



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:08 AM UTC

PDB ID : 5YWC / pdb_00005ywc
EMDB ID : EMD-6852
Title : Structure of pancreatic ATP-sensitive potassium channel bound with Mg-ADP
(CTD class1 at 4.3Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-11-29
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

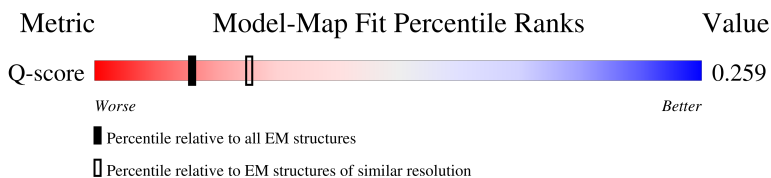
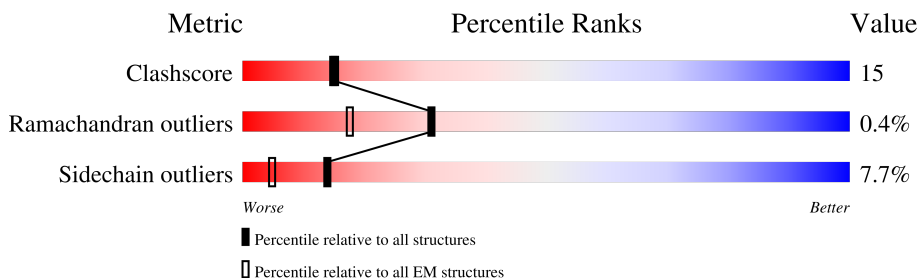
1 Overall quality at a glance

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	390	 48% 31% 5% 17%
1	C	390	 53% 30% 17%
1	E	390	 48% 31% 5% 17%
1	G	390	 48% 31% 5% 17%

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Mol	Chain	Length	Quality of chain
2	B	1582	
2	D	1582	
2	F	1582	
2	H	1582	

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
3	ADP	A	401	-	-	X	-
3	ADP	C	401	-	-	X	-
3	ADP	E	401	-	-	X	-
3	ADP	G	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51108 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	C	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	E	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	G	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0
			10231	6664	1727	1787	53		
2	D	1322	Total	C	N	O	S	0	0
			10231	6664	1727	1787	53		
2	F	1322	Total	C	N	O	S	0	0
			10231	6664	1727	1787	53		
2	H	1322	Total	C	N	O	S	0	0
			10231	6664	1727	1787	53		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

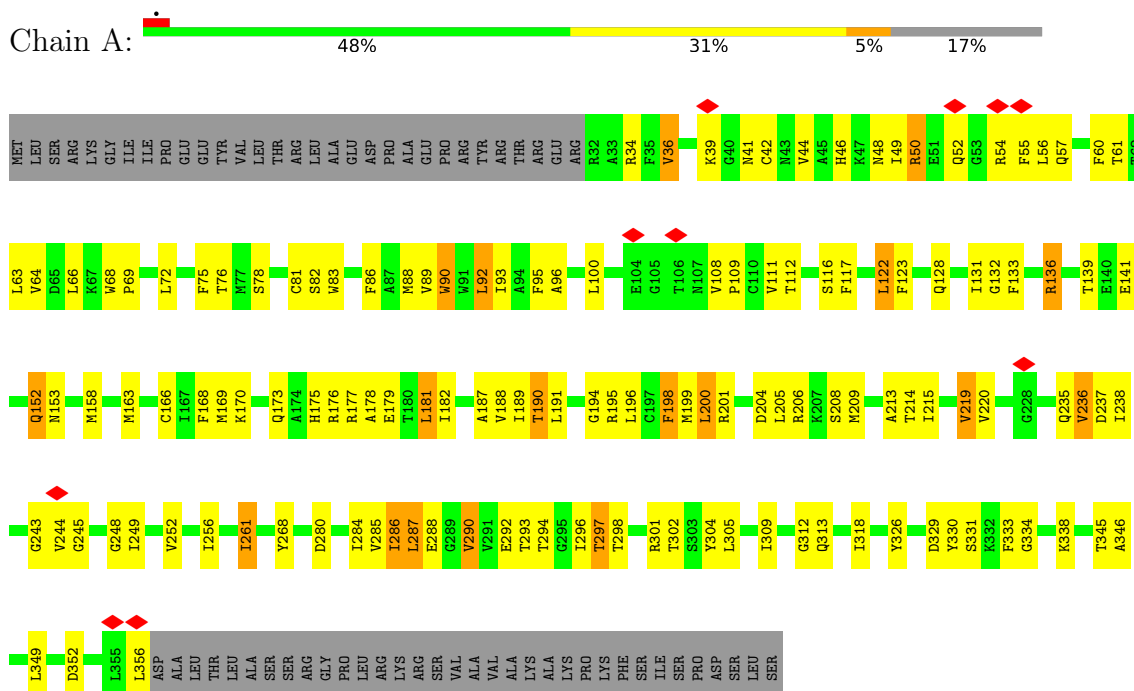
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total 2	Mg 2	0
4	D	2	Total 2	Mg 2	0
4	F	2	Total 2	Mg 2	0
4	H	2	Total 2	Mg 2	0

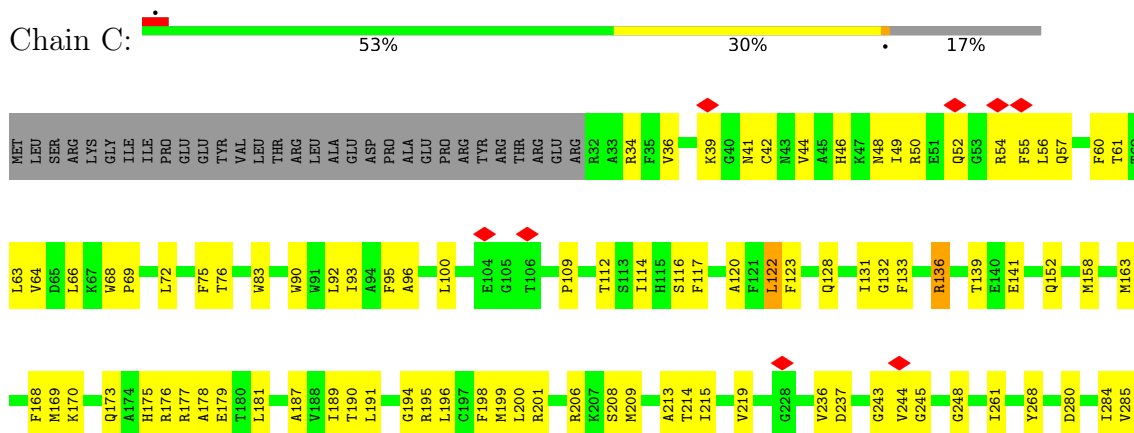
3 Residue-property plots

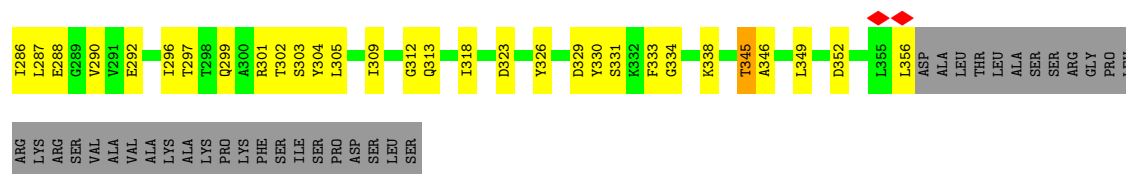
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-sensitive inward rectifier potassium channel 11



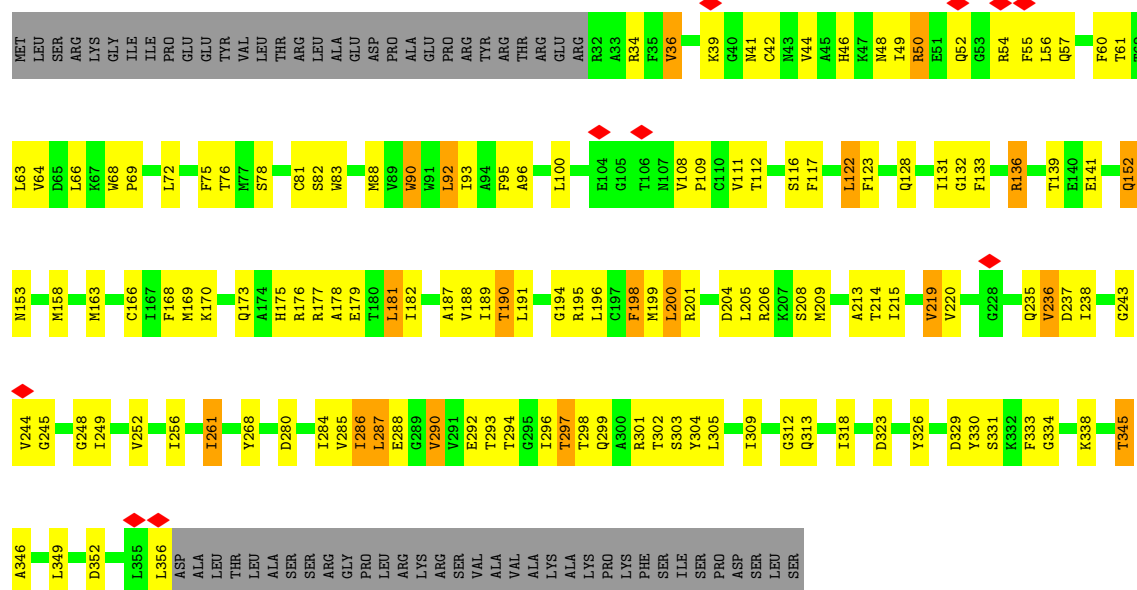
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





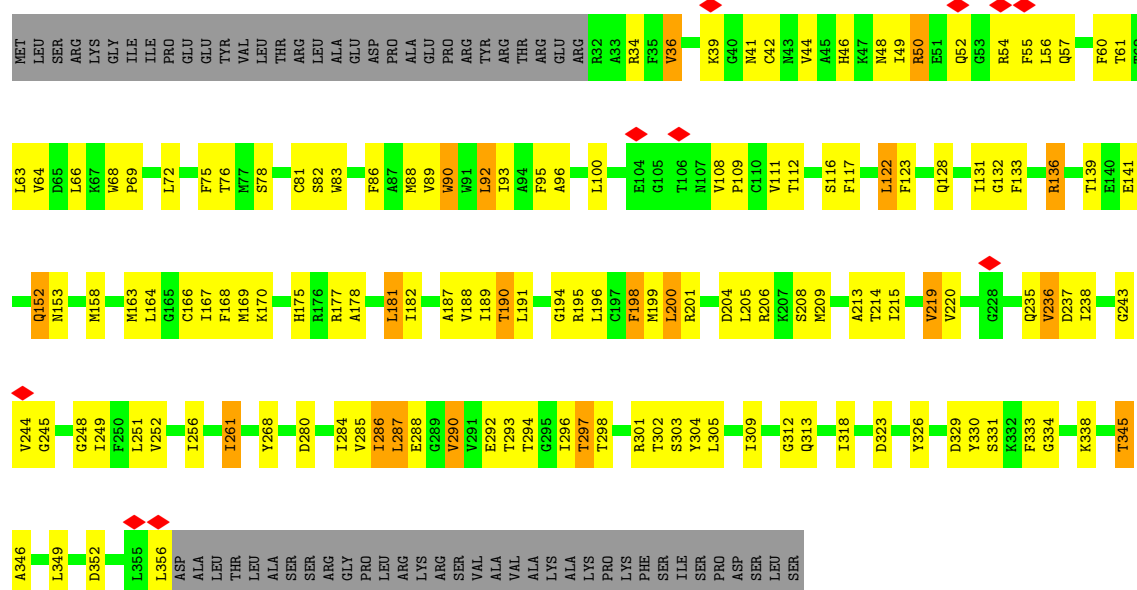
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E: 48% 31% 5% 17%



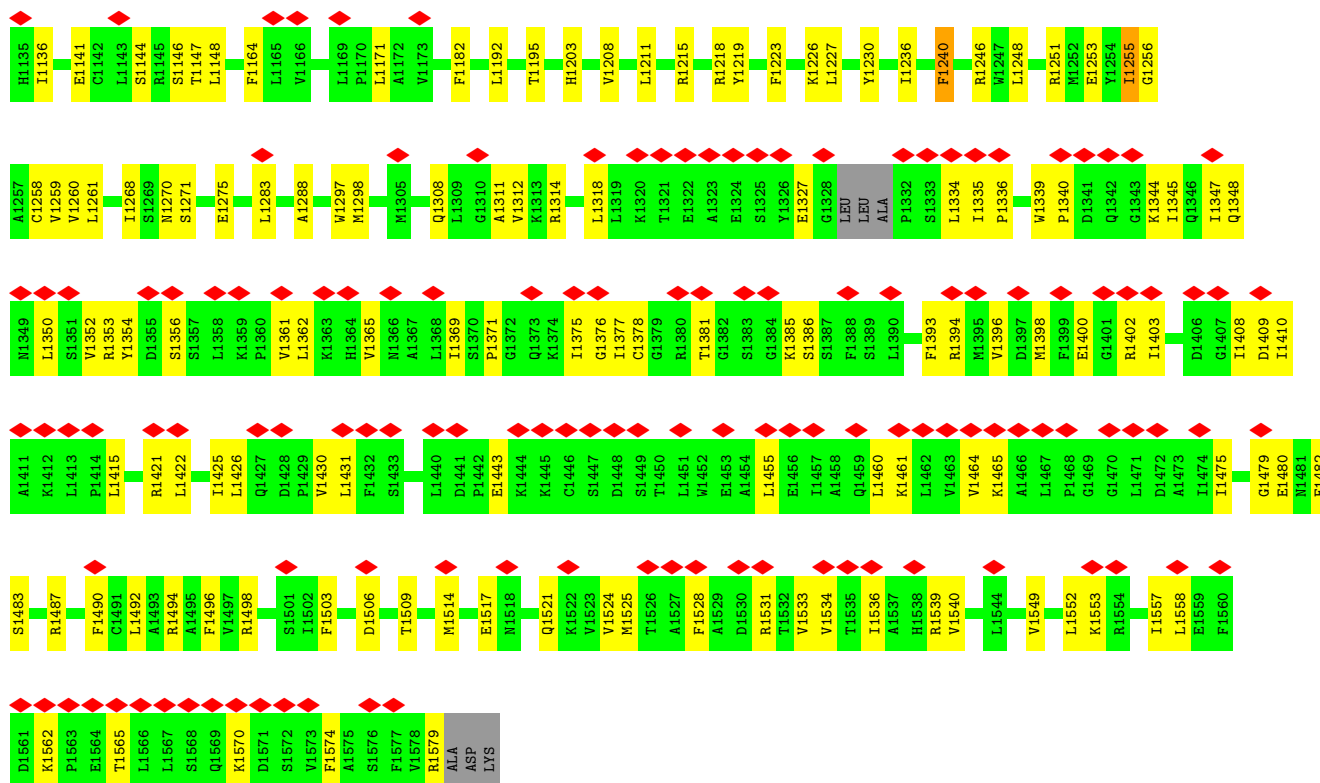
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain G: 48% 31% 5% 17%

