Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:50 AM EDT

PDB ID	:	4C2M
Title	:	Structure of RNA polymerase I at 2.8 A 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 (i) 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 (i)) were used in the production of this report:

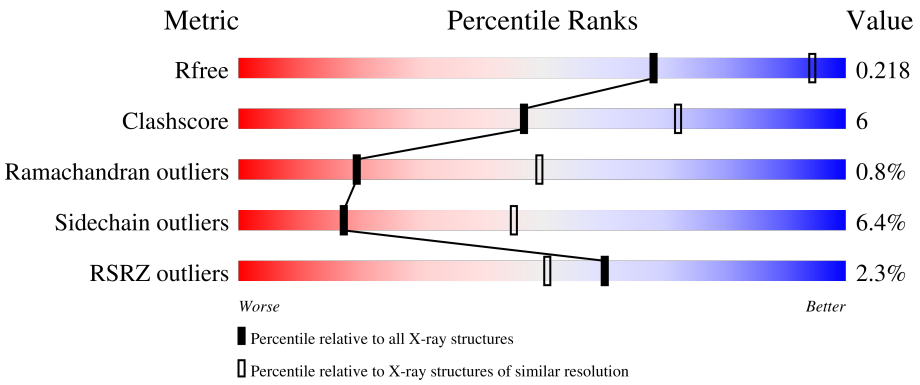
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	7% 41% 19% • 37%
1	L	70	4% 41% 19% • 37%
2	2	415	3% 19% 5% 75%
2	M	415	% 20% 6% 74%
3	3	233	4% 50% 12% 38%

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Mol	Chain	Length	Quality of chain
3	N	233	%, 49%, 13%, 38%
4	4	326	%, 14%, 83%
4	G	326	9%, 47%, 12%, 41%
4	O	326	2%, 13%, 84%
4	V	326	2%, 49%, 11%, 40%
5	A	1664	%, 74%, 16%, 9%
5	P	1664	%, 73%, 16%, 9%
6	B	1203	%, 78%, 17%
6	Q	1203	2%, 76%, 18%
7	C	335	%, 73%, 16%, 9%
7	R	335	2%, 72%, 17%, 9%
8	D	137	31%, 10%, 58%
8	S	137	%, 31%, 10%, 57%
9	E	215	4%, 80%, 16%
9	T	215	3%, 78%, 18%
10	F	155	59%, 5%, 35%
10	U	155	59%, 5%, 35%
11	H	146	75%, 14%, 10%
11	W	146	%, 78%, 11%, 10%
12	I	125	3%, 73%, 26%
12	X	125	3%, 70%, 24%, 5%
13	J	70	74%, 20%
13	Y	70	70%, 24%
14	K	142	%, 54%, 15%, 29%
14	Z	142	3%, 49%, 20%, 30%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	1	44	352	217	70	61	4	0	0	0
1	L	44	352	217	70	61	4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

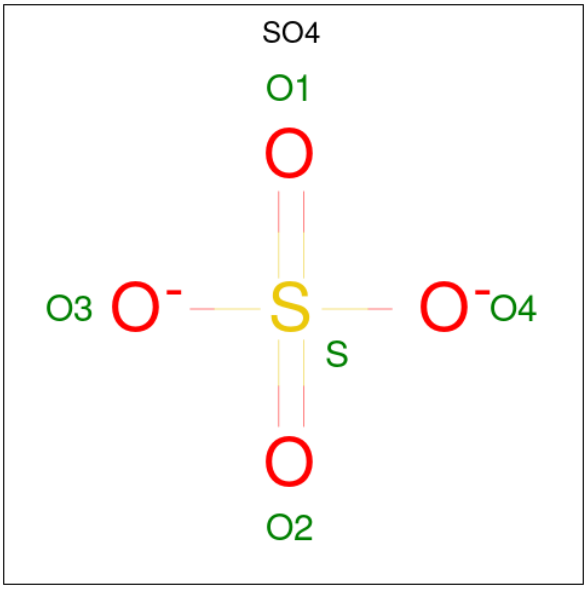
- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

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

- Molecule 15 is ZINC ION (three-letter code: 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 (three-letter code: SO4) (formula: O_4S).



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.

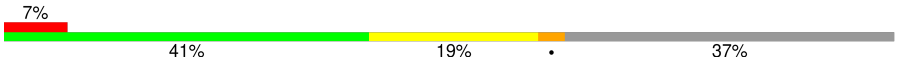
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	3	1	Total O 1 1	0	0
17	A	96	Total O 96 96	0	0
17	B	62	Total O 62 62	0	0
17	C	1	Total O 1 1	0	0
17	D	3	Total O 3 3	0	0
17	E	4	Total O 4 4	0	0
17	F	4	Total O 4 4	0	0
17	G	1	Total O 1 1	0	0
17	H	10	Total O 10 10	0	0
17	I	3	Total O 3 3	0	0
17	N	3	Total O 3 3	0	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

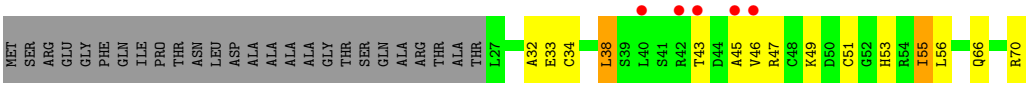
3 Residue-property plots (i)

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

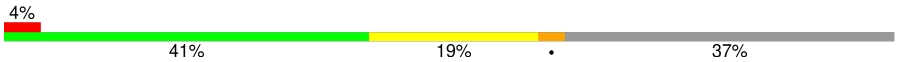
Chain 1:

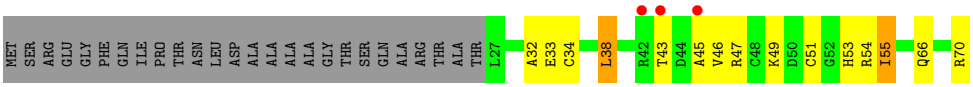




• Molecule 1: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

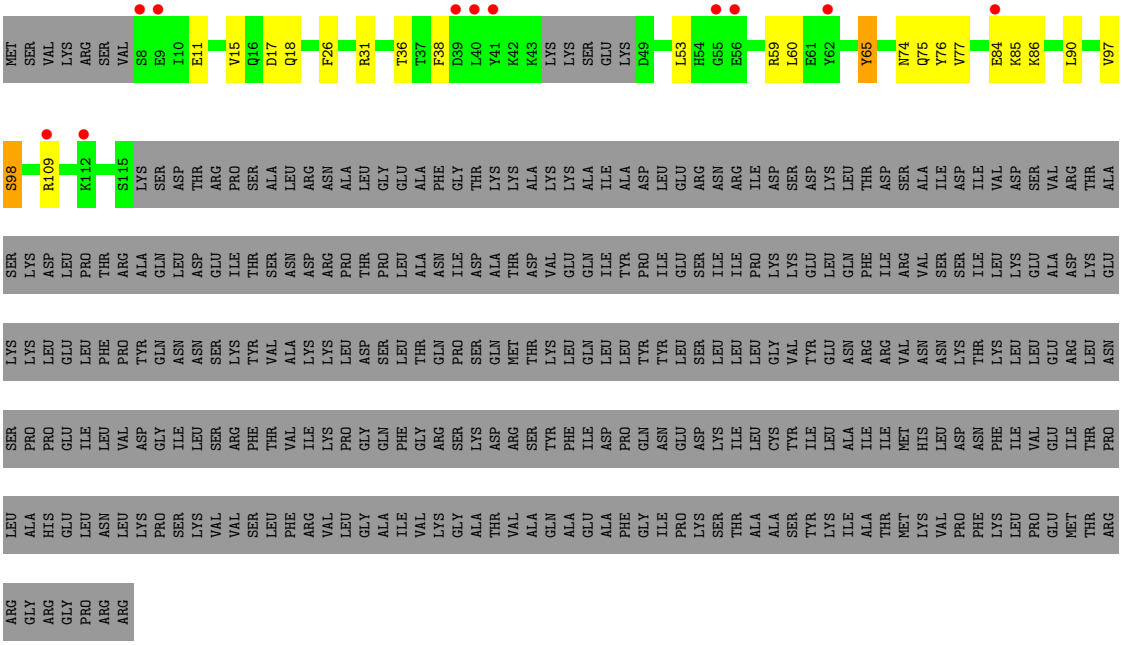
Chain L:





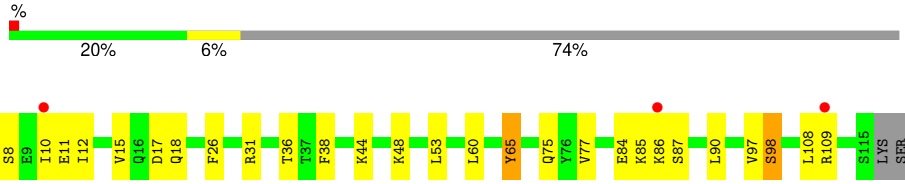
• Molecule 2: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49

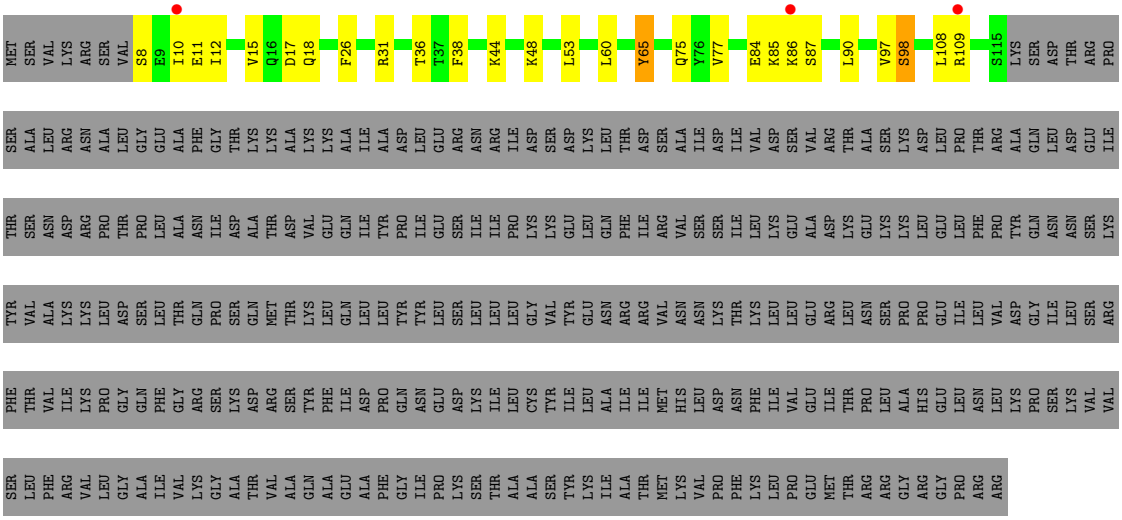
Chain 2:



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

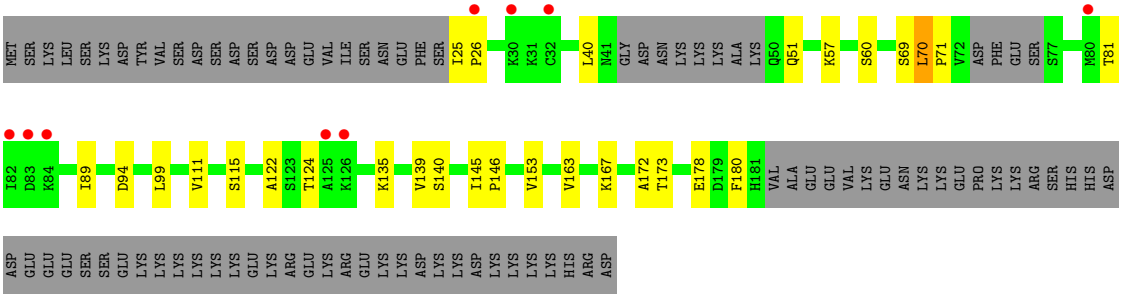
Chain M:





