



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 07:25 PM JST

PDB ID : 9KCF / pdb\_00009kcf  
EMDB ID : EMD-62249  
Title : Bovine Flagellar TRiC  
Authors : Cong, Y.; Meng, X.  
Deposited on : 2024-11-01  
Resolution : 3.40 Å(reported)  
Based on initial models : 4A0V, .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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

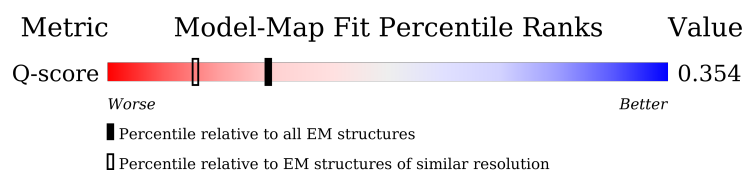
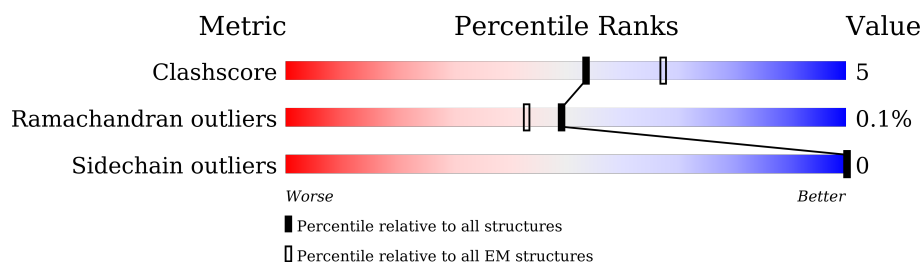
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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.



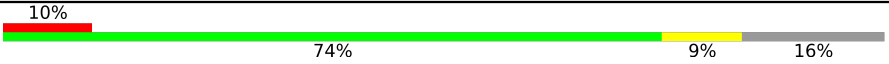
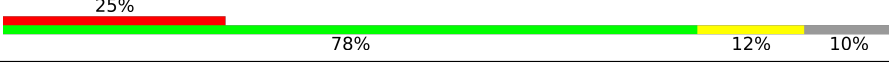



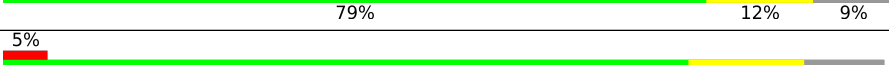
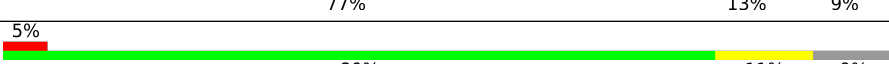
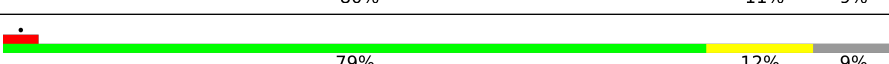
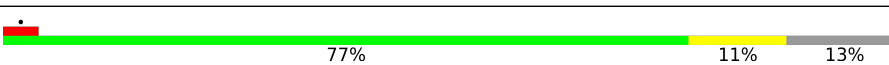
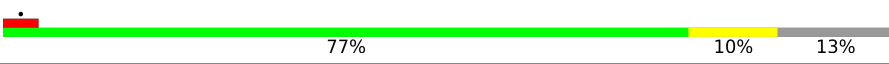


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 ( 2.90 - 3.90 )

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  $\geq 3$ , 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	A	531	
2	F	543	
2	N	543	
3	H	556	

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Mol	Chain	Length	Quality of chain
3	I	556	
4	B	535	
4	J	535	
5	C	545	
5	K	545	
6	D	542	
6	L	542	
7	E	541	
7	M	541	
8	G	548	
8	O	548	
9	P	531	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ADP	A	602	-	-	X	-
11	ADP	G	602	-	-	X	-
11	ADP	K	602	-	-	X	-
11	ADP	O	602	-	-	X	-
11	ADP	P	602	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 58930 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 Probable T-complex protein 1 subunit zeta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	484	Total	C	N	O	S	0	0
			3713	2342	656	695	20		

- Molecule 2 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	470	Total	C	N	O	S	0	0
			3603	2283	622	673	25		
2	N	476	Total	C	N	O	S	0	0
			3652	2312	630	685	25		

- Molecule 3 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	465	Total	C	N	O	S	0	0
			3523	2212	620	671	20		
3	I	465	Total	C	N	O	S	0	0
			3523	2212	620	671	20		

- Molecule 4 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	479	Total	C	N	O	S	0	0
			3599	2258	630	693	18		
4	J	479	Total	C	N	O	S	0	0
			3599	2258	630	693	18		

- Molecule 5 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	487	Total	C	N	O	S	0	0
			3783	2362	670	723	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	487	Total	C	N	O	S	0	0
			3783	2362	670	723	28		

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	491	Total	C	N	O	S	0	0
			3698	2316	641	720	21		
6	L	491	Total	C	N	O	S	0	0
			3698	2316	641	720	21		

- Molecule 7 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	490	Total	C	N	O	S	0	0
			3762	2353	660	720	29		
7	M	490	Total	C	N	O	S	0	0
			3762	2353	660	720	29		

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	479	Total	C	N	O	S	0	0
			3662	2306	625	707	24		
8	O	479	Total	C	N	O	S	0	0
			3662	2306	625	707	24		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	489	Total	C	N	O	S	0	0
			3740	2352	654	714	20		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

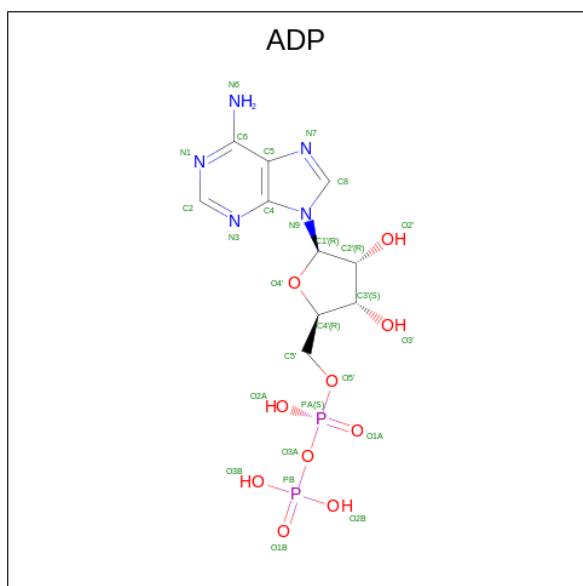
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
10	G	1	Total	Mg	0
			1	1	
10	K	1	Total	Mg	0
			1	1	
10	O	1	Total	Mg	0
			1	1	
10	P	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

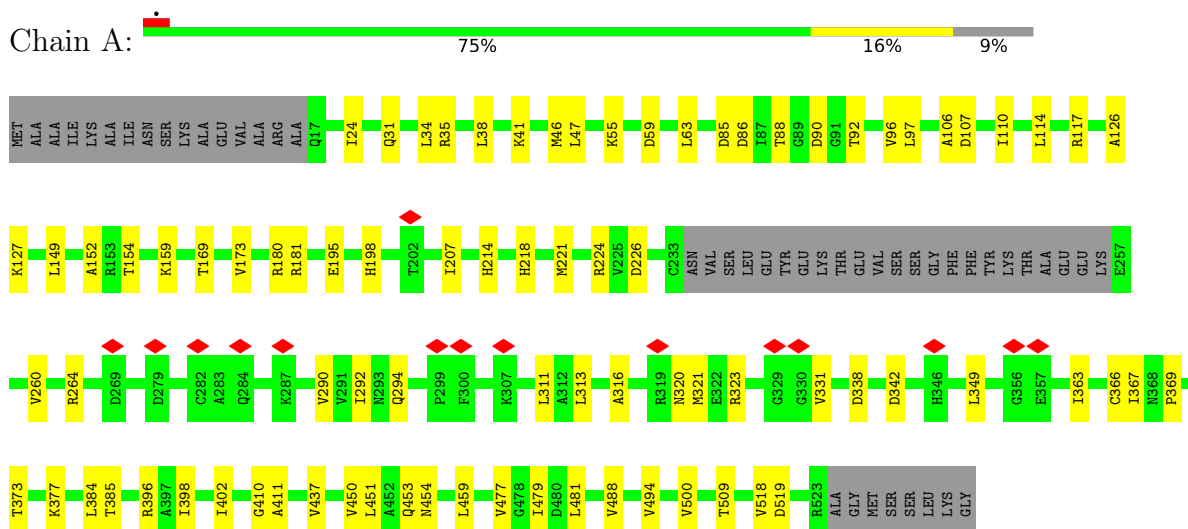


Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	P	1	Total	C	N	O	P	0
			27	10	5	10	2	

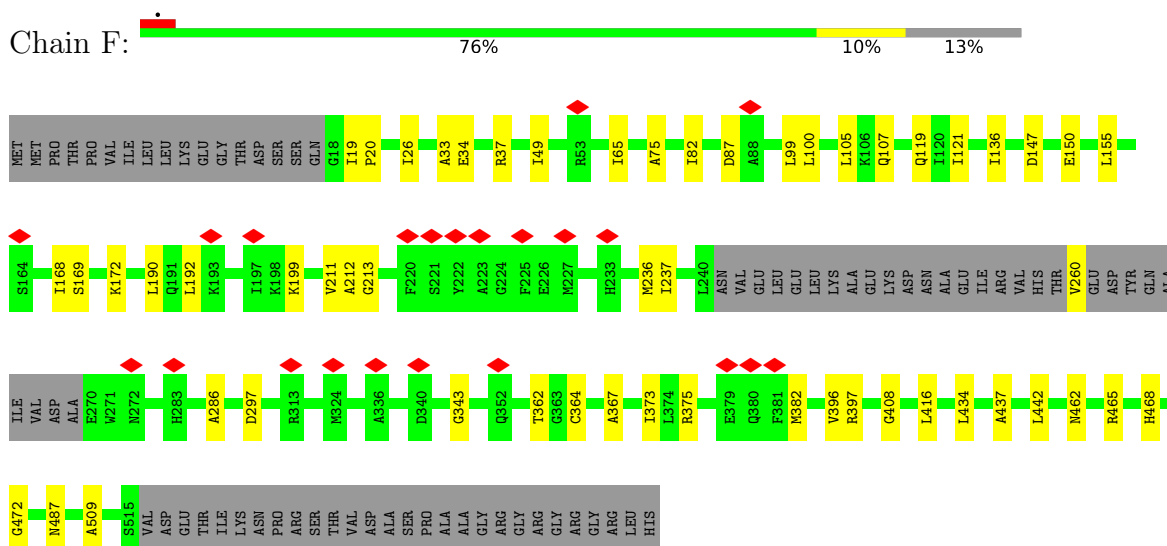
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

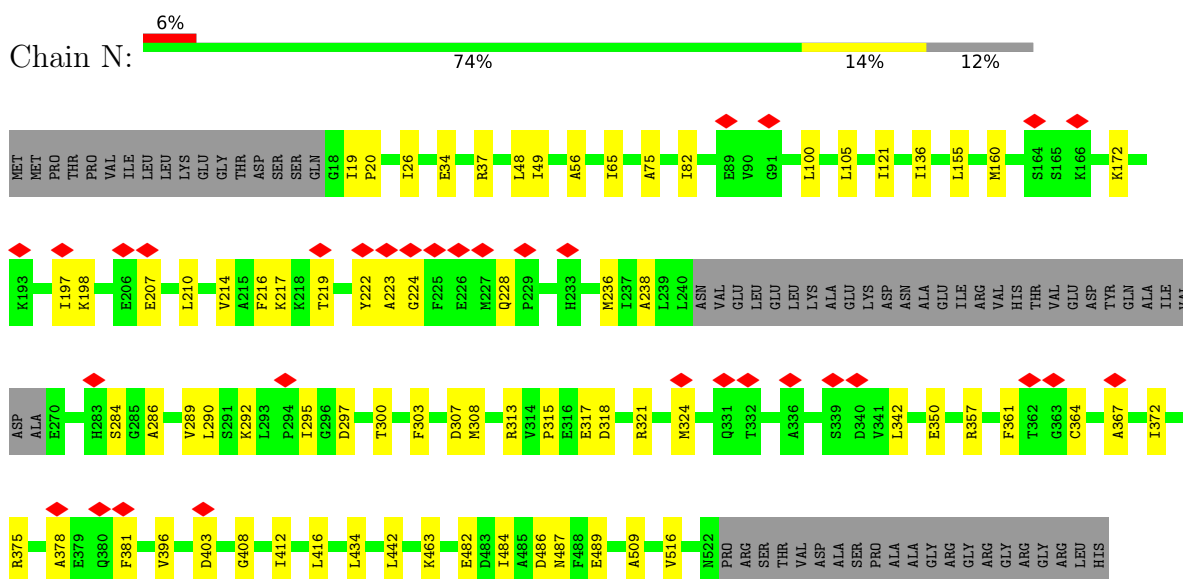
- Molecule 1: Probable T-complex protein 1 subunit zeta-2



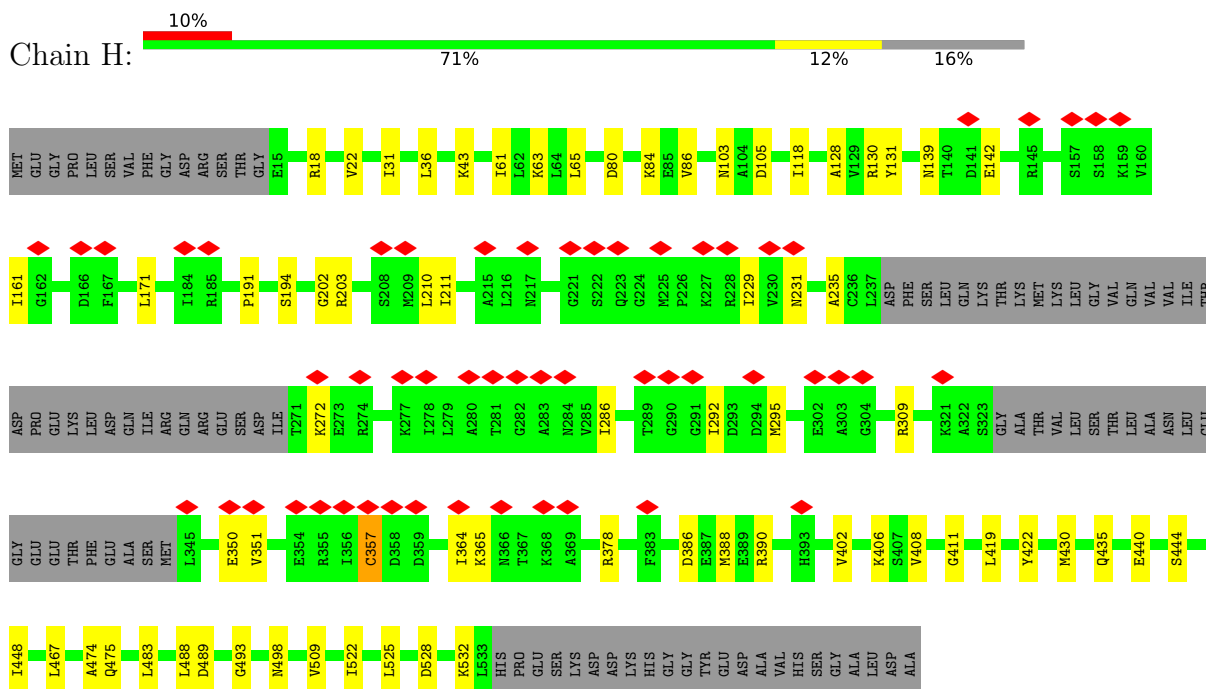
- Molecule 2: T-complex protein 1 subunit eta



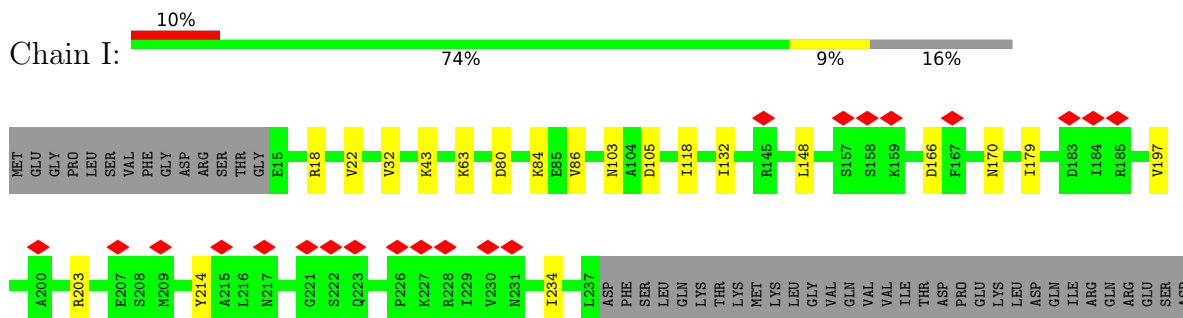
- Molecule 2: T-complex protein 1 subunit eta



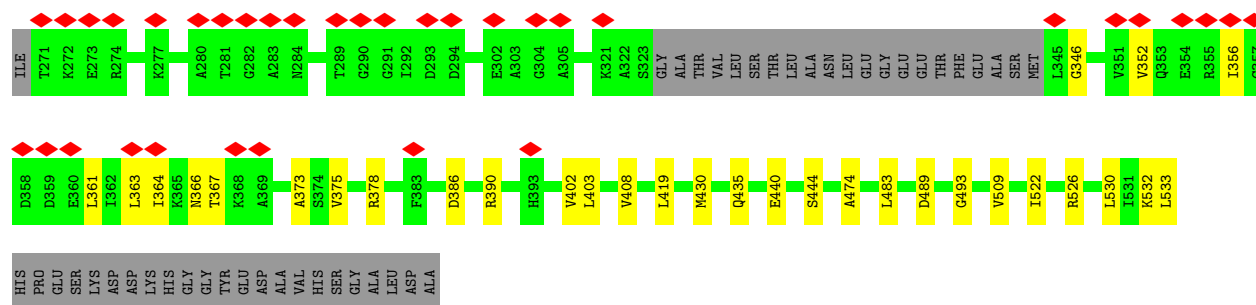
- Molecule 3: T-complex protein 1 subunit alpha