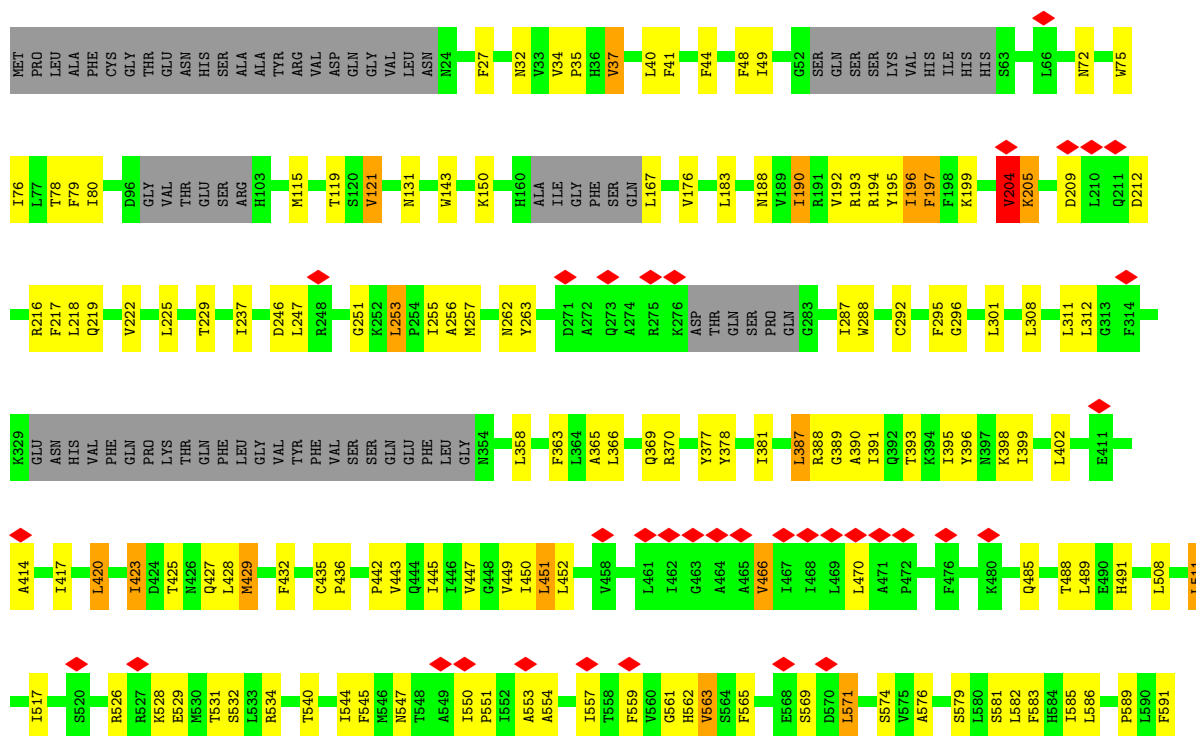


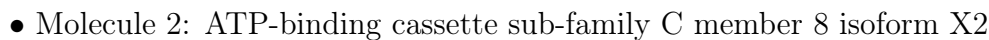
Chain B: 15% 60% 22% 3%

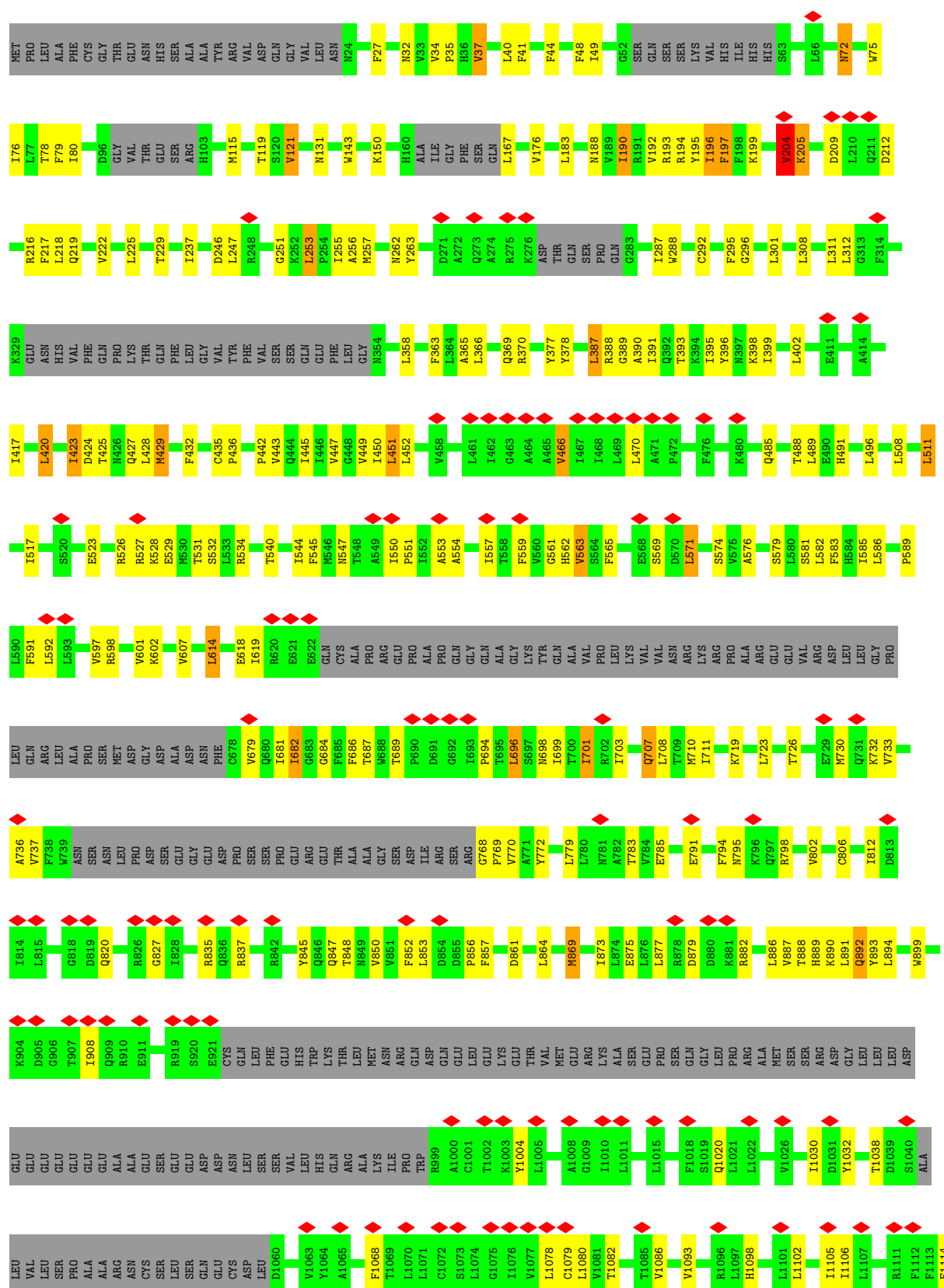


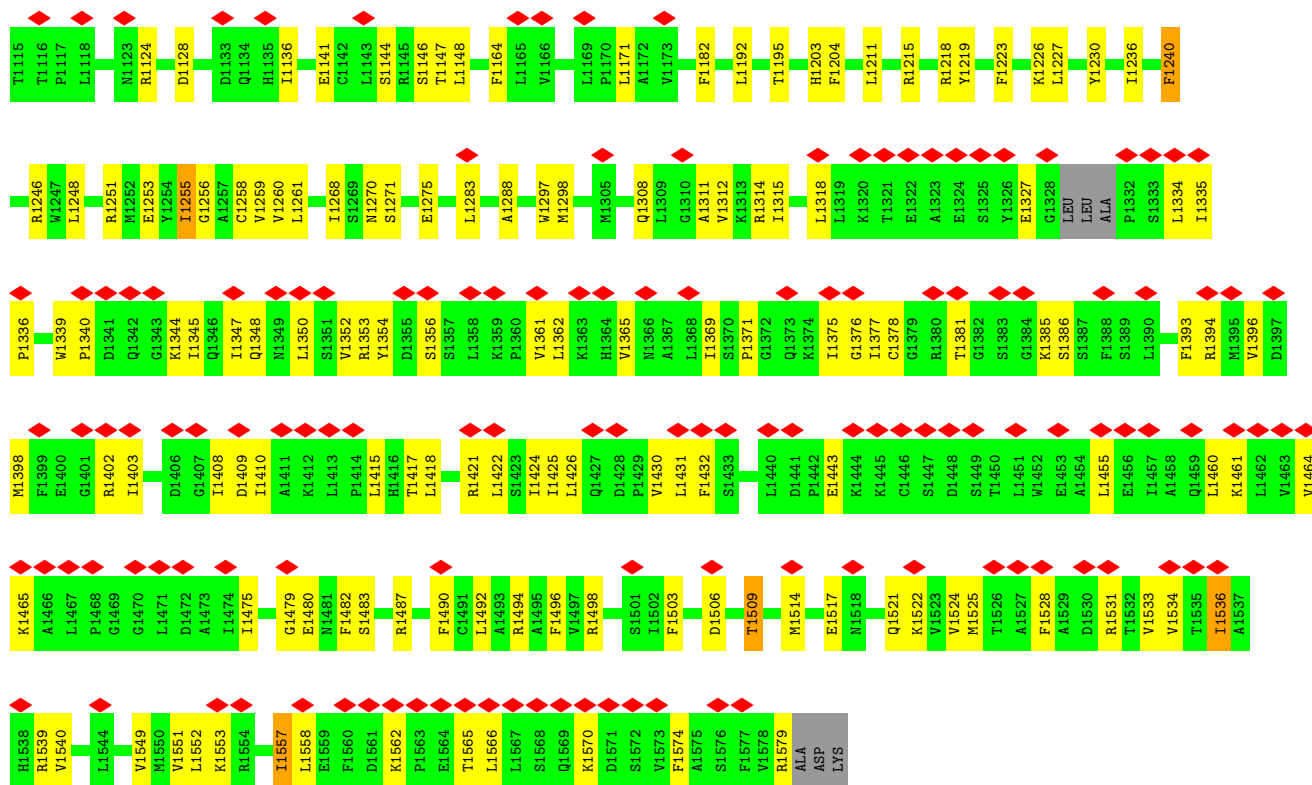


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

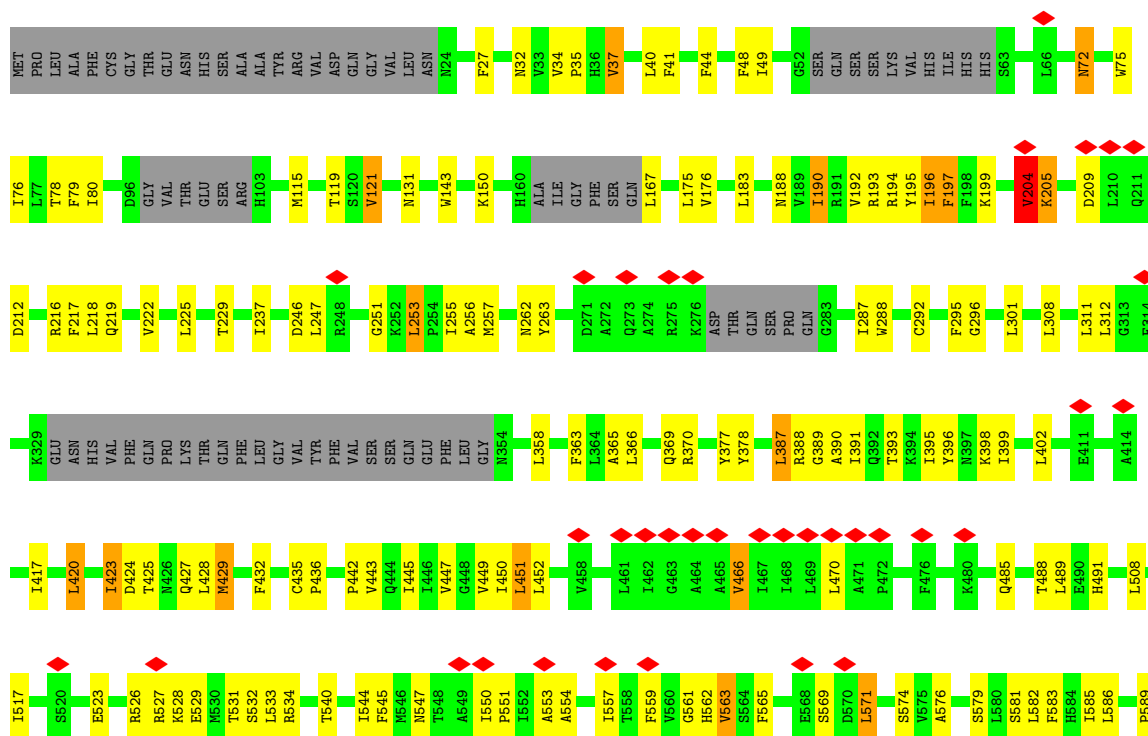








• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55214	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.33	0/2518	0.56	0/3430
1	C	0.33	0/2518	0.56	0/3430
1	E	0.33	0/2518	0.56	0/3430
1	G	0.33	0/2518	0.56	0/3430
2	B	0.19	0/10436	0.42	3/14176 (0.0%)
2	D	0.19	0/10436	0.42	3/14176 (0.0%)
2	F	0.19	0/10436	0.42	3/14176 (0.0%)
2	H	0.19	0/10436	0.42	3/14176 (0.0%)
All	All	0.23	0/51816	0.45	12/70424 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	GLY	N-CA-C	6.29	122.90	110.77
2	D	296	GLY	N-CA-C	6.29	122.90	110.77
2	F	296	GLY	N-CA-C	6.29	122.90	110.77
2	H	296	GLY	N-CA-C	6.29	122.90	110.77
2	B	194	ARG	N-CA-C	6.13	120.83	109.24
2	D	194	ARG	N-CA-C	6.13	120.83	109.24
2	F	194	ARG	N-CA-C	6.13	120.83	109.24
2	H	194	ARG	N-CA-C	6.13	120.83	109.24
2	B	204	VAL	N-CA-C	5.25	115.97	110.62
2	D	204	VAL	N-CA-C	5.25	115.97	110.62
2	F	204	VAL	N-CA-C	5.25	115.97	110.62
2	H	204	VAL	N-CA-C	5.25	115.97	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2451	116	0
1	C	2463	0	2451	117	0
1	E	2463	0	2451	121	0
1	G	2463	0	2451	122	0
2	B	10231	0	10474	281	0
2	D	10231	0	10474	279	0
2	F	10231	0	10474	279	0
2	H	10231	0	10474	280	0
3	A	27	0	12	10	0
3	B	54	0	24	5	0
3	C	27	0	12	9	0
3	D	54	0	24	4	0
3	E	27	0	12	9	0
3	F	54	0	24	4	0
3	G	27	0	12	9	0
3	H	54	0	24	5	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
All	All	51108	0	51844	1529	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 15.

