



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 8XGC / pdb_00008xgc
EMDB ID : EMD-38317
Title : Structure of yeast replisome associated with FACT and histone hexamer, Composite map
Authors : Li, N.; Gao, Y.; Yu, D.; Gao, N.; Zhai, Y.
Deposited on : 2023-12-15
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

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

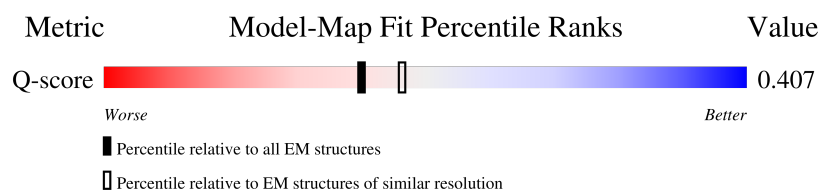
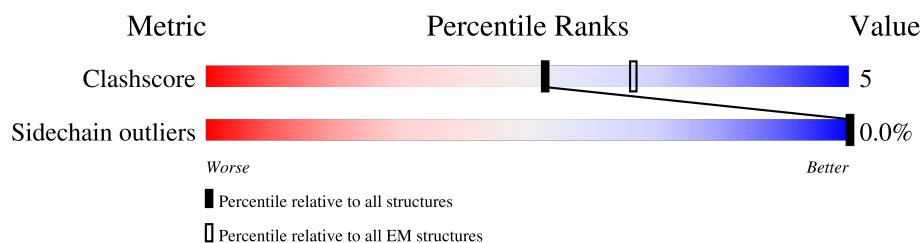
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	16% 75% 14% 10%
2	3	971	10% 54% 9% 37%
3	4	933	24% 60% 12% 27%
4	5	775	13% 75% 13% 13%
5	6	1017	9% 53% 9% 38%

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Mol	Chain	Length	Quality of chain
6	7	845	
7	8	2222	
8	9	689	
9	A	208	
10	B	251	
11	C	194	
12	D	294	
13	E	650	
14	F	927	
14	G	927	
14	H	927	
15	I	1238	
16	J	317	
17	K	1096	
18	L	1035	
19	M	552	
20	N	136	
20	R	136	
21	O	103	
21	S	103	
22	P	132	
23	Q	131	
24	X	51	
25	Y	39	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 82765 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	778	Total	C	N	O	S	0	0
			6161	3835	1105	1198	23		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	613	Total	C	N	O	S	0	0
			4795	3026	854	902	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	679	Total	C	N	O	S	0	0
			5269	3313	922	1005	29		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	678	Total	C	N	O	S	0	0
			5376	3379	937	1036	24		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	634	Total	C	N	O	S	0	0
			4991	3151	875	940	25		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	635	Total	C	N	O	S	0	0
			4919	3112	860	923	24		

- Molecule 7 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	857	Total	C	N	O	S	0	0
			6945	4496	1137	1274	38		

- Molecule 8 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	573	Total	C	N	O	S	0	0
			4594	2947	788	840	19		

- Molecule 9 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	197	Total	C	N	O	S	0	0
			1611	1012	277	313	9		

- Molecule 10 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	192	Total	C	N	O	S	0	0
			1609	1034	285	286	4		

- Molecule 11 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	171	Total	C	N	O	S	0	0
			1379	899	222	252	6		

- Molecule 12 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	241	Total	C	N	O	S	0	0
			1988	1266	325	385	12		

- Molecule 13 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	562	Total	C	N	O	S	0	0
			4550	2906	766	864	14		

- Molecule 14 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	424	Total	C	N	O	S	0	0
			3404	2188	564	637	15		
14	G	422	Total	C	N	O	S	0	0
			3380	2172	557	636	15		
14	H	425	Total	C	N	O	S	0	0
			3411	2193	565	638	15		

- Molecule 15 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	745	Total	C	N	O	S	0	0
			6057	3897	1027	1114	19		

- Molecule 16 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	94	Total	C	N	O	S	0	0
			788	507	144	133	4		

- Molecule 17 is a protein called Mediator of replication checkpoint protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	K	20	Total	C	N	O	0	0
			163	102	23	38		

- Molecule 18 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	493	Total	C	N	O	S	0	0
			3474	2177	616	671	10		

- Molecule 19 is a protein called FACT complex subunit POB3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	M	379	Total	C	N	O	0	0
			1876	1118	379	379		

- Molecule 20 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	N	77	Total	C	N	O	0	0
			629	399	118	112		

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Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	90	Total	C	N	O	0	0
			741	469	142	130		

- Molecule 21 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	O	73	Total	C	N	O	0	0
			583	365	114	104		
21	S	85	Total	C	N	O	0	0
			684	431	135	118		

- Molecule 22 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	P	91	Total	C	N	O	0	0
			703	439	139	125		

- Molecule 23 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	91	Total	C	N	O	S	0	0
			706	444	121	140	1		

- Molecule 24 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	51	Total	C	N	O	P	0	0
			1041	507	156	327	51		

- Molecule 25 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	39	Total	C	N	O	P	0	0
			796	382	149	226	39		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

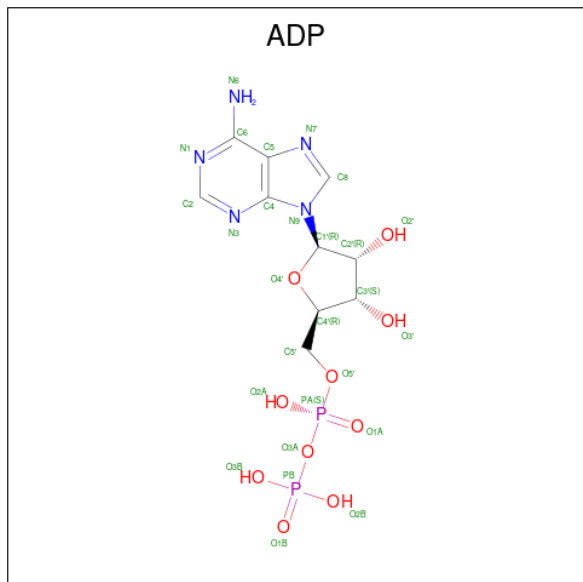
Mol	Chain	Residues	Atoms		AltConf
26	2	1	Total	Zn	0
			1	1	

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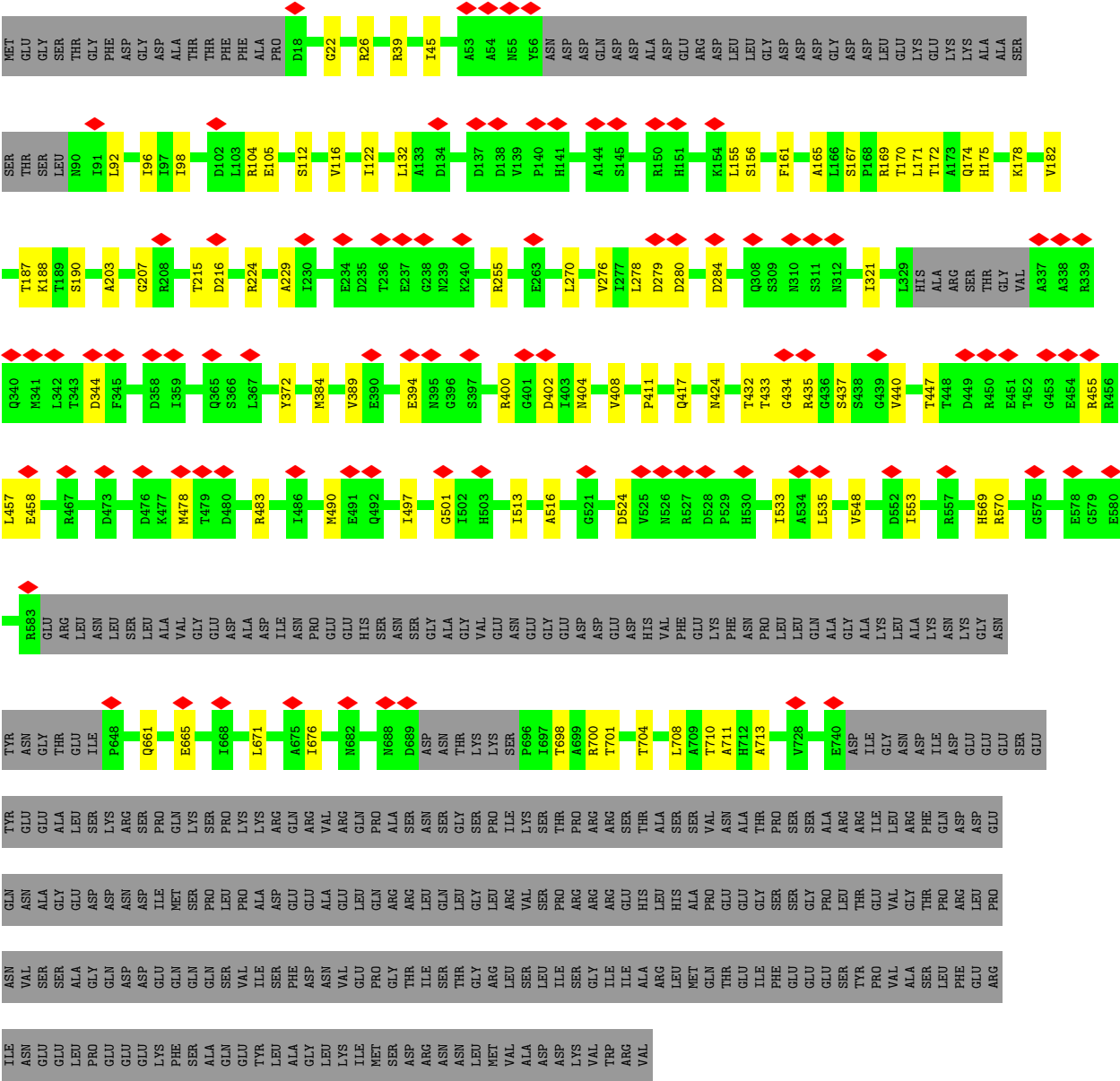
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Mol	Chain	Residues	Atoms		AltConf
26	4	1	Total	Zn	0
			1	1	
26	5	1	Total	Zn	0
			1	1	
26	6	1	Total	Zn	0
			1	1	
26	7	1	Total	Zn	0
			1	1	
26	8	2	Total	Zn	0
			2	2	

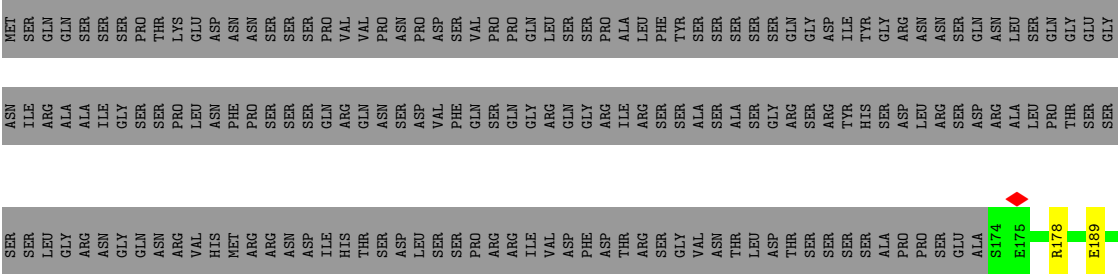
- Molecule 27 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

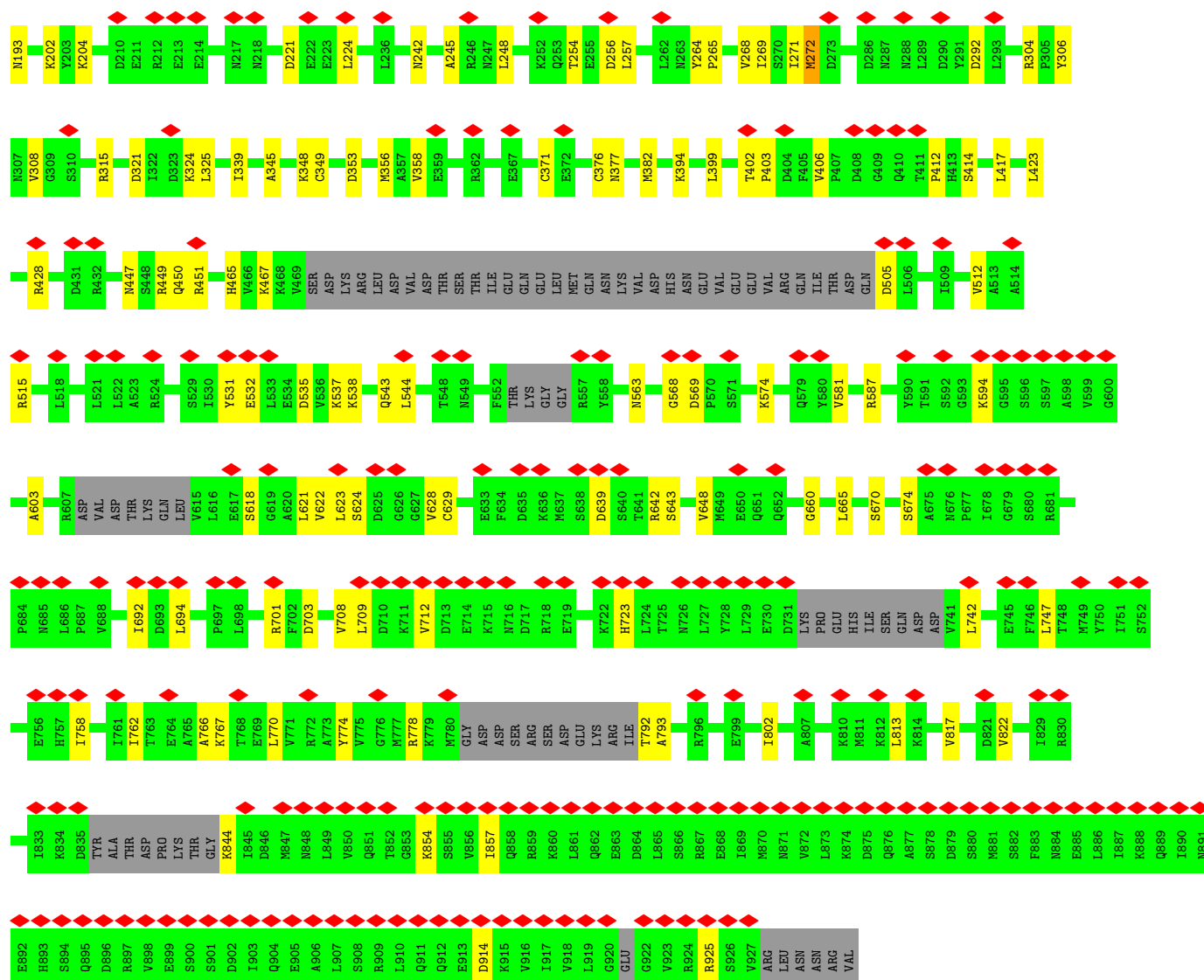


Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
27	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
27	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
27	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
27	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

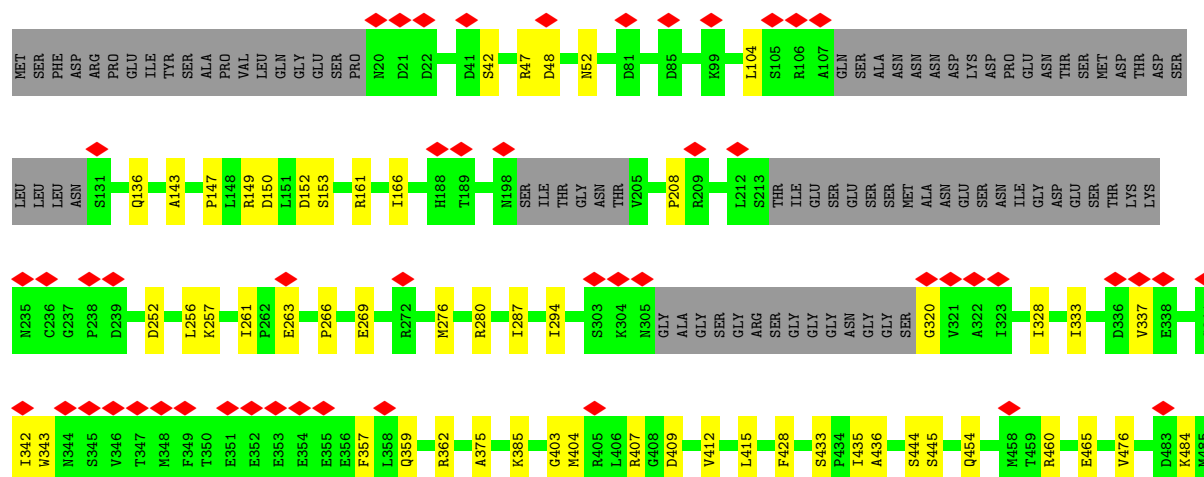
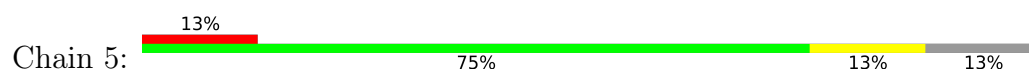


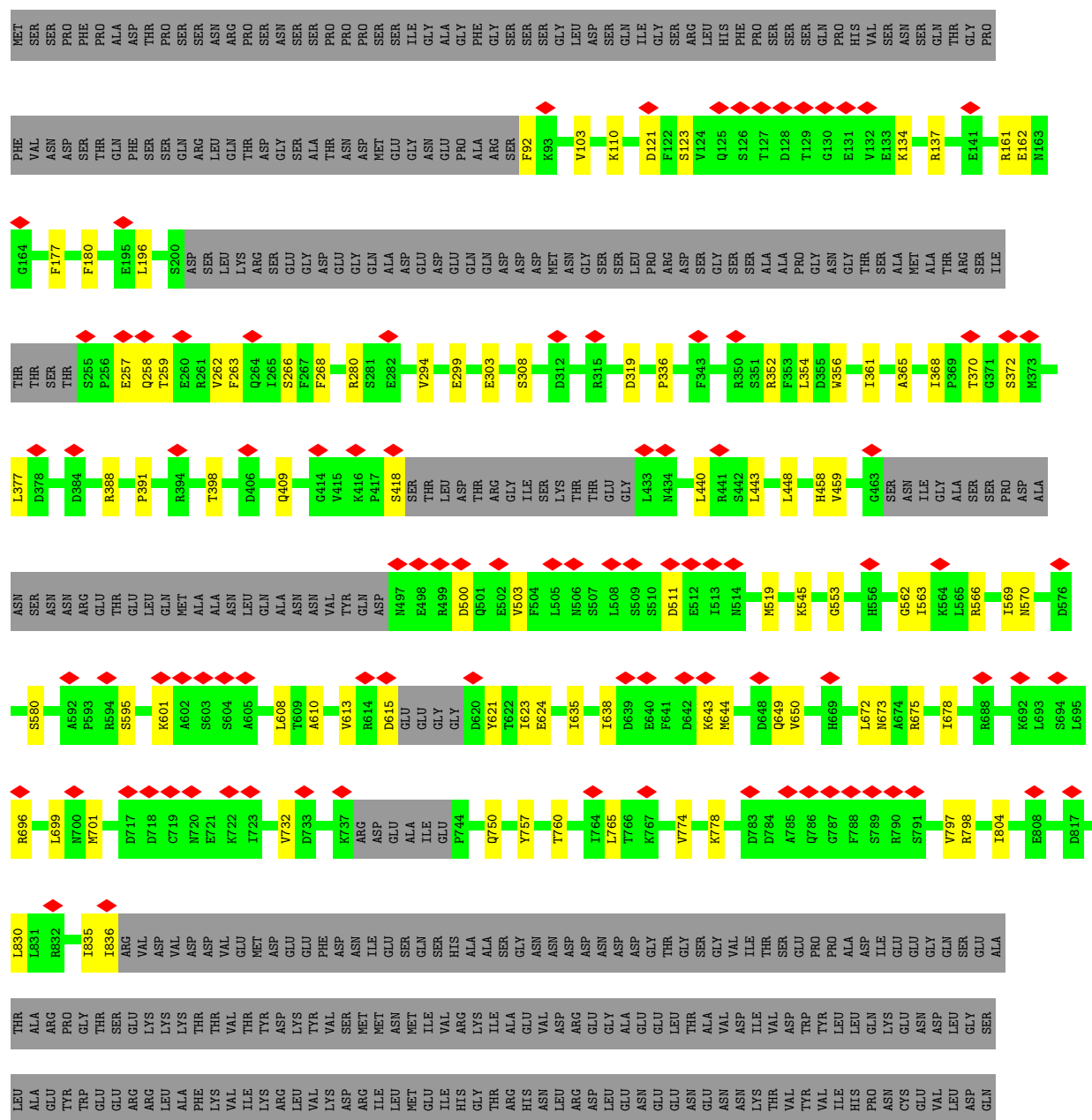
• Molecule 3: DNA replication licensing factor MCM4





