



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:26 PM UTC

PDB ID : 7YKZ / pdb_00007ykh
EMDB ID : EMD-32402
Title : Cryo-EM structure of Drg1 hexamer in the planar state treated with ADP/A
MPPNP/Diazaborine
Authors : Ma, C.Y.; Wu, D.M.; Chen, Q.; Gao, N.
Deposited on : 2022-07-25
Resolution : 4.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

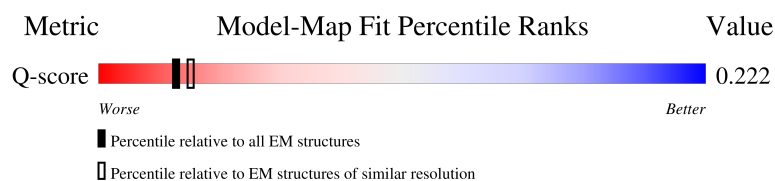
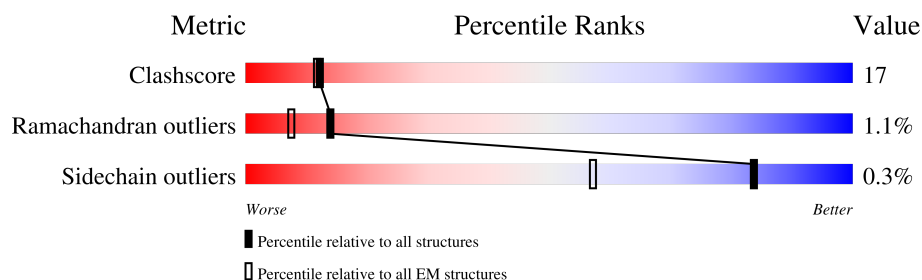
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	A	780	34% 67% 27% 6%
1	B	780	37% 68% 25% 6%
1	C	780	31% 62% 31% 6%
1	D	780	28% 65% 28% 6%

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Mol	Chain	Length	Quality of chain
1	E	780	
1	F	780	

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
2	ADP	F	801	-	-	X	-
3	ATP	C	802	-	-	X	-
3	ATP	D	802	-	-	X	-
3	ATP	E	802	-	-	X	-
4	NDT	A	803	X	-	-	-
4	NDT	B	803	X	-	-	-
4	NDT	D	803	X	-	X	-
4	NDT	D	804	X	-	-	-
4	NDT	E	803	X	-	X	-
4	NDT	F	803	X	-	X	-

2 Entry composition [i](#)

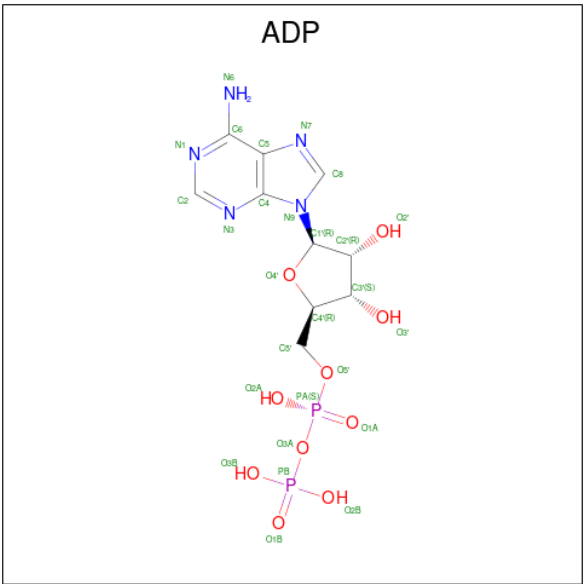
There are 4 unique types of molecules in this entry. The entry contains 34146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATPase family gene 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	734	Total 5613	3535	959	1095	24	0	0
1	F	734	Total 5613	3535	959	1095	24	0	0
1	B	734	Total 5613	3535	959	1095	24	0	0
1	E	734	Total 5613	3535	959	1095	24	0	0
1	A	734	Total 5613	3535	959	1095	24	0	0
1	C	734	Total 5613	3535	959	1095	24	0	0

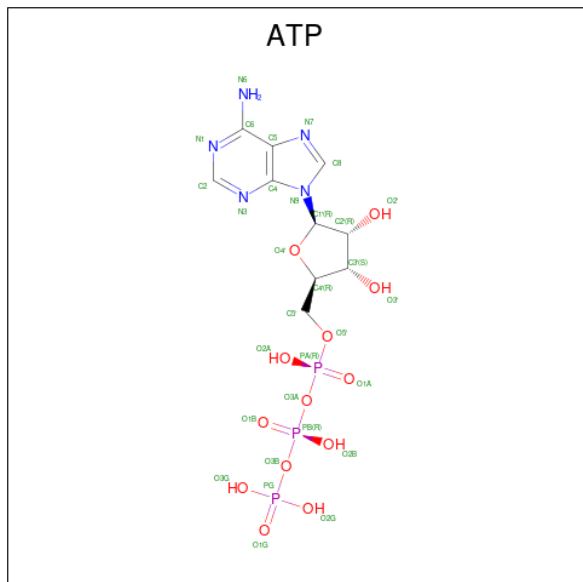
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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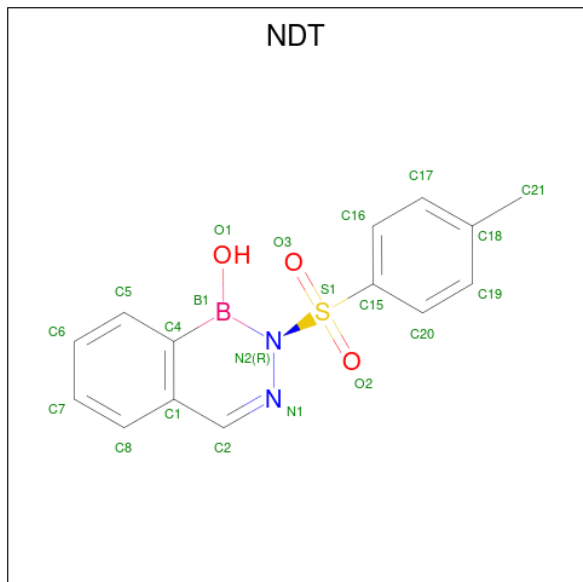
Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is 2-(TOLUENE-4-SULFONYL)-2H-BENZO[D][1,2,3]DIAZABORININ-1-OL (CCD ID: NDT) (formula: $C_{14}H_{13}BN_2O_3S$) (labeled as "Ligand of Interest" by depositor).

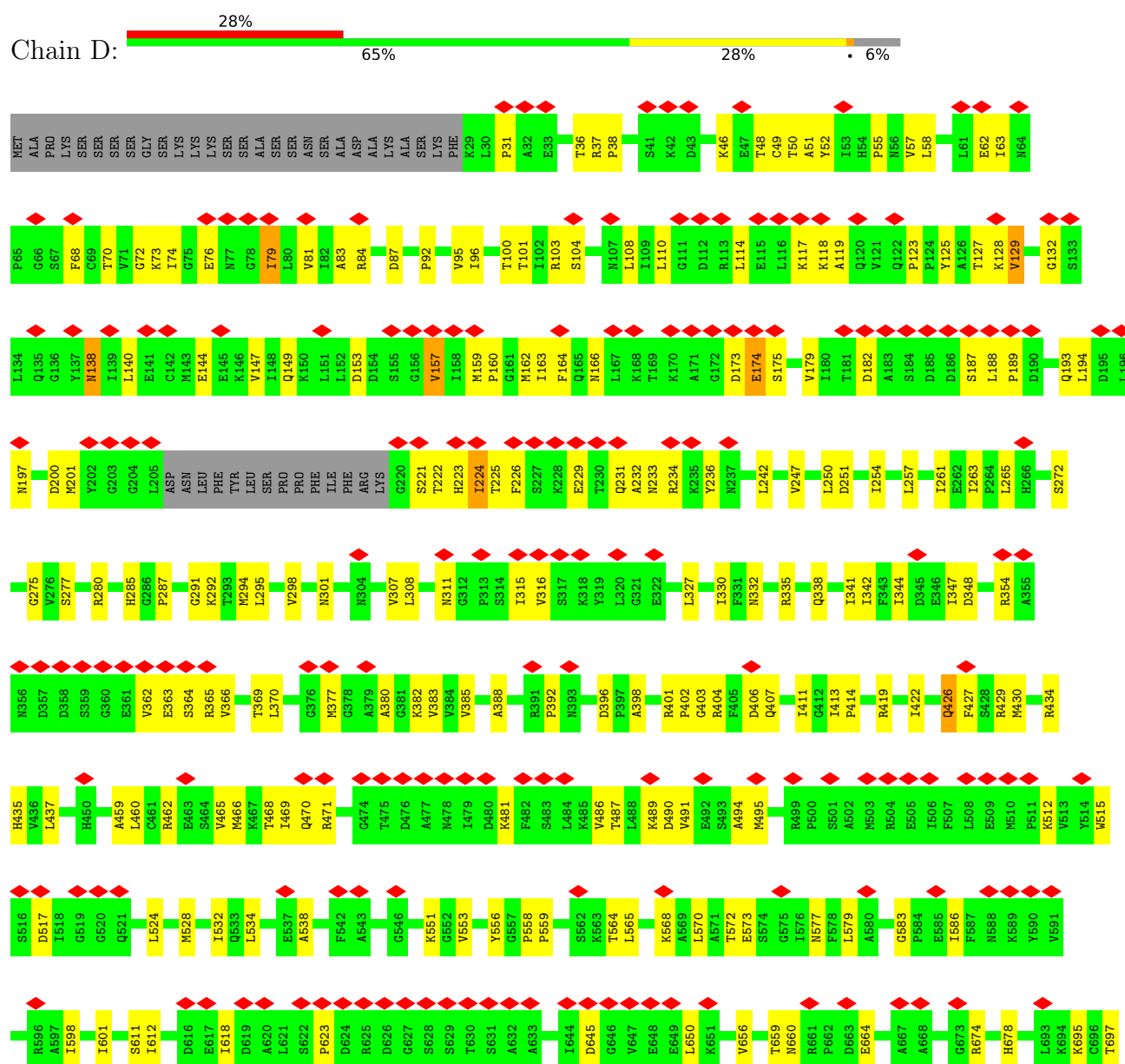


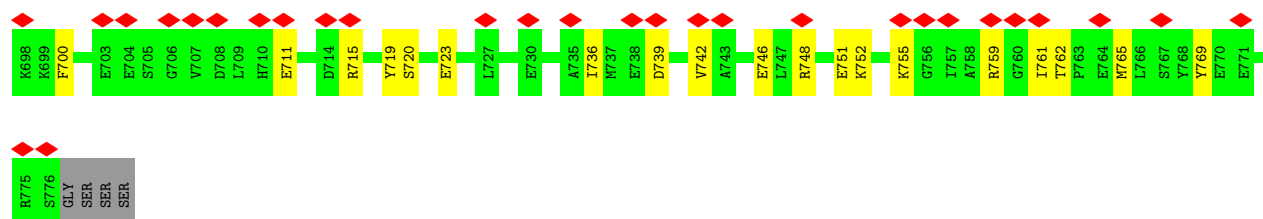
Mol	Chain	Residues	Atoms						AltConf
4	D	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	
4	D	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	
4	F	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	
4	B	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	
4	E	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	
4	A	1	Total	B	C	N	O	S	0
			20	1	14	2	2	1	

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.

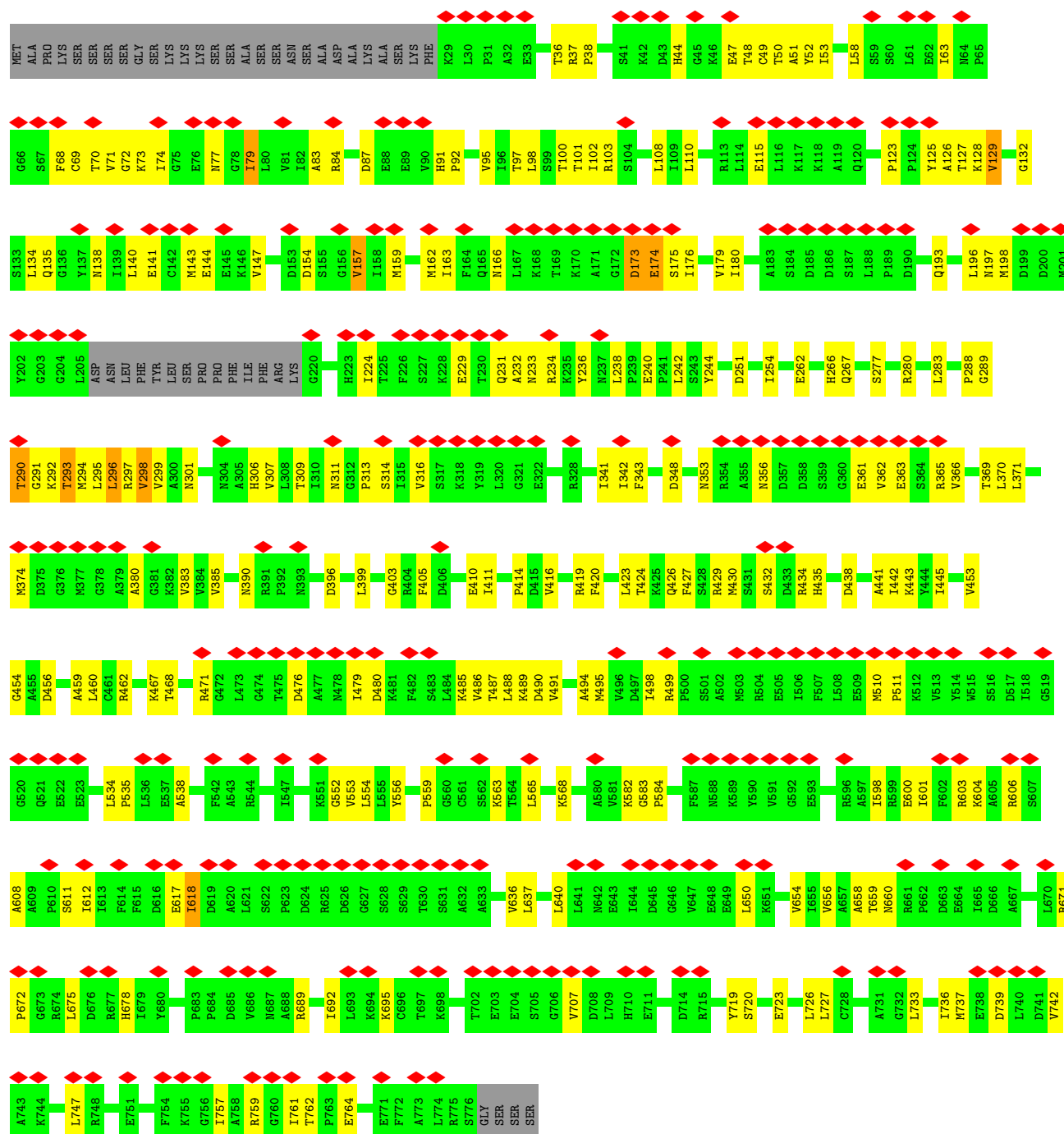
• Molecule 1: ATPase family gene 2 protein



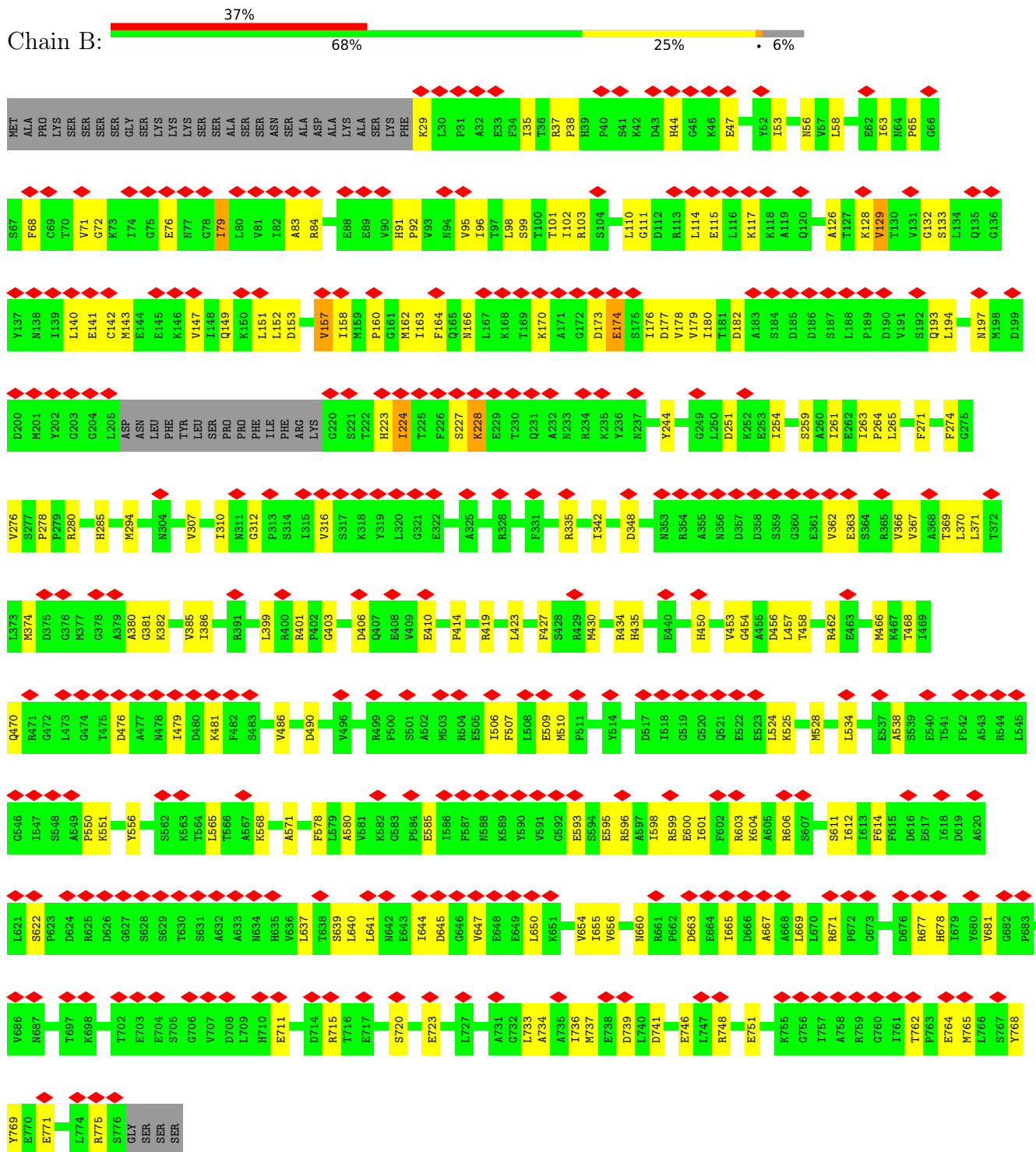


• Molecule 1: ATPase family gene 2 protein

Chain F: 33% 64% 29% 6%

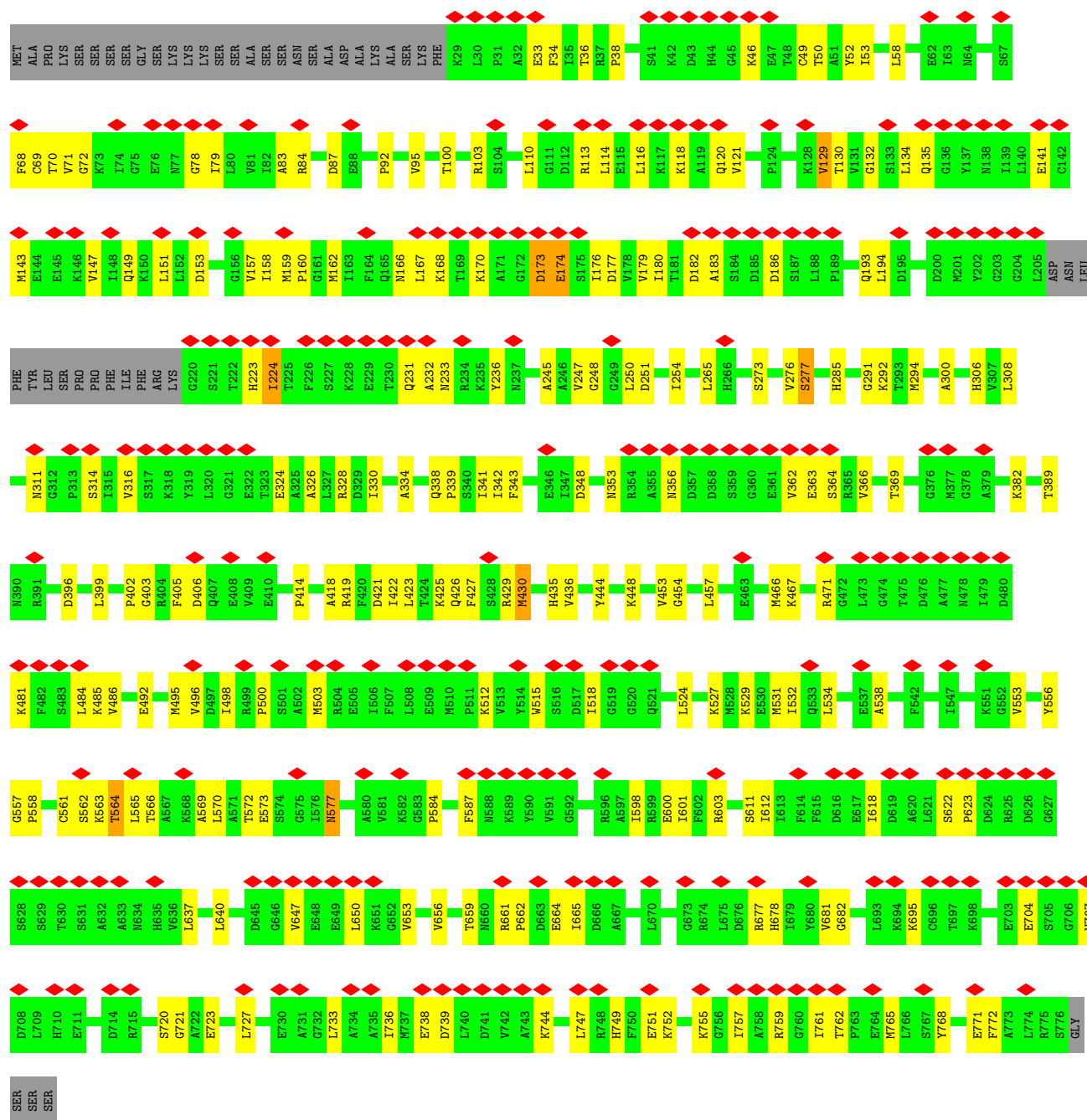


Chain B:

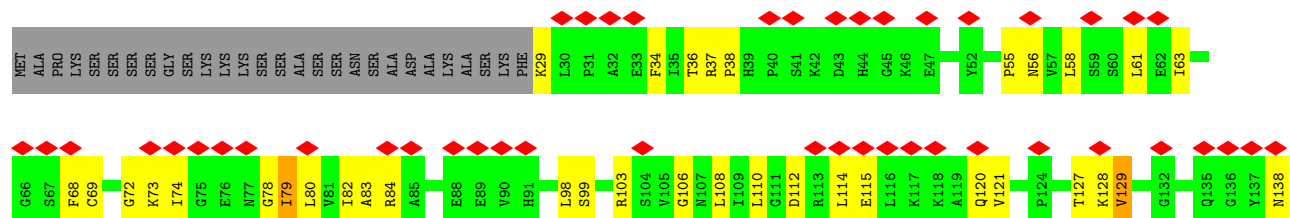


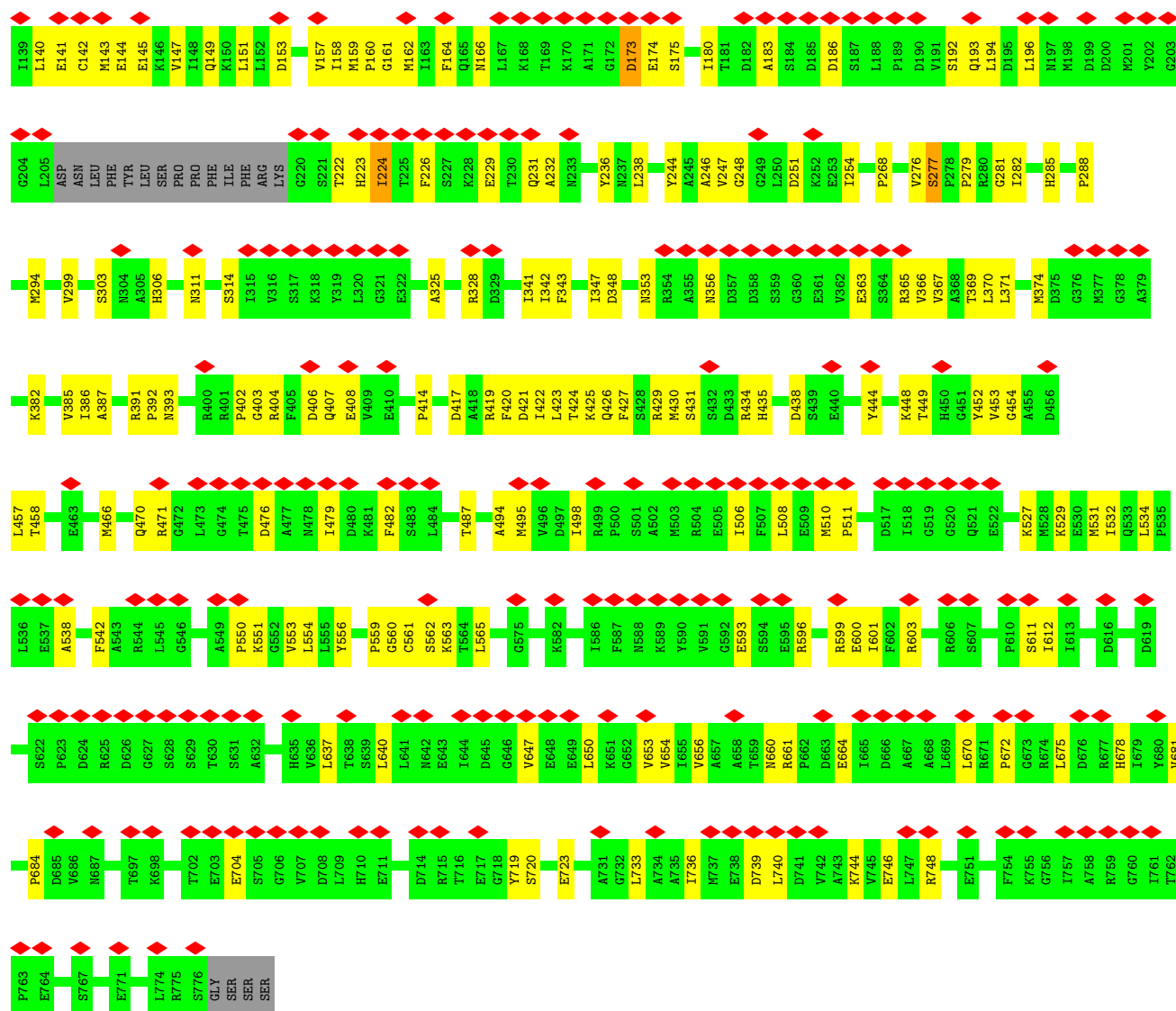
Chain E:



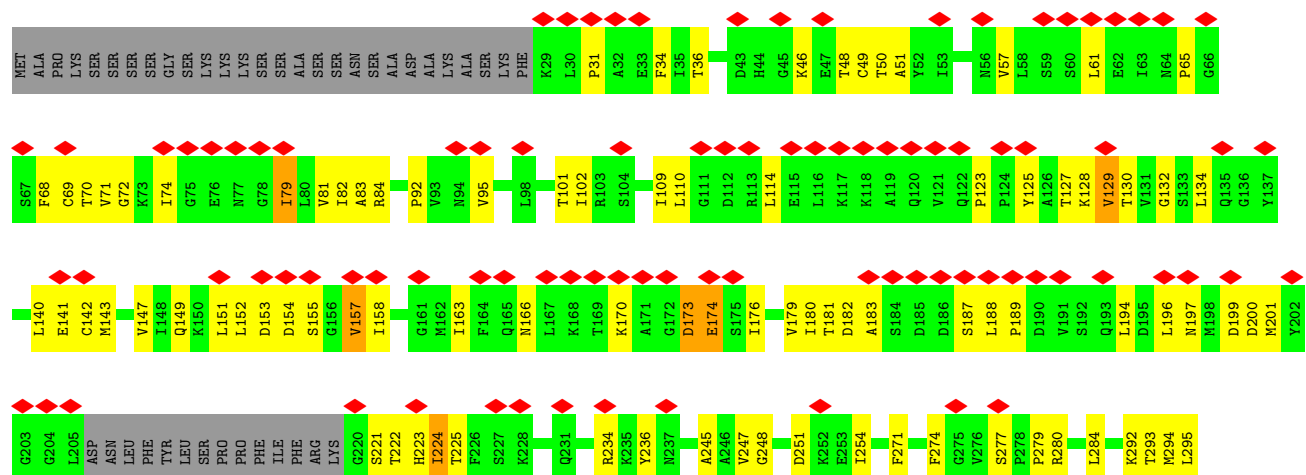


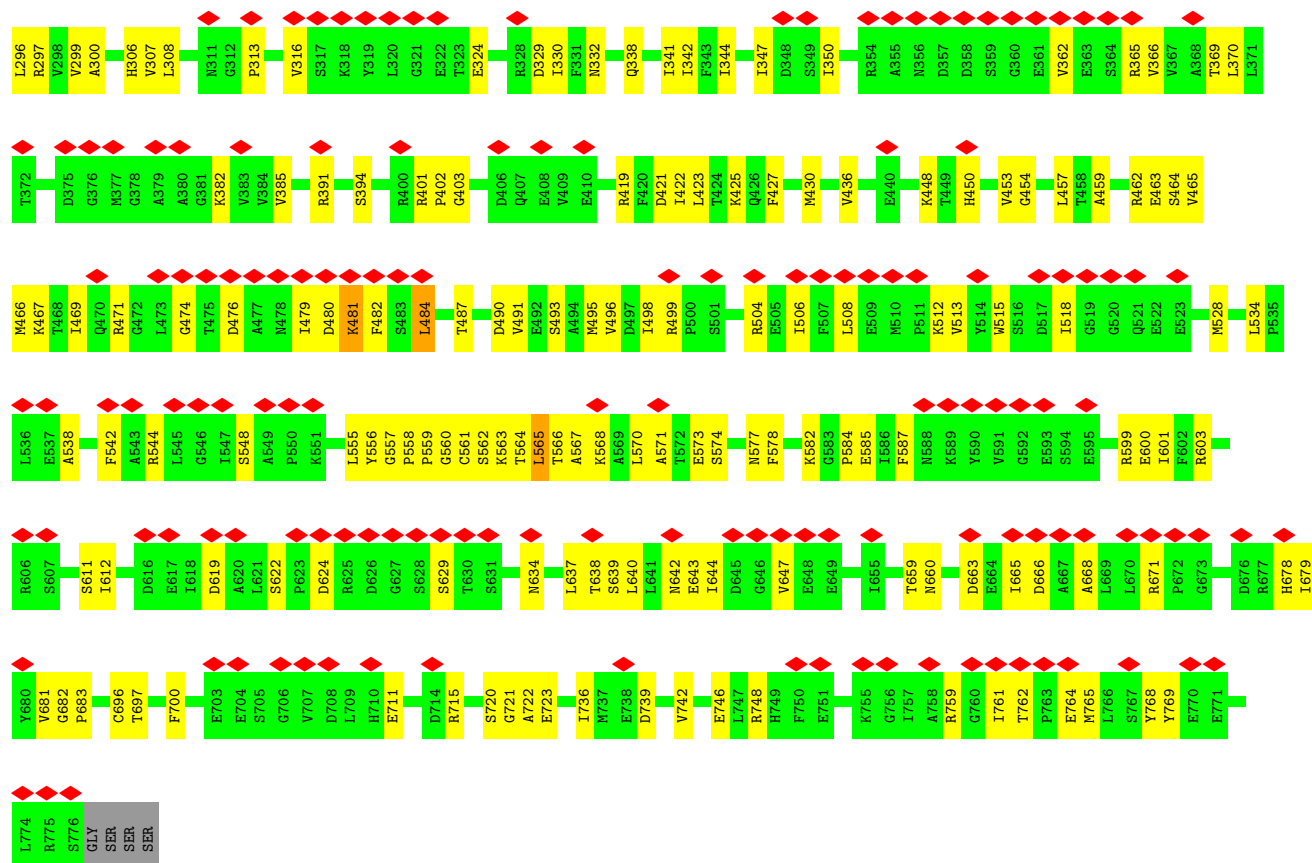
• Molecule 1: ATPase family gene 2 protein





• Molecule 1: ATPase family gene 2 protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	252.48001, 252.48001, 252.48001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.052, 1.052, 1.052	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: ATP, NDT, 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	A	0.20	0/5706	0.42	1/7725 (0.0%)
1	B	0.16	0/5706	0.41	0/7725
1	C	0.27	0/5706	0.53	5/7725 (0.1%)
1	D	0.19	0/5706	0.42	1/7725 (0.0%)
1	E	0.25	0/5706	0.48	1/7725 (0.0%)
1	F	0.26	0/5706	0.50	1/7725 (0.0%)
All	All	0.23	0/34236	0.46	9/46350 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	484	LEU	CA-C-N	6.18	133.34	121.54
1	C	484	LEU	C-N-CA	6.18	133.34	121.54
1	F	618	ILE	N-CA-C	-6.15	106.72	113.43
1	E	430	MET	CA-C-O	-5.44	114.79	120.55
1	D	138	ASN	CB-CA-C	-5.42	110.34	116.63
1	C	474	GLY	CA-C-N	-5.31	113.99	122.17
1	C	474	GLY	C-N-CA	-5.31	113.99	122.17
1	C	565	LEU	N-CA-C	-5.13	106.71	112.87
1	A	740	LEU	CB-CA-C	-5.09	110.31	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5613	0	5678	159	0
1	B	5613	0	5678	152	0
1	C	5613	0	5678	226	0
1	D	5613	0	5678	202	0
1	E	5613	0	5678	207	0
1	F	5613	0	5678	245	0
2	A	27	0	12	3	0
2	B	27	0	12	0	0
2	C	27	0	12	2	0
2	D	27	0	12	1	0
2	E	27	0	12	4	0
2	F	27	0	12	20	0
3	A	31	0	11	4	0
3	B	31	0	11	4	0
3	C	31	0	11	12	0
3	D	31	0	11	18	0
3	E	31	0	11	14	0
3	F	31	0	11	1	0
4	A	20	0	12	4	0
4	B	20	0	12	1	0
4	D	40	0	24	32	0
4	E	20	0	12	22	0
4	F	20	0	12	23	0
All	All	34146	0	34278	1171	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 17.