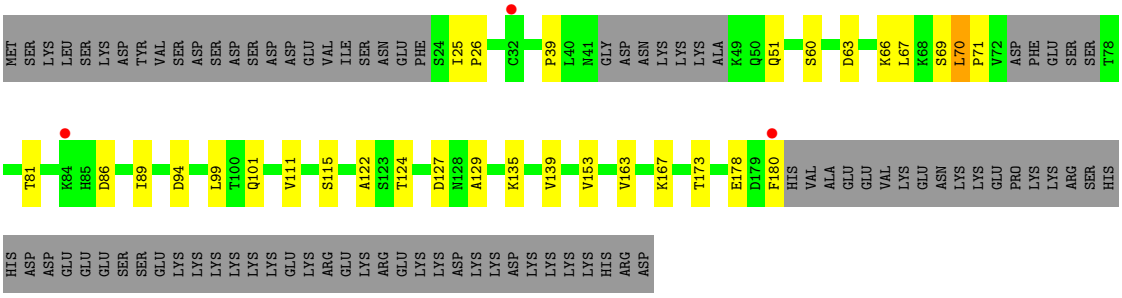
- Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain 3:



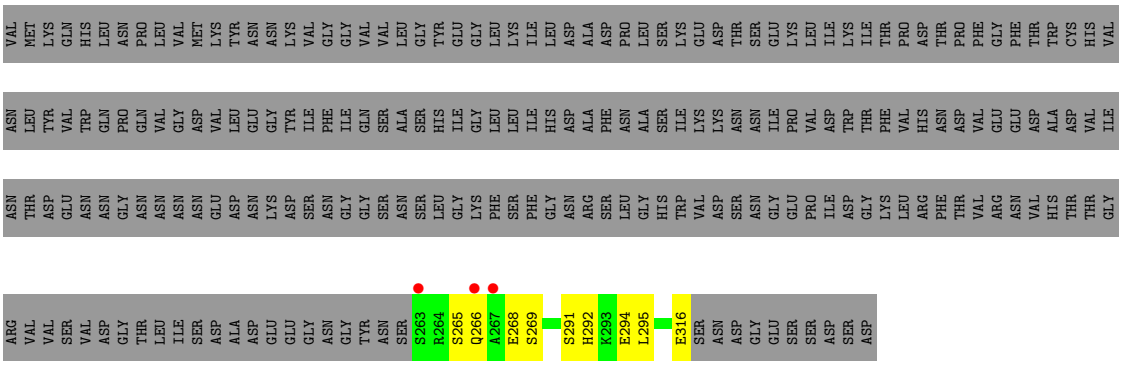
- Molecule 3: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34

Chain N:



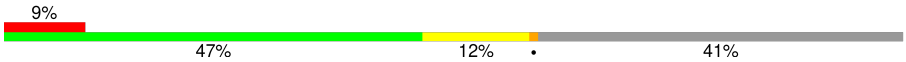
- Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

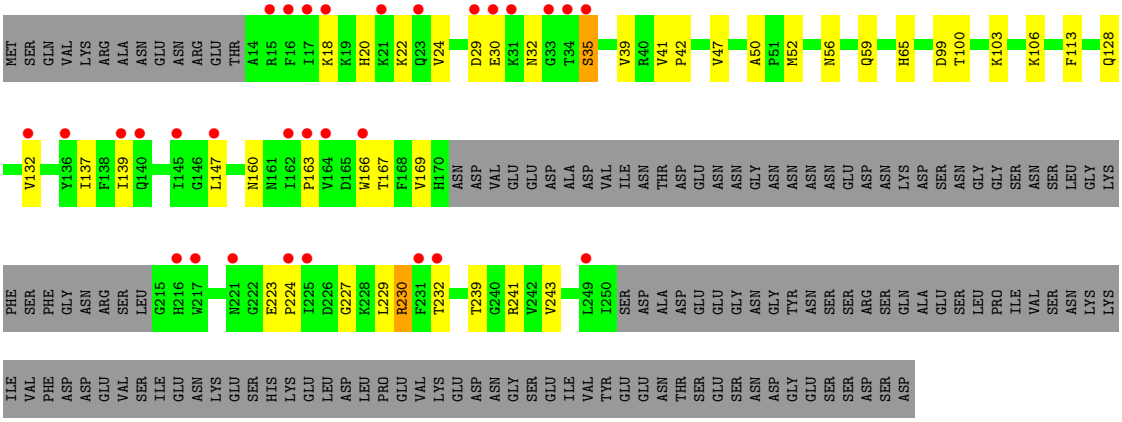
Chain 4:



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

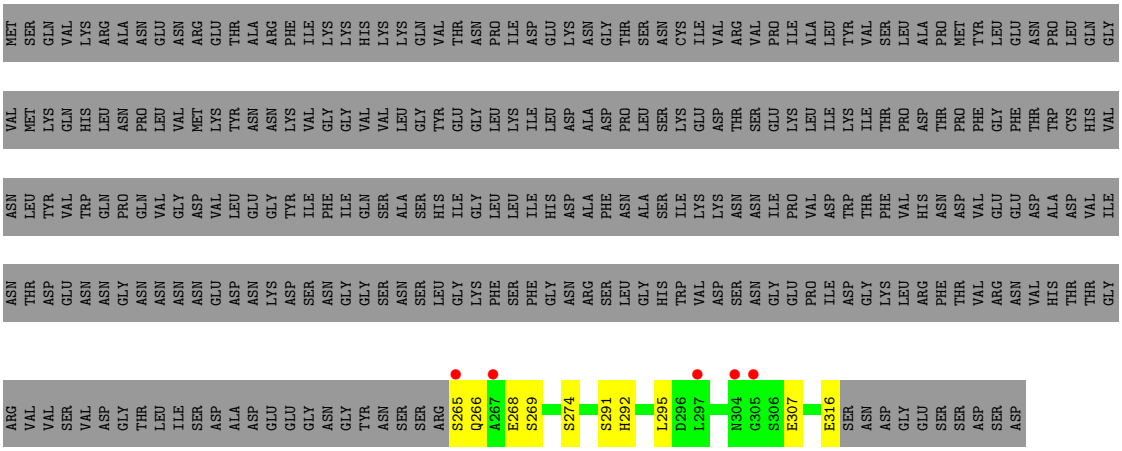
Chain G:





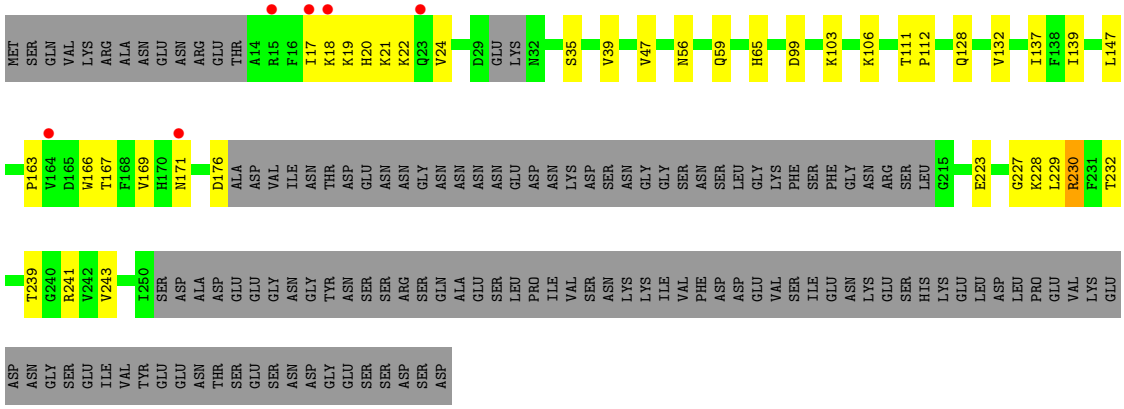
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

Chain O:



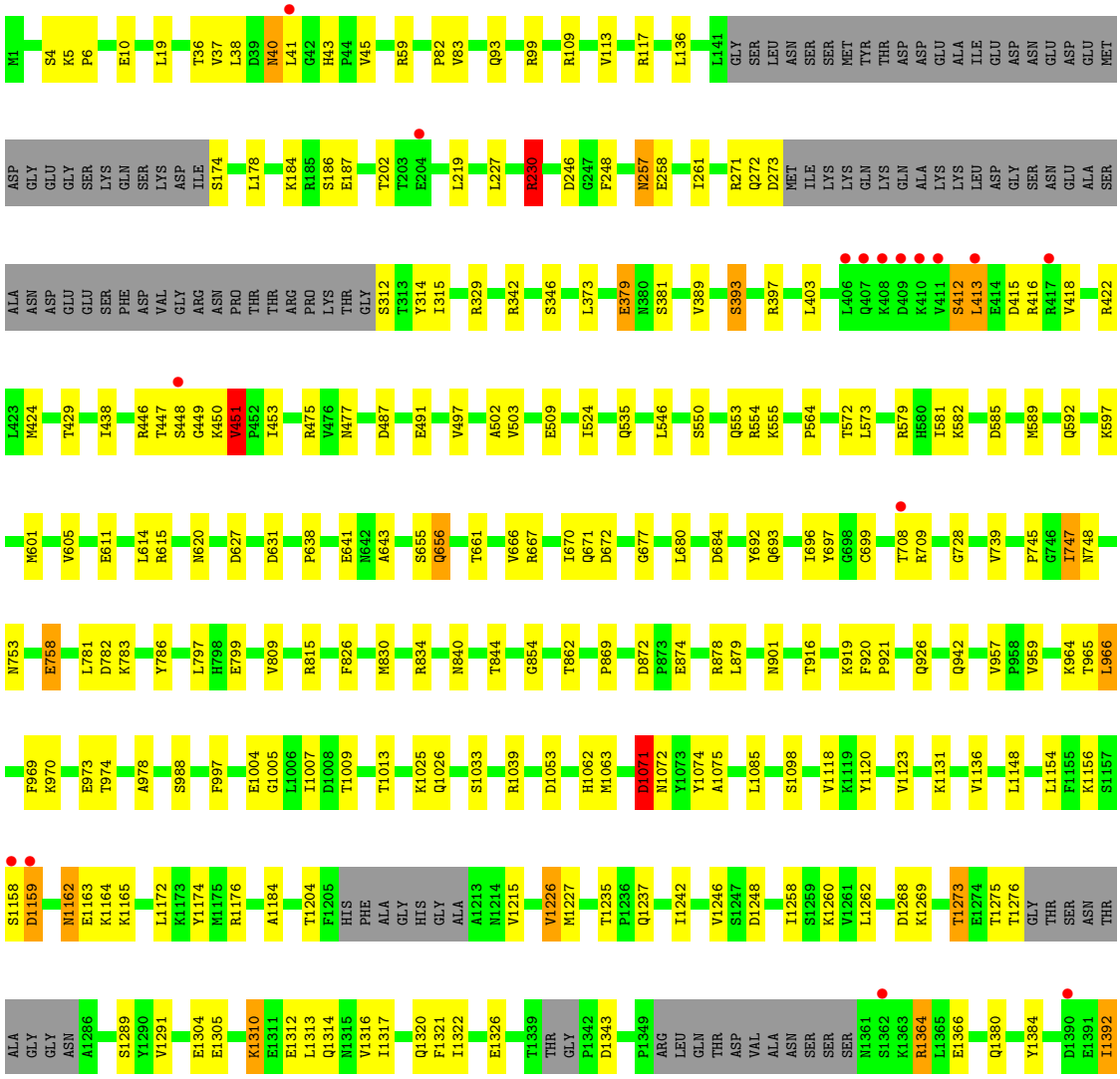
• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43