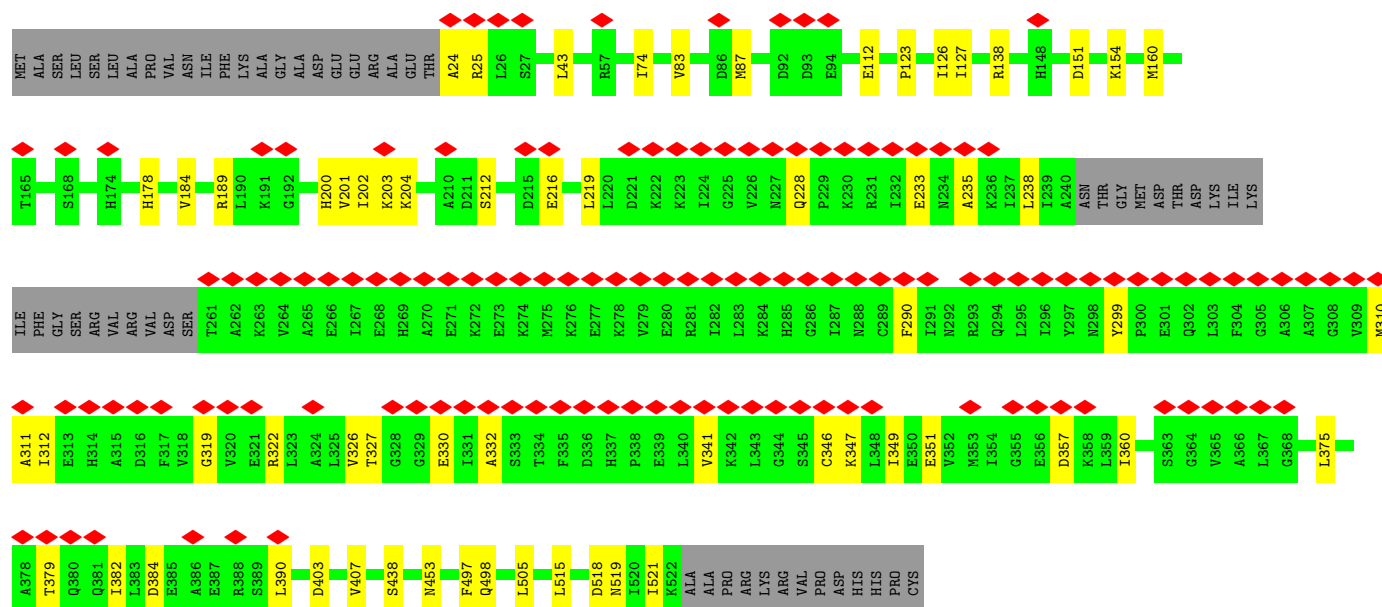
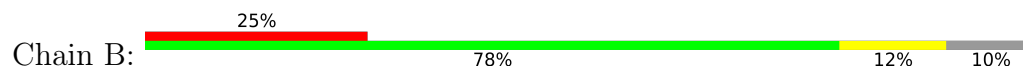
- Molecule 3: T-complex protein 1 subunit alpha



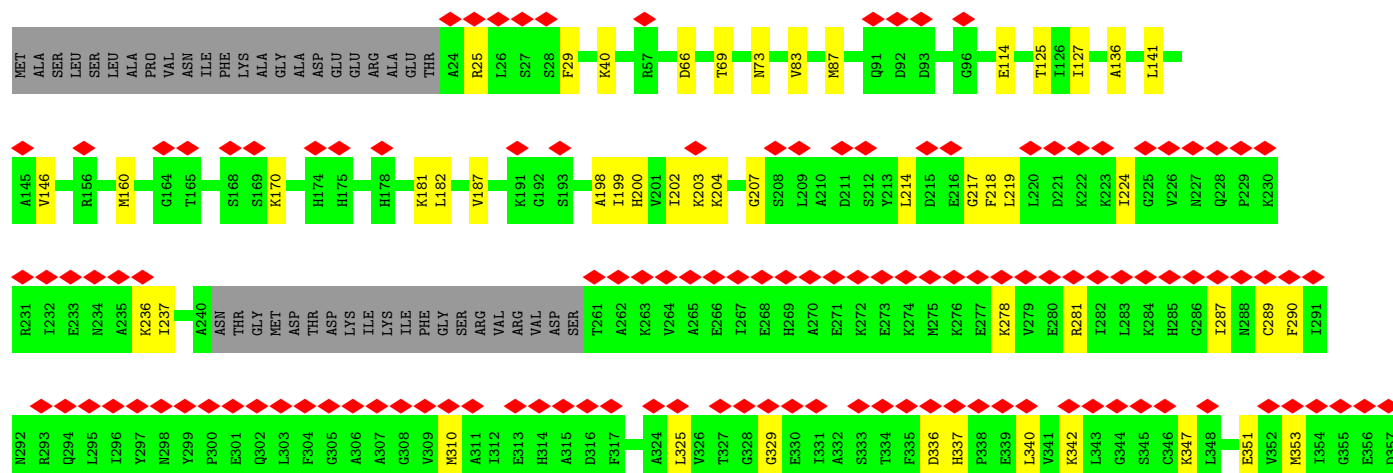
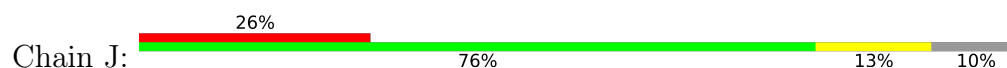


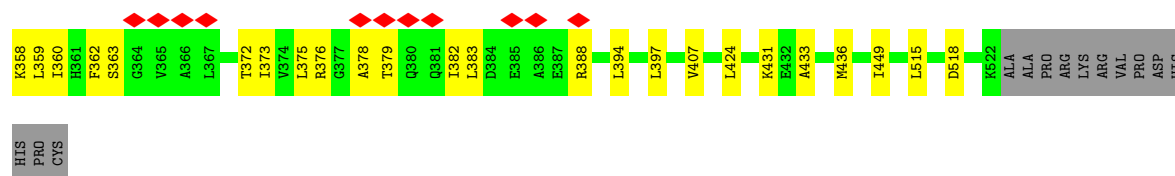


• Molecule 4: T-complex protein 1 subunit beta

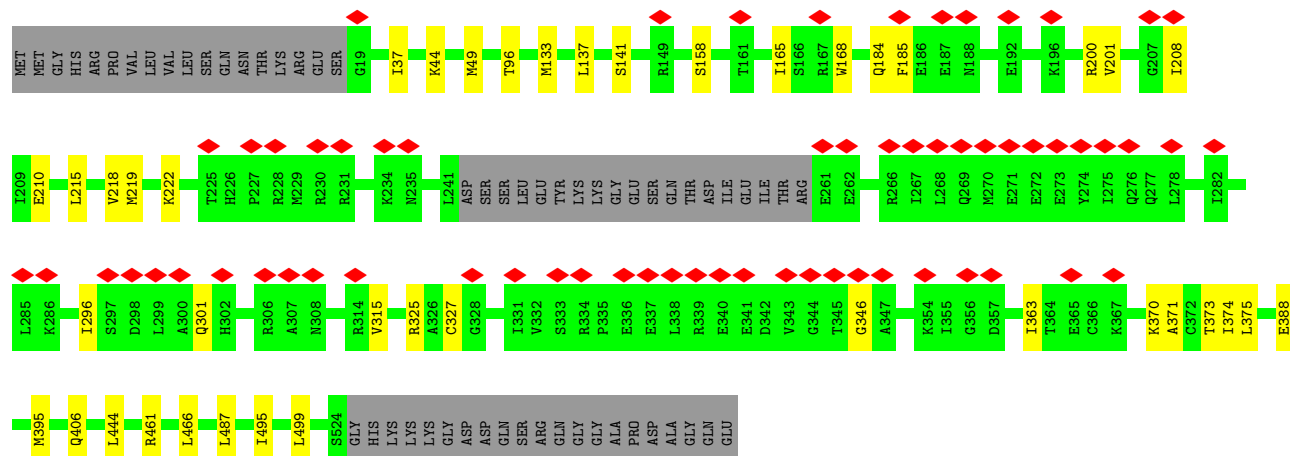
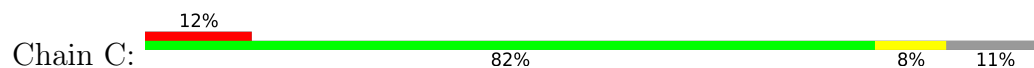


• Molecule 4: T-complex protein 1 subunit beta

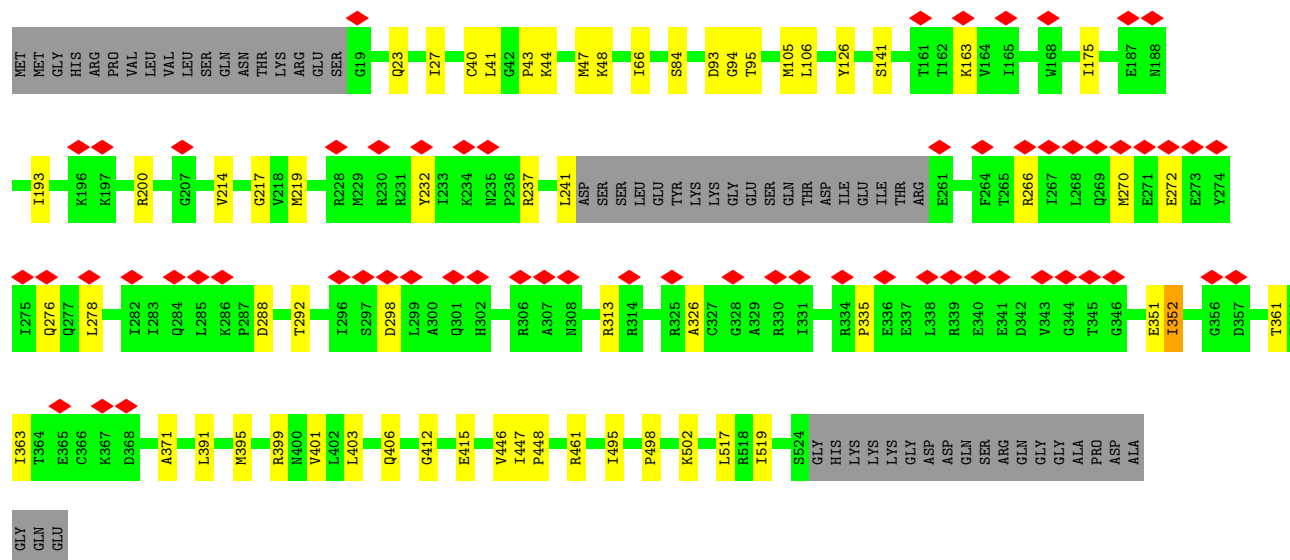
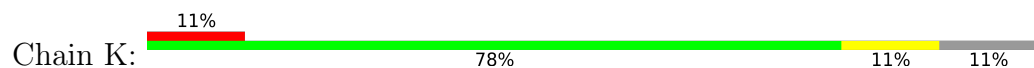




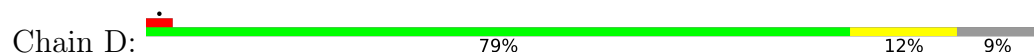
• Molecule 5: T-complex protein 1 subunit gamma



• Molecule 5: T-complex protein 1 subunit gamma



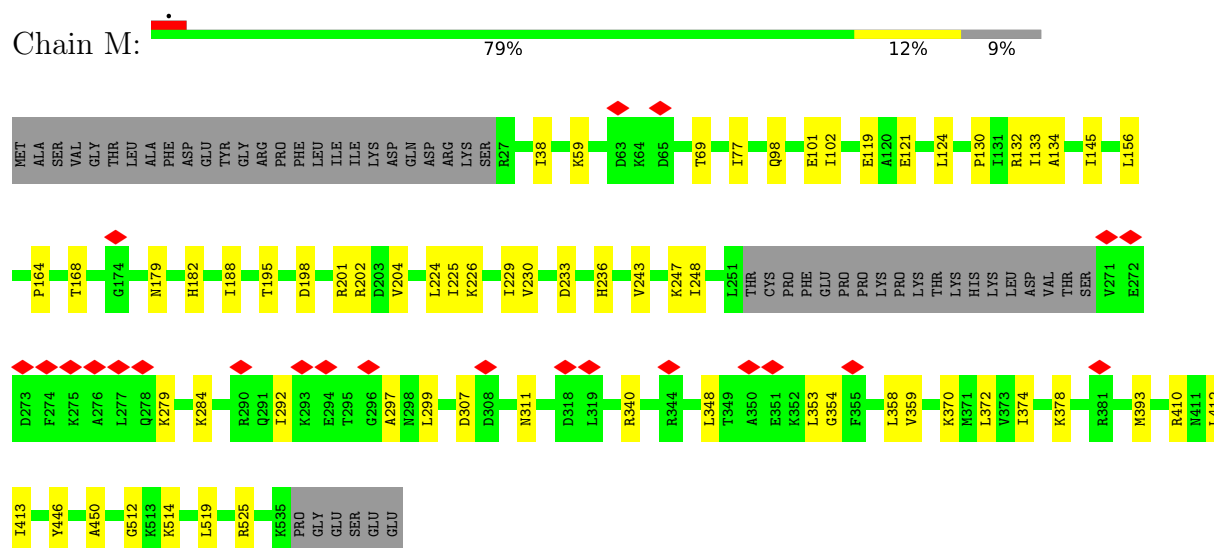
• Molecule 6: T-complex protein 1 subunit delta





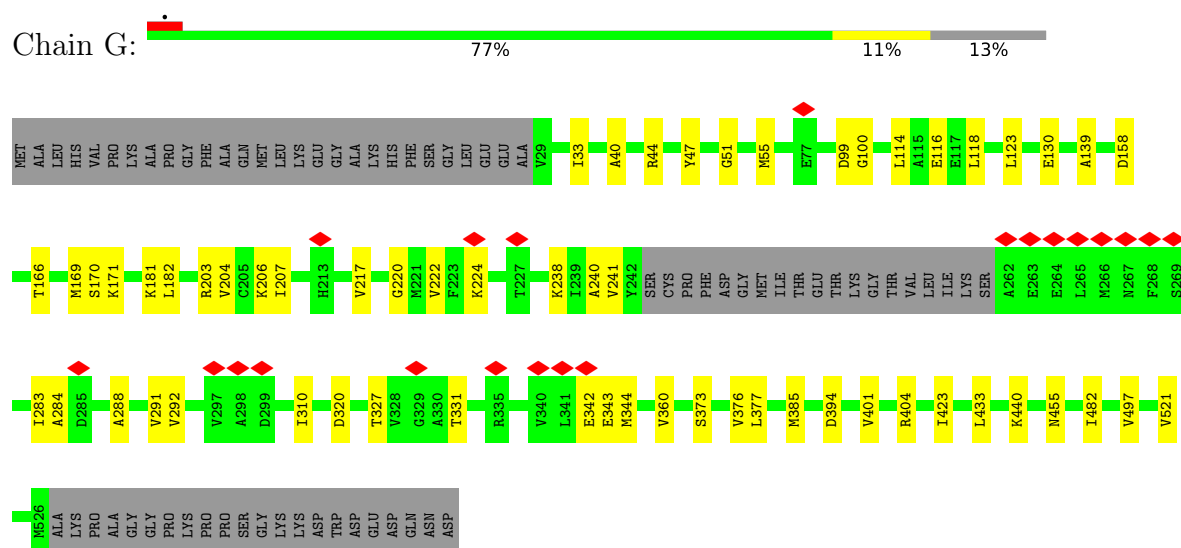
- Molecule 7: T-complex protein 1 subunit epsilon

Chain M:



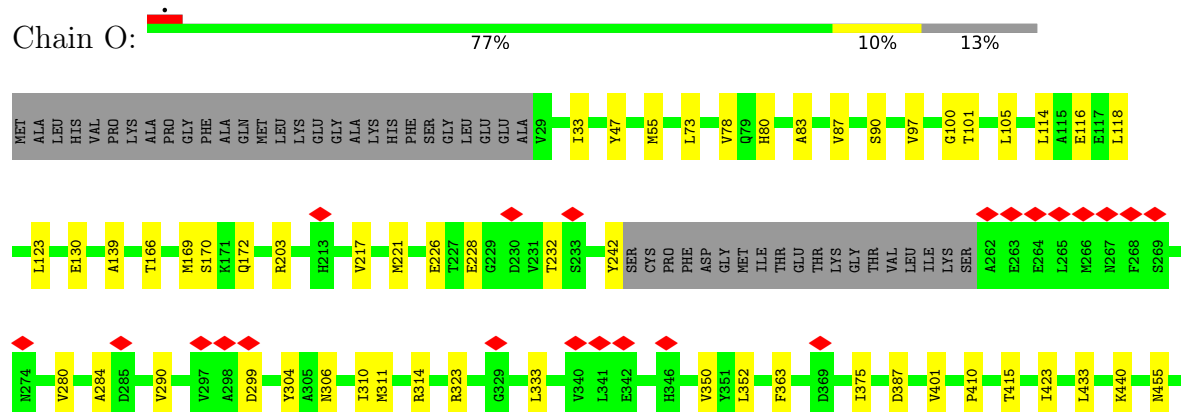
- Molecule 8: T-complex protein 1 subunit theta

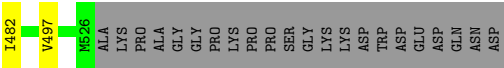
Chain G:



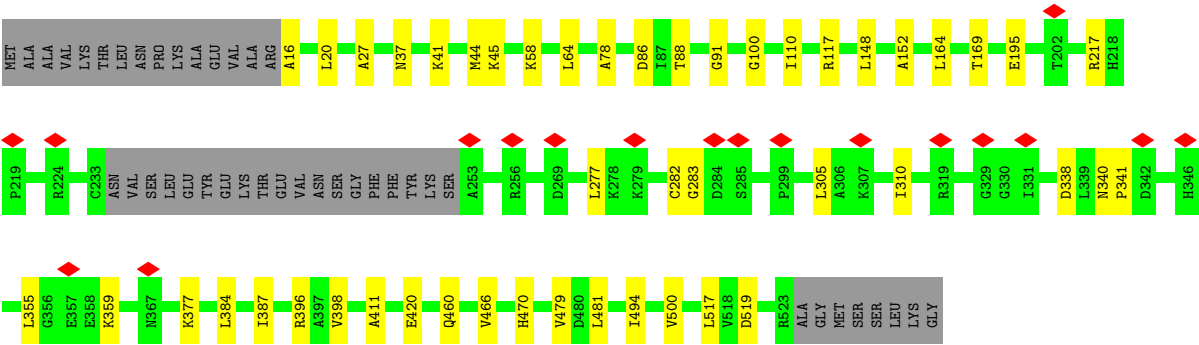
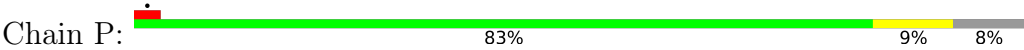
- Molecule 8: T-complex protein 1 subunit theta

Chain O:





• Molecule 9: T-complex protein 1 subunit zeta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130150	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	15.250	Depositor
Minimum map value	0.000	Depositor
Average map value	0.096	Depositor
Map value standard deviation	0.692	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	346.28, 346.28, 346.28	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8657, 0.8657, 0.8657	Depositor

## 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: ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.09	0/3757	0.24	0/5074
2	F	0.10	0/3652	0.27	0/4921
2	N	0.11	0/3702	0.31	0/4990
3	H	0.10	0/3555	0.27	0/4800
3	I	0.09	0/3555	0.26	0/4800
4	B	0.09	0/3637	0.24	0/4901
4	J	0.10	0/3637	0.26	0/4901
5	C	0.10	0/3825	0.28	0/5164
5	K	0.10	0/3825	0.29	2/5164 (0.0%)
6	D	0.10	0/3726	0.28	0/5028
6	L	0.10	0/3726	0.26	0/5028
7	E	0.09	0/3801	0.24	0/5116
7	M	0.09	0/3801	0.26	0/5116
8	G	0.09	0/3712	0.22	0/5020
8	O	0.09	0/3712	0.24	0/5020
9	P	0.09	0/3780	0.24	0/5095
All	All	0.10	0/59403	0.26	2/80138 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	446	VAL	CA-C-N	5.78	132.81	122.13
5	K	446	VAL	C-N-CA	5.78	132.81	122.13

