1275	THR
5	A	1276	THR
5	A	1304	GLU
5	A	1310	LYS
5	A	1314	GLN
5	A	1320	GLN
5	A	1364	ARG
5	A	1392	ILE
5	A	1441	LYS
5	A	1455	ARG
5	A	1508	VAL
5	A	1518	VAL
5	A	1531	ASP
5	A	1533	GLU
5	A	1536	ILE
5	A	1601	GLN
5	A	1604	GLU
5	A	1605	THR
5	A	1607	THR
5	A	1609	SER
5	A	1611	MET
5	A	1616	GLU

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Mol	Chain	Res	Type
5	A	1633	GLN
5	A	1635	ASP
6	B	13	THR
6	B	17	ARG
6	B	22	GLU
6	B	37	LEU
6	B	53	THR
6	B	57	ASP
6	B	65	VAL
6	B	79	LEU
6	B	81	SER
6	B	87	ASN
6	B	97	VAL
6	B	117	VAL
6	B	187	SER
6	B	202	LEU
6	B	207	ILE
6	B	221	SER
6	B	228	SER
6	B	231	HIS
6	B	236	ILE
6	B	239	VAL
6	B	276	ILE
6	B	305	ARG
6	B	306	LEU
6	B	311	ARG
6	B	315	LYS
6	B	357	ILE
6	B	481	VAL
6	B	486	VAL
6	B	490	LYS
6	B	523	GLU
6	B	537	SER
6	B	583	LEU
6	B	622	ILE
6	B	658	LEU
6	B	720	GLN
6	B	725	THR
6	B	731	VAL
6	B	753	LYS
6	B	782	ASP
6	B	811	LEU

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Mol	Chain	Res	Type
6	B	813	LEU
6	B	822	THR
6	B	824	HIS
6	B	829	ASN
6	B	833	PRO
6	B	835	GLU
6	B	858	ILE
6	B	871	ILE
6	B	883	GLU
6	B	897	GLU
6	B	977	ILE
6	B	998	GLU
6	B	1026	ILE
6	B	1038	HIS
6	B	1042	ASP
6	B	1047	ARG
6	B	1060	VAL
6	B	1064	LYS
6	B	1075	GLU
6	B	1103	VAL
6	B	1125	THR
6	B	1136	GLU
6	B	1141	LEU
6	B	1153	ILE
6	B	1163	GLN
6	B	1165	ASN
6	B	1174	THR
7	C	38	LYS
7	C	43	ASN
7	C	61	THR
7	C	77	SER
7	C	91	VAL
7	C	97	LEU
7	C	118	SER
7	C	138	VAL
7	C	142	ARG
7	C	181	ASP
7	C	193	LEU
7	C	224	THR
7	C	243	SER
7	C	277	ARG
7	C	279	VAL

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Mol	Chain	Res	Type
8	D	15	THR
8	D	29	GLN
8	D	38	GLN
8	D	80	THR
8	D	99	LEU
9	E	4	GLU
9	E	31	THR
9	E	33	GLU
9	E	74	ASP
9	E	90	VAL
9	E	92	THR
9	E	93	MET
9	E	107	THR
9	E	131	THR
9	E	136	ASN
9	E	142	VAL
9	E	162	ARG
9	E	163	GLU
9	E	177	ARG
10	F	59	GLN
10	F	87	LYS
10	F	99	LEU
10	F	109	VAL
4	G	21	LYS
4	G	24	VAL
4	G	35	SER
4	G	39	VAL
4	G	139	ILE
4	G	147	LEU
4	G	167	THR
4	G	169	VAL
4	G	223	GLU
4	G	230	ARG
4	G	239	THR
4	G	241	ARG
4	G	243	VAL
11	H	3	ASN
11	H	9	ILE
11	H	39	THR
11	H	108	SER
11	H	111	LEU
11	H	112	ILE