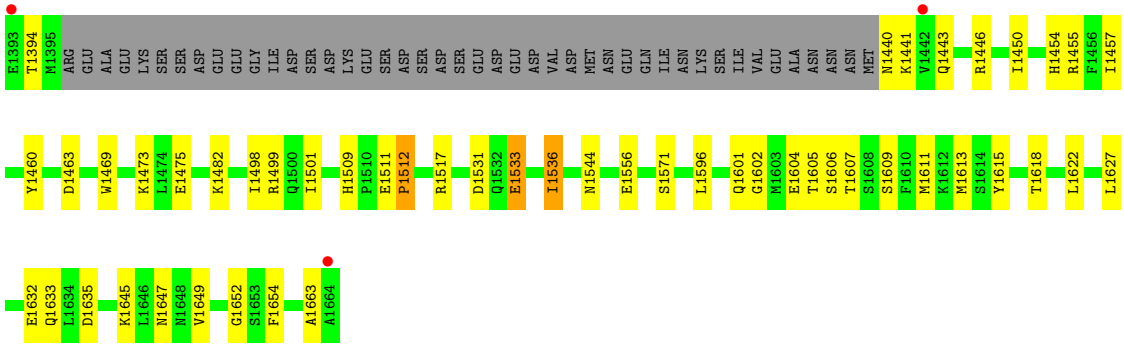
Chain V:



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

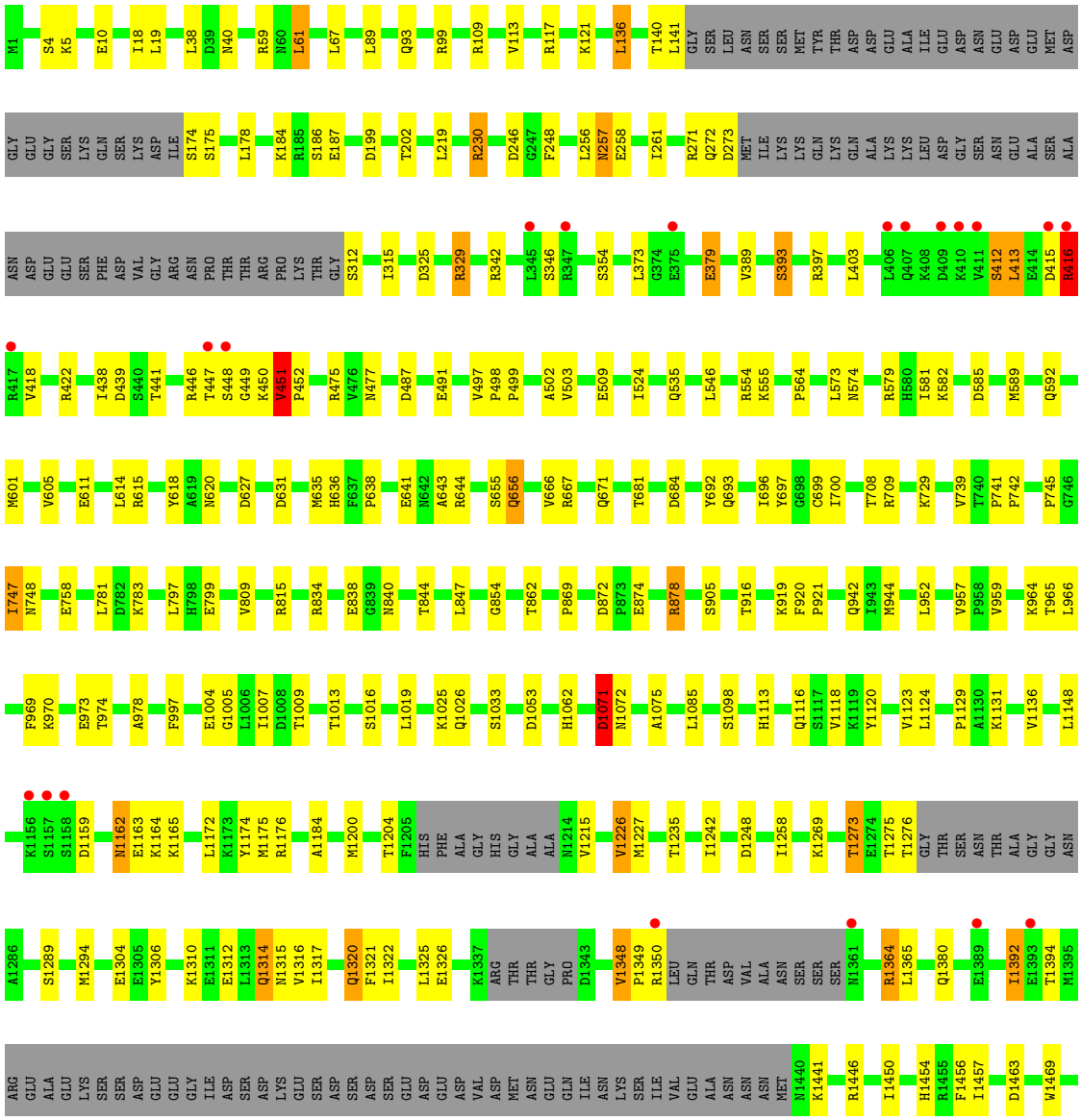
Chain A:

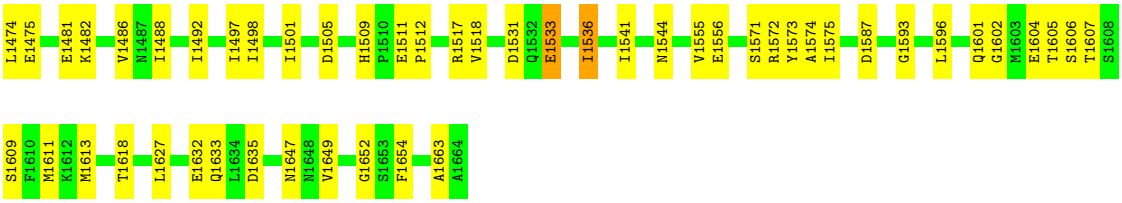




• Molecule 5: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190

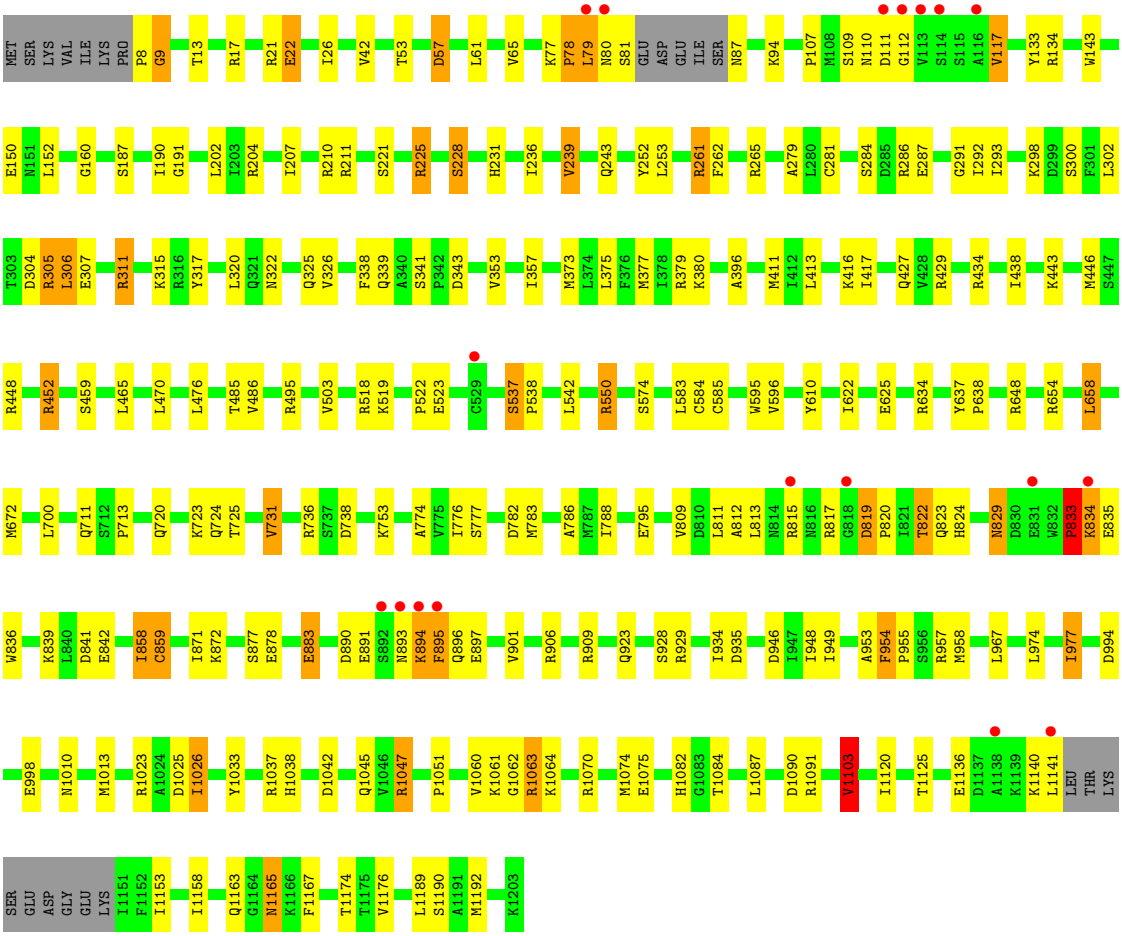
Chain P:





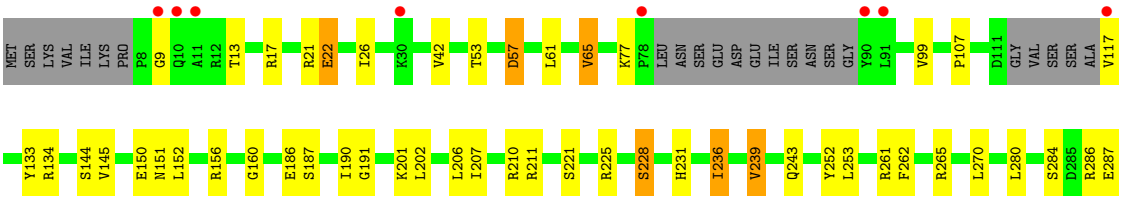
• Molecule 6: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135