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	A	3713	0	3875	65	0
2	F	3603	0	3711	33	0
2	N	3652	0	3759	44	0
3	H	3523	0	3683	37	0
3	I	3523	0	3683	30	0
4	B	3599	0	3718	35	0
4	J	3599	0	3718	40	0
5	C	3783	0	3917	23	0
5	K	3783	0	3917	44	0
6	D	3698	0	3909	39	0
6	L	3698	0	3909	43	0
7	E	3762	0	3879	36	0
7	M	3762	0	3879	38	0
8	G	3662	0	3705	56	0
8	O	3662	0	3705	55	0
9	P	3740	0	3888	38	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
10	G	1	0	0	0	0
10	K	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
11	A	27	0	12	18	0
11	C	27	0	12	0	0
11	G	27	0	12	23	0
11	K	27	0	12	14	0
11	O	27	0	12	25	0
11	P	27	0	12	11	0
All	All	58930	0	60927	625	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 (625) 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)
8:G:169:MET:CE	11:G:602:ADP:N7	1.81	1.41
1:A:481:LEU:HD21	11:A:602:ADP:C2	1.56	1.34
8:G:169:MET:HE1	11:G:602:ADP:C5	1.63	1.33
8:O:169:MET:CE	11:O:602:ADP:N7	1.96	1.26
8:O:169:MET:HE1	11:O:602:ADP:C5	1.70	1.25
8:G:169:MET:HE2	11:G:602:ADP:N7	1.48	1.18
1:A:90:ASP:OD1	11:A:602:ADP:O2B	1.59	1.17
8:G:169:MET:CE	11:G:602:ADP:C5	2.25	1.15
8:G:169:MET:HE1	11:G:602:ADP:N7	1.51	1.15
8:O:169:MET:CE	11:O:602:ADP:C5	2.31	1.11
8:O:169:MET:HE2	11:O:602:ADP:N7	1.59	1.10
1:A:481:LEU:CD2	11:A:602:ADP:H2	1.63	1.07
8:O:169:MET:HE1	11:O:602:ADP:C6	1.89	1.06
5:K:93:ASP:OD1	11:K:602:ADP:PB	2.16	1.04
1:A:90:ASP:OD1	11:A:602:ADP:PB	2.18	1.00
8:G:170:SER:HB3	11:G:602:ADP:H5'2	1.40	1.00
8:G:169:MET:HE1	11:G:602:ADP:C6	1.97	1.00
1:A:38:LEU:HD12	11:A:602:ADP:O1A	1.62	0.99
1:A:38:LEU:HD12	11:A:602:ADP:PA	2.05	0.94
8:O:169:MET:HE1	11:O:602:ADP:N7	1.70	0.94
5:K:93:ASP:OD1	11:K:602:ADP:O1B	1.88	0.91
8:G:169:MET:HE2	11:G:602:ADP:C8	2.05	0.90
9:P:494:ILE:HD12	11:P:602:ADP:C6	2.12	0.84
8:O:100:GLY:HA2	11:O:602:ADP:O1B	1.77	0.84
1:A:90:ASP:OD1	11:A:602:ADP:O3B	1.98	0.82
8:O:169:MET:HE1	11:O:602:ADP:N6	1.94	0.81
8:G:170:SER:CB	11:G:602:ADP:H5'2	2.11	0.80
9:P:481:LEU:HD11	11:P:602:ADP:C2	2.16	0.80
1:A:38:LEU:CD1	11:A:602:ADP:PA	2.72	0.76
9:P:91:GLY:HA2	11:P:602:ADP:O1B	1.85	0.76
8:O:166:THR:HG23	11:O:602:ADP:C8	2.22	0.75
2:N:303:PHE:HB2	2:N:308:MET:HB2	1.69	0.74
8:O:166:THR:HG23	11:O:602:ADP:H8	1.52	0.74
5:K:237:ARG:H	5:K:288:ASP:HB2	1.54	0.73
5:K:495:ILE:HD13	11:K:602:ADP:C6	2.25	0.72
8:O:100:GLY:HA2	11:O:602:ADP:PB	2.30	0.71
1:A:481:LEU:CD2	11:A:602:ADP:C2	2.37	0.71
5:K:495:ILE:CD1	11:K:602:ADP:C6	2.74	0.71
8:G:169:MET:CE	11:G:602:ADP:C8	2.70	0.70
1:A:38:LEU:CD1	11:A:602:ADP:O1A	2.41	0.68
8:O:170:SER:CB	11:O:602:ADP:H5'2	2.22	0.68
8:G:169:MET:HE1	11:G:602:ADP:N6	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:LEU:HD21	11:A:602:ADP:H2	0.68	0.68
1:A:38:LEU:HD12	11:A:602:ADP:O5'	1.95	0.67
7:M:134:ALA:HB1	7:M:525:ARG:HG2	1.77	0.67
6:L:346:LYS:HD2	6:L:358:MET:HG2	1.76	0.67
4:J:236:LYS:HB2	4:J:287:ILE:HA	1.77	0.66
2:N:223:ALA:H	2:N:300:THR:HG21	1.59	0.66
7:E:119:GLU:HB3	7:E:450:ALA:HB1	1.78	0.65
1:A:38:LEU:CD1	11:A:602:ADP:O5'	2.44	0.65
7:M:354:GLY:HA2	7:M:378:LYS:HE2	1.78	0.65
8:O:169:MET:HE2	11:O:602:ADP:C8	2.31	0.65
2:N:364:CYS:HB2	2:N:367:ALA:HB2	1.79	0.64
5:K:84:SER:HB3	5:K:95:THR:HG23	1.80	0.64
9:P:282:CYS:SG	9:P:283:GLY:N	2.71	0.64
7:M:145:ILE:HD12	7:M:514:LYS:HG2	1.80	0.64
5:K:93:ASP:CG	11:K:602:ADP:PB	2.82	0.63
2:F:364:CYS:HB2	2:F:367:ALA:HB2	1.81	0.63
5:K:141:SER:HB2	5:K:406:GLN:HB3	1.80	0.63
7:M:230:VAL:HB	7:M:372:LEU:HB2	1.80	0.63
5:K:193:ILE:HG21	5:K:403:LEU:HD21	1.80	0.62
7:E:145:ILE:HD12	7:E:514:LYS:HG2	1.80	0.62
3:I:203:ARG:HD2	3:I:378:ARG:HD3	1.80	0.62
3:I:18:ARG:HH22	6:L:60:MET:HE1	1.65	0.62
7:E:170:LYS:O	7:E:182:HIS:NE2	2.33	0.61
8:G:284:ALA:HB2	8:G:310:ILE:HD11	1.81	0.61
7:M:204:VAL:HB	7:M:410:ARG:HG3	1.82	0.61
9:P:494:ILE:HD12	11:P:602:ADP:C5	2.36	0.61
4:B:178:HIS:HB3	4:B:212:SER:HB2	1.81	0.61
8:O:33:ILE:HG21	8:O:116:GLU:HB2	1.83	0.61
4:B:349:ILE:HG12	4:B:360:ILE:HG22	1.82	0.60
8:O:170:SER:HB2	11:O:602:ADP:H5'2	1.82	0.60
8:G:207:ILE:HA	8:G:224:LYS:HD2	1.84	0.60
1:A:152:ALA:HB2	1:A:398:ILE:HD11	1.83	0.60
9:P:481:LEU:CD1	11:P:602:ADP:N1	2.65	0.60
8:O:170:SER:HB3	11:O:602:ADP:H5'2	1.82	0.59
8:G:433:LEU:HD11	5:K:461:ARG:HG2	1.83	0.59
6:D:162:ASP:HA	6:D:166:LEU:HB2	1.84	0.59
8:G:170:SER:HB2	11:G:602:ADP:PA	2.42	0.59
6:L:154:MET:HG2	6:L:492:LYS:HD3	1.85	0.59
7:M:119:GLU:HB3	7:M:450:ALA:HB1	1.84	0.59
5:C:208:ILE:HG23	5:C:210:GLU:H	1.68	0.59
6:L:296:THR:HG1	6:L:298:CYS:HG	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:ILE:HD11	2:F:416:LEU:HD11	1.85	0.58
4:B:332:ALA:HB2	4:B:341:VAL:HG21	1.85	0.58
2:N:155:LEU:HD22	2:N:396:VAL:HG13	1.84	0.58
5:K:41:LEU:HA	11:K:602:ADP:O1A	2.04	0.58
6:L:159:GLU:HB3	6:L:162:ASP:HB2	1.85	0.58
1:A:349:LEU:HB3	1:A:363:ILE:HG23	1.84	0.58
8:G:100:GLY:HA2	11:G:602:ADP:O1B	2.04	0.58
8:O:203:ARG:HD2	8:O:323:ARG:HD3	1.84	0.58
4:B:310:MET:HE2	4:B:312:ILE:HD11	1.85	0.58
6:D:223:ASP:O	6:D:394:ARG:NH1	2.37	0.58
7:E:247:LYS:HB2	7:E:297:ALA:HA	1.86	0.58
8:O:482:ILE:CG2	11:O:602:ADP:C2	2.87	0.58
1:A:180:ARG:HD2	1:A:402:ILE:HD13	1.86	0.57
7:E:184:GLN:NE2	7:E:222:THR:O	2.37	0.57
7:M:358:LEU:HB3	7:M:374:ILE:HG23	1.87	0.57
3:H:411:GLY:O	3:H:498:ASN:ND2	2.38	0.57
3:I:103:ASN:ND2	3:I:440:GLU:OE1	2.38	0.57
6:L:97:LEU:HD11	6:L:524:LEU:HB3	1.86	0.57
8:O:169:MET:HE1	11:O:602:ADP:HN61	1.69	0.57
4:J:207:GLY:HA3	4:J:376:ARG:HB3	1.87	0.56
6:D:51:ILE:HG22	6:D:110:THR:HG23	1.86	0.56
7:E:134:ALA:HB1	7:E:525:ARG:HG2	1.85	0.56
6:L:248:LYS:H	6:L:299:ASN:HB2	1.70	0.56
2:N:100:LEU:HD11	2:N:442:LEU:HD23	1.88	0.56
4:J:83:VAL:HG12	4:J:87:MET:HE2	1.87	0.56
8:O:169:MET:CE	11:O:602:ADP:C6	2.74	0.56
7:E:124:LEU:HD21	7:E:130:PRO:HG3	1.87	0.56
7:M:292:ILE:HB	7:M:297:ALA:HB3	1.88	0.56
7:E:280:TYR:HA	7:E:284:LYS:HB3	1.88	0.56
4:J:198:ALA:HB2	4:J:325:LEU:HD12	1.88	0.56
4:J:337:HIS:HB3	4:J:340:LEU:HB2	1.86	0.56
3:H:22:VAL:HG21	3:H:105:ASP:HB2	1.85	0.56
3:H:489:ASP:HB3	3:H:493:GLY:H	1.71	0.56
4:J:224:ILE:HG13	4:J:360:ILE:HG12	1.87	0.56
8:O:280:VAL:HG11	8:O:304:TYR:HB3	1.85	0.56
8:O:482:ILE:HG23	11:O:602:ADP:C2	2.41	0.56
6:L:166:LEU:HD21	6:L:415:ILE:HG12	1.88	0.56
3:H:161:ILE:HD13	3:H:388:MET:HG3	1.88	0.56
6:D:41:ILE:HG12	6:D:120:LEU:HD22	1.88	0.55
5:K:93:ASP:OD1	11:K:602:ADP:O3B	2.23	0.55
4:B:326:VAL:HG13	4:B:327:THR:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:332:GLU:HG3	6:L:334:GLU:H	1.72	0.55
3:I:22:VAL:HG21	3:I:105:ASP:HB2	1.87	0.55
4:J:203:LYS:HB2	4:J:383:LEU:HD21	1.87	0.55
7:M:233:ASP:HB3	7:M:370:LYS:HB2	1.89	0.55
1:A:477:VAL:HG12	1:A:488:VAL:HG22	1.89	0.55
5:C:37:ILE:HG22	5:C:96:THR:HG23	1.89	0.55
2:F:121:ILE:HA	2:F:434:LEU:HD13	1.89	0.55
3:H:292:ILE:O	3:H:309:ARG:NH2	2.40	0.55
2:F:408:GLY:O	2:F:487:ASN:ND2	2.39	0.55
9:P:91:GLY:CA	11:P:602:ADP:O1B	2.55	0.55
3:I:386:ASP:OD2	3:I:390:ARG:NH1	2.40	0.54
5:K:278:LEU:HD13	5:K:335:PRO:HB2	1.89	0.54
8:G:241:VAL:HA	8:G:292:VAL:HB	1.90	0.54
3:I:118:ILE:HG23	3:I:522:ILE:HG12	1.88	0.54
5:K:495:ILE:CD1	11:K:602:ADP:N1	2.70	0.54
2:N:315:PRO:HB2	2:N:318:ASP:HB2	1.89	0.54
5:K:495:ILE:HD11	11:K:602:ADP:C6	2.42	0.54
6:L:276:ASP:OD2	6:L:280:ARG:NH1	2.40	0.54
5:C:461:ARG:HG2	8:O:433:LEU:HD11	1.89	0.54
2:N:160:MET:HB3	2:N:172:LYS:HE2	1.90	0.54
4:J:160:MET:HE1	4:J:181:LYS:HG3	1.88	0.54
8:G:401:VAL:HG22	8:G:404:ARG:HH21	1.72	0.54
1:A:38:LEU:O	1:A:454:ASN:ND2	2.39	0.54
3:I:489:ASP:HB3	3:I:493:GLY:H	1.72	0.54
9:P:195:GLU:HB2	9:P:384:LEU:HD22	1.89	0.54
5:C:141:SER:HB2	5:C:406:GLN:HB3	1.90	0.54
5:K:200:ARG:NH1	5:K:219:MET:O	2.41	0.54
2:N:48:LEU:HD11	2:N:56:ALA:HB1	1.90	0.54
2:N:317:GLU:OE2	2:N:321:ARG:NH2	2.40	0.54
3:H:31:ILE:O	3:H:43:LYS:NZ	2.36	0.54
4:J:40:LYS:HE3	4:J:449:ILE:HG12	1.90	0.54
3:H:386:ASP:OD2	3:H:390:ARG:NH1	2.41	0.53
7:M:279:LYS:O	7:M:284:LYS:N	2.37	0.53
3:H:139:ASN:HB3	3:H:142:GLU:HG2	1.90	0.53
4:B:351:GLU:HA	4:B:360:ILE:HA	1.90	0.53
2:F:462:ASN:OD1	2:F:465:ARG:NH2	2.41	0.53
2:F:26:ILE:HG12	2:F:105:LEU:HB3	1.90	0.53
2:N:224:GLY:HA2	7:M:340:ARG:HH21	1.73	0.53
2:N:516:VAL:HG21	8:O:55:MET:HE3	1.90	0.53
7:M:247:LYS:HB3	7:M:353:LEU:HD11	1.89	0.53
5:C:219:MET:HB3	5:C:373:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:278:LYS:NZ	4:J:336:ASP:OD1	2.42	0.53
6:D:206:VAL:HB	6:D:416:ARG:HG3	1.91	0.53
8:G:331:THR:HB	8:G:343:GLU:HG2	1.91	0.53
7:M:124:LEU:HD21	7:M:130:PRO:HG3	1.91	0.53
1:A:320:ASN:OD1	1:A:323:ARG:NH2	2.40	0.53
4:B:201:VAL:HG13	4:B:390:LEU:HD23	1.90	0.53
6:L:234:GLN:NE2	6:L:330:ASP:O	2.40	0.53
1:A:264:ARG:NH1	8:G:342:GLU:OE1	2.42	0.53
2:N:408:GLY:O	2:N:487:ASN:ND2	2.41	0.53
2:N:236:MET:HB2	2:N:286:ALA:HA	1.91	0.52
8:O:130:GLU:OE2	9:P:41:LYS:NZ	2.42	0.52
8:O:232:THR:HG23	8:O:352:LEU:HB2	1.91	0.52
2:N:19:ILE:HG13	2:N:20:PRO:HD3	1.92	0.52
8:O:172:GLN:NE2	8:O:387:ASP:OD2	2.42	0.52
7:E:367:THR:OG1	7:E:388:ARG:NH2	2.42	0.52
1:A:181:ARG:NH2	1:A:369:PRO:O	2.41	0.52
7:E:208:LEU:HD12	7:E:382:ALA:HB2	1.89	0.52
2:N:197:ILE:HG12	2:N:372:ILE:HB	1.92	0.52
4:J:204:LYS:HE2	4:J:359:LEU:HD12	1.92	0.52
1:A:46:MET:HE3	8:G:521:VAL:HG21	1.91	0.52
4:B:228:GLN:NE2	4:B:311:ALA:O	2.42	0.52
4:B:112:GLU:HB3	4:B:438:SER:HB3	1.91	0.52
2:N:82:ILE:HG21	2:N:509:ALA:HB2	1.92	0.52
4:J:281:ARG:NH1	4:J:336:ASP:O	2.42	0.52
5:K:93:ASP:OD2	11:K:602:ADP:O2B	2.28	0.52
1:A:35:ARG:HA	1:A:97:LEU:HD21	1.92	0.52
7:E:148:LEU:HD22	7:E:419:VAL:HG11	1.90	0.52
7:E:279:LYS:O	7:E:284:LYS:N	2.37	0.52
2:F:211:VAL:HG12	2:F:213:GLY:H	1.74	0.52
6:D:194:VAL:HG21	6:D:415:ILE:HG21	1.92	0.52
3:I:63:LYS:NZ	3:I:80:ASP:OD1	2.43	0.52
3:I:366:ASN:ND2	3:I:367:THR:O	2.42	0.52
6:L:227:VAL:HG11	6:L:378:LYS:HD2	1.91	0.52
8:O:139:ALA:HB2	8:O:423:ILE:HD11	1.92	0.52
9:P:355:LEU:HD21	9:P:377:LYS:HE2	1.92	0.52
9:P:481:LEU:HD11	11:P:602:ADP:N1	2.25	0.52
6:D:370:LEU:HB2	6:D:375:LYS:HE2	1.92	0.51
9:P:277:LEU:HD22	9:P:341:PRO:HG3	1.92	0.51
8:G:33:ILE:HG21	8:G:116:GLU:HB2	1.92	0.51
5:K:193:ILE:HB	5:K:399:ARG:HD2	1.92	0.51
1:A:88:THR:HB	1:A:500:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ILE:HD11	2:F:65:ILE:HG23	1.92	0.51
7:M:248:ILE:HG13	7:M:299:LEU:HD12	1.92	0.51
9:P:481:LEU:CD1	11:P:602:ADP:C2	2.90	0.51
6:D:55:LEU:O	6:D:471:ASN:ND2	2.44	0.51
4:J:66:ASP:HB3	4:J:388:ARG:HH21	1.75	0.51
8:G:482:ILE:HG23	11:G:602:ADP:C2	2.45	0.51
2:N:219:THR:HB	2:N:222:TYR:HE2	1.76	0.51
1:A:126:ALA:HB2	1:A:437:VAL:HG22	1.93	0.51
2:F:236:MET:HB2	2:F:286:ALA:HA	1.91	0.51
6:L:41:ILE:HG23	6:L:120:LEU:HB3	1.93	0.51
4:B:74:ILE:HG12	6:D:539:VAL:HG11	1.93	0.50
6:D:275:MET:HA	6:D:278:VAL:HB	1.93	0.50
9:P:148:LEU:HD22	9:P:398:VAL:HG13	1.93	0.50
5:C:374:ILE:HG13	5:C:395:MET:HE1	1.92	0.50
3:H:211:ILE:HB	3:H:365:LYS:HE2	1.93	0.50
8:G:204:VAL:HG13	8:G:377:LEU:HD12	1.93	0.50
5:K:48:LYS:HD2	5:K:66:ILE:HD13	1.93	0.50
8:O:217:VAL:HG22	8:O:375:ILE:HG12	1.93	0.50
9:P:88:THR:HB	9:P:500:VAL:HG22	1.94	0.50
4:B:25:ARG:HH22	7:E:57:LEU:HD13	1.76	0.50
9:P:20:LEU:HD13	9:P:110:ILE:HD13	1.94	0.50
8:G:203:ARG:NH2	8:G:327:THR:OG1	2.40	0.50
8:G:224:LYS:HA	8:G:360:VAL:HG12	1.94	0.50
2:N:238:ALA:HB3	2:N:289:VAL:HG22	1.93	0.50
2:N:482:GLU:OE1	7:M:132:ARG:NH2	2.44	0.50
3:H:272:LYS:HB2	3:H:295:MET:HE2	1.94	0.50
6:D:314:ASP:OD1	6:D:314:ASP:N	2.45	0.50
3:I:356:ILE:HD12	3:I:361:LEU:HB2	1.94	0.50
6:L:45:LYS:NZ	6:L:49:ASP:OD2	2.40	0.50
8:O:80:HIS:HD2	8:O:83:ALA:H	1.60	0.50
8:O:226:GLU:O	8:O:314:ARG:NH2	2.45	0.50
5:C:215:LEU:HD11	5:C:375:LEU:HD12	1.94	0.50
8:G:139:ALA:HB2	8:G:423:ILE:HD11	1.93	0.50
2:N:297:ASP:OD1	2:N:297:ASP:N	2.45	0.50
4:J:170:LYS:HE3	4:J:382:ILE:HA	1.93	0.50
2:F:468:HIS:ND1	2:F:472:GLY:O	2.45	0.49
3:H:63:LYS:NZ	3:H:80:ASP:OD1	2.45	0.49
6:D:216:LYS:NZ	6:D:217:LEU:O	2.45	0.49
7:E:50:THR:OG1	7:E:59:LYS:NZ	2.44	0.49
3:H:118:ILE:HG23	3:H:522:ILE:HG12	1.93	0.49
6:L:64:ILE:HD11	6:L:80:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:82:ILE:HG21	2:F:509:ALA:HB2	1.94	0.49
2:N:210:LEU:HD11	2:N:372:ILE:HG12	1.94	0.49
8:O:242:TYR:HA	8:O:333:LEU:H	1.77	0.49
3:H:202:GLY:O	3:H:203:ARG:NH1	2.46	0.49
2:N:136:ILE:HG12	2:N:412:ILE:HD11	1.94	0.49
2:N:284:SER:HB3	2:N:342:LEU:HD11	1.95	0.49
3:H:430:MET:O	3:H:435:GLN:NE2	2.43	0.49
7:E:188:ILE:HG12	7:E:224:LEU:HG	1.94	0.49
2:N:292:LYS:O	2:N:313:ARG:NH1	2.44	0.49
3:I:80:ASP:OD2	3:I:84:LYS:NZ	2.45	0.49
5:C:200:ARG:HB3	5:C:373:THR:HG23	1.95	0.49
2:N:49:ILE:HD11	2:N:65:ILE:HG23	1.95	0.49
4:J:199:ILE:HG12	4:J:394:LEU:HD22	1.94	0.49
1:A:86:ASP:O	1:A:396:ARG:NH2	2.45	0.49
6:D:320:LEU:HD13	6:D:327:VAL:HG21	1.94	0.49
7:E:235:SER:N	7:E:321:ALA:O	2.44	0.49
1:A:24:ILE:HD13	1:A:107:ASP:HB2	1.94	0.49
1:A:518:VAL:HG21	5:C:49:MET:HE3	1.95	0.49
8:O:482:ILE:HG23	11:O:602:ADP:H2	1.76	0.49
2:F:373:ILE:HG22	2:F:375:ARG:HG2	1.94	0.49
4:B:379:THR:HB	4:B:382:ILE:HG22	1.95	0.49
3:I:430:MET:O	3:I:435:GLN:NE2	2.46	0.49
4:J:353:MET:HB2	4:J:358:LYS:HE2	1.94	0.49
6:L:214:VAL:HG21	6:L:231:VAL:HB	1.94	0.49
9:P:86:ASP:O	9:P:396:ARG:NH2	2.46	0.49
4:J:187:VAL:HG21	4:J:397:LEU:HD13	1.95	0.48
6:D:434:GLU:OE2	6:D:438:ARG:NH1	2.46	0.48
6:L:304:GLN:HB2	6:L:307:ILE:HD11	1.94	0.48
2:F:119:GLN:NE2	8:G:51:GLY:O	2.46	0.48
2:F:260:VAL:N	7:E:281:GLU:OE2	2.46	0.48
2:F:297:ASP:N	2:F:297:ASP:OD1	2.45	0.48
6:D:50:ALA:O	6:D:62:LYS:NZ	2.45	0.48
7:E:361:GLU:HB3	7:E:370:LYS:HD2	1.95	0.48
3:I:402:VAL:HG13	3:I:408:VAL:HG11	1.95	0.48
9:P:411:ALA:HB1	9:P:479:VAL:H	1.78	0.48
2:N:214:VAL:HB	2:N:361:PHE:H	1.79	0.48
1:A:366:CYS:SG	1:A:367:ILE:N	2.87	0.48
6:D:155:SER:HB2	6:D:423:ALA:HB1	1.95	0.48
6:D:225:GLU:OE2	6:D:378:LYS:NZ	2.45	0.48
4:J:373:ILE:HG22	4:J:375:LEU:HG	1.95	0.48
7:E:443:LEU:HD11	6:L:478:SER:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:497:VAL:HG13	11:G:602:ADP:C8	2.48	0.48
3:I:532:LYS:HA	6:L:65:GLN:HB3	1.95	0.48
8:O:228:GLU:OE1	8:O:306:ASN:ND2	2.40	0.48
1:A:316:ALA:HB1	1:A:321:MET:HE3	1.96	0.48
4:B:407:VAL:HG13	4:B:497:PHE:HB2	1.96	0.48
6:L:434:GLU:OE1	6:L:487:HIS:ND1	2.46	0.48
7:M:38:ILE:HG21	7:M:121:GLU:HB2	1.96	0.48
7:E:51:SER:HB3	7:E:107:THR:HG21	1.96	0.48
8:G:171:LYS:NZ	8:G:394:ASP:OD2	2.43	0.48
7:M:225:ILE:HD13	7:M:229:ILE:HD11	1.96	0.48
6:D:326:MET:HE2	6:D:377:ILE:HD13	1.96	0.48
7:E:248:ILE:HG12	7:E:299:LEU:HD22	1.94	0.48
8:G:166:THR:HG23	11:G:602:ADP:C8	2.48	0.48
8:G:220:GLY:H	8:G:373:SER:HA	1.78	0.48
8:O:221:MET:HB2	8:O:363:PHE:HB2	1.95	0.48
1:A:34:LEU:HD12	1:A:96:VAL:HG11	1.96	0.47
3:H:61:ILE:O	3:H:65:LEU:HG	2.14	0.47
5:C:201:VAL:HG21	5:C:388:GLU:HG3	1.97	0.47
7:E:344:ARG:HA	7:E:349:THR:HB	1.95	0.47
2:N:228:GLN:NE2	2:N:307:ASP:OD1	2.46	0.47
3:I:179:ILE:HD13	3:I:373:ALA:HB3	1.95	0.47
5:K:40:CYS:O	11:K:602:ADP:O1A	2.32	0.47
5:K:93:ASP:CG	11:K:602:ADP:O2B	2.56	0.47
8:O:47:TYR:O	8:O:455:ASN:ND2	2.47	0.47
8:O:97:VAL:HG13	8:O:401:VAL:HG21	1.97	0.47
9:P:16:ALA:N	9:P:519:ASP:O	2.47	0.47
9:P:27:ALA:HB1	9:P:100:GLY:HA2	1.96	0.47
2:F:19:ILE:HG13	2:F:20:PRO:HD3	1.95	0.47
7:M:69:THR:HG23	7:M:393:MET:HE1	1.96	0.47
7:M:195:THR:OG1	7:M:226:LYS:NZ	2.42	0.47
2:F:107:GLN:HB3	2:F:437:ALA:HB1	1.96	0.47
4:B:202:ILE:HG13	4:B:219:LEU:HB2	1.96	0.47
6:L:104:GLU:OE2	6:L:420:LYS:NZ	2.47	0.47
8:O:299:ASP:OD1	8:O:299:ASP:N	2.46	0.47
1:A:41:LYS:NZ	8:G:130:GLU:OE2	2.44	0.47
2:F:100:LEU:HD11	2:F:442:LEU:HD23	1.97	0.47
4:B:83:VAL:HG12	4:B:87:MET:HE2	1.96	0.47
6:D:312:LEU:HD12	6:D:329:LYS:HE2	1.96	0.47
5:K:94:GLY:N	11:K:602:ADP:O1B	2.36	0.47
6:L:486:ARG:HD3	6:L:494:THR:HG21	1.96	0.47
8:O:482:ILE:HG21	11:O:602:ADP:C2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:402:VAL:HG13	3:H:408:VAL:HG11	1.96	0.47
3:H:474:ALA:HB2	3:H:483:LEU:HB2	1.96	0.47
6:D:214:VAL:HG21	6:D:231:VAL:HB	1.97	0.47
6:D:232:LEU:HB3	6:D:377:ILE:HB	1.96	0.47
8:G:166:THR:HG23	11:G:602:ADP:H8	1.80	0.47
2:N:26:ILE:HG12	2:N:105:LEU:HB3	1.96	0.47
5:K:266:ARG:NH1	5:K:270:MET:SD	2.88	0.47
6:L:249:ILE:HB	6:L:343:ILE:HG21	1.97	0.47
1:A:195:GLU:HG2	1:A:384:LEU:HD22	1.97	0.47
5:C:222:LYS:HE3	5:C:315:VAL:HA	1.97	0.47
6:L:483:LEU:HD11	6:L:496:ILE:HG13	1.96	0.47
1:A:198:HIS:HB2	1:A:377:LYS:HB2	1.97	0.47
4:B:160:MET:HG3	4:B:184:VAL:HG21	1.96	0.47
5:K:175:ILE:HG23	5:K:214:VAL:HG22	1.97	0.47
5:K:415:GLU:OE2	5:K:502:LYS:NZ	2.44	0.47
6:L:300:VAL:HG22	6:L:326:MET:HB3	1.96	0.47
1:A:224:ARG:NH1	1:A:226:ASP:OD2	2.47	0.47
5:C:218:VAL:HB	5:C:363:ILE:HD12	1.96	0.47
6:D:247:ALA:HB3	6:D:362:ALA:HB3	1.96	0.47
4:J:69:THR:O	4:J:73:ASN:ND2	2.43	0.47
4:J:182:LEU:HD22	4:J:214:LEU:HD23	1.97	0.47
9:P:466:VAL:HG21	9:P:479:VAL:HG22	1.97	0.47
1:A:38:LEU:HD11	11:A:602:ADP:O5'	2.14	0.46
4:B:24:ALA:HB3	4:B:519:ASN:HA	1.97	0.46
1:A:331:VAL:HB	1:A:342:ASP:HB2	1.98	0.46
2:F:190:LEU:HB3	2:F:397:ARG:HG3	1.97	0.46
2:F:465:ARG:NE	3:I:435:GLN:OE1	2.42	0.46
7:E:145:ILE:HG23	7:E:514:LYS:HE2	1.97	0.46
8:G:238:LYS:HB3	8:G:344:MET:HB3	1.96	0.46
2:N:136:ILE:HD11	2:N:416:LEU:HD11	1.97	0.46
8:O:284:ALA:HB2	8:O:310:ILE:HD11	1.97	0.46
1:A:207:ILE:HB	1:A:373:THR:HB	1.97	0.46
2:N:300:THR:HA	2:N:303:PHE:CE2	2.51	0.46
4:J:329:GLY:HA2	4:J:342:LYS:HB3	1.98	0.46
6:L:174:LEU:HD13	6:L:183:SER:HB2	1.97	0.46
6:L:370:LEU:HB2	6:L:376:LEU:HD13	1.96	0.46
9:P:494:ILE:CD1	11:P:602:ADP:C5	2.98	0.46
4:B:43:LEU:O	4:B:453:ASN:ND2	2.48	0.46
8:G:169:MET:HE3	11:G:602:ADP:C5	2.38	0.46
4:J:202:ILE:HG21	4:J:219:LEU:HD23	1.98	0.46
1:A:106:ALA:O	1:A:110:ILE:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:LYS:HB3	2:F:382:MET:HE1	1.96	0.46
2:N:290:LEU:HD11	2:N:361:PHE:HE2	1.80	0.46
2:N:350:GLU:OE2	2:N:357:ARG:NE	2.43	0.46
5:C:184:GLN:HG2	5:C:370:LYS:HA	1.97	0.46
6:D:232:LEU:HD11	6:D:328:VAL:HG11	1.97	0.46
7:M:156:LEU:HB3	7:M:164:PRO:HG3	1.98	0.46
7:M:179:ASN:HA	7:M:182:HIS:HB3	1.97	0.46
3:H:235:ALA:HB3	3:H:286:ILE:HG12	1.98	0.46
7:E:434:SER:HB3	6:L:444:ARG:HH21	1.80	0.46
4:J:353:MET:HA	4:J:358:LYS:HG2	1.98	0.46
4:B:330:GLU:HB2	4:B:341:VAL:HG13	1.96	0.46
5:C:296:ILE:HG21	5:C:301:GLN:HE21	1.81	0.46
2:N:121:ILE:HA	2:N:434:LEU:HD13	1.97	0.46
9:P:217:ARG:HA	9:P:359:LYS:HD2	1.98	0.46
6:D:232:LEU:HD22	6:D:377:ILE:HD12	1.97	0.46
5:K:23:GLN:NE2	5:K:517:LEU:O	2.43	0.46
2:F:212:ALA:HB3	2:F:362:THR:HB	1.97	0.46
4:B:189:ARG:NH1	4:B:216:GLU:OE1	2.45	0.46
4:J:136:ALA:HB2	4:J:424:LEU:HD22	1.97	0.46
4:J:141:LEU:HD22	4:J:407:VAL:HG11	1.97	0.46
6:L:226:LEU:HD21	6:L:391:ILE:HG12	1.97	0.46
7:M:101:GLU:HA	7:M:410:ARG:HH22	1.80	0.46
7:M:145:ILE:HG23	7:M:514:LYS:HE2	1.98	0.46
8:O:78:VAL:HG21	8:O:87:VAL:HG21	1.98	0.46
1:A:451:LEU:CD2	11:A:602:ADP:N3	2.79	0.45
9:P:91:GLY:HA2	11:P:602:ADP:PB	2.56	0.45
3:H:532:LYS:HA	6:D:65:GLN:HB3	1.98	0.45
5:K:391:LEU:HG	5:K:395:MET:HE2	1.98	0.45
2:F:237:ILE:O	2:F:343:GLY:N	2.44	0.45
3:H:103:ASN:OD1	3:H:444:SER:OG	2.34	0.45
7:E:152:SER:HB2	7:E:417:ARG:HB3	1.98	0.45
4:J:379:THR:O	4:J:383:LEU:N	2.38	0.45
2:N:324:MET:HE3	2:N:324:MET:HB3	1.85	0.45
4:J:224:ILE:HD12	4:J:351:GLU:HB2	1.98	0.45
4:B:233:GLU:OE1	4:B:347:LYS:NZ	2.48	0.45
8:O:114:LEU:HD22	8:O:440:LYS:HD2	1.97	0.45
1:A:451:LEU:HD22	11:A:602:ADP:C2	2.52	0.45
9:P:37:ASN:HD21	9:P:45:LYS:HG3	1.82	0.45
1:A:152:ALA:HB3	1:A:169:THR:HG23	1.97	0.45
5:C:325:ARG:HD2	5:C:370:LYS:HD2	1.99	0.45
6:D:131:ILE:HG23	6:D:449:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:474:ALA:HB2	3:I:483:LEU:HB2	1.98	0.45
4:J:125:THR:HG21	4:J:431:LYS:HB2	1.99	0.45
5:K:326:ALA:HB2	5:K:371:ALA:HB3	1.99	0.45
6:L:51:ILE:HG22	6:L:110:THR:HG23	1.99	0.45
6:L:194:VAL:HG21	6:L:415:ILE:HG21	1.98	0.45
9:P:338:ASP:OD1	9:P:340:ASN:ND2	2.48	0.45
9:P:481:LEU:HD12	11:P:602:ADP:N1	2.32	0.45
2:F:136:ILE:HG13	2:F:416:LEU:HD21	1.99	0.45
7:E:480:ARG:HB3	7:E:489:LEU:HD13	1.98	0.45
7:M:38:ILE:HD13	7:M:121:GLU:HB2	1.99	0.45
7:M:102:ILE:HG22	7:M:512:GLY:HA2	1.99	0.45
8:O:114:LEU:HB3	8:O:440:LYS:HD2	1.99	0.45
8:O:290:VAL:HG11	8:O:350:VAL:HG11	1.99	0.45
5:C:466:LEU:HD13	5:C:487:LEU:HD22	1.98	0.45
6:D:62:LYS:HD3	6:D:80:ILE:HD13	1.99	0.45
7:M:348:LEU:HD21	7:M:353:LEU:HD13	1.98	0.45
9:P:152:ALA:HB3	9:P:169:THR:HG23	1.99	0.45
8:G:320:ASP:N	8:G:320:ASP:OD1	2.44	0.45
2:F:192:LEU:HG	2:F:397:ARG:HD2	1.98	0.44
3:H:118:ILE:HG13	3:H:525:LEU:HD23	1.98	0.44
1:A:451:LEU:HD22	11:A:602:ADP:N3	2.31	0.44
3:H:229:ILE:HG22	3:H:231:ASN:H	1.82	0.44
4:B:151:ASP:HB3	4:B:154:LYS:HB2	1.99	0.44
8:G:40:ALA:O	8:G:44:ARG:HG3	2.16	0.44
2:N:217:LYS:HG3	2:N:315:PRO:HA	1.99	0.44
3:I:197:VAL:HG22	3:I:375:VAL:HB	1.99	0.44
3:I:352:VAL:HG23	3:I:363:LEU:HB3	1.99	0.44
1:A:59:ASP:OD1	1:A:159:LYS:NZ	2.46	0.44
3:H:36:LEU:HD21	3:H:448:ILE:HG23	1.97	0.44
5:C:137:LEU:HB3	5:C:499:LEU:HD11	2.00	0.44
6:D:462:GLU:OE2	7:M:446:TYR:OH	2.28	0.44
4:J:217:GLY:HA3	4:J:363:SER:HA	1.99	0.44
4:B:521:ILE:HG21	7:E:81:MET:HA	1.99	0.44
5:K:105:MET:O	5:K:126:TYR:OH	2.36	0.44
9:P:44:MET:HG2	9:P:58:LYS:HD2	2.00	0.44
7:E:235:SER:O	7:E:311:ASN:ND2	2.50	0.44
5:K:352:ILE:HD13	5:K:361:THR:HA	2.00	0.44
8:O:290:VAL:HG12	8:O:311:MET:HB3	1.99	0.44
1:A:47:LEU:HD11	1:A:63:LEU:HD23	1.99	0.44
3:I:530:LEU:HD11	6:L:65:GLN:HB2	1.99	0.44
6:D:41:ILE:HG23	6:D:120:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:198:ILE:HD13	6:D:206:VAL:HG22	1.99	0.44
2:N:207:GLU:O	2:N:375:ARG:NH2	2.48	0.44
3:H:130:ARG:NH2	3:H:422:TYR:OH	2.51	0.44
4:J:200:HIS:HB3	4:J:372:THR:HG23	1.99	0.44
8:O:100:GLY:CA	11:O:602:ADP:O1B	2.59	0.44
2:F:168:ILE:HB	2:F:172:LYS:HD3	1.99	0.44
3:H:103:ASN:HB3	3:H:440:GLU:HB3	1.99	0.44
3:H:191:PRO:HB2	3:H:194:SER:HB2	2.00	0.44
8:G:47:TYR:O	8:G:455:ASN:ND2	2.51	0.44
6:L:166:LEU:HD13	6:L:418:LEU:HG	1.99	0.44
7:M:168:THR:HG21	7:M:412:LEU:HD11	2.00	0.44
9:P:64:LEU:HB3	9:P:78:ALA:HB1	2.00	0.44
4:B:238:LEU:HD23	4:B:290:PHE:HE1	1.82	0.43
6:L:41:ILE:HG12	6:L:120:LEU:HD22	1.99	0.43
8:O:410:PRO:O	8:O:415:THR:OG1	2.33	0.43
4:B:375:LEU:HD21	4:B:390:LEU:HD22	2.01	0.43
2:N:378:ALA:HB1	2:N:381:PHE:HB3	1.99	0.43
4:J:218:PHE:HB3	4:J:362:PHE:HB2	2.00	0.43
1:A:97:LEU:HD13	1:A:450:VAL:HG21	2.01	0.43
6:D:210:ASP:HB3	6:D:388:THR:HG22	2.00	0.43
8:G:482:ILE:CG2	11:G:602:ADP:C2	3.02	0.43
3:I:533:LEU:HD21	6:L:84:MET:HG2	1.99	0.43
5:K:43:PRO:O	5:K:163:LYS:NZ	2.42	0.43
7:M:179:ASN:O	7:M:182:HIS:ND1	2.51	0.43
2:F:34:GLU:OE2	2:F:37:ARG:NE	2.52	0.43
4:B:123:PRO:HA	4:B:126:ILE:HD12	2.00	0.43
4:B:203:LYS:NZ	4:B:384:ASP:OD1	2.52	0.43
4:J:347:LYS:HD3	4:J:362:PHE:HB3	2.00	0.43
5:K:241:LEU:HD11	5:K:335:PRO:HG3	2.00	0.43
5:K:272:GLU:OE2	5:K:276:GLN:NE2	2.51	0.43
7:E:248:ILE:HD12	7:E:337:THR:HG21	2.01	0.43
2:F:147:ASP:HB3	2:F:150:GLU:HB2	2.01	0.43
3:H:350:GLU:HB2	3:H:365:LYS:HB2	2.00	0.43
8:G:182:LEU:HD22	8:G:217:VAL:HG23	2.01	0.43
3:I:148:LEU:HD21	3:I:403:LEU:HD21	2.01	0.43
8:O:90:SER:HB3	8:O:101:THR:HG23	2.00	0.43
1:A:154:THR:HG23	11:A:602:ADP:N7	2.34	0.43
4:B:127:ILE:HG13	4:B:515:LEU:HD23	2.00	0.43
6:D:304:GLN:HA	6:D:331:ILE:HB	2.00	0.43
7:E:99:ASP:OD1	7:E:99:ASP:N	2.52	0.43
8:G:170:SER:CB	11:G:602:ADP:C5'	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:132:ILE:HD11	3:I:419:LEU:HD11	2.00	0.43
8:O:169:MET:HE3	11:O:602:ADP:C5	2.41	0.43
7:E:38:ILE:HD13	7:E:121:GLU:HB2	2.00	0.43
5:K:495:ILE:HD11	11:K:602:ADP:N6	2.33	0.43
8:G:222:VAL:HG11	8:G:376:VAL:HG22	2.01	0.43
5:K:292:THR:HB	5:K:313:ARG:HA	2.00	0.43
1:A:214:HIS:HB2	1:A:313:LEU:HG	2.01	0.42
4:B:138:ARG:HD2	4:B:505:LEU:HD21	2.01	0.42
7:E:59:LYS:HD2	7:E:77:ILE:HD13	2.01	0.42
5:K:47:MET:H	9:P:517:LEU:HB3	1.84	0.42
1:A:411:ALA:HB1	1:A:479:ILE:H	1.84	0.42
7:E:212:GLU:HG3	7:E:386:PHE:HD1	1.84	0.42
3:I:214:TYR:HB2	3:I:364:ILE:HB	2.00	0.42
8:G:99:ASP:OD1	11:G:602:ADP:O2B	2.36	0.42
8:G:206:LYS:HA	8:G:385:MET:HE2	2.01	0.42
9:P:305:LEU:HD22	9:P:310:ILE:HG21	2.01	0.42
7:E:251:LEU:HB2	7:E:344:ARG:HD3	2.01	0.42
3:I:234:ILE:O	3:I:346:GLY:N	2.51	0.42
1:A:31:GLN:HG3	1:A:97:LEU:HD23	2.00	0.42
1:A:292:ILE:HG23	1:A:313:LEU:HD22	2.00	0.42
7:E:38:ILE:HG21	7:E:121:GLU:HB2	2.00	0.42
2:F:33:ALA:HB1	2:F:99:LEU:HD23	2.02	0.42
3:H:131:TYR:OH	3:H:475:GLN:OE1	2.37	0.42
3:I:103:ASN:OD1	3:I:444:SER:OG	2.35	0.42
8:O:73:LEU:HD11	8:O:105:LEU:HD11	2.02	0.42
4:B:403:ASP:OD2	4:B:498:GLN:NE2	2.48	0.42
6:D:479:THR:HG23	6:D:503:ILE:HD11	2.01	0.42
8:G:169:MET:HE1	11:G:602:ADP:HN61	1.80	0.42
2:N:34:GLU:OE2	2:N:37:ARG:NE	2.52	0.42
2:N:486:ASP:HB3	2:N:489:GLU:HB2	2.01	0.42
4:J:25:ARG:HB2	4:J:518:ASP:HA	2.01	0.42
4:J:127:ILE:HG13	4:J:515:LEU:HD23	2.02	0.42
1:A:338:ASP:OD1	1:A:338:ASP:N	2.52	0.42
3:H:86:VAL:HG11	3:H:509:VAL:HG13	2.01	0.42
8:G:114:LEU:HD22	8:G:440:LYS:HD2	2.01	0.42
6:L:224:CYS:HA	6:L:394:ARG:HD3	2.02	0.42
7:M:236:HIS:HD2	7:M:311:ASN:HD21	1.68	0.42
8:O:100:GLY:CA	11:O:602:ADP:PB	3.05	0.42
1:A:294:GLN:HA	1:A:316:ALA:H	1.85	0.42
5:C:158:SER:HB3	5:C:495:ILE:HA	2.02	0.42
6:D:320:LEU:O	6:D:324:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:378:ALA:HB3	4:J:383:LEU:HB2	2.02	0.42
6:L:141:GLN:OE1	6:L:530:ARG:NH1	2.52	0.42
7:M:98:GLN:HB2	7:M:519:LEU:HD22	2.01	0.42
7:M:188:ILE:HG23	7:M:224:LEU:HD12	2.01	0.42
7:M:307:ASP:OD1	7:M:307:ASP:N	2.53	0.42
1:A:149:LEU:HA	1:A:173:VAL:HG21	2.02	0.42
2:N:198:LYS:HD3	2:N:216:PHE:HB2	2.02	0.42
2:N:295:ILE:HD13	2:N:303:PHE:HE2	1.85	0.41
4:J:290:PHE:N	4:J:310:MET:O	2.53	0.41
7:M:202:ARG:NH2	7:M:413:ILE:O	2.49	0.41
7:M:243:VAL:HB	7:M:359:VAL:HB	2.02	0.41
2:F:155:LEU:HD22	2:F:396:VAL:HG13	2.01	0.41
5:C:325:ARG:HH21	5:C:371:ALA:HA	1.86	0.41
8:G:238:LYS:HB2	8:G:288:ALA:HA	2.01	0.41
2:N:75:ALA:HA	8:O:55:MET:HE1	2.02	0.41
4:J:29:PHE:HD2	4:J:114:GLU:HG3	1.84	0.41
4:J:237:ILE:HG12	4:J:289:CYS:HB3	2.02	0.41
5:K:217:GLY:HA3	5:K:363:ILE:HG22	2.01	0.41
5:K:232:TYR:HD1	5:K:351:GLU:HA	1.85	0.41
6:L:438:ARG:NH1	6:L:441:GLU:OE1	2.49	0.41
3:H:406:LYS:HD3	3:H:406:LYS:HA	1.92	0.41
4:B:204:LYS:HD2	4:B:357:ASP:HB2	2.02	0.41
6:D:212:LYS:HB3	6:D:390:THR:HG23	2.01	0.41
8:G:240:ALA:HB3	8:G:291:VAL:HG22	2.01	0.41
3:I:86:VAL:HG11	3:I:509:VAL:HG13	2.02	0.41
4:J:433:ALA:HA	4:J:436:MET:HE3	2.02	0.41
1:A:114:LEU:HD11	9:P:460:GLN:HG3	2.03	0.41
1:A:218:HIS:HB3	1:A:221:MET:HG3	2.02	0.41
8:G:118:LEU:HD22	8:G:123:LEU:HD12	2.02	0.41
7:M:59:LYS:HD2	7:M:77:ILE:HG21	2.02	0.41
7:M:198:ASP:HB3	7:M:201:ARG:HG2	2.01	0.41
1:A:55:LYS:HD2	1:A:385:THR:HG21	2.03	0.41
2:F:75:ALA:HA	8:G:55:MET:HE1	2.03	0.41
3:H:171:LEU:HG	3:H:210:LEU:HD22	2.01	0.41
8:G:158:ASP:OD1	8:G:181:LYS:NZ	2.54	0.41
3:I:32:VAL:HA	3:I:43:LYS:HE3	2.01	0.41
1:A:519:ASP:OD1	1:A:519:ASP:N	2.52	0.41
5:C:133:MET:HE2	5:C:444:LEU:HD11	2.02	0.41
8:G:440:LYS:HD3	8:G:440:LYS:HA	1.89	0.41
5:K:23:GLN:NE2	5:K:519:ILE:O	2.54	0.41
5:K:412:GLY:HA3	5:K:448:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:80:ASP:OD2	3:H:84:LYS:NZ	2.53	0.41
6:D:313:SER:OG	6:D:314:ASP:N	2.52	0.41
8:G:114:LEU:HB3	8:G:440:LYS:HD2	2.03	0.41
1:A:117:ARG:HD3	5:C:44:LYS:HD2	2.01	0.41
1:A:127:LYS:HD3	1:A:509:THR:HG21	2.02	0.41
3:H:18:ARG:HH22	3:H:528:ASP:HB3	1.86	0.41
2:N:403:ASP:OD1	2:N:403:ASP:N	2.51	0.41
5:K:298:ASP:OD1	5:K:298:ASP:N	2.45	0.41
1:A:85:ASP:OD1	1:A:92:THR:OG1	2.38	0.41
1:A:290:VAL:HG12	1:A:311:LEU:HB2	2.03	0.41
1:A:410:GLY:HA3	1:A:494:VAL:HG12	2.03	0.41
2:F:168:ILE:HG13	2:F:169:SER:N	2.36	0.41
3:H:128:ALA:HB1	3:H:419:LEU:HD13	2.02	0.41
3:H:467:LEU:HD22	3:H:488:LEU:HG	2.03	0.41
4:B:518:ASP:OD1	4:B:518:ASP:N	2.54	0.41
5:C:327:CYS:HA	5:C:346:GLY:HA3	2.03	0.41
8:G:100:GLY:HA2	11:G:602:ADP:PB	2.61	0.41
3:I:526:ARG:O	6:L:61:ASP:N	2.54	0.41
5:K:401:VAL:HG12	5:K:498:PRO:HB3	2.03	0.41
8:O:118:LEU:HD22	8:O:123:LEU:HD12	2.03	0.41
8:O:497:VAL:HG13	11:O:602:ADP:C8	2.56	0.41
6:D:446:LEU:HD12	6:D:454:ILE:HG13	2.03	0.41
8:G:283:ILE:HD12	8:G:291:VAL:HG21	2.02	0.41
5:K:27:ILE:HG12	5:K:106:LEU:HB3	2.02	0.41
6:L:320:LEU:HD13	6:L:325:ILE:HD11	2.03	0.41
8:O:242:TYR:HD1	8:O:333:LEU:HB2	1.86	0.41
1:A:260:VAL:HB	1:A:264:ARG:HH21	1.86	0.40
2:N:463:LYS:HB3	2:N:484:ILE:HD13	2.01	0.40
3:H:351:VAL:HG13	3:H:364:ILE:HG13	2.02	0.40
4:B:200:HIS:NE2	4:B:322:ARG:HB2	2.35	0.40
6:D:193:ALA:HB1	6:D:389:VAL:HG21	2.04	0.40
7:E:37:HIS:CG	7:E:87:ILE:HG13	2.56	0.40
3:I:166:ASP:O	3:I:170:ASN:ND2	2.48	0.40
5:K:44:LYS:HD3	9:P:117:ARG:HG2	2.03	0.40
9:P:88:THR:HG21	9:P:500:VAL:HA	2.03	0.40
2:F:87:ASP:OD1	2:F:87:ASP:N	2.54	0.40
6:L:283:ARG:HG2	6:L:315:LEU:HD22	2.03	0.40
4:B:200:HIS:CE1	4:B:319:GLY:HA2	2.57	0.40
6:D:249:ILE:HB	6:D:343:ILE:HG21	2.04	0.40
6:L:223:ASP:O	6:L:394:ARG:NH1	2.54	0.40
9:P:164:LEU:HD21	9:P:387:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:420:GLU:HG3	9:P:470:HIS:HD2	1.86	0.40
9:P:519:ASP:N	9:P:519:ASP:OD1	2.53	0.40
1:A:453:GLN:HG3	1:A:459:LEU:HD12	2.04	0.40
3:H:357:CYS:SG	3:H:378:ARG:NH2	2.95	0.40
4:B:235:ALA:N	4:B:346:CYS:O	2.51	0.40
5:C:165:ILE:HG22	5:C:168:TRP:HE1	1.86	0.40
4:J:200:HIS:NE2	4:J:219:LEU:O	2.54	0.40
6:L:55:LEU:O	6:L:471:ASN:ND2	2.54	0.40
7:M:130:PRO:HA	7:M:133:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/531 (90%)	465 (97%)	15 (3%)	0	100	100
2	F	465/543 (86%)	458 (98%)	7 (2%)	0	100	100
2	N	472/543 (87%)	454 (96%)	18 (4%)	0	100	100
3	H	459/556 (83%)	445 (97%)	13 (3%)	1 (0%)	43	71
3	I	459/556 (83%)	450 (98%)	9 (2%)	0	100	100
4	B	475/535 (89%)	467 (98%)	7 (2%)	1 (0%)	43	71
4	J	475/535 (89%)	461 (97%)	13 (3%)	1 (0%)	43	71
5	C	483/545 (89%)	466 (96%)	16 (3%)	1 (0%)	43	71
5	K	483/545 (89%)	470 (97%)	11 (2%)	2 (0%)	30	59
6	D	487/542 (90%)	473 (97%)	13 (3%)	1 (0%)	43	71
6	L	487/542 (90%)	480 (99%)	7 (1%)	0	100	100
7	E	486/541 (90%)	465 (96%)	21 (4%)	0	100	100
7	M	486/541 (90%)	472 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	475/548 (87%)	469 (99%)	6 (1%)	0	100	100
8	O	475/548 (87%)	466 (98%)	9 (2%)	0	100	100
9	P	485/531 (91%)	476 (98%)	9 (2%)	0	100	100
All	All	7632/8682 (88%)	7437 (97%)	188 (2%)	7 (0%)	49	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	K	447	ILE
4	B	299	TYR
3	H	357	CYS
4	J	146	VAL
5	C	185	PHE
5	K	352	ILE
6	D	178	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	406/442 (92%)	406 (100%)	0	100	100
2	F	384/445 (86%)	384 (100%)	0	100	100
2	N	390/445 (88%)	390 (100%)	0	100	100
3	H	385/461 (84%)	385 (100%)	0	100	100
3	I	385/461 (84%)	385 (100%)	0	100	100
4	B	383/429 (89%)	383 (100%)	0	100	100
4	J	383/429 (89%)	383 (100%)	0	100	100
5	C	421/470 (90%)	421 (100%)	0	100	100
5	K	421/470 (90%)	421 (100%)	0	100	100
6	D	417/454 (92%)	417 (100%)	0	100	100
6	L	417/454 (92%)	417 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	409/455 (90%)	409 (100%)	0	100	100
7	M	409/455 (90%)	409 (100%)	0	100	100
8	G	398/452 (88%)	398 (100%)	0	100	100
8	O	398/452 (88%)	398 (100%)	0	100	100
9	P	406/440 (92%)	406 (100%)	0	100	100
All	All	6412/7214 (89%)	6412 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	37	ASN
1	A	61	ASN
1	A	286	ASN
2	F	21	GLN
2	F	380	GLN
3	H	164	ASN
3	H	284	ASN
4	B	65	ASN
4	B	78	ASN
4	B	91	GLN
4	B	124	GLN
4	B	148	HIS
4	B	380	GLN
4	B	399	GLN
5	C	148	ASN
5	C	235	ASN
5	C	390	ASN
5	C	442	GLN
5	C	504	GLN
6	D	65	GLN
6	D	274	GLN
6	D	299	ASN
6	D	409	HIS
6	D	475	ASN
7	E	376	GLN
7	E	379	ASN
7	E	469	ASN