All (1171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:GLY:HA3	1:E:563:LYS:NZ	1.33	1.36
1:F:565:LEU:HD13	2:F:801:ADP:C8	1.71	1.25
1:C:559:PRO:HG3	1:C:660:ASN:OD1	1.36	1.23
1:F:565:LEU:HD22	2:F:801:ADP:N7	1.54	1.22
1:B:423:LEU:CD1	1:B:427:PHE:HE1	1.53	1.20
1:B:423:LEU:HD12	1:B:427:PHE:CE1	1.77	1.18
4:D:803:NDT:H7	1:E:403:GLY:HA2	1.21	1.14
1:F:288:PRO:O	1:F:453:VAL:HG21	1.48	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:518:ILE:HG23	1:E:565:LEU:HD21	1.16	1.13
1:C:284:LEU:HD12	1:C:296:LEU:HD11	1.27	1.12
1:C:561:CYS:CB	1:C:721:GLY:HA3	1.79	1.12
1:D:294:MET:HE3	3:D:802:ATP:C3'	1.79	1.12
1:D:294:MET:HE3	3:D:802:ATP:H3'	1.33	1.11
1:C:561:CYS:HB3	1:C:721:GLY:HA3	1.34	1.07
1:B:423:LEU:HD12	1:B:427:PHE:HE1	0.89	1.05
4:F:803:NDT:H7	1:A:403:GLY:HA2	1.10	1.04
1:F:618:ILE:HG22	1:F:658:ALA:O	1.55	1.03
1:F:565:LEU:HD13	2:F:801:ADP:N7	1.72	1.02
1:E:557:GLY:HA3	1:E:563:LYS:HZ3	1.20	1.02
1:F:297:ARG:HA	1:F:297:ARG:HH11	1.23	1.02
1:F:291:GLY:O	1:F:295:LEU:HG	1.58	1.02
4:F:803:NDT:H7	1:A:403:GLY:CA	1.89	1.01
1:E:515:TRP:HE1	1:E:573:GLU:HG3	1.26	0.99
1:F:565:LEU:HD13	2:F:801:ADP:C5	1.97	0.99
1:D:429:ARG:CZ	4:D:803:NDT:C17	2.40	0.99
1:F:565:LEU:CD2	2:F:801:ADP:N7	2.25	0.99
1:F:429:ARG:HH21	4:F:803:NDT:C19	1.76	0.98
1:F:429:ARG:HD2	4:F:803:NDT:H212	1.43	0.98
1:C:296:LEU:O	1:C:299:VAL:HG12	1.64	0.98
1:C:284:LEU:CD1	1:C:296:LEU:HD11	1.93	0.97
1:C:247:VAL:HG23	3:C:802:ATP:N6	1.78	0.97
1:B:423:LEU:O	1:B:427:PHE:HD1	1.48	0.95
1:E:557:GLY:CA	1:E:563:LYS:NZ	2.28	0.95
1:B:423:LEU:CD1	1:B:427:PHE:CE1	2.42	0.94
1:E:532:ILE:HG21	1:E:570:LEU:HD11	1.49	0.94
1:E:534:LEU:O	1:E:538:ALA:HB3	1.67	0.93
1:F:242:LEU:H	1:F:301:ASN:ND2	1.65	0.93
1:E:563:LYS:NZ	1:E:681:VAL:HG13	1.83	0.93
1:D:294:MET:HE1	4:D:803:NDT:O2	1.69	0.92
1:E:291:GLY:HA2	3:E:802:ATP:H5'2	1.50	0.92
1:D:534:LEU:O	1:D:538:ALA:HB3	1.70	0.91
1:F:242:LEU:H	1:F:301:ASN:HD22	1.18	0.91
1:F:565:LEU:CD1	2:F:801:ADP:C8	2.52	0.91
1:C:292:LYS:HD2	3:C:802:ATP:O3G	1.70	0.91
1:F:295:LEU:O	1:F:298:VAL:HG13	1.70	0.90
1:D:294:MET:HE3	3:D:802:ATP:C2'	2.02	0.90
1:E:248:GLY:HA3	1:E:425:LYS:CD	2.02	0.89
1:E:557:GLY:HA3	1:E:563:LYS:HZ1	1.07	0.89
1:E:247:VAL:C	1:E:425:LYS:HE2	1.98	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:VAL:HG11	1:C:295:LEU:HD21	1.55	0.88
1:E:292:LYS:HD2	3:E:802:ATP:O3G	1.74	0.88
1:E:421:ASP:O	1:E:425:LYS:HG3	1.74	0.88
1:E:429:ARG:HD3	4:E:803:NDT:C21	2.04	0.87
1:F:295:LEU:HA	1:F:298:VAL:CG1	2.03	0.87
1:F:429:ARG:HH21	4:F:803:NDT:C18	1.87	0.87
4:D:803:NDT:H7	1:E:403:GLY:CA	2.04	0.87
1:F:244:TYR:CE1	1:F:298:VAL:CG2	2.58	0.87
4:F:803:NDT:C7	1:A:403:GLY:HA2	2.03	0.87
1:F:565:LEU:CD1	2:F:801:ADP:N7	2.38	0.86
1:D:294:MET:CE	3:D:802:ATP:H2'	2.06	0.85
1:A:534:LEU:O	1:A:538:ALA:HB3	1.74	0.85
1:E:248:GLY:HA3	1:E:425:LYS:HD3	1.58	0.85
1:C:481:LYS:H	1:C:481:LYS:HD3	1.41	0.85
1:C:423:LEU:CD1	1:C:427:PHE:HE1	1.89	0.84
1:C:528:MET:HE3	1:C:570:LEU:HD22	1.58	0.84
1:F:294:MET:O	1:F:298:VAL:HG12	1.79	0.83
1:F:565:LEU:HD13	2:F:801:ADP:C4	2.13	0.83
1:D:160:PRO:HB2	1:D:194:LEU:HD12	1.58	0.83
1:B:423:LEU:O	1:B:427:PHE:CD1	2.32	0.83
1:C:534:LEU:O	1:C:538:ALA:HB3	1.79	0.82
1:F:242:LEU:N	1:F:301:ASN:HD22	1.78	0.82
1:C:562:SER:HA	1:C:565:LEU:HB3	1.60	0.82
1:D:294:MET:HE3	3:D:802:ATP:H2'	1.61	0.82
1:B:534:LEU:O	1:B:538:ALA:HB3	1.80	0.81
1:D:275:GLY:O	4:D:804:NDT:H19	1.80	0.81
1:D:435:HIS:HB2	1:D:486:VAL:HB	1.61	0.81
1:F:426:GLN:HA	1:F:426:GLN:HE21	1.46	0.81
1:F:244:TYR:CD1	1:F:298:VAL:HG21	2.15	0.81
1:C:423:LEU:HD12	1:C:427:PHE:HE1	1.44	0.80
1:E:248:GLY:CA	1:E:425:LYS:HE2	2.11	0.80
1:E:563:LYS:HZ2	1:E:681:VAL:HG13	1.47	0.80
1:C:247:VAL:HG11	1:C:295:LEU:CD2	2.12	0.80
1:C:423:LEU:O	1:C:427:PHE:HD1	1.62	0.80
1:E:248:GLY:N	1:E:425:LYS:HE2	1.96	0.80
1:E:429:ARG:NH1	4:E:803:NDT:C19	2.46	0.79
1:E:518:ILE:CG2	1:E:565:LEU:HD21	2.07	0.79
1:C:561:CYS:CB	1:C:721:GLY:CA	2.60	0.79
1:C:563:LYS:NZ	1:C:660:ASN:HA	1.98	0.78
1:A:559:PRO:HD3	1:A:660:ASN:OD1	1.83	0.78
1:C:284:LEU:HD12	1:C:296:LEU:CD1	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:565:LEU:HD13	2:F:801:ADP:N9	1.99	0.77
1:D:751:GLU:HG3	1:D:755:LYS:HZ3	1.48	0.77
1:F:426:GLN:HE22	4:F:803:NDT:C17	1.97	0.77
1:C:423:LEU:HD12	1:C:427:PHE:CE1	2.19	0.77
1:D:429:ARG:HG2	4:D:803:NDT:C21	2.15	0.77
1:F:429:ARG:NH2	4:F:803:NDT:C20	2.48	0.77
1:A:247:VAL:C	1:A:425:LYS:HE3	2.10	0.76
1:E:532:ILE:HG21	1:E:570:LEU:CD1	2.14	0.76
1:E:557:GLY:CA	1:E:563:LYS:HZ1	1.95	0.76
1:F:429:ARG:NH2	4:F:803:NDT:C19	2.49	0.75
1:F:429:ARG:HH22	4:F:803:NDT:C15	2.00	0.75
1:D:430:MET:HE1	1:E:276:VAL:HG13	1.68	0.75
1:F:244:TYR:CE1	1:F:298:VAL:HG21	2.21	0.75
1:F:565:LEU:CB	2:F:801:ADP:C8	2.69	0.75
1:D:429:ARG:HG2	4:D:803:NDT:H213	1.69	0.74
1:F:565:LEU:CD1	2:F:801:ADP:C5	2.69	0.74
1:C:559:PRO:HG3	1:C:660:ASN:CG	2.11	0.74
1:F:565:LEU:CG	2:F:801:ADP:N7	2.50	0.74
1:C:561:CYS:HB2	1:C:721:GLY:CA	2.17	0.74
3:E:802:ATP:N3	3:E:802:ATP:H2'	2.02	0.74
1:C:294:MET:HE3	3:C:802:ATP:H3'	1.69	0.74
1:D:294:MET:CE	4:D:803:NDT:O2	2.36	0.74
1:B:37:ARG:HE	1:B:38:PRO:HD2	1.53	0.74
1:C:565:LEU:O	1:C:565:LEU:HD23	1.88	0.74
1:D:68:PHE:HA	1:D:83:ALA:HA	1.70	0.74
1:D:430:MET:HG3	1:D:434:ARG:HB2	1.70	0.73
1:A:282:ILE:HG13	1:A:407:GLN:HE21	1.53	0.73
1:C:247:VAL:HG21	1:C:295:LEU:HD21	1.69	0.73
1:D:247:VAL:HG13	3:D:802:ATP:N6	2.02	0.73
1:E:68:PHE:HA	1:E:83:ALA:HA	1.69	0.73
1:C:558:PRO:HG2	1:C:683:PRO:HD3	1.71	0.73
1:C:561:CYS:HB2	1:C:721:GLY:HA3	1.67	0.73
1:F:403:GLY:HA2	4:E:803:NDT:H7	1.71	0.72
1:D:265:LEU:HD13	1:D:382:LYS:HB2	1.71	0.72
1:C:464:SER:OG	1:C:491:VAL:HA	1.89	0.72
1:C:463:GLU:O	1:C:467:LYS:HG2	1.89	0.72
1:F:534:LEU:O	1:F:538:ALA:HB3	1.88	0.72
1:E:553:VAL:HB	1:E:656:VAL:HG12	1.71	0.72
1:A:563:LYS:NZ	1:A:660:ASN:OD1	2.23	0.71
1:B:251:ASP:HA	1:B:254:ILE:HG22	1.72	0.71
1:C:563:LYS:NZ	1:C:659:THR:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LYS:H	1:C:481:LYS:CD	2.03	0.71
1:F:68:PHE:HA	1:F:83:ALA:HA	1.71	0.71
1:F:295:LEU:O	1:F:298:VAL:CG1	2.38	0.71
1:E:563:LYS:CE	1:E:681:VAL:HG13	2.20	0.71
1:D:429:ARG:CD	4:D:803:NDT:C21	2.69	0.71
1:F:288:PRO:O	1:F:453:VAL:CG2	2.35	0.71
1:E:557:GLY:HA3	1:E:563:LYS:CE	2.21	0.71
1:F:244:TYR:CE1	1:F:298:VAL:HG22	2.26	0.70
1:E:557:GLY:CA	1:E:563:LYS:HZ3	2.00	0.70
1:C:292:LYS:CD	3:C:802:ATP:O3G	2.40	0.70
1:F:251:ASP:HA	1:F:254:ILE:HG22	1.74	0.70
1:B:263:ILE:HG13	1:B:264:PRO:HD3	1.72	0.70
1:C:401:ARG:HD3	1:C:402:PRO:HD2	1.72	0.70
1:D:307:VAL:HG12	1:D:341:ILE:HB	1.73	0.70
1:E:294:MET:HE1	3:E:802:ATP:C4	2.27	0.69
1:C:480:ASP:HB3	1:C:482:PHE:HD1	1.57	0.69
1:C:561:CYS:HB2	1:C:722:ALA:N	2.07	0.69
1:A:466:MET:O	1:A:470:GLN:NE2	2.26	0.69
1:C:512:LYS:HE3	1:C:571:ALA:HB1	1.74	0.69
1:E:292:LYS:NZ	1:E:389:THR:O	2.26	0.68
1:E:565:LEU:C	1:E:565:LEU:HD23	2.17	0.68
1:B:466:MET:O	1:B:470:GLN:NE2	2.25	0.68
1:A:458:THR:HG21	3:A:802:ATP:H1'	1.74	0.68
1:D:247:VAL:HG13	3:D:802:ATP:HN62	1.57	0.68
1:D:471:ARG:HH12	1:D:490:ASP:HB3	1.56	0.68
1:F:297:ARG:HH11	1:F:297:ARG:CA	2.04	0.68
1:D:435:HIS:HD1	1:D:437:LEU:HD23	1.58	0.68
1:C:284:LEU:CD1	1:C:296:LEU:CD1	2.70	0.68
1:E:454:GLY:HA3	3:E:802:ATP:C8	2.28	0.68
1:A:494:ALA:O	1:A:498:ILE:HB	1.94	0.68
1:C:506:ILE:HD11	1:C:601:ILE:HB	1.76	0.68
1:F:403:GLY:O	4:E:803:NDT:H7	1.93	0.67
1:F:494:ALA:O	1:F:498:ILE:HB	1.93	0.67
1:C:515:TRP:HE1	1:C:573:GLU:HG3	1.60	0.67
1:F:295:LEU:HA	1:F:298:VAL:HG11	1.74	0.67
1:C:556:TYR:HE1	1:C:678:HIS:HB3	1.60	0.67
1:C:467:LYS:HB2	1:C:490:ASP:HB3	1.77	0.67
1:D:398:ALA:O	1:D:404:ARG:NH2	2.27	0.67
1:C:561:CYS:HB2	1:C:721:GLY:C	2.19	0.67
1:C:132:GLY:N	1:C:179:VAL:O	2.28	0.66
1:D:466:MET:O	1:D:470:GLN:NE2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ASN:ND2	1:E:174:GLU:O	2.29	0.66
1:A:426:GLN:HG3	4:A:803:NDT:H213	1.78	0.66
1:C:68:PHE:HA	1:C:83:ALA:HA	1.77	0.66
1:C:296:LEU:O	1:C:299:VAL:CG1	2.42	0.66
1:C:560:GLY:HA3	1:C:720:SER:HB2	1.78	0.66
1:B:149:GLN:O	1:B:153:ASP:HB2	1.95	0.66
1:A:68:PHE:HA	1:A:83:ALA:HA	1.76	0.66
1:C:247:VAL:C	1:C:425:LYS:HE2	2.21	0.66
1:C:558:PRO:CD	1:C:682:GLY:HA2	2.25	0.66
1:C:720:SER:H	1:C:723:GLU:HB2	1.60	0.65
1:D:435:HIS:ND1	1:D:437:LEU:HD23	2.12	0.65
1:F:462:ARG:NH1	1:A:277:SER:O	2.29	0.65
1:E:71:VAL:HB	1:E:114:LEU:HD12	1.78	0.65
1:C:391:ARG:NH2	1:C:394:SER:OG	2.28	0.65
1:D:435:HIS:CE1	1:D:437:LEU:HB2	2.32	0.65
1:D:645:ASP:HB2	1:D:674:ARG:HE	1.61	0.65
1:B:423:LEU:HD13	1:B:427:PHE:CE1	2.31	0.65
1:B:506:ILE:HD12	1:B:604:LYS:HE3	1.79	0.65
1:D:365:ARG:HG3	1:C:313:PRO:HB2	1.79	0.65
1:D:429:ARG:HD3	4:D:803:NDT:C18	2.26	0.65
1:D:294:MET:HE1	3:D:802:ATP:H2'	1.78	0.65
1:F:244:TYR:CD1	1:F:298:VAL:CG2	2.79	0.65
1:E:245:ALA:O	1:E:425:LYS:NZ	2.29	0.65
1:C:421:ASP:O	1:C:425:LYS:HG3	1.96	0.65
1:F:100:THR:HG22	1:F:103:ARG:HH21	1.62	0.65
1:E:159:MET:HE2	1:E:183:ALA:HB2	1.79	0.65
1:E:294:MET:HE1	3:E:802:ATP:C5	2.31	0.65
1:C:479:ILE:CG2	1:C:484:LEU:HD11	2.27	0.65
1:F:429:ARG:NH2	4:F:803:NDT:C18	2.60	0.64
1:B:265:LEU:HA	1:B:382:LYS:HB2	1.79	0.64
1:E:515:TRP:NE1	1:E:573:GLU:HG3	2.06	0.64
1:F:297:ARG:HA	1:F:297:ARG:NH1	2.06	0.64
1:D:277:SER:O	1:C:462:ARG:NH1	2.31	0.64
1:D:247:VAL:HA	3:D:802:ATP:N1	2.13	0.64
1:A:559:PRO:HB3	1:A:660:ASN:ND2	2.13	0.64
1:C:599:ARG:HH22	1:C:639:SER:HB3	1.62	0.64
1:D:429:ARG:CG	4:D:803:NDT:C21	2.76	0.63
1:D:491:VAL:HG12	1:D:495:MET:HE1	1.81	0.63
1:F:429:ARG:NH2	4:F:803:NDT:C16	2.61	0.63
1:D:62:GLU:O	1:D:62:GLU:HG2	1.98	0.63
1:D:125:TYR:O	1:D:197:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:ARG:HD2	4:F:803:NDT:C21	2.25	0.63
1:F:429:ARG:NH2	4:F:803:NDT:C15	2.61	0.63
1:F:460:LEU:HD22	1:F:498:ILE:HG12	1.79	0.63
1:E:36:THR:HG23	1:E:110:LEU:HD13	1.81	0.63
1:A:236:TYR:HB3	1:A:238:LEU:HD23	1.81	0.63
1:A:281:GLY:O	1:A:407:GLN:NE2	2.32	0.63
1:F:429:ARG:NH2	4:F:803:NDT:C17	2.61	0.63
1:B:525:LYS:HA	1:B:528:MET:HE2	1.81	0.63
1:E:158:ILE:HD11	1:E:194:LEU:HB3	1.80	0.63
1:E:563:LYS:HE3	1:E:681:VAL:CG1	2.27	0.63
1:C:564:THR:C	1:C:566:THR:H	2.06	0.63
1:A:251:ASP:O	1:A:254:ILE:N	2.32	0.63
1:B:734:ALA:HA	1:B:737:MET:HE3	1.79	0.63
1:E:759:ARG:HG2	1:E:761:ILE:HG22	1.81	0.63
1:A:510:MET:HG2	1:A:511:PRO:HD2	1.80	0.63
1:F:37:ARG:HE	1:F:38:PRO:HD2	1.63	0.63
1:F:426:GLN:NE2	4:F:803:NDT:H17	2.14	0.63
1:D:532:ILE:HG21	1:D:570:LEU:HD11	1.81	0.62
1:D:553:VAL:HB	1:D:656:VAL:HG12	1.80	0.62
1:E:429:ARG:HD3	4:E:803:NDT:H212	1.80	0.62
1:C:158:ILE:HD12	1:C:196:LEU:HB3	1.79	0.62
1:B:71:VAL:HB	1:B:114:LEU:HD12	1.81	0.62
1:C:127:THR:HG22	1:C:128:LYS:HE3	1.81	0.62
1:F:280:ARG:NH2	1:F:380:ALA:O	2.33	0.62
1:B:550:PRO:HB2	1:B:677:ARG:HH22	1.63	0.62
1:A:563:LYS:HE3	2:A:801:ADP:O1B	1.99	0.62
1:F:424:THR:HG22	1:F:442:ILE:HG21	1.82	0.62
1:D:76:GLU:O	1:D:193:GLN:NE2	2.33	0.62
1:D:618:ILE:HG22	1:D:659:THR:HB	1.82	0.62
1:F:71:VAL:HG11	1:F:98:LEU:HD21	1.82	0.62
1:C:308:LEU:HD13	1:C:330:ILE:HG23	1.82	0.62
1:F:36:THR:HG23	1:F:110:LEU:HD13	1.80	0.62
1:A:553:VAL:HB	1:A:656:VAL:HG12	1.82	0.62
1:E:577:ASN:N	1:E:577:ASN:HD22	1.97	0.62
1:F:295:LEU:CA	1:F:298:VAL:CG1	2.76	0.62
1:F:426:GLN:HA	1:F:426:GLN:NE2	2.14	0.62
1:A:370:LEU:O	1:A:374:MET:HG3	2.00	0.62
1:C:294:MET:HE3	3:C:802:ATP:C3'	2.30	0.62
1:E:33:GLU:HG3	1:E:113:ARG:HE	1.65	0.61
1:C:292:LYS:CE	3:C:802:ATP:O3G	2.49	0.61
1:B:720:SER:H	1:B:723:GLU:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:O	1:A:341:ILE:N	2.32	0.61
1:F:403:GLY:HA2	4:E:803:NDT:C7	2.29	0.61
1:D:166:ASN:ND2	1:D:174:GLU:O	2.29	0.61
1:A:559:PRO:HB3	1:A:660:ASN:HD21	1.65	0.61
1:B:403:GLY:HA2	4:A:803:NDT:H6	1.82	0.61
1:D:101:THR:HG23	1:D:163:ILE:H	1.66	0.61
3:D:802:ATP:H2'	3:D:802:ATP:N3	2.15	0.61
1:F:159:MET:SD	1:F:197:ASN:ND2	2.73	0.61
1:F:166:ASN:ND2	1:F:174:GLU:O	2.34	0.61
1:D:123:PRO:HB2	1:D:197:ASN:HA	1.82	0.60
1:C:125:TYR:O	1:C:197:ASN:ND2	2.34	0.60
1:E:130:THR:HB	1:E:182:ASP:HB3	1.84	0.60
1:D:251:ASP:HA	1:D:254:ILE:HG22	1.82	0.60
1:F:618:ILE:HG22	1:F:658:ALA:C	2.26	0.60
1:C:306:HIS:O	1:C:341:ILE:N	2.32	0.60
1:A:420:PHE:O	1:A:424:THR:HG23	2.02	0.60
1:D:291:GLY:HA2	3:D:802:ATP:O1A	2.02	0.60
1:F:295:LEU:O	1:F:299:VAL:HG22	2.01	0.60
1:F:598:ILE:HD13	1:F:636:VAL:HG13	1.84	0.60
1:D:149:GLN:O	1:D:153:ASP:HB2	2.02	0.60
1:D:429:ARG:HD3	4:D:803:NDT:C21	2.32	0.60
1:B:599:ARG:HH22	1:B:639:SER:HB3	1.66	0.60
1:E:423:LEU:HD21	1:E:457:LEU:HD12	1.83	0.60
1:C:149:GLN:O	1:C:153:ASP:HB2	2.01	0.60
1:D:138:ASN:HD22	1:D:229:GLU:HG3	1.67	0.60
1:F:427:PHE:HA	1:F:430:MET:CE	2.32	0.60
1:F:565:LEU:HB2	2:F:801:ADP:C8	2.36	0.60
1:E:338:GLN:HE22	1:E:382:LYS:HE3	1.67	0.60
1:A:422:ILE:HD13	3:A:802:ATP:HN62	1.67	0.59
1:C:481:LYS:O	1:C:484:LEU:HB2	2.02	0.59
1:D:36:THR:HG23	1:D:110:LEU:HD13	1.84	0.59
1:B:132:GLY:N	1:B:179:VAL:O	2.35	0.59
1:E:248:GLY:HA3	1:E:425:LYS:CE	2.32	0.59
1:A:248:GLY:N	1:A:425:LYS:HE3	2.17	0.59
1:A:402:PRO:HA	1:A:406:ASP:HB3	1.83	0.59
1:C:92:PRO:HG2	1:C:95:VAL:HG12	1.85	0.59
1:F:491:VAL:O	1:F:495:MET:HG3	2.02	0.59
1:E:294:MET:SD	3:E:802:ATP:C2	2.96	0.59
1:D:429:ARG:CG	4:D:803:NDT:H211	2.32	0.59
1:C:147:VAL:HG12	1:C:151:LEU:HG	1.83	0.59
1:E:429:ARG:HD3	4:E:803:NDT:H211	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:727:LEU:HD21	1:E:757:ILE:HG21	1.85	0.59
1:F:101:THR:HG23	1:F:163:ILE:H	1.67	0.59
1:C:324:GLU:OE2	1:C:365:ARG:NH1	2.29	0.59
1:C:556:TYR:CE1	1:C:678:HIS:HB3	2.38	0.59
1:F:553:VAL:HB	1:F:656:VAL:HG12	1.84	0.59
1:F:295:LEU:HA	1:F:298:VAL:HG12	1.85	0.58
1:B:58:LEU:HD22	1:B:84:ARG:HH21	1.67	0.58
1:E:294:MET:SD	3:E:802:ATP:N3	2.76	0.58
1:A:29:LYS:HZ2	1:A:56:ASN:HB2	1.68	0.58
1:C:565:LEU:HD12	2:C:801:ADP:H2'	1.83	0.58
1:D:711:GLU:OE1	1:D:715:ARG:NH1	2.36	0.58
1:A:434:ARG:HH12	1:A:482:PHE:HA	1.67	0.58
1:C:188:LEU:HD23	1:C:189:PRO:HD3	1.85	0.58
1:F:565:LEU:CG	2:F:801:ADP:C8	2.85	0.58
1:E:426:GLN:HB2	4:E:803:NDT:H213	1.85	0.58
1:A:73:LYS:NZ	1:A:106:GLY:O	2.36	0.58
1:F:737:MET:HE1	1:A:534:LEU:HD21	1.84	0.58
1:F:234:ARG:NH2	1:F:240:GLU:OE2	2.34	0.58
1:F:242:LEU:HD22	1:F:297:ARG:HB2	1.86	0.58
3:F:802:ATP:N3	3:F:802:ATP:H2'	2.18	0.58
1:F:295:LEU:CA	1:F:298:VAL:HG12	2.34	0.58
1:F:692:ILE:HD11	2:F:801:ADP:N1	2.18	0.58
1:D:462:ARG:NH1	1:E:277:SER:O	2.37	0.58
1:B:76:GLU:O	1:B:193:GLN:NE2	2.37	0.58
1:E:515:TRP:HE1	1:E:573:GLU:CG	2.10	0.58
1:F:426:GLN:NE2	4:F:803:NDT:C17	2.65	0.58
1:B:251:ASP:O	1:B:254:ILE:N	2.36	0.58
1:D:414:PRO:O	1:D:419:ARG:NH1	2.37	0.57
1:F:92:PRO:HG2	1:F:95:VAL:HG12	1.86	0.57
1:F:236:TYR:HB3	1:F:238:LEU:HD23	1.85	0.57
1:A:37:ARG:O	1:A:103:ARG:NH2	2.30	0.57
1:D:429:ARG:CZ	4:D:803:NDT:C16	2.81	0.57
1:D:751:GLU:HG3	1:D:755:LYS:NZ	2.18	0.57
1:A:72:GLY:HA2	1:A:79:ILE:HG23	1.86	0.57
1:D:316:VAL:HG13	1:D:362:VAL:HG21	1.87	0.57
3:D:802:ATP:H2'	4:D:803:NDT:O2	2.03	0.57
1:A:34:PHE:HB2	1:A:114:LEU:HB2	1.84	0.57
1:F:37:ARG:HH22	1:F:306:HIS:HB2	1.68	0.57
1:E:563:LYS:CE	1:E:681:VAL:CG1	2.82	0.57
1:A:554:LEU:HD12	1:A:675:LEU:HD23	1.84	0.57
1:E:429:ARG:CD	4:E:803:NDT:H212	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:HD11	1:A:601:ILE:HB	1.86	0.57
1:F:292:LYS:NZ	1:F:390:ASN:HA	2.19	0.57
1:F:403:GLY:CA	4:E:803:NDT:H7	2.34	0.57
1:B:29:LYS:HZ2	1:B:56:ASN:HB2	1.70	0.57
1:B:468:THR:OG1	1:B:490:ASP:OD2	2.22	0.57
1:D:73:LYS:HA	1:D:114:LEU:HA	1.86	0.57
1:B:595:GLU:OE2	1:B:599:ARG:NH1	2.38	0.56
1:A:720:SER:H	1:A:723:GLU:HB2	1.70	0.56
1:B:166:ASN:ND2	1:B:174:GLU:O	2.37	0.56
1:B:612:ILE:HG22	1:B:654:VAL:HB	1.86	0.56
1:C:423:LEU:HD13	1:C:427:PHE:HE1	1.69	0.56
1:D:430:MET:CE	1:E:276:VAL:HG13	2.35	0.56
1:D:746:GLU:OE1	1:D:748:ARG:NE	2.36	0.56
1:B:663:ASP:OD1	1:B:775:ARG:NH2	2.39	0.56
1:C:560:GLY:O	1:C:722:ALA:HB2	2.05	0.56
1:D:127:THR:HG22	1:D:128:LYS:HE3	1.88	0.56
1:B:733:LEU:HD13	1:B:736:ILE:HD11	1.88	0.56
1:C:101:THR:HG23	1:C:163:ILE:H	1.71	0.56
1:C:247:VAL:CG1	1:C:295:LEU:HD21	2.33	0.56
1:E:353:ASN:HB3	1:E:356:ASN:HB2	1.88	0.56
1:E:500:PRO:HB2	1:E:503:MET:HE3	1.87	0.56
1:F:242:LEU:HB2	1:F:301:ASN:ND2	2.21	0.56
1:F:361:GLU:O	1:F:365:ARG:NH2	2.37	0.56
1:C:70:THR:HB	1:C:79:ILE:HG12	1.87	0.56
1:F:48:THR:HG21	1:F:157:VAL:H	1.71	0.56
1:A:733:LEU:HA	1:A:736:ILE:HG12	1.87	0.56
1:F:242:LEU:HD22	1:F:297:ARG:CB	2.36	0.55
1:B:140:LEU:HB2	1:B:143:MET:HB3	1.86	0.55
1:E:414:PRO:O	1:E:419:ARG:NH1	2.39	0.55
1:D:294:MET:HE1	3:D:802:ATP:N3	2.22	0.55
1:B:462:ARG:NH1	1:C:277:SER:O	2.29	0.55
1:D:559:PRO:HB3	1:D:660:ASN:HD21	1.71	0.55
1:F:606:ARG:HE	1:F:650:LEU:HD21	1.71	0.55
1:A:78:GLY:HA2	1:A:192:SER:HA	1.88	0.55
1:C:401:ARG:HG3	1:C:403:GLY:H	1.71	0.55
1:B:342:ILE:HB	1:B:385:VAL:HA	1.89	0.55
1:C:638:THR:O	1:C:642:ASN:ND2	2.40	0.55
1:D:429:ARG:NE	4:D:803:NDT:C17	2.70	0.55
1:B:129:VAL:HG22	1:B:180:ILE:HD11	1.89	0.55
1:B:585:GLU:OE2	1:C:642:ASN:ND2	2.39	0.55
1:F:471:ARG:HH12	1:F:489:LYS:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:O	1:C:142:CYS:N	2.39	0.55
1:E:247:VAL:O	1:E:425:LYS:HE2	2.07	0.55
1:A:371:LEU:HD22	1:A:404:ARG:HG2	1.89	0.55
1:E:46:LYS:HD3	1:E:49:CYS:HB2	1.89	0.55
1:E:291:GLY:HA3	1:E:294:MET:HE2	1.88	0.55
1:A:282:ILE:HB	1:A:386:ILE:HG22	1.89	0.55
1:F:289:GLY:HA3	1:F:453:VAL:HG22	1.88	0.55
1:E:149:GLN:O	1:E:153:ASP:HB2	2.07	0.55
1:A:414:PRO:O	1:A:419:ARG:NH1	2.40	0.55
1:A:534:LEU:O	1:A:538:ALA:CB	2.53	0.55
1:C:247:VAL:HG23	3:C:802:ATP:HN62	1.64	0.55
1:D:37:ARG:HE	1:D:38:PRO:HD2	1.72	0.55
1:D:280:ARG:NH2	1:D:380:ALA:O	2.38	0.54
1:B:280:ARG:NH2	1:B:380:ALA:O	2.40	0.54
1:E:52:TYR:HB3	1:E:87:ASP:HB3	1.89	0.54
1:C:338:GLN:HB3	1:C:382:LYS:HD2	1.86	0.54
1:F:72:GLY:HA2	1:F:79:ILE:HG13	1.88	0.54
1:A:299:VAL:O	1:A:303:SER:OG	2.22	0.54
1:F:618:ILE:HG23	1:F:659:THR:HB	1.90	0.54
1:B:450:HIS:NE2	1:B:509:GLU:O	2.41	0.54
1:E:248:GLY:CA	1:E:425:LYS:CE	2.82	0.54
1:C:561:CYS:HB3	1:C:721:GLY:CA	2.22	0.54
1:C:564:THR:C	1:C:566:THR:N	2.60	0.54
1:B:37:ARG:NE	1:B:38:PRO:HD2	2.21	0.54
1:E:466:MET:HE3	1:E:466:MET:HA	1.90	0.54
1:C:479:ILE:HG23	1:C:484:LEU:HD11	1.90	0.54
1:D:468:THR:OG1	1:D:490:ASP:OD2	2.25	0.54
1:A:127:THR:O	1:A:222:THR:OG1	2.20	0.54
1:A:611:SER:OG	1:A:612:ILE:N	2.40	0.54
1:D:275:GLY:O	4:D:804:NDT:C19	2.53	0.54
1:B:414:PRO:O	1:B:419:ARG:NH1	2.41	0.54
1:E:418:ALA:O	1:E:422:ILE:HG13	2.07	0.54
1:E:429:ARG:NH1	4:E:803:NDT:C20	2.71	0.54
1:E:453:VAL:HG22	1:E:454:GLY:H	1.72	0.54
1:C:557:GLY:HA3	1:C:681:VAL:HG13	1.90	0.54
1:D:429:ARG:CG	4:D:803:NDT:H213	2.38	0.54
1:D:532:ILE:HD13	1:D:570:LEU:HD11	1.88	0.54
1:C:110:LEU:O	1:C:307:VAL:N	2.32	0.54
1:C:746:GLU:OE1	1:C:748:ARG:NE	2.41	0.54
1:F:414:PRO:HB2	1:F:419:ARG:HG2	1.89	0.54
1:A:285:HIS:NE2	1:A:408:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HB2	1:C:179:VAL:HG21	1.88	0.54
1:D:104:SER:HB3	1:D:163:ILE:HG21	1.90	0.53
1:B:453:VAL:H	1:B:456:ASP:HB2	1.73	0.53
1:E:316:VAL:HG22	1:E:362:VAL:HG21	1.88	0.53
1:D:429:ARG:NH2	4:D:803:NDT:C17	2.70	0.53
1:F:73:LYS:HZ2	1:F:108:LEU:HA	1.73	0.53
1:F:166:ASN:HB3	1:F:175:SER:HA	1.90	0.53
1:E:564:THR:HB	2:E:801:ADP:H3'	1.90	0.53
1:A:127:THR:HG22	1:A:128:LYS:HE3	1.91	0.53
1:D:103:ARG:HA	1:D:108:LEU:HD12	1.89	0.53
1:E:92:PRO:HG2	1:E:95:VAL:HG22	1.91	0.53
1:E:707:VAL:HG12	1:E:747:LEU:HD12	1.91	0.53
1:A:129:VAL:HB	1:A:180:ILE:HD11	1.89	0.53
1:A:561:CYS:SG	1:A:684:PRO:HD3	2.48	0.53
1:C:143:MET:HA	1:C:170:LYS:HE3	1.90	0.53
1:C:634:ASN:O	1:C:638:THR:HG23	2.08	0.53
1:F:231:GLN:HG3	1:F:232:ALA:H	1.73	0.53
1:A:347:ILE:HD11	1:A:387:ALA:HB1	1.90	0.53
1:F:414:PRO:HB2	1:F:419:ARG:CG	2.39	0.53
1:F:414:PRO:O	1:F:419:ARG:NH1	2.40	0.53
1:F:426:GLN:CD	4:F:803:NDT:H17	2.34	0.53
1:B:227:SER:O	1:B:228:LYS:HG3	2.09	0.53
1:B:294:MET:HE1	3:B:802:ATP:C5	2.44	0.53
1:E:399:LEU:HD12	1:E:405:PHE:HE2	1.74	0.53
1:A:471:ARG:HH22	1:A:487:THR:HG22	1.72	0.53
1:E:427:PHE:HA	1:E:430:MET:HB2	1.91	0.53
1:E:557:GLY:N	1:E:563:LYS:HE2	2.23	0.53
1:A:159:MET:HE1	1:A:183:ALA:HB3	1.90	0.53
1:A:251:ASP:HA	1:A:254:ILE:HG22	1.91	0.53
1:C:423:LEU:O	1:C:427:PHE:CD1	2.53	0.53
1:D:250:LEU:HD11	1:D:411:ILE:HG23	1.90	0.53
1:D:429:ARG:HG2	4:D:803:NDT:H211	1.87	0.53
1:F:432:SER:HA	1:F:435:HIS:O	2.08	0.53
1:B:600:GLU:OE2	1:B:603:ARG:NH2	2.36	0.53
1:C:560:GLY:O	1:C:722:ALA:CB	2.57	0.53
1:D:427:PHE:HB3	1:D:435:HIS:NE2	2.24	0.53
1:F:342:ILE:HB	1:F:385:VAL:HA	1.90	0.53
1:B:316:VAL:HG13	1:B:362:VAL:HG21	1.90	0.53
1:C:563:LYS:HZ3	1:C:660:ASN:HA	1.70	0.53
1:F:309:THR:HA	1:F:343:PHE:HB2	1.91	0.53
1:A:61:LEU:HB3	1:A:63:ILE:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PRO:CD	1:A:660:ASN:OD1	2.56	0.53
1:F:143:MET:HE2	1:F:176:ILE:HD13	1.89	0.52
1:B:126:ALA:HB2	1:B:197:ASN:HB3	1.91	0.52
1:B:506:ILE:HG13	1:B:507:PHE:HD1	1.74	0.52
1:A:563:LYS:NZ	1:A:660:ASN:CG	2.67	0.52
1:C:466:MET:HA	1:C:469:ILE:HG12	1.91	0.52
1:F:468:THR:OG1	1:F:490:ASP:OD2	2.26	0.52
1:A:72:GLY:HA3	1:A:115:GLU:HB2	1.91	0.52
1:D:52:TYR:HD1	1:D:87:ASP:HA	1.73	0.52
1:E:265:LEU:HA	1:E:382:LYS:HB2	1.89	0.52
1:D:338:GLN:NE2	1:D:382:LYS:HG2	2.25	0.52
1:F:429:ARG:HH22	4:F:803:NDT:C16	2.20	0.52
1:B:335:ARG:HH12	1:B:381:GLY:HA3	1.74	0.52
1:B:614:PHE:HD1	1:B:656:VAL:HG13	1.74	0.52
1:F:132:GLY:HA3	1:F:179:VAL:HB	1.92	0.52
1:D:429:ARG:CD	4:D:803:NDT:C18	2.87	0.52
1:B:406:ASP:OD1	1:B:406:ASP:N	2.40	0.52
1:F:429:ARG:CD	4:F:803:NDT:H212	2.28	0.52
1:F:692:ILE:HD11	2:F:801:ADP:C2	2.45	0.52
1:B:551:LYS:HD3	1:B:655:ILE:HB	1.91	0.52
1:F:159:MET:HB2	1:F:197:ASN:HB2	1.92	0.52
1:A:149:GLN:O	1:A:153:ASP:HB2	2.10	0.52
1:C:563:LYS:HZ1	1:C:660:ASN:HA	1.73	0.52
4:F:803:NDT:H213	1:A:276:VAL:HG12	1.91	0.52
1:B:68:PHE:HA	1:B:83:ALA:HA	1.92	0.52
1:C:467:LYS:CB	1:C:490:ASP:HB3	2.40	0.52
1:C:622:SER:HB2	1:C:665:ILE:HA	1.91	0.52
1:D:660:ASN:O	1:D:769:TYR:OH	2.28	0.52
1:E:739:ASP:OD1	1:E:739:ASP:N	2.43	0.52
1:D:739:ASP:OD1	1:D:739:ASP:N	2.43	0.51
1:F:426:GLN:HE21	1:F:426:GLN:CA	2.13	0.51
1:F:556:TYR:HE1	1:F:678:HIS:HB3	1.75	0.51
1:E:444:TYR:CE2	1:E:448:LYS:HD2	2.45	0.51
1:E:695:LYS:NZ	2:E:801:ADP:HN62	2.08	0.51
1:A:406:ASP:N	1:A:406:ASP:OD1	2.42	0.51
1:D:294:MET:CE	3:D:802:ATP:N3	2.73	0.51
1:F:69:CYS:HB3	1:F:84:ARG:HH11	1.75	0.51
1:F:459:ALA:HB2	1:A:402:PRO:HB3	1.92	0.51
1:C:109:ILE:HD11	1:C:297:ARG:HH21	1.74	0.51
1:C:69:CYS:HB3	1:C:84:ARG:HB3	1.93	0.51
1:C:611:SER:OG	1:C:612:ILE:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:THR:OG1	1:B:764:GLU:OE1	2.28	0.51
1:E:251:ASP:HA	1:E:254:ILE:HG22	1.91	0.51
1:D:429:ARG:NH1	4:D:803:NDT:C16	2.73	0.51
1:F:453:VAL:HG22	1:F:454:GLY:H	1.75	0.51
1:B:162:MET:HE2	1:B:164:PHE:HD2	1.76	0.51
1:E:38:PRO:HD3	1:E:110:LEU:HD11	1.91	0.51
1:A:166:ASN:ND2	1:A:174:GLU:O	2.28	0.51
1:A:596:ARG:HA	1:A:599:ARG:HG2	1.92	0.51
1:D:70:THR:HG22	1:D:81:VAL:HA	1.92	0.51
1:F:426:GLN:HE22	4:F:803:NDT:C18	2.23	0.51
1:B:152:LEU:HA	1:B:157:VAL:HG21	1.92	0.51
1:A:559:PRO:CB	1:A:660:ASN:HD21	2.24	0.51
1:C:668:ALA:O	1:C:671:ARG:NH1	2.43	0.51
1:F:611:SER:OG	1:F:612:ILE:N	2.41	0.51
1:B:510:MET:HB3	1:B:568:LYS:HD2	1.93	0.51
1:B:660:ASN:O	1:B:769:TYR:OH	2.25	0.51
1:F:311:ASN:HB2	1:F:314:SER:HB3	1.92	0.51
1:B:435:HIS:HB2	1:B:486:VAL:HB	1.93	0.51
1:B:711:GLU:OE2	1:B:715:ARG:NH1	2.38	0.51
1:B:746:GLU:OE1	1:B:748:ARG:NE	2.42	0.51
1:A:423:LEU:HD21	1:A:457:LEU:HD12	1.92	0.51
1:A:560:GLY:H	2:A:801:ADP:PB	2.33	0.51
1:D:31:PRO:HG3	1:D:57:VAL:HG13	1.93	0.51
1:D:125:TYR:C	1:D:197:ASN:HB3	2.36	0.51
1:D:159:MET:HE1	1:D:197:ASN:HB2	1.92	0.51
1:D:406:ASP:OD1	1:D:407:GLN:N	2.43	0.51
1:F:692:ILE:HD12	1:F:695:LYS:HD3	1.93	0.51
1:F:293:THR:O	1:F:296:LEU:HB2	2.12	0.50
1:F:726:LEU:HD22	1:A:672:PRO:HB3	1.94	0.50
1:B:622:SER:HA	1:B:637:LEU:HD22	1.93	0.50
1:E:363:GLU:HG2	1:E:364:SER:H	1.75	0.50
1:F:129:VAL:HG22	1:F:180:ILE:HD11	1.92	0.50
1:C:570:LEU:O	1:C:574:SER:OG	2.21	0.50
1:F:125:TYR:HA	1:F:198:MET:HG2	1.92	0.50
1:E:515:TRP:CZ2	1:E:569:ALA:HB1	2.45	0.50
1:D:435:HIS:CB	1:D:486:VAL:HB	2.35	0.50
1:D:551:LYS:HZ2	1:D:650:LEU:H	1.59	0.50
1:F:290:THR:HG22	1:F:411:ILE:HG22	1.94	0.50
1:F:403:GLY:HA2	4:E:803:NDT:C6	2.42	0.50
1:B:44:HIS:O	1:B:47:GLU:HB2	2.12	0.50
1:D:92:PRO:HG2	1:D:95:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:GLN:NE2	1:F:426:GLN:CA	2.73	0.50
1:E:429:ARG:HH11	4:E:803:NDT:C19	2.19	0.50
1:E:534:LEU:O	1:E:538:ALA:CB	2.53	0.50
1:A:144:GLU:O	1:A:147:VAL:HG23	2.12	0.50
1:A:393:ASN:ND2	1:A:600:GLU:OE2	2.42	0.50
1:A:426:GLN:HE22	1:A:458:THR:HA	1.75	0.50
1:F:295:LEU:C	1:F:298:VAL:CG1	2.84	0.50
1:C:292:LYS:HB2	3:C:802:ATP:O2B	2.10	0.50
1:F:123:PRO:HG3	1:F:196:LEU:HG	1.92	0.50
1:C:65:PRO:HA	1:C:84:ARG:HH21	1.77	0.50
1:C:277:SER:O	1:C:277:SER:OG	2.30	0.50
1:F:316:VAL:HG22	1:F:362:VAL:HG21	1.94	0.50
1:B:274:PHE:HB3	1:B:276:VAL:HG23	1.93	0.50
1:E:223:HIS:O	1:E:224:ILE:HG22	2.12	0.50
1:E:565:LEU:HD23	1:E:565:LEU:O	2.12	0.50
1:E:762:THR:H	1:E:765:MET:HE2	1.77	0.50
1:C:476:ASP:HB2	1:C:479:ILE:HG22	1.93	0.50
1:C:558:PRO:HD2	1:C:682:GLY:HA2	1.94	0.50
1:D:188:LEU:HG	1:D:189:PRO:HD3	1.94	0.49
1:D:366:VAL:HA	1:D:369:THR:HG22	1.92	0.49
1:D:759:ARG:HB2	1:D:761:ILE:HG22	1.93	0.49
1:F:410:GLU:HG2	1:F:604:LYS:HE2	1.94	0.49
1:B:611:SER:OG	1:B:612:ILE:N	2.44	0.49
1:E:637:LEU:HD23	1:E:640:LEU:HD21	1.93	0.49
1:C:558:PRO:HD2	1:C:681:VAL:O	2.12	0.49
1:D:118:LYS:HE2	1:D:118:LYS:HA	1.94	0.49
1:D:224:ILE:HG13	1:D:225:THR:H	1.76	0.49
1:C:465:VAL:O	1:C:469:ILE:HG12	2.12	0.49
1:D:459:ALA:HB2	1:E:402:PRO:HB3	1.94	0.49
1:B:160:PRO:HG2	1:B:194:LEU:HG	1.94	0.49
1:B:667:ALA:HB1	1:B:671:ARG:HH12	1.76	0.49
1:C:123:PRO:HB2	1:C:197:ASN:HA	1.95	0.49
1:D:140:LEU:O	1:D:144:GLU:N	2.46	0.49
1:D:512:LYS:HB3	1:D:572:THR:HG23	1.94	0.49
1:B:427:PHE:HA	1:B:430:MET:HG3	1.94	0.49
1:E:129:VAL:HA	1:E:159:MET:HE1	1.93	0.49
1:E:134:LEU:O	1:E:135:GLN:HG3	2.13	0.49
1:E:248:GLY:CA	1:E:425:LYS:CD	2.85	0.49
1:E:324:GLU:HB3	1:E:328:ARG:HH21	1.77	0.49
1:C:72:GLY:HA2	1:C:79:ILE:HG13	1.95	0.49
1:C:342:ILE:HB	1:C:385:VAL:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:SER:O	1:B:263:ILE:HG12	2.13	0.49
1:B:647:VAL:HG21	1:A:508:LEU:HD21	1.95	0.49
1:A:562:SER:HB3	1:A:681:VAL:CG2	2.43	0.49
1:E:421:ASP:OD1	1:E:425:LYS:HG3	2.13	0.49
1:A:55:PRO:HA	1:A:58:LEU:HD12	1.95	0.49