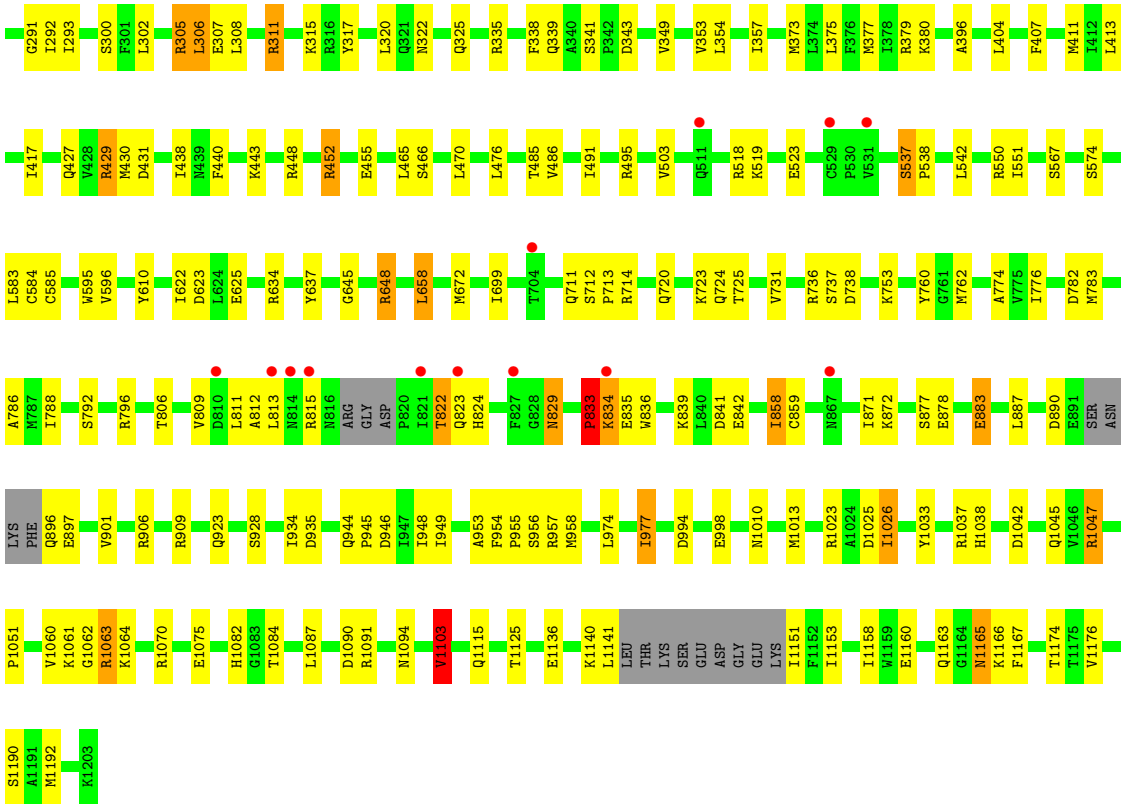
Chain B:



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

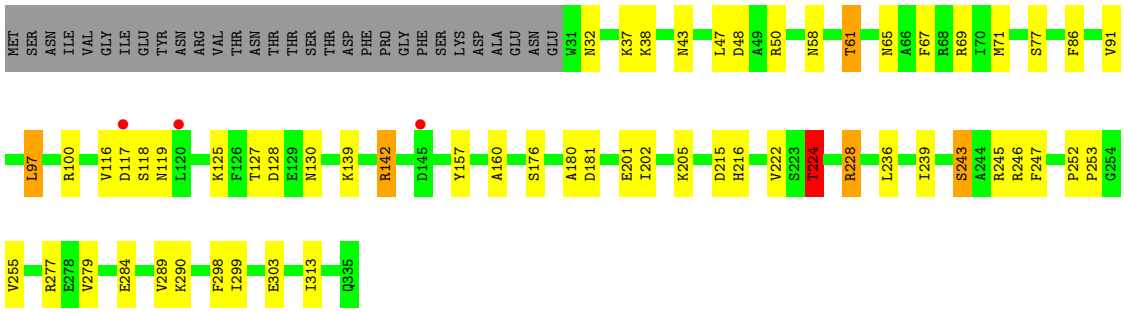
Chain Q:





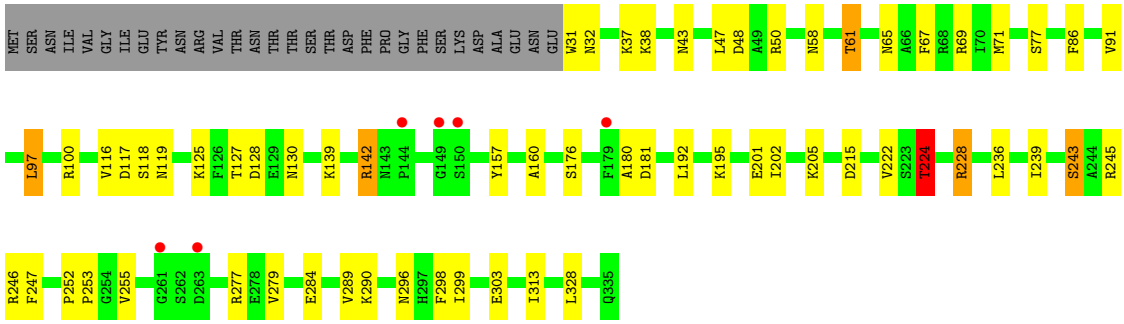
• Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain C:



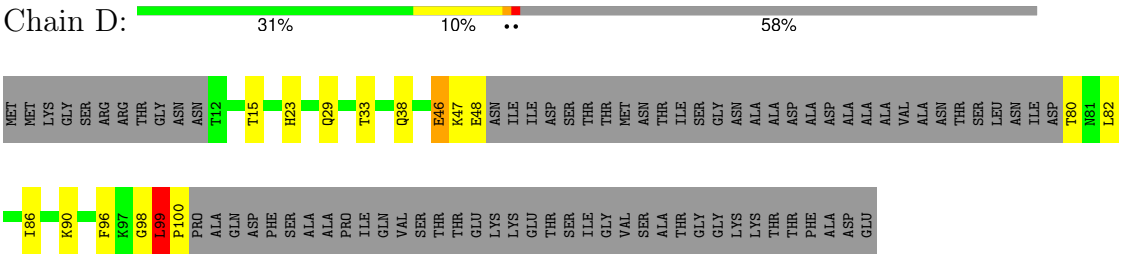
• Molecule 7: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

Chain R:



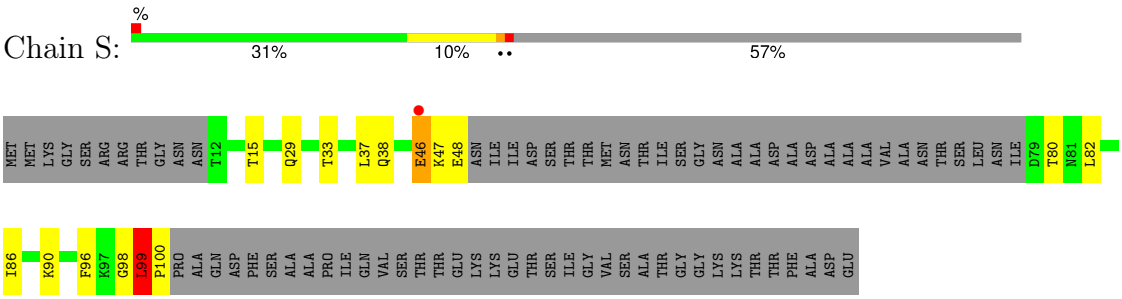
• Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain D:



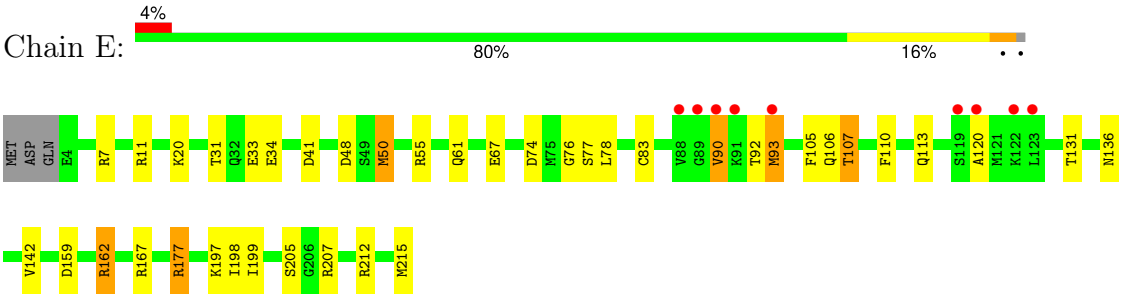
• Molecule 8: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

Chain S:



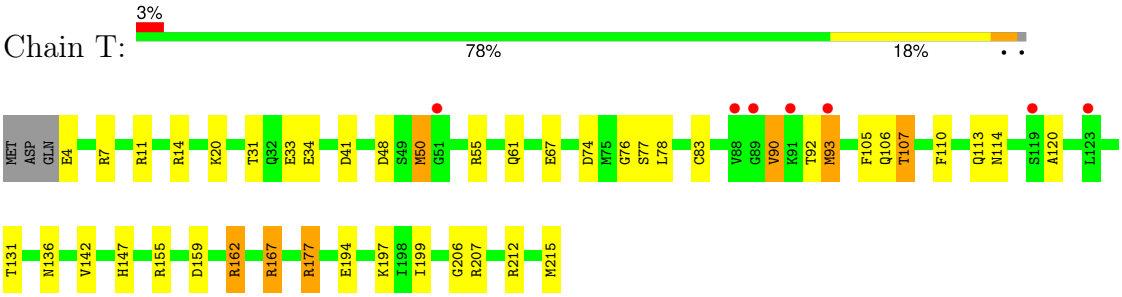
• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain E:



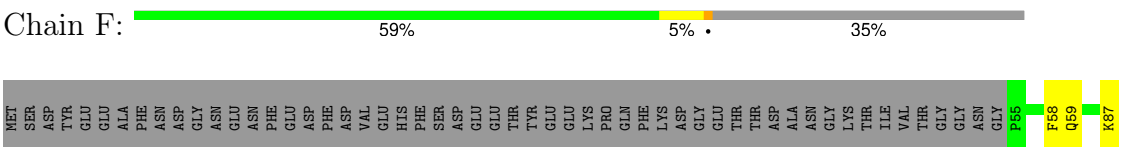
• Molecule 9: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1

Chain T:



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

Chain F:



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

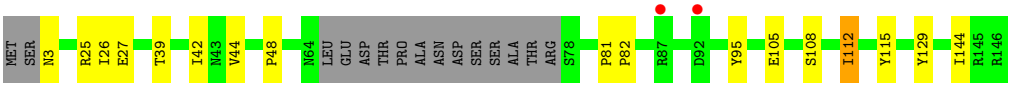
Chain U:

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

Chain H:

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

Chain W:

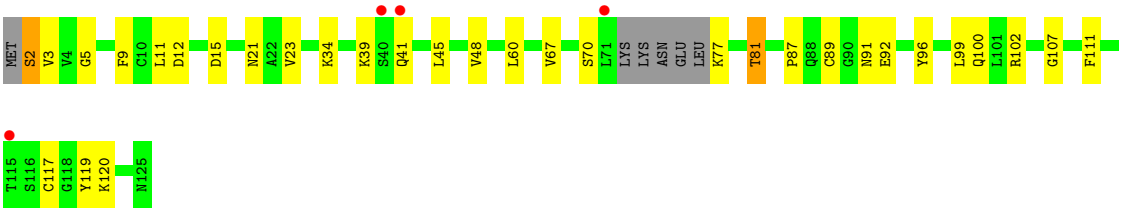


• Molecule 12: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I:

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

Chain X:

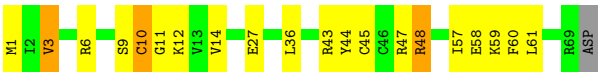


• Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:

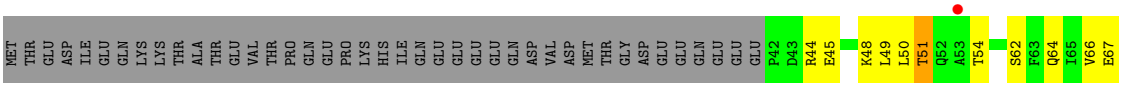
• Molecule 13: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

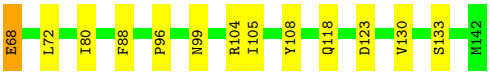
Chain Y:



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

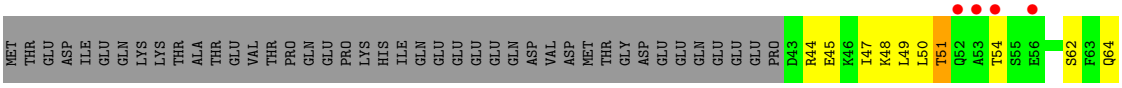
Chain K:





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

Chain Z:



4 Data and refinement statistics (i)

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 39.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.29-2.80) 99.9 (39.98-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.29 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/354	0.58	0/468
1	L	0.42	0/354	0.60	0/468
2	2	0.34	0/829	0.53	0/1114
2	M	0.40	0/872	0.55	0/1170
3	3	0.35	0/1174	0.52	0/1584
3	N	0.40	0/1172	0.55	0/1580
4	4	0.38	0/434	0.58	0/584
4	G	0.37	0/1564	0.66	3/2127 (0.1%)
4	O	0.42	0/417	0.60	0/562
4	V	0.38	0/1594	0.65	3/2168 (0.1%)
5	A	0.49	0/12236	0.75	25/16523 (0.2%)
5	P	0.45	0/12216	0.73	25/16495 (0.2%)
6	B	0.50	2/9594 (0.0%)	0.78	25/12967 (0.2%)
6	Q	0.43	0/9465	0.76	25/12789 (0.2%)
7	C	0.46	2/2475 (0.1%)	0.67	3/3354 (0.1%)
7	R	0.43	2/2475 (0.1%)	0.66	3/3354 (0.1%)
8	D	0.40	0/465	0.58	0/630
8	S	0.41	0/473	0.59	0/641
9	E	0.40	0/1771	0.66	3/2383 (0.1%)
9	T	0.41	0/1771	0.67	3/2383 (0.1%)
10	F	0.46	0/838	0.59	0/1129
10	U	0.43	0/838	0.59	0/1129
11	H	0.42	0/1070	0.61	0/1449
11	W	0.40	0/1070	0.60	0/1449
12	I	0.43	0/956	0.59	0/1288
12	X	0.42	0/912	0.58	0/1229
13	J	0.57	1/578 (0.2%)	0.59	0/775
13	Y	0.42	0/578	0.58	0/775
14	K	0.46	0/804	0.79	3/1083 (0.3%)
14	Z	0.42	0/796	0.75	3/1072 (0.3%)
All	All	0.45	7/70145 (0.0%)	0.71	124/94722 (0.1%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	10	CYS	CB-SG	7.66	1.95	1.82
6	B	281	CYS	CB-SG	-6.93	1.70	1.82
7	C	58	ASN	CG-ND2	-6.88	1.15	1.32
7	R	58	ASN	CG-OD1	-6.67	1.09	1.24
7	C	58	ASN	CG-OD1	-6.47	1.09	1.24
7	R	58	ASN	CG-ND2	-6.37	1.17	1.32
6	B	859	CYS	CB-SG	-6.18	1.71	1.82

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	1023	ARG	NE-CZ-NH2	-14.08	113.26	120.30
6	Q	550	ARG	NE-CZ-NH2	-13.79	113.41	120.30
6	B	1023	ARG	NE-CZ-NH2	-13.75	113.43	120.30
5	P	397	ARG	NE-CZ-NH1	13.48	127.04	120.30
6	Q	452	ARG	NE-CZ-NH2	-13.35	113.62	120.30
6	B	452	ARG	NE-CZ-NH2	-13.35	113.62	120.30
5	A	397	ARG	NE-CZ-NH1	13.31	126.96	120.30
6	Q	550	ARG	NE-CZ-NH1	13.09	126.84	120.30
6	B	448	ARG	NE-CZ-NH2	-12.99	113.80	120.30
5	A	329	ARG	NE-CZ-NH2	-12.94	113.83	120.30
6	Q	648	ARG	NE-CZ-NH2	-12.92	113.84	120.30
5	A	59	ARG	NE-CZ-NH1	12.84	126.72	120.30
6	Q	452	ARG	NE-CZ-NH1	12.83	126.72	120.30
5	A	329	ARG	NE-CZ-NH1	12.79	126.70	120.30
5	A	59	ARG	NE-CZ-NH2	-12.76	113.92	120.30
6	B	429	ARG	NE-CZ-NH2	-12.75	113.93	120.30
5	P	397	ARG	NE-CZ-NH2	-12.74	113.93	120.30
6	Q	634	ARG	NE-CZ-NH2	-12.74	113.93	120.30
9	T	167	ARG	NE-CZ-NH2	-12.59	114.00	120.30
5	P	342	ARG	NE-CZ-NH2	-12.58	114.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	167	ARG	NE-CZ-NH2	-12.54	114.03	120.30
9	E	167	ARG	NE-CZ-NH1	12.53	126.57	120.30
5	A	416	ARG	NE-CZ-NH2	-12.46	114.07	120.30
6	B	261	ARG	NE-CZ-NH1	12.46	126.53	120.30
6	B	448	ARG	NE-CZ-NH1	12.40	126.50	120.30
5	P	422	ARG	NE-CZ-NH2	-12.32	114.14	120.30
14	K	44	ARG	NE-CZ-NH2	-12.31	114.14	120.30
6	B	634	ARG	NE-CZ-NH2	-12.23	114.19	120.30
6	Q	634	ARG	NE-CZ-NH1	12.23	126.42	120.30
5	P	59	ARG	NE-CZ-NH2	-12.19	114.20	120.30
6	B	452	ARG	NE-CZ-NH1	12.19	126.39	120.30
6	B	261	ARG	NE-CZ-NH2	-12.14	114.23	120.30
6	B	429	ARG	NE-CZ-NH1	12.12	126.36	120.30
5	P	416	ARG	NE-CZ-NH2	-12.06	114.27	120.30
5	P	342	ARG	NE-CZ-NH1	12.04	126.32	120.30
5	P	422	ARG	NE-CZ-NH1	11.98	126.29	120.30
14	K	44	ARG	NE-CZ-NH1	11.98	126.29	120.30
6	Q	261	ARG	NE-CZ-NH1	11.93	126.27	120.30
5	P	416	ARG	NE-CZ-NH1	11.86	126.23	120.30
7	R	142	ARG	NE-CZ-NH2	-11.84	114.38	120.30
9	T	167	ARG	NE-CZ-NH1	11.84	126.22	120.30
5	A	1364	ARG	NE-CZ-NH2	-11.82	114.39	120.30
5	A	397	ARG	NE-CZ-NH2	-11.81	114.39	120.30
5	P	59	ARG	NE-CZ-NH1	11.79	126.19	120.30
5	P	329	ARG	NE-CZ-NH1	11.78	126.19	120.30
4	G	241	ARG	NE-CZ-NH1	11.78	126.19	120.30
6	Q	261	ARG	NE-CZ-NH2	-11.75	114.42	120.30
5	P	329	ARG	NE-CZ-NH2	-11.70	114.45	120.30
6	Q	648	ARG	NE-CZ-NH1	11.67	126.14	120.30
5	A	422	ARG	NE-CZ-NH2	-11.65	114.47	120.30
4	G	241	ARG	NE-CZ-NH2	-11.64	114.48	120.30
7	C	142	ARG	NE-CZ-NH2	-11.50	114.55	120.30
6	Q	429	ARG	NE-CZ-NH2	-11.50	114.55	120.30
6	Q	448	ARG	NE-CZ-NH1	11.42	126.01	120.30
7	C	142	ARG	NE-CZ-NH1	11.41	126.01	120.30
5	P	230	ARG	NE-CZ-NH2	-11.41	114.59	120.30
5	P	230	ARG	NE-CZ-NH1	11.32	125.96	120.30
7	R	142	ARG	NE-CZ-NH1	11.31	125.95	120.30
5	A	422	ARG	NE-CZ-NH1	11.30	125.95	120.30
6	Q	448	ARG	NE-CZ-NH2	-11.29	114.66	120.30
5	A	342	ARG	NE-CZ-NH2	-11.24	114.68	120.30
14	Z	44	ARG	NE-CZ-NH2	-11.20	114.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	1364	ARG	NE-CZ-NH2	-11.20	114.70	120.30
5	A	1364	ARG	NE-CZ-NH1	11.11	125.85	120.30
5	A	416	ARG	NE-CZ-NH1	11.09	125.84	120.30
6	B	634	ARG	NE-CZ-NH1	11.08	125.84	120.30
6	Q	1023	ARG	NE-CZ-NH1	10.87	125.74	120.30
14	Z	44	ARG	NE-CZ-NH1	10.82	125.71	120.30
5	A	230	ARG	NE-CZ-NH2	-10.81	114.89	120.30
5	A	230	ARG	NE-CZ-NH1	10.74	125.67	120.30
5	P	1364	ARG	NE-CZ-NH1	10.70	125.65	120.30
6	B	550	ARG	NE-CZ-NH2	-10.63	114.98	120.30
4	V	241	ARG	NE-CZ-NH2	-10.62	114.99	120.30
6	B	648	ARG	NE-CZ-NH2	-10.60	115.00	120.30
6	Q	429	ARG	NE-CZ-NH1	10.60	125.60	120.30
4	V	241	ARG	NE-CZ-NH1	10.03	125.31	120.30
6	B	550	ARG	NE-CZ-NH1	9.81	125.21	120.30
6	B	1023	ARG	NE-CZ-NH1	9.56	125.08	120.30
5	A	342	ARG	NE-CZ-NH1	9.15	124.87	120.30
6	B	648	ARG	NE-CZ-NH1	8.97	124.78	120.30
5	A	397	ARG	CD-NE-CZ	6.93	133.31	123.60
6	B	261	ARG	CD-NE-CZ	6.89	133.24	123.60
9	T	167	ARG	CD-NE-CZ	6.72	133.01	123.60
5	A	59	ARG	CD-NE-CZ	6.63	132.88	123.60
5	P	397	ARG	CD-NE-CZ	6.58	132.81	123.60
5	P	59	ARG	CD-NE-CZ	6.55	132.77	123.60
6	B	452	ARG	CD-NE-CZ	6.54	132.75	123.60
5	A	329	ARG	CD-NE-CZ	6.42	132.58	123.60
5	P	329	ARG	CD-NE-CZ	6.37	132.52	123.60
6	B	448	ARG	CD-NE-CZ	6.33	132.47	123.60
6	Q	550	ARG	CD-NE-CZ	6.29	132.41	123.60
14	K	44	ARG	CD-NE-CZ	6.26	132.37	123.60
6	Q	452	ARG	CD-NE-CZ	6.25	132.35	123.60
6	Q	634	ARG	CD-NE-CZ	6.25	132.35	123.60
5	A	416	ARG	CD-NE-CZ	6.18	132.25	123.60
5	P	422	ARG	CD-NE-CZ	6.17	132.24	123.60
6	B	634	ARG	CD-NE-CZ	6.17	132.23	123.60
7	R	142	ARG	CD-NE-CZ	6.13	132.18	123.60
6	B	429	ARG	CD-NE-CZ	6.13	132.18	123.60
5	A	422	ARG	CD-NE-CZ	6.12	132.16	123.60
4	G	241	ARG	CD-NE-CZ	6.03	132.05	123.60
5	P	416	ARG	CD-NE-CZ	6.00	131.99	123.60
7	C	142	ARG	CD-NE-CZ	5.99	131.98	123.60
6	Q	1023	ARG	CD-NE-CZ	5.95	131.93	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	167	ARG	CD-NE-CZ	5.90	131.86	123.60
14	Z	44	ARG	CD-NE-CZ	5.82	131.75	123.60
6	Q	261	ARG	CD-NE-CZ	5.81	131.74	123.60
6	Q	448	ARG	CD-NE-CZ	5.81	131.73	123.60
5	A	1364	ARG	CD-NE-CZ	5.74	131.63	123.60
6	Q	1103	VAL	CB-CA-C	-5.73	100.51	111.40
5	A	342	ARG	CD-NE-CZ	5.67	131.54	123.60
5	P	1364	ARG	CD-NE-CZ	5.67	131.53	123.60
6	B	1103	VAL	CB-CA-C	-5.60	100.76	111.40
6	Q	429	ARG	CD-NE-CZ	5.55	131.38	123.60
5	P	342	ARG	CD-NE-CZ	5.55	131.37	123.60
5	P	230	ARG	CD-NE-CZ	5.51	131.32	123.60
6	B	550	ARG	CD-NE-CZ	5.48	131.27	123.60
4	V	241	ARG	CD-NE-CZ	5.44	131.22	123.60
6	Q	648	ARG	CD-NE-CZ	5.43	131.20	123.60
6	B	648	ARG	CD-NE-CZ	5.42	131.18	123.60
6	B	1023	ARG	CD-NE-CZ	5.29	131.01	123.60
5	A	230	ARG	CD-NE-CZ	5.21	130.89	123.60
5	P	1071	ASP	N-CA-C	-5.09	97.27	111.00
5	A	1071	ASP	N-CA-C	-5.03	97.41	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	1152	0	1163	16	0
3	N	1151	0	1169	17	0
4	4	430	0	407	15	0
4	G	1526	0	1540	21	0
4	O	413	0	389	13	0
4	V	1557	0	1555	16	0
5	A	12019	0	12078	156	1
5	P	12000	0	12058	157	1
6	B	9386	0	9279	148	0
6	Q	9261	0	9161	153	0
7	C	2423	0	2412	33	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	19	0
9	T	1735	0	1764	21	0
10	F	823	0	841	5	0
10	U	823	0	841	6	0
11	H	1052	0	1021	10	0
11	W	1052	0	1021	7	0
12	I	943	0	929	20	0
12	X	900	0	879	22	0
13	J	569	0	585	12	0
13	Y	569	0	585	15	0
14	K	793	0	790	13	0
14	Z	786	0	782	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	69107	0	68760	848	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 6.