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Mol	Chain	Res	Type
11	H	114	VAL
11	H	121	LEU
12	I	2	SER
12	I	3	VAL
12	I	15	ASP
12	I	45	LEU
12	I	70	SER
12	I	74	ASN
12	I	81	THR
13	J	3	VAL
13	J	9	SER
13	J	10	CYS
13	J	14	VAL
13	J	27	GLU
13	J	34	THR
13	J	45	CYS
13	J	48	ARG
14	K	44	ARG
14	K	45	GLU
14	K	51	THR
14	K	68	GLU
14	K	99	ASN
14	K	103	ILE
14	K	118	GLN
14	K	123	ASP
14	K	133	SER
1	L	38	LEU
1	L	41	SER
1	L	55	ILE
1	L	57	LEU
1	L	66	GLN
2	M	17	ASP
2	M	18	GLN
2	M	31	ARG
2	M	44	LYS
2	M	48	LYS
2	M	52	VAL
2	M	63	GLU
2	M	65	TYR
2	M	77	VAL
2	M	84	GLU
2	M	98	SER

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Mol	Chain	Res	Type
2	M	109	ARG
3	N	51	GLN
3	N	89	ILE
3	N	124	THR
3	N	135	LYS
3	N	141	GLU
3	N	153	VAL
3	N	167	LYS
3	N	178	GLU
4	O	269	SER
4	O	272	ILE
4	O	278	ILE
5	P	10	GLU
5	P	40	ASN
5	P	61	LEU
5	P	83	VAL
5	P	136	LEU
5	P	174	SER
5	P	175	SER
5	P	186	SER
5	P	202	THR
5	P	257	ASN
5	P	262	THR
5	P	266	VAL
5	P	271	ARG
5	P	272	GLN
5	P	312	SER
5	P	315	ILE
5	P	346	SER
5	P	373	LEU
5	P	379	GLU
5	P	393	SER
5	P	397	ARG
5	P	413	LEU
5	P	416	ARG
5	P	447	THR
5	P	451	VAL
5	P	503	VAL
5	P	518	GLU
5	P	524	ILE
5	P	555	LYS
5	P	611	GLU

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Mol	Chain	Res	Type
5	P	655	SER
5	P	666	VAL
5	P	670	ILE
5	P	684	ASP
5	P	700	ILE
5	P	708	THR
5	P	709	ARG
5	P	739	VAL
5	P	747	ILE
5	P	758	GLU
5	P	783	LYS
5	P	794	VAL
5	P	815	ARG
5	P	878	ARG
5	P	955	ARG
5	P	957	VAL
5	P	966	LEU
5	P	988	SER
5	P	1009	THR
5	P	1013	THR
5	P	1021	ARG
5	P	1026	GLN
5	P	1033	SER
5	P	1071	ASP
5	P	1085	LEU
5	P	1098	SER
5	P	1102	LEU
5	P	1118	VAL
5	P	1123	VAL
5	P	1131	LYS
5	P	1136	VAL
5	P	1150	LYS
5	P	1159	ASP
5	P	1162	ASN
5	P	1204	THR
5	P	1215	VAL
5	P	1226	VAL
5	P	1273	THR
5	P	1275	THR
5	P	1276	THR
5	P	1304	GLU
5	P	1310	LYS

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Mol	Chain	Res	Type
5	P	1314	GLN
5	P	1320	GLN
5	P	1350	ARG
5	P	1392	ILE
5	P	1441	LYS
5	P	1442	VAL
5	P	1468	LYS
5	P	1480	THR
5	P	1481	GLU
5	P	1486	VAL
5	P	1492	ILE
5	P	1505	ASP
5	P	1518	VAL
5	P	1536	ILE
5	P	1584	LEU
5	P	1601	GLN
5	P	1604	GLU
5	P	1605	THR
5	P	1607	THR
5	P	1609	SER
5	P	1611	MET
5	P	1616	GLU
5	P	1633	GLN
5	P	1635	ASP
6	Q	13	THR
6	Q	17	ARG
6	Q	22	GLU
6	Q	37	LEU
6	Q	53	THR
6	Q	57	ASP
6	Q	65	VAL
6	Q	97	VAL
6	Q	117	VAL
6	Q	187	SER
6	Q	202	LEU
6	Q	207	ILE
6	Q	221	SER
6	Q	228	SER
6	Q	231	HIS
6	Q	236	ILE
6	Q	239	VAL
6	Q	276	ILE