All (1529) 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)
2:F:79:PHE:CZ	2:F:225:LEU:HD13	1.63	1.33
2:B:79:PHE:CZ	2:B:225:LEU:HD13	1.63	1.31
2:D:79:PHE:CZ	2:D:225:LEU:HD13	1.63	1.31
2:D:209:ASP:CB	2:D:255:ILE:HD13	1.60	1.31
2:B:209:ASP:CB	2:B:255:ILE:HD13	1.60	1.30
2:H:79:PHE:CZ	2:H:225:LEU:HD13	1.63	1.30
2:H:209:ASP:CB	2:H:255:ILE:HD13	1.60	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:209:ASP:CB	2:F:255:ILE:HD13	1.60	1.29
1:C:200:LEU:HD12	1:C:201:ARG:N	1.51	1.23
1:E:200:LEU:HD12	1:E:201:ARG:N	1.51	1.22
1:G:200:LEU:HD12	1:G:201:ARG:N	1.51	1.21
1:A:200:LEU:HD12	1:A:201:ARG:N	1.51	1.21
1:A:200:LEU:CD1	1:A:201:ARG:N	2.05	1.19
1:E:200:LEU:CD1	1:E:201:ARG:N	2.05	1.18
1:G:200:LEU:CD1	1:G:201:ARG:N	2.05	1.17
1:C:200:LEU:CD1	1:C:201:ARG:N	2.05	1.17
2:D:190:ILE:HG13	2:D:195:TYR:CB	1.79	1.13
2:F:190:ILE:HG13	2:F:195:TYR:CB	1.79	1.13
2:H:190:ILE:HG13	2:H:195:TYR:CB	1.79	1.12
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
2:D:79:PHE:HZ	2:D:225:LEU:CD1	1.64	1.11
1:E:198:PHE:HD1	1:E:198:PHE:C	1.56	1.11
2:B:79:PHE:HZ	2:B:225:LEU:CD1	1.64	1.10
1:G:198:PHE:HD1	1:G:198:PHE:C	1.56	1.10
1:C:198:PHE:C	1:C:198:PHE:HD1	1.56	1.09
2:F:79:PHE:HZ	2:F:225:LEU:CD1	1.64	1.09
1:A:198:PHE:HD1	1:A:198:PHE:C	1.56	1.09
2:H:79:PHE:HZ	2:H:225:LEU:CD1	1.64	1.09
1:C:198:PHE:HD1	1:C:199:MET:N	1.52	1.07
1:A:198:PHE:HD1	1:A:199:MET:N	1.52	1.06
1:E:198:PHE:HD1	1:E:199:MET:N	1.52	1.06
1:G:198:PHE:HD1	1:G:199:MET:N	1.52	1.05
1:A:198:PHE:C	1:A:198:PHE:CD1	2.30	1.04
1:E:198:PHE:C	1:E:198:PHE:CD1	2.30	1.02
2:F:79:PHE:HZ	2:F:225:LEU:HD13	0.95	1.02
1:G:198:PHE:C	1:G:198:PHE:CD1	2.30	1.01
1:C:198:PHE:C	1:C:198:PHE:CD1	2.30	1.01
2:D:79:PHE:HZ	2:D:225:LEU:HD13	0.95	1.01
1:C:200:LEU:HD13	1:C:201:ARG:H	1.25	1.01
1:A:200:LEU:HD13	1:A:201:ARG:H	1.25	1.00
1:G:200:LEU:HD13	1:G:201:ARG:H	1.25	0.99
2:B:79:PHE:HZ	2:B:225:LEU:HD13	0.95	0.98
1:E:200:LEU:HD13	1:E:201:ARG:H	1.25	0.98
3:A:401:ADP:O1A	1:C:334:GLY:HA3	1.63	0.98
3:C:401:ADP:O1A	1:E:334:GLY:HA3	1.63	0.98
2:H:79:PHE:HZ	2:H:225:LEU:HD13	0.95	0.97
1:A:334:GLY:HA3	3:G:401:ADP:O1A	1.63	0.97
3:E:401:ADP:O1A	1:G:334:GLY:HA3	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:295:PHE:CZ	2:H:387:LEU:HB2	2.01	0.95
2:D:190:ILE:CG1	2:D:195:TYR:CB	2.44	0.95
2:D:295:PHE:CZ	2:D:387:LEU:HB2	2.01	0.94
2:F:190:ILE:CG1	2:F:195:TYR:CB	2.44	0.94
2:H:190:ILE:CG1	2:H:195:TYR:CB	2.44	0.94
2:F:295:PHE:CZ	2:F:387:LEU:HB2	2.01	0.94
2:B:295:PHE:CZ	2:B:387:LEU:HB2	2.01	0.94
1:G:200:LEU:CD1	1:G:201:ARG:H	1.78	0.94
1:A:200:LEU:HD12	1:A:200:LEU:C	1.93	0.93
2:B:190:ILE:CG1	2:B:195:TYR:CB	2.44	0.93
1:E:200:LEU:HD12	1:E:200:LEU:C	1.93	0.93
2:D:209:ASP:CB	2:D:255:ILE:CD1	2.46	0.93
2:F:79:PHE:CZ	2:F:225:LEU:CD1	2.46	0.93
1:G:200:LEU:HD12	1:G:200:LEU:C	1.93	0.92
1:C:200:LEU:HD12	1:C:200:LEU:C	1.93	0.92
1:A:50:ARG:HB2	3:A:401:ADP:C6	2.05	0.92
1:C:50:ARG:HB2	3:C:401:ADP:C6	2.05	0.92
2:H:209:ASP:CB	2:H:255:ILE:CD1	2.46	0.92
1:E:50:ARG:HB2	3:E:401:ADP:C6	2.05	0.92
2:B:209:ASP:CB	2:B:255:ILE:CD1	2.46	0.92
1:G:50:ARG:HB2	3:G:401:ADP:C6	2.05	0.92
1:C:200:LEU:CD1	1:C:201:ARG:H	1.78	0.92
2:F:209:ASP:CB	2:F:255:ILE:CD1	2.46	0.92
1:A:200:LEU:CD1	1:A:201:ARG:H	1.78	0.91
2:F:209:ASP:CB	2:F:255:ILE:HG21	2.01	0.91
2:H:209:ASP:CB	2:H:255:ILE:HG21	2.01	0.90
2:H:79:PHE:CZ	2:H:225:LEU:CD1	2.46	0.90
2:D:209:ASP:CB	2:D:255:ILE:HG21	2.01	0.89
2:B:209:ASP:CB	2:B:255:ILE:HG21	2.01	0.89
2:D:79:PHE:CZ	2:D:225:LEU:CD1	2.46	0.89
1:A:198:PHE:CD1	1:A:199:MET:N	2.43	0.86
2:B:79:PHE:CZ	2:B:225:LEU:CD1	2.46	0.86
3:A:401:ADP:O1A	1:C:334:GLY:CA	2.23	0.86
1:A:334:GLY:CA	3:G:401:ADP:O1A	2.23	0.86
1:E:200:LEU:CD1	1:E:201:ARG:H	1.78	0.86
3:E:401:ADP:O1A	1:G:334:GLY:CA	2.23	0.86
3:C:401:ADP:O1A	1:E:334:GLY:CA	2.23	0.85
1:E:198:PHE:CD1	1:E:199:MET:N	2.43	0.85
1:G:198:PHE:CD1	1:G:199:MET:N	2.43	0.84
1:E:50:ARG:N	3:E:401:ADP:N1	2.25	0.83
1:G:50:ARG:N	3:G:401:ADP:N1	2.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PHE:CD1	1:C:199:MET:N	2.43	0.82
1:C:50:ARG:N	3:C:401:ADP:N1	2.25	0.81
1:A:200:LEU:HD13	1:A:201:ARG:N	1.86	0.80
1:A:50:ARG:N	3:A:401:ADP:N1	2.25	0.79
2:D:1124:ARG:HH11	2:D:1314:ARG:HD3	1.49	0.78
2:D:1271:SER:HA	2:D:1275:GLU:HB3	1.66	0.78
2:F:1271:SER:HA	2:F:1275:GLU:HB3	1.66	0.78
2:F:1124:ARG:HH11	2:F:1314:ARG:HD3	1.49	0.78
1:A:219:VAL:HG13	1:A:236:VAL:HG23	1.65	0.78
2:D:79:PHE:CE2	2:D:225:LEU:HD13	2.19	0.77
2:D:204:VAL:O	2:D:205:LYS:HB3	1.83	0.77
2:B:204:VAL:O	2:B:205:LYS:HB3	1.83	0.77
1:E:219:VAL:HG13	1:E:236:VAL:HG23	1.65	0.77
2:F:79:PHE:CE2	2:F:225:LEU:HD13	2.19	0.77
2:H:1271:SER:HA	2:H:1275:GLU:HB3	1.66	0.77
1:G:219:VAL:HG13	1:G:236:VAL:HG23	1.65	0.77
2:B:1421:ARG:HG3	2:B:1422:LEU:HG	1.67	0.77
2:B:196:ILE:O	2:B:197:PHE:O	2.03	0.77
2:B:1271:SER:HA	2:B:1275:GLU:HB3	1.66	0.77
1:C:219:VAL:HG13	1:C:236:VAL:HG23	1.65	0.76
2:D:1421:ARG:HG3	2:D:1422:LEU:HG	1.67	0.76
2:F:204:VAL:O	2:F:205:LYS:HB3	1.83	0.76
2:H:1124:ARG:HH11	2:H:1314:ARG:HD3	1.49	0.76
2:B:79:PHE:CE2	2:B:225:LEU:HD13	2.19	0.76
1:A:334:GLY:HA3	3:G:401:ADP:PA	2.26	0.76
2:F:1421:ARG:HG3	2:F:1422:LEU:HG	1.67	0.76
2:H:75:TRP:CE3	2:H:225:LEU:HB2	2.21	0.76
2:H:204:VAL:O	2:H:205:LYS:HB3	1.83	0.76
2:D:196:ILE:O	2:D:197:PHE:O	2.03	0.76
2:D:209:ASP:CB	2:D:255:ILE:CG2	2.64	0.76
2:B:209:ASP:CB	2:B:255:ILE:CG2	2.64	0.76
2:B:1124:ARG:HH11	2:B:1314:ARG:HD3	1.49	0.76
2:B:75:TRP:CE3	2:B:225:LEU:HB2	2.21	0.76
2:F:75:TRP:CE3	2:F:225:LEU:HB2	2.21	0.76
2:H:1421:ARG:HG3	2:H:1422:LEU:HG	1.67	0.76
3:A:401:ADP:PA	1:C:334:GLY:HA3	2.26	0.75
2:D:75:TRP:CE3	2:D:225:LEU:HB2	2.21	0.75
2:F:209:ASP:CB	2:F:255:ILE:CG2	2.64	0.75
2:H:79:PHE:CE2	2:H:225:LEU:HD13	2.19	0.75
2:H:209:ASP:CB	2:H:255:ILE:CG2	2.64	0.75
3:C:401:ADP:PA	1:E:334:GLY:HA3	2.26	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:401:ADP:PA	1:G:334:GLY:HA3	2.26	0.75
2:D:387:LEU:HD21	2:D:428:LEU:HB3	1.69	0.74
2:H:196:ILE:O	2:H:197:PHE:O	2.03	0.74
2:F:196:ILE:O	2:F:197:PHE:O	2.03	0.74
1:E:200:LEU:HD13	1:E:201:ARG:N	1.86	0.74
2:B:387:LEU:HD21	2:B:428:LEU:HB3	1.69	0.73
2:D:75:TRP:CZ3	2:D:225:LEU:HB2	2.24	0.73
1:E:36:VAL:HG12	1:E:42:CYS:HA	1.71	0.73
2:B:75:TRP:CZ3	2:B:225:LEU:HB2	2.24	0.73
2:H:387:LEU:HD21	2:H:428:LEU:HB3	1.69	0.72
1:C:213:ALA:HA	1:C:288:GLU:O	1.90	0.72
1:G:36:VAL:HG12	1:G:42:CYS:HA	1.71	0.72
2:H:75:TRP:CZ3	2:H:225:LEU:HB2	2.24	0.72
2:F:387:LEU:HD21	2:F:428:LEU:HB3	1.69	0.72
2:F:75:TRP:CZ3	2:F:225:LEU:HB2	2.24	0.72
2:H:1334:LEU:HD13	2:H:1408:ILE:HG23	1.72	0.72
1:A:213:ALA:HA	1:A:288:GLU:O	1.90	0.72
1:G:200:LEU:CD1	1:G:200:LEU:C	2.50	0.71
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.71	0.71
1:C:54:ARG:O	1:E:206:ARG:NH2	2.24	0.71
2:B:1334:LEU:HD13	2:B:1408:ILE:HG23	1.72	0.71
1:A:36:VAL:HG12	1:A:42:CYS:HA	1.71	0.71
1:A:54:ARG:O	1:C:206:ARG:NH2	2.24	0.71
1:G:54:ARG:HA	1:G:57:GLN:HB2	1.73	0.71
1:A:206:ARG:NH2	1:G:54:ARG:O	2.24	0.71
1:E:213:ALA:HA	1:E:288:GLU:O	1.90	0.71
2:F:1334:LEU:HD13	2:F:1408:ILE:HG23	1.72	0.71
1:E:54:ARG:HA	1:E:57:GLN:HB2	1.73	0.71
1:G:213:ALA:HA	1:G:288:GLU:O	1.90	0.71
1:E:54:ARG:O	1:G:206:ARG:NH2	2.24	0.70
2:H:301:LEU:C	2:H:301:LEU:HD23	2.16	0.70
1:A:54:ARG:HA	1:A:57:GLN:HB2	1.73	0.70
1:C:54:ARG:HA	1:C:57:GLN:HB2	1.73	0.70
2:F:682:ILE:HG23	2:F:736:ALA:HB3	1.73	0.70
2:D:1334:LEU:HD13	2:D:1408:ILE:HG23	1.72	0.70
2:F:204:VAL:O	2:F:205:LYS:CB	2.40	0.70
2:F:301:LEU:C	2:F:301:LEU:HD23	2.16	0.70
2:B:301:LEU:C	2:B:301:LEU:HD23	2.16	0.70
2:D:204:VAL:O	2:D:205:LYS:CB	2.40	0.70
2:B:682:ILE:HG23	2:B:736:ALA:HB3	1.73	0.70
2:D:301:LEU:HD23	2:D:301:LEU:C	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:682:ILE:HG23	2:D:736:ALA:HB3	1.73	0.70
2:D:1394:ARG:HD2	2:D:1410:ILE:HG21	1.73	0.69
2:H:1394:ARG:HD2	2:H:1410:ILE:HG21	1.73	0.69
1:A:200:LEU:CD1	1:A:201:ARG:O	2.41	0.69
2:B:562:HIS:NE2	2:B:569:SER:O	2.26	0.69
1:E:200:LEU:CD1	1:E:201:ARG:O	2.41	0.69
2:D:287:ILE:HD11	2:D:607:VAL:HG13	1.74	0.69
2:F:287:ILE:HD11	2:F:607:VAL:HG13	1.74	0.69
1:C:200:LEU:CD1	1:C:201:ARG:O	2.41	0.69
1:G:194:GLY:O	1:G:195:ARG:HD2	1.93	0.69
1:G:200:LEU:HD21	1:G:304:TYR:CZ	2.28	0.69
1:A:95:PHE:HD1	1:A:100:LEU:HD23	1.58	0.68
1:A:200:LEU:HD21	1:A:304:TYR:CZ	2.28	0.68
1:C:200:LEU:HD21	1:C:304:TYR:CZ	2.28	0.68
1:C:243:GLY:O	1:C:245:GLY:N	2.26	0.68
1:A:243:GLY:O	1:A:245:GLY:N	2.26	0.68
2:B:1394:ARG:HD2	2:B:1410:ILE:HG21	1.73	0.68
2:D:562:HIS:NE2	2:D:569:SER:O	2.26	0.68
1:E:200:LEU:HD21	1:E:304:TYR:CZ	2.28	0.68
1:G:200:LEU:CD1	1:G:201:ARG:O	2.41	0.68
1:G:243:GLY:O	1:G:245:GLY:N	2.26	0.68
2:B:287:ILE:HD11	2:B:607:VAL:HG13	1.74	0.68
2:F:562:HIS:NE2	2:F:569:SER:O	2.26	0.68
2:H:562:HIS:NE2	2:H:569:SER:O	2.26	0.68
2:H:682:ILE:HG23	2:H:736:ALA:HB3	1.73	0.68
1:C:95:PHE:HD1	1:C:100:LEU:HD23	1.58	0.68
1:E:243:GLY:O	1:E:245:GLY:N	2.26	0.68
2:H:287:ILE:HD11	2:H:607:VAL:HG13	1.74	0.68
2:F:1394:ARG:HD2	2:F:1410:ILE:HG21	1.73	0.68
2:B:869:MET:HA	2:B:873:ILE:HD12	1.75	0.68
1:E:194:GLY:O	1:E:195:ARG:HD2	1.93	0.67
1:A:194:GLY:O	1:A:195:ARG:HD2	1.93	0.67
1:G:200:LEU:HD13	1:G:201:ARG:N	1.86	0.67
2:D:75:TRP:HZ3	2:D:225:LEU:HD22	1.60	0.67
2:F:75:TRP:HZ3	2:F:225:LEU:HD22	1.60	0.67
2:H:869:MET:HA	2:H:873:ILE:HD12	1.75	0.67
2:B:75:TRP:HZ3	2:B:225:LEU:HD22	1.60	0.67
2:B:204:VAL:O	2:B:205:LYS:CB	2.40	0.67
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.77	0.67
1:G:95:PHE:HD1	1:G:100:LEU:HD23	1.58	0.67
2:H:75:TRP:HZ3	2:H:225:LEU:HD22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLY:O	1:C:195:ARG:HD2	1.93	0.67
2:D:869:MET:HA	2:D:873:ILE:HD12	1.75	0.67
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.77	0.67
2:F:551:PRO:HB3	2:F:583:PHE:CZ	2.30	0.67
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.77	0.67
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.77	0.67
2:H:551:PRO:HB3	2:H:583:PHE:CZ	2.30	0.67
2:F:869:MET:HA	2:F:873:ILE:HD12	1.75	0.66
2:H:466:VAL:HG11	2:H:554:ALA:HB2	1.76	0.66
2:H:204:VAL:O	2:H:205:LYS:CB	2.40	0.66
2:D:466:VAL:HG11	2:D:554:ALA:HB2	1.76	0.66
2:B:551:PRO:HB3	2:B:583:PHE:CZ	2.30	0.66
2:B:466:VAL:HG11	2:B:554:ALA:HB2	1.76	0.66
1:E:95:PHE:HD1	1:E:100:LEU:HD23	1.58	0.66
1:C:200:LEU:HD13	1:C:201:ARG:N	1.86	0.66
2:D:551:PRO:HB3	2:D:583:PHE:CZ	2.30	0.66
2:F:466:VAL:HG11	2:F:554:ALA:HB2	1.76	0.66
2:B:1509:THR:HG23	2:B:1517:GLU:HG2	1.79	0.65
2:D:511:LEU:HD23	2:D:1426:LEU:HD21	1.79	0.65
2:D:1509:THR:HG23	2:D:1517:GLU:HG2	1.79	0.65
2:H:217:PHE:HD2	2:H:1240:PHE:CE1	2.15	0.65
2:F:511:LEU:HD23	2:F:1426:LEU:HD21	1.79	0.65
1:E:50:ARG:CB	3:E:401:ADP:C6	2.79	0.65
1:G:50:ARG:CB	3:G:401:ADP:C6	2.79	0.65
2:H:1509:THR:HG23	2:H:1517:GLU:HG2	1.79	0.65
2:B:710:MET:HE3	2:B:893:TYR:HB3	1.79	0.65
1:G:177:ARG:NH1	1:G:208:SER:OG	2.30	0.65
2:H:710:MET:HE3	2:H:893:TYR:HB3	1.79	0.65
1:E:177:ARG:NH1	1:E:208:SER:OG	2.30	0.64
1:C:50:ARG:CB	3:C:401:ADP:C6	2.79	0.64
2:D:217:PHE:HD2	2:D:1240:PHE:CE1	2.15	0.64
1:A:200:LEU:HD21	1:A:304:TYR:OH	1.98	0.64
2:B:217:PHE:HD2	2:B:1240:PHE:CE1	2.15	0.64
2:F:217:PHE:HD2	2:F:1240:PHE:CE1	2.15	0.64
2:D:1480:GLU:OE1	3:D:2501:ADP:N6	2.30	0.64
2:F:217:PHE:HD2	2:F:1240:PHE:HE1	1.46	0.64
2:F:1480:GLU:OE1	3:F:2501:ADP:N6	2.30	0.64
2:B:1032:TYR:HA	2:B:1283:LEU:HD11	1.80	0.64
2:B:1480:GLU:OE1	3:B:2501:ADP:N6	2.30	0.64
2:D:217:PHE:HD2	2:D:1240:PHE:HE1	1.46	0.64
2:H:1480:GLU:OE1	3:H:2501:ADP:N6	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1032:TYR:HA	2:D:1283:LEU:HD11	1.80	0.64
2:F:710:MET:HE3	2:F:893:TYR:HB3	1.79	0.64
2:H:365:ALA:O	2:H:369:GLN:HG3	1.98	0.64
2:H:681:ILE:HB	2:H:701:ILE:HG23	1.80	0.64
1:A:50:ARG:CB	3:A:401:ADP:C6	2.79	0.64
1:C:200:LEU:HD21	1:C:304:TYR:OH	1.98	0.64
2:D:365:ALA:O	2:D:369:GLN:HG3	1.98	0.64
2:B:365:ALA:O	2:B:369:GLN:HG3	1.98	0.63
2:B:783:THR:HB	2:B:820:GLN:HA	1.80	0.63
2:D:681:ILE:HB	2:D:701:ILE:HG23	1.80	0.63
1:A:200:LEU:HD12	1:A:201:ARG:CA	2.29	0.63
1:C:177:ARG:NH1	1:C:208:SER:OG	2.30	0.63
2:D:1506:ASP:HA	2:D:1536:ILE:HG13	1.80	0.63
2:F:1509:THR:HG23	2:F:1517:GLU:HG2	1.79	0.63
2:H:190:ILE:CB	2:H:195:TYR:CB	2.77	0.63
1:A:177:ARG:NH1	1:A:208:SER:OG	2.30	0.63
2:B:190:ILE:CB	2:B:195:TYR:CB	2.77	0.63
2:D:190:ILE:CB	2:D:195:TYR:CB	2.77	0.63
2:D:710:MET:HE3	2:D:893:TYR:HB3	1.79	0.63
1:E:200:LEU:HD21	1:E:304:TYR:OH	1.98	0.63
2:F:1347:ILE:HG23	2:F:1403:ILE:HG12	1.80	0.63
1:G:200:LEU:HD21	1:G:304:TYR:OH	1.98	0.63
2:D:592:LEU:HD11	2:D:1297:TRP:HH2	1.63	0.63
2:B:1506:ASP:HA	2:B:1536:ILE:HG13	1.80	0.63
2:D:209:ASP:HA	2:D:255:ILE:CG2	2.29	0.63
2:H:1506:ASP:HA	2:H:1536:ILE:HG13	1.80	0.63
2:B:511:LEU:HD23	2:B:1426:LEU:HD21	1.79	0.63
2:H:783:THR:HB	2:H:820:GLN:HA	1.80	0.63
2:B:209:ASP:HA	2:B:255:ILE:CG2	2.29	0.63
2:F:365:ALA:O	2:F:369:GLN:HG3	1.98	0.63
2:F:681:ILE:HB	2:F:701:ILE:HG23	1.80	0.63
2:F:1506:ASP:HA	2:F:1536:ILE:HG13	1.80	0.63
2:H:511:LEU:HD23	2:H:1426:LEU:HD21	1.79	0.63
2:B:592:LEU:HD11	2:B:1297:TRP:HH2	1.63	0.63
2:H:551:PRO:HB3	2:H:583:PHE:HZ	1.64	0.63
1:C:200:LEU:HD12	1:C:201:ARG:CA	2.29	0.62
2:D:1347:ILE:HG23	2:D:1403:ILE:HG12	1.80	0.62
2:F:295:PHE:HZ	2:F:387:LEU:HB2	1.63	0.62
2:H:217:PHE:HD2	2:H:1240:PHE:HE1	1.46	0.62
2:D:295:PHE:HZ	2:D:387:LEU:HB2	1.63	0.62
2:F:1032:TYR:HA	2:F:1283:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1553:LYS:HZ1	2:B:1558:LEU:HD22	1.63	0.62
2:F:783:THR:HB	2:F:820:GLN:HA	1.80	0.62
2:D:551:PRO:HB3	2:D:583:PHE:HZ	1.64	0.62
2:D:783:THR:HB	2:D:820:GLN:HA	1.80	0.62
2:F:209:ASP:HA	2:F:255:ILE:CG2	2.29	0.62
1:G:109:PRO:HG2	1:G:112:THR:HA	1.82	0.62
2:H:592:LEU:HD11	2:H:1297:TRP:HH2	1.63	0.62
1:A:109:PRO:HG2	1:A:112:THR:HA	1.82	0.62
2:B:217:PHE:HD2	2:B:1240:PHE:HE1	1.46	0.62
2:H:1032:TYR:HA	2:H:1283:LEU:HD11	1.80	0.62
1:E:109:PRO:HG2	1:E:112:THR:HA	1.82	0.62
2:F:190:ILE:CB	2:F:195:TYR:CB	2.77	0.62
2:B:681:ILE:HB	2:B:701:ILE:HG23	1.80	0.62
2:H:369:GLN:HB2	2:H:370:ARG:NH2	2.15	0.62
1:C:109:PRO:HG2	1:C:112:THR:HA	1.82	0.62
2:D:561:GLY:HA2	2:D:565:PHE:HB3	1.82	0.61
2:F:592:LEU:HD11	2:F:1297:TRP:HH2	1.63	0.61
2:H:209:ASP:HA	2:H:255:ILE:CG2	2.29	0.61
2:H:1347:ILE:HG23	2:H:1403:ILE:HG12	1.80	0.61
2:B:551:PRO:HB3	2:B:583:PHE:HZ	1.64	0.61
1:E:200:LEU:HD12	1:E:201:ARG:CA	2.29	0.61
2:B:369:GLN:HB2	2:B:370:ARG:NH2	2.15	0.61
2:F:369:GLN:HB2	2:F:370:ARG:NH2	2.15	0.61
1:A:83:TRP:CD1	1:A:128:GLN:HG2	2.36	0.61
2:B:561:GLY:HA2	2:B:565:PHE:HB3	1.82	0.61
1:C:83:TRP:CD1	1:C:128:GLN:HG2	2.36	0.61
2:D:369:GLN:HB2	2:D:370:ARG:NH2	2.15	0.61
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.82	0.61
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	1.83	0.61
2:B:1347:ILE:HG23	2:B:1403:ILE:HG12	1.80	0.61
2:D:301:LEU:HD23	2:D:301:LEU:O	2.01	0.61
2:F:301:LEU:HD23	2:F:301:LEU:O	2.01	0.61
1:G:83:TRP:CD1	1:G:128:GLN:HG2	2.36	0.61
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	1.83	0.61
2:F:551:PRO:HB3	2:F:583:PHE:HZ	1.64	0.61
2:F:561:GLY:HA2	2:F:565:PHE:HB3	1.82	0.61
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.82	0.61
2:D:1362:LEU:HD13	2:D:1365:VAL:HG21	1.83	0.60
1:E:83:TRP:CD1	1:E:128:GLN:HG2	2.36	0.60
2:H:1171:LEU:HD11	2:H:1255:ILE:HG23	1.84	0.60
2:B:1171:LEU:HD11	2:B:1255:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:389:GLY:O	2:H:393:THR:HG22	2.02	0.60
2:H:561:GLY:HA2	2:H:565:PHE:HB3	1.82	0.60
2:F:1171:LEU:HD11	2:F:1255:ILE:HG23	1.84	0.60
1:G:200:LEU:HD11	1:G:201:ARG:O	2.02	0.60
2:D:1171:LEU:HD11	2:D:1255:ILE:HG23	1.84	0.60
2:F:699:ILE:HG23	2:F:908:ILE:HD11	1.82	0.60
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	1.83	0.60
2:H:295:PHE:HZ	2:H:387:LEU:HB2	1.63	0.60
2:H:301:LEU:HD23	2:H:301:LEU:O	2.01	0.60
2:B:301:LEU:HD23	2:B:301:LEU:O	2.01	0.60
3:C:401:ADP:H5'2	1:E:333:PHE:CD2	2.37	0.60
2:D:312:LEU:HB2	2:D:369:GLN:HG2	1.84	0.60
2:D:389:GLY:O	2:D:393:THR:HG22	2.02	0.60
3:E:401:ADP:H5'2	1:G:333:PHE:CD2	2.37	0.60
2:F:190:ILE:HB	2:F:195:TYR:CB	2.32	0.60
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	1.83	0.60
1:A:200:LEU:HD11	1:A:201:ARG:O	2.02	0.60
2:B:190:ILE:HB	2:B:195:TYR:CB	2.32	0.60
2:D:190:ILE:HB	2:D:195:TYR:CB	2.32	0.60
2:D:216:ARG:CB	2:D:251:GLY:N	2.65	0.60
1:G:200:LEU:HD12	1:G:201:ARG:CA	2.29	0.60
2:H:190:ILE:HB	2:H:195:TYR:CB	2.32	0.60
2:H:1362:LEU:HD13	2:H:1365:VAL:HG21	1.83	0.60
2:B:295:PHE:HZ	2:B:387:LEU:HB2	1.63	0.59
2:B:785:GLU:HB3	2:B:794:PHE:HZ	1.67	0.59
2:B:1553:LYS:HE3	2:B:1558:LEU:HB2	1.83	0.59
2:F:1362:LEU:HD13	2:F:1365:VAL:HG21	1.83	0.59
2:F:389:GLY:O	2:F:393:THR:HG22	2.02	0.59
2:H:785:GLU:HB3	2:H:794:PHE:HZ	1.67	0.59
2:H:216:ARG:CB	2:H:251:GLY:N	2.65	0.59
2:D:785:GLU:HB3	2:D:794:PHE:HZ	1.67	0.59
1:E:200:LEU:HD12	1:E:201:ARG:O	2.02	0.59
2:F:312:LEU:HB2	2:F:369:GLN:HG2	1.84	0.59
2:F:785:GLU:HB3	2:F:794:PHE:HZ	1.67	0.59
1:C:200:LEU:HD11	1:C:201:ARG:O	2.02	0.59
2:B:699:ILE:HG23	2:B:908:ILE:HD11	1.82	0.59
2:D:1377:ILE:HB	2:D:1536:ILE:HG23	1.85	0.59
2:D:1553:LYS:HE3	2:D:1558:LEU:HB2	1.83	0.59
3:A:401:ADP:H5'2	1:C:333:PHE:CD2	2.37	0.59
2:B:389:GLY:O	2:B:393:THR:HG22	2.02	0.59
1:E:200:LEU:HD11	1:E:201:ARG:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CD2	3:G:401:ADP:H5'2	2.37	0.59
2:B:216:ARG:CB	2:B:251:GLY:N	2.65	0.59
2:D:75:TRP:CZ3	2:D:225:LEU:CB	2.85	0.59
2:F:216:ARG:CB	2:F:251:GLY:N	2.65	0.59
2:H:1553:LYS:HE3	2:H:1558:LEU:HB2	1.83	0.59
1:A:200:LEU:HD12	1:A:201:ARG:O	2.02	0.59
2:B:1362:LEU:HD13	2:B:1365:VAL:HG21	1.83	0.59