All (848) 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
1:1:34:CYS:HB3	1:1:51: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:1366:GLU:CD	6:B:204:ARG:HH22	2.00	0.65
5:A:1322:ILE:HD12	5:A:1457:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:1200:MET:HE3	5:P:1575:ILE:HD12	1.78	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
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: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: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
6:Q:946:ASP:OD2	13:Y:48:ARG:NH2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
9:T:159:ASP:OD1	9:T:162:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:Q:737:SER:HB3	6:Q:806:THR:HG21	1.88	0.56
7:C:253:PRO:HB2	3:N:180:PHE:HD1	1.71	0.56
5:A:942:GLN:HB2	6:B:958:MET:HE1	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:ILE:HD13	6:B:377:MET:HE1	1.87	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
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
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
2:M:12:ILE:HD12	3:N:67:LEU:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:P:942:GLN:HB2	6:Q:958:MET:HE1	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
6:B:134:ARG:HD2	6:B:160:GLY:HA3	1.91	0.53
5:P:959:VAL:HG22	5:P:965:THR:HG22	1.91	0.53
5:A:589:MET:HE1	5:A:614:LEU:HD13	1.90	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
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
6:B:298:LYS:HE3	3:N:101:GLN:OE1	2.10	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
6:B:819:ASP:CG	6:B:820:PRO:HD2	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:601:MET:HE1	5:A:656:GLN:HB2	1.93	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
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
4:G:35:SER:HG	4:G:132:VAL:H	1.57	0.50
5:P:1482:LYS:HG2	6:Q:308:LEU:HD21	1.94	0.50
6:Q:431:ASP:CG	6:Q:452:ARG:HH22	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:1647:ASN:O	5:A:1652:GLY:HA3	2.13	0.49
5:P:589:MET:HE1	5:P:614:LEU:HD13	1.94	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:65:TYR:CE1	2:M:97:VAL:HB	2.48	0.48
6:Q:877:SER:HB3	6:Q:1064:LYS:HE3	1.95	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
6:B:610:TYR:HE1	6:B:658:LEU:HD11	1.77	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
7:C:215:ASP:CG	1:L:70:ARG:HH22	2.17	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
5:A:869:PRO:HG2	5:A:872:ASP:HB2	1.96	0.48
9:E:48:ASP:OD1	9:E:50:MET:HB3	2.13	0.48
6:Q:236:ILE:HD13	6:Q:377:MET:HE1	1.96	0.48
7:R:71:MET:HE3	7:R:313:ILE:HG22	1.94	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
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
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:236:ILE:HG21	6:Q:377:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:70:ARG:HH22	7:R:215:ASP:CG	2.17	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
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
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: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
5:A:1482:LYS:HE2	6:B:304:ASP:CG	2.36	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
3:3:173:THR:OG1	7:R:228:ARG:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:J:1:MET:HE3	13:J:60:PHE:CD1	2.50	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
8:D:46:GLU:OE1	8:D:47:LYS:HE2	2.15	0.46
5:P:1348:VAL:HA	5:P:1349:PRO:HD3	1.68	0.46
6:Q:427:GLN:HA	6:Q:430:MET:HE3	1.97	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
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
6:Q:1151:ILE:HG12	4:V:21:LYS:HZ2	1.80	0.46
9:T:61:GLN:HE21	9:T:105:PHE:HE1	1.63	0.46
1:1:45:ALA:O	1:1:47: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:P:1571:SER:C	5:P:1573:TYR:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:67:GLU:CD	9:T:67:GLU:H	2.20	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:758:GLU:N	17:A:2042:HOH:O	2.36	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
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:273:ASP:OD1	5:P:273:ASP:N	2.50	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
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
7:R:328:LEU:HD11	14:Z:47:ILE:HB	1.98	0.45
1:1:32:ALA:HB3	1:1:55: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1153:ILE:HA	6:B:1153:ILE:HD13	1.79	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:210:ARG:HH22	6:Q:625:GLU:CD	2.19	0.45
6:Q:1082:HIS:HB3	6:Q:1084:THR:HG23	1.99	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
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
6:Q:201:LYS:NZ	6:Q:466:SER:O	2.50	0.44
13:Y:1:MET:HE3	13:Y:60:PHE:CD1	2.52	0.44
5:A:1463:ASP:HB2	5:A:1469:TRP:CE2	2.52	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
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
7:R:222:VAL:C	7:R:224:THR:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
6:B:236:ILE:HG21	6:B:377:MET:HE1	1.99	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
6:B:107:PRO:HG2	6:B:133:TYR:CZ	2.52	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
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
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
12:X:87:PRO:HG2	12:X:119:TYR:CE2	2.55	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
4:V:17:ILE:C	4:V:19:LYS:H	2.23	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
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:681:THR:O	5:P:729:LYS:NZ	2.52	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:1314:GLN:HG3	5:P:1315:ASN:N	2.34	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
7:C:71:MET:HE3	7:C:313:ILE:HG22	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
9:E:67:GLU:H	9:E:67:GLU:CD	2.23	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: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
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
5:P:601:MET:HE1	5:P:656:GLN:HB2	2.03	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:P:1294:MET:HB2	5:P:1294:MET:HE3	1.96	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
5:A:227:LEU:HD23	5:A:227:LEU:HA	1.84	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
6:Q:760:TYR:O	6:Q:762:MET:HE2	2.19	0.41
9:T:7:ARG:O	9:T:11:ARG:HG3	2.20	0.41
7:C:222:VAL:C	7:C:224:THR:H	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: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
3:3:140: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
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
5:A:1063:MET:HE1	5:A:1174:TYR:CD2	2.55	0.41
6:B:286:ARG:HA	6:B:286:ARG:HD2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1051:PRO:HA	4:O:307:GLU:O	2.21	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
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
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: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
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
5:P:497:VAL:HG22	5:P:635:MET:HE1	2.03	0.40
6:Q:338:PHE:HZ	6:Q:357:ILE:CD1	2.33	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: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
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
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
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
5:P:916:THR:HG22	5:P:944:MET:HE1	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:58:GLU:HA	13:Y:61:LEU:HD12	2.03	0.40
5:A:1156:LYS:C	5:A:1158:SER:H	2.25	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

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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	42/70 (60%)	37 (88%)	3 (7%)	2 (5%)	2 7
1	L	42/70 (60%)	36 (86%)	4 (10%)	2 (5%)	2 7
2	2	99/415 (24%)	93 (94%)	4 (4%)	2 (2%)	7 24
2	M	106/415 (26%)	96 (91%)	8 (8%)	2 (2%)	8 26
3	3	139/233 (60%)	122 (88%)	15 (11%)	2 (1%)	11 34
3	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	6 22
4	4	52/326 (16%)	49 (94%)	3 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	189/326 (58%)	174 (92%)	13 (7%)	2 (1%)	14	41
4	O	50/326 (15%)	46 (92%)	4 (8%)	0	100	100
4	V	191/326 (59%)	175 (92%)	15 (8%)	1 (0%)	29	61
5	A	1505/1664 (90%)	1434 (95%)	62 (4%)	9 (1%)	25	56
5	P	1502/1664 (90%)	1433 (95%)	59 (4%)	10 (1%)	22	53
6	B	1176/1203 (98%)	1116 (95%)	47 (4%)	13 (1%)	14	41
6	Q	1152/1203 (96%)	1104 (96%)	42 (4%)	6 (0%)	29	61
7	C	303/335 (90%)	288 (95%)	13 (4%)	2 (1%)	22	53
7	R	303/335 (90%)	289 (95%)	12 (4%)	2 (1%)	22	53
8	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	3	11
8	S	55/137 (40%)	51 (93%)	2 (4%)	2 (4%)	3	11
9	E	210/215 (98%)	198 (94%)	11 (5%)	1 (0%)	29	61
9	T	210/215 (98%)	199 (95%)	9 (4%)	2 (1%)	15	44
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%)	5	19
12	X	115/125 (92%)	102 (89%)	10 (9%)	3 (3%)	5	18
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%)	19	49