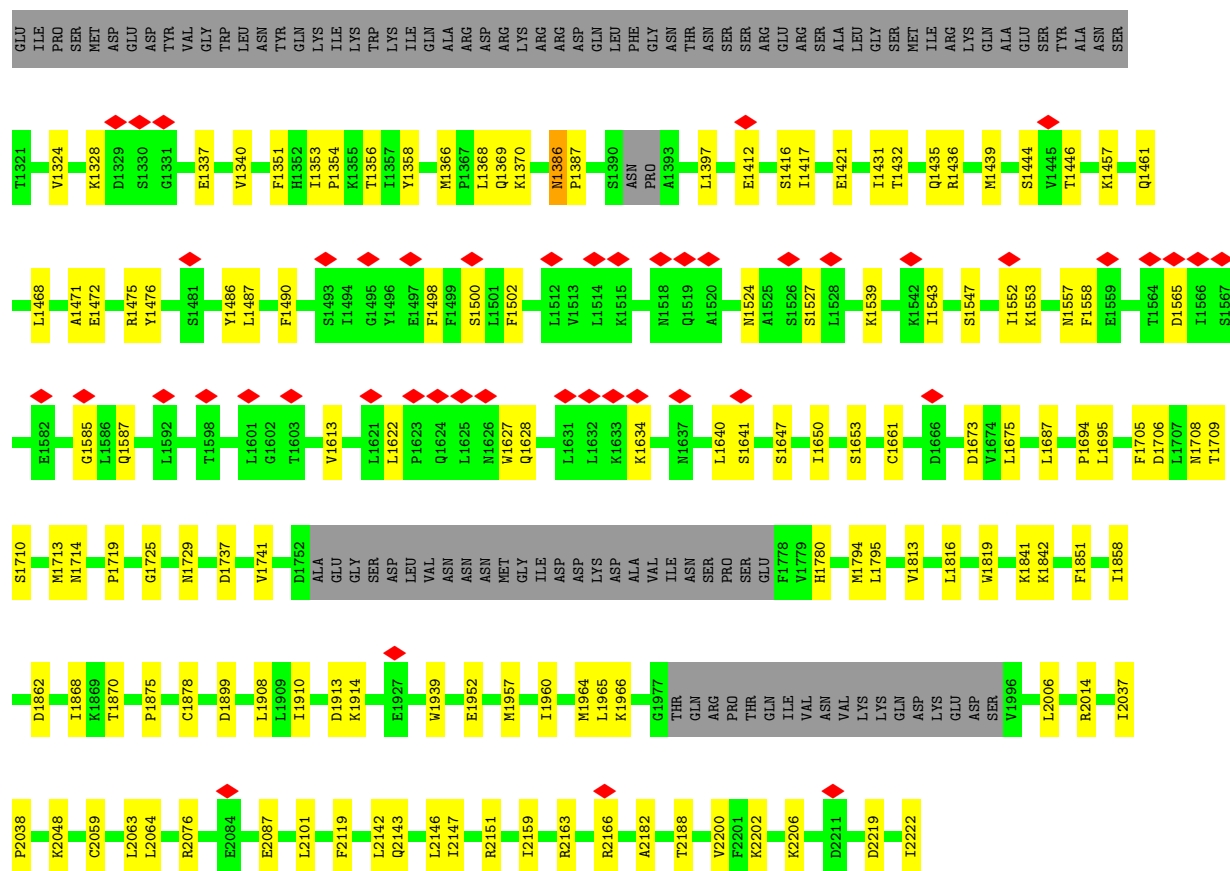
• Molecule 4: Minichromosome maintenance protein 5



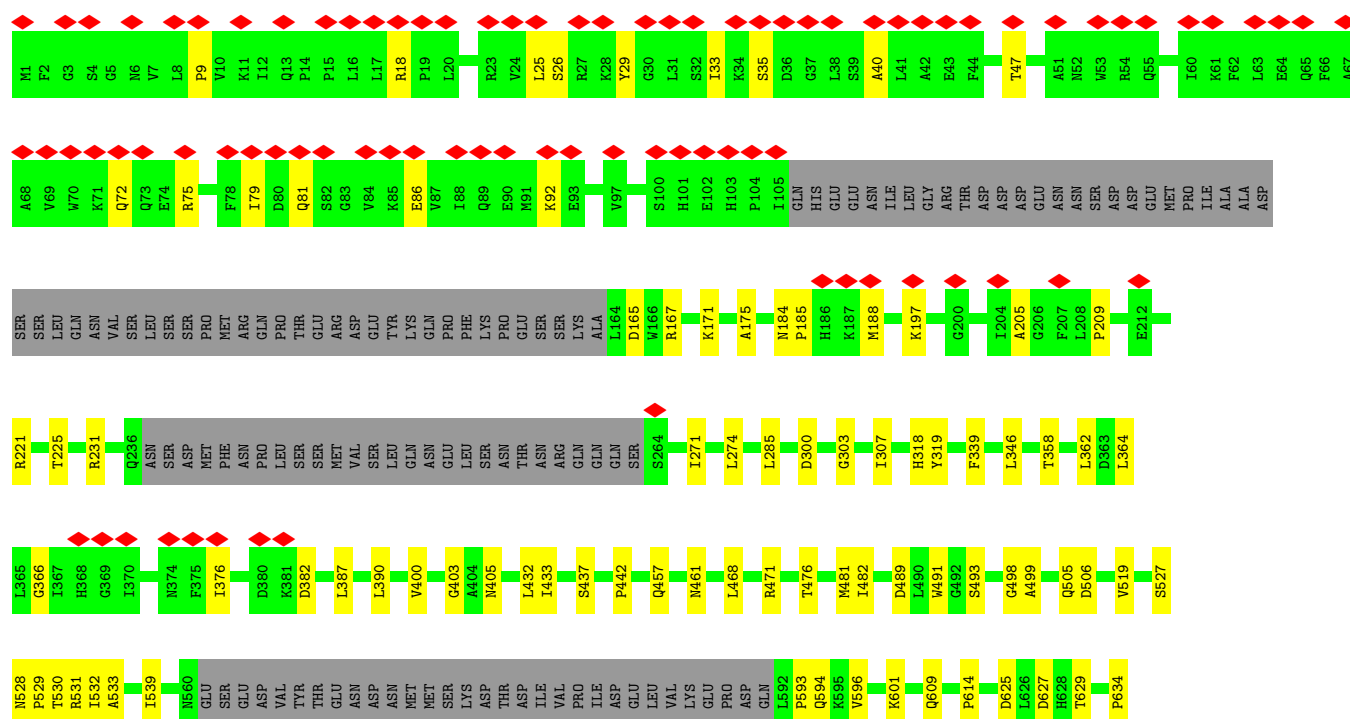


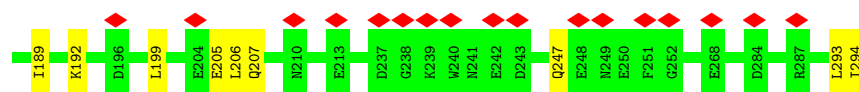
MET	MET	PHE	GLY	LYS	LYS	ASN	ASN	GLY	GLY	SER	SER	THR	ALA	ALA	ARG	TYR	SER	ASN	ASN	THR	LEU	LEU	ALA	GLN	GLN	LEU	LEU	ASP	ASP	ILE	ILE	ASP	SER	MET	MET	GLY	PHE	GLU	ARG	TYR	VAL	PRO	PRO	GLN	GLN
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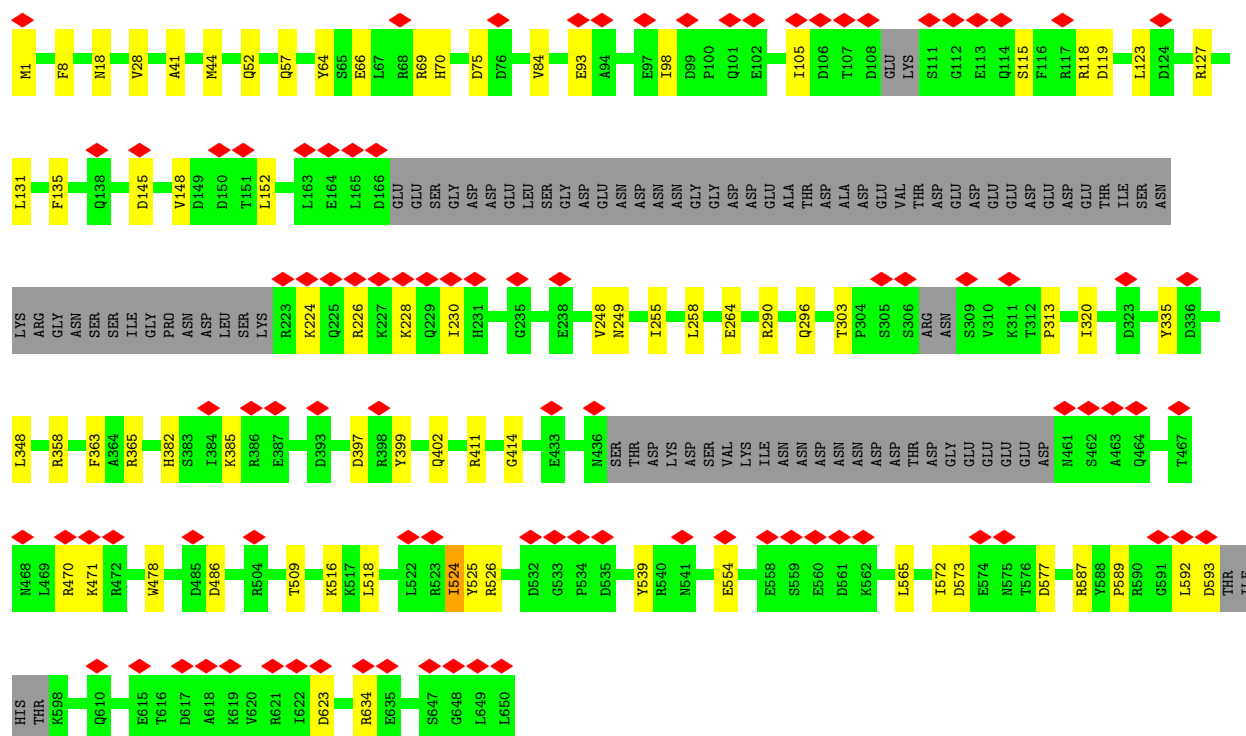
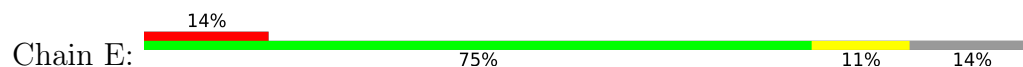


• Molecule 8: DNA polymerase epsilon subunit B

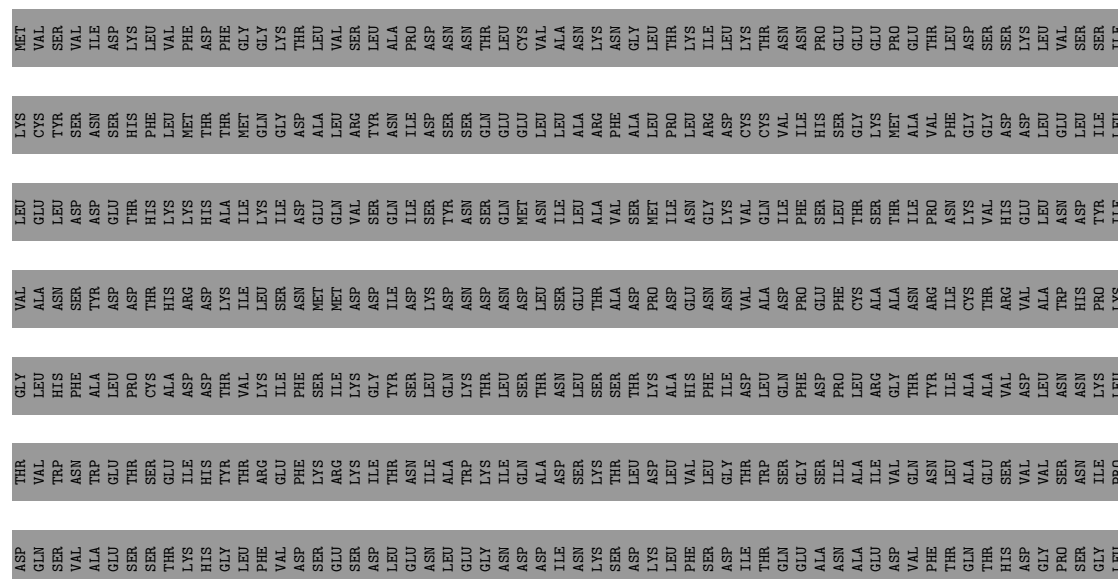
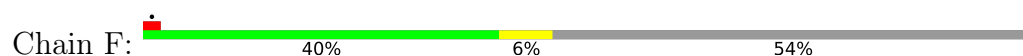


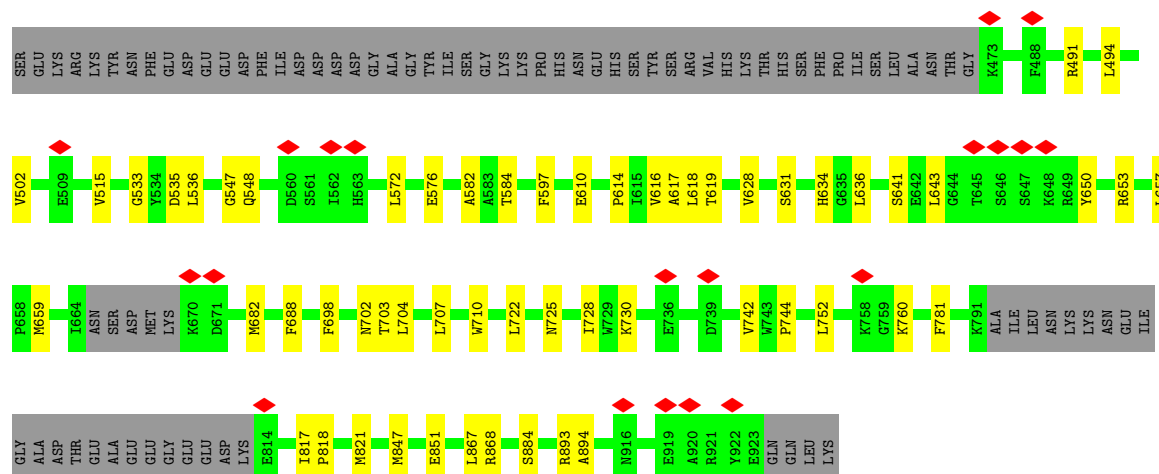


• Molecule 13: Cell division control protein 45



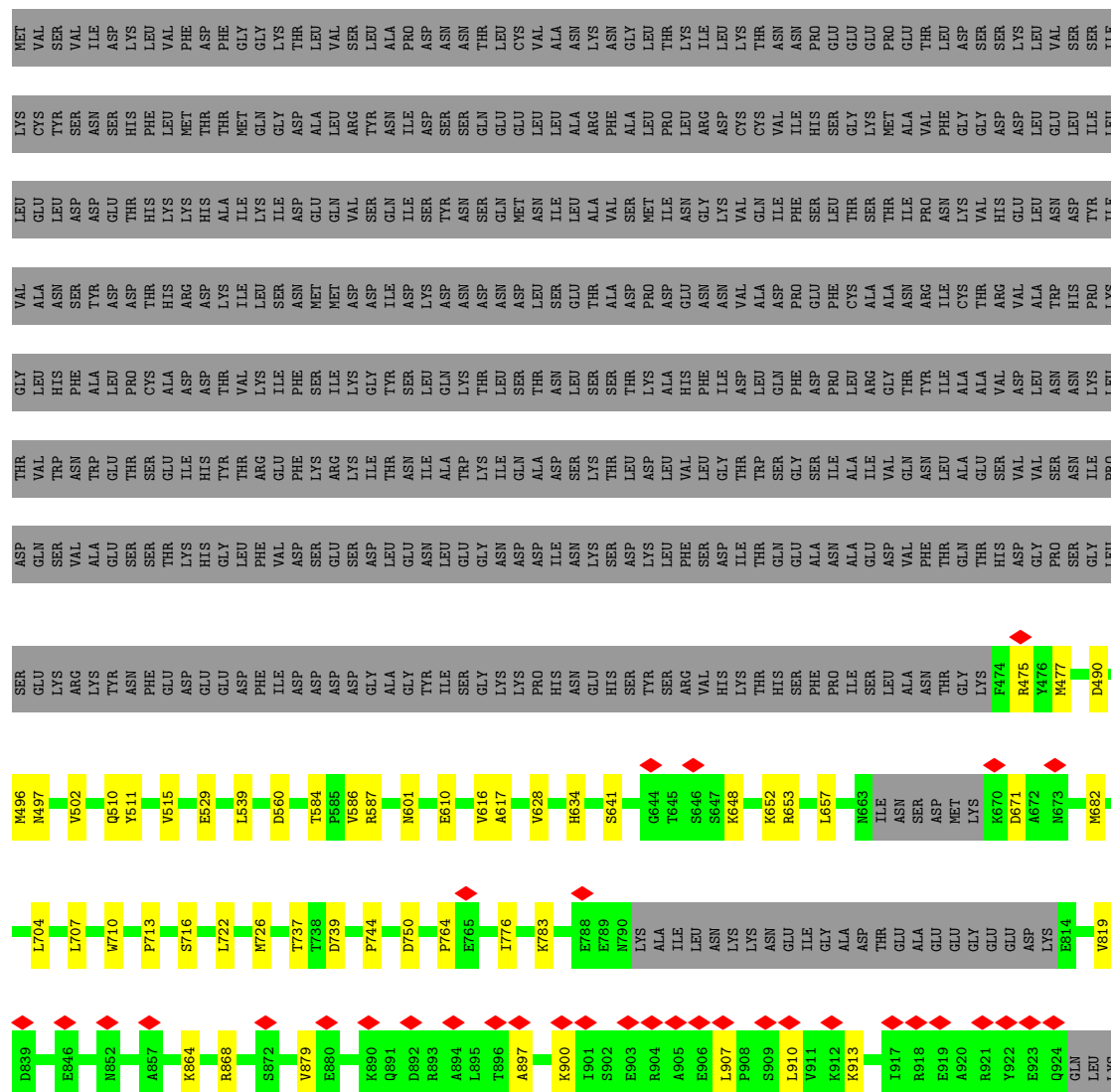
• Molecule 14: DNA polymerase alpha-binding protein



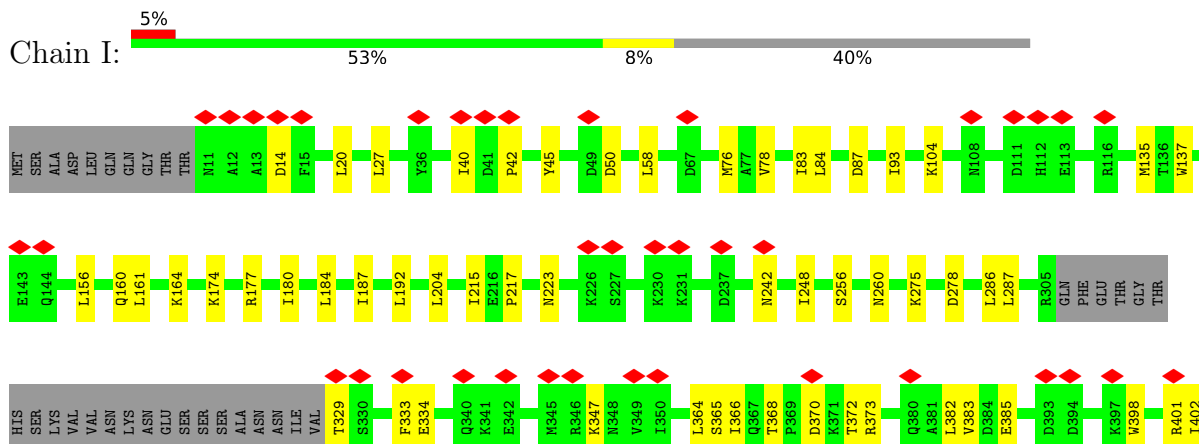


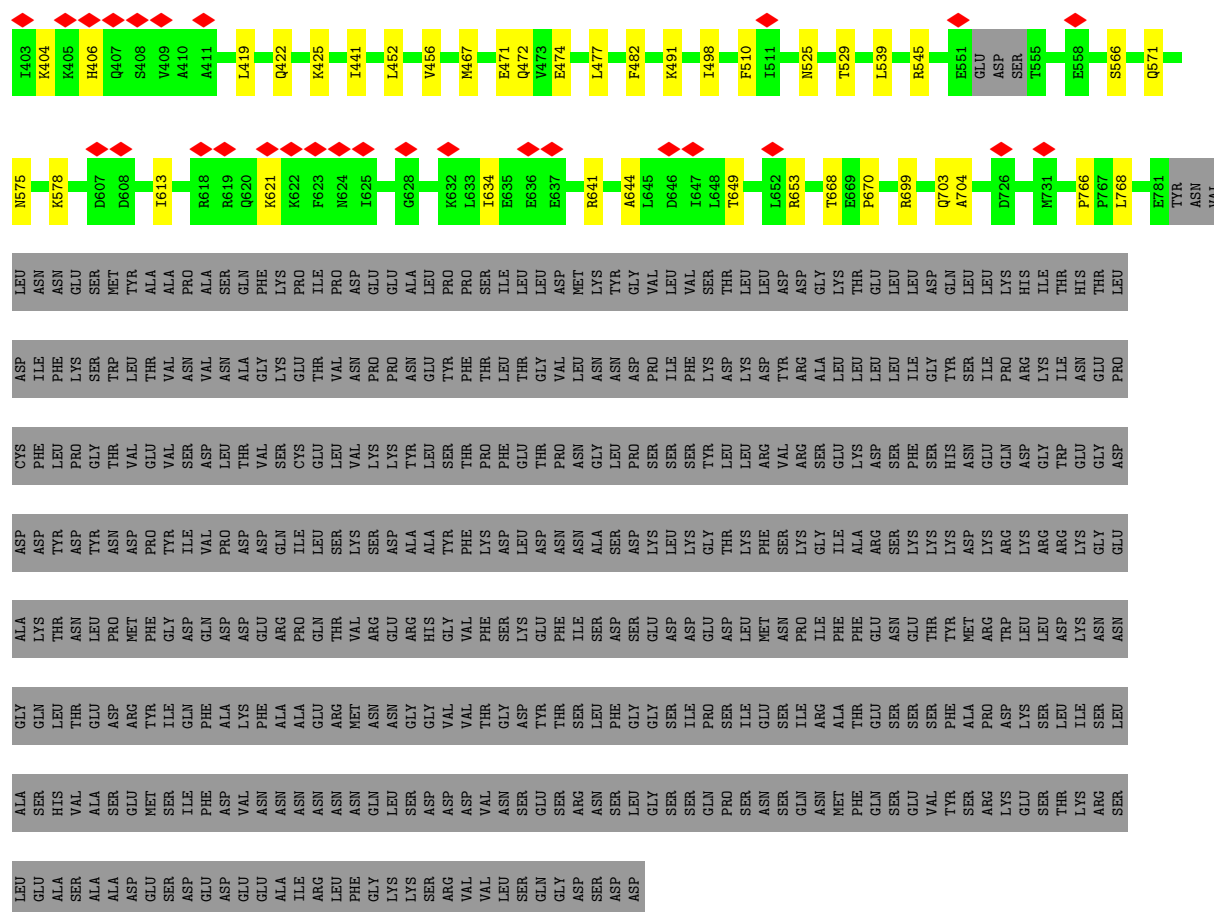
• Molecule 14: DNA polymerase alpha-binding protein