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Mol	Chain	Res	Type
7	E	522	GLN
8	G	213	HIS
2	N	233	HIS
2	N	448	GLN
3	I	187	GLN
3	I	223	GLN
3	I	353	GLN
4	J	195	ASN
5	K	174	ASN
5	K	184	GLN
5	K	221	ASN
5	K	276	GLN
5	K	301	GLN
5	K	396	GLN
6	L	83	GLN
6	L	101	GLN
6	L	274	GLN
6	L	299	ASN
6	L	409	HIS
7	M	184	GLN
7	M	236	HIS
7	M	278	GLN
7	M	298	ASN
7	M	469	ASN
7	M	481	GLN
7	M	504	GLN
8	O	279	GLN
8	O	365	HIS
9	P	71	HIS
9	P	198	HIS
9	P	346	HIS
9	P	386	GLN
9	P	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
11	ADP	P	602	10	27,29,29	0.37	0	42,45,45	0.46	0
11	ADP	K	602	10	27,29,29	0.34	0	42,45,45	0.46	0
11	ADP	C	602	-	27,29,29	1.37	4 (14%)	42,45,45	1.91	10 (23%)
11	ADP	A	602	10	27,29,29	0.46	0	42,45,45	0.63	0
11	ADP	O	602	10	27,29,29	0.43	0	42,45,45	0.57	0
11	ADP	G	602	10	27,29,29	0.42	0	42,45,45	0.56	0