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

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%)	36 (92%)	3 (8%)	13 35
1	L	39/57 (68%)	36 (92%)	3 (8%)	13 35
2	2	93/371 (25%)	85 (91%)	8 (9%)	10 30
2	M	98/371 (26%)	88 (90%)	10 (10%)	7 22
3	3	135/220 (61%)	128 (95%)	7 (5%)	23 55
3	N	135/220 (61%)	129 (96%)	6 (4%)	28 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	52/291 (18%)	51 (98%)	1 (2%)	57	85
4	G	171/291 (59%)	159 (93%)	12 (7%)	15	40
4	O	50/291 (17%)	49 (98%)	1 (2%)	55	84
4	V	175/291 (60%)	161 (92%)	14 (8%)	12	34
5	A	1345/1465 (92%)	1263 (94%)	82 (6%)	18	48
5	P	1343/1465 (92%)	1261 (94%)	82 (6%)	18	48
6	B	1033/1053 (98%)	965 (93%)	68 (7%)	16	44
6	Q	1019/1053 (97%)	956 (94%)	63 (6%)	18	47
7	C	269/296 (91%)	253 (94%)	16 (6%)	19	49
7	R	269/296 (91%)	252 (94%)	17 (6%)	18	46
8	D	55/116 (47%)	49 (89%)	6 (11%)	6	19
8	S	56/116 (48%)	50 (89%)	6 (11%)	6	20
9	E	194/197 (98%)	180 (93%)	14 (7%)	14	38
9	T	194/197 (98%)	178 (92%)	16 (8%)	11	33
10	F	90/137 (66%)	86 (96%)	4 (4%)	28	61
10	U	90/137 (66%)	86 (96%)	4 (4%)	28	61
11	H	115/128 (90%)	111 (96%)	4 (4%)	36	70
11	W	115/128 (90%)	111 (96%)	4 (4%)	36	70
12	I	109/110 (99%)	102 (94%)	7 (6%)	17	45
12	X	104/110 (94%)	98 (94%)	6 (6%)	20	50
13	J	64/65 (98%)	57 (89%)	7 (11%)	6	19
13	Y	64/65 (98%)	57 (89%)	7 (11%)	6	19
14	K	91/130 (70%)	84 (92%)	7 (8%)	13	35
14	Z	90/130 (69%)	83 (92%)	7 (8%)	12	35
All	All	7696/9854 (78%)	7204 (94%)	492 (6%)	17	45

All (492) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	38	LEU
1	1	55	ILE
1	1	66	GLN
2	2	17	ASP
2	2	18	GLN

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Mol	Chain	Res	Type
2	2	31	ARG
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	124	THR
3	3	135	LYS
3	3	153	VAL
3	3	167	LYS
3	3	178	GLU
4	4	269	SER
5	A	10	GLU
5	A	40	ASN
5	A	83	VAL
5	A	117	ARG
5	A	136	LEU
5	A	174	SER
5	A	186	SER
5	A	202	THR
5	A	230	ARG
5	A	257	ASN
5	A	271	ARG
5	A	272	GLN
5	A	273	ASP
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	446	ARG
5	A	447	THR
5	A	451	VAL
5	A	503	VAL
5	A	555	LYS
5	A	611	GLU
5	A	627	ASP
5	A	655	SER

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Mol	Chain	Res	Type
5	A	656	GLN
5	A	661	THR
5	A	666	VAL
5	A	670	ILE
5	A	684	ASP
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	957	VAL
5	A	966	LEU
5	A	988	SER
5	A	1013	THR
5	A	1026	GLN
5	A	1033	SER
5	A	1071	ASP
5	A	1085	LEU
5	A	1098	SER
5	A	1118	VAL
5	A	1123	VAL
5	A	1131	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	1509	HIS
5	A	1531	ASP
5	A	1533	GLU

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Mol	Chain	Res	Type
5	A	1536	ILE
5	A	1571	SER
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	1632	GLU
5	A	1633	GLN
5	A	1635	ASP
5	A	1645	LYS
6	B	13	THR
6	B	17	ARG
6	B	22	GLU
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	117	VAL
6	B	150	GLU
6	B	187	SER
6	B	202	LEU
6	B	221	SER
6	B	225	ARG
6	B	228	SER
6	B	231	HIS
6	B	239	VAL
6	B	300	SER
6	B	305	ARG
6	B	306	LEU
6	B	311	ARG
6	B	315	LYS
6	B	379	ARG
6	B	459	SER
6	B	486	VAL
6	B	537	SER
6	B	583	LEU
6	B	622	ILE
6	B	658	LEU

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Mol	Chain	Res	Type
6	B	720	GLN
6	B	724	GLN
6	B	725	THR
6	B	731	VAL
6	B	753	LYS
6	B	782	ASP
6	B	811	LEU
6	B	813	LEU
6	B	819	ASP
6	B	822	THR
6	B	824	HIS
6	B	829	ASN
6	B	833	PRO
6	B	835	GLU
6	B	839	LYS
6	B	858	ILE
6	B	871	ILE
6	B	883	GLU
6	B	894	LYS
6	B	897	GLU
6	B	977	ILE
6	B	998	GLU
6	B	1026	ILE
6	B	1033	TYR
6	B	1037	ARG
6	B	1038	HIS
6	B	1042	ASP
6	B	1047	ARG
6	B	1060	VAL
6	B	1075	GLU
6	B	1091	ARG
6	B	1103	VAL
6	B	1125	THR
6	B	1136	GLU
6	B	1141	LEU
6	B	1163	GLN
6	B	1165	ASN
6	B	1174	THR
7	C	38	LYS
7	C	43	ASN
7	C	50	ARG
7	C	61	THR

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Mol	Chain	Res	Type
7	C	77	SER
7	C	91	VAL
7	C	97	LEU
7	C	118	SER
7	C	142	ARG
7	C	181	ASP
7	C	224	THR
7	C	228	ARG
7	C	243	SER
7	C	245	ARG
7	C	277	ARG
7	C	279	VAL
8	D	15	THR
8	D	29	GLN
8	D	38	GLN
8	D	46	GLU
8	D	80	THR
8	D	99	LEU
9	E	31	THR
9	E	33	GLU
9	E	41	ASP
9	E	74	ASP
9	E	77	SER
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	177	ARG
10	F	59	GLN
10	F	87	LYS
10	F	99	LEU
10	F	109	VAL
4	G	18	LYS
4	G	24	VAL
4	G	35	SER
4	G	39	VAL
4	G	139	ILE
4	G	147	LEU

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Mol	Chain	Res	Type
4	G	167	THR
4	G	169	VAL
4	G	223	GLU
4	G	230	ARG
4	G	239	THR
4	G	243	VAL
11	H	3	ASN
11	H	39	THR
11	H	108	SER
11	H	112	ILE
12	I	2	SER
12	I	15	ASP
12	I	45	LEU
12	I	70	SER
12	I	74	ASN
12	I	81	THR
12	I	117	CYS
13	J	3	VAL
13	J	9	SER
13	J	10	CYS
13	J	14	VAL
13	J	27	GLU
13	J	45	CYS
13	J	48	ARG
14	K	45	GLU
14	K	51	THR
14	K	68	GLU
14	K	99	ASN
14	K	118	GLN
14	K	123	ASP
14	K	133	SER
1	L	38	LEU
1	L	55	ILE
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	65	TYR
2	M	77	VAL
2	M	84	GLU

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Mol	Chain	Res	Type
2	M	98	SER
2	M	109	ARG
3	N	51	GLN
3	N	124	THR
3	N	135	LYS
3	N	153	VAL
3	N	167	LYS
3	N	178	GLU
4	O	269	SER
5	P	10	GLU
5	P	61	LEU
5	P	117	ARG
5	P	136	LEU
5	P	174	SER
5	P	175	SER
5	P	186	SER
5	P	199	ASP
5	P	202	THR
5	P	257	ASN
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	413	LEU
5	P	416	ARG
5	P	446	ARG
5	P	447	THR
5	P	451	VAL
5	P	503	VAL
5	P	555	LYS
5	P	611	GLU
5	P	627	ASP
5	P	655	SER
5	P	656	GLN
5	P	666	VAL
5	P	684	ASP
5	P	708	THR
5	P	709	ARG

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Mol	Chain	Res	Type
5	P	739	VAL
5	P	747	ILE
5	P	758	GLU
5	P	783	LYS
5	P	878	ARG
5	P	957	VAL
5	P	1013	THR
5	P	1016	SER
5	P	1026	GLN
5	P	1033	SER
5	P	1071	ASP
5	P	1085	LEU
5	P	1098	SER
5	P	1118	VAL
5	P	1123	VAL
5	P	1131	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
5	P	1314	GLN
5	P	1320	GLN
5	P	1350	ARG
5	P	1364	ARG
5	P	1392	ILE
5	P	1441	LYS
5	P	1481	GLU
5	P	1486	VAL
5	P	1505	ASP
5	P	1509	HIS
5	P	1518	VAL
5	P	1531	ASP
5	P	1536	ILE
5	P	1587	ASP
5	P	1601	GLN
5	P	1604	GLU

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Mol	Chain	Res	Type
5	P	1605	THR
5	P	1607	THR
5	P	1609	SER
5	P	1611	MET
5	P	1632	GLU
5	P	1633	GLN
5	P	1635	ASP
6	Q	13	THR
6	Q	17	ARG
6	Q	22	GLU
6	Q	53	THR
6	Q	57	ASP
6	Q	65	VAL
6	Q	117	VAL
6	Q	150	GLU
6	Q	187	SER
6	Q	202	LEU
6	Q	221	SER
6	Q	225	ARG
6	Q	228	SER
6	Q	231	HIS
6	Q	236	ILE
6	Q	239	VAL
6	Q	300	SER
6	Q	305	ARG
6	Q	306	LEU
6	Q	311	ARG
6	Q	315	LYS
6	Q	379	ARG
6	Q	429	ARG
6	Q	486	VAL
6	Q	537	SER
6	Q	583	LEU
6	Q	622	ILE
6	Q	658	LEU
6	Q	720	GLN
6	Q	724	GLN
6	Q	725	THR
6	Q	753	LYS
6	Q	782	ASP
6	Q	811	LEU
6	Q	813	LEU

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Mol	Chain	Res	Type
6	Q	822	THR
6	Q	824	HIS
6	Q	829	ASN
6	Q	833	PRO
6	Q	835	GLU
6	Q	839	LYS
6	Q	858	ILE
6	Q	871	ILE
6	Q	883	GLU
6	Q	897	GLU
6	Q	977	ILE
6	Q	998	GLU
6	Q	1026	ILE
6	Q	1033	TYR
6	Q	1037	ARG
6	Q	1038	HIS
6	Q	1042	ASP
6	Q	1047	ARG
6	Q	1060	VAL
6	Q	1075	GLU
6	Q	1091	ARG
6	Q	1103	VAL
6	Q	1125	THR
6	Q	1136	GLU
6	Q	1141	LEU
6	Q	1163	GLN
6	Q	1165	ASN
6	Q	1174	THR
7	R	38	LYS
7	R	43	ASN
7	R	50	ARG
7	R	61	THR
7	R	77	SER
7	R	91	VAL
7	R	97	LEU
7	R	118	SER
7	R	128	ASP
7	R	142	ARG
7	R	181	ASP
7	R	224	THR
7	R	228	ARG
7	R	243	SER

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Mol	Chain	Res	Type
7	R	245	ARG
7	R	277	ARG
7	R	279	VAL
8	S	15	THR
8	S	29	GLN
8	S	38	GLN
8	S	46	GLU
8	S	80	THR
8	S	99	LEU
9	T	4	GLU
9	T	31	THR
9	T	33	GLU
9	T	41	ASP
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	167	ARG
9	T	177	ARG
10	U	59	GLN
10	U	87	LYS
10	U	99	LEU
10	U	109	VAL
4	V	18	LYS
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	171	ASN
4	V	176	ASP
4	V	223	GLU
4	V	230	ARG
4	V	239	THR