1:C:200:LEU:HD12	1:C:201:ARG:O	2.02	0.59
2:H:312:LEU:HB2	2:H:369:GLN:HG2	1.84	0.59
2:B:75:TRP:CZ3	2:B:225:LEU:CB	2.85	0.58
2:F:75:TRP:CZ3	2:F:225:LEU:CB	2.85	0.58
2:B:312:LEU:HB2	2:B:369:GLN:HG2	1.84	0.58
1:A:312:GLY:O	1:A:313:GLN:NE2	2.37	0.58
2:B:686:PHE:H	2:B:696:LEU:HB3	1.69	0.58
1:G:209:MET:HB2	1:G:292:GLU:OE2	2.04	0.58
2:H:545:PHE:HB2	2:H:1080:LEU:HD13	1.86	0.58
2:H:1377:ILE:HB	2:H:1536:ILE:HG23	1.85	0.58
1:A:169:MET:HE3	1:C:168:PHE:CE1	2.39	0.58
2:B:1377:ILE:HB	2:B:1536:ILE:HG23	1.85	0.58
2:D:366:LEU:O	2:D:370:ARG:HG2	2.04	0.58
1:E:312:GLY:O	1:E:313:GLN:NE2	2.37	0.58
2:F:1553:LYS:HE3	2:F:1558:LEU:HB2	1.83	0.58
1:C:169:MET:HE3	1:E:168:PHE:CE1	2.39	0.58
2:H:75:TRP:CZ3	2:H:225:LEU:CB	2.85	0.58
1:C:209:MET:HB2	1:C:292:GLU:OE2	2.04	0.58
2:F:686:PHE:H	2:F:696:LEU:HB3	1.69	0.58
2:F:1344:LYS:HB2	2:F:1371:PRO:HG3	1.85	0.58
2:F:1377:ILE:HB	2:F:1536:ILE:HG23	1.85	0.58
2:H:686:PHE:H	2:H:696:LEU:HB3	1.69	0.58
1:A:48:ASN:O	1:C:330:TYR:HB2	2.04	0.58
1:C:312:GLY:O	1:C:313:GLN:NE2	2.37	0.58
2:H:366:LEU:O	2:H:370:ARG:HG2	2.04	0.58
1:G:200:LEU:HD12	1:G:201:ARG:O	2.02	0.57
2:D:686:PHE:H	2:D:696:LEU:HB3	1.69	0.57
1:G:312:GLY:O	1:G:313:GLN:NE2	2.37	0.57
1:A:168:PHE:CE1	1:G:169:MET:HE3	2.39	0.57
1:G:352:ASP:O	1:G:356:LEU:N	2.38	0.57
2:B:209:ASP:CA	2:B:255:ILE:CG2	2.82	0.57
1:C:48:ASN:O	1:E:330:TYR:HB2	2.04	0.57
1:E:209:MET:HB2	1:E:292:GLU:OE2	2.04	0.57
2:B:377:TYR:HB3	2:B:1246:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.87	0.57
2:B:1344:LYS:HB2	2:B:1371:PRO:HG3	1.85	0.57
1:E:214:THR:HA	1:E:248:GLY:HA2	1.87	0.57
2:F:366:LEU:O	2:F:370:ARG:HG2	2.04	0.57
1:G:34:ARG:NE	1:G:305:LEU:HD11	2.20	0.57
2:H:681:ILE:HD11	2:H:726:THR:HG22	1.87	0.57
1:A:209:MET:HB2	1:A:292:GLU:OE2	2.04	0.57
1:C:352:ASP:O	1:C:356:LEU:N	2.38	0.57
1:E:34:ARG:NE	1:E:305:LEU:HD11	2.20	0.57
1:G:214:THR:HA	1:G:248:GLY:HA2	1.87	0.57
1:A:352:ASP:O	1:A:356:LEU:N	2.38	0.57
2:D:545:PHE:HB2	2:D:1080:LEU:HD13	1.86	0.57
2:B:366:LEU:O	2:B:370:ARG:HG2	2.04	0.57
2:B:545:PHE:HB2	2:B:1080:LEU:HD13	1.86	0.57
2:D:681:ILE:HD11	2:D:726:THR:HG22	1.87	0.57
2:F:1385:LYS:HB2	2:F:1536:ILE:HG21	1.86	0.57
1:A:330:TYR:HB2	1:G:48:ASN:O	2.04	0.57
2:F:545:PHE:HB2	2:F:1080:LEU:HD13	1.86	0.57
2:D:209:ASP:CA	2:D:255:ILE:CG2	2.82	0.57
2:H:209:ASP:CA	2:H:255:ILE:CG2	2.82	0.57
2:H:1344:LYS:HB2	2:H:1371:PRO:HG3	1.85	0.56
1:C:34:ARG:NE	1:C:305:LEU:HD11	2.20	0.56
1:E:48:ASN:O	1:G:330:TYR:HB2	2.04	0.56
2:F:681:ILE:HD11	2:F:726:THR:HG22	1.87	0.56
1:A:34:ARG:NE	1:A:305:LEU:HD11	2.20	0.56
2:B:466:VAL:HG13	2:B:550:ILE:HG22	1.87	0.56
2:B:1385:LYS:HB2	2:B:1536:ILE:HG21	1.86	0.56
1:C:214:THR:HA	1:C:248:GLY:HA2	1.87	0.56
2:D:1344:LYS:HB2	2:D:1371:PRO:HG3	1.85	0.56
1:E:352:ASP:O	1:E:356:LEU:N	2.38	0.56
2:F:209:ASP:CA	2:F:255:ILE:CG2	2.82	0.56
2:F:377:TYR:HB3	2:F:1246:ARG:HE	1.70	0.56
2:D:466:VAL:HG13	2:D:550:ILE:HG22	1.87	0.56
2:D:1475:ILE:HD12	2:D:1482:PHE:HE2	1.71	0.56
1:E:122:LEU:HD22	1:E:136:ARG:HH12	1.71	0.56
2:B:1475:ILE:HD12	2:B:1482:PHE:HE2	1.71	0.56
2:D:377:TYR:HB3	2:D:1246:ARG:HE	1.70	0.56
1:E:169:MET:HE3	1:G:168:PHE:CE1	2.39	0.56
1:G:139:THR:HG23	1:G:141:GLU:H	1.70	0.56
2:H:377:TYR:HB3	2:H:1246:ARG:HE	1.70	0.56
1:C:122:LEU:HD22	1:C:136:ARG:HH12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1475:ILE:HD12	2:H:1482:PHE:HE2	1.71	0.56
2:B:209:ASP:CA	2:B:255:ILE:HG21	2.35	0.56
1:C:139:THR:HG23	1:C:141:GLU:H	1.70	0.56
2:D:1385:LYS:HB2	2:D:1536:ILE:HG21	1.86	0.56
1:G:122:LEU:HD22	1:G:136:ARG:HH12	1.71	0.56
1:A:214:THR:HA	1:A:248:GLY:HA2	1.87	0.56
2:H:1528:PHE:HD1	2:H:1531:ARG:HD2	1.71	0.56
1:A:122:LEU:HD22	1:A:136:ARG:HH12	1.71	0.56
2:B:1528:PHE:HD1	2:B:1531:ARG:HD2	1.71	0.56
1:E:139:THR:HG23	1:E:141:GLU:H	1.70	0.56
2:F:466:VAL:HG13	2:F:550:ILE:HG22	1.87	0.56
1:A:139:THR:HG23	1:A:141:GLU:H	1.70	0.55
2:B:686:PHE:HD1	2:B:733:VAL:HG23	1.71	0.55
2:B:1540:VAL:HG11	2:B:1579:ARG:HA	1.88	0.55
1:C:200:LEU:HD12	1:C:201:ARG:C	2.32	0.55
2:D:1540:VAL:HG11	2:D:1579:ARG:HA	1.88	0.55
2:H:209:ASP:CA	2:H:255:ILE:HG21	2.35	0.55
2:H:466:VAL:HG13	2:H:550:ILE:HG22	1.87	0.55
2:H:1385:LYS:HB2	2:H:1536:ILE:HG21	1.86	0.55
1:A:331:SER:OG	1:G:48:ASN:ND2	2.39	0.55
2:B:1086:VAL:HG11	2:B:1141:GLU:HB2	1.89	0.55
1:C:63:LEU:HA	1:C:66:LEU:HG	1.89	0.55
2:D:209:ASP:CA	2:D:255:ILE:HG21	2.35	0.55
2:F:1475:ILE:HD12	2:F:1482:PHE:HE2	1.71	0.55
2:H:1455:LEU:HD13	2:H:1464:VAL:HG21	1.88	0.55
1:A:48:ASN:ND2	1:C:331:SER:OG	2.39	0.55
2:D:686:PHE:HD1	2:D:733:VAL:HG23	1.71	0.55
2:D:1455:LEU:HD13	2:D:1464:VAL:HG21	1.88	0.55
2:D:1086:VAL:HG11	2:D:1141:GLU:HB2	1.89	0.55
2:F:209:ASP:CA	2:F:255:ILE:HG21	2.35	0.55
1:G:200:LEU:HD12	1:G:201:ARG:C	2.32	0.55
1:A:333:PHE:HD2	3:G:401:ADP:H5'2	1.72	0.55
1:E:48:ASN:ND2	1:G:331:SER:OG	2.39	0.55
2:H:686:PHE:HD1	2:H:733:VAL:HG23	1.71	0.55
1:A:200:LEU:HD12	1:A:201:ARG:C	2.32	0.55
2:B:1353:ARG:HE	2:B:1398:MET:HE3	1.71	0.55
1:E:63:LEU:HA	1:E:66:LEU:HG	1.89	0.55
2:F:1086:VAL:HG11	2:F:1141:GLU:HB2	1.89	0.55
2:F:1455:LEU:HD13	2:F:1464:VAL:HG21	1.88	0.55
2:B:363:PHE:HB2	2:B:1261:LEU:HD13	1.90	0.54
1:C:48:ASN:ND2	1:E:331:SER:OG	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1353:ARG:HE	2:F:1398:MET:HE3	1.71	0.54
1:A:63:LEU:HA	1:A:66:LEU:HG	1.89	0.54
2:B:1455:LEU:HD13	2:B:1464:VAL:HG21	1.88	0.54
2:D:1353:ARG:HE	2:D:1398:MET:HE3	1.71	0.54
2:H:1086:VAL:HG11	2:H:1141:GLU:HB2	1.89	0.54
2:H:1226:LYS:HG2	2:H:1230:TYR:HE1	1.73	0.54
2:B:1226:LYS:HG2	2:B:1230:TYR:HE1	1.73	0.54
3:C:401:ADP:H5'2	1:E:333:PHE:HD2	1.72	0.54
2:D:526:ARG:HE	2:D:1098:HIS:CG	2.25	0.54
2:F:686:PHE:HD1	2:F:733:VAL:HG23	1.71	0.54
2:F:1562:LYS:HB3	2:F:1565:THR:HB	1.89	0.54
2:H:363:PHE:HB2	2:H:1261:LEU:HD13	1.90	0.54
1:E:200:LEU:HD12	1:E:201:ARG:C	2.32	0.54
2:F:1528:PHE:HD1	2:F:1531:ARG:HD2	1.71	0.54
2:B:1311:ALA:O	2:B:1314:ARG:HG2	2.08	0.54
1:C:39:LYS:HE2	1:C:41:ASN:HB2	1.89	0.54
2:D:1528:PHE:HD1	2:D:1531:ARG:HD2	1.71	0.54
2:D:1562:LYS:HB3	2:D:1565:THR:HB	1.89	0.54
2:F:526:ARG:HE	2:F:1098:HIS:CG	2.25	0.54
2:F:366:LEU:HD23	2:F:1260:VAL:HG11	1.89	0.54
2:H:1353:ARG:HE	2:H:1398:MET:HE3	1.71	0.54
2:B:719:LYS:HB3	2:B:887:VAL:HG11	1.90	0.54
2:F:719:LYS:HB3	2:F:887:VAL:HG11	1.90	0.54
2:F:791:GLU:HB3	2:F:1219:TYR:HE2	1.73	0.54
2:H:1562:LYS:HB3	2:H:1565:THR:HB	1.89	0.54
2:D:363:PHE:HB2	2:D:1261:LEU:HD13	1.90	0.54
2:D:366:LEU:HD23	2:D:1260:VAL:HG11	1.89	0.54
1:E:169:MET:HB2	1:G:168:PHE:HE1	1.73	0.54
2:F:209:ASP:HA	2:F:255:ILE:HG21	1.90	0.54
1:G:63:LEU:HA	1:G:66:LEU:HG	1.89	0.54
2:B:366:LEU:HD23	2:B:1260:VAL:HG11	1.89	0.54
2:F:1540:VAL:HG11	2:F:1579:ARG:HA	1.88	0.54
2:H:1540:VAL:HG11	2:H:1579:ARG:HA	1.88	0.54
2:B:442:PRO:O	2:B:445:ILE:HG13	2.08	0.53
2:B:526:ARG:HE	2:B:1098:HIS:CG	2.25	0.53
2:F:1311:ALA:O	2:F:1314:ARG:HG2	2.08	0.53
1:A:169:MET:HB2	1:C:168:PHE:HE1	1.73	0.53
1:C:169:MET:HB2	1:E:168:PHE:HE1	1.73	0.53
1:G:39:LYS:HE2	1:G:41:ASN:HB2	1.89	0.53
2:H:366:LEU:HD23	2:H:1260:VAL:HG11	1.89	0.53
1:A:168:PHE:HE1	1:G:169:MET:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1226:LYS:HG2	2:D:1230:TYR:HE1	1.73	0.53
2:F:363:PHE:HB2	2:F:1261:LEU:HD13	1.90	0.53
2:H:562:HIS:CD2	2:H:571:LEU:HD23	2.44	0.53
2:F:1226:LYS:HG2	2:F:1230:TYR:HE1	1.73	0.53
2:H:526:ARG:HE	2:H:1098:HIS:CG	2.25	0.53
2:H:1311:ALA:O	2:H:1314:ARG:HG2	2.08	0.53
2:H:1386:SER:OG	3:H:2502:ADP:O2B	2.26	0.53
2:B:209:ASP:HA	2:B:255:ILE:HG21	1.90	0.53
2:B:517:ILE:HD11	2:B:1443:GLU:HG2	1.91	0.53
2:D:791:GLU:HB3	2:D:1219:TYR:HE2	1.73	0.53
2:D:1311:ALA:O	2:D:1314:ARG:HG2	2.08	0.53
2:F:827:GLY:O	2:F:835:ARG:NH2	2.42	0.53
1:A:334:GLY:HA2	3:G:401:ADP:O1A	2.07	0.53
3:A:401:ADP:H5'2	1:C:333:PHE:HD2	1.72	0.53
2:B:1562:LYS:HB3	2:B:1565:THR:HB	1.89	0.53
2:F:217:PHE:CD2	2:F:1240:PHE:HE1	2.26	0.53
2:F:442:PRO:O	2:F:445:ILE:HG13	2.08	0.53
2:H:827:GLY:O	2:H:835:ARG:NH2	2.42	0.53
2:B:562:HIS:CD2	2:B:571:LEU:HD23	2.44	0.53
2:H:209:ASP:HA	2:H:255:ILE:HG21	1.90	0.53
2:H:791:GLU:HB3	2:H:1219:TYR:HE2	1.73	0.53
2:D:209:ASP:HA	2:D:255:ILE:HG21	1.90	0.53
2:D:517:ILE:HD11	2:D:1443:GLU:HG2	1.91	0.53
1:C:198:PHE:CE1	1:C:200:LEU:HB2	2.44	0.53
2:D:442:PRO:O	2:D:445:ILE:HG13	2.08	0.53
2:D:719:LYS:HB3	2:D:887:VAL:HG11	1.90	0.53
2:D:1124:ARG:NH1	2:D:1314:ARG:HD3	2.22	0.53
1:A:39:LYS:HE2	1:A:41:ASN:HB2	1.89	0.53
3:A:401:ADP:O1A	1:C:334:GLY:HA2	2.07	0.53
2:B:827:GLY:O	2:B:835:ARG:NH2	2.42	0.53
2:B:1393:PHE:CZ	2:B:1422:LEU:HB2	2.44	0.53
1:E:39:LYS:HE2	1:E:41:ASN:HB2	1.89	0.53
2:B:791:GLU:HB3	2:B:1219:TYR:HE2	1.73	0.52
2:D:1386:SER:OG	3:D:2502:ADP:O2B	2.26	0.52
3:E:401:ADP:H5'2	1:G:333:PHE:HD2	1.72	0.52
2:F:517:ILE:HD11	2:F:1443:GLU:HG2	1.91	0.52
2:H:442:PRO:O	2:H:445:ILE:HG13	2.08	0.52
2:H:719:LYS:HB3	2:H:887:VAL:HG11	1.90	0.52
2:B:559:PHE:O	2:B:563:VAL:HG22	2.10	0.52
1:C:132:GLY:HA3	1:E:131:ILE:O	2.09	0.52
2:F:1393:PHE:CZ	2:F:1422:LEU:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:517:ILE:HD11	2:H:1443:GLU:HG2	1.91	0.52
2:B:1386:SER:OG	3:B:2502:ADP:O2B	2.26	0.52
2:D:217:PHE:CD2	2:D:1240:PHE:HE1	2.26	0.52
2:D:562:HIS:CD2	2:D:571:LEU:HD23	2.44	0.52
1:E:198:PHE:CE1	1:E:200:LEU:HB2	2.44	0.52
2:H:559:PHE:O	2:H:563:VAL:HG22	2.10	0.52
1:A:131:ILE:O	1:G:132:GLY:HA3	2.09	0.52
1:E:132:GLY:HA3	1:G:131:ILE:O	2.09	0.52
1:E:190:THR:HG22	1:E:191:LEU:H	1.75	0.52
2:F:562:HIS:CD2	2:F:571:LEU:HD23	2.44	0.52
2:H:1393:PHE:CZ	2:H:1422:LEU:HB2	2.44	0.52
2:H:1528:PHE:CD1	2:H:1531:ARG:HD2	2.45	0.52
2:D:769:PRO:O	2:D:848:THR:OG1	2.26	0.52
2:H:217:PHE:CD2	2:H:1240:PHE:HE1	2.26	0.52
2:H:779:LEU:HD11	2:H:835:ARG:HG2	1.92	0.52
2:B:1528:PHE:CD1	2:B:1531:ARG:HD2	2.45	0.52
2:F:559:PHE:O	2:F:563:VAL:HG22	2.10	0.52
1:G:190:THR:HG22	1:G:191:LEU:H	1.75	0.52
2:B:143:TRP:HB3	2:B:183:LEU:HG	1.92	0.52
3:C:401:ADP:O1A	1:E:334:GLY:HA2	2.07	0.52
2:D:779:LEU:HD11	2:D:835:ARG:HG2	1.92	0.52
1:G:198:PHE:CE1	1:G:200:LEU:HB2	2.44	0.52
2:D:1393:PHE:CZ	2:D:1422:LEU:HB2	2.44	0.52
2:H:687:THR:HB	2:H:694:PRO:HA	1.92	0.52
1:A:190:THR:HG22	1:A:191:LEU:H	1.75	0.52
2:F:1528:PHE:CD1	2:F:1531:ARG:HD2	2.45	0.52
1:A:198:PHE:CE1	1:A:200:LEU:HB2	2.44	0.51
2:B:679:VAL:HB	2:B:703:ILE:HD12	1.93	0.51
2:F:679:VAL:HB	2:F:703:ILE:HD12	1.93	0.51
2:F:1124:ARG:NH1	2:F:1314:ARG:HD3	2.22	0.51
2:B:779:LEU:HD11	2:B:835:ARG:HG2	1.92	0.51
2:B:1124:ARG:NH1	2:B:1314:ARG:HD3	2.22	0.51
2:D:827:GLY:O	2:D:835:ARG:NH2	2.42	0.51
2:H:423:ILE:O	2:H:427:GLN:HG2	2.11	0.51
1:A:132:GLY:HA3	1:C:131:ILE:O	2.09	0.51
2:D:308:LEU:O	2:D:311:LEU:HG	2.11	0.51
2:F:779:LEU:HD11	2:F:835:ARG:HG2	1.92	0.51
2:F:1455:LEU:HD22	2:F:1460:LEU:HD23	1.92	0.51
2:H:1455:LEU:HD22	2:H:1460:LEU:HD23	1.92	0.51
2:D:423:ILE:O	2:D:427:GLN:HG2	2.11	0.51
2:H:308:LEU:O	2:H:311:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:679:VAL:HB	2:H:703:ILE:HD12	1.93	0.51
2:B:217:PHE:CD2	2:B:1240:PHE:HE1	2.26	0.51
2:F:687:THR:HB	2:F:694:PRO:HA	1.92	0.51
2:F:768:GLY:O	2:F:1218:ARG:NH2	2.44	0.51
1:C:72:LEU:O	1:C:76:THR:HG22	2.11	0.51
3:E:401:ADP:O1A	1:G:334:GLY:HA2	2.07	0.51
2:F:143:TRP:HB3	2:F:183:LEU:HG	1.92	0.51
2:H:295:PHE:CE1	2:H:387:LEU:HB2	2.46	0.51
2:H:686:PHE:HB2	2:H:732:LYS:HA	1.93	0.51
1:C:190:THR:HG22	1:C:191:LEU:H	1.75	0.51
2:H:686:PHE:CD1	2:H:733:VAL:HG23	2.46	0.51
1:A:175:HIS:O	1:A:178:ALA:N	2.44	0.51
1:C:175:HIS:O	1:C:178:ALA:N	2.44	0.51
2:D:679:VAL:HB	2:D:703:ILE:HD12	1.93	0.51
2:F:847:GLN:HA	2:F:882:ARG:HH12	1.76	0.51
1:G:90:TRP:HZ3	1:G:152:GLN:HE21	1.59	0.51
2:H:143:TRP:HB3	2:H:183:LEU:HG	1.92	0.51
2:H:1124:ARG:NH1	2:H:1314:ARG:HD3	2.22	0.51
1:A:96:ALA:HB2	2:B:27:PHE:HE1	1.76	0.51
2:B:768:GLY:O	2:B:1218:ARG:NH2	2.44	0.51
2:D:559:PHE:O	2:D:563:VAL:HG22	2.10	0.51
2:D:687:THR:HB	2:D:694:PRO:HA	1.92	0.51
2:D:768:GLY:O	2:D:1218:ARG:NH2	2.44	0.51
2:D:1528:PHE:CD1	2:D:1531:ARG:HD2	2.45	0.51
1:G:175:HIS:O	1:G:178:ALA:N	2.44	0.51
1:A:52:GLN:O	1:A:52:GLN:HG3	2.11	0.51
1:A:200:LEU:CD2	1:A:304:TYR:CZ	2.94	0.51
1:C:52:GLN:O	1:C:52:GLN:HG3	2.11	0.51
1:E:175:HIS:O	1:E:178:ALA:N	2.44	0.51
2:B:686:PHE:CD1	2:B:733:VAL:HG23	2.46	0.50
2:F:76:ILE:O	2:F:80:ILE:HG13	2.11	0.50
2:F:308:LEU:O	2:F:311:LEU:HG	2.11	0.50
2:F:686:PHE:HB2	2:F:732:LYS:HA	1.93	0.50
1:G:52:GLN:HG3	1:G:52:GLN:O	2.11	0.50
2:D:686:PHE:CD1	2:D:733:VAL:HG23	2.46	0.50
2:H:76:ILE:O	2:H:80:ILE:HG13	2.11	0.50
2:H:769:PRO:O	2:H:848:THR:OG1	2.26	0.50
1:A:72:LEU:O	1:A:76:THR:HG22	2.11	0.50
2:B:769:PRO:O	2:B:848:THR:OG1	2.26	0.50
1:C:96:ALA:HB2	2:D:27:PHE:HE1	1.76	0.50
2:D:76:ILE:O	2:D:80:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:GLN:HG3	1:E:52:GLN:O	2.11	0.50
1:E:72:LEU:O	1:E:76:THR:HG22	2.11	0.50
1:E:90:TRP:HZ3	1:E:152:GLN:HE21	1.59	0.50
2:H:768:GLY:O	2:H:1218:ARG:NH2	2.44	0.50
2:H:798:ARG:NH2	2:H:847:GLN:OE1	2.45	0.50
2:D:847:GLN:HA	2:D:882:ARG:HH12	1.76	0.50
1:G:72:LEU:O	1:G:76:THR:HG22	2.11	0.50
2:B:196:ILE:C	2:B:197:PHE:O	2.55	0.50
2:B:308:LEU:O	2:B:311:LEU:HG	2.11	0.50
2:B:686:PHE:HB2	2:B:732:LYS:HA	1.93	0.50
2:D:143:TRP:HB3	2:D:183:LEU:HG	1.92	0.50
2:D:402:LEU:O	2:D:1215:ARG:NH1	2.45	0.50
2:D:864:LEU:HD11	2:D:1381:THR:HG21	1.94	0.50
2:F:295:PHE:CE1	2:F:387:LEU:HB2	2.46	0.50
2:H:196:ILE:C	2:H:197:PHE:O	2.55	0.50
2:H:255:ILE:HG13	2:H:256:ALA:N	2.27	0.50
2:B:402:LEU:O	2:B:1215:ARG:NH1	2.45	0.50
2:B:423:ILE:O	2:B:427:GLN:HG2	2.11	0.50
2:B:798:ARG:NH2	2:B:847:GLN:OE1	2.45	0.50
2:B:847:GLN:HA	2:B:882:ARG:HH12	1.76	0.50
2:F:423:ILE:O	2:F:427:GLN:HG2	2.11	0.50
1:A:90:TRP:HZ3	1:A:152:GLN:HE21	1.59	0.50
2:B:216:ARG:CB	2:B:251:GLY:HA3	2.42	0.50
2:B:216:ARG:CB	2:B:251:GLY:CA	2.90	0.50
1:C:200:LEU:CD2	1:C:304:TYR:CZ	2.94	0.50
2:D:1004:TYR:HE1	2:D:1093:VAL:HG11	1.77	0.50
2:D:1455:LEU:HD22	2:D:1460:LEU:HD23	1.92	0.50
2:F:216:ARG:CB	2:F:251:GLY:HA3	2.42	0.50
2:F:1004:TYR:HE1	2:F:1093:VAL:HG11	1.77	0.50
1:A:44:VAL:HG22	1:C:326:TYR:HB2	1.94	0.50
2:B:508:LEU:HD13	2:B:1430:VAL:HG12	1.94	0.50
2:B:687:THR:HB	2:B:694:PRO:HA	1.92	0.50
2:D:216:ARG:CB	2:D:251:GLY:CA	2.90	0.50
2:D:1347:ILE:HG21	2:D:1350:LEU:HD22	1.93	0.50
2:F:769:PRO:O	2:F:848:THR:OG1	2.26	0.50
2:H:216:ARG:CB	2:H:251:GLY:CA	2.90	0.50
2:H:847:GLN:HA	2:H:882:ARG:HH12	1.76	0.50
1:A:243:GLY:HA3	1:G:237:ASP:HB3	1.94	0.50
1:A:326:TYR:HB2	1:G:44:VAL:HG22	1.94	0.50
2:B:301:LEU:C	2:B:301:LEU:CD2	2.85	0.50
1:E:34:ARG:HE	1:E:305:LEU:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:196:ILE:C	2:F:197:PHE:O	2.55	0.50
2:F:798:ARG:NH2	2:F:847:GLN:OE1	2.45	0.50
1:G:34:ARG:HE	1:G:305:LEU:HD11	1.77	0.50
1:G:200:LEU:CD2	1:G:304:TYR:CZ	2.94	0.50
2:H:508:LEU:HD13	2:H:1430:VAL:HG12	1.94	0.50
2:B:255:ILE:HG13	2:B:256:ALA:N	2.27	0.49
2:B:1455:LEU:HD22	2:B:1460:LEU:HD23	1.92	0.49
2:B:1496:PHE:HA	2:B:1528:PHE:HZ	1.77	0.49
1:C:44:VAL:HG22	1:E:326:TYR:HB2	1.94	0.49
2:D:196:ILE:C	2:D:197:PHE:O	2.55	0.49
2:D:301:LEU:C	2:D:301:LEU:CD2	2.85	0.49
2:F:508:LEU:HD13	2:F:1430:VAL:HG12	1.94	0.49
2:H:131:ASN:OD1	2:H:131:ASN:N	2.43	0.49
2:B:1004:TYR:HE1	2:B:1093:VAL:HG11	1.77	0.49
1:C:90:TRP:HZ3	1:C:152:GLN:HE21	1.59	0.49
2:F:864:LEU:HD11	2:F:1381:THR:HG21	1.94	0.49
2:H:216:ARG:CB	2:H:251:GLY:HA3	2.42	0.49
2:B:76:ILE:O	2:B:80:ILE:HG13	2.11	0.49
2:D:686:PHE:HB2	2:D:732:LYS:HA	1.93	0.49
1:E:200:LEU:CD2	1:E:304:TYR:CZ	2.94	0.49
2:F:1496:PHE:HA	2:F:1528:PHE:HZ	1.77	0.49
2:B:1347:ILE:HG21	2:B:1350:LEU:HD22	1.93	0.49
2:D:1553:LYS:HZ1	2:D:1558:LEU:HD13	1.78	0.49
2:D:1570:LYS:HD3	2:D:1574:PHE:HB2	1.95	0.49
2:F:686:PHE:CD1	2:F:733:VAL:HG23	2.46	0.49
2:F:1347:ILE:HG21	2:F:1350:LEU:HD22	1.93	0.49
2:H:301:LEU:C	2:H:301:LEU:CD2	2.85	0.49
2:H:1353:ARG:HE	2:H:1398:MET:HB3	1.77	0.49
1:A:237:ASP:HB3	1:C:243:GLY:HA3	1.94	0.49
1:C:34:ARG:HE	1:C:305:LEU:HD11	1.77	0.49
1:E:44:VAL:HG22	1:G:326:TYR:HB2	1.94	0.49
2:B:1570:LYS:HD3	2:B:1574:PHE:HB2	1.95	0.49
2:D:216:ARG:CB	2:D:251:GLY:HA3	2.42	0.49
2:D:255:ILE:HG13	2:D:256:ALA:N	2.27	0.49
2:F:255:ILE:HG13	2:F:256:ALA:N	2.27	0.49
1:A:60:PHE:O	1:A:64:VAL:HG13	2.13	0.49
2:B:864:LEU:HD11	2:B:1381:THR:HG21	1.94	0.49
2:B:1182:PHE:CD2	2:B:1248:LEU:HD22	2.48	0.49
2:B:1353:ARG:NE	2:B:1398:MET:HE3	2.28	0.49
1:C:237:ASP:HB3	1:E:243:GLY:HA3	1.94	0.49
2:D:798:ARG:NH2	2:D:847:GLN:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1353:ARG:NE	2:D:1398:MET:HE3	2.28	0.49
1:E:237:ASP:HB3	1:G:243:GLY:HA3	1.94	0.49
2:F:216:ARG:CB	2:F:251:GLY:CA	2.90	0.49
2:H:864:LEU:HD11	2:H:1381:THR:HG21	1.94	0.49
1:C:95:PHE:CD1	1:C:100:LEU:HD23	2.45	0.49
2:D:508:LEU:HD13	2:D:1430:VAL:HG12	1.94	0.49
2:F:1339:TRP:CD2	2:F:1340:PRO:HD2	2.48	0.49
1:G:96:ALA:HB2	2:H:27:PHE:HE1	1.76	0.49
2:B:363:PHE:CD1	2:B:1261:LEU:HB2	2.48	0.49
2:B:1353:ARG:HE	2:B:1398:MET:HB3	1.77	0.49
1:E:96:ALA:HB2	2:F:27:PHE:HE1	1.76	0.49
2:F:363:PHE:CD1	2:F:1261:LEU:HB2	2.48	0.49
2:F:402:LEU:O	2:F:1215:ARG:NH1	2.45	0.49
2:F:1553:LYS:HZ1	2:F:1558:LEU:HD13	1.78	0.49
1:G:60:PHE:O	1:G:64:VAL:HG13	2.13	0.49
2:H:526:ARG:NH1	2:H:529:GLU:OE1	2.46	0.49
2:H:1004:TYR:HE1	2:H:1093:VAL:HG11	1.77	0.49
2:H:1182:PHE:CD2	2:H:1248:LEU:HD22	2.48	0.49
2:B:526:ARG:NH1	2:B:529:GLU:OE1	2.46	0.48
1:E:123:PHE:HD2	1:E:136:ARG:HG3	1.78	0.48
2:F:785:GLU:OE1	2:F:820:GLN:NE2	2.41	0.48
2:F:1570:LYS:HD3	2:F:1574:PHE:HB2	1.95	0.48
1:G:123:PHE:HD2	1:G:136:ARG:HG3	1.78	0.48
1:A:280:ASP:OD1	1:A:280:ASP:N	2.46	0.48
2:B:795:ASN:HB2	2:B:798:ARG:HB3	1.95	0.48
2:B:1339:TRP:CD2	2:B:1340:PRO:HD2	2.48	0.48
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.95	0.48