1:C:696:CYS:SG	2:C:801:ADP:N6	2.86	0.49
1:F:427:PHE:HA	1:F:430:MET:HE1	1.94	0.49
1:A:527:LYS:HB3	1:A:531:MET:HE1	1.94	0.49
1:F:138:ASN:HB2	1:F:229:GLU:HB3	1.95	0.49
1:F:727:LEU:HD21	1:F:757:ILE:HG21	1.94	0.49
1:F:759:ARG:HB2	1:F:761:ILE:HG22	1.95	0.49
1:B:733:LEU:HA	1:B:736:ILE:HG12	1.95	0.49
1:A:476:ASP:HB3	1:A:479:ILE:HB	1.93	0.49
1:C:481:LYS:HD3	1:C:481:LYS:N	2.20	0.49
1:D:430:MET:O	1:D:434:ARG:HG2	2.13	0.49
1:F:144:GLU:OE2	1:F:147:VAL:N	2.45	0.49
1:F:424:THR:CG2	1:F:442:ILE:HG21	2.42	0.49
1:E:110:LEU:HG	1:E:306:HIS:HA	1.94	0.49
1:E:471:ARG:HE	1:E:484:LEU:HD21	1.78	0.49
1:A:367:VAL:O	1:A:371:LEU:HG	2.13	0.49
1:C:248:GLY:HA3	1:C:425:LYS:CD	2.42	0.49
1:C:344:ILE:HG22	1:C:347:ILE:HG12	1.95	0.49
1:D:128:LYS:O	1:D:129:VAL:HG22	2.12	0.48
1:D:272:SER:O	1:C:234:ARG:NH2	2.42	0.48
1:F:132:GLY:N	1:F:179:VAL:O	2.46	0.48
1:F:290:THR:HB	1:F:411:ILE:HG21	1.94	0.48
1:E:661:ARG:HB3	1:E:664:GLU:OE1	2.13	0.48
1:C:183:ALA:O	1:C:236:TYR:OH	2.30	0.48
1:A:223:HIS:O	1:A:224:ILE:HG22	2.13	0.48
1:A:612:ILE:HG22	1:A:654:VAL:HB	1.95	0.48
1:C:453:VAL:HG22	1:C:454:GLY:H	1.78	0.48
1:C:736:ILE:HG22	1:C:742:VAL:HG22	1.94	0.48
1:D:287:PRO:HG2	1:D:413:ILE:HG23	1.95	0.48
1:F:290:THR:HB	1:F:411:ILE:CG2	2.43	0.48
1:F:396:ASP:HB3	1:F:399:LEU:HD23	1.94	0.48
1:F:692:ILE:CD1	2:F:801:ADP:N1	2.76	0.48
1:E:577:ASN:HB2	1:E:611:SER:HB2	1.94	0.48
1:C:166:ASN:HB3	1:C:176:ILE:H	1.78	0.48
1:D:173:ASP:O	1:D:174:GLU:HG2	2.14	0.48
1:D:182:ASP:OD1	1:D:182:ASP:N	2.46	0.48
1:D:465:VAL:O	1:D:469:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:SER:H	1:D:723:GLU:HB3	1.78	0.48
1:F:584:PRO:HD3	1:F:617:GLU:HB2	1.95	0.48
1:B:91:HIS:NE2	1:B:95:VAL:HG23	2.29	0.48
1:E:600:GLU:O	1:E:603:ARG:HG3	2.13	0.48
1:A:158:ILE:HD11	1:A:194:LEU:HB3	1.94	0.48
1:C:223:HIS:O	1:C:224:ILE:HG22	2.13	0.48
1:A:294:MET:HE2	3:A:802:ATP:H3'	1.96	0.48
1:A:353:ASN:HB3	1:A:356:ASN:HB2	1.95	0.48
1:A:363:GLU:O	1:A:366:VAL:HG12	2.13	0.48
1:C:187:SER:HB3	1:C:189:PRO:HD2	1.95	0.48
1:C:296:LEU:C	1:C:299:VAL:HG12	2.37	0.48
1:C:316:VAL:HG13	1:C:362:VAL:HG21	1.96	0.48
1:C:660:ASN:O	1:C:769:TYR:OH	2.31	0.48
1:D:200:ASP:C	1:D:201:MET:HE2	2.38	0.48
1:F:267:GLN:O	1:F:267:GLN:HG2	2.13	0.48
1:B:556:TYR:HE1	1:B:678:HIS:HB3	1.79	0.48
1:C:459:ALA:HB1	1:C:498:ILE:HD11	1.94	0.48
1:B:223:HIS:O	1:B:224:ILE:HG22	2.13	0.48
1:E:120:GLN:NE2	1:E:121:VAL:HG12	2.28	0.48
1:E:147:VAL:HG12	1:E:151:LEU:HG	1.96	0.48
1:C:487:THR:O	1:C:491:VAL:HG23	2.13	0.48
1:C:513:VAL:HG22	1:C:568:LYS:HB3	1.96	0.48
1:D:736:ILE:HG22	1:D:742:VAL:HG22	1.95	0.48
1:B:571:ALA:HB2	1:B:612:ILE:HD11	1.95	0.48
1:A:268:PRO:HG3	1:A:382:LYS:HE2	1.95	0.48
1:A:348:ASP:OD1	1:A:348:ASP:N	2.47	0.48
1:A:366:VAL:HA	1:A:369:THR:HG22	1.96	0.48
1:C:247:VAL:CG2	3:C:802:ATP:N6	2.66	0.48
1:D:247:VAL:CG1	3:D:802:ATP:HN62	2.26	0.48
1:D:697:THR:HA	1:D:700:PHE:HD2	1.78	0.48
1:B:133:SER:HA	1:B:178:VAL:HG12	1.95	0.48
1:B:565:LEU:HA	1:B:568:LYS:HE2	1.94	0.48
1:E:565:LEU:C	1:E:565:LEU:CD2	2.86	0.48
1:A:158:ILE:HG23	1:A:160:PRO:HD2	1.96	0.48
1:A:438:ASP:OD1	1:A:438:ASP:N	2.46	0.48
1:D:577:ASN:O	1:D:611:SER:OG	2.23	0.48
1:F:426:GLN:OE1	4:F:803:NDT:H17	2.14	0.48
1:B:466:MET:HE1	1:C:271:PHE:HE2	1.79	0.48
1:E:52:TYR:HD2	1:E:87:ASP:HA	1.79	0.48
1:E:162:MET:HE2	1:E:180:ILE:HG21	1.94	0.48
1:D:223:HIS:O	1:D:224:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:GLY:HA3	3:E:802:ATP:H8	1.79	0.47
1:E:752:LYS:HA	1:E:755:LYS:HE2	1.95	0.47
1:A:140:LEU:HB2	1:A:143:MET:HE3	1.96	0.47
1:D:132:GLY:HA3	1:D:179:VAL:HB	1.95	0.47
1:A:193:GLN:HG3	1:A:194:LEU:HD22	1.96	0.47
1:F:127:THR:HG22	1:F:128:LYS:HE3	1.96	0.47
1:B:53:ILE:HB	1:B:58:LEU:HD21	1.96	0.47
1:E:396:ASP:HB3	1:E:399:LEU:HD23	1.97	0.47
1:A:37:ARG:HE	1:A:38:PRO:HD2	1.78	0.47
1:A:161:GLY:HA2	1:A:180:ILE:HG22	1.95	0.47
1:C:251:ASP:O	1:C:254:ILE:N	2.47	0.47
1:C:558:PRO:HG2	1:C:683:PRO:CD	2.42	0.47
1:E:186:ASP:OD1	1:E:186:ASP:N	2.45	0.47
1:B:147:VAL:HG12	1:B:151:LEU:HG	1.96	0.47
1:B:550:PRO:HB2	1:B:677:ARG:NH2	2.30	0.47
1:A:556:TYR:HE1	1:A:678:HIS:HB3	1.80	0.47
1:C:200:ASP:O	1:C:201:MET:HE2	2.15	0.47
1:C:482:PHE:C	1:C:484:LEU:H	2.21	0.47
1:C:666:ASP:N	1:C:666:ASP:OD1	2.48	0.47
1:D:719:TYR:CD1	1:D:759:ARG:HB3	2.49	0.47
1:E:577:ASN:H	1:E:577:ASN:ND2	2.12	0.47
1:C:600:GLU:O	1:C:603:ARG:HG3	2.13	0.47
1:D:429:ARG:CD	4:D:803:NDT:H213	2.44	0.47
1:D:564:THR:HB	2:D:801:ADP:H3'	1.97	0.47
1:F:53:ILE:HG13	1:F:84:ARG:HD2	1.95	0.47
1:F:123:PRO:HG2	1:F:198:MET:SD	2.55	0.47
1:F:233:ASN:HB3	1:F:236:TYR:HD2	1.79	0.47
1:B:665:ILE:HG23	1:B:669:LEU:HD23	1.97	0.47
1:A:173:ASP:O	1:A:174:GLU:HG2	2.15	0.47
1:A:600:GLU:O	1:A:603:ARG:HG3	2.15	0.47
1:C:329:ASP:O	1:C:332:ASN:N	2.48	0.47
1:C:739:ASP:OD1	1:C:739:ASP:N	2.47	0.47
1:E:135:GLN:HE21	1:E:176:ILE:HA	1.79	0.47
1:C:49:CYS:SG	1:C:83:ALA:HB3	2.55	0.47
1:C:129:VAL:HG13	1:C:180:ILE:HD11	1.97	0.47
1:C:245:ALA:O	1:C:425:LYS:NZ	2.36	0.47
1:D:515:TRP:HE1	1:D:573:GLU:HG3	1.80	0.47
1:F:671:ARG:HG3	1:F:672:PRO:HD2	1.97	0.47
1:B:524:LEU:HD22	1:B:681:VAL:HG23	1.97	0.47
1:B:593:GLU:O	1:B:596:ARG:HG3	2.15	0.47
1:E:326:ALA:O	1:E:330:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:MET:HE1	1:D:383:VAL:HG21	1.96	0.47
1:D:429:ARG:NE	4:D:803:NDT:C18	2.77	0.47
1:F:134:LEU:O	1:F:135:GLN:HG3	2.14	0.47
1:B:739:ASP:OD1	1:B:739:ASP:N	2.48	0.47
1:C:46:LYS:HB2	1:C:50:THR:HG22	1.97	0.47
1:D:294:MET:CE	3:D:802:ATP:H3'	2.24	0.46
1:B:244:TYR:CD1	1:B:254:ILE:HD11	2.50	0.46
1:A:69:CYS:N	1:A:82:ILE:O	2.30	0.46
1:A:103:ARG:HD2	1:A:108:LEU:HD12	1.96	0.46
1:A:417:ASP:OD1	1:A:417:ASP:N	2.49	0.46
1:D:396:ASP:OD1	1:D:396:ASP:N	2.45	0.46
1:F:534:LEU:HB2	1:F:535:PRO:HD3	1.96	0.46
1:E:173:ASP:O	1:E:174:GLU:HG2	2.16	0.46
1:E:426:GLN:HA	4:E:803:NDT:H212	1.97	0.46
1:A:593:GLU:O	1:A:596:ARG:HG3	2.15	0.46
1:F:441:ALA:HB1	1:F:488:LEU:HD11	1.97	0.46
1:F:559:PRO:HB3	1:F:660:ASN:HD21	1.81	0.46
1:B:72:GLY:N	1:B:115:GLU:O	2.30	0.46
1:B:72:GLY:HA3	1:B:117:LYS:HE3	1.98	0.46
1:A:444:TYR:CE2	1:A:448:LYS:HD2	2.49	0.46
1:A:650:LEU:HB3	1:A:653:VAL:HG22	1.97	0.46
1:C:697:THR:HA	1:C:700:PHE:HD2	1.79	0.46
1:D:460:LEU:HG	1:D:494:ALA:HB1	1.96	0.46
1:F:98:LEU:O	1:F:102:ILE:HB	2.15	0.46
1:C:48:THR:HG23	1:C:102:ILE:HD11	1.97	0.46
1:C:166:ASN:ND2	1:C:174:GLU:O	2.41	0.46
1:D:565:LEU:HA	1:D:568:LYS:HD3	1.98	0.46
1:F:399:LEU:HD12	1:F:405:PHE:HE2	1.80	0.46
1:F:476:ASP:HB3	1:F:479:ILE:HB	1.96	0.46
1:F:565:LEU:HB3	2:F:801:ADP:C8	2.50	0.46
1:E:495:MET:O	1:E:498:ILE:HG22	2.16	0.46
1:A:244:TYR:HD1	1:A:254:ILE:HD11	1.81	0.46
1:F:366:VAL:HA	1:F:369:THR:HG22	1.97	0.46
1:E:414:PRO:HB2	1:E:419:ARG:HG3	1.98	0.46
1:E:429:ARG:HD3	4:E:803:NDT:C18	2.46	0.46
1:E:527:LYS:HB3	1:E:531:MET:HE1	1.98	0.46
1:A:162:MET:HB3	1:A:164:PHE:CE2	2.51	0.46
1:C:224:ILE:HG13	1:C:225:THR:H	1.80	0.46
1:C:294:MET:HE3	3:C:802:ATP:H2'	1.97	0.46
1:D:752:LYS:HA	1:D:755:LYS:HE2	1.97	0.46
1:F:293:THR:HA	1:F:296:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:GLY:CA	1:E:563:LYS:CE	2.90	0.46
1:C:71:VAL:HG23	1:C:114:LEU:HB3	1.98	0.46
1:C:496:VAL:O	1:C:499:ARG:NH2	2.49	0.46
1:C:565:LEU:HD23	1:C:565:LEU:C	2.40	0.46
1:D:311:ASN:H	1:D:315:ILE:HD11	1.81	0.46
1:B:101:THR:HG23	1:B:163:ILE:H	1.81	0.46
1:B:762:THR:O	1:B:765:MET:HG3	2.16	0.46
1:C:221:SER:OG	1:C:222:THR:N	2.48	0.46
1:C:493:SER:O	1:C:496:VAL:N	2.48	0.46
1:C:762:THR:HG22	1:C:765:MET:HE1	1.98	0.46
1:D:46:LYS:HB2	1:D:50:THR:HG22	1.96	0.46
1:D:48:THR:HG21	1:D:157:VAL:H	1.81	0.46
1:D:63:ILE:HG12	1:D:84:ARG:HE	1.81	0.46
1:F:134:LEU:HB2	1:F:179:VAL:HG23	1.97	0.46
1:F:293:THR:HA	1:F:296:LEU:HD22	1.98	0.46
1:F:403:GLY:HA2	4:E:803:NDT:H6	1.97	0.46
1:B:158:ILE:HG12	1:B:160:PRO:HD2	1.96	0.46
1:D:558:PRO:HB3	1:D:765:MET:HE1	1.97	0.46
1:F:50:THR:OG1	1:F:51:ALA:N	2.49	0.46
1:F:420:PHE:CD1	1:F:443:LYS:HA	2.51	0.46
1:F:510:MET:SD	1:F:511:PRO:HD2	2.56	0.46
1:F:720:SER:H	1:F:723:GLU:HB2	1.80	0.46
1:B:348:ASP:OD1	1:B:348:ASP:N	2.47	0.46
1:E:78:GLY:HA3	1:E:193:GLN:H	1.80	0.46
1:E:577:ASN:N	1:E:577:ASN:ND2	2.60	0.46
1:E:768:TYR:O	1:E:771:GLU:HG3	2.15	0.46
1:D:63:ILE:HG23	1:D:84:ARG:HH21	1.80	0.45
1:D:294:MET:SD	3:D:802:ATP:C2	3.09	0.45
1:B:294:MET:HE1	3:B:802:ATP:C8	2.50	0.45
1:B:363:GLU:O	1:B:366:VAL:HG12	2.15	0.45
1:E:300:ALA:HB2	1:E:343:PHE:CE1	2.51	0.45
1:E:423:LEU:HD21	1:E:457:LEU:CD1	2.46	0.45
1:C:251:ASP:HA	1:C:254:ILE:HG22	1.98	0.45
1:C:582:LYS:HB2	1:C:585:GLU:HB2	1.98	0.45
1:D:100:THR:HG22	1:D:103:ARG:HH21	1.81	0.45
1:D:140:LEU:HD23	1:D:140:LEU:H	1.81	0.45
1:D:354:ARG:HH21	1:D:364:SER:HB2	1.80	0.45
1:F:126:ALA:HB2	1:F:197:ASN:HB3	1.99	0.45
1:F:173:ASP:O	1:F:174:GLU:HG2	2.16	0.45
1:F:719:TYR:CE1	1:F:759:ARG:HB3	2.50	0.45
3:E:802:ATP:H2'	4:E:803:NDT:O2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:PRO:HG3	1:A:660:ASN:HD21	1.81	0.45
1:C:50:THR:OG1	1:C:51:ALA:N	2.50	0.45
1:D:118:LYS:HD3	1:D:119:ALA:H	1.80	0.45
1:D:512:LYS:HE3	1:D:572:THR:HA	1.98	0.45
1:F:313:PRO:HB3	1:A:365:ARG:HB2	1.98	0.45
1:B:142:CYS:SG	1:B:170:LYS:NZ	2.79	0.45
1:B:285:HIS:NE2	1:B:410:GLU:OE2	2.48	0.45
1:B:450:HIS:NE2	1:B:509:GLU:HB2	2.31	0.45
1:E:618:ILE:HG22	1:E:659:THR:HB	1.98	0.45
1:A:147:VAL:HG12	1:A:151:LEU:HG	1.98	0.45
1:C:476:ASP:HB2	1:C:479:ILE:CG2	2.47	0.45
1:F:48:THR:HA	1:F:102:ILE:HD11	1.98	0.45
1:F:637:LEU:HD23	1:F:640:LEU:HD21	1.97	0.45
1:F:736:ILE:HG22	1:F:742:VAL:HG22	1.97	0.45
4:B:803:NDT:C7	1:C:403:GLY:HA2	2.46	0.45
1:A:80:LEU:HD13	1:A:194:LEU:HG	1.98	0.45
1:A:427:PHE:HB3	1:A:435:HIS:NE2	2.31	0.45
1:C:109:ILE:HG21	1:C:300:ALA:HB1	1.99	0.45
1:D:426:GLN:HE21	1:D:426:GLN:HB2	1.57	0.45
1:E:132:GLY:N	1:E:179:VAL:O	2.49	0.45
1:E:251:ASP:O	1:E:254:ILE:N	2.47	0.45
1:D:144:GLU:O	1:D:147:VAL:HG13	2.16	0.45
1:D:187:SER:HB3	1:D:189:PRO:HD2	1.99	0.45
1:D:231:GLN:CD	1:D:232:ALA:H	2.24	0.45
1:F:58:LEU:HD22	1:F:84:ARG:HE	1.82	0.45
1:F:242:LEU:HB2	1:F:301:ASN:HD22	1.82	0.45
1:F:295:LEU:C	1:F:298:VAL:HG12	2.41	0.45
1:E:72:GLY:HA2	1:E:79:ILE:HG23	1.99	0.45
1:A:69:CYS:HB3	1:A:84:ARG:HD3	1.97	0.45
1:C:34:PHE:N	1:C:114:LEU:O	2.46	0.45
1:D:429:ARG:NE	4:D:803:NDT:H213	2.32	0.45
1:B:481:LYS:HB2	1:B:481:LYS:HE3	1.81	0.45
1:E:426:GLN:HB2	4:E:803:NDT:C21	2.47	0.45
1:E:429:ARG:HD3	4:E:803:NDT:C19	2.46	0.45
1:D:401:ARG:HH21	1:D:404:ARG:HH12	1.65	0.45
1:F:434:ARG:HH21	1:F:485:LYS:HA	1.81	0.45
1:F:565:LEU:CB	2:F:801:ADP:H8	2.25	0.45
1:B:476:ASP:HB3	1:B:479:ILE:HB	1.98	0.45
1:E:556:TYR:HE1	1:E:678:HIS:HB3	1.82	0.45
1:C:453:VAL:O	1:C:457:LEU:HG	2.17	0.45
1:D:327:LEU:HD21	1:D:370:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:O	1:B:374:MET:HG2	2.17	0.45
1:A:449:THR:HB	1:A:452:TYR:HB2	1.99	0.45
1:A:550:PRO:O	1:A:551:LYS:HG2	2.16	0.45
1:C:663:ASP:OD2	1:C:768:TYR:OH	2.32	0.45
1:D:435:HIS:O	1:D:435:HIS:CG	2.70	0.45
1:B:98:LEU:H	1:B:103:ARG:HH21	1.64	0.45
1:E:492:GLU:O	1:E:496:VAL:HG23	2.17	0.45
1:E:558:PRO:CD	1:E:682:GLY:HA2	2.46	0.45
1:E:720:SER:H	1:E:723:GLU:HB2	1.82	0.45
1:A:453:VAL:HG22	1:A:454:GLY:H	1.82	0.45
1:E:512:LYS:HG3	1:E:572:THR:OG1	2.17	0.44
1:E:751:GLU:HG3	1:E:755:LYS:HZ2	1.82	0.44
1:C:152:LEU:HA	1:C:157:VAL:HG21	1.98	0.44
1:C:173:ASP:O	1:C:174:GLU:HG2	2.17	0.44
1:B:37:ARG:N	1:B:96:ILE:O	2.47	0.44
1:B:263:ILE:HG13	1:B:264:PRO:CD	2.43	0.44
1:E:348:ASP:N	1:E:348:ASP:OD1	2.48	0.44
1:E:515:TRP:CH2	1:E:569:ALA:HB1	2.53	0.44
1:E:650:LEU:HB3	1:E:653:VAL:HG22	1.99	0.44
1:A:36:THR:HG23	1:A:110:LEU:HA	2.00	0.44
1:A:138:ASN:HD22	1:A:229:GLU:HB3	1.81	0.44
1:A:565:LEU:HD12	2:A:801:ADP:C8	2.53	0.44
1:C:366:VAL:O	1:C:370:LEU:HD23	2.17	0.44
1:D:294:MET:CE	3:D:802:ATP:C3'	2.72	0.44
1:D:429:ARG:CZ	4:D:803:NDT:H17	2.39	0.44
1:B:166:ASN:HB3	1:B:176:ILE:H	1.82	0.44
1:E:251:ASP:N	1:E:251:ASP:OD1	2.48	0.44
1:E:467:LYS:HD3	1:E:467:LYS:HA	1.74	0.44
1:A:448:LYS:HB3	1:A:495:MET:HE1	1.98	0.44
1:C:759:ARG:NH1	1:C:761:ILE:O	2.51	0.44
1:E:300:ALA:HB2	1:E:343:PHE:HE1	1.83	0.44
1:E:406:ASP:OD1	1:E:406:ASP:N	2.50	0.44
1:A:99:SER:O	1:A:103:ARG:HD3	2.17	0.44
1:A:429:ARG:NE	4:A:803:NDT:C19	2.80	0.44
1:E:100:THR:HA	1:E:103:ARG:HE	1.82	0.44
1:E:751:GLU:HG3	1:E:755:LYS:NZ	2.32	0.44
1:C:296:LEU:HA	1:C:299:VAL:HG12	1.99	0.44
1:F:63:ILE:HG12	1:F:84:ARG:HH12	1.82	0.44
1:F:128:LYS:O	1:F:129:VAL:HG12	2.18	0.44
1:F:198:MET:SD	1:F:198:MET:N	2.90	0.44
1:F:582:LYS:HG2	1:F:584:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:689:ARG:HA	1:F:692:ILE:HG22	1.99	0.44
1:B:92:PRO:HG2	1:B:95:VAL:HG22	2.00	0.44
1:E:247:VAL:HA	3:E:802:ATP:N1	2.32	0.44
1:D:123:PRO:HB2	1:D:197:ASN:CA	2.45	0.44
1:D:363:GLU:HG2	1:D:364:SER:H	1.82	0.44
1:F:363:GLU:OE2	1:F:365:ARG:HG3	2.17	0.44
1:F:565:LEU:HB2	2:F:801:ADP:H8	1.83	0.44
1:B:251:ASP:HA	1:B:254:ILE:CG2	2.46	0.44
1:E:69:CYS:HB3	1:E:84:ARG:HD3	1.99	0.44
1:E:160:PRO:HG2	1:E:194:LEU:HG	1.99	0.44
1:A:138:ASN:HD21	1:A:226:PHE:HE1	1.66	0.44
1:A:294:MET:HE1	3:A:802:ATP:C4	2.53	0.44
1:F:173:ASP:CG	1:F:174:GLU:H	2.26	0.44
1:F:733:LEU:O	1:F:737:MET:HG2	2.17	0.44
1:E:524:LEU:HD22	1:E:681:VAL:HG23	2.00	0.44
1:D:419:ARG:HA	1:D:422:ILE:HG22	1.98	0.44
1:D:429:ARG:NH1	4:D:803:NDT:C17	2.81	0.44
1:F:77:ASN:O	1:F:193:GLN:HG2	2.18	0.44
1:F:707:VAL:HG12	1:F:747:LEU:HD12	1.99	0.44
1:E:233:ASN:HB3	1:E:236:TYR:HD2	1.83	0.44
1:E:733:LEU:HD23	1:E:736:ILE:HD11	2.00	0.44
1:C:450:HIS:HE1	1:C:508:LEU:HG	1.83	0.44
1:C:556:TYR:O	1:C:556:TYR:CG	2.70	0.44
1:D:487:THR:HG23	1:D:489:LYS:H	1.83	0.43
1:F:48:THR:OG1	1:F:154:ASP:OD2	2.25	0.43
1:F:100:THR:HG22	1:F:103:ARG:NH2	2.30	0.43
1:B:98:LEU:O	1:B:102:ILE:HB	2.18	0.43
1:E:34:PHE:O	1:E:114:LEU:N	2.36	0.43
1:E:366:VAL:HA	1:E:369:THR:HG22	2.00	0.43
1:E:402:PRO:HA	1:E:406:ASP:HB3	1.99	0.43
1:C:280:ARG:O	1:C:385:VAL:N	2.38	0.43
1:F:280:ARG:NH1	1:F:383:VAL:H	2.16	0.43
1:B:162:MET:SD	1:B:178:VAL:HG23	2.58	0.43
1:B:294:MET:HE1	3:B:802:ATP:C4	2.53	0.43
1:B:316:VAL:HG22	1:B:362:VAL:HG11	2.01	0.43
1:B:419:ARG:HG2	1:B:457:LEU:HD11	2.00	0.43
1:E:143:MET:HA	1:E:170:LYS:HD2	2.00	0.43
1:E:611:SER:OG	1:E:612:ILE:N	2.51	0.43
1:A:37:ARG:NE	1:A:38:PRO:HD2	2.34	0.43
1:C:448:LYS:HB3	1:C:495:MET:HE1	2.00	0.43
1:C:476:ASP:OD2	1:C:484:LEU:HD21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:NH1	1:E:273:SER:O	2.52	0.43
1:F:242:LEU:N	1:F:301:ASN:ND2	2.43	0.43
1:F:348:ASP:OD1	1:F:348:ASP:N	2.50	0.43
1:F:423:LEU:HD12	1:F:423:LEU:HA	1.90	0.43
1:B:768:TYR:O	1:B:771:GLU:HG3	2.18	0.43
1:E:435:HIS:HB2	1:E:486:VAL:HB	2.00	0.43
1:E:695:LYS:HZ1	2:E:801:ADP:HN62	1.66	0.43
1:A:231:GLN:CD	1:A:232:ALA:H	2.27	0.43
1:A:637:LEU:HD23	1:A:640:LEU:HD21	2.00	0.43
1:C:31:PRO:HG3	1:C:57:VAL:HG22	2.00	0.43
1:C:567:ALA:HB1	1:C:578:PHE:CZ	2.53	0.43
1:C:577:ASN:O	1:C:611:SER:OG	2.26	0.43
1:D:70:THR:OG1	1:D:117:LYS:O	2.36	0.43
1:F:52:TYR:HD2	1:F:87:ASP:HA	1.83	0.43
1:F:91:HIS:NE2	1:F:95:VAL:O	2.50	0.43
1:F:307:VAL:HG23	1:F:341:ILE:HB	2.00	0.43
1:B:58:LEU:HD22	1:B:84:ARG:HE	1.82	0.43
1:B:173:ASP:O	1:B:174:GLU:HG2	2.18	0.43
1:E:70:THR:O	1:E:116:LEU:HD23	2.19	0.43
1:A:98:LEU:H	1:A:103:ARG:CZ	2.30	0.43
1:A:343:PHE:CE2	1:A:386:ILE:HD11	2.54	0.43
1:C:158:ILE:HD11	1:C:194:LEU:HB3	2.00	0.43
1:C:599:ARG:HH21	1:C:643:GLU:HG3	1.83	0.43
1:F:456:ASP:O	1:F:460:LEU:HD23	2.18	0.43
1:F:759:ARG:HH11	1:F:761:ILE:HG23	1.84	0.43
1:B:366:VAL:O	1:B:370:LEU:HD23	2.18	0.43
1:E:251:ASP:O	1:E:254:ILE:HG22	2.19	0.43
1:E:363:GLU:O	1:E:366:VAL:HG22	2.19	0.43
1:C:476:ASP:CB	1:C:479:ILE:CG2	2.96	0.43
1:D:556:TYR:HE1	1:D:678:HIS:HB3	1.82	0.43
1:F:435:HIS:HB2	1:F:486:VAL:HB	2.00	0.43
1:B:63:ILE:HG12	1:B:84:ARG:HH12	1.84	0.43
1:E:308:LEU:N	1:E:341:ILE:O	2.50	0.43
1:C:61:LEU:HD23	1:C:61:LEU:O	2.18	0.43
1:C:481:LYS:HE2	1:C:482:PHE:CZ	2.53	0.43
1:D:55:PRO:HA	1:D:58:LEU:HD12	1.99	0.43
1:D:342:ILE:HB	1:D:385:VAL:HG22	2.00	0.43
1:D:429:ARG:HD3	4:D:803:NDT:H211	2.00	0.43
1:F:110:LEU:HB2	1:F:307:VAL:HG12	2.00	0.43
1:B:741:ASP:OD1	1:C:544:ARG:NH2	2.51	0.43
1:E:265:LEU:HD13	1:E:382:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:SER:OG	1:E:665:ILE:HG13	2.18	0.43
1:A:120:GLN:HG3	1:A:121:VAL:H	1.84	0.43
1:A:529:LYS:HA	1:A:532:ILE:HG12	2.00	0.43
1:E:248:GLY:O	3:E:802:ATP:N6	2.52	0.43
1:E:291:GLY:HA2	3:E:802:ATP:PA	2.58	0.43
1:E:556:TYR:C	1:E:563:LYS:CE	2.92	0.43
1:E:704:GLU:HB2	1:E:744:LYS:HD3	2.01	0.43
1:A:166:ASN:HB3	1:A:175:SER:HA	2.01	0.43
1:A:563:LYS:HZ1	1:A:660:ASN:CG	2.25	0.43
1:A:719:TYR:HB3	1:A:723:GLU:HB2	2.01	0.43
1:C:247:VAL:CG2	1:C:295:LEU:HD21	2.43	0.43
1:D:579:LEU:HD12	1:D:601:ILE:HD11	2.01	0.43
1:F:53:ILE:HB	1:F:58:LEU:HD21	2.00	0.43
1:F:552:GLY:HA3	1:F:675:LEU:H	1.84	0.43
1:B:58:LEU:HD13	1:B:65:PRO:HG3	2.00	0.43
1:E:285:HIS:HA	1:E:292:LYS:HZ3	1.84	0.43
1:E:426:GLN:HG3	1:E:427:PHE:HD2	1.83	0.43
1:E:50:THR:HB	1:E:52:TYR:CE1	2.54	0.43
1:E:429:ARG:CD	4:E:803:NDT:C21	2.85	0.43
1:E:598:ILE:HA	1:E:601:ILE:HG22	2.00	0.43
1:C:637:LEU:HD23	1:C:637:LEU:HA	1.91	0.43
1:D:623:PRO:HD3	1:D:664:GLU:HB3	2.01	0.42
1:B:271:PHE:CD2	1:B:278:PRO:HB3	2.54	0.42
1:E:69:CYS:HB3	1:E:84:ARG:HB2	2.01	0.42
1:E:529:LYS:HA	1:E:532:ILE:HG12	2.01	0.42
1:A:186:ASP:OD1	1:A:186:ASP:N	2.51	0.42
1:A:421:ASP:O	1:A:424:THR:OG1	2.34	0.42
1:C:561:CYS:HB2	1:C:722:ALA:H	1.84	0.42
1:D:257:LEU:O	1:D:261:ILE:HG12	2.19	0.42
1:D:429:ARG:CD	4:D:803:NDT:H211	2.47	0.42
1:F:403:GLY:C	4:E:803:NDT:H7	2.43	0.42
1:F:462:ARG:HD3	1:A:279:PRO:HD3	2.01	0.42
1:E:738:GLU:HG3	1:E:749:HIS:HE2	1.84	0.42
1:D:430:MET:CE	1:E:276:VAL:CG1	2.98	0.42
1:F:72:GLY:HA3	1:F:115:GLU:HB2	2.01	0.42
1:F:97:THR:C	1:F:98:LEU:HD12	2.44	0.42
1:F:583:GLY:HA3	1:F:617:GLU:O	2.19	0.42
1:B:110:LEU:O	1:B:307:VAL:HG22	2.19	0.42
1:B:177:ASP:N	1:B:177:ASP:OD1	2.52	0.42
1:B:430:MET:SD	1:B:435:HIS:ND1	2.92	0.42
1:C:70:THR:HG22	1:C:81:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:MET:O	1:C:430:MET:HG2	2.19	0.42
1:D:50:THR:OG1	1:D:51:ALA:N	2.51	0.42
1:B:367:VAL:HG13	1:B:399:LEU:HG	2.01	0.42
1:E:134:LEU:N	1:E:177:ASP:O	2.52	0.42
1:E:311:ASN:OD1	1:E:314:SER:HB3	2.19	0.42
1:E:695:LYS:NZ	2:E:801:ADP:N6	2.66	0.42
1:C:247:VAL:CG2	3:C:802:ATP:HN62	2.30	0.42
1:C:619:ASP:OD1	1:C:619:ASP:N	2.51	0.42
1:D:344:ILE:HG21	1:D:347:ILE:HD13	2.01	0.42
1:F:554:LEU:HD22	1:F:678:HIS:CD2	2.54	0.42
1:B:79:ILE:H	1:B:193:GLN:HE21	1.68	0.42
1:B:606:ARG:HE	1:B:650:LEU:HD21	1.83	0.42
1:A:391:ARG:HH21	1:A:392:PRO:HD2	1.84	0.42
1:F:70:THR:HB	1:F:79:ILE:HG23	2.02	0.42
1:E:53:ILE:HB	1:E:58:LEU:HD21	2.01	0.42
1:A:140:LEU:O	1:A:142:CYS:N	2.53	0.42
1:A:434:ARG:HA	1:A:434:ARG:NH1	2.34	0.42
1:C:69:CYS:N	1:C:82:ILE:O	2.32	0.42
1:C:640:LEU:O	1:C:644:ILE:HG12	2.19	0.42
1:D:285:HIS:HB2	1:D:392:PRO:HG3	2.02	0.42
1:D:403:GLY:HA2	4:D:804:NDT:H6	2.01	0.42
1:F:140:LEU:HB2	1:F:143:MET:HB3	2.01	0.42
1:F:162:MET:HE2	1:F:180:ILE:HG21	2.01	0.42
1:F:251:ASP:O	1:F:254:ILE:HG22	2.20	0.42
1:B:251:ASP:O	1:B:254:ILE:HG22	2.20	0.42
1:B:578:PHE:HE2	1:B:580:ALA:HB2	1.83	0.42
1:A:246:ALA:C	1:A:425:LYS:HD3	2.44	0.42
1:C:436:VAL:O	1:C:436:VAL:HG13	2.19	0.42
1:D:49:CYS:SG	1:D:83:ALA:HB3	2.60	0.42
1:F:283:LEU:HD21	1:F:405:PHE:CG	2.55	0.42
1:F:297:ARG:CA	1:F:297:ARG:NH1	2.75	0.42
1:F:480:ASP:OD1	1:F:480:ASP:N	2.52	0.42
1:F:739:ASP:OD1	1:F:739:ASP:N	2.52	0.42
1:F:762:THR:HG23	1:F:764:GLU:HG3	2.00	0.42
1:A:562:SER:HB2	1:A:681:VAL:HG22	2.02	0.42
1:D:138:ASN:HD21	1:D:226:PHE:HE1	1.68	0.42
1:D:263:ILE:HD13	1:C:469:ILE:HG21	2.00	0.42
1:D:427:PHE:CD1	1:D:435:HIS:CE1	3.08	0.42
1:F:598:ILE:HA	1:F:601:ILE:HG12	2.01	0.42
1:B:35:ILE:HG23	1:B:111:GLY:HA2	2.01	0.42
1:B:71:VAL:O	1:B:79:ILE:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:GLN:HB3	1:E:339:PRO:HD3	2.02	0.42
1:C:36:THR:HB	1:C:114:LEU:HD11	2.02	0.42
1:C:463:GLU:OE2	1:C:463:GLU:HA	2.20	0.42
1:D:38:PRO:HD3	1:D:110:LEU:HD11	2.01	0.42
1:D:348:ASP:OD1	1:D:348:ASP:N	2.52	0.42
1:D:611:SER:OG	1:D:612:ILE:N	2.53	0.42
1:F:49:CYS:SG	1:F:83:ALA:HB3	2.60	0.42
1:F:510:MET:HG3	1:F:568:LYS:HD3	2.01	0.42
1:B:462:ARG:HH11	1:C:279:PRO:HD3	1.84	0.42
1:E:448:LYS:HB3	1:E:495:MET:HE1	2.01	0.42
1:E:584:PRO:HA	1:E:587:PHE:HD2	1.83	0.42
1:A:311:ASN:HB2	1:A:314:SER:HB3	2.01	0.42
1:C:419:ARG:HA	1:C:422:ILE:HG22	2.01	0.42
1:C:423:LEU:CD1	1:C:427:PHE:CE1	2.80	0.42
1:C:471:ARG:CZ	1:C:484:LEU:HD22	2.49	0.42
1:C:759:ARG:H	1:C:759:ARG:HG2	1.72	0.42
1:D:598:ILE:O	1:D:601:ILE:HG22	2.21	0.41
1:F:487:THR:OG1	1:F:488:LEU:N	2.53	0.41
1:B:140:LEU:O	1:B:142:CYS:N	2.53	0.41
1:B:401:ARG:HH12	1:A:288:PRO:HB2	1.85	0.41
1:A:342:ILE:HB	1:A:385:VAL:HA	2.02	0.41
1:A:661:ARG:HB3	1:A:664:GLU:OE1	2.20	0.41
1:C:134:LEU:HB2	1:C:179:VAL:CG2	2.50	0.41
1:C:152:LEU:HD23	1:C:199:ASP:HB3	2.02	0.41
1:D:583:GLY:O	1:D:586:ILE:HG12	2.20	0.41
1:B:434:ARG:HB3	1:C:274:PHE:CE1	2.55	0.41
1:B:641:LEU:HD12	1:B:644:ILE:HD11	2.02	0.41
1:E:118:LYS:H	1:E:118:LYS:HG2	1.70	0.41
1:A:112:ASP:OD1	1:A:112:ASP:N	2.51	0.41
1:C:481:LYS:CD	1:C:481:LYS:N	2.79	0.41
1:F:262:GLU:HG2	1:F:266:HIS:CG	2.55	0.41
1:B:274:PHE:HE1	1:A:434:ARG:HH21	1.67	0.41
1:E:231:GLN:CD	1:E:232:ALA:H	2.29	0.41
1:A:138:ASN:ND2	1:A:229:GLU:HB3	2.35	0.41
1:C:102:ILE:HD12	1:C:102:ILE:H	1.85	0.41
1:C:324:GLU:OE1	1:C:369:THR:HG21	2.20	0.41
1:C:555:LEU:HD13	1:C:679:ILE:HB	2.02	0.41
1:C:560:GLY:HA3	1:C:720:SER:CB	2.46	0.41
1:C:711:GLU:OE1	1:C:715:ARG:NH1	2.53	0.41
1:D:96:ILE:HD11	1:D:114:LEU:HD22	2.01	0.41
1:D:481:LYS:HA	1:D:481:LYS:HD2	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:LYS:HA	1:F:467:LYS:HD3	1.84	0.41
1:F:612:ILE:HG22	1:F:654:VAL:HB	2.02	0.41
1:B:366:VAL:HA	1:B:369:THR:HG22	2.02	0.41
1:A:36:THR:OG1	1:A:103:ARG:NH2	2.52	0.41
1:C:109:ILE:HD11	1:C:297:ARG:NH2	2.35	0.41
1:C:542:PHE:HB3	1:C:548:SER:HA	2.02	0.41
1:D:233:ASN:HB3	1:D:236:TYR:CD2	2.56	0.41
1:D:292:LYS:HD2	1:D:388:ALA:HB1	2.02	0.41
1:D:489:LYS:HA	1:D:489:LYS:HD2	1.77	0.41
1:F:91:HIS:CE1	1:F:95:VAL:HG13	2.56	0.41
1:B:644:ILE:HG13	1:B:645:ASP:N	2.36	0.41
1:E:167:LEU:HB3	1:E:168:LYS:H	1.73	0.41
1:A:144:GLU:O	1:A:145:GLU:HG3	2.21	0.41
1:A:704:GLU:HB3	1:A:744:LYS:HD3	2.03	0.41
1:C:130:THR:O	1:C:180:ILE:HD12	2.21	0.41
1:D:762:THR:O	1:D:765:MET:HG3	2.20	0.41
1:F:370:LEU:O	1:F:374:MET:HG3	2.20	0.41
1:F:600:GLU:O	1:F:603:ARG:HD3	2.20	0.41
1:A:431:SER:O	1:A:435:HIS:CD2	2.73	0.41
1:A:534:LEU:HD22	1:A:542:PHE:HZ	1.85	0.41
1:D:402:PRO:HA	1:D:406:ASP:HB3	2.03	0.41
1:D:403:GLY:HA2	4:D:804:NDT:H7	2.01	0.41
1:F:63:ILE:HG23	1:F:84:ARG:NH2	2.35	0.41
1:F:499:ARG:HD2	1:F:499:ARG:O	2.21	0.41
1:E:429:ARG:HD3	4:E:803:NDT:H19	2.02	0.41
1:E:561:CYS:SG	1:E:721:GLY:N	2.87	0.41
1:E:662:PRO:HB2	1:E:772:PHE:CZ	2.55	0.41
1:D:517:ASP:CG	1:D:695:LYS:HE2	2.46	0.41
1:D:524:LEU:O	1:D:528:MET:HG3	2.20	0.41
1:F:251:ASP:CA	1:F:254:ILE:HG22	2.48	0.41
1:F:363:GLU:O	1:F:366:VAL:HG22	2.20	0.41
1:B:453:VAL:HG22	1:B:454:GLY:H	1.85	0.41
1:B:534:LEU:O	1:B:538:ALA:CB	2.61	0.41
1:E:338:GLN:NE2	1:E:382:LYS:HG2	2.35	0.41
1:C:762:THR:HG23	1:C:764:GLU:HG3	2.03	0.41
1:D:72:GLY:HA2	1:D:79:ILE:HA	2.02	0.41
1:D:166:ASN:HB3	1:D:175:SER:HA	2.02	0.41
1:D:332:ASN:HA	1:D:335:ARG:HG2	2.03	0.41
1:F:460:LEU:HD11	1:F:495:MET:HA	2.02	0.41
1:F:563:LYS:NZ	1:F:660:ASN:HA	2.36	0.41
1:B:63:ILE:HG23	1:B:84:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:THR:OG1	3:B:802:ATP:H1'	2.20	0.41
1:B:551:LYS:HG2	1:B:655:ILE:H	1.86	0.41
1:B:595:GLU:CD	1:B:639:SER:HG	2.27	0.41
1:B:715:ARG:NH2	1:B:751:GLU:OE1	2.53	0.41
1:E:250:LEU:HD23	3:E:802:ATP:N6	2.35	0.41
1:E:553:VAL:HA	1:E:677:ARG:HB2	2.02	0.41
1:E:623:PRO:HB3	1:E:664:GLU:HB3	2.02	0.41
1:A:158:ILE:HA	1:A:196:LEU:HG	2.01	0.41
1:C:154:ASP:OD1	1:C:155:SER:N	2.53	0.41
1:C:173:ASP:CG	1:C:174:GLU:H	2.28	0.41
1:C:347:ILE:HA	1:C:350:ILE:HB	2.02	0.41
1:D:242:LEU:H	1:D:301:ASN:HD22	1.68	0.41
1:B:128:LYS:O	1:B:129:VAL:HG12	2.22	0.41
1:B:310:ILE:HG22	1:B:312:GLY:H	1.85	0.41
1:E:481:LYS:HE2	1:E:481:LYS:HB2	1.93	0.41
1:E:600:GLU:OE2	1:E:603:ARG:NH2	2.48	0.41
1:A:391:ARG:NH2	1:A:392:PRO:HD2	2.35	0.41
1:A:554:LEU:HD13	1:A:670:LEU:HD21	2.03	0.41
1:C:504:ARG:NH1	1:C:585:GLU:OE2	2.54	0.41
1:C:518:ILE:HD13	1:C:565:LEU:HD21	2.02	0.41
1:D:162:MET:HB3	1:D:164:PHE:CE2	2.56	0.40
1:F:371:LEU:HA	1:F:374:MET:HG3	2.02	0.40
1:B:261:ILE:HD11	1:B:386:ILE:HD11	2.03	0.40
1:B:598:ILE:O	1:B:601:ILE:HG22	2.22	0.40
1:E:173:ASP:CG	1:E:174:GLU:H	2.30	0.40
1:C:624:ASP:HA	1:C:629:SER:HB2	2.03	0.40
1:D:63:ILE:O	1:D:84:ARG:NH2	2.54	0.40
1:D:308:LEU:HD23	1:D:330:ILE:HG23	2.04	0.40
1:B:182:ASP:OD1	1:B:182:ASP:N	2.54	0.40
1:B:640:LEU:O	1:B:644:ILE:HG12	2.21	0.40
1:E:334:ALA:HB1	1:E:342:ILE:HD11	2.02	0.40
1:A:746:GLU:OE1	1:A:748:ARG:NE	2.46	0.40
1:C:110:LEU:HB3	1:C:306:HIS:HA	2.04	0.40
1:D:159:MET:CE	1:D:197:ASN:HB2	2.51	0.40
1:F:438:ASP:N	1:F:438:ASP:OD1	2.45	0.40
1:F:604:LYS:HZ2	1:F:608:ALA:HB2	1.87	0.40
1:F:723:GLU:O	1:F:727:LEU:HD23	2.21	0.40
1:B:367:VAL:O	1:B:371:LEU:HG	2.22	0.40
1:E:436:VAL:HG13	1:E:485:LYS:HD2	2.04	0.40
1:A:325:ALA:HA	1:A:328:ARG:HG2	2.02	0.40
1:A:739:ASP:N	1:A:739:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LYS:HD3	1:D:119:ALA:N	2.36	0.40
1:D:221:SER:OG	1:D:222:THR:N	2.55	0.40
1:D:295:LEU:HA	1:D:298:VAL:HG12	2.03	0.40
1:D:429:ARG:NH2	4:D:803:NDT:H17	2.35	0.40
1:F:353:ASN:HB3	1:F:356:ASN:HB2	2.03	0.40
1:F:423:LEU:HD21	1:F:445:ILE:HG21	2.03	0.40
1:C:181:THR:OG1	1:C:182:ASP:N	2.54	0.40
1:C:584:PRO:HA	1:C:587:PHE:HD2	1.86	0.40
1:D:117:LYS:HD2	1:D:117:LYS:HA	1.95	0.40
1:D:401:ARG:NH2	1:D:404:ARG:HH22	2.19	0.40
1:F:44:HIS:O	1:F:47:GLU:HB2	2.22	0.40
1:F:233:ASN:HB3	1:F:236:TYR:CD2	2.57	0.40
1:A:282:ILE:HG13	1:A:407:GLN:NE2	2.30	0.40
1:A:429:ARG:HB3	4:A:803:NDT:H212	2.04	0.40
1:C:294:MET:HE3	3:C:802:ATP:C2'	2.52	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	730/780 (94%)	653 (90%)	68 (9%)	9 (1%)	10	42
1	B	730/780 (94%)	659 (90%)	63 (9%)	8 (1%)	11	45
1	C	730/780 (94%)	648 (89%)	73 (10%)	9 (1%)	10	42
1	D	730/780 (94%)	658 (90%)	66 (9%)	6 (1%)	16	52
1	E	730/780 (94%)	652 (89%)	69 (10%)	9 (1%)	10	42
1	F	730/780 (94%)	660 (90%)	61 (8%)	9 (1%)	10	42
All	All	4380/4680 (94%)	3930 (90%)	400 (9%)	50 (1%)	14	45