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Mol	Chain	Res	Type
4	V	243	VAL
11	W	3	ASN
11	W	39	THR
11	W	108	SER
11	W	112	ILE
12	X	2	SER
12	X	15	ASP
12	X	45	LEU
12	X	70	SER
12	X	81	THR
12	X	117	CYS
13	Y	3	VAL
13	Y	9	SER
13	Y	10	CYS
13	Y	14	VAL
13	Y	27	GLU
13	Y	45	CYS
13	Y	48	ARG
14	Z	45	GLU
14	Z	51	THR
14	Z	68	GLU
14	Z	99	ASN
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	43	HIS
5	A	1162	ASN
6	B	1163	GLN
5	P	1162	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	5 (11%)	5	3	79, 117, 154, 193	0
1	L	44/70 (62%)	-0.25	3 (6%)	17	10	65, 88, 134, 175	0
2	2	103/415 (24%)	0.54	11 (10%)	6	3	96, 128, 160, 171	0
2	M	108/415 (26%)	0.09	3 (2%)	53	43	66, 94, 134, 156	0
3	3	145/233 (62%)	0.22	9 (6%)	20	13	76, 121, 161, 187	0
3	N	145/233 (62%)	-0.18	3 (2%)	63	54	56, 93, 133, 160	0
4	4	54/326 (16%)	0.06	3 (5%)	24	16	74, 103, 143, 158	0
4	G	193/326 (59%)	0.35	30 (15%)	2	1	51, 107, 168, 189	0
4	O	52/326 (15%)	0.20	5 (9%)	8	4	64, 100, 145, 155	0
4	V	197/326 (60%)	-0.06	6 (3%)	50	40	57, 89, 140, 164	0
5	A	1521/1664 (91%)	-0.38	19 (1%)	79	73	40, 63, 117, 161	0
5	P	1518/1664 (91%)	-0.35	20 (1%)	77	72	48, 72, 123, 182	0
6	B	1182/1203 (98%)	-0.39	18 (1%)	73	68	37, 59, 108, 187	0
6	Q	1164/1203 (96%)	-0.24	21 (1%)	68	61	40, 83, 132, 165	0
7	C	305/335 (91%)	-0.25	3 (0%)	82	77	60, 81, 127, 148	0
7	R	305/335 (91%)	-0.13	6 (1%)	65	56	68, 95, 137, 151	0
8	D	58/137 (42%)	-0.22	0	100	100	56, 107, 136, 149	0
8	S	59/137 (43%)	-0.24	1 (1%)	70	63	62, 96, 128, 134	0
9	E	212/215 (98%)	-0.06	9 (4%)	36	26	49, 92, 149, 164	0
9	T	212/215 (98%)	-0.06	7 (3%)	46	36	57, 94, 147, 169	0
10	F	100/155 (64%)	-0.61	0	100	100	42, 60, 93, 129	0
10	U	100/155 (64%)	-0.57	0	100	100	51, 70, 107, 119	0
11	H	131/146 (89%)	-0.38	0	100	100	60, 80, 113, 125	0
11	W	131/146 (89%)	-0.26	2 (1%)	73	68	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%)	-0.22	4 (3%) 47 37	52, 81, 129, 155	0
12	X	119/125 (95%)	0.09	4 (3%) 45 35	65, 103, 152, 177	0
13	J	69/70 (98%)	-0.36	0 100 100	56, 68, 91, 106	0
13	Y	69/70 (98%)	-0.22	0 100 100	72, 85, 114, 128	0
14	K	101/142 (71%)	-0.37	1 (0%) 82 77	58, 72, 121, 148	0
14	Z	100/142 (70%)	-0.29	4 (4%) 38 28	63, 83, 133, 164	0
All	All	8665/11124 (77%)	-0.25	197 (2%) 60 51	37, 77, 136, 193	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	893	ASN	6.2
3	3	84	LYS	5.9
5	P	448	SER	5.8
1	1	43	THR	5.6
4	G	23	GLN	5.2
14	Z	53	ALA	5.1
6	Q	815	ARG	4.9
6	B	894	LYS	4.8
4	G	31	LYS	4.7
5	A	411	VAL	4.7
9	T	123	LEU	4.6
4	G	15	ARG	4.4
5	A	410	LYS	4.2
6	Q	814	ASN	4.1
9	E	91	LYS	4.0
4	O	305	GLY	4.0
6	B	112	GLY	4.0
4	V	15	ARG	4.0
4	G	162	ILE	4.0
1	L	43	THR	3.9
4	V	23	GLN	3.9
6	Q	821	ILE	3.8
4	G	147	LEU	3.8
6	B	114	SER	3.8
6	B	892	SER	3.8
6	B	895	PHE	3.7
3	3	83	ASP	3.7
9	E	90	VAL	3.6
4	G	21	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
6	B	818	GLY	3.6
5	A	407	GLN	3.5
6	Q	90	TYR	3.5
6	B	113	VAL	3.5
2	2	112	LYS	3.5
4	4	267	ALA	3.4
5	P	447	THR	3.4
4	G	30	GLU	3.4
12	X	40	SER	3.4
2	2	62	TYR	3.4
4	G	17	ILE	3.3
7	R	179	PHE	3.3
5	A	409	ASP	3.3
9	E	119	SER	3.3
6	Q	827	PHE	3.3
1	1	46	VAL	3.2
2	M	86	LYS	3.2
4	G	164	VAL	3.2
6	Q	529	CYS	3.2
12	I	24	LEU	3.2
1	1	45	ALA	3.1
4	G	16	PHE	3.1
5	A	1158	SER	3.1
6	Q	9	GLY	3.1
11	W	87	ARG	3.1
4	G	221	ASN	3.1
4	G	29	ASP	3.1
4	4	263	SER	3.0
9	T	89	GLY	3.0
2	2	41	TYR	3.0
4	V	171	ASN	3.0
4	G	166	TRP	3.0
6	B	834	LYS	3.0
4	4	266	GLN	3.0
12	X	41	GLN	3.0
4	G	139	ILE	3.0
5	A	1664	ALA	2.9
9	E	120	ALA	2.9
5	P	406	LEU	2.9
9	E	123	LEU	2.9
5	P	1393	GLU	2.9
4	V	17	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
6	B	116	ALA	2.9
6	Q	91	LEU	2.9
5	P	410	LYS	2.9
6	Q	10	GLN	2.8
2	2	39	ASP	2.8
4	G	224	PRO	2.8
5	A	1159	ASP	2.8
6	Q	823	GLN	2.8
5	P	1158	SER	2.8
1	1	42	ARG	2.8
5	A	1362	SER	2.8
5	P	1156	LYS	2.8
6	B	1138	ALA	2.8
4	G	163	PRO	2.8
3	3	82	ILE	2.8
4	G	33	GLY	2.7
7	R	261	GLY	2.7
2	2	56	GLU	2.7
5	A	448	SER	2.7
2	2	55	GLY	2.7
6	Q	813	LEU	2.7
4	G	145	ILE	2.7
4	G	225	ILE	2.7
5	P	409	ASP	2.7
14	Z	52	GLN	2.7
14	K	53	ALA	2.7
6	Q	834	LYS	2.7
4	O	304	ASN	2.7
5	A	417	ARG	2.7
7	R	150	SER	2.6
4	G	136	TYR	2.6
4	G	140	GLN	2.6
6	Q	78	PRO	2.6
2	2	9	GLU	2.6
5	A	204	GLU	2.6
5	P	345	LEU	2.6
2	M	109	ARG	2.6
14	Z	54	THR	2.6
3	N	180	PHE	2.6
4	G	132	VAL	2.6
3	N	32	CYS	2.6
5	A	1390	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
5	A	41	LEU	2.6
4	G	217	TRP	2.6
6	Q	11	ALA	2.6
2	2	8	SER	2.6
4	V	18	LYS	2.5
2	2	109	ARG	2.5
6	B	111	ASP	2.5
12	X	115	THR	2.5
5	P	1361	ASN	2.5
4	G	249	LEU	2.5
5	A	406	LEU	2.5
5	A	708	THR	2.4
2	2	40	LEU	2.4
3	3	80	MET	2.4
6	Q	30	LYS	2.4
3	3	32	CYS	2.4
6	Q	810	ASP	2.4
4	G	216	HIS	2.4
5	A	408	LYS	2.4
14	Z	56	GLU	2.4
5	A	413	LEU	2.4
7	R	149	GLY	2.4
12	X	71	LEU	2.4
12	I	42	PHE	2.4
11	W	92	ASP	2.4
9	E	89	GLY	2.4
4	G	232	THR	2.4
5	P	1157	SER	2.4
5	A	1393	GLU	2.3
4	V	164	VAL	2.3
5	P	407	GLN	2.3
9	E	122	LYS	2.3
5	P	416	ARG	2.3
6	B	831	GLU	2.3
9	T	119	SER	2.3
5	P	417	ARG	2.3
6	Q	511	GLN	2.3
7	R	263	ASP	2.3
4	O	267	ALA	2.3
4	G	231	PHE	2.3
6	Q	117	VAL	2.3
3	3	26	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
5	A	1442	VAL	2.3
9	E	93	MET	2.3
12	I	75	GLU	2.3
7	R	144	PRO	2.3
5	P	415	ASP	2.2
6	B	529	CYS	2.2
9	T	88	VAL	2.2
5	P	347	ARG	2.2
4	O	265	SER	2.2
7	C	120	LEU	2.2
3	N	84	LYS	2.2
4	G	18	LYS	2.2
2	2	84	GLU	2.2
5	P	1389	GLU	2.2
6	Q	867	ASN	2.2
9	T	51	GLY	2.2
1	L	42	ARG	2.2
6	B	1141	LEU	2.2
3	3	125	ALA	2.2
3	3	126	LYS	2.2
1	1	40	LEU	2.2
6	Q	704	THR	2.2
8	S	46	GLU	2.2
9	T	91	LYS	2.2
6	B	79	LEU	2.1
9	T	93	MET	2.1
4	O	297	LEU	2.1
6	B	815	ARG	2.1
7	C	145	ASP	2.1
6	B	80	ASN	2.1
5	P	411	VAL	2.1
9	E	88	VAL	2.1
3	3	30	LYS	2.1
7	C	117	ASP	2.1
4	G	35	SER	2.1
12	I	43	SER	2.1
4	G	34	THR	2.1
2	M	10	ILE	2.0
5	P	1350	ARG	2.0
1	L	45	ALA	2.0
6	Q	531	VAL	2.0
5	P	375	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	SO4	Q	2204	5/5	0.93	0.32	133,139,142,147	0
16	SO4	B	2204	5/5	0.94	0.30	123,124,132,137	0
15	ZN	X	3002	1/1	0.97	0.04	89,89,89,89	1
15	ZN	X	3001	1/1	0.98	0.08	113,113,113,113	0
15	ZN	I	3002	1/1	0.98	0.06	77,77,77,77	1
15	ZN	P	3002	1/1	0.99	0.11	83,83,83,83	0
15	ZN	Q	3001	1/1	0.99	0.10	64,64,64,64	0
15	ZN	A	3001	1/1	0.99	0.11	75,75,75,75	0
15	ZN	I	3001	1/1	0.99	0.11	73,73,73,73	0
15	ZN	Y	3001	1/1	0.99	0.19	489,489,489,489	0
15	ZN	1	3001	1/1	0.99	0.10	120,120,120,120	0
15	ZN	J	3001	1/1	0.99	0.21	547,547,547,547	0
15	ZN	P	3001	1/1	1.00	0.09	70,70,70,70	0
15	ZN	B	3001	1/1	1.00	0.10	53,53,53,53	0
15	ZN	A	3002	1/1	1.00	0.11	77,77,77,77	0
15	ZN	L	3001	1/1	1.00	0.08	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.