2:D:526:ARG:NH1	2:D:529:GLU:OE1	2.46	0.48
2:D:795:ASN:HB2	2:D:798:ARG:HB3	1.95	0.48
2:D:1353:ARG:HE	2:D:1398:MET:HB3	1.77	0.48
2:F:253:LEU:HD13	2:F:1236:ILE:HB	1.95	0.48
2:F:301:LEU:C	2:F:301:LEU:CD2	2.85	0.48
1:A:68:TRP:CE2	1:A:170:LYS:HE2	2.48	0.48
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.95	0.48
1:C:290:VAL:HG23	1:C:296:ILE:O	2.13	0.48
2:D:253:LEU:HD13	2:D:1236:ILE:HB	1.95	0.48
2:D:1182:PHE:CD2	2:D:1248:LEU:HD22	2.48	0.48
2:F:449:VAL:HA	2:F:452:LEU:HG	1.96	0.48
2:F:1353:ARG:HE	2:F:1398:MET:HB3	1.77	0.48
1:G:290:VAL:HG23	1:G:296:ILE:O	2.13	0.48
1:G:345:THR:O	1:G:349:LEU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:HD2	1:A:136:ARG:HG3	1.78	0.48
1:A:290:VAL:HG23	1:A:296:ILE:O	2.13	0.48
1:C:60:PHE:O	1:C:64:VAL:HG13	2.13	0.48
1:E:290:VAL:HG23	1:E:296:ILE:O	2.13	0.48
2:F:526:ARG:NH1	2:F:529:GLU:OE1	2.46	0.48
2:F:1353:ARG:NE	2:F:1398:MET:HE3	2.28	0.48
2:H:402:LEU:O	2:H:1215:ARG:NH1	2.45	0.48
2:H:449:VAL:HA	2:H:452:LEU:HG	1.96	0.48
2:H:1347:ILE:HG21	2:H:1350:LEU:HD22	1.93	0.48
2:H:1353:ARG:NE	2:H:1398:MET:HE3	2.28	0.48
2:H:1496:PHE:HA	2:H:1528:PHE:HZ	1.77	0.48
2:D:363:PHE:CD1	2:D:1261:LEU:HB2	2.48	0.48
2:D:581:SER:O	2:D:585:ILE:HG12	2.14	0.48
2:D:711:ILE:HB	2:D:887:VAL:HG13	1.96	0.48
1:E:280:ASP:OD1	1:E:280:ASP:N	2.46	0.48
2:F:1182:PHE:CD2	2:F:1248:LEU:HD22	2.48	0.48
2:F:1461:LYS:HE2	2:F:1465:LYS:HE2	1.95	0.48
2:H:1226:LYS:HG2	2:H:1230:TYR:CE1	2.49	0.48
2:H:1339:TRP:CD2	2:H:1340:PRO:HD2	2.48	0.48
1:A:34:ARG:HE	1:A:305:LEU:HD11	1.77	0.48
2:B:449:VAL:HA	2:B:452:LEU:HG	1.96	0.48
2:D:449:VAL:HA	2:D:452:LEU:HG	1.96	0.48
2:H:1553:LYS:HZ1	2:H:1558:LEU:HD13	1.78	0.48
2:D:1339:TRP:CD2	2:D:1340:PRO:HD2	2.48	0.48
1:G:49:ILE:HG21	1:G:55:PHE:HZ	1.79	0.48
2:H:526:ARG:HE	2:H:1098:HIS:CD2	2.32	0.48
2:B:32:ASN:O	2:B:35:PRO:HD2	2.14	0.48
1:C:68:TRP:CE2	1:C:170:LYS:HE2	2.48	0.48
2:D:526:ARG:HE	2:D:1098:HIS:CD2	2.32	0.48
2:D:1496:PHE:HA	2:D:1528:PHE:HZ	1.77	0.48
1:E:60:PHE:O	1:E:64:VAL:HG13	2.13	0.48
1:G:68:TRP:CE2	1:G:170:LYS:HE2	2.48	0.48
2:H:32:ASN:O	2:H:35:PRO:HD2	2.14	0.48
2:H:363:PHE:CD1	2:H:1261:LEU:HB2	2.48	0.48
2:H:1128:ASP:OD1	2:H:1311:ALA:HB1	2.14	0.48
2:H:1570:LYS:HD3	2:H:1574:PHE:HB2	1.95	0.48
2:B:131:ASN:OD1	2:B:131:ASN:N	2.43	0.48
2:B:1226:LYS:HG2	2:B:1230:TYR:CE1	2.49	0.48
1:C:280:ASP:OD1	1:C:280:ASP:N	2.46	0.48
2:F:581:SER:O	2:F:585:ILE:HG12	2.14	0.48
1:G:280:ASP:OD1	1:G:280:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:488:THR:OG1	2:H:532:SER:HB3	2.14	0.48
2:B:253:LEU:HD13	2:B:1236:ILE:HB	1.95	0.48
2:B:550:ILE:HB	2:B:551:PRO:HD3	1.96	0.48
1:E:68:TRP:CE2	1:E:170:LYS:HE2	2.48	0.48
1:A:198:PHE:HE1	1:A:200:LEU:HB2	1.79	0.47
2:D:32:ASN:O	2:D:35:PRO:HD2	2.14	0.47
2:D:550:ILE:HB	2:D:551:PRO:HD3	1.96	0.47
2:D:1246:ARG:HA	2:D:1246:ARG:HD3	1.65	0.47
2:H:581:SER:O	2:H:585:ILE:HG12	2.14	0.47
2:B:396:TYR:CD1	2:B:1227:LEU:HD13	2.49	0.47
2:D:396:TYR:CD1	2:D:1227:LEU:HD13	2.49	0.47
2:D:1078:LEU:O	2:D:1082:THR:HG23	2.15	0.47
2:F:526:ARG:HE	2:F:1098:HIS:CD2	2.32	0.47
2:F:711:ILE:HB	2:F:887:VAL:HG13	1.96	0.47
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.95	0.47
2:B:869:MET:HE3	2:B:869:MET:HB3	1.77	0.47
1:E:90:TRP:HA	1:E:93:ILE:HG22	1.95	0.47
2:F:550:ILE:HB	2:F:551:PRO:HD3	1.96	0.47
1:G:90:TRP:HA	1:G:93:ILE:HG22	1.95	0.47
2:H:550:ILE:HB	2:H:551:PRO:HD3	1.96	0.47
2:H:553:ALA:O	2:H:557:ILE:HG12	2.15	0.47
2:H:1078:LEU:O	2:H:1082:THR:HG23	2.15	0.47
2:B:526:ARG:HE	2:B:1098:HIS:CD2	2.32	0.47
2:D:295:PHE:CE1	2:D:387:LEU:HB2	2.46	0.47
2:D:488:THR:OG1	2:D:532:SER:HB3	2.14	0.47
2:D:1079:CYS:O	2:D:1082:THR:OG1	2.27	0.47
1:E:169:MET:HE3	1:G:168:PHE:HE1	1.79	0.47
2:H:802:VAL:HG11	2:H:845:TYR:HB2	1.97	0.47
1:A:49:ILE:HG21	1:A:55:PHE:HZ	1.79	0.47
1:A:95:PHE:CD1	1:A:100:LEU:HD23	2.45	0.47
2:B:1078:LEU:O	2:B:1082:THR:HG23	2.15	0.47
2:B:1128:ASP:OD1	2:B:1311:ALA:HB1	2.14	0.47
2:D:553:ALA:O	2:D:557:ILE:HG12	2.15	0.47
2:F:485:GLN:HE22	2:F:598:ARG:HG3	1.79	0.47
2:F:1375:ILE:HB	2:F:1534:VAL:HG22	1.97	0.47
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	1.97	0.47
2:H:253:LEU:HD13	2:H:1236:ILE:HB	1.95	0.47
2:H:396:TYR:CD1	2:H:1227:LEU:HD13	2.49	0.47
2:H:1461:LYS:HE2	2:H:1465:LYS:HE2	1.95	0.47
1:C:49:ILE:HG21	1:C:55:PHE:HZ	1.79	0.47
1:C:189:ILE:HA	1:C:198:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1425:ILE:HD13	2:D:1492:LEU:HD12	1.97	0.47
2:F:795:ASN:HB2	2:F:798:ARG:HB3	1.95	0.47
2:H:370:ARG:HD2	2:H:1253:GLU:CD	2.40	0.47
2:H:795:ASN:HB2	2:H:798:ARG:HB3	1.95	0.47
2:H:1345:ILE:HD11	2:H:1369:ILE:HD12	1.97	0.47
2:B:370:ARG:HD2	2:B:1253:GLU:CD	2.40	0.47
2:B:488:THR:OG1	2:B:532:SER:HB3	2.14	0.47
1:C:123:PHE:HD2	1:C:136:ARG:HG3	1.78	0.47
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.97	0.47
2:F:32:ASN:O	2:F:35:PRO:HD2	2.14	0.47
2:F:592:LEU:HD11	2:F:1297:TRP:CH2	2.48	0.47
2:F:1128:ASP:OD1	2:F:1311:ALA:HB1	2.14	0.47
2:F:1226:LYS:HG2	2:F:1230:TYR:CE1	2.49	0.47
2:F:1345:ILE:HD11	2:F:1369:ILE:HD12	1.97	0.47
2:H:711:ILE:HB	2:H:887:VAL:HG13	1.96	0.47
2:D:370:ARG:HD2	2:D:1253:GLU:CD	2.40	0.47
2:D:785:GLU:OE1	2:D:820:GLN:NE2	2.41	0.47
2:B:581:SER:O	2:B:585:ILE:HG12	2.14	0.47
2:B:853:LEU:HB2	2:B:886:LEU:HG	1.97	0.47
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	1.97	0.47
2:F:370:ARG:HD2	2:F:1253:GLU:CD	2.40	0.47
2:F:396:TYR:OH	2:F:1223:PHE:HB3	2.15	0.47
1:C:169:MET:HE3	1:E:168:PHE:HE1	1.79	0.47
2:D:853:LEU:HB2	2:D:886:LEU:HG	1.97	0.47
2:D:1128:ASP:OD1	2:D:1311:ALA:HB1	2.14	0.47
2:F:388:ARG:HD3	2:F:429:MET:SD	2.55	0.47
2:F:489:LEU:HD11	2:F:602:LYS:HE3	1.97	0.47
2:F:853:LEU:HB2	2:F:886:LEU:HG	1.97	0.47
1:G:92:LEU:HD22	2:H:34:VAL:HG21	1.97	0.47
1:G:189:ILE:HA	1:G:198:PHE:HA	1.96	0.47
1:G:198:PHE:HE1	1:G:200:LEU:HB2	1.79	0.47
2:B:396:TYR:OH	2:B:1223:PHE:HB3	2.15	0.46
2:B:553:ALA:O	2:B:557:ILE:HG12	2.15	0.46
2:B:1503:PHE:HB2	2:B:1533:VAL:HG22	1.97	0.46
1:C:198:PHE:HE1	1:C:200:LEU:HB2	1.79	0.46
2:D:1345:ILE:HD11	2:D:1369:ILE:HD12	1.97	0.46
2:F:488:THR:OG1	2:F:532:SER:HB3	2.14	0.46
2:H:253:LEU:HD12	2:H:253:LEU:HA	1.77	0.46
2:H:1375:ILE:HB	2:H:1534:VAL:HG22	1.97	0.46
2:H:1503:PHE:HB2	2:H:1533:VAL:HG22	1.97	0.46
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.96	0.46
2:D:388:ARG:HD3	2:D:429:MET:SD	2.55	0.46
2:D:1503:PHE:HB2	2:D:1533:VAL:HG22	1.97	0.46
1:E:49:ILE:HG21	1:E:55:PHE:HZ	1.79	0.46
2:H:447:VAL:HA	2:H:450:ILE:HG22	1.98	0.46
2:H:701:ILE:HD11	2:H:703:ILE:HD11	1.98	0.46
2:B:1375:ILE:HB	2:B:1534:VAL:HG22	1.97	0.46
2:D:396:TYR:OH	2:D:1223:PHE:HB3	2.15	0.46
2:D:701:ILE:HD11	2:D:703:ILE:HD11	1.98	0.46
2:D:1260:VAL:HG23	2:D:1288:ALA:HB1	1.98	0.46
2:D:1375:ILE:HB	2:D:1534:VAL:HG22	1.97	0.46
2:H:190:ILE:CD1	2:H:195:TYR:CB	2.94	0.46
2:B:485:GLN:HE22	2:B:598:ARG:HG3	1.79	0.46
2:D:398:LYS:CD	2:D:614:LEU:HA	2.45	0.46
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.95	0.46
1:E:92:LEU:HD22	2:F:34:VAL:HG21	1.97	0.46
2:F:396:TYR:CD1	2:F:1227:LEU:HD13	2.49	0.46
2:F:1490:PHE:O	2:F:1494:ARG:HG3	2.16	0.46
2:H:398:LYS:HE3	2:H:398:LYS:HB3	1.81	0.46
2:H:853:LEU:HB2	2:H:886:LEU:HG	1.97	0.46
2:B:388:ARG:HD3	2:B:429:MET:SD	2.55	0.46
2:B:398:LYS:CD	2:B:614:LEU:HA	2.45	0.46
2:B:802:VAL:HG11	2:B:845:TYR:HB2	1.97	0.46
2:B:1345:ILE:HD11	2:B:1369:ILE:HD12	1.97	0.46
2:H:396:TYR:OH	2:H:1223:PHE:HB3	2.15	0.46
2:H:1352:VAL:HG13	2:H:1361:VAL:HB	1.97	0.46
2:B:190:ILE:CD1	2:B:195:TYR:CB	2.94	0.46
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.98	0.46
2:B:1356:SER:HA	2:B:1398:MET:HE2	1.98	0.46
2:B:1514:MET:HG2	2:B:1539:ARG:NH2	2.31	0.46
2:D:263:TYR:HB2	2:D:393:THR:HG21	1.98	0.46
2:D:802:VAL:HG11	2:D:845:TYR:HB2	1.97	0.46
2:D:1226:LYS:HG2	2:D:1230:TYR:CE1	2.49	0.46
2:D:1352:VAL:HG13	2:D:1361:VAL:HB	1.97	0.46
1:E:189:ILE:HA	1:E:198:PHE:HA	1.96	0.46
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.97	0.46
2:F:398:LYS:CD	2:F:614:LEU:HA	2.45	0.46
2:F:553:ALA:O	2:F:557:ILE:HG12	2.15	0.46
2:F:1260:VAL:HG23	2:F:1288:ALA:HB1	1.98	0.46
2:F:1514:MET:HG2	2:F:1539:ARG:NH2	2.31	0.46
2:H:1356:SER:HA	2:H:1398:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HD13	1:A:215:ILE:HA	1.83	0.46
2:B:1260:VAL:HG23	2:B:1288:ALA:HB1	1.98	0.46
2:B:1490:PHE:O	2:B:1494:ARG:HG3	2.16	0.46
1:E:158:MET:HE1	1:G:75:PHE:HD2	1.81	0.46
2:F:209:ASP:CA	2:F:255:ILE:HG23	2.46	0.46
2:F:701:ILE:HD11	2:F:703:ILE:HD11	1.98	0.46
2:F:1503:PHE:HB2	2:F:1533:VAL:HG22	1.97	0.46
2:H:485:GLN:HE22	2:H:598:ARG:HG3	1.79	0.46
1:A:158:MET:HE1	1:C:75:PHE:HD2	1.81	0.46
2:B:209:ASP:CB	2:B:255:ILE:CG1	2.94	0.46
2:B:785:GLU:OE1	2:B:820:GLN:NE2	2.41	0.46
2:B:1352:VAL:HG13	2:B:1361:VAL:HB	1.97	0.46
2:D:489:LEU:HD11	2:D:602:LYS:HE3	1.97	0.46
1:E:198:PHE:HE1	1:E:200:LEU:HB2	1.79	0.46
2:F:802:VAL:HG11	2:F:845:TYR:HB2	1.97	0.46
2:F:1078:LEU:O	2:F:1082:THR:HG23	2.15	0.46
2:H:489:LEU:HD11	2:H:602:LYS:HE3	1.97	0.46
2:H:1425:ILE:HD13	2:H:1492:LEU:HD12	1.97	0.46
1:A:189:ILE:HA	1:A:198:PHE:HA	1.96	0.46
1:C:158:MET:HE1	1:E:75:PHE:HD2	1.81	0.46
2:D:209:ASP:CA	2:D:255:ILE:HG23	2.46	0.46
2:H:253:LEU:HG	2:H:257:MET:HB3	1.98	0.46
2:B:447:VAL:HA	2:B:450:ILE:HG22	1.98	0.46
2:F:447:VAL:HA	2:F:450:ILE:HG22	1.98	0.46
2:F:511:LEU:HD12	2:F:511:LEU:HA	1.72	0.46
2:F:1356:SER:HA	2:F:1398:MET:HE2	1.98	0.46
2:H:209:ASP:CA	2:H:255:ILE:HG23	2.46	0.46
2:H:388:ARG:HD3	2:H:429:MET:SD	2.55	0.46
2:H:398:LYS:CD	2:H:614:LEU:HA	2.45	0.46
2:H:1353:ARG:NH1	2:H:1400:GLU:OE2	2.45	0.46
2:B:253:LEU:HG	2:B:257:MET:HB3	1.98	0.45
2:D:253:LEU:HG	2:D:257:MET:HB3	1.98	0.45
2:D:485:GLN:HE22	2:D:598:ARG:HG3	1.79	0.45
2:D:1102:LEU:HD23	2:D:1102:LEU:HA	1.76	0.45
2:H:209:ASP:CB	2:H:255:ILE:CG1	2.94	0.45
2:H:1327:GLU:HB3	2:H:1415:LEU:H	1.82	0.45
1:A:75:PHE:HD2	1:G:158:MET:HE1	1.81	0.45
2:D:1514:MET:HG2	2:D:1539:ARG:NH2	2.31	0.45
2:F:263:TYR:HB2	2:F:393:THR:HG21	1.98	0.45
2:F:1352:VAL:HG13	2:F:1361:VAL:HB	1.97	0.45
2:H:1260:VAL:HG23	2:H:1288:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD22	2:B:34:VAL:HG21	1.97	0.45
2:B:312:LEU:CB	2:B:369:GLN:HG2	2.47	0.45
2:B:489:LEU:HD11	2:B:602:LYS:HE3	1.97	0.45
2:B:576:ALA:O	2:B:579:SER:OG	2.34	0.45
1:C:92:LEU:HD22	2:D:34:VAL:HG21	1.97	0.45
2:D:209:ASP:CB	2:D:255:ILE:CG1	2.94	0.45
2:D:447:VAL:HA	2:D:450:ILE:HG22	1.98	0.45
2:D:1490:PHE:O	2:D:1494:ARG:HG3	2.16	0.45
2:F:190:ILE:CD1	2:F:195:TYR:CB	2.94	0.45
2:F:892:GLN:H	2:F:892:GLN:HG3	1.41	0.45
2:H:216:ARG:CB	2:H:251:GLY:H	2.30	0.45
2:H:1490:PHE:O	2:H:1494:ARG:HG3	2.16	0.45
1:A:169:MET:HE3	1:C:168:PHE:HE1	1.79	0.45
2:B:288:TRP:CE3	2:B:607:VAL:HG11	2.52	0.45
2:B:1327:GLU:HB3	2:B:1415:LEU:H	1.82	0.45
1:C:170:LYS:O	1:C:173:GLN:N	2.48	0.45
2:D:1356:SER:HA	2:D:1398:MET:HE2	1.98	0.45
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.97	0.45
2:D:511:LEU:HD12	2:D:511:LEU:HA	1.72	0.45
1:E:196:LEU:CB	1:E:261:ILE:HD11	2.47	0.45
2:F:37:VAL:HG13	2:F:41:PHE:CE2	2.52	0.45
2:H:1030:ILE:HD11	2:H:1068:PHE:CE1	2.52	0.45
2:H:1102:LEU:HD23	2:H:1102:LEU:HA	1.76	0.45
2:H:1514:MET:HG2	2:H:1539:ARG:NH2	2.31	0.45
2:D:37:VAL:HG13	2:D:41:PHE:CE2	2.52	0.45
2:D:190:ILE:CD1	2:D:195:TYR:CB	2.94	0.45
2:D:288:TRP:CE3	2:D:607:VAL:HG11	2.52	0.45
2:D:1327:GLU:HB3	2:D:1415:LEU:H	1.82	0.45
1:E:345:THR:O	1:E:349:LEU:N	2.40	0.45
2:F:1353:ARG:O	2:F:1398:MET:HB2	2.17	0.45
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.52	0.45
2:B:209:ASP:CA	2:B:255:ILE:HG23	2.46	0.45
2:D:398:LYS:HE3	2:D:398:LYS:HB3	1.81	0.45
2:D:540:THR:O	2:D:544:ILE:HG12	2.17	0.45
2:F:216:ARG:CB	2:F:251:GLY:H	2.30	0.45
2:F:253:LEU:HG	2:F:257:MET:HB3	1.98	0.45
2:F:1079:CYS:O	2:F:1082:THR:OG1	2.27	0.45
2:H:785:GLU:OE1	2:H:820:GLN:NE2	2.41	0.45
1:A:158:MET:HE1	1:C:75:PHE:CD2	2.52	0.45
2:D:196:ILE:O	2:D:197:PHE:C	2.60	0.45
2:D:246:ASP:OD1	2:D:247:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:592:LEU:HD21	2:D:1297:TRP:CH2	2.52	0.45
2:F:312:LEU:CB	2:F:369:GLN:HG2	2.47	0.45
2:F:540:THR:O	2:F:544:ILE:HG12	2.17	0.45
2:B:75:TRP:HZ3	2:B:225:LEU:CD2	2.29	0.45
2:B:592:LEU:HD21	2:B:1297:TRP:CH2	2.52	0.45
2:D:312:LEU:CB	2:D:369:GLN:HG2	2.47	0.45
2:F:209:ASP:CB	2:F:255:ILE:CG1	2.94	0.45
2:H:1353:ARG:O	2:H:1398:MET:HB2	2.17	0.45
1:A:116:SER:OG	1:A:117:PHE:N	2.50	0.45
2:B:1020:GLN:HB3	2:B:1148:LEU:HD11	1.99	0.45
2:D:395:ILE:O	2:D:399:ILE:HG13	2.17	0.45
1:E:170:LYS:O	1:E:173:GLN:N	2.48	0.45
1:G:95:PHE:CD1	1:G:100:LEU:HD23	2.45	0.45
2:H:540:THR:O	2:H:544:ILE:HG12	2.17	0.45
2:H:1460:LEU:HD21	2:H:1490:PHE:CE1	2.52	0.45
2:B:37:VAL:HG13	2:B:41:PHE:CE2	2.52	0.44
2:B:1246:ARG:HD3	2:B:1246:ARG:HA	1.65	0.44
1:C:116:SER:OG	1:C:117:PHE:N	2.50	0.44
2:D:853:LEU:HD23	2:D:856:PRO:HG3	1.99	0.44
2:F:219:GLN:HG2	2:F:378:TYR:CZ	2.52	0.44
2:F:288:TRP:CE3	2:F:607:VAL:HG11	2.52	0.44
2:F:395:ILE:O	2:F:399:ILE:HG13	2.17	0.44
2:H:263:TYR:HB2	2:H:393:THR:HG21	1.98	0.44
2:H:592:LEU:HD11	2:H:1297:TRP:CH2	2.48	0.44
2:H:869:MET:HE3	2:H:869:MET:HB3	1.77	0.44
2:B:295:PHE:CE1	2:B:387:LEU:HB2	2.46	0.44
2:B:892:GLN:H	2:B:892:GLN:HG3	1.41	0.44
2:B:1030:ILE:HD11	2:B:1068:PHE:CE1	2.52	0.44
2:D:219:GLN:HG2	2:D:378:TYR:CZ	2.52	0.44
2:D:1020:GLN:HB3	2:D:1148:LEU:HD11	1.99	0.44
2:D:1353:ARG:O	2:D:1398:MET:HB2	2.17	0.44
2:D:1460:LEU:HD21	2:D:1490:PHE:CE1	2.52	0.44
1:E:116:SER:OG	1:E:117:PHE:N	2.50	0.44
2:F:196:ILE:O	2:F:197:PHE:C	2.60	0.44
1:G:116:SER:OG	1:G:117:PHE:N	2.50	0.44
1:G:196:LEU:CB	1:G:261:ILE:HD11	2.47	0.44
2:H:288:TRP:CE3	2:H:607:VAL:HG11	2.52	0.44
2:H:312:LEU:CB	2:H:369:GLN:HG2	2.47	0.44
2:H:395:ILE:O	2:H:399:ILE:HG13	2.17	0.44
2:H:853:LEU:HD23	2:H:856:PRO:HG3	1.99	0.44
2:D:1004:TYR:CE1	2:D:1093:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:592:LEU:HD21	2:F:1297:TRP:CH2	2.52	0.44
2:H:730:MET:HE3	2:H:730:MET:HB3	1.89	0.44
1:A:75:PHE:CD2	1:G:158:MET:HE1	2.52	0.44
2:B:219:GLN:HG2	2:B:378:TYR:CZ	2.52	0.44
2:B:246:ASP:OD1	2:B:247:LEU:N	2.49	0.44
2:B:263:TYR:HB2	2:B:393:THR:HG21	1.98	0.44
2:B:853:LEU:HD23	2:B:856:PRO:HG3	1.99	0.44
2:B:1256:GLY:O	2:B:1260:VAL:HG12	2.18	0.44
2:B:1353:ARG:O	2:B:1398:MET:HB2	2.17	0.44
1:C:158:MET:HE1	1:E:75:PHE:CD2	2.52	0.44
1:C:196:LEU:CB	1:C:261:ILE:HD11	2.47	0.44
2:F:75:TRP:HZ3	2:F:225:LEU:CD2	2.29	0.44
2:F:853:LEU:HD23	2:F:856:PRO:HG3	1.99	0.44
2:F:1460:LEU:HD21	2:F:1490:PHE:CE1	2.52	0.44
2:H:219:GLN:HG2	2:H:378:TYR:CZ	2.52	0.44
2:B:391:ILE:O	2:B:395:ILE:HG23	2.18	0.44
2:D:1030:ILE:HD11	2:D:1068:PHE:CE1	2.52	0.44
2:D:1256:GLY:O	2:D:1260:VAL:HG12	2.18	0.44
2:H:196:ILE:O	2:H:197:PHE:C	2.60	0.44
2:H:246:ASP:OD1	2:H:247:LEU:N	2.49	0.44
2:H:491:HIS:CE1	2:H:528:LYS:HB3	2.53	0.44
2:H:819:ASP:OD1	2:H:820:GLN:N	2.41	0.44
2:H:1004:TYR:CE1	2:H:1093:VAL:HG11	2.52	0.44
2:B:1460:LEU:HD21	2:B:1490:PHE:CE1	2.52	0.44
2:B:1483:SER:O	2:B:1487:ARG:HG3	2.18	0.44
2:D:391:ILE:O	2:D:395:ILE:HG23	2.18	0.44
2:F:40:LEU:O	2:F:44:PHE:HD2	2.01	0.44
2:F:576:ALA:O	2:F:579:SER:OG	2.34	0.44
2:F:1030:ILE:HD11	2:F:1068:PHE:CE1	2.52	0.44
2:F:1256:GLY:O	2:F:1260:VAL:HG12	2.18	0.44
2:F:1369:ILE:HD13	2:F:1375:ILE:HG13	2.00	0.44
2:F:1509:THR:HG21	2:F:1539:ARG:HB2	2.00	0.44
2:H:1431:LEU:HD12	2:H:1487:ARG:HG2	2.00	0.44
1:A:46:HIS:HD2	1:C:330:TYR:OH	2.01	0.44
1:A:56:LEU:HD22	2:B:49:ILE:CG2	2.48	0.44
1:A:68:TRP:N	1:A:69:PRO:HD2	2.33	0.44
1:C:46:HIS:HD2	1:E:330:TYR:OH	2.01	0.44
2:D:1369:ILE:HD13	2:D:1375:ILE:HG13	2.00	0.44
2:D:1479:GLY:O	2:D:1487:ARG:NH1	2.51	0.44
2:D:1509:THR:HG21	2:D:1539:ARG:HB2	2.00	0.44
2:F:684:GLY:O	2:F:698:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HD22	2:H:49:ILE:CG2	2.48	0.44
2:H:40:LEU:O	2:H:44:PHE:HD2	2.01	0.44
2:H:175:LEU:HA	2:H:175:LEU:HD23	1.81	0.44
2:H:684:GLY:O	2:H:698:ASN:N	2.51	0.44
2:H:1256:GLY:O	2:H:1260:VAL:HG12	2.18	0.44
2:B:216:ARG:CB	2:B:251:GLY:H	2.30	0.44
2:B:295:PHE:HZ	2:B:387:LEU:CD1	2.30	0.44
2:B:491:HIS:CE1	2:B:528:LYS:HB3	2.53	0.44
1:C:215:ILE:HD13	1:C:215:ILE:HA	1.83	0.44
2:D:1255:ILE:HD13	2:D:1255:ILE:HA	1.93	0.44
2:F:1105:ILE:HD11	2:F:1318:LEU:HD21	2.00	0.44
2:F:1479:GLY:O	2:F:1487:ARG:NH1	2.51	0.44
1:G:268:TYR:O	1:G:346:ALA:HB3	2.18	0.44
2:H:1479:GLY:O	2:H:1487:ARG:NH1	2.51	0.44
1:A:196:LEU:CB	1:A:261:ILE:HD11	2.47	0.44
1:A:313:GLN:HE22	1:A:338:LYS:HD2	1.83	0.44
2:B:40:LEU:O	2:B:44:PHE:HD2	2.01	0.44
1:C:68:TRP:N	1:C:69:PRO:HD2	2.33	0.44
1:C:313:GLN:HE22	1:C:338:LYS:HD2	1.83	0.44
2:D:40:LEU:O	2:D:44:PHE:HD2	2.01	0.44
2:F:131:ASN:OD1	2:F:131:ASN:N	2.43	0.44
2:F:1192:LEU:HA	2:F:1195:THR:HG22	2.00	0.44
2:F:1483:SER:O	2:F:1487:ARG:HG3	2.18	0.44
2:B:395:ILE:O	2:B:399:ILE:HG13	2.17	0.43
2:B:540:THR:O	2:B:544:ILE:HG12	2.17	0.43
2:B:1004:TYR:CE1	2:B:1093:VAL:HG11	2.52	0.43
2:B:1479:GLY:O	2:B:1487:ARG:NH1	2.51	0.43
1:E:68:TRP:N	1:E:69:PRO:HD2	2.33	0.43
2:F:1386:SER:OG	3:F:2502:ADP:O1A	2.36	0.43
1:G:284:ILE:HA	1:G:302:THR:O	2.18	0.43
2:H:1345:ILE:HG12	2:H:1369:ILE:HB	2.00	0.43
2:D:592:LEU:HD21	2:D:1297:TRP:CZ2	2.54	0.43
2:D:892:GLN:H	2:D:892:GLN:HG3	1.41	0.43
1:E:284:ILE:HA	1:E:302:THR:O	2.18	0.43
2:F:288:TRP:HE3	2:F:607:VAL:HG11	1.83	0.43
2:F:1327:GLU:HB3	2:F:1415:LEU:H	1.82	0.43
2:H:806:CYS:O	2:H:837:ARG:HD2	2.18	0.43
2:H:1105:ILE:HD11	2:H:1318:LEU:HD21	2.00	0.43
1:A:168:PHE:HE1	1:G:169:MET:HE3	1.79	0.43
1:A:330:TYR:OH	1:G:46:HIS:HD2	2.01	0.43
2:B:262:ASN:HB3	2:B:390:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:819:ASP:OD1	2:B:820:GLN:N	2.41	0.43
2:B:1354:TYR:HA	2:B:1396:VAL:HG13	2.00	0.43