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
11	ADP	P	602	10	-	3/16/32/32	0/3/3/3
11	ADP	K	602	10	-	2/16/32/32	0/3/3/3
11	ADP	C	602	-	-	7/16/32/32	0/3/3/3
11	ADP	A	602	10	-	3/16/32/32	0/3/3/3
11	ADP	O	602	10	-	7/16/32/32	0/3/3/3
11	ADP	G	602	10	-	5/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	602	ADP	C5-C4	4.56	1.47	1.39
11	C	602	ADP	C5-C6	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	602	ADP	C8-N7	2.35	1.36	1.31
11	C	602	ADP	C5-N7	-2.24	1.34	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	602	ADP	C5-C4-N3	-6.08	118.82	126.75
11	C	602	ADP	N3-C4-N9	4.79	134.97	127.08
11	C	602	ADP	C2-N3-C4	3.79	120.70	111.75
11	C	602	ADP	N3-C2-N1	-3.18	123.63	128.60
11	C	602	ADP	C4-C5-N7	-2.98	106.98	110.62
11	C	602	ADP	O3B-PB-O2B	2.87	118.59	107.64
11	C	602	ADP	C3'-C2'-C1'	2.57	106.30	101.43
11	C	602	ADP	C5-N7-C8	2.47	107.02	103.51
11	C	602	ADP	C4-N9-C8	2.36	108.29	105.73
11	C	602	ADP	PA-O3A-PB	-2.01	125.93	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	602	ADP	C3'-C4'-C5'-O5'
11	C	602	ADP	C5'-O5'-PA-O2A
11	C	602	ADP	C3'-C4'-C5'-O5'
11	G	602	ADP	C5'-O5'-PA-O1A
11	G	602	ADP	C5'-O5'-PA-O2A
11	G	602	ADP	C3'-C4'-C5'-O5'
11	O	602	ADP	C5'-O5'-PA-O1A
11	O	602	ADP	C5'-O5'-PA-O2A
11	O	602	ADP	C3'-C4'-C5'-O5'
11	G	602	ADP	O4'-C4'-C5'-O5'
11	O	602	ADP	O4'-C4'-C5'-O5'
11	A	602	ADP	O4'-C4'-C5'-O5'
11	C	602	ADP	O4'-C4'-C5'-O5'
11	C	602	ADP	C5'-O5'-PA-O3A
11	G	602	ADP	C5'-O5'-PA-O3A
11	O	602	ADP	C5'-O5'-PA-O3A
11	P	602	ADP	C5'-O5'-PA-O3A
11	K	602	ADP	PB-O3A-PA-O2A
11	P	602	ADP	PB-O3A-PA-O2A
11	A	602	ADP	PB-O3A-PA-O2A
11	C	602	ADP	PB-O3A-PA-O1A

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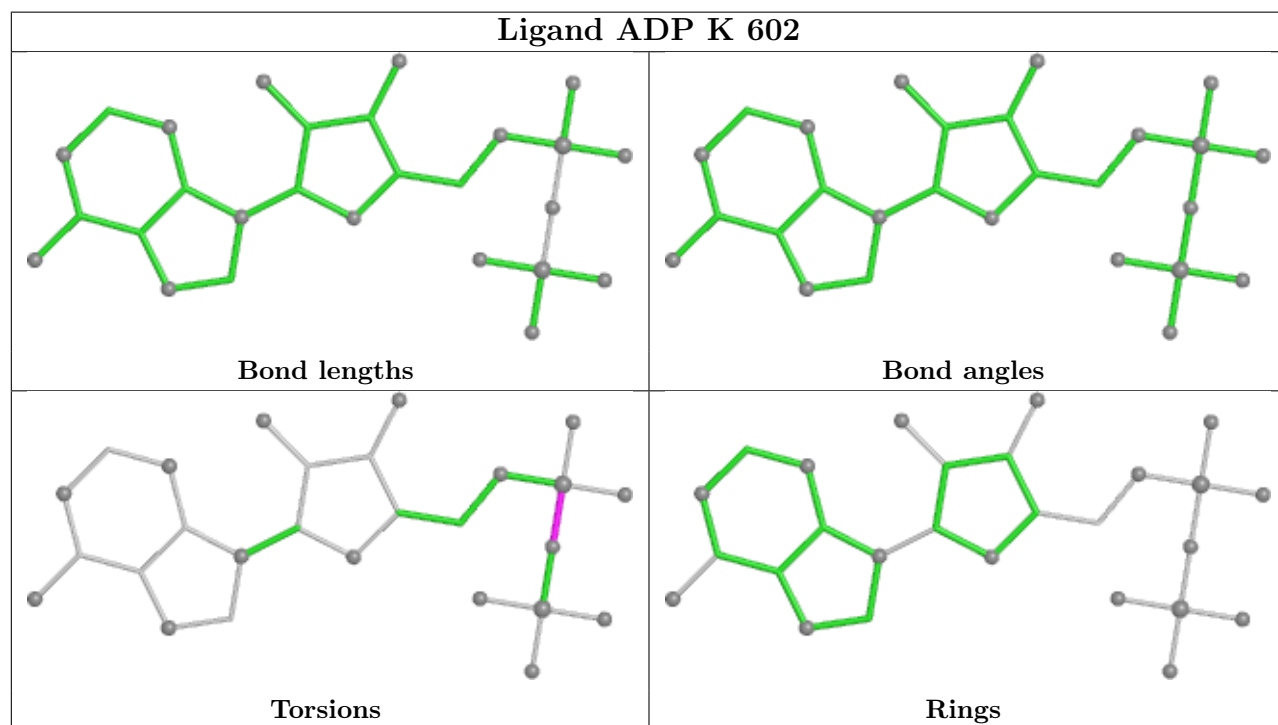
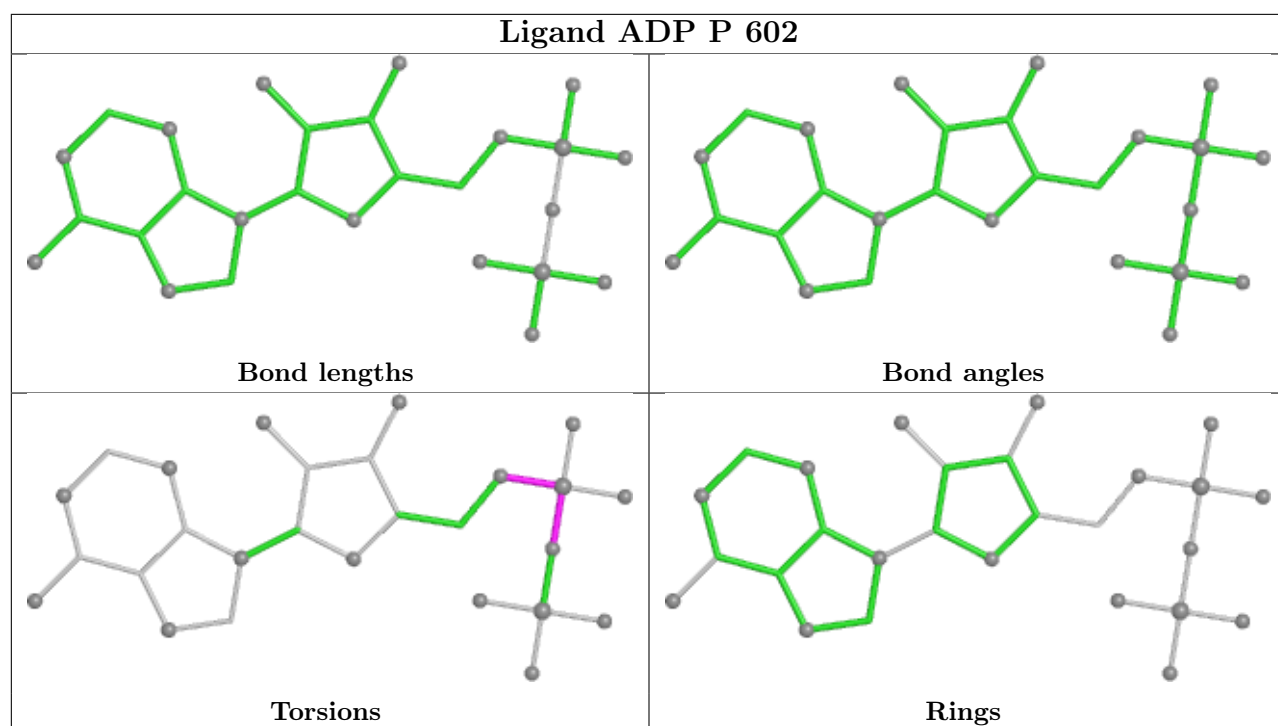
Mol	Chain	Res	Type	Atoms
11	C	602	ADP	PB-O3A-PA-O2A
11	K	602	ADP	PB-O3A-PA-O1A
11	O	602	ADP	PB-O3A-PA-O1A
11	O	602	ADP	PB-O3A-PA-O2A
11	P	602	ADP	PB-O3A-PA-O1A
11	C	602	ADP	C5'-O5'-PA-O1A

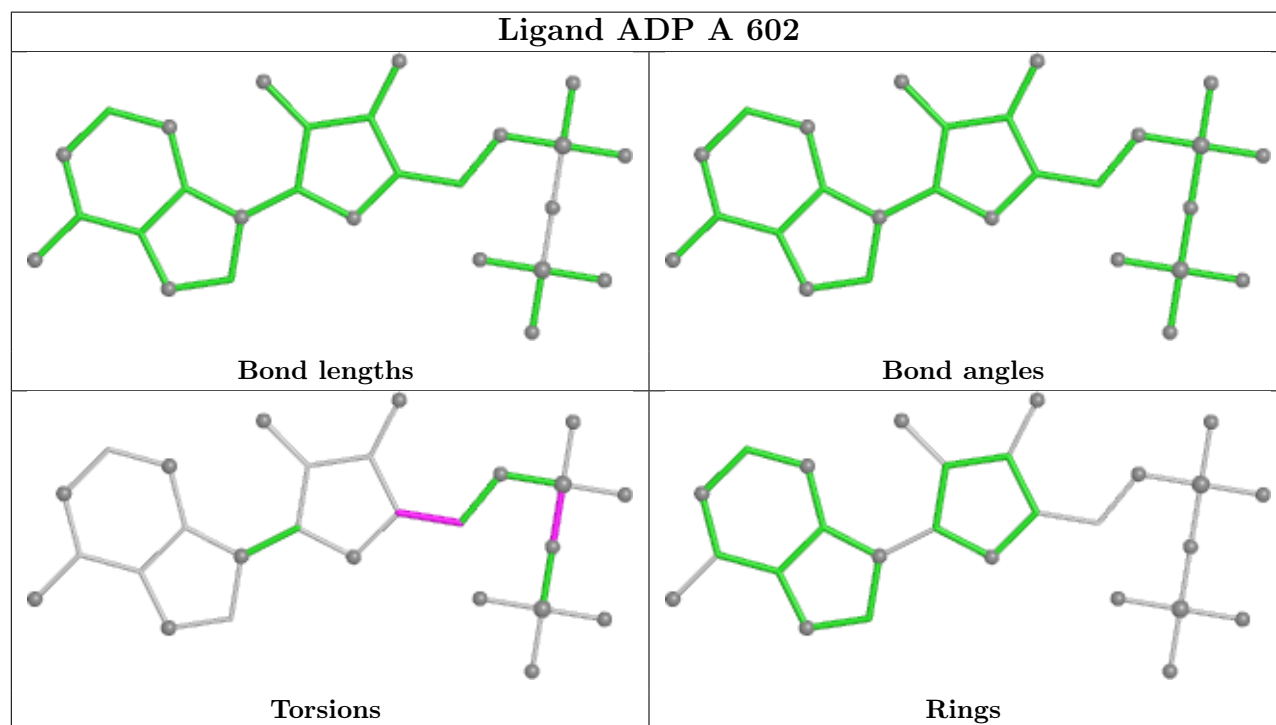
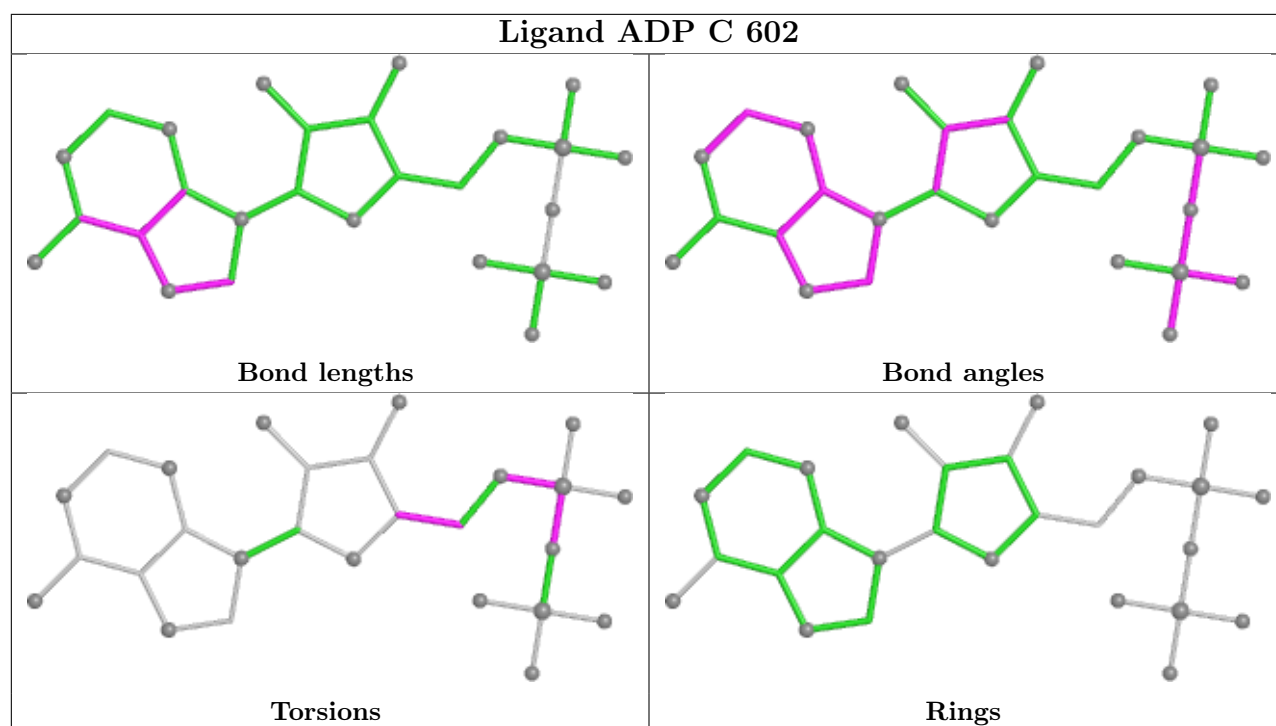
There are no ring outliers.