Chain G: 40% 6% 54%

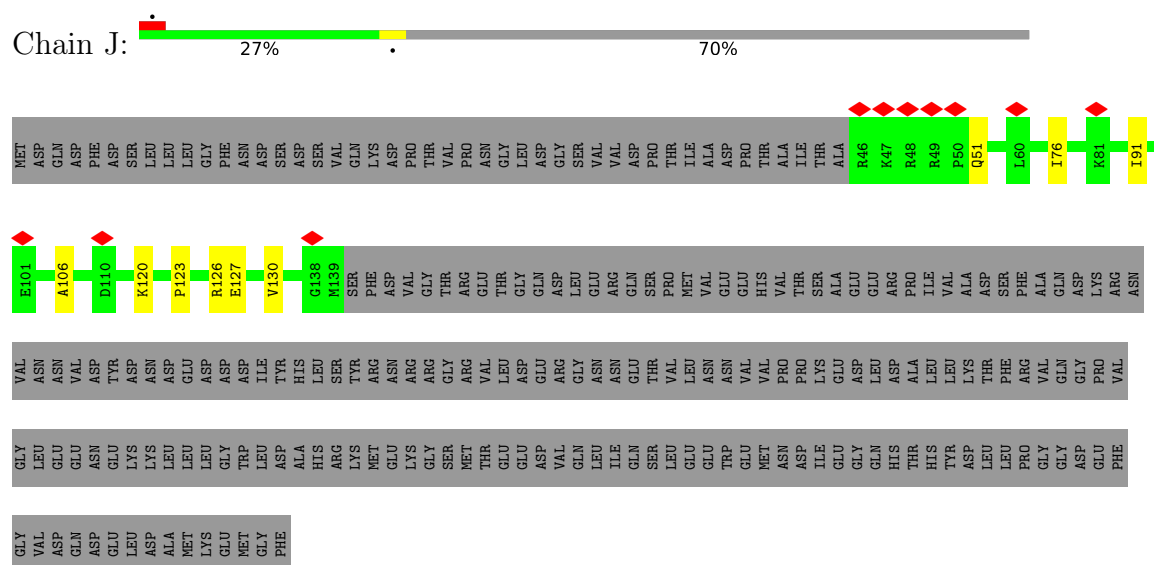


Chain H:





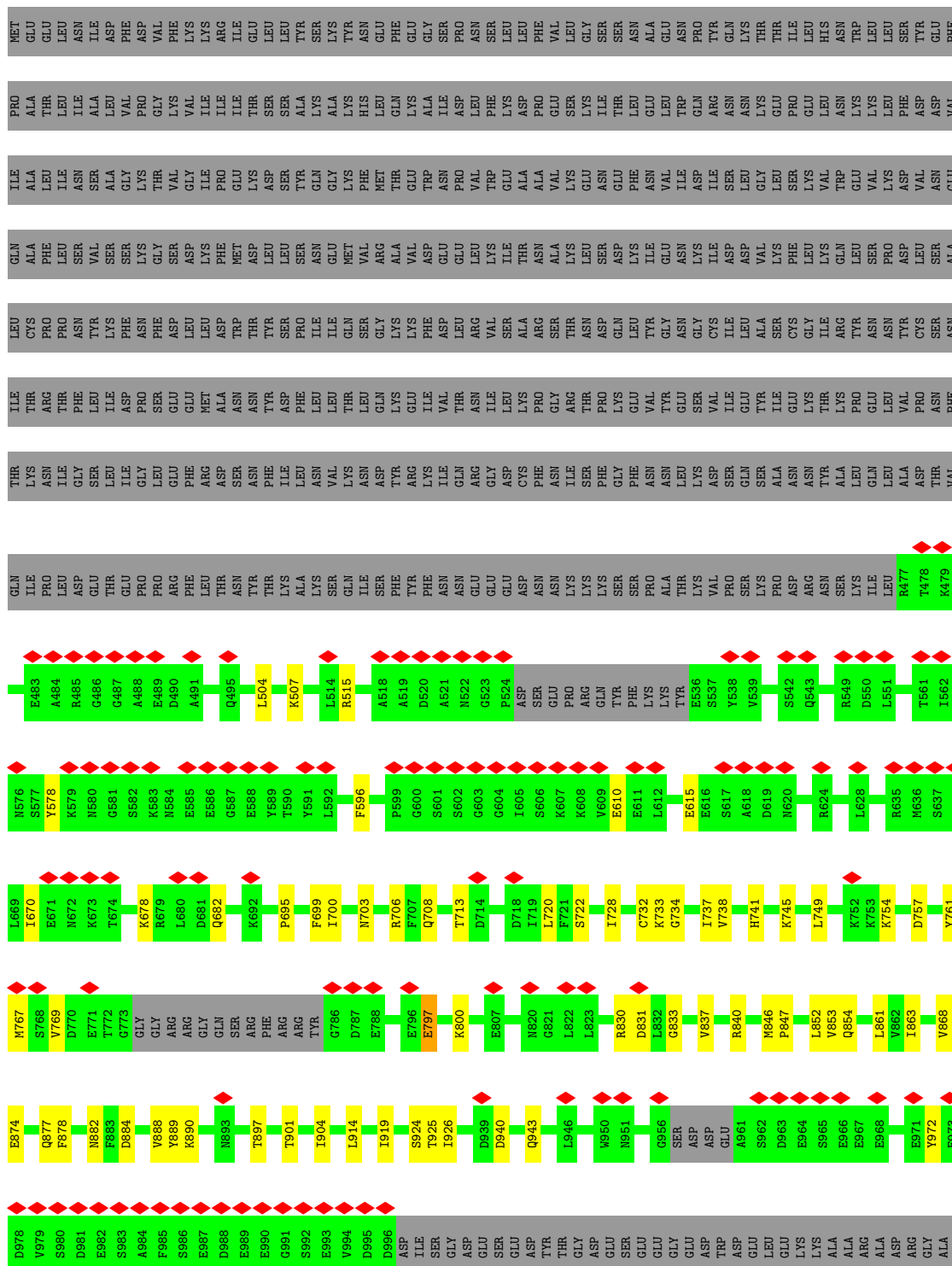
- Molecule 16: Chromosome segregation in meiosis protein 3



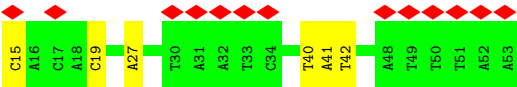
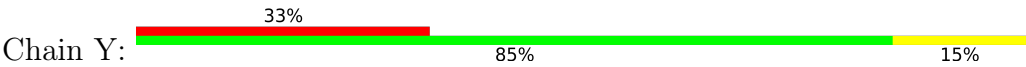
- Molecule 17: Mediator of replication checkpoint protein 1



- Molecule 18: FACT complex subunit SPT16



Chain M:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	524000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	84.549	Depositor
Minimum map value	-59.011	Depositor
Average map value	0.090	Depositor
Map value standard deviation	1.797	Depositor
Recommended contour level	10	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	2	0.19	0/6259	0.48	1/8458 (0.0%)
2	3	0.19	0/4880	0.50	0/6619
3	4	0.21	0/5337	0.56	1/7213 (0.0%)
4	5	0.22	1/5454 (0.0%)	0.52	3/7365 (0.0%)
5	6	0.20	0/5073	0.50	1/6846 (0.0%)
6	7	0.21	0/4993	0.52	0/6757
7	8	0.22	0/7097	0.52	0/9594
8	9	0.21	0/4699	0.53	1/6360 (0.0%)
9	A	0.21	0/1631	0.54	0/2194
10	B	0.21	0/1642	0.49	0/2221
11	C	0.19	0/1412	0.49	0/1908
12	D	0.22	0/2024	0.54	0/2733
13	E	0.19	0/4633	0.49	1/6269 (0.0%)
14	F	0.19	0/3489	0.47	0/4724
14	G	0.20	0/3465	0.52	0/4696
14	H	0.19	0/3496	0.46	0/4735
15	I	0.21	0/6171	0.52	2/8321 (0.0%)
16	J	0.21	0/804	0.51	0/1074
17	K	0.26	0/166	0.61	0/220
18	L	0.22	0/3522	0.59	4/4786 (0.1%)
19	M	0.13	0/1868	0.35	0/2591
20	N	0.27	0/635	0.68	0/850
20	R	0.29	0/748	0.74	1/1000 (0.1%)
21	O	0.29	0/588	0.73	0/788
21	S	0.24	0/692	0.55	0/924
22	P	0.25	0/711	0.60	0/959
23	Q	0.29	0/716	0.66	0/966
24	X	0.25	0/1159	0.58	0/1789
25	Y	0.20	0/894	0.45	0/1375
All	All	0.21	1/84258 (0.0%)	0.52	15/114335 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	208	PRO	CG-CD	-6.97	1.27	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	208	PRO	N-CD-CG	-9.33	89.21	103.20
4	5	208	PRO	CA-N-CD	-6.84	102.42	112.00
18	L	797	GLU	N-CA-CB	6.37	120.78	110.40
13	E	524	ILE	N-CA-C	-6.04	107.98	113.71
15	I	704	ALA	CA-C-N	5.94	135.47	125.02
15	I	704	ALA	C-N-CA	5.94	135.47	125.02
18	L	797	GLU	CA-CB-CG	5.88	125.85	114.10
18	L	972	TYR	CA-C-N	5.66	131.44	122.61
18	L	972	TYR	C-N-CA	5.66	131.44	122.61
1	2	815	ARG	CB-CG-CD	5.64	124.27	111.30
5	6	162	GLU	CA-CB-CG	5.41	124.92	114.10
8	9	72	GLN	N-CA-CB	5.25	117.93	110.16
20	R	116	LYS	CB-CG-CD	5.24	123.36	111.30
3	4	272	MET	CB-CG-SD	5.08	127.95	112.70
4	5	208	PRO	CA-CB-CG	-5.04	94.93	104.50

There are no chirality outliers.

There are no planarity outliers.