1:C:268:TYR:O	1:C:346:ALA:HB3	2.18	0.43
2:D:253:LEU:HA	2:D:253:LEU:HD12	1.77	0.43
2:D:295:PHE:HZ	2:D:387:LEU:CD1	2.30	0.43
2:D:592:LEU:HD11	2:D:1297:TRP:CH2	2.48	0.43
2:D:772:TYR:HD1	2:D:852:PHE:HB2	1.83	0.43
2:D:1483:SER:O	2:D:1487:ARG:HG3	2.18	0.43
1:E:46:HIS:HD2	1:G:330:TYR:OH	2.01	0.43
1:E:268:TYR:O	1:E:346:ALA:HB3	2.18	0.43
2:F:592:LEU:HD21	2:F:1297:TRP:CZ2	2.54	0.43
1:G:68:TRP:N	1:G:69:PRO:HD2	2.33	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CH2	2.52	0.43
2:B:806:CYS:O	2:B:837:ARG:HD2	2.18	0.43
2:B:1105:ILE:HD11	2:B:1318:LEU:HD21	2.00	0.43
2:D:825:GLU:OE1	2:D:825:GLU:N	2.48	0.43
2:D:1105:ILE:HD11	2:D:1318:LEU:HD21	2.00	0.43
1:G:196:LEU:HB2	1:G:261:ILE:HD11	2.01	0.43
2:H:288:TRP:HE3	2:H:607:VAL:HG11	1.83	0.43
2:H:391:ILE:O	2:H:395:ILE:HG23	2.18	0.43
2:H:825:GLU:OE1	2:H:825:GLU:N	2.48	0.43
2:H:1114:GLU:OE1	3:H:2502:ADP:N6	2.52	0.43
1:A:284:ILE:HA	1:A:302:THR:O	2.18	0.43
2:B:1431:LEU:HD12	2:B:1487:ARG:HG2	2.00	0.43
2:D:806:CYS:O	2:D:837:ARG:HD2	2.18	0.43
2:D:1354:TYR:HA	2:D:1396:VAL:HG13	2.00	0.43
1:E:176:ARG:O	1:E:179:GLU:N	2.51	0.43
2:F:491:HIS:CE1	2:F:528:LYS:HB3	2.53	0.43
2:F:1020:GLN:HB3	2:F:1148:LEU:HD11	1.99	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CZ2	2.54	0.43
2:H:892:GLN:H	2:H:892:GLN:HG3	1.41	0.43
1:A:268:TYR:O	1:A:346:ALA:HB3	2.18	0.43
2:B:398:LYS:HE3	2:B:398:LYS:HB3	1.81	0.43
1:C:196:LEU:HB2	1:C:261:ILE:HD11	2.01	0.43
2:D:216:ARG:CB	2:D:251:GLY:H	2.30	0.43
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.19	0.43
2:D:262:ASN:HB3	2:D:390:ALA:HB2	2.00	0.43
1:E:56:LEU:HD22	2:F:49:ILE:CG2	2.48	0.43
2:F:551:PRO:CB	2:F:583:PHE:HZ	2.30	0.43
1:G:313:GLN:HE22	1:G:338:LYS:HD2	1.83	0.43
2:H:295:PHE:HZ	2:H:387:LEU:CD1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:586:LEU:O	2:H:589:PRO:HD2	2.19	0.43
2:H:1020:GLN:HB3	2:H:1148:LEU:HD11	1.99	0.43
2:H:1192:LEU:HA	2:H:1195:THR:HG22	2.00	0.43
1:A:95:PHE:HE2	2:B:27:PHE:HB2	1.84	0.43
2:B:263:TYR:HB2	2:B:393:THR:CG2	2.49	0.43
2:B:592:LEU:HD21	2:B:1297:TRP:CZ2	2.54	0.43
1:C:49:ILE:HG21	1:C:55:PHE:CZ	2.54	0.43
1:C:56:LEU:HD22	2:D:49:ILE:CG2	2.48	0.43
2:D:491:HIS:CE1	2:D:528:LYS:HB3	2.53	0.43
2:D:684:GLY:O	2:D:698:ASN:N	2.51	0.43
2:D:1431:LEU:HD12	2:D:1487:ARG:HG2	2.00	0.43
1:E:158:MET:HE1	1:G:75:PHE:CD2	2.52	0.43
1:E:313:GLN:HE22	1:E:338:LYS:HD2	1.83	0.43
2:F:772:TYR:HD1	2:F:852:PHE:HB2	1.83	0.43
2:F:1106:ILE:HD13	2:F:1106:ILE:HA	1.89	0.43
2:H:1369:ILE:HD13	2:H:1375:ILE:HG13	2.00	0.43
2:B:288:TRP:HE3	2:B:607:VAL:HG11	1.83	0.43
2:B:1114:GLU:OE1	3:B:2502:ADP:N6	2.52	0.43
2:F:262:ASN:HB3	2:F:390:ALA:HB2	2.00	0.43
2:F:391:ILE:O	2:F:395:ILE:HG23	2.18	0.43
2:F:586:LEU:O	2:F:589:PRO:HD2	2.19	0.43
2:F:1431:LEU:HD12	2:F:1487:ARG:HG2	2.00	0.43
1:G:49:ILE:HG21	1:G:55:PHE:CZ	2.54	0.43
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.19	0.43
2:H:263:TYR:HB2	2:H:393:THR:CG2	2.49	0.43
2:B:1203:HIS:CD2	2:B:1227:LEU:HD12	2.54	0.43
2:F:295:PHE:HZ	2:F:387:LEU:CD1	2.30	0.43
2:F:1102:LEU:HD23	2:F:1102:LEU:HA	1.76	0.43
1:G:187:ALA:O	1:G:309:ILE:HG13	2.19	0.43
2:H:1494:ARG:O	2:H:1498:ARG:HG3	2.19	0.43
2:B:586:LEU:O	2:B:589:PRO:HD2	2.19	0.43
2:B:684:GLY:O	2:B:698:ASN:N	2.51	0.43
2:B:1369:ILE:HD13	2:B:1375:ILE:HG13	2.00	0.43
1:C:284:ILE:HA	1:C:302:THR:O	2.18	0.43
2:D:75:TRP:HZ3	2:D:225:LEU:CD2	2.29	0.43
2:D:1192:LEU:HA	2:D:1195:THR:HG22	2.00	0.43
2:D:1353:ARG:NH1	2:D:1400:GLU:OE2	2.45	0.43
2:F:44:PHE:HD1	2:F:48:PHE:CE2	2.37	0.43
2:F:806:CYS:O	2:F:837:ARG:HD2	2.18	0.43
2:F:1004:TYR:CE1	2:F:1093:VAL:HG11	2.52	0.43
1:G:251:LEU:HD23	1:G:251:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1483:SER:O	2:H:1487:ARG:HG3	2.18	0.43
2:D:1114:GLU:OE1	3:D:2502:ADP:N6	2.52	0.42
2:D:1345:ILE:HG12	2:D:1369:ILE:HB	2.00	0.42
2:D:1494:ARG:O	2:D:1498:ARG:HG3	2.19	0.42
1:E:187:ALA:O	1:E:309:ILE:HG13	2.19	0.42
1:E:215:ILE:HD13	1:E:215:ILE:HA	1.83	0.42
1:G:338:LYS:HB3	1:G:338:LYS:HE3	1.76	0.42
2:H:772:TYR:HD1	2:H:852:PHE:HB2	1.83	0.42
2:H:1079:CYS:O	2:H:1082:THR:OG1	2.27	0.42
2:H:1509:THR:HG21	2:H:1539:ARG:HB2	2.00	0.42
1:A:297:THR:O	1:A:297:THR:OG1	2.37	0.42
2:B:253:LEU:HA	2:B:253:LEU:HD12	1.77	0.42
2:B:1509:THR:HG21	2:B:1539:ARG:HB2	2.00	0.42
1:C:345:THR:O	1:C:349:LEU:N	2.40	0.42
2:D:263:TYR:HB2	2:D:393:THR:CG2	2.49	0.42
2:D:869:MET:HE3	2:D:869:MET:HB3	1.77	0.42
2:F:263:TYR:HB2	2:F:393:THR:CG2	2.49	0.42
2:F:875:GLU:O	2:F:879:ASP:HB2	2.20	0.42
2:F:1345:ILE:HG12	2:F:1369:ILE:HB	2.00	0.42
1:G:297:THR:O	1:G:297:THR:OG1	2.37	0.42
2:H:262:ASN:HB3	2:H:390:ALA:HB2	2.00	0.42
2:H:1521:GLN:HA	2:H:1524:VAL:HG12	2.01	0.42
1:A:49:ILE:HG21	1:A:55:PHE:CZ	2.54	0.42
1:C:95:PHE:HE2	2:D:27:PHE:HB2	1.84	0.42
2:F:1256:GLY:HA2	2:F:1259:VAL:HG12	2.02	0.42
1:G:169:MET:HE3	1:G:169:MET:HB2	1.96	0.42
2:D:288:TRP:HE3	2:D:607:VAL:HG11	1.83	0.42
2:D:576:ALA:O	2:D:579:SER:OG	2.34	0.42
2:D:1521:GLN:HA	2:D:1524:VAL:HG12	2.01	0.42
1:E:338:LYS:HB3	1:E:338:LYS:HE3	1.76	0.42
2:F:1494:ARG:O	2:F:1498:ARG:HG3	2.19	0.42
2:B:772:TYR:HD1	2:B:852:PHE:HB2	1.83	0.42
2:B:1192:LEU:HA	2:B:1195:THR:HG22	2.00	0.42
2:B:1345:ILE:HG12	2:B:1369:ILE:HB	2.00	0.42
2:D:78:THR:HG21	2:D:121:VAL:HG23	2.02	0.42
2:D:586:LEU:O	2:D:589:PRO:HD2	2.19	0.42
2:D:875:GLU:O	2:D:879:ASP:HB2	2.20	0.42
2:D:1256:GLY:HA2	2:D:1259:VAL:HG12	2.02	0.42
2:D:1521:GLN:O	2:D:1525:MET:HG2	2.20	0.42
1:E:49:ILE:HG21	1:E:55:PHE:CZ	2.54	0.42
1:E:181:LEU:HD23	1:E:287:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:THR:HG21	2:F:121:VAL:HG23	2.02	0.42
2:H:44:PHE:HD1	2:H:48:PHE:CE2	2.37	0.42
2:H:78:THR:HG21	2:H:121:VAL:HG23	2.02	0.42
1:A:187:ALA:O	1:A:309:ILE:HG13	2.19	0.42
1:A:196:LEU:HB2	1:A:261:ILE:HD11	2.01	0.42
2:B:1020:GLN:HB3	2:B:1148:LEU:CD1	2.50	0.42
2:B:1308:GLN:O	2:B:1312:VAL:HG23	2.20	0.42
2:D:1020:GLN:HB3	2:D:1148:LEU:CD1	2.50	0.42
2:B:875:GLU:O	2:B:879:ASP:HB2	2.20	0.42
1:C:181:LEU:HD23	1:C:287:LEU:HD21	2.02	0.42
1:C:297:THR:O	1:C:297:THR:OG1	2.37	0.42
2:D:44:PHE:HD1	2:D:48:PHE:CE2	2.37	0.42
2:D:1164:PHE:HZ	2:D:1259:VAL:HG23	1.85	0.42
2:D:1203:HIS:CD2	2:D:1227:LEU:HD12	2.54	0.42
2:D:1335:ILE:N	2:D:1336:PRO:HD2	2.35	0.42
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.19	0.42
2:F:1146:SER:HB3	2:F:1298:MET:HB2	2.02	0.42
2:F:1521:GLN:HA	2:F:1524:VAL:HG12	2.01	0.42
1:G:95:PHE:HE2	2:H:27:PHE:HB2	1.84	0.42
2:H:571:LEU:HD12	2:H:571:LEU:O	2.20	0.42
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.19	0.42
2:B:592:LEU:HD11	2:B:1297:TRP:CH2	2.48	0.42
2:B:857:PHE:HE2	2:B:886:LEU:HD21	1.85	0.42
2:B:1079:CYS:O	2:B:1082:THR:OG1	2.27	0.42
1:C:187:ALA:O	1:C:309:ILE:HG13	2.19	0.42
2:D:217:PHE:HB2	2:D:1240:PHE:HE1	1.85	0.42
2:D:1308:GLN:O	2:D:1312:VAL:HG23	2.20	0.42
1:E:261:ILE:H	1:E:261:ILE:HG13	1.55	0.42
2:F:571:LEU:O	2:F:571:LEU:HD12	2.20	0.42
2:F:1255:ILE:HD13	2:F:1255:ILE:HA	1.93	0.42
1:G:318:ILE:HD12	1:G:329:ASP:O	2.20	0.42
2:H:217:PHE:HB2	2:H:1240:PHE:HE1	1.85	0.42
2:H:531:THR:O	2:H:534:ARG:HG2	2.20	0.42
2:H:1020:GLN:HB3	2:H:1148:LEU:CD1	2.50	0.42
2:H:1335:ILE:N	2:H:1336:PRO:HD2	2.35	0.42
1:A:181:LEU:HD23	1:A:287:LEU:HD21	2.02	0.42
2:B:44:PHE:HD1	2:B:48:PHE:CE2	2.37	0.42
2:B:1335:ILE:N	2:B:1336:PRO:HD2	2.35	0.42
2:B:1386:SER:OG	3:B:2502:ADP:O1A	2.36	0.42
1:E:318:ILE:HD12	1:E:329:ASP:O	2.20	0.42
2:F:417:ILE:O	2:F:420:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1203:HIS:CD2	2:F:1227:LEU:HD12	2.54	0.42
2:F:1354:TYR:HA	2:F:1396:VAL:HG13	2.00	0.42
2:H:576:ALA:O	2:H:579:SER:OG	2.34	0.42
2:H:1354:TYR:HA	2:H:1396:VAL:HG13	2.00	0.42
1:A:61:THR:HA	1:A:64:VAL:HG22	2.02	0.42
1:A:176:ARG:O	1:A:179:GLU:N	2.51	0.42
1:A:345:THR:O	1:A:349:LEU:N	2.40	0.42
2:B:1494:ARG:O	2:B:1498:ARG:HG3	2.19	0.42
2:D:857:PHE:HE2	2:D:886:LEU:HD21	1.85	0.42
2:D:1226:LYS:O	2:D:1230:TYR:HD1	2.03	0.42
1:E:195:ARG:HG3	1:E:195:ARG:HH11	1.85	0.42
2:F:869:MET:HB3	2:F:869:MET:HE3	1.77	0.42
1:G:220:VAL:HG12	1:G:235:GLN:HG2	2.02	0.42
2:H:888:THR:OG1	2:H:889:HIS:N	2.53	0.42
2:H:1226:LYS:O	2:H:1230:TYR:HD1	2.03	0.42
2:B:1521:GLN:O	2:B:1525:MET:HG2	2.20	0.41
2:D:435:CYS:HB3	2:D:436:PRO:HD3	2.02	0.41
2:D:451:LEU:HD13	2:D:582:LEU:HD21	2.01	0.41
2:F:188:ASN:O	2:F:192:VAL:HG23	2.20	0.41
2:F:1020:GLN:HB3	2:F:1148:LEU:CD1	2.50	0.41
2:H:417:ILE:O	2:H:420:LEU:HB3	2.20	0.41
2:H:435:CYS:HB3	2:H:436:PRO:HD3	2.02	0.41
2:H:451:LEU:HD13	2:H:582:LEU:HD21	2.01	0.41
2:H:1203:HIS:CD2	2:H:1227:LEU:HD12	2.54	0.41
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.65	0.41
2:B:435:CYS:HB3	2:B:436:PRO:HD3	2.02	0.41
2:B:531:THR:O	2:B:534:ARG:HG2	2.20	0.41
2:B:825:GLU:OE1	2:B:825:GLU:N	2.48	0.41
2:D:40:LEU:HD11	2:D:115:MET:HB2	2.03	0.41
2:D:571:LEU:HD12	2:D:571:LEU:O	2.20	0.41
1:E:95:PHE:HE2	2:F:27:PHE:HB2	1.84	0.41
2:F:531:THR:O	2:F:534:ARG:HG2	2.20	0.41
2:F:857:PHE:HE2	2:F:886:LEU:HD21	1.85	0.41
2:F:1164:PHE:HZ	2:F:1259:VAL:HG23	1.85	0.41
1:G:61:THR:HA	1:G:64:VAL:HG22	2.02	0.41
2:H:150:LYS:HB3	2:H:176:VAL:HG22	2.01	0.41
2:H:188:ASN:O	2:H:192:VAL:HG23	2.20	0.41
2:D:417:ILE:O	2:D:420:LEU:HB3	2.20	0.41
1:E:297:THR:O	1:E:297:THR:OG1	2.37	0.41
1:G:181:LEU:HD12	1:G:181:LEU:HA	1.89	0.41
2:H:1124:ARG:O	2:H:1128:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1146:SER:HB3	2:H:1298:MET:HB2	2.02	0.41
2:H:1308:GLN:O	2:H:1312:VAL:HG23	2.20	0.41
1:A:220:VAL:HG12	1:A:235:GLN:HG2	2.02	0.41
1:A:318:ILE:HD12	1:A:329:ASP:O	2.20	0.41
2:B:40:LEU:HD11	2:B:115:MET:HB2	2.03	0.41
2:B:188:ASN:O	2:B:192:VAL:HG23	2.20	0.41
2:B:196:ILE:O	2:B:197:PHE:C	2.60	0.41
2:B:217:PHE:HB2	2:B:1240:PHE:HE1	1.85	0.41
2:B:547:ASN:O	2:B:551:PRO:HG2	2.21	0.41
2:B:571:LEU:HD12	2:B:571:LEU:O	2.20	0.41
2:B:888:THR:OG1	2:B:889:HIS:N	2.53	0.41
2:B:1144:SER:O	2:B:1147:THR:HG22	2.21	0.41
2:B:1553:LYS:CE	2:B:1558:LEU:HB2	2.50	0.41
2:D:890:LYS:HB2	2:D:893:TYR:CE2	2.55	0.41
2:D:1348:GLN:CG	2:D:1402:ARG:HB2	2.51	0.41
1:E:75:PHE:HB3	1:E:163:MET:SD	2.61	0.41
2:F:435:CYS:HB3	2:F:436:PRO:HD3	2.02	0.41
2:F:812:ILE:HD13	2:F:812:ILE:HA	1.91	0.41
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.65	0.41
1:G:181:LEU:HD23	1:G:287:LEU:HD21	2.02	0.41
1:A:75:PHE:HB3	1:A:163:MET:SD	2.61	0.41
1:A:86:PHE:HA	1:A:89:VAL:HG12	2.03	0.41
2:B:1124:ARG:O	2:B:1128:ASP:HB2	2.21	0.41
2:B:1353:ARG:NH1	2:B:1400:GLU:OE2	2.45	0.41
2:B:1521:GLN:HA	2:B:1524:VAL:HG12	2.01	0.41
1:C:61:THR:HA	1:C:64:VAL:HG22	2.02	0.41
2:D:1394:ARG:HE	2:D:1415:LEU:HD11	1.86	0.41
1:E:100:LEU:HD12	1:E:100:LEU:HA	1.89	0.41
2:F:1144:SER:O	2:F:1147:THR:HG22	2.21	0.41
2:F:1394:ARG:HE	2:F:1415:LEU:HD11	1.86	0.41
2:F:1521:GLN:O	2:F:1525:MET:HG2	2.20	0.41
1:G:86:PHE:HA	1:G:89:VAL:HG12	2.03	0.41
2:H:875:GLU:O	2:H:879:ASP:HB2	2.20	0.41
2:H:890:LYS:HB2	2:H:893:TYR:CE2	2.55	0.41
2:H:1256:GLY:HA2	2:H:1259:VAL:HG12	2.02	0.41
2:B:150:LYS:HB3	2:B:176:VAL:HG22	2.01	0.41
2:B:175:LEU:HD23	2:B:175:LEU:HA	1.81	0.41
2:B:1552:LEU:HD23	2:B:1557:ILE:HG12	2.03	0.41
2:D:150:LYS:HB3	2:D:176:VAL:HG22	2.01	0.41
2:D:427:GLN:OE1	2:D:602:LYS:HD3	2.21	0.41
2:D:547:ASN:O	2:D:551:PRO:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:THR:HA	1:E:64:VAL:HG22	2.02	0.41
1:E:196:LEU:HB2	1:E:261:ILE:HD11	2.01	0.41
2:F:217:PHE:HB2	2:F:1240:PHE:HE1	1.85	0.41
2:F:1114:GLU:OE1	3:F:2502:ADP:N6	2.52	0.41
2:F:1308:GLN:O	2:F:1312:VAL:HG23	2.20	0.41
2:F:1552:LEU:HD23	2:F:1557:ILE:HG12	2.03	0.41
1:G:75:PHE:HB3	1:G:163:MET:SD	2.61	0.41
2:B:78:THR:HG21	2:B:121:VAL:HG23	2.02	0.41
2:B:427:GLN:OE1	2:B:602:LYS:HD3	2.21	0.41
2:B:890:LYS:HB2	2:B:893:TYR:CE2	2.55	0.41
2:B:1256:GLY:HA2	2:B:1259:VAL:HG12	2.02	0.41
2:F:246:ASP:OD1	2:F:247:LEU:N	2.49	0.41
1:G:195:ARG:HH11	1:G:195:ARG:HG3	1.85	0.41
2:H:1164:PHE:HZ	2:H:1259:VAL:HG23	1.85	0.41
1:C:318:ILE:HD12	1:C:329:ASP:O	2.20	0.41
2:D:131:ASN:OD1	2:D:131:ASN:N	2.43	0.41
2:D:531:THR:O	2:D:534:ARG:HG2	2.20	0.41
2:D:1146:SER:HB3	2:D:1298:MET:HB2	2.02	0.41
1:E:36:VAL:HG23	1:E:303:SER:OG	2.21	0.41
2:F:888:THR:OG1	2:F:889:HIS:N	2.53	0.41
2:F:1335:ILE:N	2:F:1336:PRO:HD2	2.35	0.41
1:G:286:ILE:HG23	1:G:301:ARG:HG2	2.03	0.41
2:H:40:LEU:HD11	2:H:115:MET:HB2	2.03	0.41
2:B:451:LEU:HD13	2:B:582:LEU:HD21	2.01	0.41
2:B:523:GLU:O	2:B:527:ARG:HG3	2.21	0.41
2:B:1102:LEU:HD23	2:B:1102:LEU:HA	1.76	0.41
2:B:1164:PHE:HZ	2:B:1259:VAL:HG23	1.85	0.41
2:B:1226:LYS:O	2:B:1230:TYR:HD1	2.03	0.41
2:B:1394:ARG:HE	2:B:1415:LEU:HD11	1.86	0.41
1:C:195:ARG:HG3	1:C:195:ARG:HH11	1.85	0.41
1:C:299:GLN:HE21	1:C:301:ARG:HD3	1.86	0.41
2:D:188:ASN:O	2:D:192:VAL:HG23	2.20	0.41
2:D:414:ALA:HA	2:D:1208:VAL:HG11	2.03	0.41
2:D:1552:LEU:HD23	2:D:1557:ILE:HG12	2.03	0.41
1:E:220:VAL:HG12	1:E:235:GLN:HG2	2.02	0.41
1:E:286:ILE:HG23	1:E:301:ARG:HG2	2.03	0.41
1:E:299:GLN:HE21	1:E:301:ARG:HD3	1.86	0.41
2:F:40:LEU:HD11	2:F:115:MET:HB2	2.03	0.41
2:F:427:GLN:OE1	2:F:602:LYS:HD3	2.21	0.41
2:F:451:LEU:HD13	2:F:582:LEU:HD21	2.01	0.41
2:F:496:LEU:HD23	2:F:496:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1348:GLN:CG	2:F:1402:ARG:HB2	2.51	0.41
2:F:1376:GLY:O	2:F:1549:VAL:HA	2.21	0.41
2:F:1415:LEU:HA	2:F:1418:LEU:HD12	2.03	0.41
1:G:36:VAL:HG23	1:G:303:SER:OG	2.21	0.41
1:G:198:PHE:HD1	1:G:199:MET:CA	2.31	0.41
2:H:489:LEU:HD21	2:H:602:LYS:HG2	2.03	0.41
2:H:547:ASN:O	2:H:551:PRO:HG2	2.21	0.41
2:H:1144:SER:O	2:H:1147:THR:HG22	2.21	0.41
2:H:1386:SER:OG	3:H:2502:ADP:O1A	2.36	0.41
2:H:1521:GLN:O	2:H:1525:MET:HG2	2.20	0.41
1:C:75:PHE:HB3	1:C:163:MET:SD	2.61	0.41
2:H:423:ILE:HG13	2:H:424:ASP:N	2.36	0.41
2:H:707:GLN:HE21	2:H:899:TRP:CD1	2.39	0.41
2:H:1348:GLN:CG	2:H:1402:ARG:HB2	2.51	0.41
1:A:50:ARG:HB2	3:A:401:ADP:C5	2.55	0.40
1:A:170:LYS:O	1:A:173:GLN:HG2	2.22	0.40
2:B:597:VAL:O	2:B:601:VAL:HG12	2.21	0.40
2:B:1146:SER:HB3	2:B:1298:MET:HB2	2.02	0.40
2:D:618:GLU:HG2	2:D:619:ILE:H	1.87	0.40
2:D:1144:SER:O	2:D:1147:THR:HG22	2.21	0.40
2:D:1415:LEU:HA	2:D:1418:LEU:HD12	2.03	0.40
2:F:72:ASN:OD1	2:F:72:ASN:N	2.54	0.40
2:F:150:LYS:HB3	2:F:176:VAL:HG22	2.01	0.40
2:F:423:ILE:HG13	2:F:424:ASP:N	2.36	0.40
2:F:489:LEU:HD21	2:F:602:LYS:HG2	2.03	0.40
2:F:1226:LYS:O	2:F:1230:TYR:HD1	2.03	0.40
2:H:533:LEU:HD23	2:H:533:LEU:HA	1.96	0.40
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.85	0.40
2:B:417:ILE:O	2:B:420:LEU:HB3	2.20	0.40
2:B:894:LEU:HB2	2:B:895:PRO:HD3	2.03	0.40
2:B:1348:GLN:CG	2:B:1402:ARG:HB2	2.51	0.40
1:C:36:VAL:HG23	1:C:303:SER:OG	2.21	0.40
1:C:114:ILE:HD11	1:C:120:ALA:HA	2.04	0.40
1:C:286:ILE:HG23	1:C:301:ARG:HG2	2.03	0.40
2:D:1376:GLY:O	2:D:1549:VAL:HA	2.21	0.40
2:D:1386:SER:OG	3:D:2502:ADP:O1A	2.36	0.40
1:E:170:LYS:O	1:E:173:GLN:HG2	2.22	0.40
2:F:618:GLU:HG2	2:F:619:ILE:H	1.87	0.40
1:G:215:ILE:HD13	1:G:215:ILE:HA	1.83	0.40
1:G:261:ILE:H	1:G:261:ILE:HG13	1.55	0.40
2:H:1480:GLU:HB2	3:H:2501:ADP:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1552:LEU:HD23	2:H:1557:ILE:HG12	2.03	0.40
1:A:286:ILE:HG23	1:A:301:ARG:HG2	2.03	0.40
2:B:414:ALA:HA	2:B:1208:VAL:HG11	2.03	0.40
2:B:485:GLN:NE2	2:B:598:ARG:HG3	2.37	0.40
2:B:489:LEU:HD21	2:B:602:LYS:HG2	2.03	0.40
2:B:812:ILE:HD13	2:B:812:ILE:HA	1.91	0.40
2:B:871:ALA:O	2:B:875:GLU:HB2	2.22	0.40
2:B:1480:GLU:HB2	3:B:2501:ADP:C6	2.57	0.40
1:C:56:LEU:HD22	2:D:49:ILE:HG21	2.04	0.40
2:D:489:LEU:HD21	2:D:602:LYS:HG2	2.03	0.40
2:D:544:ILE:HD12	2:D:591:PHE:CE2	2.56	0.40
2:D:597:VAL:O	2:D:601:VAL:HG12	2.21	0.40
1:E:56:LEU:HD22	2:F:49:ILE:HG21	2.04	0.40
1:E:181:LEU:HA	1:E:181:LEU:HD12	1.89	0.40
2:F:523:GLU:O	2:F:527:ARG:HG3	2.21	0.40
2:F:547:ASN:O	2:F:551:PRO:HG2	2.21	0.40
2:F:890:LYS:HB2	2:F:893:TYR:CE2	2.55	0.40
1:G:164:LEU:O	1:G:167:ILE:HG13	2.22	0.40
2:H:857:PHE:HE2	2:H:886:LEU:HD21	1.85	0.40
1:A:338:LYS:HB3	1:A:338:LYS:HE3	1.76	0.40
2:B:551:PRO:CB	2:B:583:PHE:HZ	2.30	0.40
2:B:1376:GLY:O	2:B:1549:VAL:HA	2.21	0.40
1:C:198:PHE:CE1	1:C:199:MET:C	3.00	0.40
2:D:381:ILE:HG21	2:D:1242:THR:HG21	2.04	0.40
2:D:707:GLN:HE21	2:D:899:TRP:CD1	2.39	0.40
2:D:730:MET:HE3	2:D:730:MET:HB3	1.89	0.40
1:E:95:PHE:CD1	1:E:100:LEU:HD23	2.45	0.40
2:F:544:ILE:HD12	2:F:591:PHE:CE2	2.56	0.40
2:F:597:VAL:O	2:F:601:VAL:HG12	2.21	0.40
1:G:198:PHE:CE1	1:G:199:MET:C	3.00	0.40
2:H:72:ASN:OD1	2:H:72:ASN:N	2.54	0.40
2:H:75:TRP:HZ3	2:H:225:LEU:CD2	2.29	0.40
2:H:427:GLN:OE1	2:H:602:LYS:HD3	2.21	0.40
2:H:1394:ARG:HE	2:H:1415:LEU:HD11	1.86	0.40
2:H:1558:LEU:HD12	2:H:1558:LEU:HA	1.99	0.40
2:B:685:PHE:O	2:B:732:LYS:HB3	2.22	0.40
1:C:176:ARG:O	1:C:179:GLU:N	2.51	0.40
2:D:485:GLN:NE2	2:D:598:ARG:HG3	2.37	0.40
2:D:1486:GLN:O	2:D:1490:PHE:HD1	2.05	0.40
2:F:707:GLN:HE21	2:F:899:TRP:CD1	2.39	0.40
2:F:1124:ARG:O	2:F:1128:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1480:GLU:HB2	3:F:2501:ADP:C6	2.57	0.40
2:H:523:GLU:O	2:H:527:ARG:HG3	2.21	0.40
2:H:618:GLU:HG2	2:H:619:ILE:H	1.87	0.40
2:H:685:PHE:O	2:H:732:LYS:HB3	2.22	0.40
2:H:1486:GLN:O	2:H:1490:PHE:HD1	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	323/390 (83%)	303 (94%)	19 (6%)	1 (0%)	36	71
1	C	323/390 (83%)	303 (94%)	19 (6%)	1 (0%)	36	71
1	E	323/390 (83%)	303 (94%)	19 (6%)	1 (0%)	36	71
1	G	323/390 (83%)	303 (94%)	19 (6%)	1 (0%)	36	71
2	B	1300/1582 (82%)	1243 (96%)	52 (4%)	5 (0%)	30	66
2	D	1300/1582 (82%)	1243 (96%)	52 (4%)	5 (0%)	30	66
2	F	1246/1582 (79%)	1191 (96%)	50 (4%)	5 (0%)	30	66
2	H	1300/1582 (82%)	1243 (96%)	52 (4%)	5 (0%)	30	66
All	All	6438/7888 (82%)	6132 (95%)	282 (4%)	24 (0%)	31	66