5 monomers are involved in 91 short contacts:

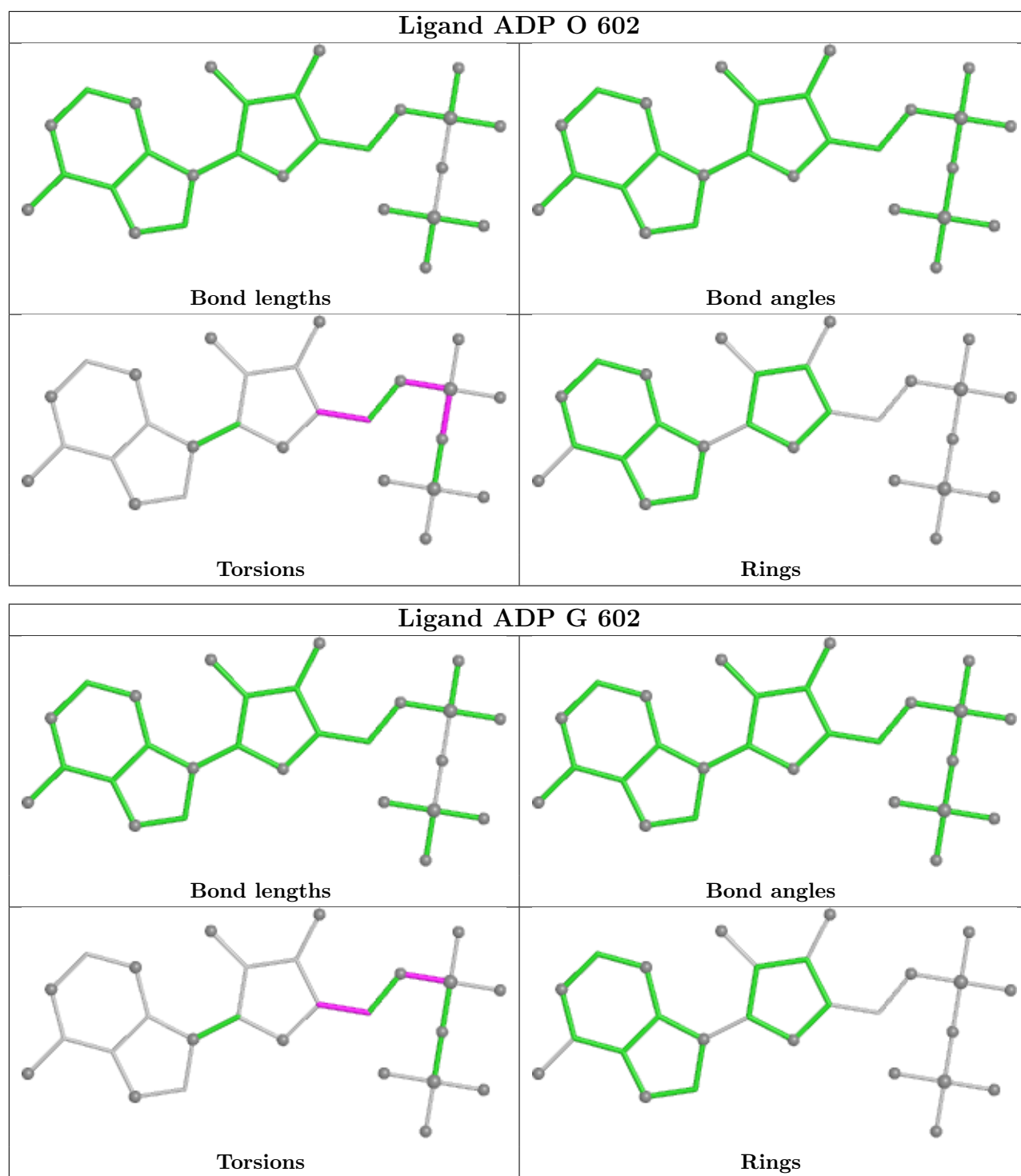
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	602	ADP	11	0
11	K	602	ADP	14	0
11	A	602	ADP	18	0
11	O	602	ADP	25	0
11	G	602	ADP	23	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

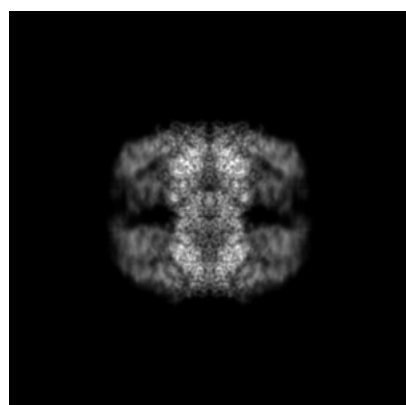
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62249. These allow visual inspection of the internal detail of the map and identification of artifacts.

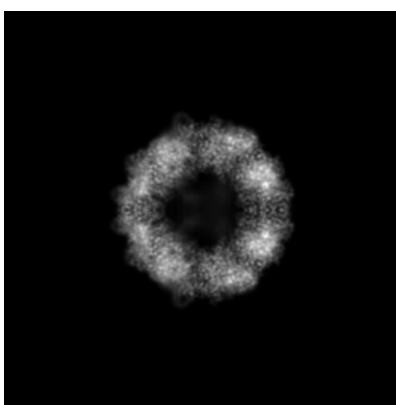
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

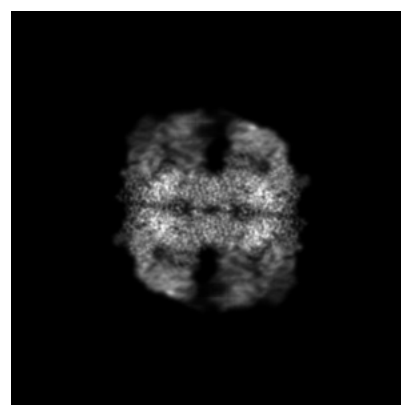
#### 6.1.1 Primary map



X



Y

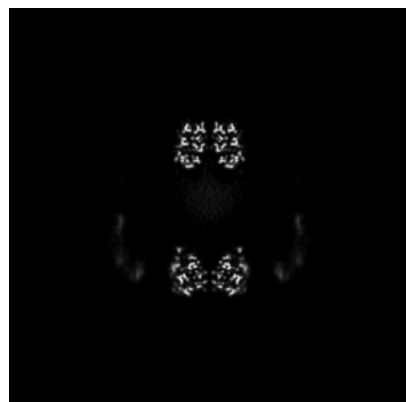


Z

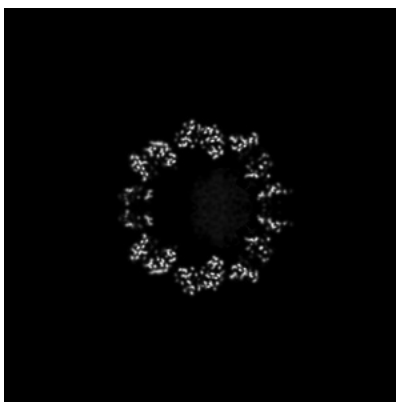
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

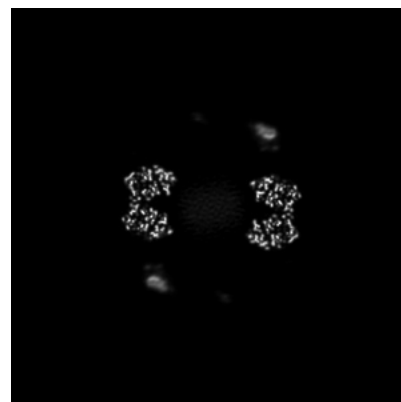
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

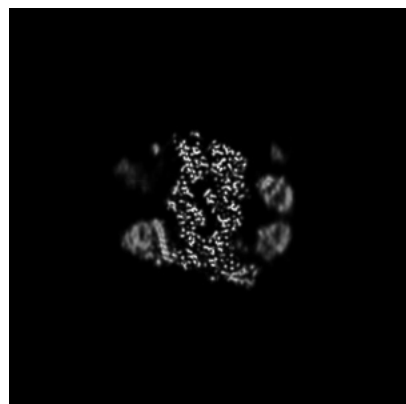


Z Index: 200

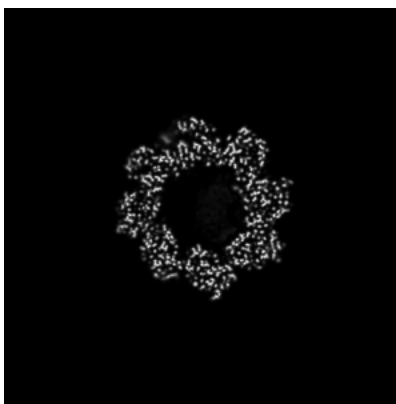
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

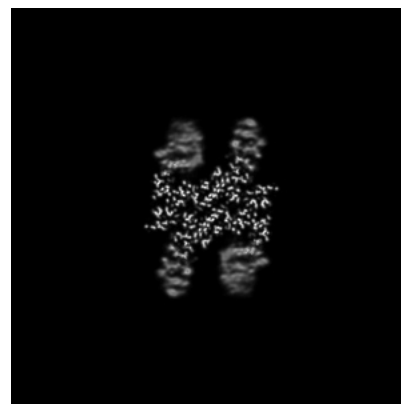
### 6.3.1 Primary map



X Index: 254



Y Index: 218

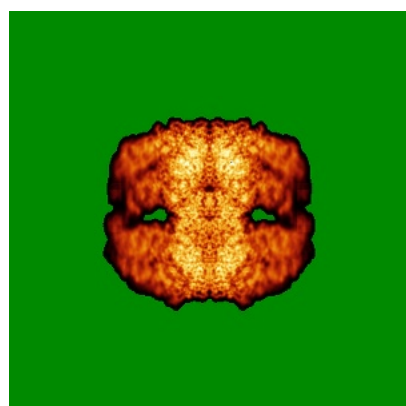


Z Index: 260

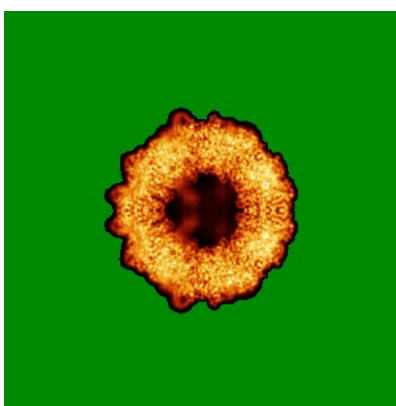
The images above show the largest variance slices of the map in three orthogonal directions.

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

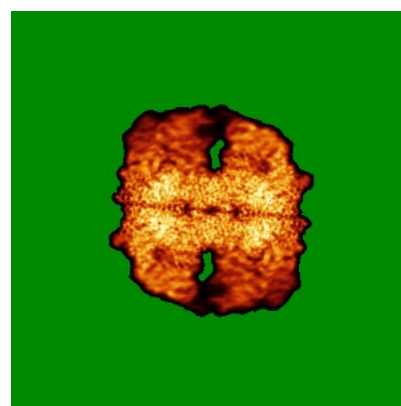
### 6.4.1 Primary map



X



Y

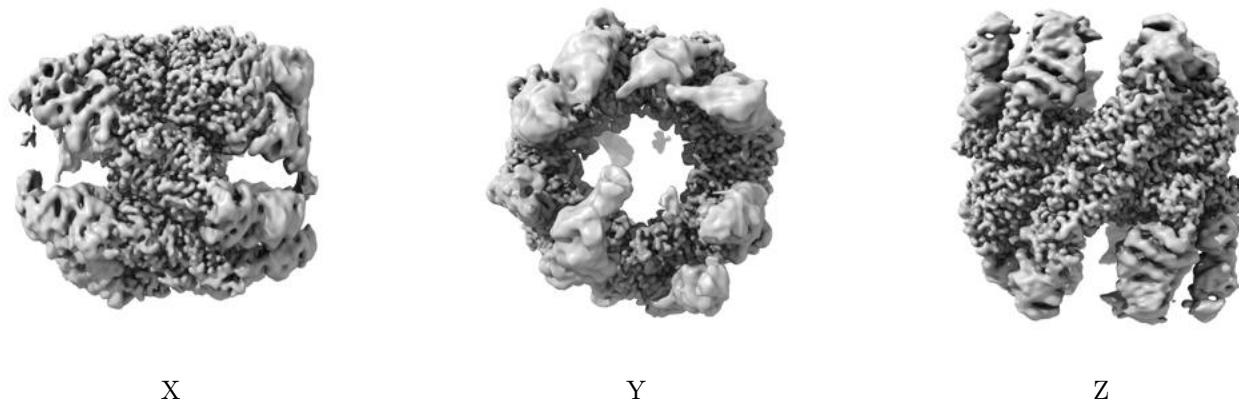


Z

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 [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

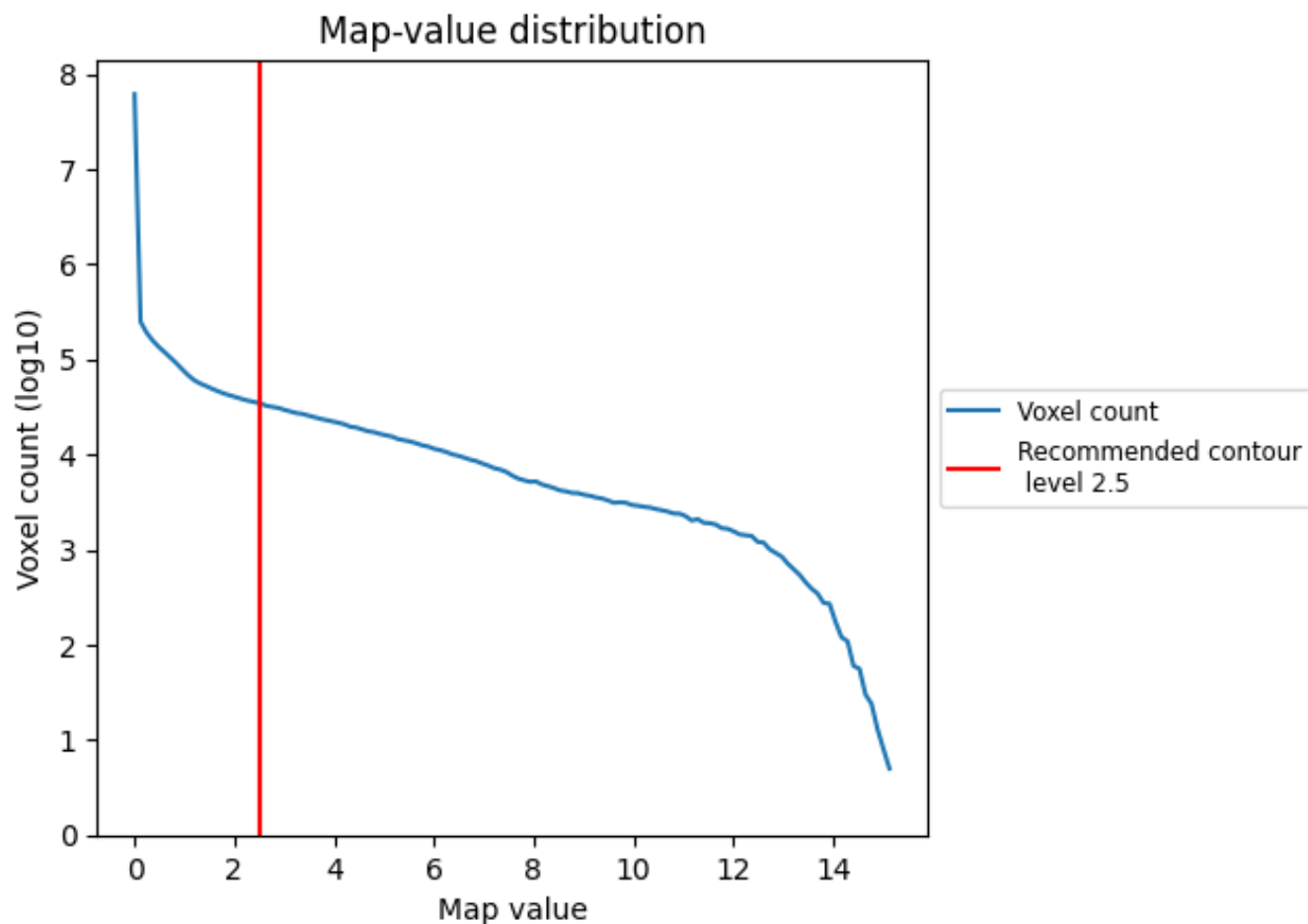
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