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Mol	Chain	Res	Type
6	Q	300	SER
6	Q	305	ARG
6	Q	306	LEU
6	Q	311	ARG
6	Q	315	LYS
6	Q	357	ILE
6	Q	477	ASP
6	Q	486	VAL
6	Q	490	LYS
6	Q	523	GLU
6	Q	537	SER
6	Q	582	SER
6	Q	583	LEU
6	Q	622	ILE
6	Q	658	LEU
6	Q	720	GLN
6	Q	725	THR
6	Q	731	VAL
6	Q	753	LYS
6	Q	782	ASP
6	Q	811	LEU
6	Q	813	LEU
6	Q	822	THR
6	Q	824	HIS
6	Q	829	ASN
6	Q	833	PRO
6	Q	835	GLU
6	Q	858	ILE
6	Q	871	ILE
6	Q	883	GLU
6	Q	934	ILE
6	Q	977	ILE
6	Q	998	GLU
6	Q	1026	ILE
6	Q	1038	HIS
6	Q	1042	ASP
6	Q	1047	ARG
6	Q	1060	VAL
6	Q	1064	LYS
6	Q	1075	GLU
6	Q	1091	ARG
6	Q	1103	VAL

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Mol	Chain	Res	Type
6	Q	1125	THR
6	Q	1136	GLU
6	Q	1141	LEU
6	Q	1153	ILE
6	Q	1163	GLN
6	Q	1165	ASN
6	Q	1174	THR
7	R	38	LYS
7	R	43	ASN
7	R	61	THR
7	R	77	SER
7	R	91	VAL
7	R	97	LEU
7	R	118	SER
7	R	138	VAL
7	R	142	ARG
7	R	181	ASP
7	R	193	LEU
7	R	224	THR
7	R	243	SER
7	R	277	ARG
7	R	279	VAL
8	S	15	THR
8	S	29	GLN
8	S	38	GLN
8	S	80	THR
8	S	99	LEU
9	T	4	GLU
9	T	31	THR
9	T	33	GLU
9	T	74	ASP
9	T	77	SER
9	T	90	VAL
9	T	92	THR
9	T	93	MET
9	T	107	THR
9	T	131	THR
9	T	136	ASN
9	T	142	VAL
9	T	162	ARG
9	T	163	GLU
9	T	167	ARG

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Mol	Chain	Res	Type
9	T	177	ARG
9	T	213	ILE
10	U	59	GLN
10	U	87	LYS
10	U	99	LEU
10	U	109	VAL
4	V	24	VAL
4	V	35	SER
4	V	39	VAL
4	V	139	ILE
4	V	147	LEU
4	V	167	THR
4	V	169	VAL
4	V	176	ASP
4	V	223	GLU
4	V	230	ARG
4	V	239	THR
4	V	243	VAL
11	W	3	ASN
11	W	9	ILE
11	W	39	THR
11	W	108	SER
11	W	112	ILE
11	W	114	VAL
11	W	121	LEU
12	X	2	SER
12	X	3	VAL
12	X	15	ASP
12	X	45	LEU
12	X	70	SER
12	X	81	THR
13	Y	3	VAL
13	Y	9	SER
13	Y	10	CYS
13	Y	14	VAL
13	Y	27	GLU
13	Y	34	THR
13	Y	45	CYS
13	Y	48	ARG
14	Z	45	GLU
14	Z	51	THR
14	Z	68	GLU