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	2	6161	0	6082	85	0
2	3	4795	0	4858	65	0
3	4	5269	0	5238	77	0
4	5	5376	0	5440	65	0
5	6	4991	0	5001	61	0
6	7	4919	0	4913	54	0
7	8	6945	0	7025	87	0
8	9	4594	0	4631	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1611	0	1615	26	0
10	B	1609	0	1662	26	0
11	C	1379	0	1393	13	0
12	D	1988	0	1986	21	0
13	E	4550	0	4536	49	0
14	F	3404	0	3352	36	0
14	G	3380	0	3310	33	0
14	H	3411	0	3355	29	0
15	I	6057	0	6200	68	0
16	J	788	0	827	7	0
17	K	163	0	136	1	0
18	L	3474	0	3005	46	0
19	M	1876	0	802	2	0
20	N	629	0	668	12	0
20	R	741	0	791	20	0
21	O	583	0	626	14	0
21	S	684	0	732	17	0
22	P	703	0	737	10	0
23	Q	706	0	722	8	0
24	X	1041	0	593	5	0
25	Y	796	0	440	6	0
26	2	1	0	0	0	0
26	4	1	0	0	0	0
26	5	1	0	0	0	0
26	6	1	0	0	0	0
26	7	1	0	0	0	0
26	8	2	0	0	0	0
27	2	27	0	12	1	0
27	3	27	0	12	3	0
27	5	27	0	12	0	0
27	6	27	0	12	2	0
27	7	27	0	12	2	0
All	All	82765	0	80736	868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (868) 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)
18:L:874:GLU:HB3	18:L:884:ASP:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:2059:CYS:O	7:8:2063:LEU:HB2	1.89	0.71
7:8:1490:PHE:HB2	7:8:1498:PHE:HB2	1.73	0.68
3:4:563:ASN:H	3:4:703:ASP:HB2	1.60	0.67
6:7:614:GLU:O	6:7:618:TYR:HB2	1.93	0.67
1:2:129:ILE:HG21	15:I:204:LEU:HB2	1.78	0.66
4:5:717:GLU:O	4:5:721:ARG:HB2	1.95	0.66
14:F:730:LYS:HD3	14:F:817:ILE:HD11	1.77	0.66
18:L:515:ARG:HH12	18:L:890:LYS:HB3	1.61	0.66
7:8:1386:ASN:C	7:8:1386:ASN:HD22	2.04	0.65
5:6:601:LYS:HD3	5:6:643:LYS:HE3	1.79	0.65
14:F:619:THR:HG21	14:F:688:PHE:HA	1.78	0.64
8:9:362:LEU:HD11	8:9:376:ILE:HD12	1.80	0.64
1:2:341:CYS:HB3	1:2:344:CYS:SG	2.36	0.64
5:6:610:ALA:HA	5:6:624:GLU:O	1.99	0.63
7:8:2151:ARG:NH1	8:9:491:TRP:O	2.31	0.63
14:G:704:LEU:HB3	14:G:722:LEU:HB3	1.81	0.63
1:2:581:ARG:HH22	1:2:584:PRO:HD3	1.62	0.63
8:9:648:GLN:HA	8:9:660:ASN:O	1.99	0.63
3:4:304:ARG:HD3	3:4:423:LEU:HD11	1.81	0.62
21:O:78:LYS:HG3	23:Q:96:ARG:HH12	1.65	0.62
10:B:27:ILE:HG13	10:B:87:ILE:HA	1.82	0.62
18:L:678:LYS:HB2	18:L:700:ILE:HD12	1.80	0.62
2:3:457:LEU:HD21	2:3:497:ILE:HG21	1.81	0.62
4:5:769:ASN:ND2	7:8:1708:ASN:OD1	2.32	0.61
7:8:1457:LYS:O	7:8:1461:GLN:HB2	2.01	0.61
8:9:9:PRO:HB3	8:9:47:THR:HA	1.81	0.61
18:L:797:GLU:HA	18:L:800:LYS:HG2	1.83	0.61
1:2:629:ILE:HB	1:2:640:LEU:HB2	1.82	0.60
18:L:667:ASP:H	18:L:720:LEU:HD11	1.65	0.60
6:7:465:ALA:HA	27:7:902:ADP:H5'2	1.83	0.60
5:6:570:ASN:HD22	5:6:678:ILE:H	1.50	0.60
1:2:136:GLN:HB3	1:2:139:ALA:HB2	1.84	0.60
5:6:644:MET:HE3	5:6:649:GLN:HG2	1.84	0.60
8:9:673:MET:SD	8:9:684:GLN:NE2	2.74	0.60
8:9:307:ILE:HG22	8:9:339:PHE:HB3	1.84	0.60
15:I:768:LEU:HD21	16:J:130:VAL:HG12	1.83	0.60
20:R:121:GLN:H	20:R:124:ASP:HB2	1.65	0.60
15:I:634:ILE:HD11	15:I:641:ARG:HB3	1.84	0.60
7:8:1431:ILE:HG12	7:8:1436:ARG:HE	1.67	0.59
18:L:833:GLY:HA2	18:L:847:PRO:HD2	1.83	0.59
7:8:1673:ASP:OD1	7:8:1819:TRP:NE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:70:ARG:HH12	21:O:25:ASP:HA	1.67	0.59
3:4:178:ARG:NH1	15:I:383:VAL:O	2.34	0.59
23:Q:117:GLU:HG3	23:Q:120:ARG:HH12	1.66	0.59
3:4:428:ARG:HH22	5:6:372:SER:HB3	1.68	0.59
13:E:84:VAL:HG22	13:E:123:LEU:HD12	1.84	0.59
9:A:47:LEU:HD13	9:A:79:MET:HG2	1.85	0.59
14:F:616:VAL:HG11	14:F:682:MET:HE3	1.85	0.59
15:I:40:ILE:HG22	15:I:42:PRO:HD2	1.85	0.59
1:2:569:GLN:OE1	1:2:613:ASN:ND2	2.35	0.59
1:2:618:THR:OG1	4:5:484:LYS:NZ	2.34	0.59
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.68	0.59
7:8:1486:TYR:HB3	7:8:1502:PHE:HB3	1.84	0.59
18:L:837:VAL:HG11	20:R:113:ILE:HD13	1.85	0.59
20:R:121:GLN:HB2	20:R:124:ASP:H	1.68	0.58
1:2:662:PRO:HG3	1:2:850:LYS:HD2	1.85	0.58
6:7:584:ILE:HG23	6:7:586:LEU:H	1.66	0.58
20:N:110:LEU:HA	20:N:113:ILE:HG12	1.84	0.58
1:2:785:LYS:NZ	7:8:2087:GLU:OE1	2.36	0.58
13:E:526:ARG:HE	13:E:565:LEU:HB2	1.68	0.58
3:4:531:TYR:OH	3:4:723:HIS:ND1	2.37	0.58
18:L:871:CYS:HB3	18:L:914:LEU:HD11	1.85	0.58
7:8:2163:ARG:HE	7:8:2188:THR:HG22	1.66	0.58
18:L:868:VAL:HA	18:L:889:TYR:HA	1.85	0.58
18:L:722:SER:O	18:L:745:LYS:NZ	2.36	0.58
7:8:1421:GLU:OE1	8:9:594:GLN:NE2	2.37	0.58
21:S:27:ILE:HB	21:S:56:ARG:HD3	1.85	0.58
10:B:23:GLU:OE1	10:B:118:ASN:ND2	2.37	0.58
14:H:489:THR:HG22	14:H:491:ARG:H	1.68	0.58
1:2:577:THR:HG23	1:2:629:ILE:HD12	1.86	0.57
1:2:341:CYS:CB	1:2:344:CYS:SG	2.92	0.57
7:8:1431:ILE:HG21	7:8:1436:ARG:HH21	1.69	0.57
2:3:417:GLN:HG2	27:3:1001:ADP:H5'2	1.86	0.57
8:9:493:SER:HB2	8:9:498:GLY:H	1.70	0.57
8:9:531:ARG:NH1	8:9:629:THR:O	2.37	0.57
15:I:422:GLN:HB3	15:I:425:LYS:HG2	1.86	0.57
18:L:854:GLN:HB3	18:L:861:LEU:HB3	1.85	0.57
27:3:1001:ADP:O2A	4:5:651:ARG:NH2	2.38	0.57
13:E:8:PHE:HB3	13:E:258:LEU:HD12	1.87	0.57
5:6:123:SER:HA	5:6:134:LYS:H	1.70	0.57
8:9:505:GLN:HB2	8:9:528:ASN:HB2	1.86	0.57
6:7:262:CYS:HB3	6:7:265:CYS:SG	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:422:ILE:HD13	6:7:469:LEU:HD21	1.86	0.57
18:L:830:ARG:HG2	18:L:846:MET:HE1	1.87	0.57
10:B:34:ARG:HG3	10:B:64:VAL:HG22	1.87	0.56
11:C:166:LEU:HD13	11:C:169:LEU:HD12	1.87	0.56
11:C:188:LYS:O	11:C:192:PHE:HB2	2.05	0.56
6:7:451:ARG:HH12	6:7:455:ASN:HD21	1.53	0.56
14:G:510:GLN:NE2	14:G:511:TYR:O	2.38	0.56
1:2:631:ILE:O	1:2:637:VAL:HA	2.06	0.56
1:2:641:GLN:OE1	1:2:643:ARG:NH2	2.39	0.56
2:3:533:ILE:HD12	2:3:535:LEU:HB2	1.86	0.56
3:4:532:GLU:O	3:4:537:LYS:NZ	2.37	0.56
8:9:432:LEU:HB3	8:9:481:MET:HG2	1.88	0.56
20:R:62:LEU:O	21:S:37:ARG:NH1	2.38	0.56
9:A:150:ASP:OD1	12:D:141:ARG:NH1	2.38	0.56
14:H:493:TYR:HE2	14:H:768:LEU:HD13	1.69	0.56
3:4:204:LYS:HB3	3:4:221:ASP:HB3	1.88	0.56
8:9:221:ARG:NH2	8:9:627:ASP:OD2	2.38	0.56
1:2:119:ARG:NH1	15:I:278:ASP:OD2	2.39	0.56
5:6:443:LEU:HD21	5:6:448:LEU:HB2	1.88	0.56
20:R:62:LEU:HD22	21:S:38:LEU:HD23	1.88	0.56
1:2:426:VAL:HG22	1:2:456:ILE:HG12	1.88	0.56
1:2:438:LEU:O	1:2:442:ASN:HB2	2.06	0.56
1:2:613:ASN:O	1:2:617:ARG:N	2.36	0.56
2:3:45:ILE:HG12	2:3:92:LEU:HD13	1.88	0.56
16:J:123:PRO:HA	16:J:126:ARG:HD3	1.87	0.56
1:2:500:SER:HB2	1:2:757:PRO:HD2	1.88	0.55
2:3:216:ASP:HB2	6:7:370:LEU:HD12	1.88	0.55
3:4:349:CYS:HB2	3:4:371:CYS:SG	2.45	0.55
8:9:209:PRO:HB3	8:9:625:ASP:HB2	1.87	0.55
1:2:343:LYS:NZ	1:2:369:SER:OG	2.39	0.55
4:5:493:ILE:HG22	4:5:497:MET:HG3	1.87	0.55
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.88	0.55
4:5:656:ILE:HA	4:5:659:ILE:HD12	1.87	0.55
14:H:601:ASN:HD21	14:H:605:VAL:HB	1.70	0.55
14:H:751:THR:HB	14:H:773:GLU:HB2	1.86	0.55
7:8:2101:LEU:HD22	7:8:2119:PHE:HB2	1.88	0.55
15:I:365:SER:HB3	15:I:373:ARG:HE	1.71	0.55
4:5:149:ARG:NH1	4:5:269:GLU:OE1	2.40	0.55
4:5:436:ALA:HA	4:5:476:VAL:O	2.07	0.55
13:E:303:THR:O	14:F:491:ARG:NH1	2.40	0.55
18:L:728:ILE:HG12	18:L:853:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:665:GLN:HG3	3:4:925:ARG:HH12	1.71	0.55
1:2:83:ALA:O	15:I:641:ARG:NH2	2.39	0.55
7:8:1358:TYR:HB3	7:8:1397:LEU:HD11	1.87	0.55
14:G:716:SER:O	14:H:653:ARG:NH2	2.40	0.55
15:I:368:THR:OG1	15:I:370:ASP:O	2.25	0.55
1:2:116:LEU:HD11	21:S:72:THR:HG21	1.87	0.55
7:8:2101:LEU:HD12	7:8:2200:VAL:HG12	1.88	0.55
22:P:104:ILE:HG22	21:S:99:TYR:HB2	1.89	0.55
14:G:584:THR:HB	14:G:587:ARG:H	1.71	0.55
20:R:130:ARG:HA	20:R:135:ARG:HD3	1.88	0.55
14:G:641:SER:HB3	14:G:648:LYS:HE2	1.88	0.54
2:3:455:ARG:HH12	24:X:51:DT:H1'	1.71	0.54
14:H:511:TYR:HB2	14:H:530:ASP:HB3	1.89	0.54
21:S:27:ILE:O	21:S:56:ARG:NH1	2.41	0.54
1:2:247:ARG:NH1	1:2:469:GLU:OE1	2.40	0.54
18:L:699:PHE:HB2	18:L:706:ARG:HB3	1.88	0.54
3:4:348:LYS:NZ	3:4:353:ASP:OD1	2.41	0.54
3:4:447:ASN:HB3	3:4:450:GLN:HB2	1.89	0.54
14:G:616:VAL:HG21	14:G:682:MET:HE2	1.88	0.54
3:4:543:GLN:HE21	3:4:670:SER:HB2	1.73	0.54
3:4:594:LYS:NZ	6:7:535:THR:O	2.40	0.54
13:E:248:VAL:O	13:E:290:ARG:NH2	2.41	0.54
13:E:572:ILE:HD11	13:E:634:ARG:HH21	1.72	0.54
14:F:641:SER:OG	14:F:653:ARG:NH1	2.41	0.54
15:I:256:SER:O	15:I:260:ASN:ND2	2.41	0.54
2:3:433:THR:OG1	4:5:503:SER:OG	2.24	0.54
5:6:294:VAL:HB	5:6:391:PRO:HA	1.90	0.54
10:B:51:GLN:HB2	12:D:129:MET:HE1	1.89	0.54
14:G:726:MET:HE1	14:G:783:LYS:HG3	1.90	0.54
7:8:1524:ASN:ND2	7:8:1628:GLN:OE1	2.37	0.54
14:G:610:GLU:OE2	14:G:653:ARG:NH2	2.41	0.54
14:G:879:VAL:HG22	14:G:907:LEU:HD21	1.90	0.54
13:E:348:LEU:O	13:E:358:ARG:NH1	2.40	0.54
4:5:412:VAL:HG13	4:5:552:MET:HB2	1.90	0.53
10:B:108:HIS:O	10:B:155:LYS:NZ	2.38	0.53
10:B:130:ALA:HB1	10:B:133:ASP:HB2	1.90	0.53
21:O:79:ARG:NH2	21:O:86:ASP:OD2	2.41	0.53
3:4:406:VAL:HG11	3:4:412:PRO:HG3	1.90	0.53
7:8:1353:ILE:HD12	7:8:1354:PRO:HD2	1.89	0.53
13:E:226:ARG:HG3	13:E:230:ILE:HD12	1.88	0.53
14:G:657:LEU:O	14:H:634:HIS:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:571:GLN:O	15:I:575:ASN:ND2	2.39	0.53
6:7:599:LEU:H	6:7:726:SER:HB3	1.73	0.53
7:8:1875:PRO:HA	7:8:1878:CYS:HB3	1.90	0.53
1:2:527:VAL:HB	1:2:531:HIS:HB3	1.90	0.53
3:4:914:ASP:OD2	5:6:696:ARG:NH1	2.38	0.53
11:C:169:LEU:HD22	11:C:173:GLU:HB3	1.91	0.53
21:O:27:ILE:O	21:O:56:ARG:NE	2.41	0.53
6:7:249:SER:O	6:7:311:GLN:NE2	2.40	0.53
7:8:1552:ILE:HG22	7:8:1553:LYS:HG2	1.91	0.53
5:6:336:PRO:O	15:I:223:ASN:ND2	2.41	0.53
7:8:1622:LEU:HD13	7:8:1627:TRP:HB2	1.91	0.53
1:2:321:THR:HG22	1:2:425:GLU:HG2	1.90	0.53
3:4:264:TYR:HE1	6:7:303:ARG:HD3	1.74	0.53
8:9:457:GLN:OE1	8:9:461:ASN:ND2	2.42	0.53
13:E:18:ASN:ND2	13:E:119:ASP:OD2	2.42	0.53
13:E:411:ARG:NH2	13:E:486:ASP:OD1	2.41	0.53
13:E:573:ASP:O	13:E:577:ASP:HA	2.08	0.53
1:2:113:ASP:O	1:2:117:ASN:ND2	2.42	0.53
5:6:103:VAL:HG22	15:I:422:GLN:HE22	1.74	0.53
14:G:617:ALA:HB3	14:G:628:VAL:HB	1.90	0.53
1:2:404:ARG:HD2	5:6:299:GLU:HG3	1.91	0.53
3:4:265:PRO:HB3	3:4:325:LEU:HD12	1.91	0.53
7:8:1613:VAL:HG12	7:8:1661:CYS:HA	1.91	0.53
15:I:93:ILE:HG12	15:I:174:LYS:HB3	1.91	0.53
2:3:104:ARG:NH2	2:3:105:GLU:OE2	2.40	0.52
2:3:447:THR:OG1	2:3:458:GLU:OE2	2.24	0.52
2:3:553:ILE:HG23	4:5:630:ARG:HE	1.73	0.52
5:6:258:GLN:O	15:I:242:ASN:ND2	2.41	0.52
3:4:854:LYS:HA	3:4:857:ILE:HG22	1.91	0.52
18:L:840:ARG:NH2	20:R:116:LYS:O	2.42	0.52
2:3:39:ARG:HG2	2:3:132:LEU:HD21	1.91	0.52
3:4:569:ASP:O	3:4:574:LYS:NZ	2.40	0.52
8:9:489:ASP:O	8:9:493:SER:OG	2.27	0.52
9:A:1:MET:SD	9:A:2:TYR:N	2.82	0.52
15:I:575:ASN:HA	15:I:578:LYS:HD3	1.91	0.52
4:5:454:GLN:NE2	4:5:465:GLU:OE1	2.43	0.52
8:9:319:TYR:HE2	8:9:601:LYS:HE2	1.74	0.52
13:E:52:GLN:NE2	13:E:264:GLU:OE2	2.42	0.52
13:E:123:LEU:HD13	13:E:255:ILE:HD11	1.90	0.52
1:2:528:ASN:ND2	4:5:584:GLN:OE1	2.42	0.52
3:4:315:ARG:HH22	3:4:412:PRO:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:1543:ILE:HG22	7:8:1547:SER:HB2	1.92	0.52
11:C:30:LEU:HD12	11:C:46:LEU:HD22	1.92	0.52
15:I:566:SER:HA	15:I:613:ILE:HG23	1.92	0.52
4:5:654:GLU:HA	4:5:657:ILE:HD12	1.92	0.52
6:7:429:LYS:HD2	6:7:432:LEU:HD12	1.91	0.52
13:E:313:PRO:HA	13:E:414:GLY:HA2	1.90	0.52
23:Q:119:THR:HA	23:Q:122:VAL:HG12	1.91	0.52
1:2:558:LYS:HD2	5:6:562:GLY:HA3	1.91	0.52
5:6:409:GLN:NE2	5:6:418:SER:O	2.43	0.52
7:8:1862:ASP:OD2	7:8:1914:LYS:NZ	2.42	0.52
8:9:165:ASP:OD2	8:9:167:ARG:NH1	2.43	0.52
14:H:617:ALA:HB3	14:H:628:VAL:HB	1.91	0.52
13:E:145:ASP:OD1	13:E:249:ASN:ND2	2.42	0.52
20:R:107:ASP:OD2	20:R:132:ARG:NH1	2.43	0.52
10:B:115:LEU:HD11	10:B:148:LEU:HD13	1.91	0.51
14:F:617:ALA:HB3	14:F:628:VAL:HB	1.92	0.51
5:6:266:SER:HB3	5:6:458:HIS:HB2	1.93	0.51
11:C:135:LEU:HD11	11:C:177:TYR:HB2	1.92	0.51
14:H:489:THR:HG23	14:H:491:ARG:HH21	1.75	0.51
15:I:161:LEU:HD22	15:I:248:ILE:HD13	1.90	0.51
1:2:113:ASP:OD1	21:S:73:TYR:OH	2.25	0.51
1:2:230:ARG:NH1	1:2:243:GLU:O	2.43	0.51
3:4:802:ILE:HD11	5:6:732:VAL:HG12	1.92	0.51
13:E:554:GLU:HG2	13:E:587:ARG:HH21	1.75	0.51
16:J:76:ILE:HD12	16:J:91:ILE:HD13	1.92	0.51
1:2:262:LYS:NZ	5:6:257:GLU:OE2	2.43	0.51
5:6:303:GLU:HG3	5:6:356:TRP:HB2	1.92	0.51
7:8:1908:LEU:HD23	7:8:1965:LEU:HD22	1.92	0.51
13:E:75:ASP:O	13:E:118:ARG:NH2	2.43	0.51
13:E:365:ARG:NH1	13:E:399:TYR:OH	2.43	0.51
3:4:315:ARG:O	6:7:341:ARG:NH1	2.44	0.51
3:4:587:ARG:NH2	3:4:623:LEU:O	2.43	0.51
6:7:618:TYR:HA	6:7:621:MET:HG2	1.92	0.51
11:C:134:GLU:OE2	11:C:138:HIS:NE2	2.43	0.51
15:I:27:LEU:HD23	15:I:58:LEU:HD22	1.93	0.51
15:I:401:ARG:NH1	15:I:402:ILE:O	2.44	0.51
18:L:940:ASP:HB3	18:L:943:GLN:HB3	1.92	0.51
20:N:70:ARG:HB2	20:N:73:ARG:HH21	1.75	0.51
23:Q:58:ILE:HG21	23:Q:63:MET:HE2	1.93	0.51
2:3:203:ALA:O	2:3:207:GLY:N	2.44	0.51
2:3:501:GLY:O	6:7:247:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:192:LEU:HD21	21:S:75:GLU:HG3	1.93	0.51
15:I:467:MET:HG3	15:I:472:GLN:HE21	1.76	0.51
3:4:268:VAL:HA	3:4:271:ILE:HD12	1.93	0.51
7:8:1366:MET:HG3	7:8:1368:LEU:HD22	1.92	0.51
18:L:749:LEU:HA	18:L:754:LYS:HA	1.93	0.51
18:L:767:MET:HE3	18:L:769:VAL:H	1.75	0.51
18:L:869:GLU:HB2	18:L:890:LYS:HA	1.93	0.51
21:S:71:VAL:HA	21:S:74:THR:HG22	1.93	0.51
1:2:578:ALA:HB3	1:2:631:ILE:HD11	1.93	0.51
7:8:1908:LEU:HD21	7:8:1964:MET:HB3	1.93	0.51
9:A:193:GLN:O	9:A:197:GLU:HB2	2.11	0.51
14:F:572:LEU:HD22	14:F:576:GLU:HG2	1.93	0.51
4:5:639:GLU:OE2	4:5:750:LYS:NZ	2.44	0.50
5:6:570:ASN:HA	5:6:678:ILE:O	2.11	0.50
7:8:1585:GLY:O	7:8:1587:GLN:NE2	2.44	0.50
18:L:874:GLU:OE1	18:L:924:SER:OG	2.29	0.50
2:3:483:ARG:HD3	2:3:535:LEU:HD22	1.92	0.50
3:4:292:ASP:OD1	3:4:292:ASP:N	2.44	0.50
4:5:143:ALA:O	4:5:161:ARG:NH1	2.42	0.50
9:A:77:LEU:HD21	11:C:53:ILE:HD11	1.93	0.50
14:F:728:ILE:HD11	14:F:742:VAL:HG23	1.93	0.50
18:L:504:LEU:HA	18:L:507:LYS:HG2	1.93	0.50
18:L:877:GLN:NE2	18:L:925:THR:O	2.43	0.50
7:8:1432:THR:OG1	7:8:1435:GLN:OE1	2.25	0.50
8:9:643:ASP:HB3	8:9:660:ASN:HD21	1.76	0.50
10:B:152:ARG:NH1	10:B:177:GLU:OE1	2.44	0.50
11:C:27:LEU:HB3	11:C:30:LEU:HD23	1.93	0.50
18:L:682:GLN:HA	18:L:695:PRO:HB3	1.94	0.50
4:5:685:GLN:HA	4:5:689:MET:HB2	1.93	0.50
7:8:1795:LEU:HD13	7:8:1816:LEU:HD13	1.93	0.50
21:O:74:THR:HG21	21:O:82:VAL:HA	1.92	0.50
2:3:279:ASP:OD1	2:3:280:ASP:N	2.42	0.50
5:6:613:VAL:O	5:6:621:TYR:HA	2.12	0.50
8:9:75:ARG:NH1	8:9:86:GLU:OE2	2.45	0.50
1:2:152:ARG:NH2	15:I:50:ASP:OD2	2.44	0.50
2:3:671:LEU:HG	2:3:676:ILE:HD11	1.94	0.50
1:2:738:LEU:N	1:2:742:GLN:OE1	2.45	0.50
2:3:175:HIS:HA	2:3:178:LYS:HD2	1.92	0.50
2:3:389:VAL:HG12	2:3:710:THR:HG21	1.93	0.50
10:B:82:GLN:HB3	10:B:84:LYS:HG2	1.94	0.50
12:D:171:LEU:HD23	12:D:175:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:589:PRO:HG2	13:E:592:LEU:HD23	1.94	0.50
1:2:618:THR:HB	1:2:621:HIS:HE1	1.77	0.50
2:3:394:GLU:HB2	6:7:624:LYS:HB2	1.93	0.50
8:9:26:SER:OG	9:A:198:ARG:NH1	2.44	0.50
18:L:578:TYR:HA	18:L:596:PHE:HA	1.94	0.50
18:L:682:GLN:OE1	18:L:762:ARG:NH2	2.44	0.50
1:2:772:THR:HG23	1:2:773:LYS:HG2	1.92	0.50
2:3:708:LEU:O	2:3:711:ALA:HB3	2.12	0.50
10:B:20:VAL:HG11	10:B:121:VAL:HG21	1.94	0.50
1:2:394:PRO:HB2	5:6:672:LEU:HD21	1.94	0.49
6:7:114:THR:HG23	6:7:202:LEU:HD23	1.95	0.49
6:7:262:CYS:CB	6:7:265:CYS:SG	3.00	0.49
13:E:224:LYS:O	13:E:228:LYS:HB2	2.12	0.49
2:3:39:ARG:HE	2:3:132:LEU:HD11	1.77	0.49
1:2:84:ALA:HA	15:I:641:ARG:HH12	1.77	0.49
1:2:118:GLU:OE2	1:2:121:ARG:NH2	2.38	0.49
6:7:495:ALA:HB3	6:7:546:ILE:HG21	1.92	0.49
7:8:1647:SER:HA	7:8:1650:ILE:HD12	1.95	0.49
7:8:2076:ARG:NH2	7:8:2087:GLU:O	2.45	0.49
13:E:127:ARG:HD2	13:E:248:VAL:HG22	1.93	0.49
7:8:1476:TYR:HE2	7:8:1653:SER:HB3	1.77	0.49
7:8:2119:PHE:HZ	7:8:2142:LEU:HD22	1.77	0.49
9:A:146:LEU:HD23	9:A:151:LEU:HD21	1.93	0.49
15:I:104:LYS:HD3	17:K:340:SER:HA	1.94	0.49
8:9:185:PRO:HA	8:9:188:MET:HA	1.95	0.49
12:D:199:LEU:HD22	12:D:207:GLN:HA	1.94	0.49
7:8:1524:ASN:HB3	7:8:1527:SER:HB3	1.95	0.49
15:I:398:TRP:HD1	16:J:106:ALA:HA	1.77	0.49
15:I:649:THR:HB	15:I:653:ARG:HH12	1.77	0.49
2:3:411:PRO:HG3	4:5:545:THR:HG22	1.94	0.49
3:4:792:THR:N	3:4:844:LYS:O	2.45	0.49
4:5:375:ALA:HB3	4:5:385:LYS:HE2	1.94	0.49
6:7:700:ALA:HB2	6:7:708:VAL:HG22	1.94	0.49
7:8:1675:LEU:HB3	7:8:1794:MET:HE1	1.94	0.49
8:9:271:ILE:HA	8:9:274:LEU:HD23	1.94	0.49
21:S:48:SER:OG	21:S:49:GLY:N	2.46	0.49
9:A:171:ALA:HB3	9:A:183:LEU:HG	1.94	0.49
14:H:665:ASN:O	14:H:670:LYS:NZ	2.46	0.49
1:2:147:LEU:HD11	15:I:20:LEU:HD12	1.94	0.49
3:4:202:LYS:HG2	3:4:224:LEU:HD23	1.95	0.49
3:4:449:ARG:NH2	24:X:46:DT:O5'	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:1858:ILE:HG22	7:8:1868:ILE:HG22	1.95	0.49
8:9:491:TRP:CD1	8:9:506:ASP:HB2	2.47	0.49
13:E:93:GLU:HA	13:E:98:ILE:HB	1.95	0.49
14:F:636:LEU:HD21	14:F:659:MET:HE2	1.94	0.49
14:H:490:ASP:OD1	14:H:490:ASP:N	2.44	0.49
3:4:178:ARG:HD3	15:I:385:GLU:HG2	1.94	0.49
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.95	0.49
3:4:774:TYR:OH	3:4:778:ARG:NH1	2.45	0.49
6:7:479:ARG:NH2	6:7:517:ASP:OD1	2.46	0.49
8:9:609:GLN:HG3	8:9:614:PRO:HG3	1.95	0.49
3:4:304:ARG:HB3	3:4:465:HIS:HD2	1.78	0.48
14:F:533:GLY:O	14:F:548:GLN:NE2	2.46	0.48
1:2:181:LEU:O	1:2:209:ARG:NH2	2.44	0.48
7:8:1709:THR:O	7:8:1713:MET:HB3	2.13	0.48
8:9:171:LYS:HG2	8:9:533:ALA:HB3	1.96	0.48
18:L:882:ASN:HB2	18:L:901:THR:HA	1.94	0.48
5:6:262:VAL:HG21	5:6:354:LEU:HD21	1.95	0.48
6:7:483:THR:HG1	6:7:493:LEU:N	2.11	0.48
7:8:1539:LYS:NZ	7:8:1641:SER:OG	2.43	0.48
18:L:733:LYS:O	18:L:830:ARG:NH1	2.46	0.48
1:2:811:GLU:HB3	1:2:815:ARG:NH1	2.28	0.48
3:4:465:HIS:HE1	3:4:467:LYS:HE2	1.79	0.48
4:5:343:TRP:HE1	4:5:435:ILE:HD11	1.78	0.48
4:5:407:ARG:HA	4:5:500:GLN:HE21	1.78	0.48
6:7:435:LEU:HD13	6:7:456:VAL:HG12	1.96	0.48
7:8:1356:THR:O	7:8:1436:ARG:NH2	2.47	0.48
1:2:237:MET:SD	1:2:237:MET:N	2.85	0.48
2:3:698:THR:HG22	2:3:700:ARG:H	1.78	0.48
3:4:254:THR:HA	3:4:257:LEU:HD13	1.96	0.48
6:7:619:VAL:HA	6:7:626:PRO:HG3	1.94	0.48
14:G:737:THR:OG1	14:G:739:ASP:OD1	2.32	0.48
18:L:757:ASP:N	18:L:757:ASP:OD1	2.46	0.48
2:3:203:ALA:O	2:3:207:GLY:CA	2.62	0.48
20:R:120:ILE:HD11	21:S:47:ILE:HG13	1.96	0.48
5:6:440:LEU:HB2	5:6:443:LEU:HB2	1.95	0.48
7:8:1966:LYS:HD2	7:8:2006:LEU:HD21	1.95	0.48
9:A:186:ASP:HB3	13:E:478:TRP:HD1	1.79	0.48
13:E:335:TYR:HD1	13:E:363:PHE:HE2	1.60	0.48
15:I:287:LEU:HD13	15:I:456:VAL:HG11	1.96	0.48
1:2:667:VAL:HG21	1:2:674:LEU:HD11	1.94	0.48
4:5:663:LEU:HD23	4:5:666:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:84:ARG:NH2	11:C:8:ASP:OD2	2.46	0.48
14:G:560:ASP:OD1	14:G:560:ASP:N	2.45	0.48
14:H:671:ASP:OD1	14:H:671:ASP:N	2.47	0.48
7:8:1412:GLU:OE1	8:9:667:ASN:ND2	2.47	0.48
15:I:364:LEU:HB2	15:I:382:LEU:HD23	1.96	0.48
2:3:344:ASP:OD1	2:3:344:ASP:N	2.47	0.48
2:3:432:THR:OG1	2:3:437:SER:OG	2.29	0.48
3:4:568:GLY:HA2	3:4:709:LEU:HD12	1.95	0.48
5:6:259:THR:HB	5:6:352:ARG:HD2	1.96	0.48
9:A:102:TRP:NE1	9:A:134:TYR:OH	2.43	0.48
12:D:69:ASN:HA	12:D:293:LEU:HB2	1.96	0.48
1:2:618:THR:HB	1:2:621:HIS:CE1	2.48	0.47
6:7:532:SER:O	6:7:535:THR:OG1	2.32	0.47
3:4:544:LEU:HD21	3:4:581:VAL:HG23	1.97	0.47
7:8:1444:SER:HB2	7:8:1471:ALA:HB3	1.96	0.47
8:9:364:LEU:HD13	8:9:634:PRO:HG3	1.96	0.47
13:E:573:ASP:O	13:E:577:ASP:CA	2.62	0.47
14:H:726:MET:HG3	14:H:730:LYS:HE3	1.96	0.47
13:E:573:ASP:O	13:E:577:ASP:N	2.47	0.47
20:N:110:LEU:HD21	20:R:130:ARG:HH22	1.80	0.47
5:6:177:PHE:HA	5:6:180:PHE:HD2	1.80	0.47
5:6:361:ILE:HD11	5:6:377:LEU:HD23	1.96	0.47
7:8:1939:TRP:HE1	7:8:1957:MET:HE2	1.79	0.47
14:F:535:ASP:OD1	14:F:535:ASP:N	2.48	0.47
18:L:670:ILE:H	18:L:703:ASN:HD21	1.62	0.47
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.96	0.47
20:N:121:GLN:N	20:N:124:ASP:OD2	2.46	0.47
1:2:508:HIS:HB3	1:2:511:ILE:HB	1.97	0.47
2:3:187:THR:HG22	2:3:188:LYS:HG3	1.97	0.47
4:5:166:ILE:HD12	4:5:256:LEU:HD23	1.97	0.47
7:8:1705:PHE:HZ	7:8:2159:ILE:HD13	1.80	0.47
7:8:1795:LEU:HD11	7:8:1813:VAL:HG23	1.95	0.47
11:C:88:ILE:HG23	11:C:127:LEU:HD13	1.96	0.47
1:2:95:GLN:OE1	20:R:73:ARG:NH1	2.48	0.47
3:4:643:SER:HA	5:6:601:LYS:HE2	1.95	0.47
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.97	0.47
7:8:2048:LYS:HA	7:8:2048:LYS:HD3	1.70	0.47
10:B:174:SER:HB3	10:B:177:GLU:HG3	1.96	0.47
11:C:53:ILE:HG22	11:C:56:ILE:HD12	1.97	0.47
1:2:562:ARG:HH21	1:2:600:ASP:H	1.62	0.47
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:254:THR:HG22	3:4:257:LEU:HD22	1.96	0.47
8:9:18:ARG:HH22	9:A:176:THR:H	1.63	0.47
15:I:441:ILE:HG23	15:I:482:PHE:HE1	1.80	0.47
14:G:475:ARG:HB3	14:G:477:MET:HE3	1.97	0.47
14:H:775:GLU:OE1	14:H:777:ARG:NH2	2.48	0.47
18:L:852:LEU:HB3	18:L:863:ILE:HB	1.96	0.47
2:3:524:ASP:OD1	2:3:524:ASP:N	2.42	0.47
3:4:622:VAL:HG21	3:4:665:LEU:HB3	1.97	0.47
8:9:171:LYS:NZ	8:9:366:GLY:O	2.45	0.47
14:F:698:PHE:CG	14:F:744:PRO:HG3	2.50	0.47
18:L:831:ASP:OD1	18:L:831:ASP:N	2.47	0.47
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.98	0.46
2:3:122:ILE:HG23	2:3:155:LEU:HD12	1.97	0.46
2:3:404:ASN:HD22	2:3:490:MET:HE1	1.80	0.46
7:8:1741:VAL:HG13	7:8:1795:LEU:HD21	1.96	0.46
12:D:205:GLU:HB3	12:D:206:LEU:HD12	1.97	0.46
14:F:781:PHE:HD1	14:F:821:MET:HE2	1.79	0.46
15:I:184:LEU:HA	15:I:187:ILE:HB	1.97	0.46
22:P:78:THR:HG23	22:P:79:ARG:HG2	1.97	0.46
7:8:1356:THR:HB	7:8:1436:ARG:HH12	1.80	0.46
12:D:156:LEU:HA	12:D:159:ARG:HG2	1.98	0.46
14:F:818:PRO:HG2	14:F:821:MET:HG2	1.97	0.46
18:L:732:CYS:HB2	18:L:738:VAL:HB	1.96	0.46
6:7:335:VAL:HG12	6:7:378:ALA:HB3	1.96	0.46
7:8:1324:VAL:HA	7:8:1340:VAL:HG12	1.97	0.46
7:8:1557:ASN:OD1	7:8:1558:PHE:N	2.48	0.46
7:8:1719:PRO:HD3	7:8:1841:LYS:HE2	1.98	0.46
7:8:1729:ASN:ND2	7:8:1870:THR:O	2.48	0.46
12:D:92:SER:O	12:D:96:GLN:OE1	2.32	0.46
13:E:470:ARG:NH2	13:E:623:ASP:OD2	2.41	0.46
18:L:863:ILE:HD11	18:L:897:THR:HG21	1.97	0.46
1:2:305:SER:OG	1:2:392:GLU:OE2	2.31	0.46
3:4:639:ASP:HA	3:4:642:ARG:HE	1.79	0.46
4:5:48:ASP:OD2	4:5:52:ASN:ND2	2.47	0.46
5:6:835:ILE:HG23	5:6:836:ILE:HG23	1.97	0.46
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.81	0.46
7:8:1710:SER:O	7:8:1714:ASN:HB2	2.16	0.46
7:8:1910:ILE:HD11	7:8:1964:MET:HE1	1.97	0.46
7:8:2202:LYS:HG2	7:8:2206:LYS:HE2	1.96	0.46
1:2:693:GLU:HB2	5:6:778:LYS:HE3	1.97	0.46
4:5:682:ARG:HG3	7:8:2182:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:E:524:ILE:HG23	13:E:525:TYR:HD1	1.81	0.46
15:I:286:LEU:HD23	15:I:452:LEU:HD13	1.98	0.46
16:J:51:GLN:HE22	25:Y:27:DA:H4'	1.81	0.46
7:8:1706:ASP:HB3	7:8:1709:THR:HG22	1.98	0.46
7:8:1913:ASP:OD1	7:8:1913:ASP:N	2.48	0.46
14:G:584:THR:HG22	14:G:586:VAL:H	1.80	0.46
15:I:404:LYS:HG3	15:I:406:HIS:H	1.80	0.46
1:2:66:GLU:OE1	20:R:121:GLN:NE2	2.48	0.46
1:2:330:VAL:HG13	1:2:415:VAL:HG21	1.97	0.46
4:5:287:ILE:HD11	4:5:342:ILE:HA	1.97	0.46
4:5:715:GLU:HG2	4:5:755:LEU:HD21	1.98	0.46
5:6:610:ALA:HB1	5:6:623:ILE:HG23	1.97	0.46
8:9:400:VAL:HA	8:9:673:MET:O	2.16	0.46
15:I:164:LYS:HD2	15:I:215:ILE:HB	1.97	0.46
18:L:766:ASP:OD1	18:L:766:ASP:N	2.49	0.46
21:O:48:SER:OG	21:O:49:GLY:N	2.48	0.46
23:Q:97:GLU:HA	23:Q:100:THR:HG22	1.98	0.46
3:4:628:VAL:HA	3:4:670:SER:O	2.16	0.46
5:6:615:ASP:OD1	5:6:615:ASP:N	2.48	0.46
6:7:122:ASP:OD2	6:7:198:ARG:NH1	2.49	0.46
6:7:453:ASP:O	6:7:694:ARG:NH1	2.49	0.46
13:E:397:ASP:OD1	13:E:402:GLN:NE2	2.48	0.46
14:G:671:ASP:OD1	14:G:671:ASP:N	2.48	0.46
14:G:707:LEU:HG	14:G:710:TRP:HB3	1.96	0.46
14:H:862:TYR:OH	14:H:888:GLU:OE2	2.33	0.46
9:A:149:ILE:HD13	12:D:140:ILE:HG22	1.98	0.46
13:E:382:HIS:HA	13:E:385:LYS:HG2	1.98	0.46
14:H:707:LEU:HG	14:H:710:TRP:HB3	1.97	0.46
15:I:14:ASP:N	15:I:14:ASP:OD1	2.46	0.46
18:L:749:LEU:HB3	18:L:754:LYS:HG3	1.97	0.46
22:P:56:VAL:HG21	23:Q:102:VAL:HG21	1.97	0.46
7:8:1737:ASP:HB3	7:8:1899:ASP:HB2	1.98	0.46
8:9:433:ILE:HG12	8:9:482:ILE:HB	1.97	0.46
12:D:128:CYS:O	12:D:132:GLU:HB2	2.16	0.46
13:E:66:GLU:OE2	13:E:70:HIS:NE2	2.48	0.46
21:S:30:ILE:HD11	21:S:59:LEU:HD22	1.98	0.46
5:6:511:ASP:OD1	5:6:511:ASP:N	2.47	0.45
7:8:1851:PHE:HD2	7:8:1868:ILE:HG21	1.81	0.45
14:G:496:MET:HE1	14:G:764:PRO:HG2	1.98	0.45
3:4:535:ASP:HA	3:4:538:LYS:HG2	1.97	0.45
5:6:673:ASN:OD1	5:6:675:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:149:ARG:NH2	15:I:372:THR:OG1	2.39	0.45
6:7:454:ILE:HG12	6:7:694:ARG:HB3	1.97	0.45
9:A:186:ASP:O	13:E:478:TRP:NE1	2.47	0.45
11:C:58:GLY:HA3	11:C:70:PRO:HA	1.98	0.45
13:E:84:VAL:HA	13:E:123:LEU:HB2	1.98	0.45
14:F:867:LEU:HD11	14:F:894:ALA:HB1	1.97	0.45
14:H:722:LEU:HD12	14:H:776:ILE:HA	1.96	0.45
2:3:440:VAL:HG11	24:X:53:DT:H3'	1.98	0.45
3:4:376:CYS:SG	3:4:377:ASN:N	2.89	0.45
4:5:47:ARG:NH2	10:B:150:GLU:OE1	2.44	0.45
5:6:699:LEU:HD23	5:6:701:MET:HE3	1.98	0.45
8:9:25:LEU:HA	8:9:29:TYR:HD2	1.81	0.45
1:2:175:ASP:HB3	1:2:178:ARG:HB3	1.99	0.45
7:8:1710:SER:O	7:8:1714:ASN:CB	2.65	0.45
8:9:387:LEU:HD23	8:9:390:LEU:HD21	1.97	0.45
14:F:610:GLU:HG3	14:H:717:LYS:HB2	1.99	0.45
18:L:734:GLY:HA3	18:L:830:ARG:HH22	1.81	0.45
6:7:703:ARG:NH2	6:7:712:ASP:OD2	2.44	0.45
8:9:318:HIS:CE1	8:9:346:LEU:HB2	2.52	0.45
10:B:15:GLU:OE2	12:D:71:ARG:NH2	2.49	0.45
10:B:57:ASP:OD1	10:B:57:ASP:N	2.46	0.45
12:D:192:LYS:HE2	12:D:192:LYS:HB3	1.84	0.45
20:N:96:SER:HB2	21:O:91:LEU:HD11	1.98	0.45
1:2:173:ASP:OD1	1:2:173:ASP:N	2.49	0.45
3:4:254:THR:O	3:4:257:LEU:HB2	2.16	0.45
5:6:608:LEU:HD21	5:6:638:ILE:HD13	1.99	0.45
8:9:300:ASP:OD1	8:9:303:GLY:N	2.49	0.45
15:I:471:GLU:HA	15:I:474:GLU:HG2	1.97	0.45
20:N:123:LYS:HG3	20:R:114:HIS:HE1	1.82	0.45
1:2:387:ARG:HH12	4:5:320:GLY:HA3	1.82	0.45
9:A:185:LYS:HD3	13:E:471:LYS:HD2	1.97	0.45
14:G:502:VAL:HG13	14:G:515:VAL:HG12	1.98	0.45
20:N:71:LEU:HD11	21:O:30:ILE:HD11	1.97	0.45
2:3:229:ALA:HB2	6:7:370:LEU:HD23	1.99	0.45
2:3:400:ARG:NH2	2:3:490:MET:O	2.50	0.45
3:4:256:ASP:N	3:4:256:ASP:OD1	2.49	0.45
3:4:345:ALA:HB3	3:4:358:VAL:HG23	1.98	0.45
3:4:603:ALA:HA	3:4:618:SER:HA	1.98	0.45
4:5:359:GLN:OE1	4:5:362:ARG:NH2	2.49	0.45
13:E:28:VAL:HG22	13:E:57:GLN:HB3	1.99	0.45
1:2:477:THR:HG23	1:2:480:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:172:THR:OG1	4:5:252:ASP:OD2	2.34	0.45
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.99	0.45
2:3:434:GLY:HA2	2:3:478:MET:SD	2.57	0.45
6:7:497:VAL:O	6:7:550:LYS:NZ	2.49	0.45
9:A:107:LEU:HB3	9:A:201:GLN:HG2	1.97	0.45
12:D:15:GLU:O	14:F:893:ARG:NH1	2.50	0.45
14:H:542:LYS:HG3	14:H:585:PRO:HB3	1.99	0.45
20:R:118:VAL:HG12	21:S:46:ARG:HG2	1.98	0.45
1:2:431:LYS:HE3	1:2:431:LYS:HB2	1.82	0.45
3:4:399:LEU:O	3:4:414:SER:HA	2.17	0.45
4:5:337:VAL:HG23	4:5:600:LYS:HD3	1.99	0.45
4:5:407:ARG:HG2	4:5:409:ASP:H	1.82	0.45
5:6:798:ARG:HH11	5:6:798:ARG:HG2	1.81	0.45
13:E:509:THR:HG21	13:E:539:TYR:HE2	1.81	0.45
14:H:776:ILE:HD11	14:H:833:LEU:HD11	1.99	0.45
4:5:587:GLN:NE2	4:5:593:GLU:OE2	2.50	0.44
5:6:121:ASP:O	5:6:161:ARG:NH1	2.50	0.44
8:9:40:ALA:HB2	8:9:81:GLN:HG3	2.00	0.44
8:9:382:ASP:OD1	8:9:382:ASP:N	2.48	0.44
14:F:502:VAL:HG22	14:F:515:VAL:HG13	1.99	0.44
14:G:897:ALA:HA	14:G:900:LYS:HE3	1.99	0.44
18:L:926:ILE:HD12	20:R:59:THR:HG22	2.00	0.44
2:3:701:THR:O	2:3:704:THR:HB	2.17	0.44
3:4:189:GLU:O	3:4:193:ASN:ND2	2.50	0.44
6:7:614:GLU:O	6:7:618:TYR:CB	2.65	0.44
7:8:1351:PHE:HE2	7:8:1468:LEU:HD11	1.81	0.44
8:9:197:LYS:HA	8:9:205:ALA:HB1	1.99	0.44
14:G:750:ASP:HA	14:G:776:ILE:HD12	1.99	0.44
22:P:104:ILE:HD12	23:Q:65:ILE:HD13	1.99	0.44
2:3:96:ILE:O	2:3:156:SER:OG	2.30	0.44
6:7:204:PHE:H	6:7:379:GLN:HB3	1.82	0.44
7:8:1387:PRO:HB3	7:8:1780:HIS:HB3	2.00	0.44
10:B:132:ASP:OD1	10:B:132:ASP:N	2.49	0.44
12:D:186:HIS:HA	12:D:189:ILE:HG22	1.98	0.44
15:I:217:PRO:HD3	15:I:248:ILE:HG21	1.99	0.44
2:3:112:SER:O	2:3:116:VAL:HB	2.17	0.44
3:4:178:ARG:HG2	15:I:366:ILE:HG22	2.00	0.44
5:6:134:LYS:HB3	5:6:137:ARG:HG3	2.00	0.44
5:6:566:ARG:NH1	5:6:570:ASN:OD1	2.51	0.44
8:9:225:THR:HG22	8:9:285:LEU:HD11	1.98	0.44
1:2:585:ILE:HG22	1:2:586:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:620:ILE:HD12	1:2:646:ILE:HD13	1.99	0.44
5:6:545:LYS:HE3	5:6:830:LEU:HD21	1.99	0.44
7:8:1446:THR:HG23	7:8:1471:ALA:HB2	1.99	0.44
7:8:1960:ILE:HG22	7:8:1964:MET:HE2	1.98	0.44
14:F:634:HIS:NE2	14:H:657:LEU:O	2.48	0.44
15:I:510:PHE:HE1	15:I:539:LEU:HD11	1.82	0.44
19:M:9:TYR:HA	19:M:16:SER:HA	1.99	0.44
1:2:311:GLU:HA	1:2:314:LEU:HD23	1.99	0.44
1:2:472:ASP:HB3	1:2:475:SER:HB2	1.98	0.44
2:3:190:SER:HG	2:3:255:ARG:H	1.64	0.44
2:3:215:THR:HG21	2:3:224:ARG:HD2	1.98	0.44
8:9:476:THR:OG1	8:9:519:VAL:O	2.36	0.44
20:R:72:VAL:HG21	20:R:93:LEU:HD13	1.98	0.44
2:3:700:ARG:NH1	27:7:902:ADP:O3'	2.50	0.44
7:8:1565:ASP:OD1	7:8:1565:ASP:N	2.49	0.44
14:H:476:TYR:OH	14:H:630:TYR:O	2.34	0.44
1:2:249:LEU:HB3	1:2:257:ALA:HB2	2.00	0.44
2:3:167:SER:HB3	2:3:170:THR:HG22	2.00	0.44
4:5:149:ARG:HG2	4:5:266:PRO:HG3	1.99	0.44
7:8:1416:SER:OG	7:8:1417:ILE:N	2.50	0.44
18:L:737:ILE:HD12	18:L:761:TYR:HB2	2.00	0.44
1:2:623:ALA:HB2	1:2:629:ILE:HD11	2.00	0.44
3:4:178:ARG:HB3	15:I:364:LEU:HD11	1.98	0.44
13:E:1:MET:HB2	13:E:148:VAL:HG21	2.00	0.44
15:I:45:TYR:OH	15:I:87:ASP:OD1	2.33	0.44
19:M:418:SER:H	19:M:441:LEU:HA	1.83	0.44
4:5:724:ILE:HB	7:8:1842:LYS:HE2	2.00	0.43
5:6:500:ASP:HB3	5:6:503:VAL:HG22	2.00	0.43
5:6:595:SER:HA	5:6:635:ILE:O	2.18	0.43
10:B:92:TRP:HA	10:B:97:GLU:HG2	1.99	0.43
10:B:178:ILE:O	10:B:182:ARG:HB2	2.18	0.43
13:E:148:VAL:HG23	13:E:152:LEU:HD23	1.99	0.43
20:N:67:PRO:O	21:O:26:ASN:ND2	2.51	0.43
1:2:259:PHE:HB3	1:2:267:MET:HE3	2.00	0.43
5:6:765:LEU:HD21	5:6:804:ILE:HD11	2.00	0.43
2:3:384:MET:HE2	2:3:513:ILE:HB	1.99	0.43
2:3:490:MET:HE3	2:3:490:MET:HB3	1.83	0.43
4:5:294:ILE:HG12	4:5:333:ILE:HD13	1.99	0.43
5:6:92:PHE:HE2	5:6:336:PRO:HB2	1.82	0.43
7:8:2037:ILE:HD12	7:8:2038:PRO:HD2	1.99	0.43
12:D:152:ASP:OD2	12:D:182:TYR:OH	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:490:ASP:OD1	14:G:490:ASP:N	2.50	0.43
14:G:819:VAL:HG23	14:G:868:ARG:HH22	1.81	0.43
15:I:419:LEU:HD13	15:I:477:LEU:HD11	2.00	0.43
5:6:196:LEU:HG	5:6:263:PHE:HZ	1.84	0.43
8:9:657:LYS:HB2	8:9:680:LYS:HE2	1.99	0.43
9:A:54:LEU:HD11	9:A:71:GLN:HE21	1.84	0.43
13:E:64:TYR:N	13:E:623:ASP:O	2.51	0.43
13:E:131:LEU:HD21	13:E:152:LEU:HD11	2.00	0.43
1:2:663:LEU:HD22	1:2:848:ALA:HB1	2.00	0.43
2:3:284:ASP:OD2	6:7:329:ARG:NH2	2.52	0.43
3:4:399:LEU:HD22	3:4:417:LEU:HD22	1.99	0.43
3:4:742:LEU:HD23	3:4:747:LEU:HG	2.00	0.43
4:5:357:PHE:HZ	4:5:601:ARG:HB3	1.83	0.43
4:5:648:ILE:HA	4:5:652:GLN:HG3	2.00	0.43
6:7:263:ASP:OD1	6:7:263:ASP:N	2.50	0.43
8:9:593:PRO:HG2	8:9:596:VAL:HB	1.99	0.43
10:B:134:PHE:HD2	10:B:138:ILE:HG12	1.84	0.43
14:F:707:LEU:HG	14:F:710:TRP:HB3	1.99	0.43
18:L:870:ILE:HG22	18:L:888:VAL:HB	2.00	0.43
22:P:45:ILE:HA	23:Q:93:ILE:HB	1.99	0.43
1:2:355:SER:OG	1:2:383:ARG:NH2	2.52	0.43
2:3:400:ARG:HG2	2:3:402:ASP:H	1.83	0.43
2:3:435:ARG:HD2	2:3:435:ARG:HA	1.71	0.43
4:5:444:SER:OG	4:5:445:SER:N	2.51	0.43
9:A:55:LYS:HA	9:A:55:LYS:HD3	1.76	0.43
14:G:698:PHE:CG	14:G:744:PRO:HG3	2.54	0.43
18:L:878:PHE:CD2	22:P:86:GLN:HB3	2.53	0.43
3:4:451:ARG:NH1	25:Y:19:DC:OP2	2.51	0.43
6:7:366:LEU:HB3	25:Y:15:DC:H6	1.84	0.43
7:8:2166:ARG:NH2	7:8:2182:ALA:O	2.45	0.43
13:E:131:LEU:O	13:E:135:PHE:HB2	2.18	0.43
13:E:593:ASP:N	13:E:593:ASP:OD1	2.50	0.43
14:F:851:GLU:OE2	14:F:851:GLU:N	2.52	0.43
2:3:171:LEU:HD11	2:3:182:VAL:HG11	2.00	0.43
3:4:242:ASN:HB3	3:4:306:TYR:HE2	1.83	0.43
8:9:18:ARG:NH2	9:A:179:GLY:O	2.51	0.43
8:9:33:ILE:HG12	8:9:79:ILE:HD12	2.01	0.43
14:F:582:ALA:HB2	14:F:618:LEU:HB3	2.00	0.43
14:F:614:PRO:HD2	14:F:631:SER:HB2	1.99	0.43
14:F:650:TYR:HB3	14:F:653:ARG:HD3	2.01	0.43
14:F:703:THR:HA	14:F:722:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:847:MET:HE2	14:F:847:MET:HB3	1.94	0.43
14:H:570:ILE:HD13	14:H:590:VAL:HG11	2.01	0.43
20:R:94:GLN:O	20:R:98:GLU:HG3	2.19	0.43
2:3:161:PHE:HB2	2:3:165:ALA:HB2	2.00	0.43
4:5:504:ILE:O	4:5:510:THR:HA	2.18	0.43
4:5:626:PHE:HB2	4:5:653:LEU:HD13	2.00	0.43
5:6:110:LYS:HE2	15:I:334:GLU:HB3	2.01	0.43
7:8:1487:LEU:HA	7:8:1500:SER:O	2.19	0.43
8:9:527:SER:O	8:9:530:THR:OG1	2.37	0.43
14:G:497:ASN:ND2	14:G:539:LEU:O	2.51	0.43
15:I:78:VAL:HG22	15:I:83:ILE:HD12	2.00	0.43
21:O:74:THR:HG22	21:O:79:ARG:HH22	1.83	0.43
1:2:749:ARG:HA	1:2:752:GLU:HG2	2.00	0.43
1:2:854:ARG:O	1:2:858:ARG:HB2	2.19	0.43
13:E:66:GLU:OE1	13:E:69:ARG:NH1	2.51	0.43
13:E:296:GLN:HG2	13:E:320:ILE:HD13	2.00	0.43
14:F:657:LEU:O	14:G:634:HIS:NE2	2.49	0.43
15:I:525:ASN:O	15:I:529:THR:OG1	2.32	0.43
18:L:904:ILE:HD11	22:P:90:ARG:HH11	1.83	0.43
1:2:339:PHE:HD2	1:2:348:LEU:HD23	1.84	0.42
2:3:169:ARG:NH2	2:3:270:LEU:O	2.46	0.42
3:4:512:VAL:HA	3:4:515:ARG:HD3	2.00	0.42
5:6:388:ARG:HD3	5:6:459:VAL:HB	2.00	0.42
5:6:519:MET:HE1	5:6:750:GLN:HB3	2.00	0.42
6:7:82:LEU:HD21	6:7:106:ILE:HG21	2.00	0.42
8:9:184:ASN:O	8:9:188:MET:N	2.51	0.42
9:A:32:TYR:CD1	9:A:124:SER:HB2	2.54	0.42
10:B:177:GLU:HA	10:B:180:GLU:HG2	2.00	0.42
12:D:88:LEU:HA	12:D:91:ILE:HG22	2.01	0.42
14:F:760:LYS:HB2	14:F:760:LYS:HE2	1.89	0.42
21:S:88:VAL:HG23	21:S:98:LEU:HB3	2.01	0.42
2:3:372:TYR:H	27:3:1001:ADP:N6	2.17	0.42
3:4:568:GLY:HA3	3:4:708:VAL:HB	2.00	0.42
3:4:624:SER:OG	3:4:629:CYS:SG	2.76	0.42
3:4:766:ALA:HB1	3:4:822:VAL:HG21	2.01	0.42
13:E:105:ILE:O	13:E:115:SER:OG	2.36	0.42
14:F:702:ASN:HD22	14:F:725:ASN:HD21	1.67	0.42
15:I:184:LEU:HD23	15:I:187:ILE:HD12	2.01	0.42
15:I:766:PRO:HG3	16:J:120:LYS:HG3	2.00	0.42
20:R:117:ARG:NH1	20:R:124:ASP:OD1	2.51	0.42
1:2:625:GLU:OE1	1:2:808:ARG:NE	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:570:ARG:NH1	4:5:614:LEU:O	2.48	0.42
14:H:768:LEU:HD12	14:H:768:LEU:HA	1.92	0.42
18:L:914:LEU:HD13	18:L:919:ILE:HG23	2.01	0.42
20:N:110:LEU:HD21	20:R:130:ARG:NH2	2.34	0.42
2:3:661:GLN:O	2:3:665:GLU:HG2	2.19	0.42
3:4:245:ALA:HB3	3:4:308:VAL:HA	2.01	0.42
7:8:1472:GLU:HB3	7:8:1475:ARG:HD2	2.02	0.42
7:8:1695:LEU:HD11	8:9:499:ALA:HB2	2.01	0.42
9:A:186:ASP:HB3	13:E:478:TRP:CD1	2.55	0.42
14:F:597:PHE:HB3	14:F:610:GLU:HB3	2.01	0.42
15:I:84:LEU:HD12	15:I:135:MET:HE3	2.00	0.42
1:2:499:SER:HB3	1:2:509:ARG:HH12	1.84	0.42
2:3:203:ALA:O	2:3:207:GLY:HA2	2.19	0.42
5:6:268:PHE:HA	5:6:398:THR:HG21	2.02	0.42
5:6:365:ALA:HA	5:6:368:ILE:HD12	2.02	0.42
6:7:459:MET:HB2	6:7:597:LEU:HD12	2.01	0.42
7:8:1694:PRO:HD2	8:9:442:PRO:HG2	2.01	0.42
14:H:576:GLU:HG3	14:H:594:LEU:HG	2.01	0.42
15:I:137:TRP:O	15:I:160:GLN:NE2	2.52	0.42
1:2:402:LEU:HG	3:4:660:GLY:HA3	2.00	0.42
5:6:553:GLY:HA2	5:6:569:ILE:HD12	2.01	0.42
14:G:864:LYS:O	14:G:868:ARG:HG3	2.20	0.42
3:4:269:ILE:HA	3:4:272:MET:HE2	2.01	0.42
5:6:757:TYR:O	5:6:760:THR:OG1	2.32	0.42
15:I:699:ARG:HA	15:I:703:GLN:HG3	2.00	0.42
2:3:424:ASN:HD22	4:5:403:GLY:HA3	1.85	0.42
3:4:505:ASP:OD1	3:4:505:ASP:N	2.52	0.42
3:4:778:ARG:NH1	3:4:793:ALA:O	2.53	0.42
4:5:261:ILE:HG22	4:5:263:GLU:H	1.84	0.42
6:7:252:LYS:HD2	6:7:252:LYS:HA	1.77	0.42
21:O:30:ILE:HD13	21:O:30:ILE:HA	1.93	0.42
21:O:33:PRO:HA	21:O:36:ARG:HB2	2.00	0.42
1:2:73:LEU:HD12	21:S:40:ARG:HG3	2.02	0.42
3:4:339:ILE:HB	3:4:394:LYS:O	2.20	0.42
7:8:1952:GLU:OE2	7:8:2014:ARG:NH2	2.45	0.42
8:9:92:LYS:HB2	8:9:92:LYS:HE2	1.88	0.42
11:C:166:LEU:HD21	11:C:177:TYR:CZ	2.55	0.42
13:E:41:ALA:HB1	13:E:255:ILE:HD12	2.02	0.42
16:J:127:GLU:HA	16:J:130:VAL:HG22	2.01	0.42
18:L:728:ILE:HD13	18:L:741:HIS:HD2	1.84	0.42
2:3:98:ILE:HG13	2:3:155:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:712:VAL:HG21	6:7:668:ARG:HB3	2.02	0.42
5:6:280:ARG:HA	5:6:280:ARG:HD3	1.87	0.42
8:9:532:ILE:HG13	8:9:539:ILE:HB	2.02	0.42
14:H:519:ASP:N	14:H:519:ASP:OD1	2.50	0.42
1:2:530:LYS:HB3	4:5:428:PHE:HE1	1.84	0.41
3:4:701:ARG:NH2	27:6:1102:ADP:O2B	2.49	0.41
4:5:415:LEU:O	4:5:555:ILE:HA	2.19	0.41
6:7:451:ARG:HG2	6:7:453:ASP:H	1.84	0.41
6:7:596:ILE:HD12	6:7:598:PHE:HE2	1.85	0.41
7:8:1369:GLN:HG2	7:8:1370:LYS:H	1.85	0.41
9:A:68:ALA:O	9:A:72:TYR:HB2	2.20	0.41
14:F:536:LEU:HB2	14:F:547:GLY:O	2.19	0.41
14:G:652:LYS:NZ	14:G:713:PRO:O	2.53	0.41
2:3:408:VAL:HA	2:3:516:ALA:O	2.20	0.41
7:8:1439:MET:HE1	7:8:1687:LEU:HD11	2.02	0.41
8:9:468:LEU:HA	8:9:471:ARG:HH11	1.84	0.41
14:G:913:LYS:HE3	14:G:913:LYS:HB3	1.89	0.41
14:H:537:CYS:HA	14:H:545:LEU:O	2.20	0.41
2:3:22:GLY:O	2:3:26:ARG:HG2	2.21	0.41
3:4:402:THR:HA	3:4:403:PRO:HD3	1.94	0.41
3:4:692:ILE:HG22	3:4:694:LEU:H	1.85	0.41
4:5:722:LEU:HA	4:5:723:PRO:HD3	1.92	0.41
5:6:308:SER:HA	5:6:319:ASP:HA	2.03	0.41
7:8:2219:ASP:HA	7:8:2222:ILE:HG22	2.02	0.41
10:B:182:ARG:NH2	12:D:294:ILE:OXT	2.50	0.41
14:G:879:VAL:HG13	14:G:910:LEU:HG	2.02	0.41
10:B:73:LEU:HD12	10:B:76:ALA:HB3	2.02	0.41
12:D:5:ILE:HD11	14:F:868:ARG:HG3	2.01	0.41
12:D:98:ILE:HD11	12:D:130:GLU:HG3	2.02	0.41
14:F:704:LEU:HD22	14:F:752:LEU:HD13	2.01	0.41
15:I:161:LEU:HD11	15:I:217:PRO:HA	2.01	0.41
22:P:81:ILE:HG22	22:P:84:HIS:ND1	2.36	0.41
1:2:813:ILE:HG12	1:2:841:VAL:HG21	2.01	0.41
2:3:710:THR:O	2:3:713:ALA:HB3	2.20	0.41
3:4:245:ALA:O	3:4:248:LEU:HB2	2.21	0.41
3:4:428:ARG:NH2	5:6:370:THR:O	2.52	0.41
3:4:574:LYS:HD3	3:4:674:SER:HB2	2.02	0.41
4:5:104:LEU:HD23	4:5:104:LEU:HA	1.96	0.41
4:5:631:LYS:HA	4:5:634:LEU:HD23	2.01	0.41
6:7:484:THR:OG1	6:7:486:LYS:NZ	2.51	0.41
7:8:1328:LYS:HD3	7:8:1337:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:9:405:ASN:OD1	8:9:437:SER:OG	2.31	0.41
9:A:149:ILE:HG22	12:D:137:LYS:HG2	2.02	0.41
10:B:141:LEU:HD23	10:B:141:LEU:HA	1.94	0.41
15:I:621:LYS:NZ	25:Y:42:DT:OP1	2.54	0.41
25:Y:40:DT:H2"	25:Y:41:DA:C8	2.55	0.41
1:2:504:SER:HB3	5:6:563:ILE:HD12	2.03	0.41
1:2:799:SER:HB3	1:2:802:SER:HB3	2.03	0.41
6:7:534:ARG:O	6:7:538:HIS:CE1	2.74	0.41
7:8:1543:ILE:HD11	7:8:1640:LEU:HB3	2.03	0.41
9:A:97:LEU:HD23	9:A:97:LEU:HA	1.94	0.41
1:2:569:GLN:H	5:6:650:VAL:HG21	1.85	0.41
1:2:662:PRO:O	1:2:666:ASN:ND2	2.52	0.41
2:3:278:LEU:HD23	2:3:278:LEU:HA	1.91	0.41
4:5:152:ASP:N	4:5:152:ASP:OD1	2.53	0.41
4:5:755:LEU:HD13	4:5:761:ILE:HD12	2.02	0.41
7:8:1858:ILE:HA	7:8:1868:ILE:HA	2.03	0.41
13:E:44:MET:HE3	13:E:44:MET:HB2	1.93	0.41
15:I:347:LYS:HE2	15:I:347:LYS:HB3	1.91	0.41
1:2:82:TYR:CZ	21:S:37:ARG:HG2	2.55	0.41
2:3:172:THR:HG23	2:3:174:GLN:HG2	2.03	0.41
2:3:408:VAL:O	2:3:548:VAL:HA	2.20	0.41
3:4:356:MET:HE3	3:4:382:MET:HE1	2.02	0.41
4:5:733:LEU:O	4:5:737:PHE:HB2	2.21	0.41
6:7:231:LYS:HE3	6:7:231:LYS:HB3	1.96	0.41
8:9:659:ILE:HG22	8:9:673:MET:HE1	2.03	0.41
13:E:516:LYS:HG3	13:E:518:LEU:HG	2.03	0.41
15:I:275:LYS:HE2	15:I:275:LYS:HB2	1.82	0.41
15:I:329:THR:O	15:I:333:PHE:N	2.51	0.41
15:I:498:ILE:HD12	15:I:498:ILE:HA	1.93	0.41
1:2:382:TYR:HB3	4:5:153:SER:HB3	2.02	0.41
27:2:902:ADP:N3	5:6:797:VAL:HG21	2.36	0.41
3:4:758:ILE:HG13	3:4:813:LEU:HD22	2.02	0.41
4:5:42:SER:OG	10:B:142:ARG:NH1	2.53	0.41
4:5:717:GLU:O	4:5:721:ARG:CB	2.68	0.41
5:6:580:SER:HB3	27:6:1102:ADP:C8	2.55	0.41
7:8:1634:LYS:HE3	7:8:1634:LYS:HB2	1.86	0.41
7:8:1725:GLY:HA2	7:8:2064:LEU:HB3	2.03	0.41
8:9:35:SER:HA	9:A:175:GLN:HE22	1.86	0.41
10:B:105:GLU:HG2	10:B:113:SER:HB3	2.02	0.41
14:F:584:THR:HG21	14:F:643:LEU:HD11	2.02	0.41
14:G:510:GLN:HE21	14:G:529:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:76:MET:HE2	15:I:76:MET:HB3	1.82	0.41
18:L:610:GLU:O	18:L:615:GLU:N	2.50	0.41
18:L:878:PHE:HZ	22:P:87:LEU:HD23	1.86	0.41
21:S:74:THR:OG1	21:S:81:THR:O	2.30	0.41
3:4:767:LYS:HA	3:4:770:LEU:HD12	2.03	0.41
6:7:363:PHE:HE2	25:Y:15:DC:H5	1.69	0.41
6:7:648:LYS:NZ	6:7:704:LEU:HD22	2.35	0.41
9:A:192:ARG:HE	9:A:192:ARG:HB2	1.73	0.41
14:F:494:LEU:N	14:F:502:VAL:O	2.54	0.41
14:F:884:SER:OG	14:G:601:ASN:ND2	2.54	0.41
15:I:668:THR:HG22	15:I:670:PRO:HD2	2.02	0.41
20:N:68:PHE:HA	20:N:71:LEU:HD12	2.03	0.41
20:N:114:HIS:NE2	20:R:124:ASP:OD2	2.47	0.41
21:O:80:LYS:HA	21:O:80:LYS:HD2	1.94	0.41
3:4:321:ASP:HA	3:4:324:LYS:HD2	2.03	0.40
6:7:533:ASP:O	6:7:537:ILE:HG12	2.21	0.40
15:I:156:LEU:HD12	15:I:156:LEU:HA	1.87	0.40
18:L:708:GLN:HE21	18:L:713:THR:HA	1.86	0.40
21:O:55:VAL:HA	21:O:58:VAL:HG12	2.03	0.40
2:3:417:GLN:NE2	4:5:404:MET:SD	2.74	0.40
10:B:53:ILE:HD13	12:D:94:GLN:HG3	2.03	0.40
14:H:879:VAL:HG22	14:H:907:LEU:HD21	2.04	0.40
15:I:491:LYS:HB2	15:I:545:ARG:HH22	1.86	0.40
22:P:85:LEU:O	22:P:89:ILE:HG12	2.21	0.40
1:2:326:ARG:HH21	1:2:584:PRO:HD2	1.87	0.40
4:5:257:LYS:HE2	4:5:257:LYS:HB2	1.84	0.40
4:5:276:MET:HG2	4:5:328:ILE:HB	2.03	0.40
7:8:2101:LEU:HD21	7:8:2146:LEU:HD11	2.04	0.40
8:9:231:ARG:HD3	8:9:358:THR:HG21	2.02	0.40
8:9:403:GLY:HA2	8:9:661:PRO:HB2	2.02	0.40
10:B:160:LEU:HD23	10:B:160:LEU:HA	1.86	0.40
1:2:566:ALA:HB1	1:2:571:ALA:HB2	2.04	0.40
4:5:147:PRO:HG2	4:5:150:ASP:HB2	2.03	0.40
4:5:460:ARG:HG3	24:X:50:DT:H71	2.02	0.40
7:8:2143:GLN:O	7:8:2147:ILE:HG12	2.21	0.40
14:G:907:LEU:HD23	14:G:910:LEU:HD12	2.02	0.40
15:I:641:ARG:HA	15:I:644:ALA:HB3	2.02	0.40
24:X:21:DT:H2"	24:X:22:DA:C8	2.56	0.40
3:4:762:ILE:HD13	3:4:817:VAL:HG21	2.03	0.40
6:7:417:SER:HA	6:7:633:VAL:HG12	2.03	0.40
6:7:451:ARG:HH22	6:7:455:ASN:HD21	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:1386:ASN:C	7:8:1386:ASN:ND2	2.77	0.40
8:9:175:ALA:HB2	8:9:529:PRO:HG2	2.02	0.40
14:H:491:ARG:HD2	14:H:766:PHE:CG	2.55	0.40
15:I:78:VAL:HG13	15:I:83:ILE:HB	2.03	0.40
15:I:177:ARG:HA	15:I:180:ILE:HG12	2.04	0.40
15:I:477:LEU:HD23	15:I:477:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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 PDB entries followed by that with respect to all EM entries.