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	129	VAL
1	D	224	ILE
1	F	74	ILE
1	F	129	VAL
1	F	224	ILE
1	B	79	ILE
1	B	224	ILE
1	E	224	ILE
1	A	129	VAL
1	A	224	ILE
1	C	74	ILE
1	C	141	GLU
1	C	224	ILE
1	B	129	VAL
1	B	141	GLU
1	E	129	VAL
1	E	173	ASP
1	A	141	GLU
1	A	173	ASP
1	C	129	VAL
1	C	173	ASP
1	F	173	ASP
1	B	228	LYS
1	E	141	GLU
1	E	562	SER
1	F	141	GLU
1	E	174	GLU
1	C	79	ILE
1	D	157	VAL
1	D	174	GLU
1	F	174	GLU
1	B	99	SER
1	B	174	GLU
1	C	174	GLU
1	D	79	ILE
1	E	157	VAL
1	E	647	VAL
1	F	79	ILE
1	F	157	VAL
1	B	157	VAL
1	A	157	VAL
1	D	74	ILE
1	A	79	ILE

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Mol	Chain	Res	Type
1	A	277	SER
1	A	647	VAL
1	F	277	SER
1	E	277	SER
1	A	74	ILE
1	C	157	VAL
1	C	647	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	618/657 (94%)	617 (100%)	1 (0%)	87	85
1	B	618/657 (94%)	618 (100%)	0	100	100
1	C	618/657 (94%)	616 (100%)	2 (0%)	86	84
1	D	618/657 (94%)	617 (100%)	1 (0%)	87	85
1	E	618/657 (94%)	615 (100%)	3 (0%)	81	81
1	F	618/657 (94%)	613 (99%)	5 (1%)	73	77
All	All	3708/3942 (94%)	3696 (100%)	12 (0%)	84	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	426	GLN
1	F	290	THR
1	F	293	THR
1	F	296	LEU
1	F	298	VAL
1	F	416	VAL
1	E	564	THR
1	E	566	THR
1	E	577	ASN
1	A	430	MET
1	C	293	THR