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	PHE
2	B	199	LYS
2	D	197	PHE
2	D	199	LYS
2	F	197	PHE

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Mol	Chain	Res	Type
2	F	199	LYS
2	H	197	PHE
2	H	199	LYS
1	A	244	VAL
1	C	244	VAL
1	E	244	VAL
1	G	244	VAL
2	B	212	ASP
2	D	212	ASP
2	F	212	ASP
2	H	212	ASP
2	B	205	LYS
2	D	205	LYS
2	F	205	LYS
2	H	205	LYS
2	B	196	ILE
2	D	196	ILE
2	F	196	ILE
2	H	196	ILE

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	213/339 (63%)	175 (82%)	38 (18%)	2	11
1	C	60/339 (18%)	55 (92%)	5 (8%)	10	31
1	E	258/339 (76%)	218 (84%)	40 (16%)	2	13
1	G	258/339 (76%)	218 (84%)	40 (16%)	2	13
2	B	754/1371 (55%)	707 (94%)	47 (6%)	16	39
2	D	1097/1371 (80%)	1029 (94%)	68 (6%)	16	39
2	F	1097/1371 (80%)	1029 (94%)	68 (6%)	16	39
2	H	1097/1371 (80%)	1029 (94%)	68 (6%)	16	39
All	All	4834/6840 (71%)	4460 (92%)	374 (8%)	14	33