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	2	434/770 (56%)	434 (100%)	0	100	100
2	3	528/835 (63%)	528 (100%)	0	100	100
3	4	573/848 (68%)	573 (100%)	0	100	100
4	5	609/688 (88%)	609 (100%)	0	100	100
5	6	547/886 (62%)	547 (100%)	0	100	100
6	7	532/753 (71%)	532 (100%)	0	100	100
7	8	786/2014 (39%)	785 (100%)	1 (0%)	88	88
8	9	517/629 (82%)	517 (100%)	0	100	100
9	A	182/193 (94%)	182 (100%)	0	100	100
10	B	182/228 (80%)	182 (100%)	0	100	100
11	C	154/173 (89%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	232/279 (83%)	231 (100%)	1 (0%)	84	81
13	E	505/586 (86%)	505 (100%)	0	100	100
14	F	375/825 (46%)	375 (100%)	0	100	100
14	G	372/825 (45%)	372 (100%)	0	100	100
14	H	375/825 (46%)	375 (100%)	0	100	100
15	I	681/1125 (60%)	681 (100%)	0	100	100
16	J	87/285 (30%)	87 (100%)	0	100	100
17	K	19/1003 (2%)	19 (100%)	0	100	100
18	L	297/935 (32%)	297 (100%)	0	100	100
20	N	67/113 (59%)	67 (100%)	0	100	100
20	R	79/113 (70%)	79 (100%)	0	100	100
21	O	63/81 (78%)	63 (100%)	0	100	100
21	S	72/81 (89%)	72 (100%)	0	100	100
22	P	71/99 (72%)	71 (100%)	0	100	100
23	Q	79/110 (72%)	79 (100%)	0	100	100
All	All	8418/15302 (55%)	8416 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	8	1386	ASN
12	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	439	ASN
1	2	651	ASN
1	2	849	GLN
2	3	29	GLN
2	3	151	HIS
2	3	164	HIS
2	3	293	ASN
2	3	424	ASN
2	3	492	GLN
2	3	531	GLN