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Mol	Chain	Res	Type
1	C	481	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	120	GLN
1	D	138	ASN
1	D	426	GLN
1	D	635	HIS
1	F	301	ASN
1	F	407	GLN
1	F	426	GLN
1	F	450	HIS
1	F	521	GLN
1	B	56	ASN
1	B	165	GLN
1	B	193	GLN
1	B	470	GLN
1	E	135	GLN
1	E	165	GLN
1	E	193	GLN
1	E	285	HIS
1	E	301	ASN
1	E	338	GLN
1	E	577	ASN
1	E	588	ASN
1	A	165	GLN
1	A	426	GLN
1	A	588	ASN
1	C	165	GLN
1	C	470	GLN
1	C	642	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	E	801	-	28,29,29	1.41	4 (14%)	43,45,45	1.83	9 (20%)
3	ATP	A	802	4	32,33,33	1.95	7 (21%)	48,52,52	2.72	13 (27%)
2	ADP	F	801	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
3	ATP	F	802	4	32,33,33	1.75	7 (21%)	48,52,52	2.71	12 (25%)
2	ADP	A	801	-	28,29,29	1.45	5 (17%)	43,45,45	1.83	9 (20%)
2	ADP	D	801	-	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	C	801	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	8 (18%)
3	ATP	B	802	4	32,33,33	1.93	7 (21%)	48,52,52	2.72	12 (25%)
4	NDT	A	803	3	20,22,23	2.14	4 (20%)	26,32,34	3.17	10 (38%)
4	NDT	F	803	3	20,22,23	2.11	4 (20%)	26,32,34	3.23	10 (38%)
3	ATP	E	802	4	32,33,33	1.77	7 (21%)	48,52,52	2.72	12 (25%)
4	NDT	D	804	3	20,22,23	2.40	5 (25%)	26,32,34	3.31	10 (38%)
4	NDT	E	803	3	20,22,23	2.19	4 (20%)	26,32,34	3.29	11 (42%)
3	ATP	C	802	4	32,33,33	1.92	7 (21%)	48,52,52	2.74	12 (25%)
3	ATP	D	802	4	32,33,33	1.73	7 (21%)	48,52,52	2.71	11 (22%)
4	NDT	D	803	3	20,22,23	2.13	3 (15%)	26,32,34	3.28	11 (42%)
2	ADP	B	801	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	9 (20%)
4	NDT	B	803	3	20,22,23	2.32	4 (20%)	26,32,34	3.24	11 (42%)

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
2	ADP	E	801	-	-	3/16/32/32	0/3/3/3
3	ATP	A	802	4	-	3/22/38/38	0/3/3/3
2	ADP	F	801	-	-	2/16/32/32	0/3/3/3
3	ATP	F	802	4	-	8/22/38/38	0/3/3/3
3	ATP	C	802	4	-	3/22/38/38	0/3/3/3
2	ADP	A	801	-	-	3/16/32/32	0/3/3/3
2	ADP	C	801	-	-	1/16/32/32	0/3/3/3
4	NDT	A	803	3	1/1/2/4	3/9/21/25	0/3/3/3
3	ATP	B	802	4	-	7/22/38/38	0/3/3/3
4	NDT	F	803	3	1/1/2/4	3/9/21/25	0/3/3/3
4	NDT	D	804	3	1/1/2/4	2/9/21/25	0/3/3/3
3	ATP	E	802	4	-	6/22/38/38	0/3/3/3
4	NDT	E	803	3	1/1/2/4	5/9/21/25	0/3/3/3
2	ADP	B	801	-	-	2/16/32/32	0/3/3/3
4	NDT	D	803	3	1/1/2/4	0/9/21/25	0/3/3/3
3	ATP	D	802	4	-	6/22/38/38	0/3/3/3
2	ADP	D	801	-	-	3/16/32/32	0/3/3/3
4	NDT	B	803	3	1/1/2/4	1/9/21/25	0/3/3/3

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	804	NDT	C15-S1	6.40	1.85	1.76
4	B	803	NDT	C15-S1	6.38	1.85	1.76
4	D	804	NDT	S1-N2	6.34	1.81	1.67
4	E	803	NDT	C15-S1	6.25	1.84	1.76
4	D	803	NDT	C15-S1	6.16	1.84	1.76
4	B	803	NDT	S1-N2	5.87	1.80	1.67
4	F	803	NDT	C15-S1	5.79	1.84	1.76
4	A	803	NDT	C15-S1	5.62	1.84	1.76
4	A	803	NDT	S1-N2	5.39	1.79	1.67
4	F	803	NDT	S1-N2	4.97	1.78	1.67
3	B	802	ATP	C5-C4	4.92	1.47	1.39
4	E	803	NDT	S1-N2	4.91	1.78	1.67
3	A	802	ATP	C5-C4	4.89	1.47	1.39
2	A	801	ADP	C5-C4	4.85	1.47	1.39
3	C	802	ATP	C5-C4	4.79	1.47	1.39
2	D	801	ADP	C5-C4	4.77	1.47	1.39
2	F	801	ADP	C5-C4	4.74	1.47	1.39
2	B	801	ADP	C5-C4	4.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ADP	C5-C4	4.71	1.47	1.39
2	E	801	ADP	C5-C4	4.69	1.47	1.39
4	D	803	NDT	S1-N2	4.63	1.78	1.67
3	E	802	ATP	C5-C4	4.61	1.47	1.39
3	D	802	ATP	C5-C4	4.56	1.47	1.39
3	B	802	ATP	PA-O1A	4.50	1.66	1.50
3	F	802	ATP	C5-C4	4.50	1.47	1.39
3	C	802	ATP	PA-O1A	4.49	1.66	1.50
3	F	802	ATP	PA-O1A	4.46	1.66	1.50
3	E	802	ATP	PA-O1A	4.45	1.66	1.50
3	A	802	ATP	PA-O1A	4.44	1.66	1.50
3	D	802	ATP	PA-O1A	4.38	1.66	1.50
3	A	802	ATP	PA-O3A	3.79	1.63	1.59
3	C	802	ATP	PA-O3A	3.56	1.63	1.59
3	B	802	ATP	PA-O3A	3.45	1.63	1.59
3	D	802	ATP	PG-O2G	-3.07	1.43	1.54
3	E	802	ATP	PG-O2G	-3.06	1.43	1.54
3	F	802	ATP	PG-O2G	-3.04	1.43	1.54
3	A	802	ATP	PG-O2G	-3.03	1.43	1.54
3	B	802	ATP	PG-O2G	-3.03	1.43	1.54
3	C	802	ATP	PG-O2G	-3.02	1.43	1.54
2	A	801	ADP	C5-C6	2.78	1.48	1.41
2	D	801	ADP	C5-C6	2.74	1.48	1.41
2	C	801	ADP	C5-C6	2.73	1.48	1.41
2	E	801	ADP	C5-C6	2.73	1.48	1.41
2	F	801	ADP	C5-C6	2.72	1.48	1.41
2	B	801	ADP	C5-C6	2.70	1.48	1.41
3	A	802	ATP	PG-O1G	2.57	1.58	1.50
3	C	802	ATP	PG-O1G	2.56	1.58	1.50
3	B	802	ATP	PG-O1G	2.55	1.58	1.50
3	E	802	ATP	PG-O1G	2.53	1.58	1.50
3	A	802	ATP	C8-N9	2.51	1.41	1.37
3	F	802	ATP	PA-O3A	2.51	1.62	1.59
3	B	802	ATP	C8-N9	2.50	1.41	1.37
3	F	802	ATP	PG-O1G	2.49	1.58	1.50
3	D	802	ATP	PG-O1G	2.48	1.58	1.50
3	C	802	ATP	C8-N9	2.45	1.41	1.37
2	C	801	ADP	C8-N7	2.40	1.36	1.31
2	E	801	ADP	C8-N7	2.37	1.36	1.31
2	A	801	ADP	C8-N7	2.35	1.36	1.31
3	D	802	ATP	PA-O2A	-2.34	1.44	1.55
2	D	801	ADP	C8-N7	2.33	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ADP	C5-N7	-2.33	1.34	1.39
4	D	804	NDT	C16-C15	2.33	1.42	1.38
2	F	801	ADP	C8-N7	2.31	1.36	1.31
3	E	802	ATP	PA-O2A	-2.31	1.44	1.55
2	B	801	ADP	C8-N7	2.31	1.36	1.31
3	D	802	ATP	C8-N9	2.30	1.41	1.37
3	C	802	ATP	PA-O2A	-2.28	1.44	1.55
3	B	802	ATP	PA-O2A	-2.28	1.44	1.55
3	F	802	ATP	PA-O2A	-2.27	1.44	1.55
2	B	801	ADP	C5-N7	-2.27	1.34	1.39
3	A	802	ATP	PA-O2A	-2.27	1.44	1.55
3	E	802	ATP	C8-N9	2.26	1.41	1.37
3	F	802	ATP	C8-N9	2.26	1.41	1.37
2	E	801	ADP	C5-N7	-2.24	1.35	1.39
2	D	801	ADP	C5-N7	-2.23	1.35	1.39
2	F	801	ADP	C5-N7	-2.22	1.35	1.39
2	C	801	ADP	C5-N7	-2.22	1.35	1.39
3	E	802	ATP	PA-O3A	2.21	1.61	1.59
4	B	803	NDT	O2-S1	-2.19	1.41	1.43
4	D	804	NDT	O2-S1	-2.14	1.41	1.43
4	E	803	NDT	O2-S1	-2.12	1.41	1.43
3	D	802	ATP	PA-O3A	2.08	1.61	1.59
4	B	803	NDT	C16-C15	2.07	1.42	1.38
4	F	803	NDT	O3-S1	-2.06	1.41	1.43
4	A	803	NDT	C2-N1	2.06	1.32	1.29
4	D	804	NDT	C2-N1	2.05	1.32	1.29
4	D	803	NDT	O2-S1	-2.05	1.41	1.43
2	A	801	ADP	PA-O3A	2.04	1.61	1.59
4	A	803	NDT	O2-S1	-2.03	1.41	1.43
4	F	803	NDT	C2-N1	2.02	1.32	1.29
4	E	803	NDT	C16-C15	2.01	1.42	1.38

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	ATP	O3G-PG-O1G	-9.43	74.09	110.83
3	D	802	ATP	O3G-PG-O1G	-9.41	74.17	110.83
3	A	802	ATP	O3G-PG-O1G	-9.37	74.33	110.83
3	B	802	ATP	O3G-PG-O1G	-9.36	74.36	110.83
3	C	802	ATP	O3G-PG-O1G	-9.36	74.36	110.83
3	F	802	ATP	O3G-PG-O1G	-9.34	74.42	110.83
3	E	802	ATP	O3A-PA-O1A	-8.67	84.63	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	ATP	O3A-PA-O1A	-8.64	84.72	110.70
3	C	802	ATP	O3A-PA-O1A	-8.57	84.93	110.70
3	F	802	ATP	O3A-PA-O1A	-8.54	85.01	110.70
3	B	802	ATP	O3A-PA-O1A	-8.54	85.02	110.70
3	A	802	ATP	O3A-PA-O1A	-8.43	85.35	110.70
4	D	804	NDT	C2-N1-N2	8.34	126.56	117.61
4	B	803	NDT	C2-N1-N2	8.21	126.43	117.61
4	E	803	NDT	C2-N1-N2	7.91	126.11	117.61
4	D	803	NDT	C2-N1-N2	7.84	126.03	117.61
4	A	803	NDT	C2-N1-N2	7.77	125.95	117.61
4	F	803	NDT	C2-N1-N2	7.68	125.86	117.61
3	D	802	ATP	O2B-PB-O3A	-6.65	89.31	107.27
3	E	802	ATP	O2B-PB-O3A	-6.65	89.31	107.27
3	C	802	ATP	O2B-PB-O3A	-6.54	89.61	107.27
3	A	802	ATP	O3B-PB-O1B	-6.51	91.11	110.70
3	F	802	ATP	O3B-PB-O1B	-6.50	91.16	110.70
3	B	802	ATP	O3B-PB-O1B	-6.49	91.17	110.70
3	F	802	ATP	O2B-PB-O3A	-6.48	89.75	107.27
3	C	802	ATP	O3B-PB-O1B	-6.48	91.20	110.70
3	B	802	ATP	O2B-PB-O3A	-6.48	89.77	107.27
3	D	802	ATP	O3B-PB-O1B	-6.46	91.28	110.70
3	A	802	ATP	O2B-PB-O3A	-6.44	89.85	107.27
4	E	803	NDT	C20-C15-C16	-6.37	112.16	120.47
4	B	803	NDT	C20-C15-C16	-6.35	112.19	120.47
4	D	803	NDT	C20-C15-C16	-6.34	112.20	120.47
4	D	804	NDT	C20-C15-C16	-6.30	112.25	120.47
3	E	802	ATP	O3B-PB-O1B	-6.27	91.83	110.70
4	F	803	NDT	C20-C15-C16	-6.23	112.34	120.47
4	A	803	NDT	C20-C15-C16	-6.18	112.41	120.47
4	D	803	NDT	C4-C1-C2	-6.09	114.44	118.29
4	D	804	NDT	C4-C1-C2	-6.05	114.47	118.29
4	F	803	NDT	C4-C1-C2	-6.02	114.48	118.29
4	E	803	NDT	C4-C1-C2	-5.96	114.53	118.29
4	A	803	NDT	C4-C1-C2	-5.93	114.54	118.29
2	F	801	ADP	C5-C4-N3	-5.87	118.63	126.72
2	D	801	ADP	C5-C4-N3	-5.83	118.68	126.72
4	B	803	NDT	C4-C1-C2	-5.83	114.60	118.29
2	A	801	ADP	C5-C4-N3	-5.83	118.70	126.72
2	C	801	ADP	C5-C4-N3	-5.82	118.70	126.72
2	B	801	ADP	C5-C4-N3	-5.81	118.71	126.72
2	E	801	ADP	C5-C4-N3	-5.81	118.72	126.72
3	D	802	ATP	O2G-PG-O3B	5.07	121.63	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	804	NDT	C19-C20-C15	5.06	124.36	119.44
4	F	803	NDT	C19-C20-C15	5.04	124.34	119.44
4	B	803	NDT	C19-C20-C15	5.03	124.33	119.44
3	E	802	ATP	O2G-PG-O3B	5.03	121.50	104.64
4	E	803	NDT	C19-C20-C15	5.03	124.33	119.44
3	F	802	ATP	O2G-PG-O3B	5.02	121.48	104.64
3	C	802	ATP	O2G-PG-O3B	5.02	121.46	104.64
3	A	802	ATP	O2G-PG-O3B	5.01	121.42	104.64
3	B	802	ATP	O2G-PG-O3B	5.00	121.41	104.64
4	D	803	NDT	C19-C20-C15	4.98	124.28	119.44
4	D	804	NDT	C17-C16-C15	4.93	124.24	119.44
4	A	803	NDT	C19-C20-C15	4.89	124.20	119.44
4	E	803	NDT	C17-C16-C15	4.89	124.19	119.44
4	D	803	NDT	C17-C16-C15	4.88	124.18	119.44
4	B	803	NDT	C17-C16-C15	4.87	124.17	119.44
2	A	801	ADP	N3-C4-N9	4.71	135.18	127.17
4	A	803	NDT	C17-C16-C15	4.70	124.01	119.44
4	F	803	NDT	C17-C16-C15	4.67	123.99	119.44
2	B	801	ADP	N3-C4-N9	4.67	135.10	127.17
2	F	801	ADP	N3-C4-N9	4.66	135.09	127.17
2	D	801	ADP	N3-C4-N9	4.63	135.04	127.17
2	E	801	ADP	N3-C4-N9	4.62	135.03	127.17
4	D	803	NDT	C20-C15-S1	4.57	124.28	119.73
4	B	803	NDT	C20-C15-S1	4.53	124.23	119.73
4	E	803	NDT	C20-C15-S1	4.50	124.21	119.73
2	C	801	ADP	N3-C4-N9	4.49	134.81	127.17
4	E	803	NDT	C15-S1-N2	4.34	114.59	107.06
4	B	803	NDT	O3-S1-O2	-4.34	112.82	119.59
4	D	803	NDT	C15-S1-N2	4.33	114.56	107.06
4	A	803	NDT	C20-C15-S1	4.31	124.02	119.73
4	D	803	NDT	O3-S1-O2	-4.31	112.87	119.59
4	F	803	NDT	C15-S1-N2	4.28	114.49	107.06
4	F	803	NDT	C20-C15-S1	4.28	123.99	119.73
4	D	804	NDT	O3-S1-O2	-4.27	112.92	119.59
4	E	803	NDT	O3-S1-O2	-4.26	112.95	119.59
4	D	804	NDT	C20-C15-S1	4.25	123.96	119.73
4	A	803	NDT	O3-S1-O2	-4.19	113.05	119.59
4	F	803	NDT	O3-S1-O2	-4.18	113.06	119.59
4	D	804	NDT	C16-C15-S1	4.09	123.80	119.73
4	D	804	NDT	C15-S1-N2	4.04	114.07	107.06
4	F	803	NDT	C16-C15-S1	3.97	123.67	119.73
4	E	803	NDT	C16-C15-S1	3.93	123.64	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	NDT	C16-C15-S1	3.87	123.58	119.73
4	A	803	NDT	C16-C15-S1	3.86	123.57	119.73
4	D	803	NDT	C16-C15-S1	3.81	123.52	119.73
2	C	801	ADP	C2-N3-C4	3.71	120.88	111.83
2	E	801	ADP	C2-N3-C4	3.70	120.86	111.83
2	A	801	ADP	C2-N3-C4	3.69	120.83	111.83
2	F	801	ADP	C2-N3-C4	3.69	120.83	111.83
2	B	801	ADP	C2-N3-C4	3.68	120.82	111.83
2	D	801	ADP	C2-N3-C4	3.68	120.81	111.83
2	C	801	ADP	C4-C5-N7	-3.55	106.53	110.58
2	D	801	ADP	C4-C5-N7	-3.47	106.61	110.58
2	F	801	ADP	C4-C5-N7	-3.44	106.65	110.58
2	E	801	ADP	C4-C5-N7	-3.41	106.68	110.58
2	B	801	ADP	C4-C5-N7	-3.40	106.69	110.58
2	A	801	ADP	C4-C5-N7	-3.36	106.74	110.58
2	C	801	ADP	N3-C2-N1	-3.28	123.62	128.58
2	E	801	ADP	N3-C2-N1	-3.26	123.65	128.58
4	A	803	NDT	C15-S1-N2	3.23	112.66	107.06
2	B	801	ADP	N3-C2-N1	-3.20	123.74	128.58
2	A	801	ADP	N3-C2-N1	-3.18	123.77	128.58
2	F	801	ADP	N3-C2-N1	-3.17	123.78	128.58
2	D	801	ADP	N3-C2-N1	-3.17	123.78	128.58
3	A	802	ATP	O2B-PB-O3B	3.15	115.78	107.27
3	C	802	ATP	O5'-C5'-C4'	3.14	119.70	108.99
3	E	802	ATP	O2B-PB-O3B	3.14	115.76	107.27
3	B	802	ATP	O5'-C5'-C4'	3.14	119.67	108.99
3	F	802	ATP	O2A-PA-O3A	3.12	115.70	107.27
3	F	802	ATP	O2B-PB-O3B	3.11	115.67	107.27
3	B	802	ATP	O2B-PB-O3B	3.10	115.65	107.27
3	C	802	ATP	O2B-PB-O3B	3.10	115.64	107.27
3	D	802	ATP	O2B-PB-O3B	3.07	115.56	107.27
4	B	803	NDT	C15-S1-N2	3.06	112.37	107.06
3	A	802	ATP	O2A-PA-O3A	3.04	115.50	107.27
3	C	802	ATP	O2A-PA-O3A	3.01	115.42	107.27
3	A	802	ATP	O5'-C5'-C4'	2.84	118.67	108.99
3	D	802	ATP	O2A-PA-O3A	2.83	114.92	107.27
3	B	802	ATP	O2A-PA-O3A	2.82	114.89	107.27
3	D	802	ATP	O3A-PB-O1B	2.79	119.11	110.70
3	E	802	ATP	O3A-PB-O1B	2.73	118.93	110.70
3	E	802	ATP	O5'-C5'-C4'	2.73	118.30	108.99
3	C	802	ATP	O3A-PB-O1B	2.71	118.84	110.70
3	E	802	ATP	O2G-PG-O1G	2.70	121.35	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	ATP	O5'-C5'-C4'	2.70	118.17	108.99
2	B	801	ADP	C4-N9-C8	2.68	108.56	105.74
3	F	802	ATP	O2G-PG-O1G	2.68	121.27	110.83
2	E	801	ADP	C4-N9-C8	2.68	108.55	105.74
3	C	802	ATP	O2G-PG-O1G	2.67	121.22	110.83
3	D	802	ATP	O2G-PG-O1G	2.65	121.17	110.83
3	B	802	ATP	O2G-PG-O1G	2.65	121.16	110.83
3	A	802	ATP	O2G-PG-O1G	2.65	121.16	110.83
2	A	801	ADP	C4-N9-C8	2.64	108.51	105.74
2	D	801	ADP	C4-N9-C8	2.63	108.50	105.74
3	F	802	ATP	O5'-C5'-C4'	2.62	117.91	108.99
3	B	802	ATP	O3A-PB-O1B	2.60	118.52	110.70
3	A	802	ATP	O3A-PB-O1B	2.59	118.50	110.70
3	E	802	ATP	O2A-PA-O3A	2.59	114.26	107.27
3	F	802	ATP	O3A-PB-O1B	2.56	118.40	110.70
2	A	801	ADP	C3'-C2'-C1'	2.56	106.30	101.46
2	F	801	ADP	C3'-C2'-C1'	2.55	106.29	101.46
2	F	801	ADP	C4-N9-C8	2.55	108.42	105.74
2	D	801	ADP	C5-N7-C8	2.52	107.42	103.45
2	B	801	ADP	C5-N7-C8	2.52	107.41	103.45
2	C	801	ADP	C5-N7-C8	2.52	107.41	103.45
2	E	801	ADP	C5-N7-C8	2.51	107.40	103.45
2	F	801	ADP	C5-N7-C8	2.51	107.40	103.45
2	C	801	ADP	C4-N9-C8	2.51	108.37	105.74
2	A	801	ADP	C5-N7-C8	2.50	107.39	103.45
4	D	803	NDT	C8-C1-C4	2.42	121.83	119.82
4	E	803	NDT	C8-C1-C4	2.41	121.83	119.82
2	B	801	ADP	C3'-C2'-C1'	2.40	106.01	101.46
2	E	801	ADP	C3'-C2'-C1'	2.40	106.00	101.46
2	D	801	ADP	C3'-C2'-C1'	2.38	105.96	101.46
4	B	803	NDT	C8-C1-C4	2.32	121.75	119.82
4	D	804	NDT	C8-C1-C4	2.30	121.73	119.82
4	F	803	NDT	C8-C1-C4	2.27	121.71	119.82
3	A	802	ATP	O2'-C2'-C3'	2.23	118.96	111.82
3	C	802	ATP	O2'-C2'-C3'	2.23	118.95	111.82
3	A	802	ATP	C2'-C3'-C4'	2.22	106.91	102.61
3	A	802	ATP	O3G-PG-O3B	2.22	112.08	104.64
4	A	803	NDT	C8-C1-C4	2.21	121.66	119.82
3	B	802	ATP	O3G-PG-O3B	2.20	112.00	104.64
3	B	802	ATP	O2'-C2'-C3'	2.18	118.81	111.82
3	F	802	ATP	C2'-C3'-C4'	2.18	106.81	102.61
3	E	802	ATP	C2'-C3'-C4'	2.17	106.81	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	ATP	O3G-PG-O3B	2.16	111.89	104.64
3	D	802	ATP	O3G-PG-O3B	2.15	111.85	104.64
2	C	801	ADP	C6-C5-N7	2.15	136.23	132.09
3	E	802	ATP	O3G-PG-O3B	2.13	111.79	104.64
3	F	802	ATP	O3G-PG-O3B	2.12	111.74	104.64
2	D	801	ADP	C6-C5-N7	2.07	136.08	132.09
2	B	801	ADP	C6-C5-N7	2.05	136.04	132.09
2	E	801	ADP	C6-C5-N7	2.03	136.01	132.09
4	E	803	NDT	C19-C18-C17	-2.03	114.17	118.11
2	F	801	ADP	C6-C5-N7	2.02	135.98	132.09
2	A	801	ADP	C6-C5-N7	2.02	135.98	132.09
4	D	803	NDT	C19-C18-C17	-2.01	114.21	118.11
4	B	803	NDT	C19-C18-C17	-2.01	114.21	118.11