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Mol	Chain	Res	Type
14	Z	99	ASN
14	Z	103	ILE
14	Z	118	GLN
14	Z	123	ASP
14	Z	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	61	ASN
4	4	292	HIS
5	A	43	HIS
5	A	126	GLN
5	A	382	GLN
5	A	407	GLN
5	A	590	ASN
5	A	1026	GLN
5	A	1162	ASN
6	B	87	ASN
6	B	235	GLN
6	B	636	GLN
6	B	1008	HIS
6	B	1163	GLN
7	C	58	ASN
7	C	232	GLN
7	C	323	ASN
8	D	23	HIS
9	E	5	ASN
10	F	59	GLN
4	G	23	GLN
12	I	97	HIS
2	M	18	GLN
3	N	61	ASN
3	N	132	GLN
4	O	292	HIS
5	P	407	GLN
5	P	590	ASN
5	P	1026	GLN
5	P	1162	ASN
5	P	1527	GLN
6	Q	224	ASN
6	Q	235	GLN

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Mol	Chain	Res	Type
6	Q	321	GLN
6	Q	351	GLN
6	Q	673	ASN
7	R	99	HIS
7	R	232	GLN
8	S	23	HIS
9	T	5	ASN
4	V	23	GLN
4	V	56	ASN
4	V	59	GLN
4	V	75	ASN
4	V	171	ASN
12	X	44	ASN
12	X	97	HIS
13	Y	26	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	$\# Z > 2$
16	SO4	B	2204	-	4,4,4	0.33	0	6,6,6	0.34	0
16	SO4	Q	2204	-	4,4,4	0.31	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	2204	SO4	1	0
16	Q	2204	SO4	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	1	44/70 (62%)	0.13	0 100 100	79, 117, 154, 193	0
1	L	44/70 (62%)	-0.16	2 (4%) 38 30	65, 88, 134, 175	0
2	2	103/415 (24%)	0.17	1 (0%) 79 72	96, 128, 160, 171	0
2	M	108/415 (26%)	-0.13	0 100 100	66, 94, 134, 156	0
3	3	145/233 (62%)	0.27	2 (1%) 73 64	76, 121, 161, 187	0
3	N	145/233 (62%)	-0.11	3 (2%) 63 54	56, 93, 133, 160	0
4	4	54/326 (16%)	0.06	0 100 100	74, 103, 143, 158	0
4	G	193/326 (59%)	0.01	0 100 100	51, 107, 168, 189	0
4	O	52/326 (15%)	0.28	3 (5%) 29 22	64, 100, 145, 155	0
4	V	197/326 (60%)	-0.04	5 (2%) 58 48	57, 89, 140, 164	0
5	A	1521/1664 (91%)	-0.54	13 (0%) 81 74	40, 63, 117, 161	0
5	P	1518/1664 (91%)	-0.41	9 (0%) 85 80	48, 72, 123, 182	0
6	B	1182/1203 (98%)	-0.60	4 (0%) 90 86	37, 59, 108, 187	0
6	Q	1164/1203 (96%)	-0.29	5 (0%) 88 84	40, 83, 132, 165	0
7	C	305/335 (91%)	-0.42	0 100 100	60, 81, 127, 148	0
7	R	305/335 (91%)	-0.28	0 100 100	68, 95, 137, 151	0
8	D	58/137 (42%)	-0.19	0 100 100	56, 107, 136, 149	0
8	S	59/137 (43%)	-0.28	1 (1%) 69 60	62, 96, 128, 134	0
9	E	212/215 (98%)	-0.21	1 (0%) 87 82	49, 92, 149, 164	0
9	T	212/215 (98%)	-0.14	1 (0%) 87 82	57, 94, 147, 169	0
10	F	100/155 (64%)	-0.78	2 (2%) 65 56	42, 60, 93, 129	0
10	U	100/155 (64%)	-0.57	1 (1%) 79 72	51, 70, 107, 119	0
11	H	131/146 (89%)	-0.41	0 100 100	60, 80, 113, 125	0
11	W	131/146 (89%)	-0.35	0 100 100	66, 91, 121, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
12	I	124/125 (99%)	-0.12	4 (3%)	50	40	52, 81, 129, 155	0
12	X	119/125 (95%)	0.30	2 (1%)	69	60	65, 103, 152, 177	0
13	J	69/70 (98%)	-0.58	0	100	100	56, 68, 91, 106	0
13	Y	69/70 (98%)	-0.38	0	100	100	72, 85, 114, 128	0
14	K	101/142 (71%)	-0.46	1 (0%)	79	72	58, 72, 121, 148	0
14	Z	100/142 (70%)	-0.36	1 (1%)	79	72	63, 83, 133, 164	0
All	All	8665/11124 (77%)	-0.36	61 (0%)	84	77	37, 77, 136, 193	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	F	55	PRO	4.2
3	3	72	VAL	4.1
5	P	1286	ALA	4.0
3	N	72	VAL	3.9
5	A	1342	PRO	3.9
5	P	1205	PHE	3.8
5	P	141	LEU	3.6
5	A	1286	ALA	3.5
12	I	42	PHE	3.4
5	A	141	LEU	3.3
5	A	1205	PHE	3.3
10	U	55	PRO	3.3
12	X	125	ASN	3.2
4	V	20	HIS	3.2
5	A	40	ASN	3.0
3	N	84	LYS	3.0
6	B	1138	ALA	3.0
5	A	41	LEU	2.9
4	O	310	TYR	2.9
2	2	22	ALA	2.8
6	Q	1152	PHE	2.8
5	A	1204	THR	2.8
4	V	136	TYR	2.7
5	A	706	HIS	2.7
1	L	43	THR	2.6
5	P	1202	LEU	2.5
3	3	50	GLN	2.5
6	B	1152	PHE	2.5
12	X	40	SER	2.5