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Mol	Chain	Res	Type
2	3	682	ASN
2	3	688	ASN
3	4	465	HIS
3	4	912	GLN
4	5	33	ASN
4	5	58	ASN
4	5	64	ASN
4	5	185	ASN
4	5	245	HIS
4	5	344	ASN
4	5	363	ASN
4	5	514	ASN
4	5	576	HIS
4	5	587	GLN
4	5	652	GLN
4	5	769	ASN
5	6	514	ASN
5	6	540	HIS
5	6	669	HIS
6	7	19	ASN
6	7	30	GLN
6	7	112	HIS
6	7	264	GLN
6	7	379	GLN
6	7	455	ASN
6	7	538	HIS
6	7	544	GLN
7	8	1587	GLN
7	8	1638	HIS
7	8	1708	ASN
7	8	1780	HIS
7	8	1864	ASN
7	8	1975	ASN
7	8	2021	ASN
8	9	179	GLN
8	9	226	ASN
8	9	280	GLN
8	9	478	ASN
9	A	58	GLN
9	A	82	ASN
9	A	90	GLN
9	A	122	ASN

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Mol	Chain	Res	Type
9	A	128	GLN
9	A	201	GLN
9	A	202	GLN
10	B	82	GLN
10	B	135	HIS
10	B	153	GLN
10	B	169	GLN
10	B	179	ASN
13	E	133	ASN
13	E	273	ASN
13	E	604	ASN
13	E	610	GLN
13	E	611	GLN
14	F	548	GLN
14	F	673	ASN
14	F	761	HIS
14	F	915	ASN
14	G	510	GLN
14	G	555	GLN
14	G	563	HIS
14	G	843	ASN
14	G	878	ASN
14	H	850	ASN
14	H	852	ASN
15	I	97	ASN
15	I	108	ASN
15	I	130	GLN
15	I	344	GLN
15	I	399	ASN
15	I	406	HIS
15	I	407	GLN
15	I	436	HIS
15	I	450	ASN
15	I	454	HIS
15	I	472	GLN
15	I	550	GLN
18	L	492	GLN
18	L	500	ASN
18	L	741	HIS
18	L	756	GLN
18	L	793	GLN
18	L	827	ASN

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Mol	Chain	Res	Type
18	L	893	ASN
18	L	900	ASN
18	L	938	GLN
22	P	91	ASN
20	R	77	GLN
20	R	114	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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$
27	ADP	6	1102	-	28,29,29	1.44	4 (14%)	43,45,45	1.82	8 (18%)
27	ADP	2	902	-	28,29,29	1.38	4 (14%)	43,45,45	1.87	9 (20%)
27	ADP	3	1001	-	28,29,29	1.34	5 (17%)	43,45,45	1.89	10 (23%)
27	ADP	5	802	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
27	ADP	7	902	-	28,29,29	1.42	5 (17%)	43,45,45	1.81	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	ADP	6	1102	-	-	3/16/32/32	0/3/3/3
27	ADP	2	902	-	-	4/16/32/32	0/3/3/3
27	ADP	3	1001	-	-	7/16/32/32	0/3/3/3
27	ADP	5	802	-	-	3/16/32/32	0/3/3/3
27	ADP	7	902	-	-	4/16/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	1102	ADP	C5-C4	4.78	1.47	1.39
27	5	802	ADP	C5-C4	4.72	1.47	1.39
27	7	902	ADP	C5-C4	4.66	1.47	1.39
27	2	902	ADP	C5-C4	4.51	1.47	1.39
27	3	1001	ADP	C5-C4	4.32	1.46	1.39
27	7	902	ADP	C5-C6	2.75	1.48	1.41
27	2	902	ADP	C5-C6	2.71	1.48	1.41
27	6	1102	ADP	C5-C6	2.71	1.48	1.41
27	5	802	ADP	C5-C6	2.65	1.48	1.41
27	2	902	ADP	C8-N7	2.41	1.36	1.31
27	3	1001	ADP	C5-C6	2.38	1.47	1.41
27	5	802	ADP	C5-N7	-2.37	1.34	1.39
27	3	1001	ADP	C5-N7	-2.37	1.34	1.39
27	6	1102	ADP	C5-N7	-2.36	1.34	1.39
27	7	902	ADP	C8-N7	2.33	1.36	1.31
27	6	1102	ADP	C8-N7	2.31	1.36	1.31
27	2	902	ADP	C5-N7	-2.30	1.34	1.39
27	5	802	ADP	C8-N7	2.25	1.36	1.31
27	7	902	ADP	C5-N7	-2.23	1.35	1.39
27	3	1001	ADP	C4-N9	-2.12	1.33	1.37
27	3	1001	ADP	C8-N7	2.11	1.35	1.31
27	7	902	ADP	PA-O3A	2.00	1.61	1.59