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	803	NDT	N2
4	D	804	NDT	N2
4	F	803	NDT	N2
4	B	803	NDT	N2
4	E	803	NDT	N2
4	A	803	NDT	N2

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	C5'-O5'-PA-O1A
3	D	802	ATP	C5'-O5'-PA-O3A
3	F	802	ATP	PB-O3B-PG-O3G
3	F	802	ATP	C5'-O5'-PA-O3A
3	F	802	ATP	O4'-C4'-C5'-O5'
3	F	802	ATP	C3'-C4'-C5'-O5'
3	B	802	ATP	PB-O3B-PG-O2G
3	B	802	ATP	PB-O3B-PG-O3G
3	B	802	ATP	C5'-O5'-PA-O1A
3	B	802	ATP	C5'-O5'-PA-O2A
3	B	802	ATP	C5'-O5'-PA-O3A
3	E	802	ATP	C5'-O5'-PA-O1A
3	E	802	ATP	C2'-C1'-N9-C4
3	A	802	ATP	PB-O3B-PG-O2G
3	A	802	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	F	803	NDT	N1-N2-S1-O2
4	B	803	NDT	N1-N2-S1-O2
4	E	803	NDT	N1-N2-S1-O2
4	E	803	NDT	N1-N2-S1-O3
4	E	803	NDT	N1-N2-S1-C15
4	A	803	NDT	N1-N2-S1-O2
4	A	803	NDT	N1-N2-S1-O3
4	A	803	NDT	N1-N2-S1-C15
2	A	801	ADP	O4'-C4'-C5'-O5'
3	E	802	ATP	C3'-C4'-C5'-O5'
3	E	802	ATP	C2'-C1'-N9-C8
2	A	801	ADP	C3'-C4'-C5'-O5'
2	B	801	ADP	O4'-C4'-C5'-O5'
2	B	801	ADP	C3'-C4'-C5'-O5'
3	E	802	ATP	O4'-C4'-C5'-O5'
3	D	802	ATP	C2'-C1'-N9-C4
3	F	802	ATP	C2'-C1'-N9-C4
3	D	802	ATP	C2'-C1'-N9-C8
3	F	802	ATP	C2'-C1'-N9-C8
4	F	803	NDT	C16-C15-S1-O2
2	D	801	ADP	C5'-O5'-PA-O1A
2	E	801	ADP	C5'-O5'-PA-O1A
2	C	801	ADP	C5'-O5'-PA-O1A
3	F	802	ATP	C5'-O5'-PA-O1A
3	F	802	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	C5'-O5'-PA-O1A
4	F	803	NDT	C20-C15-S1-O2
2	D	801	ADP	O4'-C4'-C5'-O5'
2	E	801	ADP	O4'-C4'-C5'-O5'
3	C	802	ATP	O4'-C4'-C5'-O5'
4	E	803	NDT	C16-C15-S1-O2
3	B	802	ATP	PB-O3A-PA-O2A
4	E	803	NDT	C20-C15-S1-O2
3	E	802	ATP	C4'-C5'-O5'-PA
2	F	801	ADP	PB-O3A-PA-O2A
3	D	802	ATP	PB-O3B-PG-O1G
3	D	802	ATP	O4'-C4'-C5'-O5'
2	F	801	ADP	PB-O3A-PA-O1A
3	D	802	ATP	PB-O3A-PA-O2A
3	C	802	ATP	PB-O3A-PA-O1A
3	C	802	ATP	PB-O3A-PA-O2A
2	D	801	ADP	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

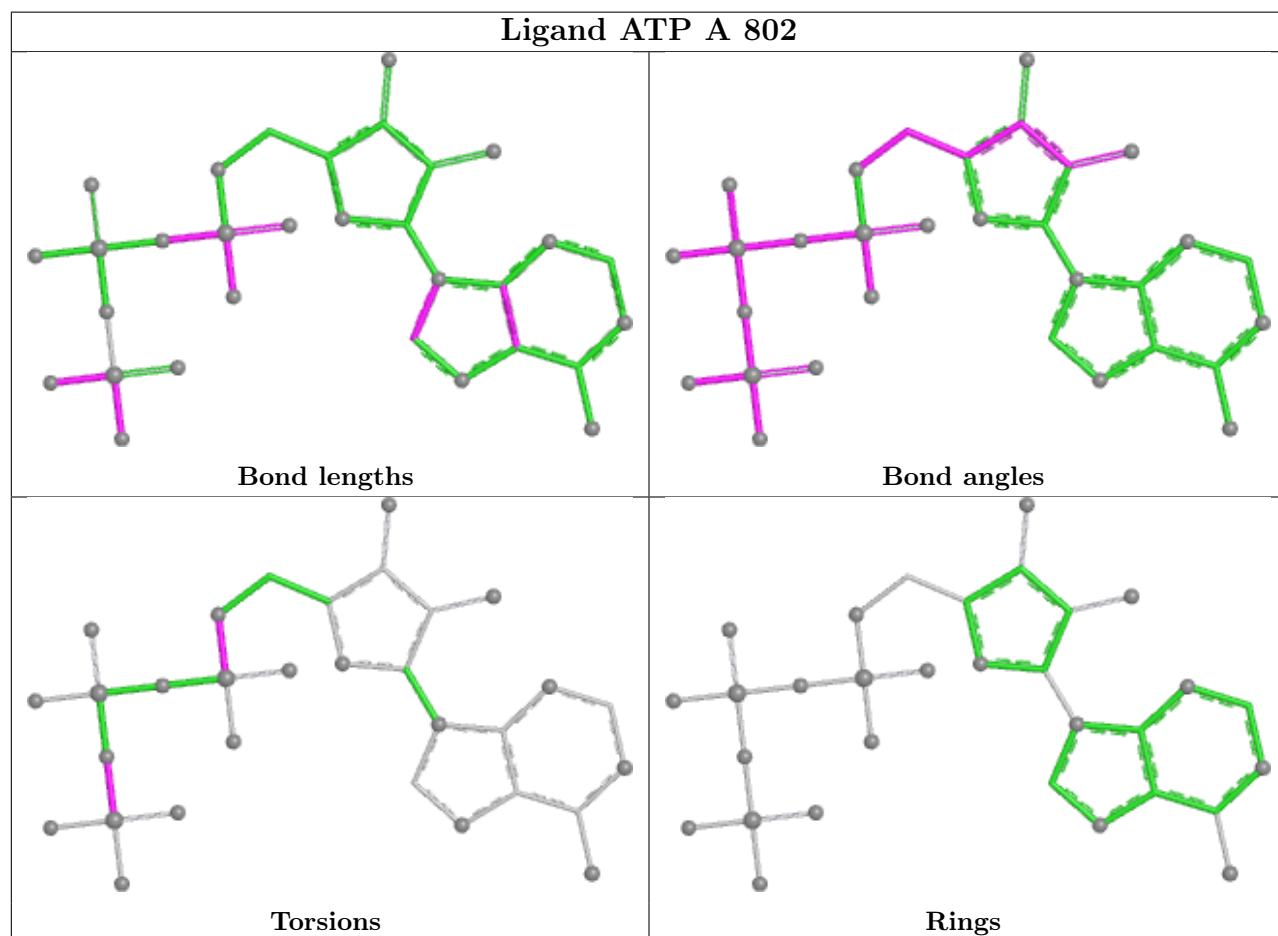
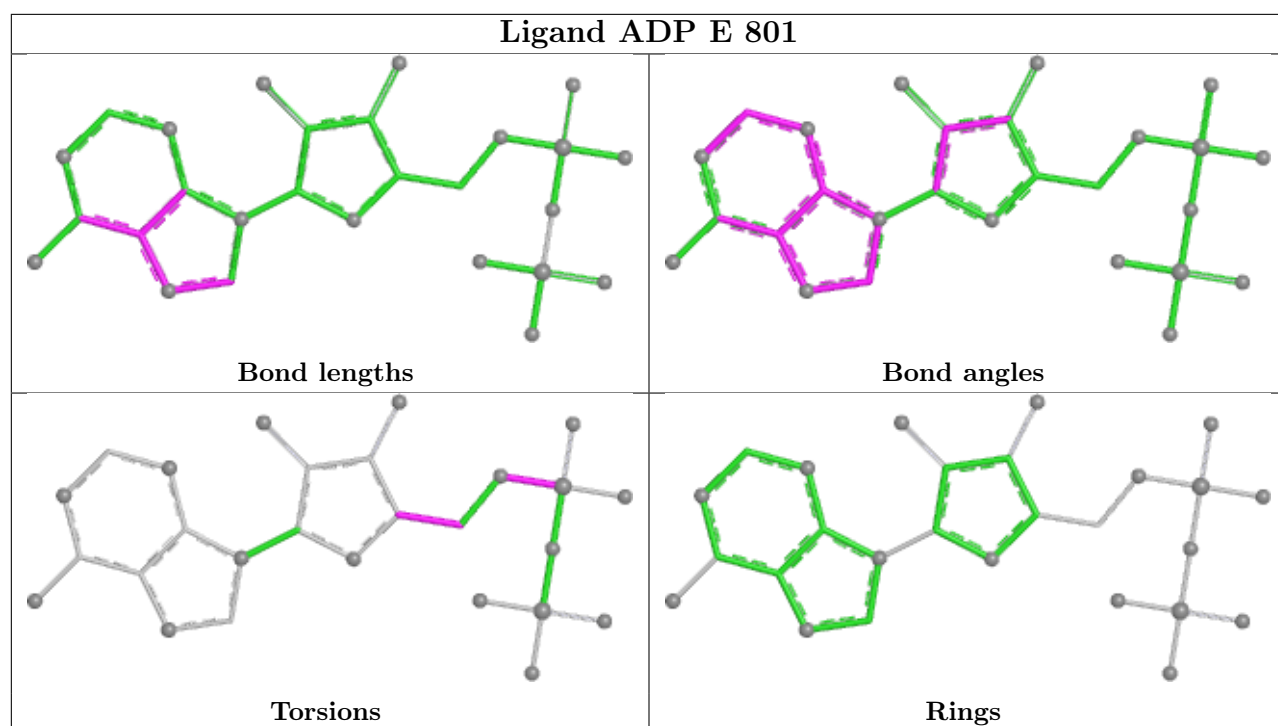
Mol	Chain	Res	Type	Atoms
2	E	801	ADP	C3'-C4'-C5'-O5'
3	B	802	ATP	O4'-C4'-C5'-O5'
4	D	804	NDT	C16-C15-S1-O3
4	D	804	NDT	C20-C15-S1-O3

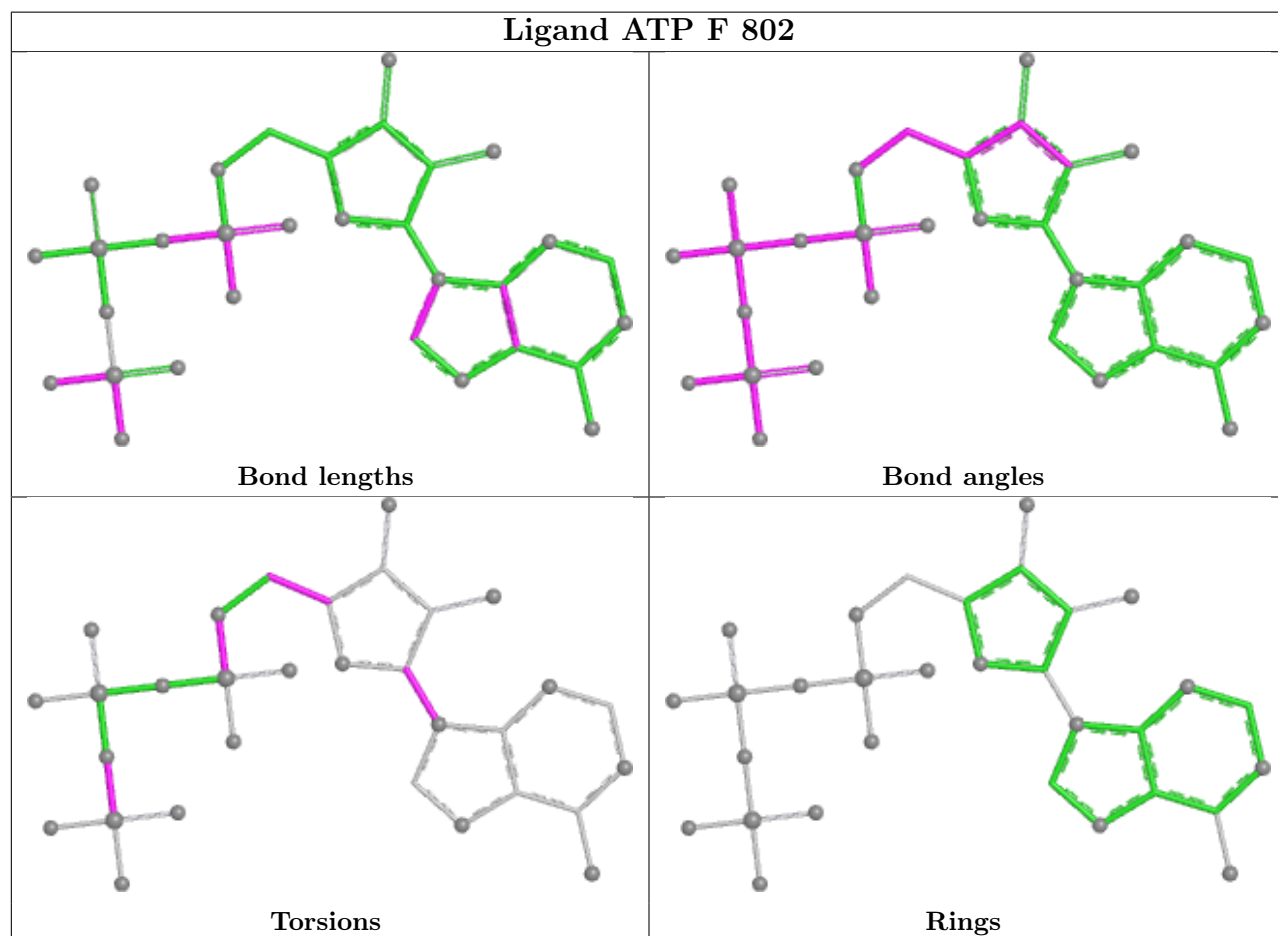
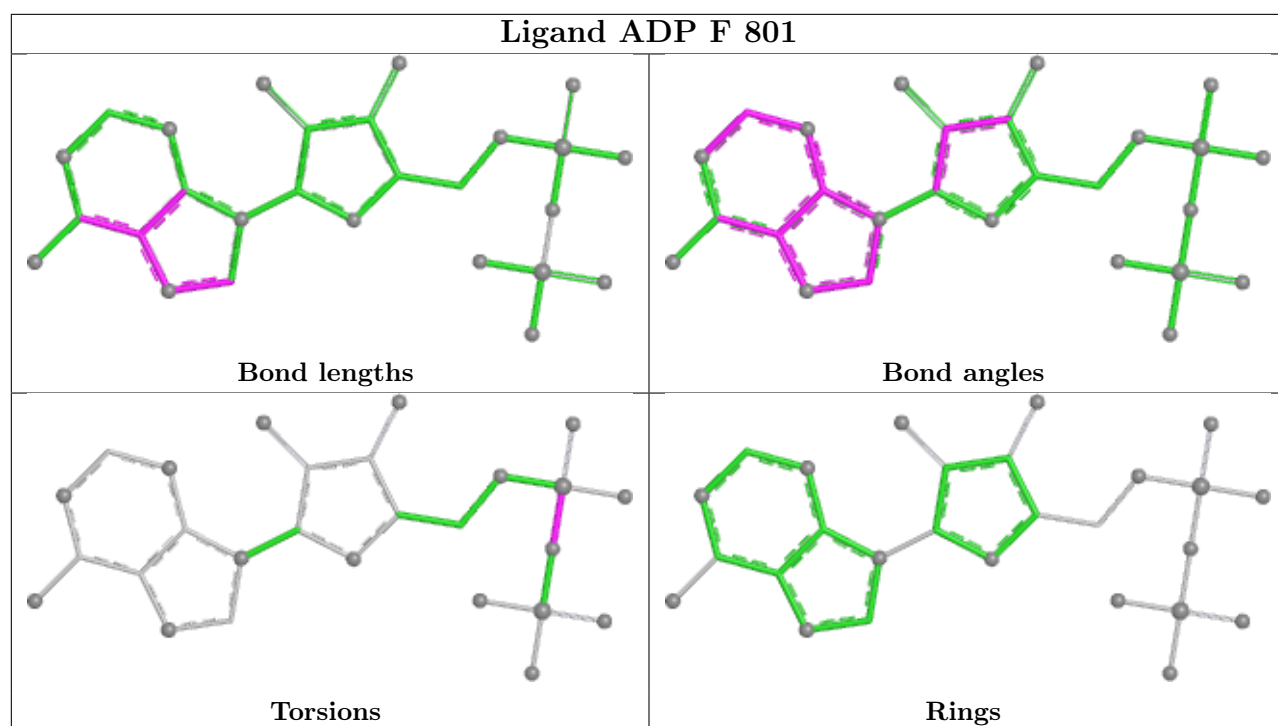
There are no ring outliers.

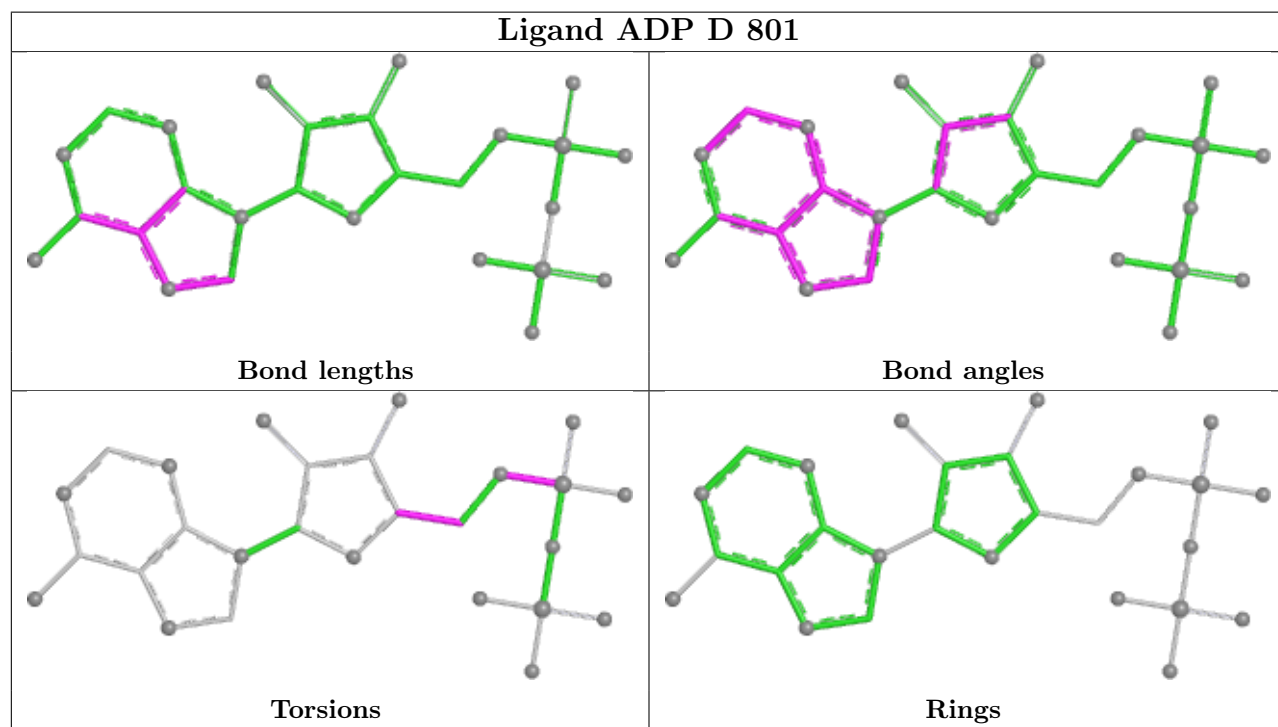
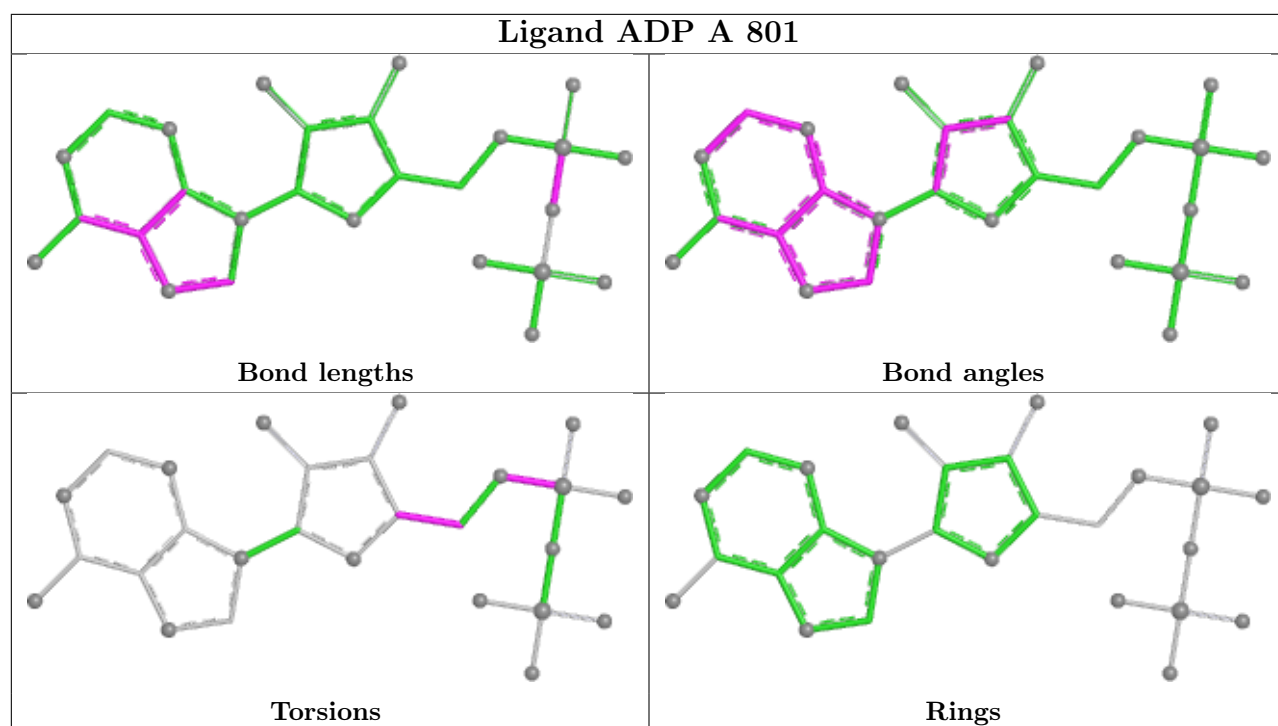
17 monomers are involved in 163 short contacts:

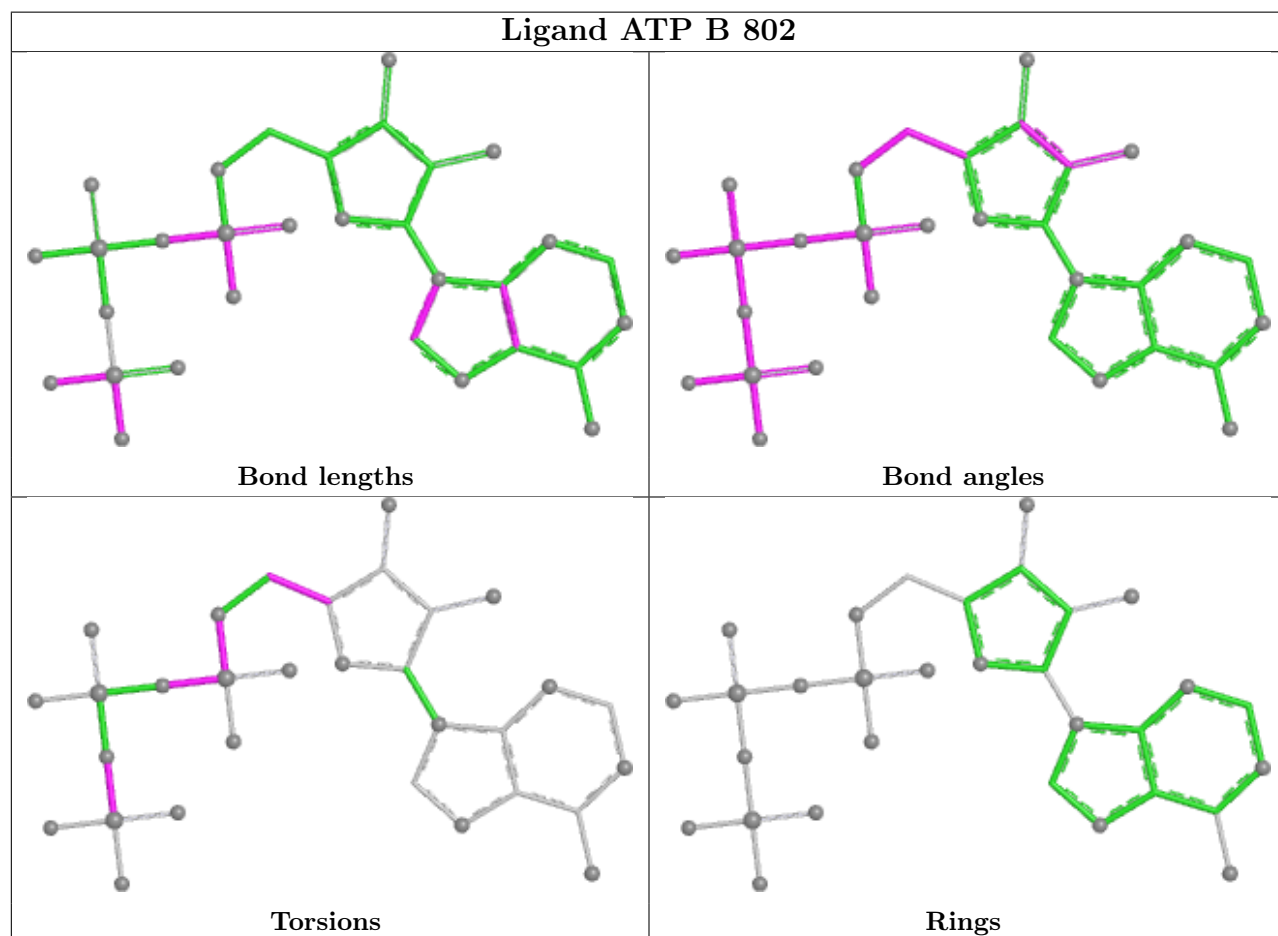
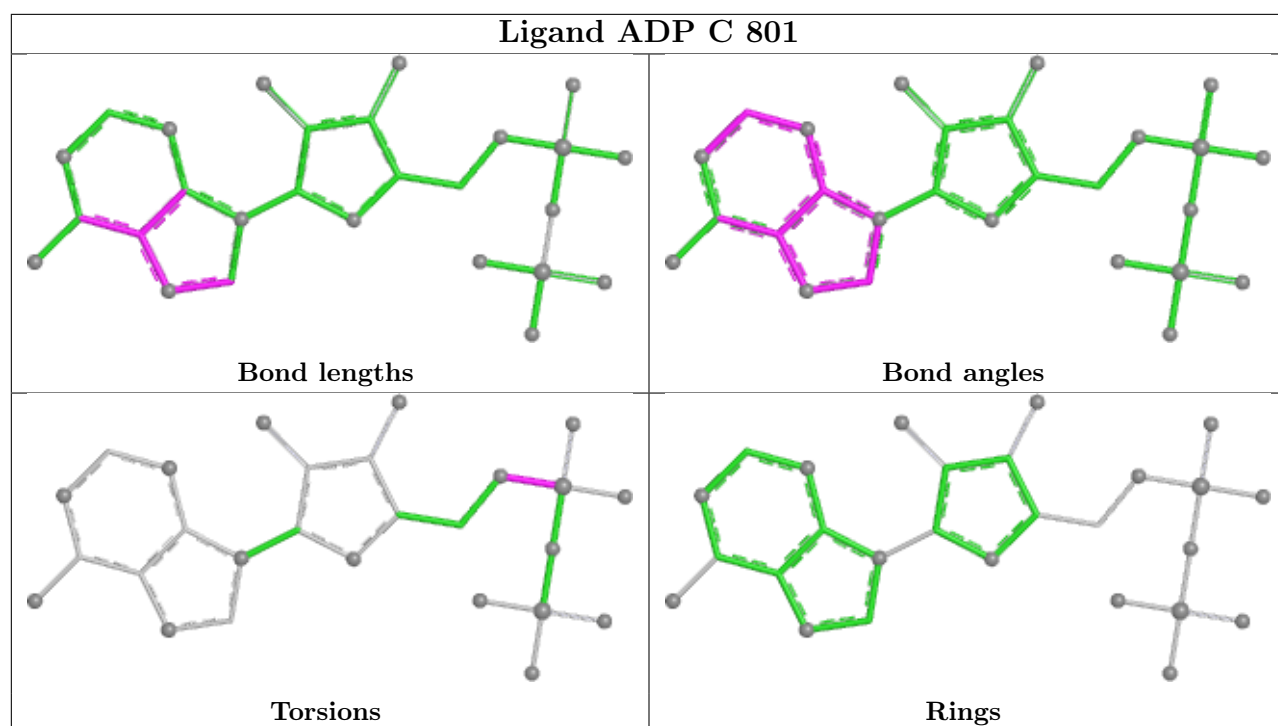
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	ADP	4	0
3	A	802	ATP	4	0
2	F	801	ADP	20	0
3	F	802	ATP	1	0
2	A	801	ADP	3	0
2	D	801	ADP	1	0
2	C	801	ADP	2	0
3	B	802	ATP	4	0
4	A	803	NDT	4	0
4	F	803	NDT	23	0
3	E	802	ATP	14	0
4	D	804	NDT	4	0
4	E	803	NDT	22	0
3	C	802	ATP	12	0
3	D	802	ATP	18	0
4	D	803	NDT	28	0
4	B	803	NDT	1	0