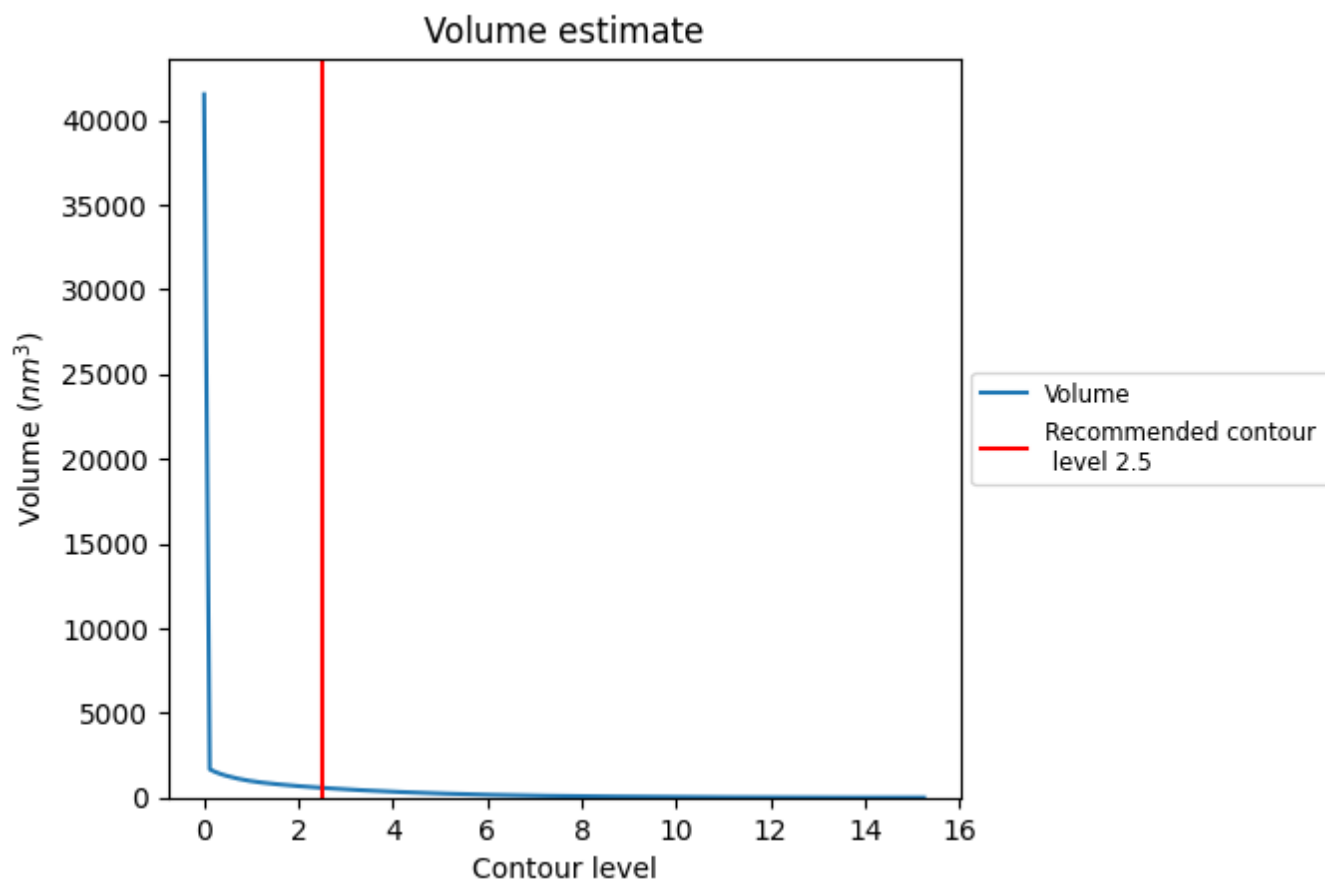
This section contains the results of statistical analysis of the map.

### 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.

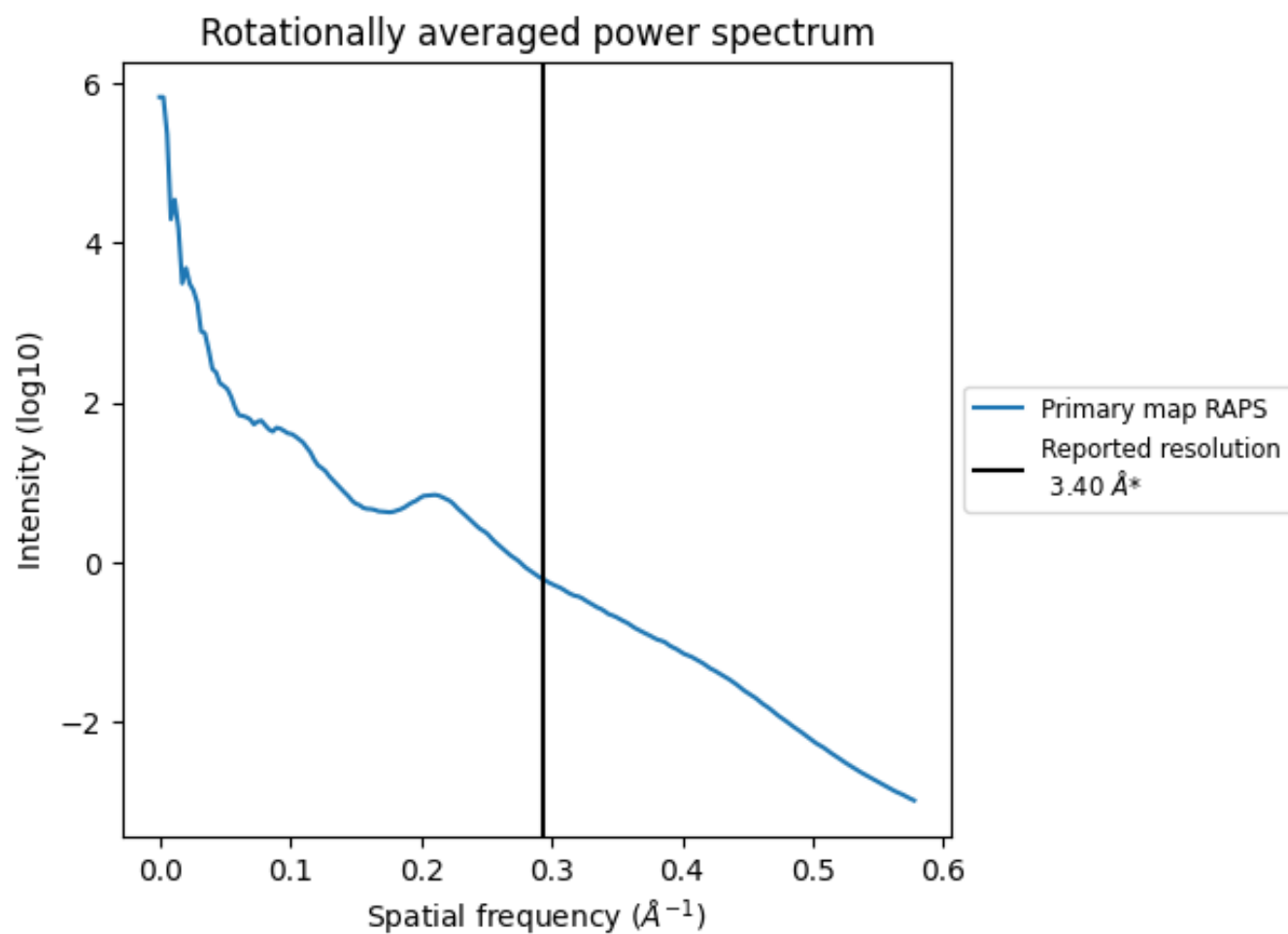
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 574 nm<sup>3</sup>; this corresponds to an approximate mass of 518 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 0.294 Å<sup>-1</sup>



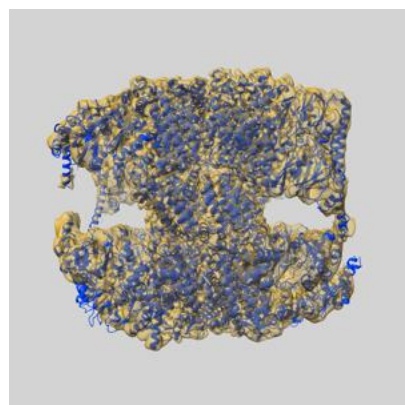
## 8 Fourier-Shell correlation

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

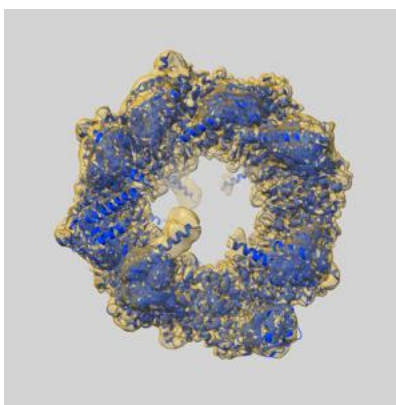
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62249 and PDB model 9KCF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

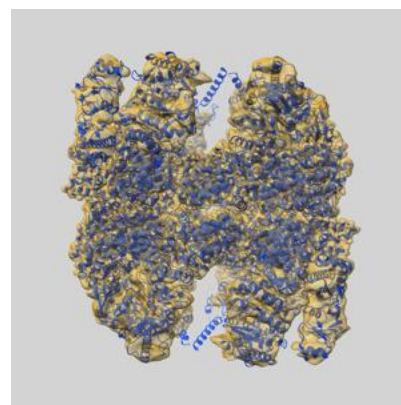
### 9.1 Map-model overlay [i](#)



X



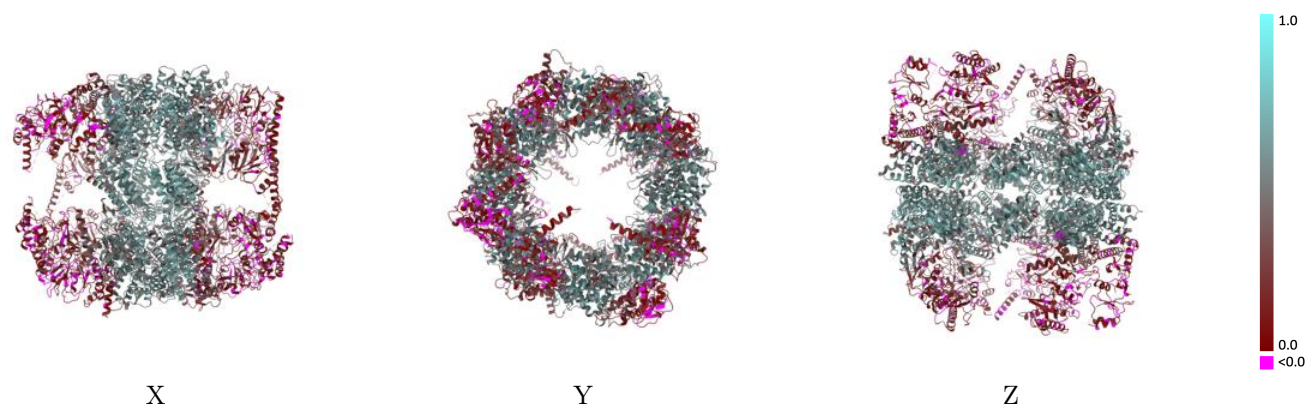
Y



Z

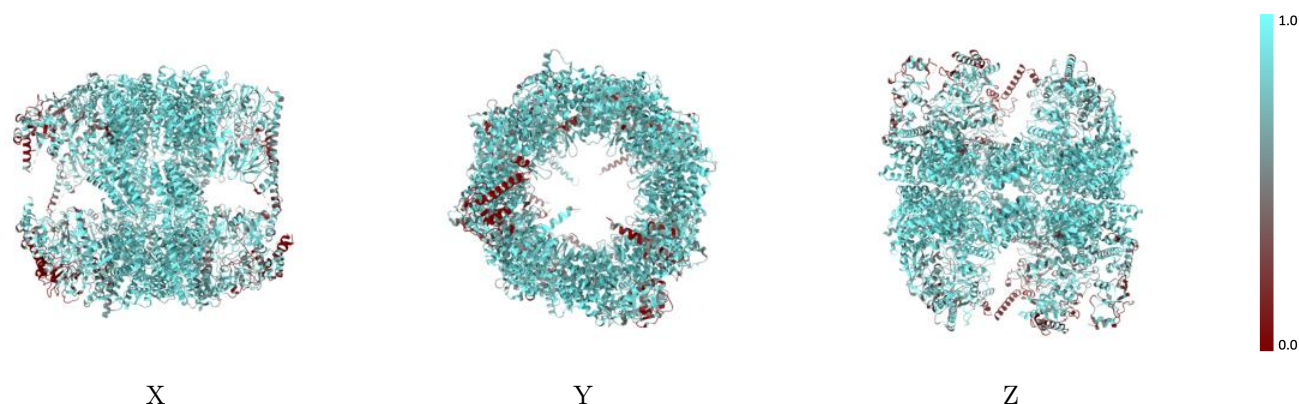
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



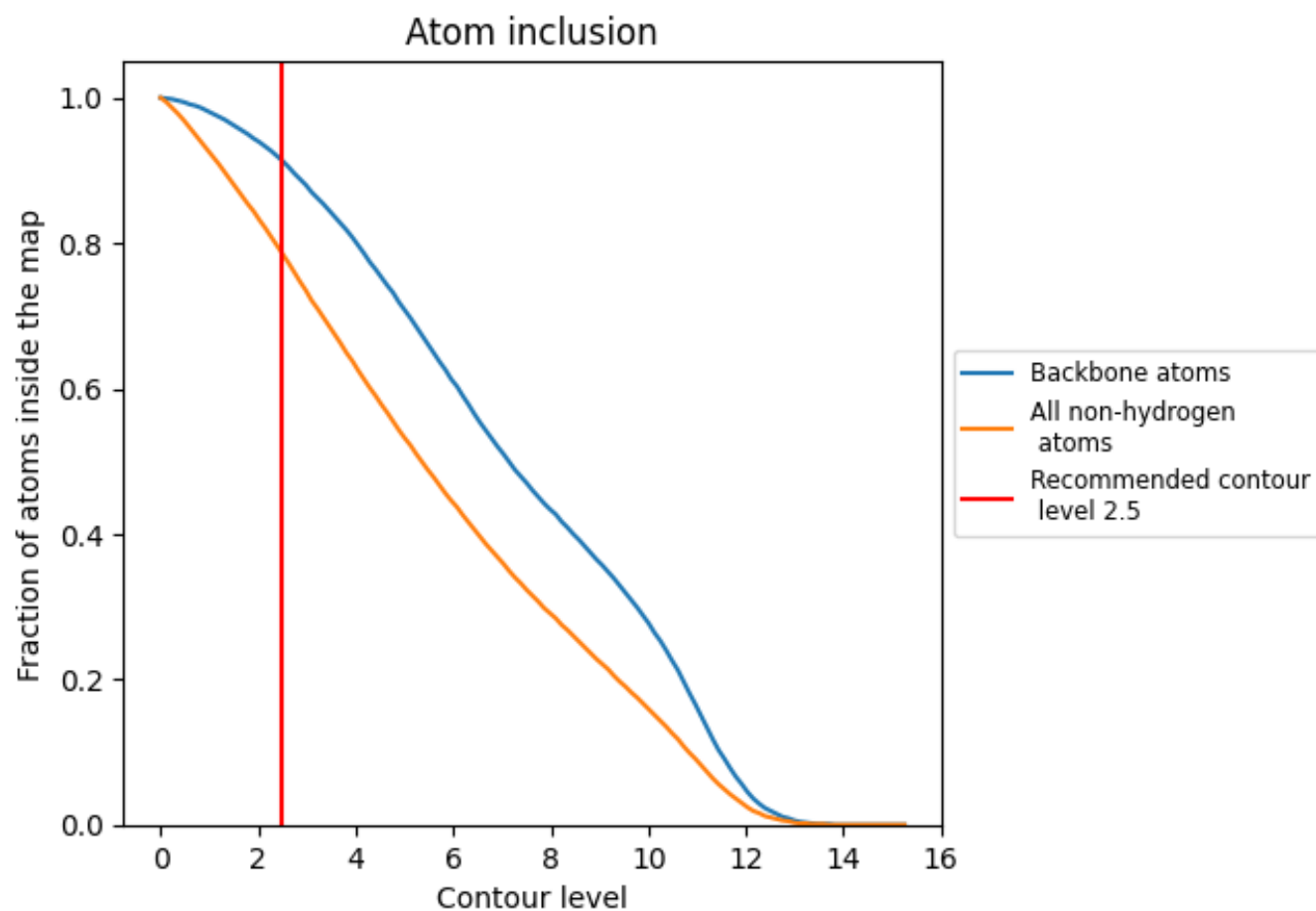
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.3540
A	 0.8500	 0.4080
B	 0.6290	 0.2890
C	 0.7530	 0.3300
D	 0.8170	 0.3360
E	 0.7960	 0.3480
F	 0.8270	 0.3540
G	 0.8530	 0.4370
H	 0.7730	 0.3420
I	 0.7630	 0.3370
J	 0.6210	 0.2730
K	 0.7530	 0.3280
L	 0.8100	 0.3280
M	 0.7950	 0.3490
N	 0.8180	 0.3520
O	 0.8500	 0.4340
P	 0.8460	 0.4070