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	902	ADP	C5-C4-N3	-6.04	118.40	126.72
27	5	802	ADP	C5-C4-N3	-5.86	118.65	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	6	1102	ADP	C5-C4-N3	-5.81	118.72	126.72
27	7	902	ADP	C5-C4-N3	-5.80	118.74	126.72
27	3	1001	ADP	C5-C4-N3	-5.49	119.16	126.72
27	3	1001	ADP	N3-C4-N9	4.68	135.13	127.17
27	5	802	ADP	N3-C4-N9	4.65	135.07	127.17
27	2	902	ADP	N3-C4-N9	4.59	134.98	127.17
27	6	1102	ADP	N3-C4-N9	4.59	134.97	127.17
27	7	902	ADP	N3-C4-N9	4.56	134.92	127.17
27	2	902	ADP	C2-N3-C4	4.00	121.61	111.83
27	7	902	ADP	C2-N3-C4	3.73	120.94	111.83
27	6	1102	ADP	C2-N3-C4	3.64	120.72	111.83
27	5	802	ADP	C2-N3-C4	3.63	120.71	111.83
27	3	1001	ADP	C2-N3-C4	3.62	120.68	111.83
27	2	902	ADP	N3-C2-N1	-3.52	123.25	128.58
27	2	902	ADP	C4-C5-N7	-3.49	106.59	110.58
27	7	902	ADP	C4-C5-N7	-3.47	106.61	110.58
27	6	1102	ADP	C4-C5-N7	-3.38	106.72	110.58
27	3	1001	ADP	N3-C2-N1	-3.37	123.49	128.58
27	5	802	ADP	C4-C5-N7	-3.36	106.73	110.58
27	3	1001	ADP	O4'-C1'-N9	3.31	114.45	108.09
27	7	902	ADP	N3-C2-N1	-3.30	123.59	128.58
27	6	1102	ADP	N3-C2-N1	-3.15	123.82	128.58
27	5	802	ADP	N3-C2-N1	-3.11	123.88	128.58
27	3	1001	ADP	C4-N9-C8	3.09	108.98	105.74
27	6	1102	ADP	C3'-C2'-C1'	2.81	106.78	101.46
27	3	1001	ADP	C4-C5-N7	-2.79	107.39	110.58
27	5	802	ADP	C3'-C2'-C1'	2.65	106.48	101.46
27	7	902	ADP	C4-N9-C8	2.61	108.47	105.74
27	2	902	ADP	O4'-C1'-N9	2.58	113.05	108.09
27	7	902	ADP	C5-N7-C8	2.52	107.41	103.45
27	2	902	ADP	C5-N7-C8	2.47	107.33	103.45
27	6	1102	ADP	C4-N9-C8	2.45	108.31	105.74
27	5	802	ADP	C4-N9-C8	2.43	108.29	105.74
27	6	1102	ADP	C5-N7-C8	2.41	107.24	103.45
27	2	902	ADP	C4-N9-C8	2.41	108.27	105.74
27	5	802	ADP	C5-N7-C8	2.39	107.20	103.45
27	2	902	ADP	C6-C5-N7	2.27	136.47	132.09
27	3	1001	ADP	C5-N7-C8	2.23	106.95	103.45
27	7	902	ADP	C6-C5-N7	2.15	136.23	132.09
27	3	1001	ADP	N9-C8-N7	-2.09	110.97	113.94
27	7	902	ADP	C3'-C2'-C1'	2.06	105.35	101.46
27	3	1001	ADP	C2'-C3'-C4'	2.03	106.53	102.61

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	902	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C5'-O5'-PA-O2A
27	3	1001	ADP	C5'-O5'-PA-O3A
27	5	802	ADP	C5'-O5'-PA-O3A
27	6	1102	ADP	C5'-O5'-PA-O3A
27	7	902	ADP	C3'-C4'-C5'-O5'
27	7	902	ADP	C2'-C1'-N9-C8
27	7	902	ADP	O4'-C4'-C5'-O5'
27	2	902	ADP	C2'-C1'-N9-C4
27	7	902	ADP	C2'-C1'-N9-C4
27	2	902	ADP	C2'-C1'-N9-C8
27	3	1001	ADP	C2'-C1'-N9-C8
27	2	902	ADP	C5'-O5'-PA-O3A
27	5	802	ADP	C5'-O5'-PA-O1A
27	6	1102	ADP	C5'-O5'-PA-O1A
27	3	1001	ADP	C2'-C1'-N9-C4
27	3	1001	ADP	O4'-C1'-N9-C8
27	5	802	ADP	O4'-C4'-C5'-O5'
27	6	1102	ADP	O4'-C4'-C5'-O5'
27	3	1001	ADP	C4'-C5'-O5'-PA

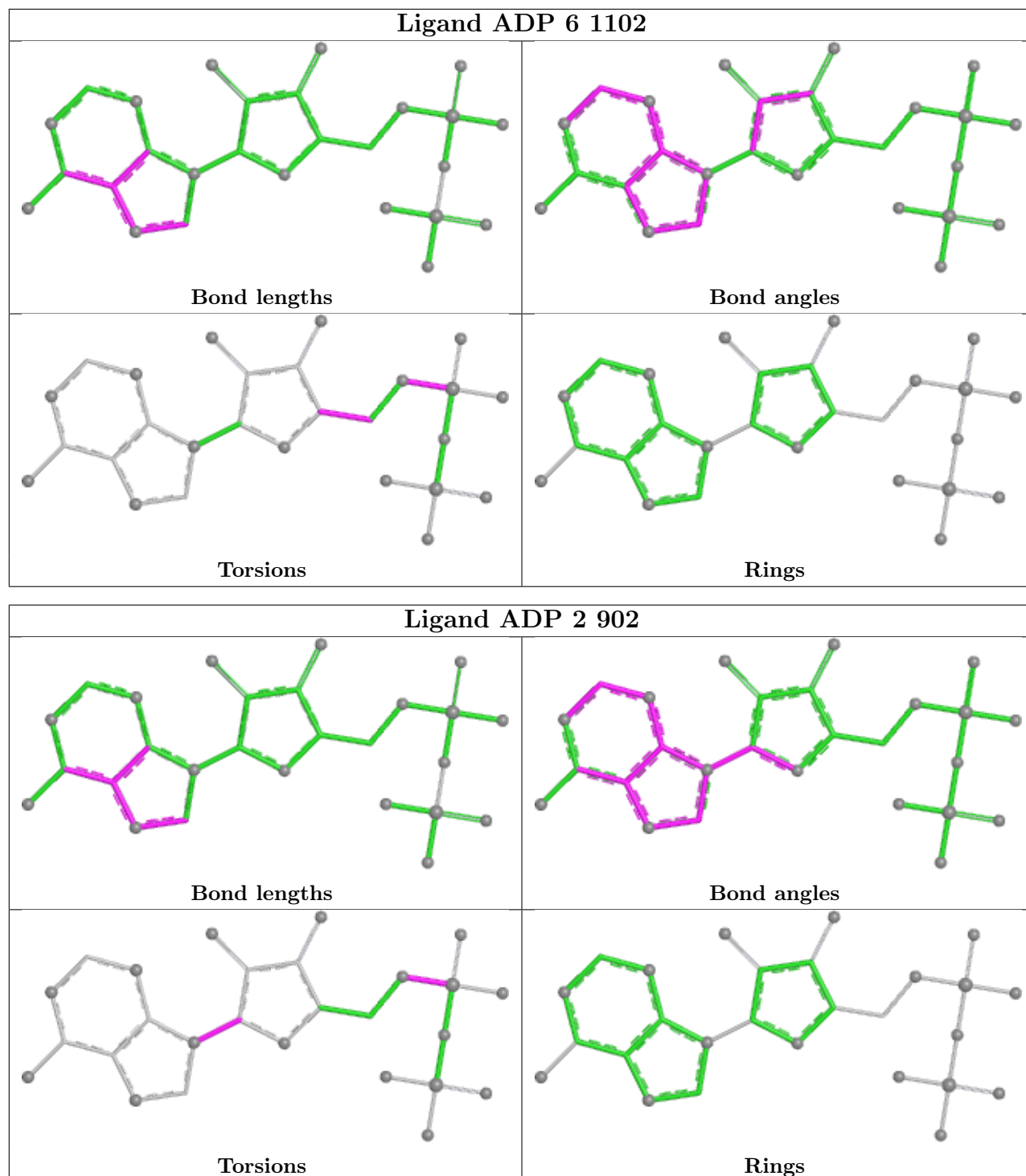
There are no ring outliers.

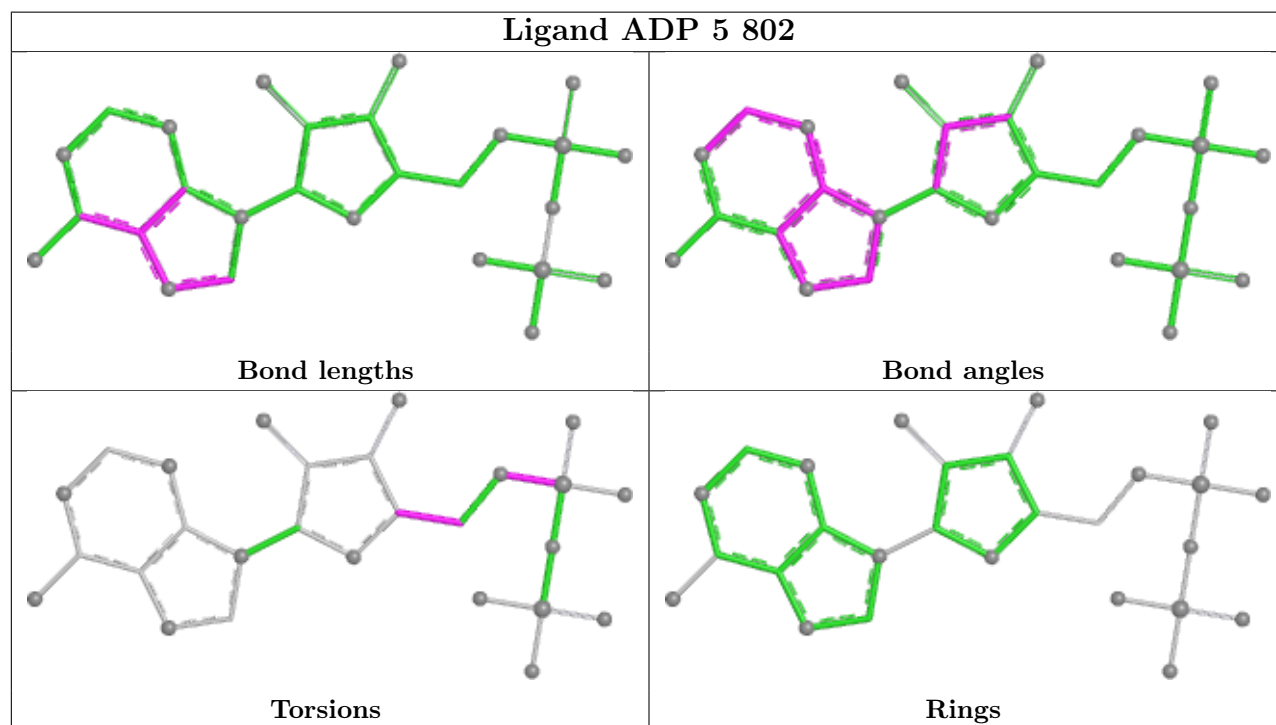
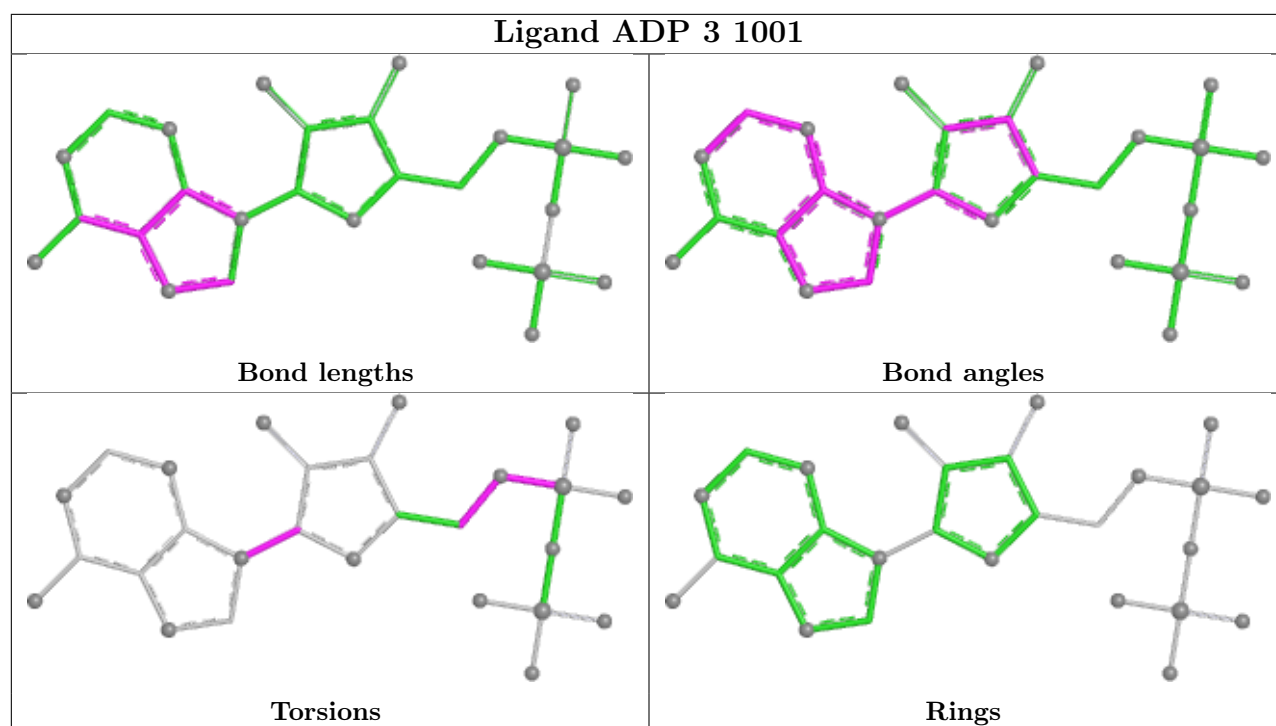
4 monomers are involved in 8 short contacts:

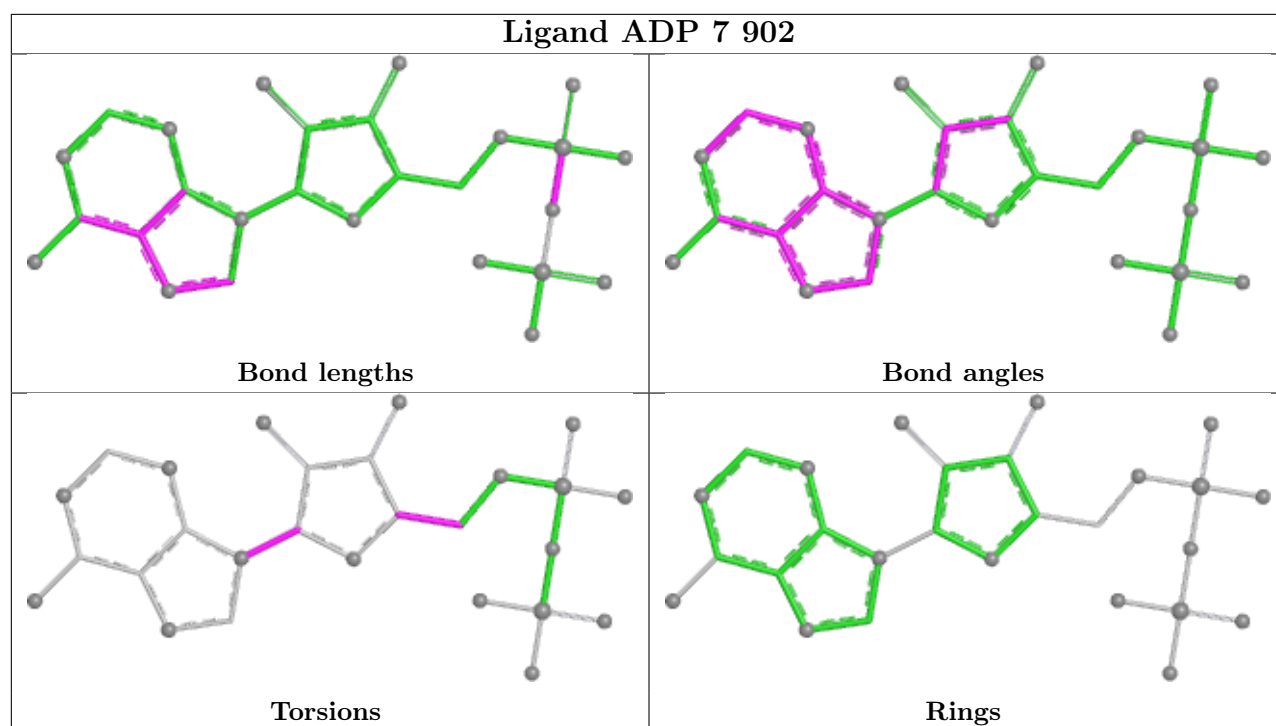
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	1102	ADP	2	0
27	2	902	ADP	1	0
27	3	1001	ADP	3	0
27	7	902	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.

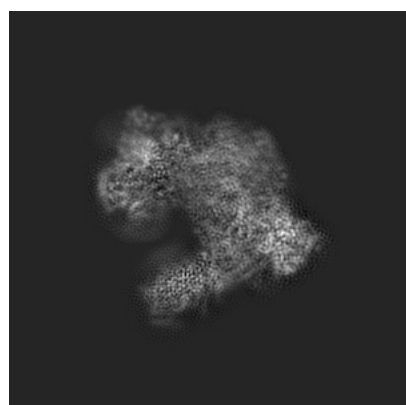
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38317. These allow visual inspection of the internal detail of the map and identification of artifacts.

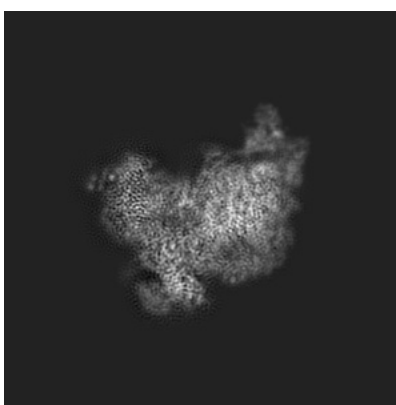
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

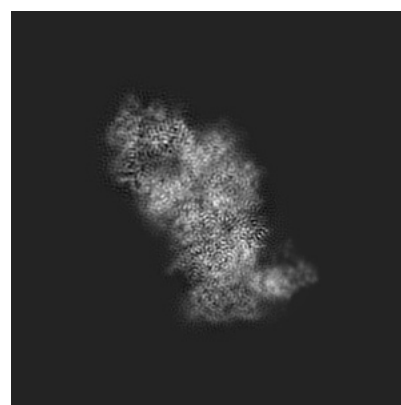
6.1.1 Primary map



X



Y

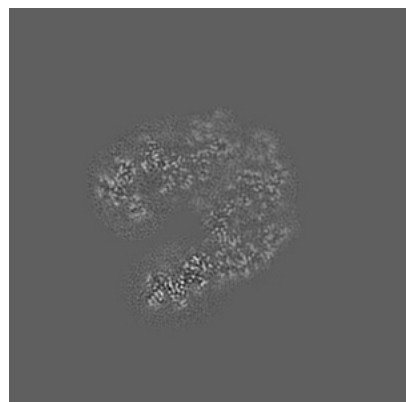


Z

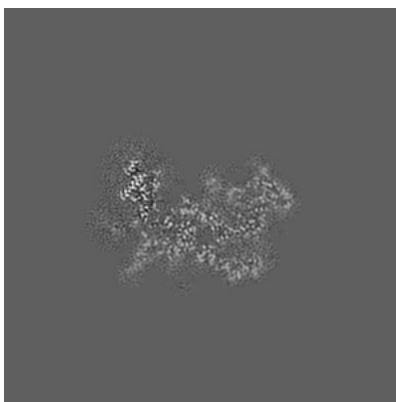
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

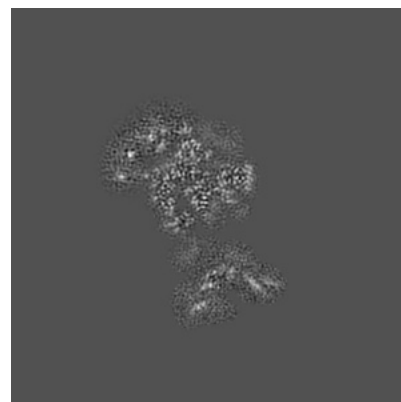
6.2.1 Primary map



X Index: 200



Y Index: 200

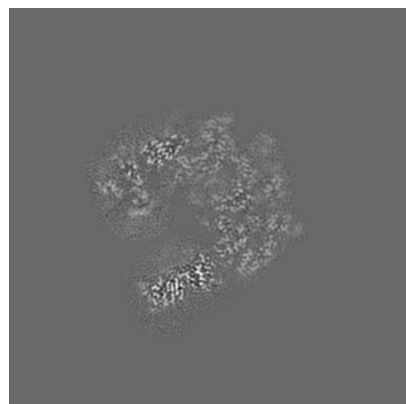


Z Index: 200

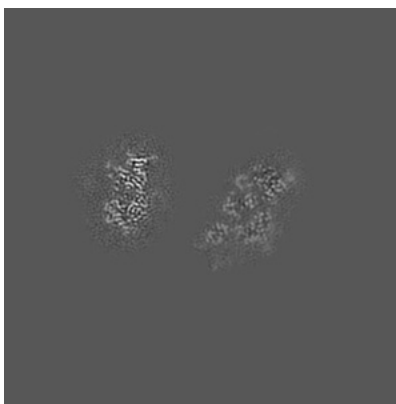
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

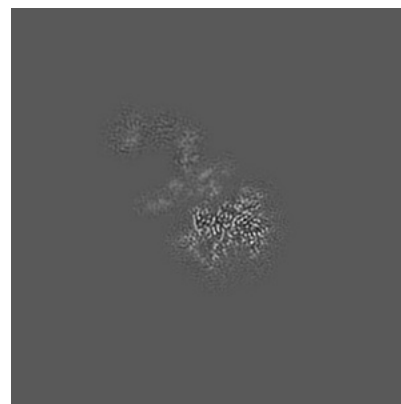
6.3.1 Primary map



X Index: 211



Y Index: 174

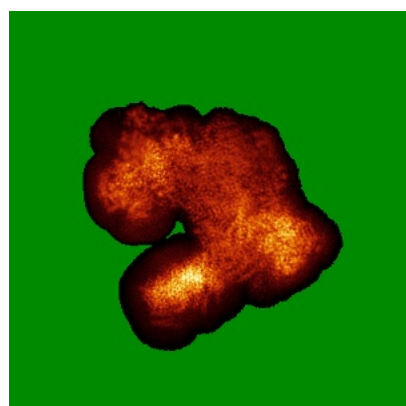


Z Index: 132

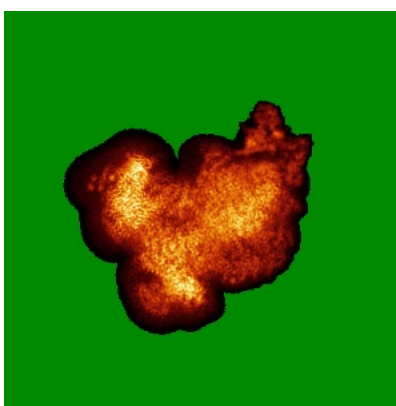
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