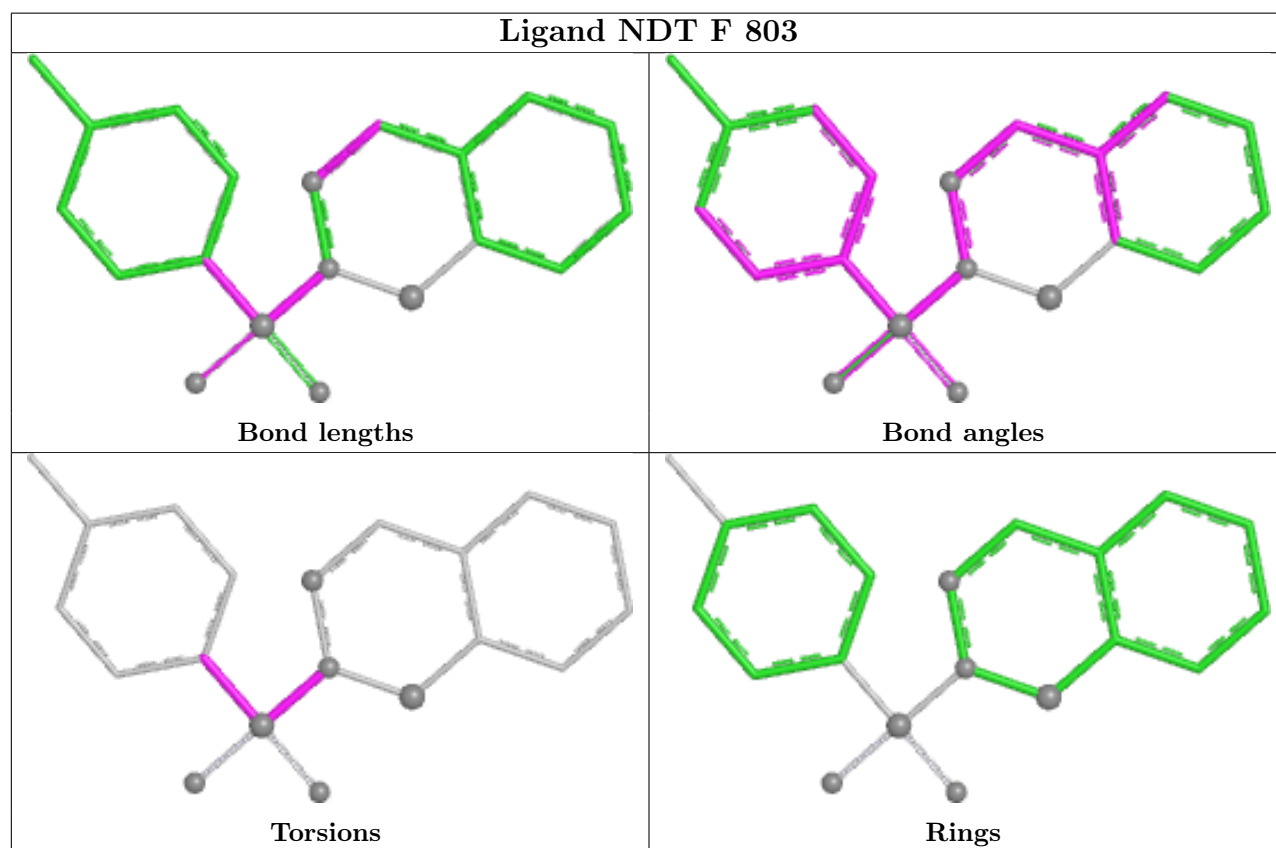
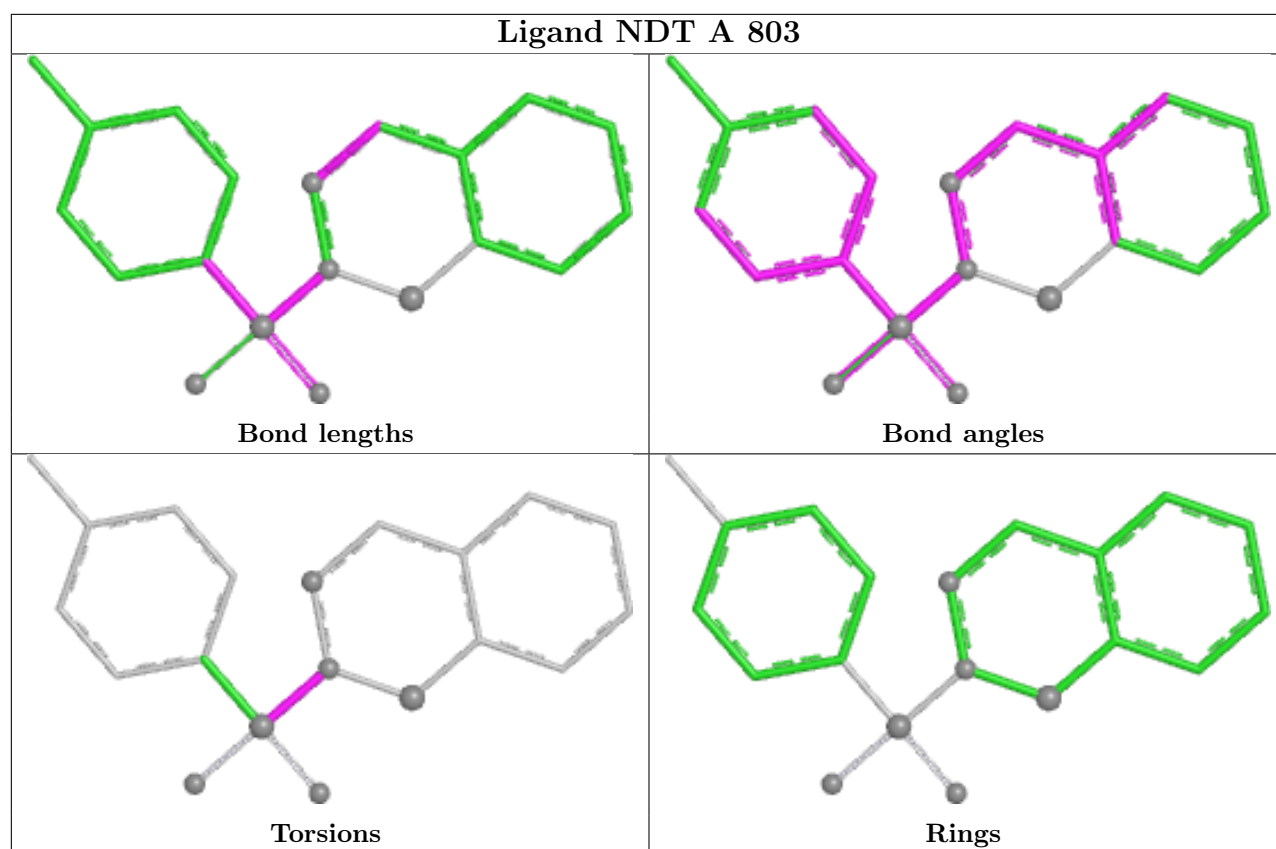
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



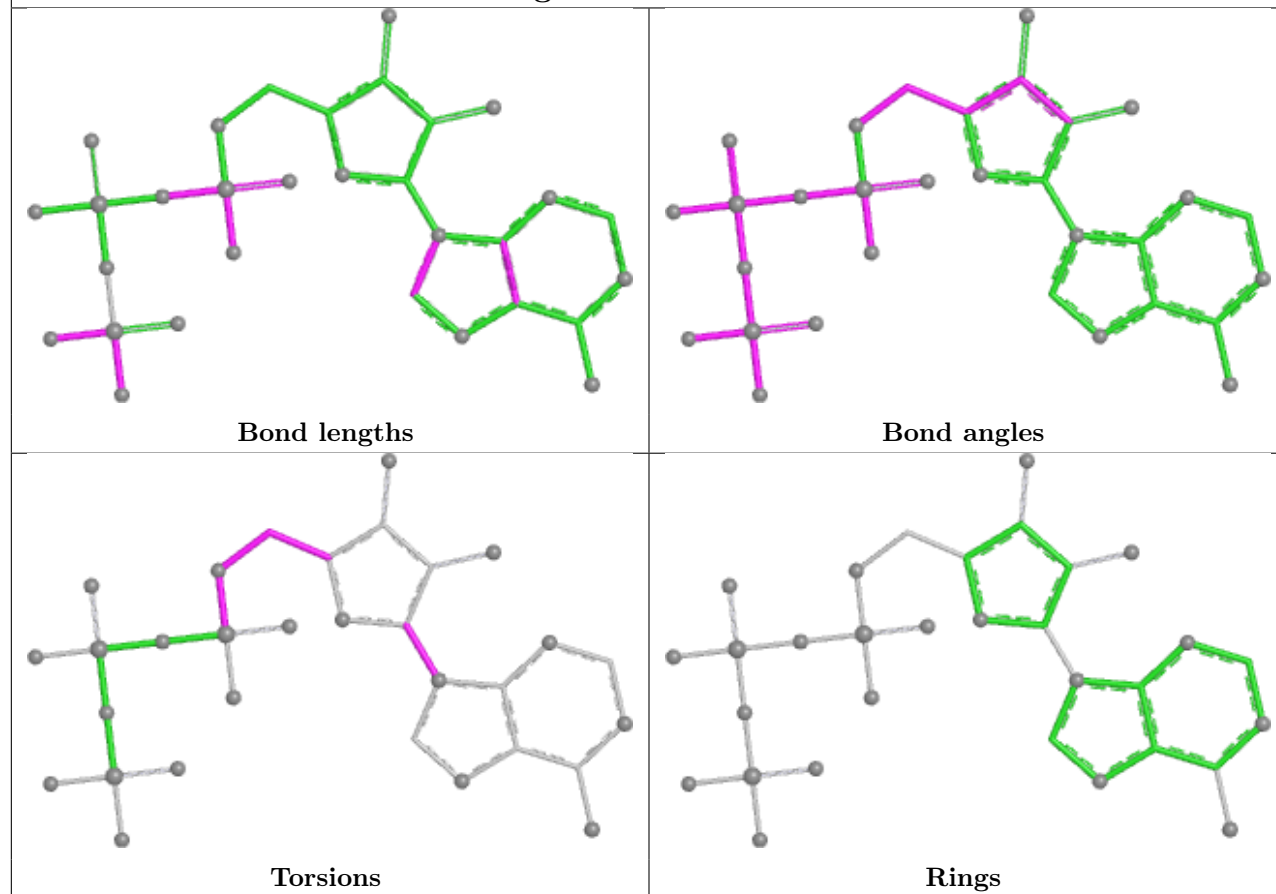




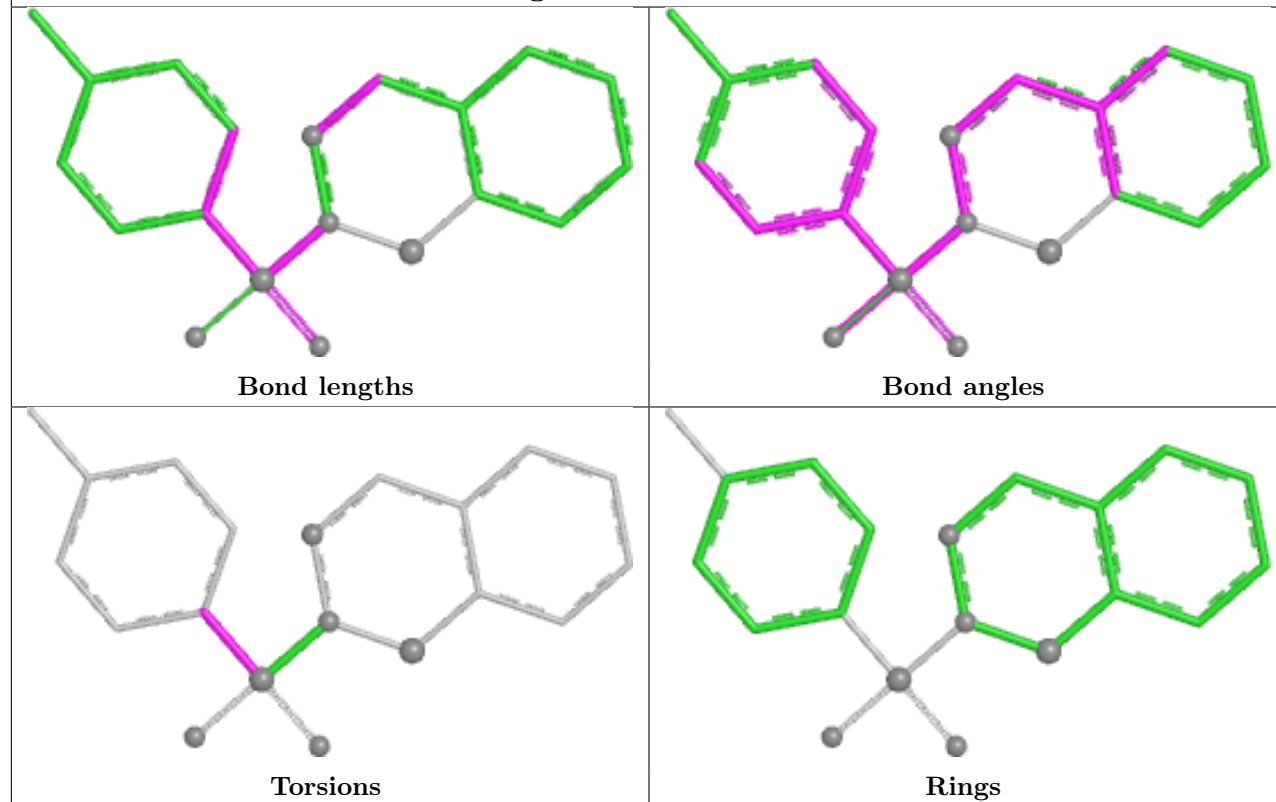




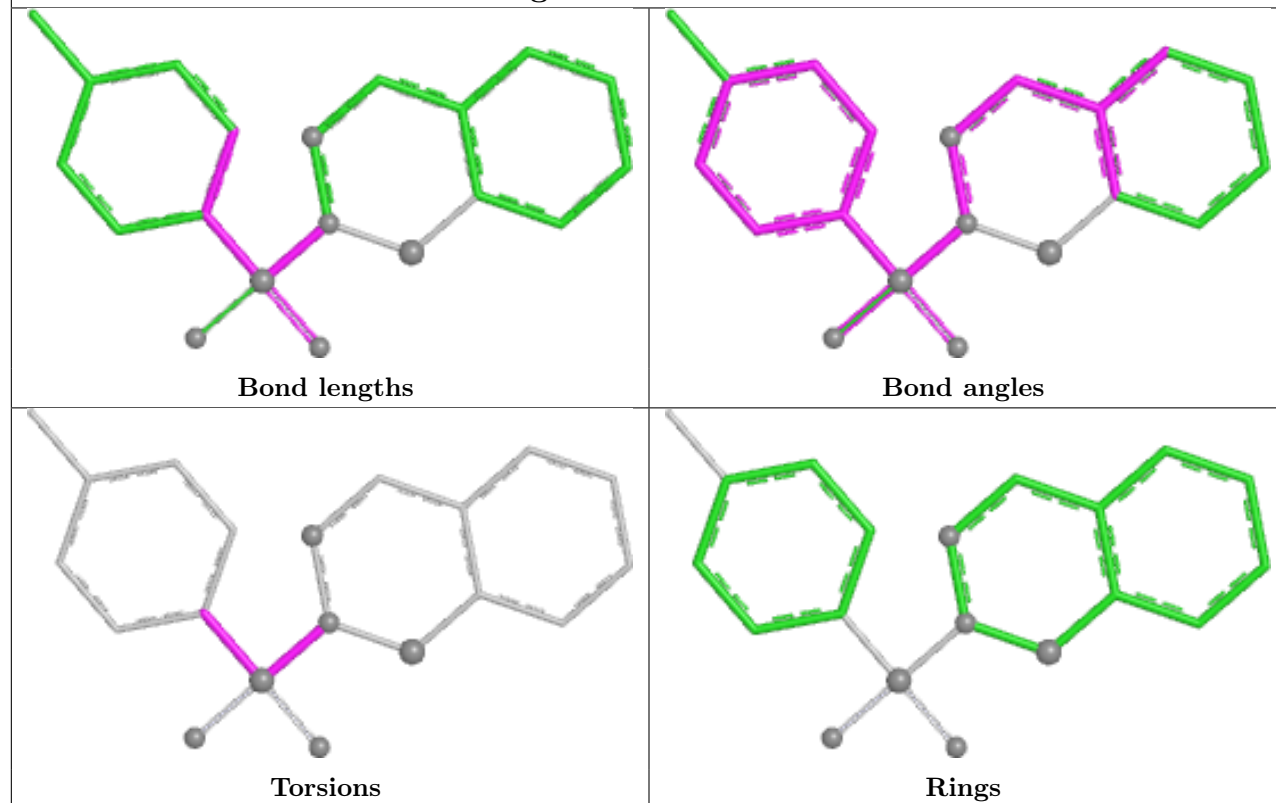
Ligand ATP E 802



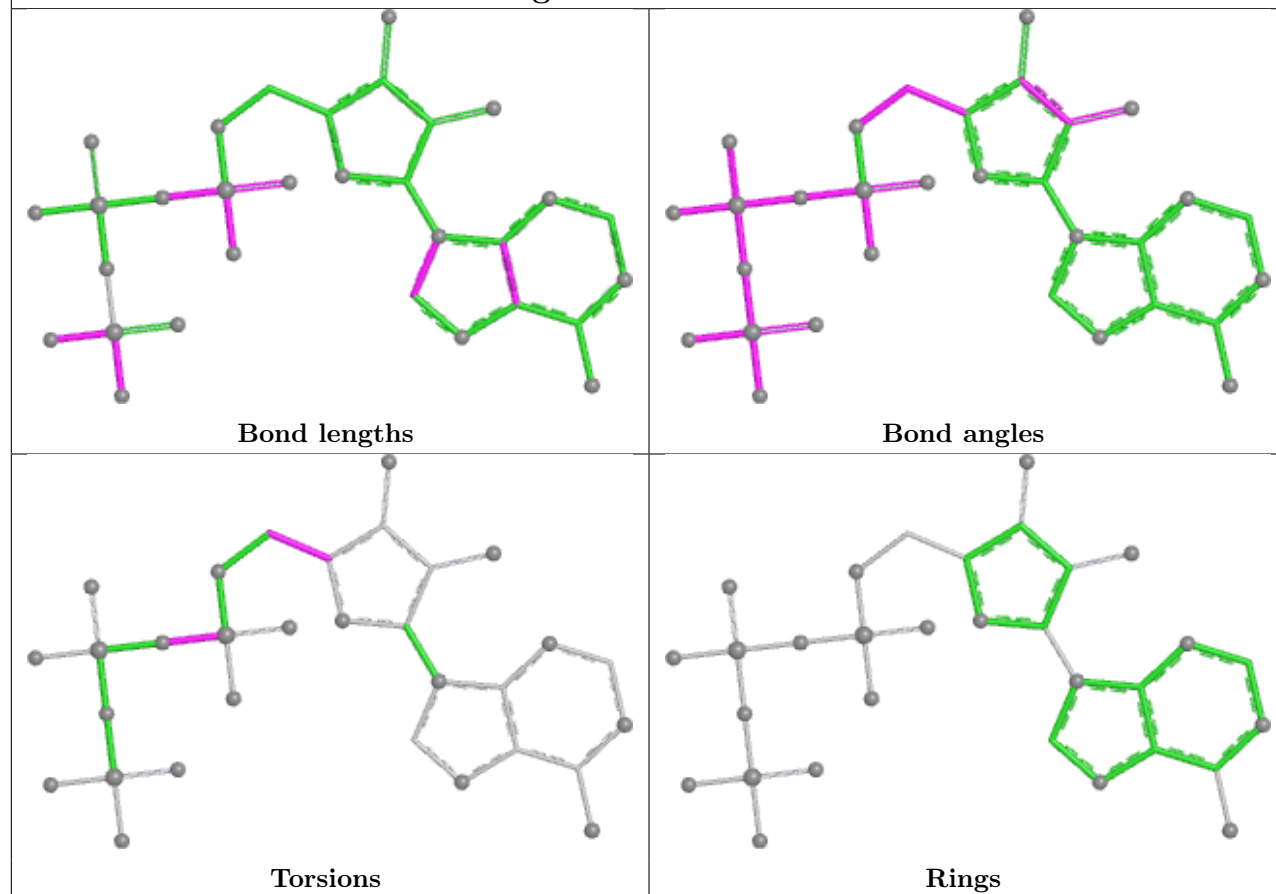
Ligand NDT D 804

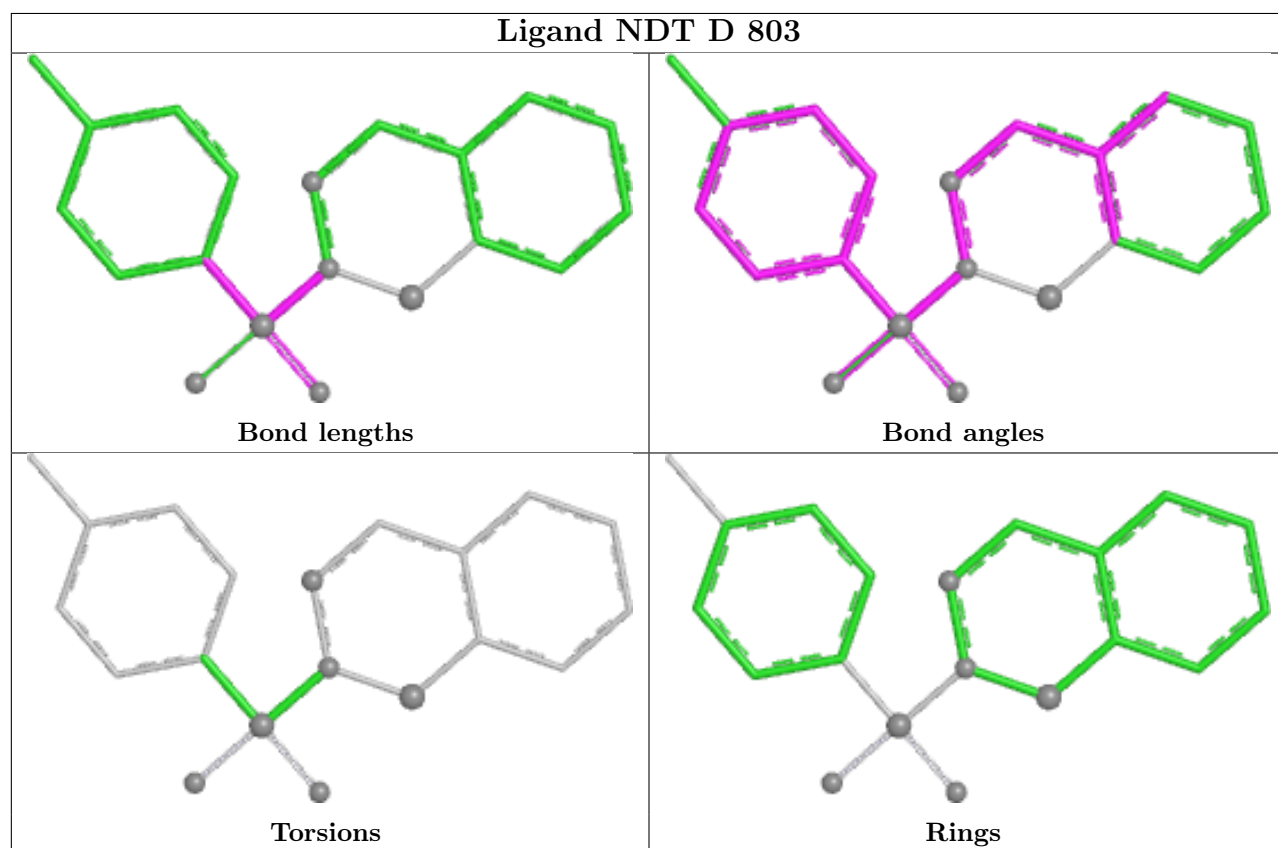
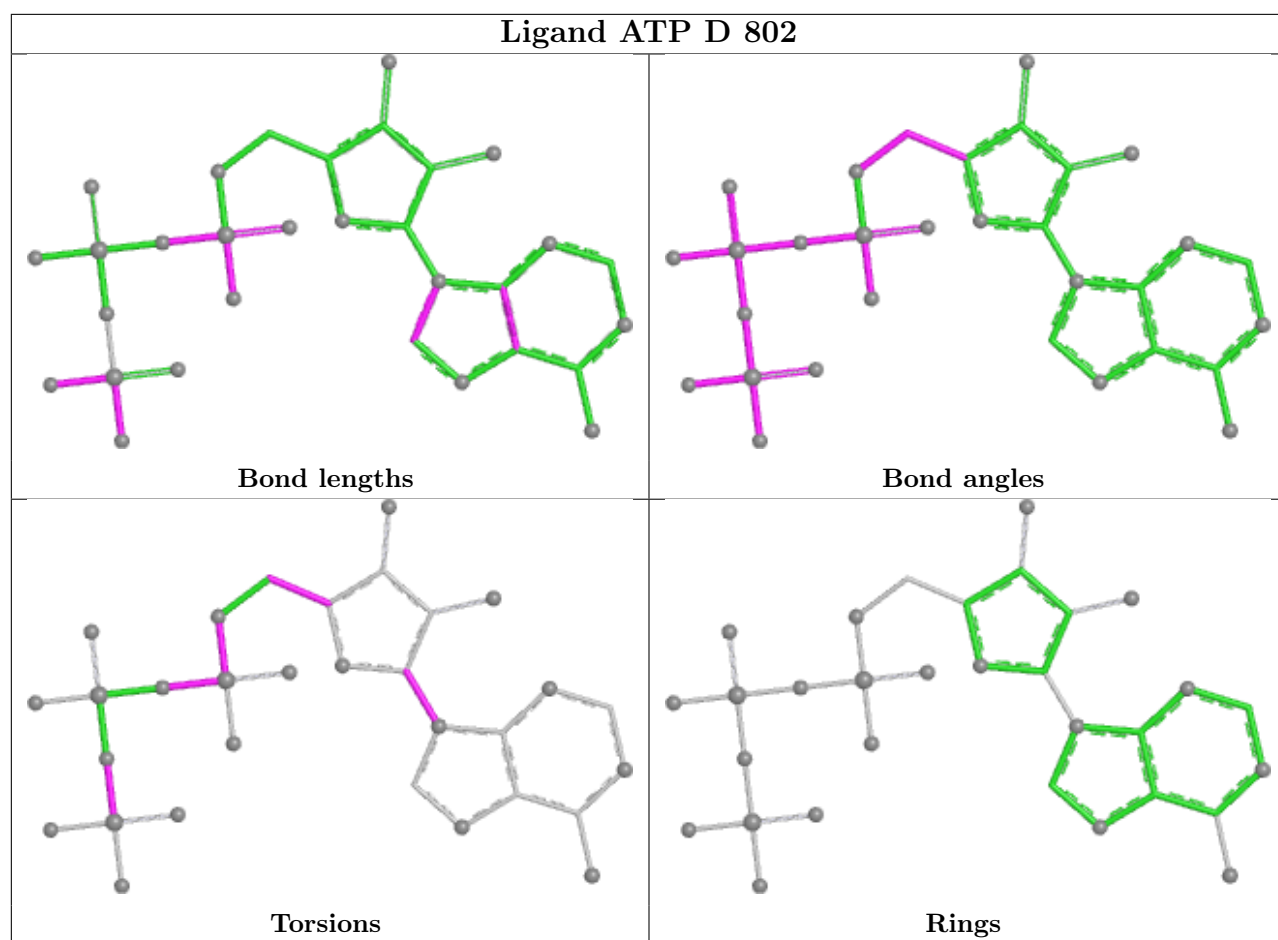


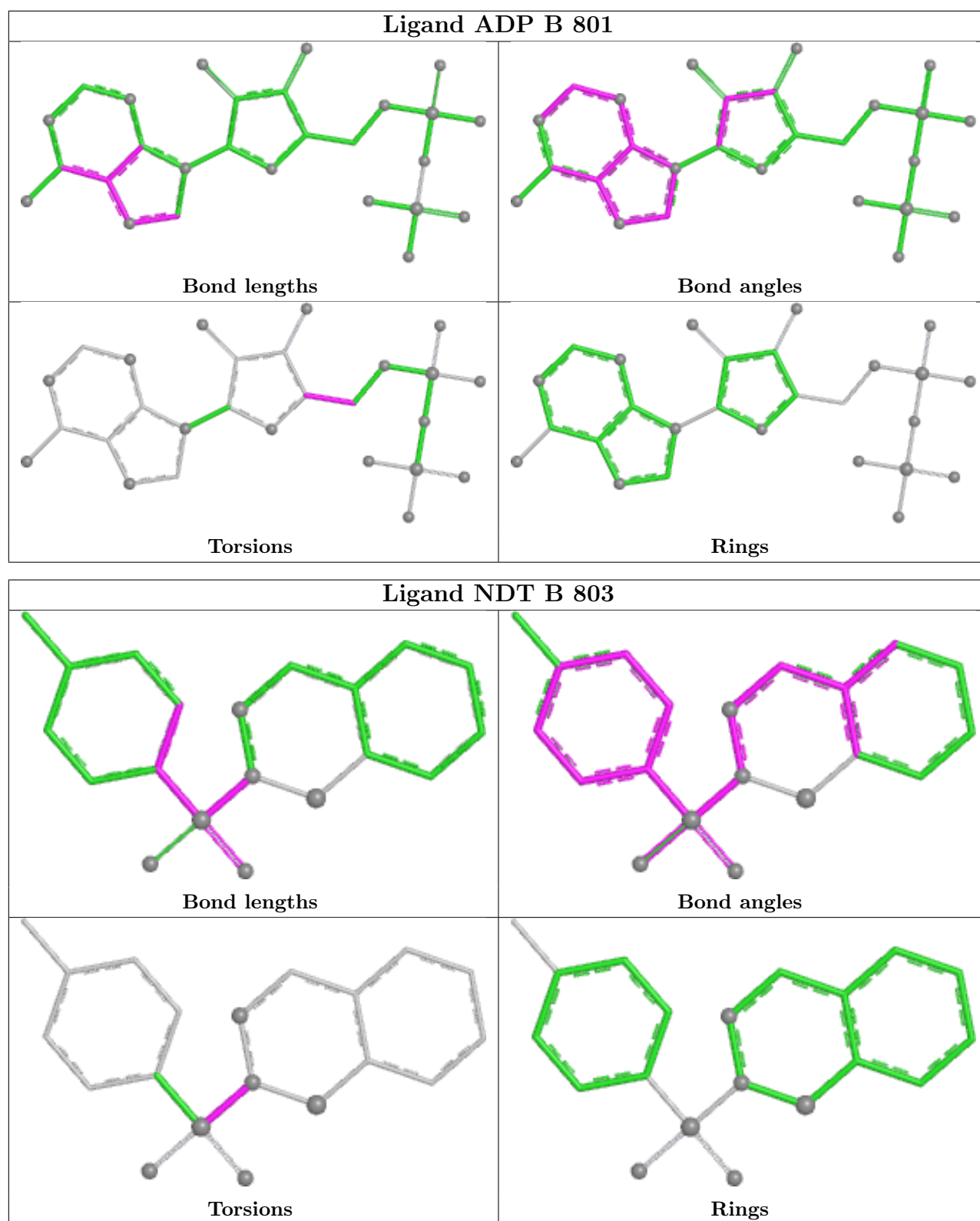
Ligand NDT E 803



Ligand ATP C 802







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

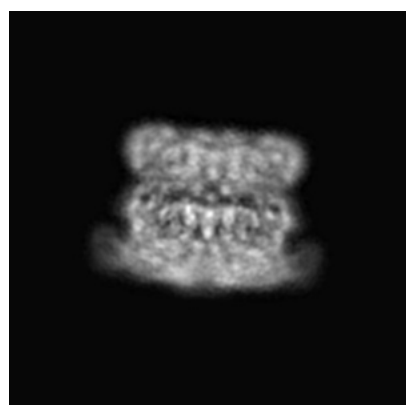
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32402. These allow visual inspection of the internal detail of the map and identification of artifacts.