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Mol	Chain	Res	Type	RSRZ
6	Q	820	PRO	2.5
6	B	116	ALA	2.4
8	S	100	PRO	2.4
4	V	14	ALA	2.4
4	O	314	THR	2.4
5	P	1276	THR	2.4
5	P	706	HIS	2.4
4	V	17	ILE	2.4
9	T	4	GLU	2.3
5	P	1664	ALA	2.3
5	P	1086	ILE	2.3
6	Q	891	GLU	2.3
5	P	1378	THR	2.3
5	A	1276	THR	2.2
5	A	1213	ALA	2.2
10	F	154	ASP	2.2
14	K	53	ALA	2.2
1	L	53	HIS	2.2
6	Q	810	ASP	2.2
5	A	1202	LEU	2.2
4	O	304	ASN	2.1
4	V	171	ASN	2.1
3	N	50	GLN	2.1
12	I	75	GLU	2.1
6	B	893	ASN	2.1
5	A	1664	ALA	2.1
14	Z	53	ALA	2.1
12	I	124	ASN	2.0
6	Q	437	ALA	2.0
5	A	710	SER	2.0
12	I	43	SER	2.0
9	E	4	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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	SO4	B	2204	5/5	0.86	0.20	123,124,132,137	0
16	SO4	Q	2204	5/5	0.87	0.20	133,139,142,147	0
15	ZN	J	3001	1/1	0.96	0.16	547,547,547,547	0
15	ZN	Y	3001	1/1	0.97	0.12	489,489,489,489	0
15	ZN	A	3001	1/1	0.99	0.03	75,75,75,75	0
15	ZN	X	3001	1/1	0.99	0.02	113,113,113,113	0
15	ZN	X	3002	1/1	0.99	0.02	89,89,89,89	1
15	ZN	L	3001	1/1	1.00	0.01	87,87,87,87	0
15	ZN	P	3001	1/1	1.00	0.02	70,70,70,70	0
15	ZN	P	3002	1/1	1.00	0.03	83,83,83,83	0
15	ZN	Q	3001	1/1	1.00	0.01	64,64,64,64	0
15	ZN	A	3002	1/1	1.00	0.02	77,77,77,77	0
15	ZN	B	3001	1/1	1.00	0.01	53,53,53,53	0
15	ZN	I	3001	1/1	1.00	0.02	73,73,73,73	0
15	ZN	I	3002	1/1	1.00	0.02	77,77,77,77	1
15	ZN	1	3001	1/1	1.00	0.04	120,120,120,120	0

6.5 Other polymers

There are no such residues in this entry.