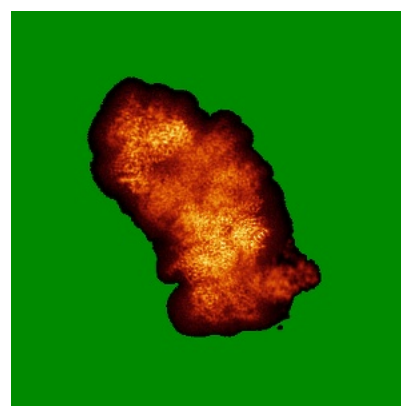
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

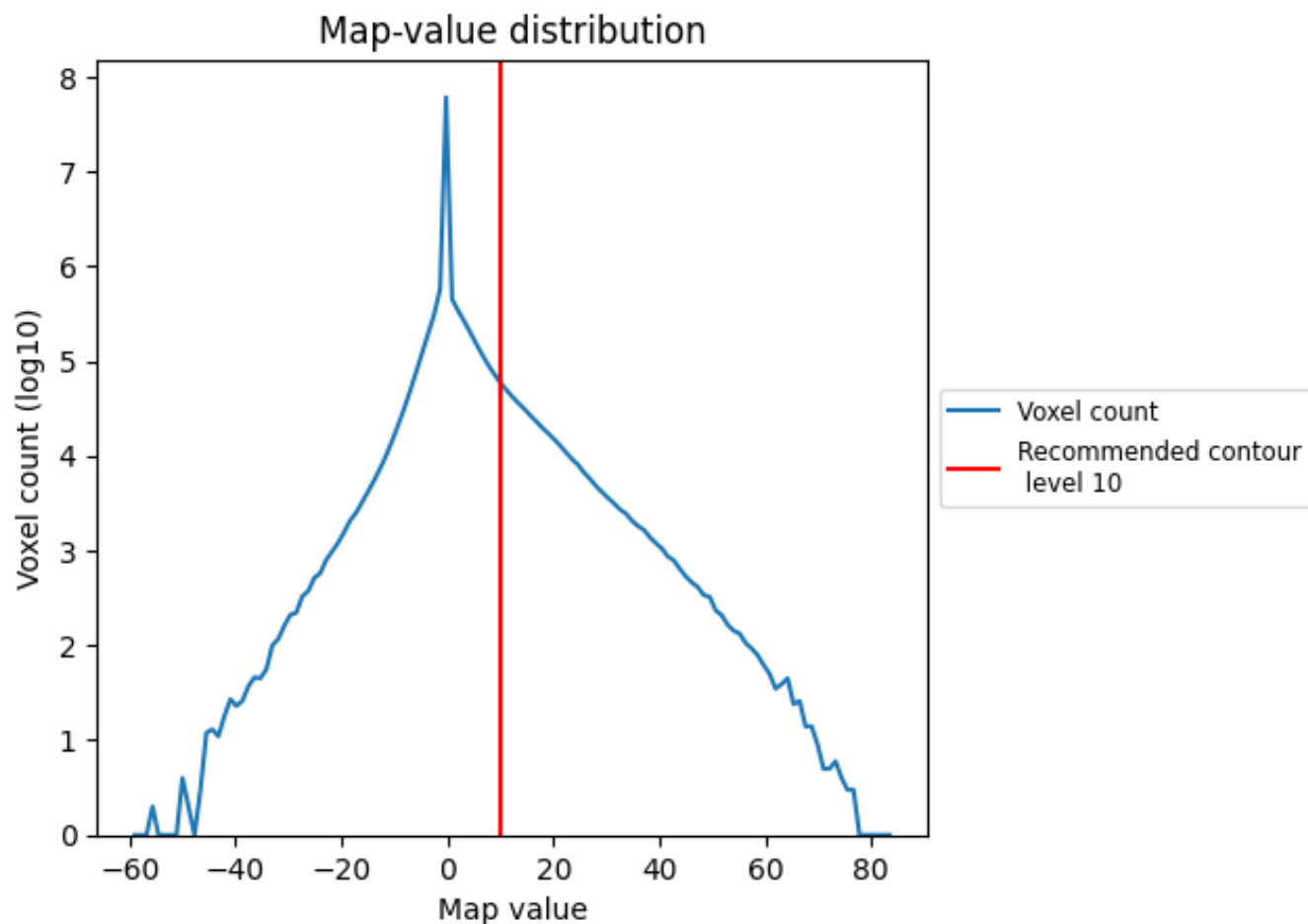
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

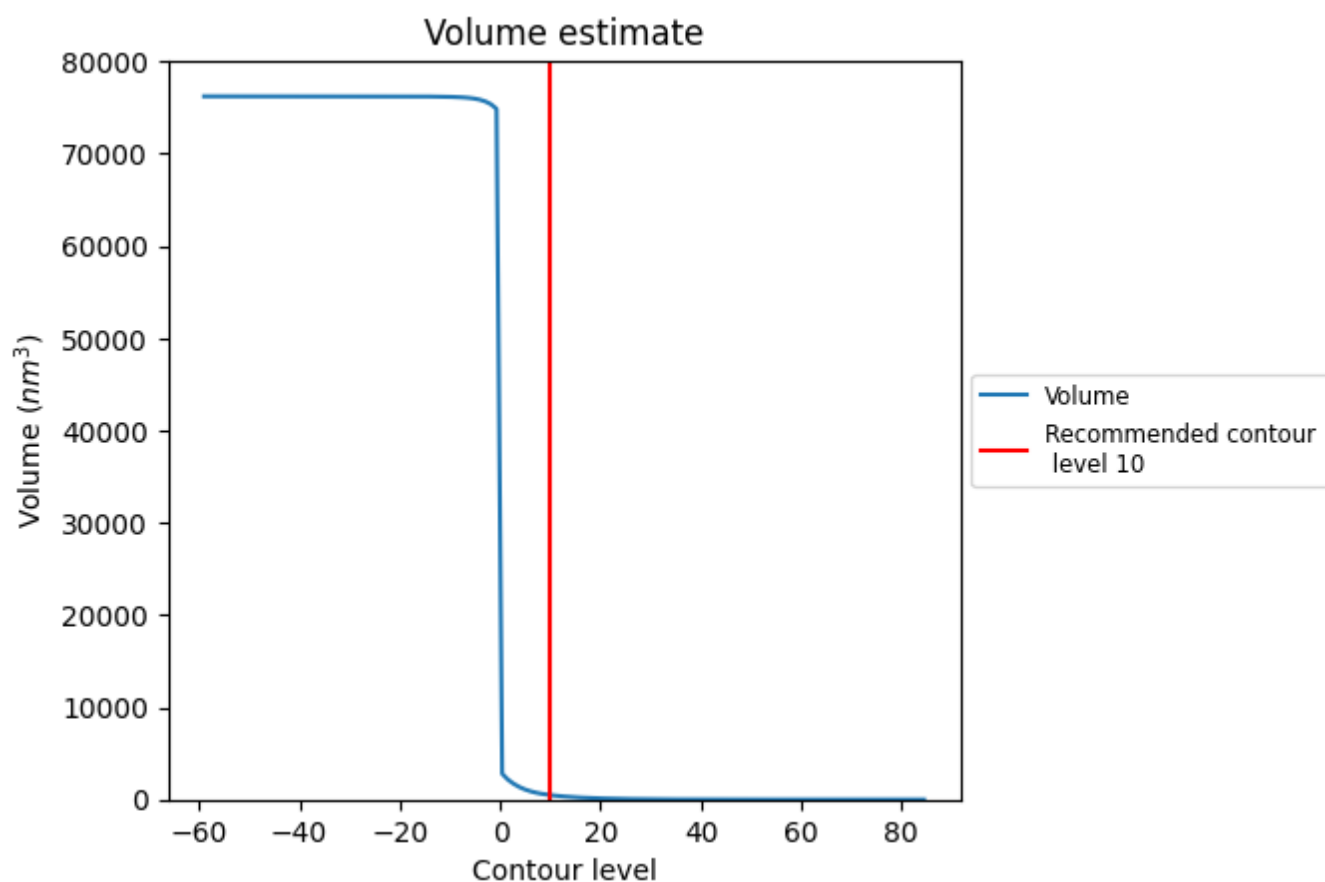
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

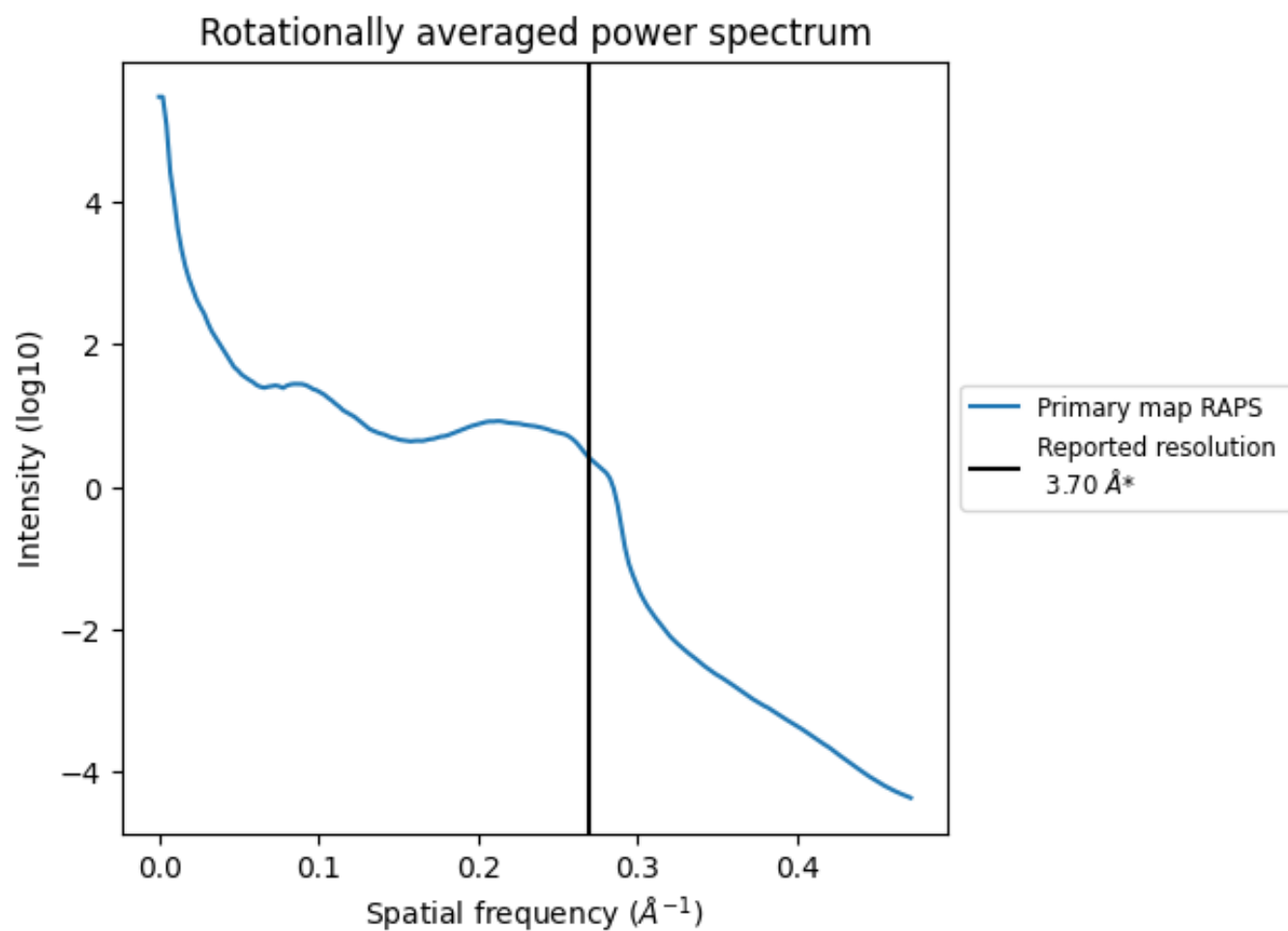
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 489 nm³; this corresponds to an approximate mass of 441 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

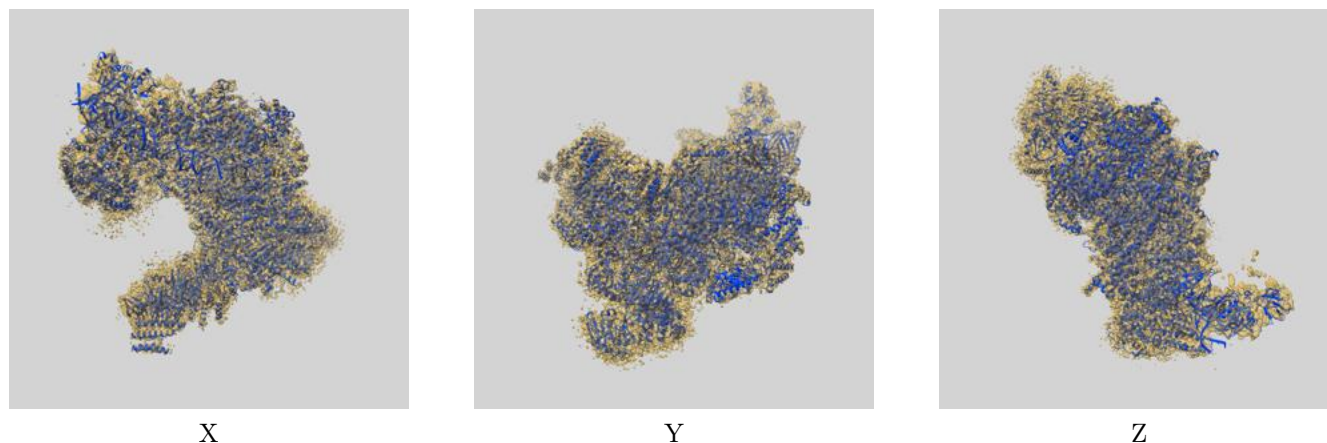
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

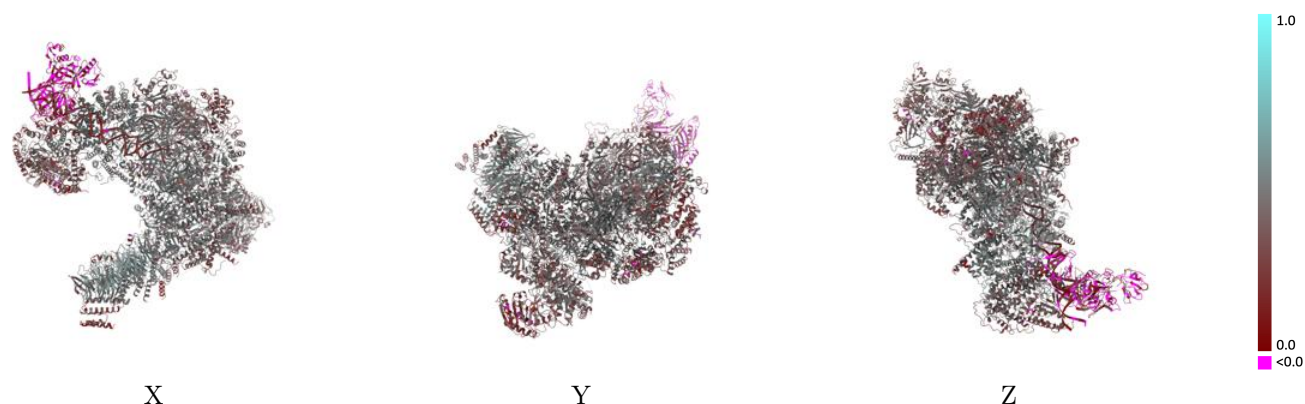
This section contains information regarding the fit between EMDB map EMD-38317 and PDB model 8XGC. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



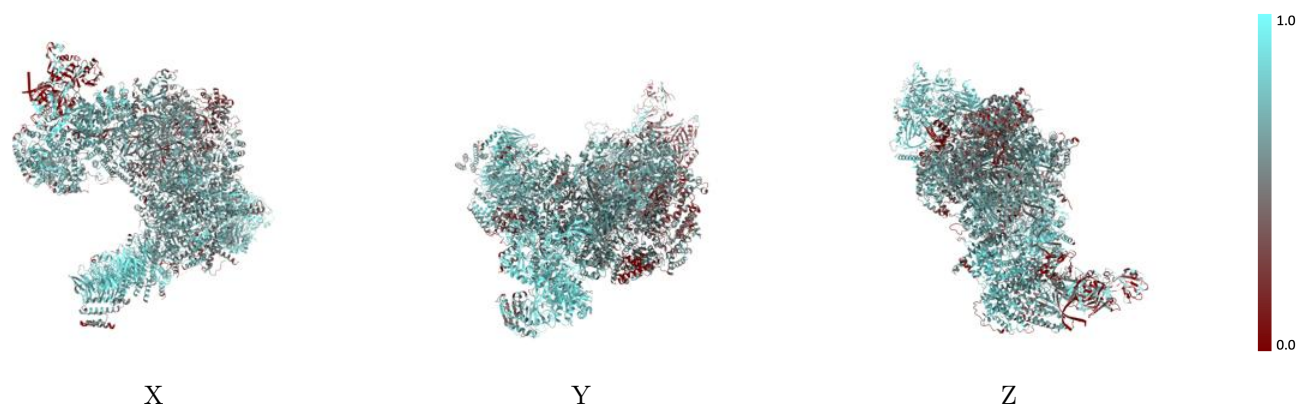
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



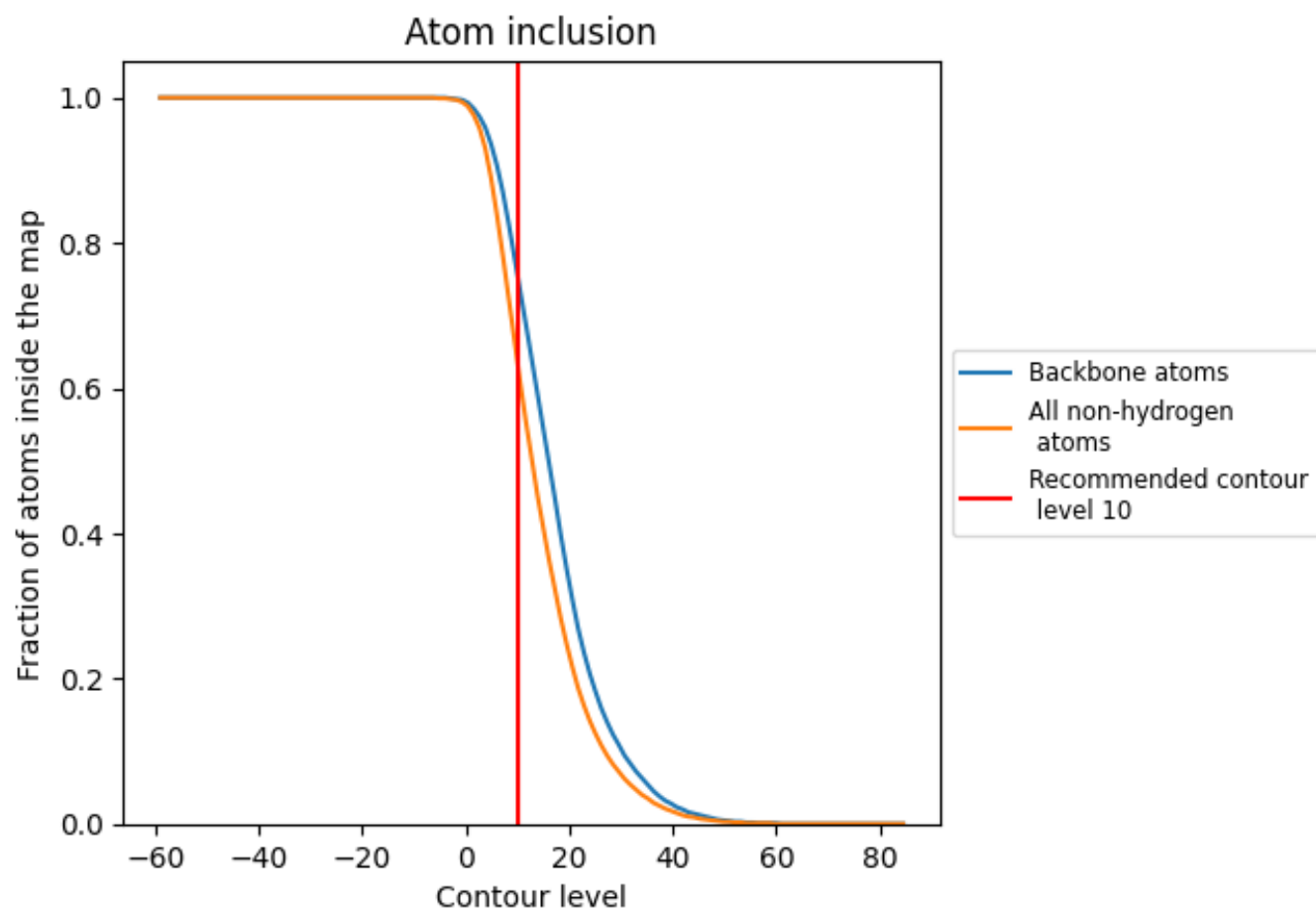
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6350	 0.4070
2	 0.6040	 0.4400
3	 0.6070	 0.4410
4	 0.4860	 0.3860
5	 0.6120	 0.4410
6	 0.6120	 0.4360
7	 0.4530	 0.3750
8	 0.7690	 0.3780
9	 0.7160	 0.3940
A	 0.5960	 0.4030
B	 0.6810	 0.4620
C	 0.6510	 0.4430
D	 0.6210	 0.4240
E	 0.6110	 0.4400
F	 0.7750	 0.4910
G	 0.7560	 0.4550
H	 0.7960	 0.4740
I	 0.7150	 0.4640
J	 0.6910	 0.4390
K	 0.4660	 0.3630
L	 0.5920	 0.2970
M	 0.2960	 0.0490
N	 0.6430	 0.3600
O	 0.6640	 0.3510
P	 0.7190	 0.4000
Q	 0.7140	 0.3890
R	 0.7400	 0.4220
S	 0.7320	 0.4500
X	 0.4680	 0.1960
Y	 0.4420	 0.1650