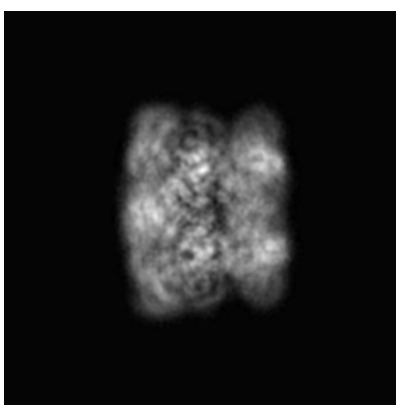
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

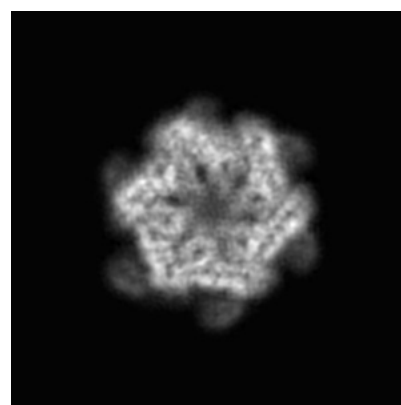
6.1.1 Primary map



X



Y

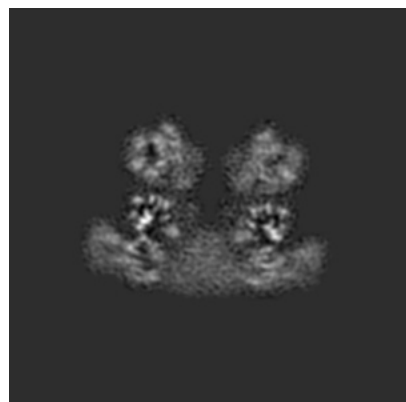


Z

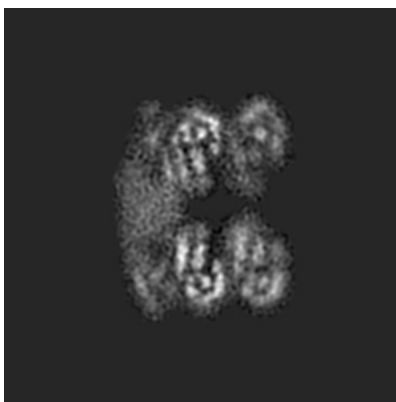
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

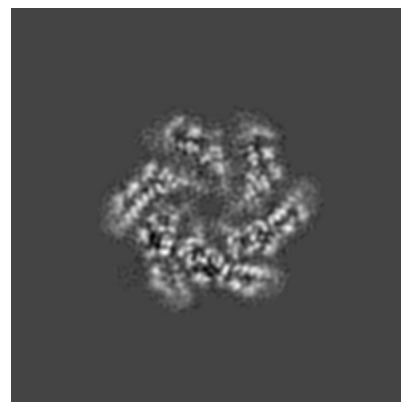
6.2.1 Primary map



X Index: 120



Y Index: 120

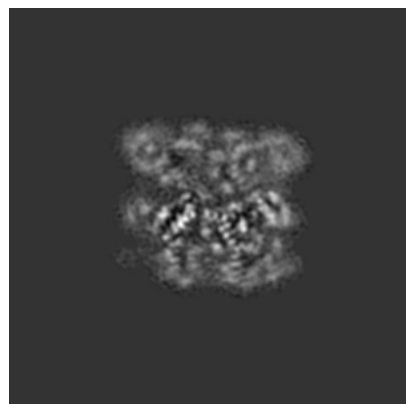


Z Index: 120

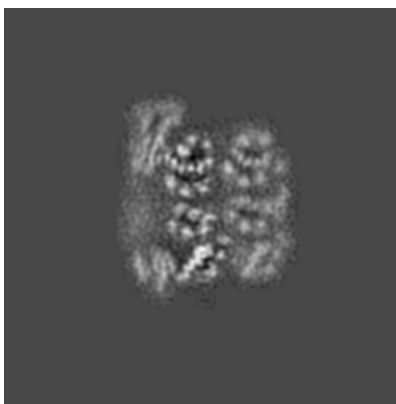
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

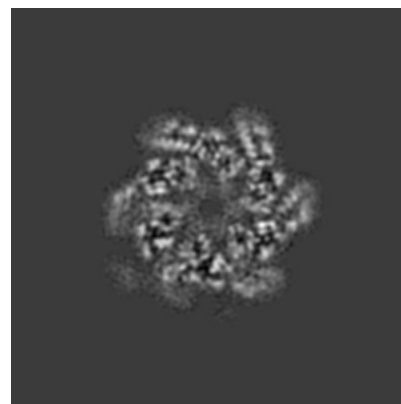
6.3.1 Primary map



X Index: 152



Y Index: 99

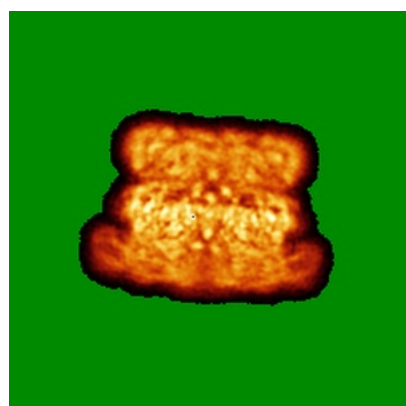


Z Index: 116

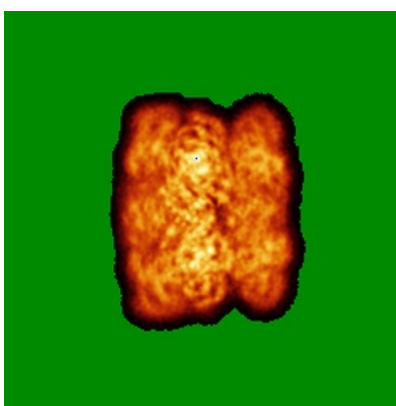
The images above show the largest variance slices of the map in three orthogonal directions.

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

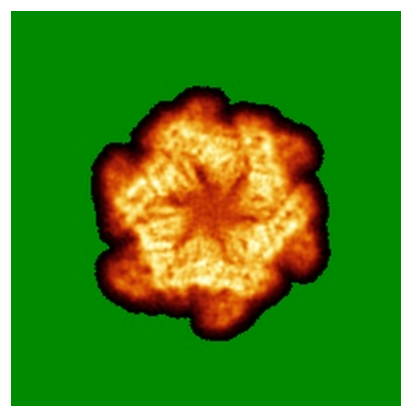
6.4.1 Primary map



X



Y

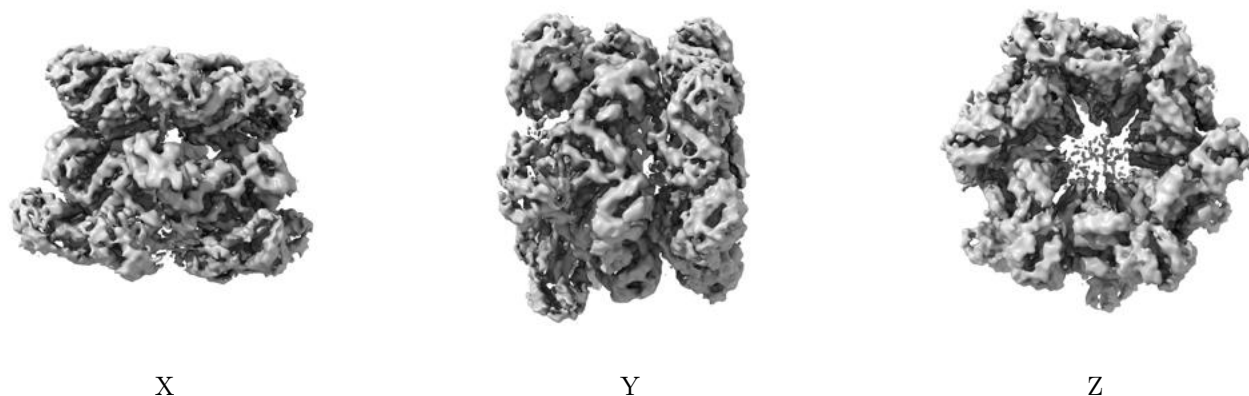


Z

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 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

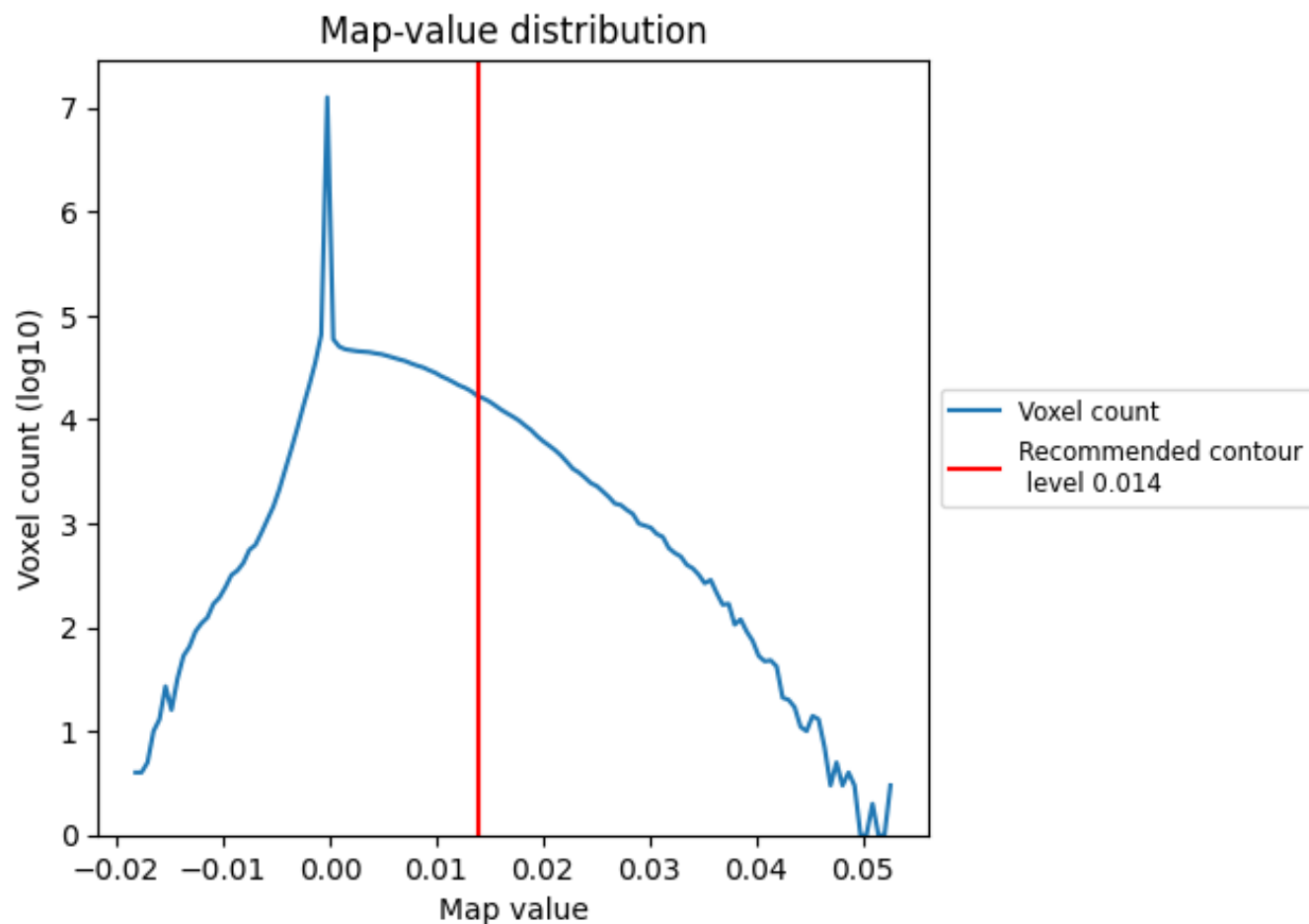
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

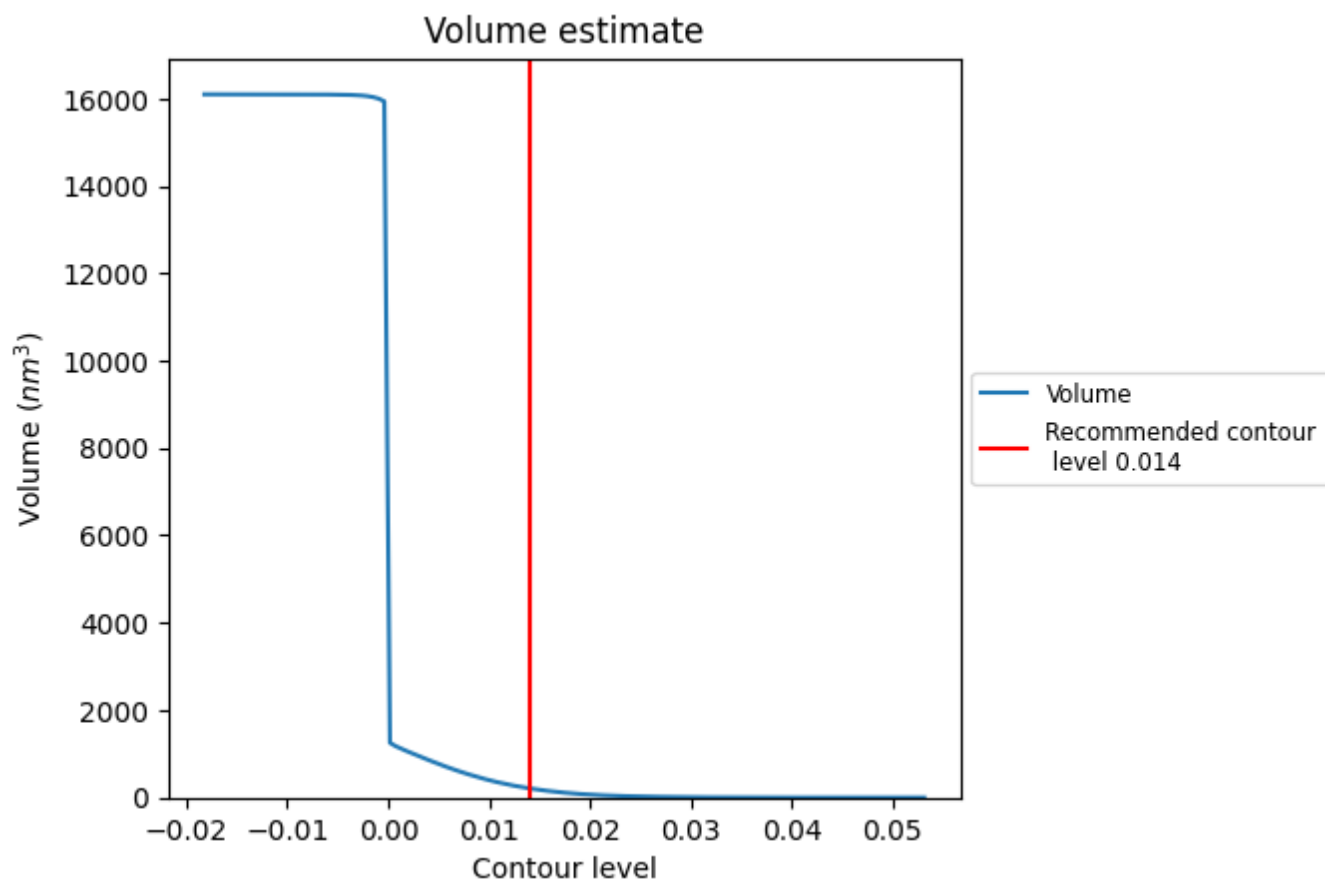
This section contains the results of statistical analysis of the map.

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.

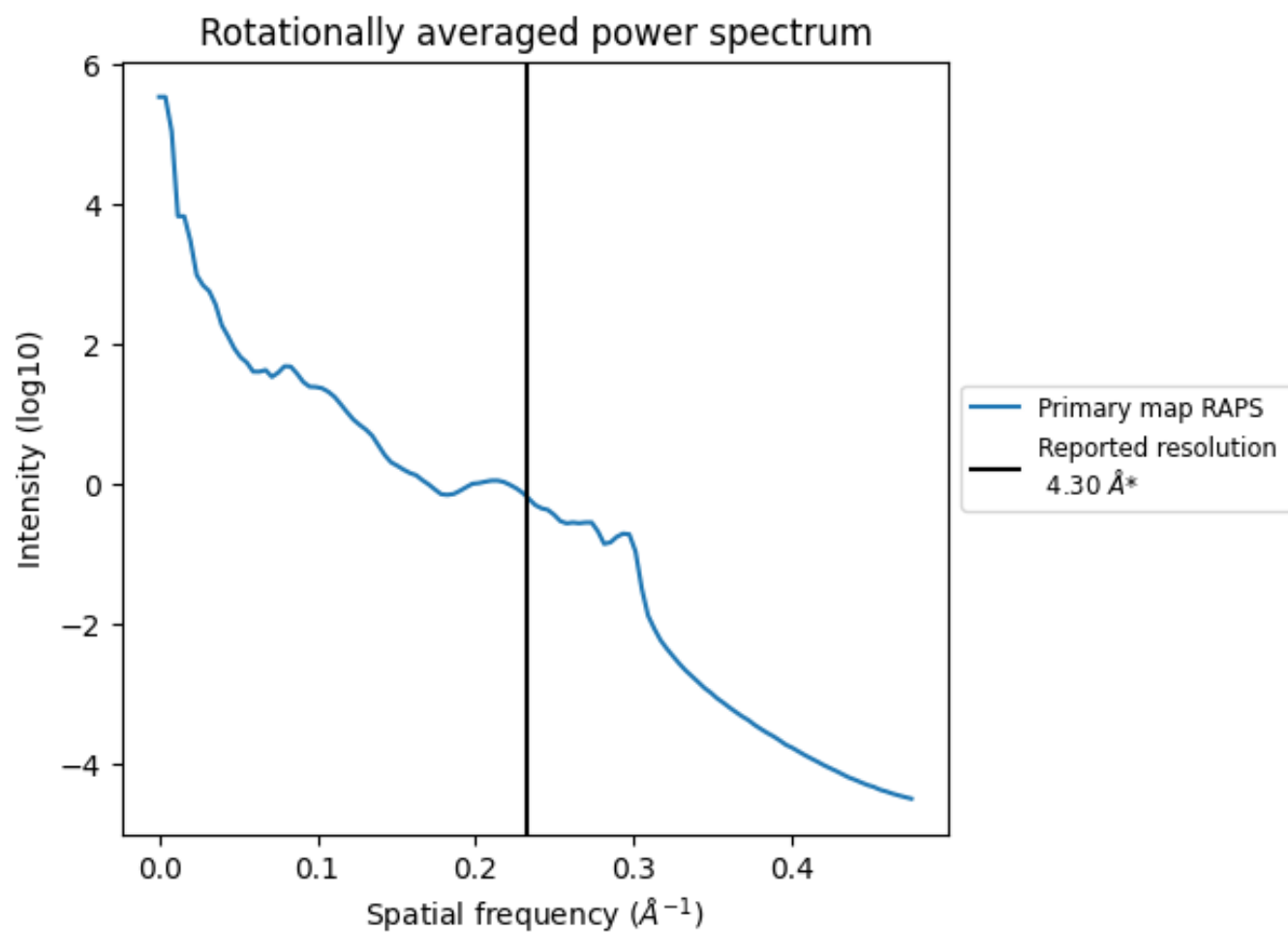
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 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 0.233 Å⁻¹

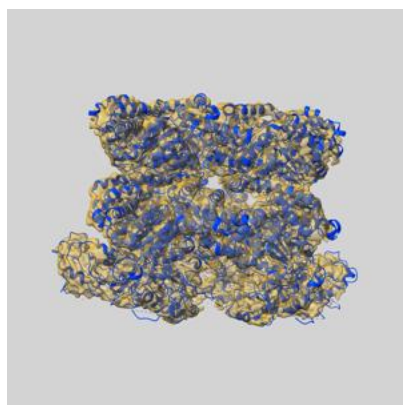
8 Fourier-Shell correlation

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

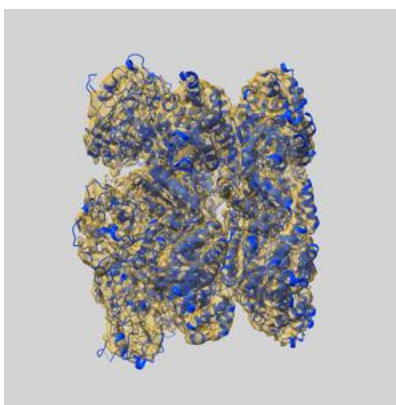
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32402 and PDB model 7YKZ. Per-residue inclusion information can be found in section 3 on page 7.

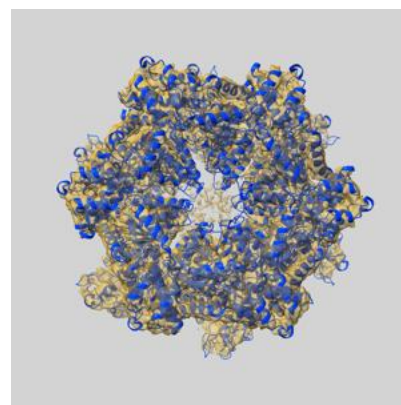
9.1 Map-model overlay [i](#)



X



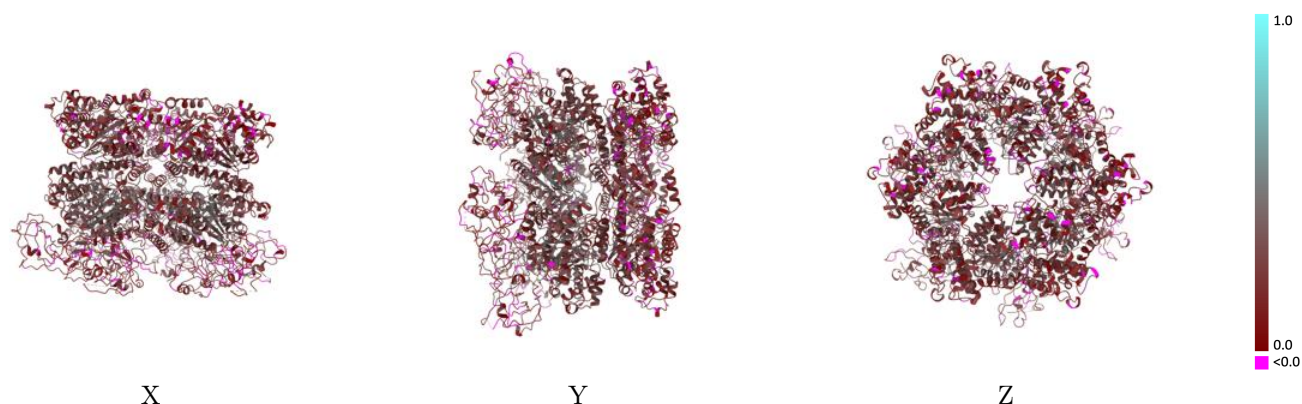
Y



Z

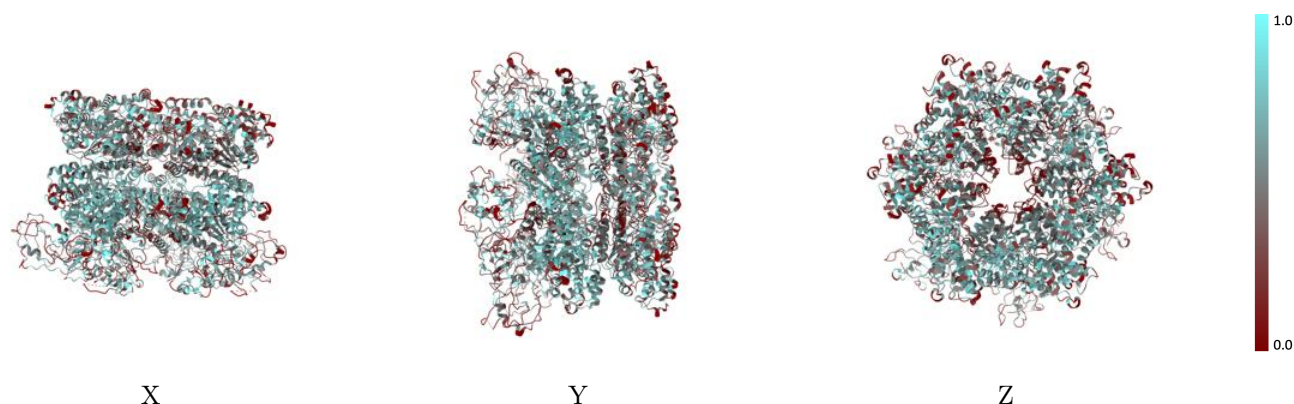
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



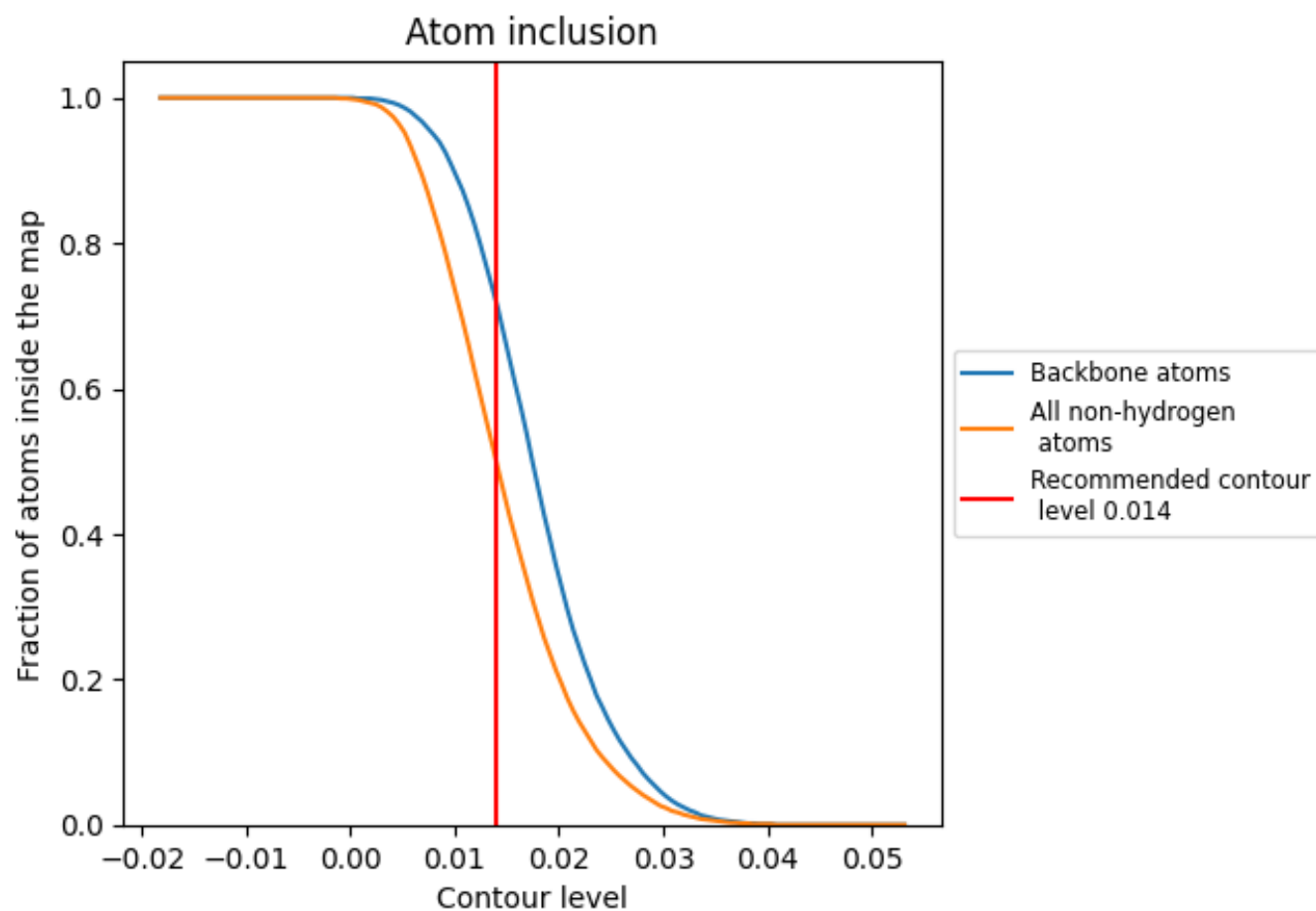
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 50% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4990	0.2220
A	0.4790	0.2130
B	0.4740	0.2140
C	0.5200	0.2270
D	0.5330	0.2400
E	0.5060	0.2260
F	0.4820	0.2120

1.0

0.0

<0.0