All (374) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	50	ARG
1	A	78	SER
1	A	81	CYS
1	A	82	SER
1	A	88	MET
1	A	90	TRP
1	A	92	LEU
1	A	108	VAL
1	A	111	VAL
1	A	122	LEU
1	A	133	PHE
1	A	136	ARG
1	A	152	GLN
1	A	153	ASN
1	A	166	CYS
1	A	181	LEU
1	A	182	ILE
1	A	188	VAL
1	A	190	THR
1	A	198	PHE
1	A	200	LEU
1	A	204	ASP
1	A	205	LEU
1	A	219	VAL
1	A	236	VAL
1	A	238	ILE
1	A	249	ILE
1	A	252	VAL
1	A	256	ILE
1	A	261	ILE
1	A	286	ILE
1	A	287	LEU
1	A	290	VAL
1	A	293	THR
1	A	294	THR
1	A	297	THR
1	A	298	THR
2	B	37	VAL
2	B	72	ASN
2	B	119	THR
2	B	121	VAL

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Mol	Chain	Res	Type
2	B	167	LEU
2	B	387	LEU
2	B	420	LEU
2	B	423	ILE
2	B	425	THR
2	B	429	MET
2	B	432	PHE
2	B	443	VAL
2	B	451	LEU
2	B	466	VAL
2	B	470	LEU
2	B	511	LEU
2	B	563	VAL
2	B	571	LEU
2	B	574	SER
2	B	614	LEU
2	B	682	ILE
2	B	689	THR
2	B	696	LEU
2	B	701	ILE
2	B	707	GLN
2	B	708	LEU
2	B	723	LEU
2	B	730	MET
2	B	737	VAL
2	B	770	VAL
2	B	850	VAL
2	B	861	ASP
2	B	869	MET
2	B	891	LEU
2	B	892	GLN
2	B	894	LEU
2	B	1038	THR
2	B	1136	ILE
2	B	1211	LEU
2	B	1240	PHE
2	B	1251	ARG
2	B	1255	ILE
2	B	1258	CYS
2	B	1268	ILE
2	B	1270	ASN
2	B	1378	CYS

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Mol	Chain	Res	Type
2	B	1409	ASP
1	C	122	LEU
1	C	133	PHE
1	C	136	ARG
1	C	323	ASP
1	C	345	THR
2	D	37	VAL
2	D	72	ASN
2	D	119	THR
2	D	121	VAL
2	D	167	LEU
2	D	190	ILE
2	D	193	ARG
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	229	THR
2	D	237	ILE
2	D	253	LEU
2	D	292	CYS
2	D	358	LEU
2	D	387	LEU
2	D	420	LEU
2	D	423	ILE
2	D	425	THR
2	D	429	MET
2	D	432	PHE
2	D	443	VAL
2	D	451	LEU
2	D	466	VAL
2	D	470	LEU
2	D	511	LEU
2	D	563	VAL
2	D	571	LEU
2	D	574	SER
2	D	614	LEU
2	D	682	ILE
2	D	689	THR
2	D	696	LEU
2	D	701	ILE
2	D	707	GLN
2	D	708	LEU

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Mol	Chain	Res	Type
2	D	723	LEU
2	D	730	MET
2	D	737	VAL
2	D	770	VAL
2	D	850	VAL
2	D	861	ASP
2	D	869	MET
2	D	891	LEU
2	D	892	GLN
2	D	894	LEU
2	D	1038	THR
2	D	1136	ILE
2	D	1204	PHE
2	D	1211	LEU
2	D	1240	PHE
2	D	1251	ARG
2	D	1255	ILE
2	D	1258	CYS
2	D	1268	ILE
2	D	1270	ASN
2	D	1315	ILE
2	D	1378	CYS
2	D	1409	ASP
2	D	1417	THR
2	D	1424	ILE
2	D	1432	PHE
2	D	1509	THR
2	D	1522	LYS
2	D	1536	ILE
2	D	1551	VAL
2	D	1557	ILE
2	D	1566	LEU
1	E	36	VAL
1	E	50	ARG
1	E	78	SER
1	E	81	CYS
1	E	82	SER
1	E	88	MET
1	E	90	TRP
1	E	92	LEU
1	E	108	VAL
1	E	111	VAL

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Mol	Chain	Res	Type
1	E	122	LEU
1	E	133	PHE
1	E	136	ARG
1	E	152	GLN
1	E	153	ASN
1	E	166	CYS
1	E	181	LEU
1	E	182	ILE
1	E	188	VAL
1	E	190	THR
1	E	198	PHE
1	E	200	LEU
1	E	204	ASP
1	E	205	LEU
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	249	ILE
1	E	252	VAL
1	E	256	ILE
1	E	261	ILE
1	E	286	ILE
1	E	287	LEU
1	E	290	VAL
1	E	293	THR
1	E	294	THR
1	E	297	THR
1	E	298	THR
1	E	323	ASP
1	E	345	THR
2	F	37	VAL
2	F	72	ASN
2	F	119	THR
2	F	121	VAL
2	F	167	LEU
2	F	190	ILE
2	F	193	ARG
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	229	THR
2	F	237	ILE

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Mol	Chain	Res	Type
2	F	253	LEU
2	F	292	CYS
2	F	358	LEU
2	F	387	LEU
2	F	420	LEU
2	F	423	ILE
2	F	425	THR
2	F	429	MET
2	F	432	PHE
2	F	443	VAL
2	F	451	LEU
2	F	466	VAL
2	F	470	LEU
2	F	511	LEU
2	F	563	VAL
2	F	571	LEU
2	F	574	SER
2	F	614	LEU
2	F	682	ILE
2	F	689	THR
2	F	696	LEU
2	F	701	ILE
2	F	707	GLN
2	F	708	LEU
2	F	723	LEU
2	F	730	MET
2	F	737	VAL
2	F	770	VAL
2	F	850	VAL
2	F	861	ASP
2	F	869	MET
2	F	891	LEU
2	F	892	GLN
2	F	894	LEU
2	F	1038	THR
2	F	1136	ILE
2	F	1204	PHE
2	F	1211	LEU
2	F	1240	PHE
2	F	1251	ARG
2	F	1255	ILE
2	F	1258	CYS

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Mol	Chain	Res	Type
2	F	1268	ILE
2	F	1270	ASN
2	F	1315	ILE
2	F	1378	CYS
2	F	1409	ASP
2	F	1417	THR
2	F	1424	ILE
2	F	1432	PHE
2	F	1509	THR
2	F	1522	LYS
2	F	1536	ILE
2	F	1551	VAL
2	F	1557	ILE
2	F	1566	LEU
1	G	36	VAL
1	G	50	ARG
1	G	78	SER
1	G	81	CYS
1	G	82	SER
1	G	88	MET
1	G	90	TRP
1	G	92	LEU
1	G	108	VAL
1	G	111	VAL
1	G	122	LEU
1	G	133	PHE
1	G	136	ARG
1	G	152	GLN
1	G	153	ASN
1	G	166	CYS
1	G	181	LEU
1	G	182	ILE
1	G	188	VAL
1	G	190	THR
1	G	198	PHE
1	G	200	LEU
1	G	204	ASP
1	G	205	LEU
1	G	219	VAL
1	G	236	VAL
1	G	238	ILE
1	G	249	ILE

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Mol	Chain	Res	Type
1	G	252	VAL
1	G	256	ILE
1	G	261	ILE
1	G	286	ILE
1	G	287	LEU
1	G	290	VAL
1	G	293	THR
1	G	294	THR
1	G	297	THR
1	G	298	THR
1	G	323	ASP
1	G	345	THR
2	H	37	VAL
2	H	72	ASN
2	H	119	THR
2	H	121	VAL
2	H	167	LEU
2	H	190	ILE
2	H	193	ARG
2	H	204	VAL
2	H	218	LEU
2	H	222	VAL
2	H	229	THR
2	H	237	ILE
2	H	253	LEU
2	H	292	CYS
2	H	358	LEU
2	H	387	LEU
2	H	420	LEU
2	H	423	ILE
2	H	425	THR
2	H	429	MET
2	H	432	PHE
2	H	443	VAL
2	H	451	LEU
2	H	466	VAL
2	H	470	LEU
2	H	511	LEU
2	H	563	VAL
2	H	571	LEU
2	H	574	SER
2	H	614	LEU

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Mol	Chain	Res	Type
2	H	682	ILE
2	H	689	THR
2	H	696	LEU
2	H	701	ILE
2	H	707	GLN
2	H	708	LEU
2	H	723	LEU
2	H	730	MET
2	H	737	VAL
2	H	770	VAL
2	H	850	VAL
2	H	861	ASP
2	H	869	MET
2	H	891	LEU
2	H	892	GLN
2	H	894	LEU
2	H	1038	THR
2	H	1136	ILE
2	H	1204	PHE
2	H	1211	LEU
2	H	1240	PHE
2	H	1251	ARG
2	H	1255	ILE
2	H	1258	CYS
2	H	1268	ILE
2	H	1270	ASN
2	H	1315	ILE
2	H	1378	CYS
2	H	1409	ASP
2	H	1417	THR
2	H	1424	ILE
2	H	1432	PHE
2	H	1509	THR
2	H	1522	LYS
2	H	1536	ILE
2	H	1551	VAL
2	H	1557	ILE
2	H	1566	LEU

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

Mol	Chain	Res	Type
1	A	46	HIS
1	A	48	ASN
1	A	128	GLN
1	A	152	GLN
1	A	173	GLN
1	A	193	HIS
1	A	259	HIS
1	A	299	GLN
2	B	416	GLN
2	B	707	GLN
1	C	128	GLN
1	C	348	GLN
2	D	223	ASN
2	D	416	GLN
2	D	863	HIS
2	D	1203	HIS
2	D	1518	ASN
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	173	GLN
1	E	259	HIS
1	E	299	GLN
1	E	313	GLN
1	E	348	GLN
2	F	223	ASN
2	F	416	GLN
2	F	707	GLN
2	F	863	HIS
2	F	1203	HIS
2	F	1373	GLN
2	F	1518	ASN
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN
1	G	152	GLN
1	G	173	GLN
1	G	193	HIS
1	G	259	HIS
1	G	299	GLN
1	G	313	GLN
1	G	348	GLN
2	H	223	ASN

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Mol	Chain	Res	Type
2	H	416	GLN
2	H	707	GLN
2	H	863	HIS
2	H	1203	HIS
2	H	1518	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	F	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	D	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	D	2501	4	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	E	401	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)
3	ADP	H	2501	4	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	H	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	B	2501	4	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	401	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)
3	ADP	B	2502	4	28,29,29	1.39	4 (14%)	43,45,45	1.78	8 (18%)
3	ADP	F	2501	4	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
3	ADP	G	401	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)
3	ADP	C	401	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)

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
3	ADP	F	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	D	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	D	2501	4	-	0/16/32/32	0/3/3/3
3	ADP	E	401	-	-	4/16/32/32	0/3/3/3
3	ADP	H	2501	4	-	0/16/32/32	0/3/3/3
3	ADP	H	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	B	2501	4	-	0/16/32/32	0/3/3/3
3	ADP	A	401	-	-	4/16/32/32	0/3/3/3
3	ADP	B	2502	4	-	4/16/32/32	0/3/3/3
3	ADP	F	2501	4	-	0/16/32/32	0/3/3/3
3	ADP	G	401	-	-	4/16/32/32	0/3/3/3
3	ADP	C	401	-	-	4/16/32/32	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2502	ADP	C5-C4	4.65	1.47	1.39
3	D	2502	ADP	C5-C4	4.65	1.47	1.39
3	F	2502	ADP	C5-C4	4.65	1.47	1.39
3	H	2502	ADP	C5-C4	4.65	1.47	1.39
3	B	2501	ADP	C5-C4	4.55	1.47	1.39
3	D	2501	ADP	C5-C4	4.55	1.47	1.39
3	F	2501	ADP	C5-C4	4.55	1.47	1.39
3	H	2501	ADP	C5-C4	4.55	1.47	1.39
3	A	401	ADP	C5-C4	4.49	1.47	1.39
3	C	401	ADP	C5-C4	4.49	1.47	1.39
3	E	401	ADP	C5-C4	4.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	401	ADP	C5-C4	4.49	1.47	1.39
3	A	401	ADP	C5-N7	-2.72	1.34	1.39
3	C	401	ADP	C5-N7	-2.72	1.34	1.39
3	E	401	ADP	C5-N7	-2.72	1.34	1.39
3	G	401	ADP	C5-N7	-2.72	1.34	1.39
3	B	2501	ADP	C5-C6	2.69	1.48	1.41
3	D	2501	ADP	C5-C6	2.69	1.48	1.41
3	F	2501	ADP	C5-C6	2.69	1.48	1.41
3	H	2501	ADP	C5-C6	2.69	1.48	1.41
3	B	2502	ADP	C5-C6	2.61	1.48	1.41
3	D	2502	ADP	C5-C6	2.61	1.48	1.41
3	F	2502	ADP	C5-C6	2.61	1.48	1.41
3	H	2502	ADP	C5-C6	2.61	1.48	1.41
3	A	401	ADP	C5-C6	2.31	1.47	1.41
3	C	401	ADP	C5-C6	2.31	1.47	1.41
3	E	401	ADP	C5-C6	2.31	1.47	1.41
3	G	401	ADP	C5-C6	2.31	1.47	1.41
3	B	2502	ADP	C5-N7	-2.31	1.34	1.39
3	D	2502	ADP	C5-N7	-2.31	1.34	1.39
3	F	2502	ADP	C5-N7	-2.31	1.34	1.39
3	H	2502	ADP	C5-N7	-2.31	1.34	1.39
3	B	2501	ADP	C8-N7	2.31	1.36	1.31
3	D	2501	ADP	C8-N7	2.31	1.36	1.31
3	F	2501	ADP	C8-N7	2.31	1.36	1.31
3	H	2501	ADP	C8-N7	2.31	1.36	1.31
3	B	2502	ADP	C8-N7	2.27	1.36	1.31
3	D	2502	ADP	C8-N7	2.27	1.36	1.31
3	F	2502	ADP	C8-N7	2.27	1.36	1.31
3	H	2502	ADP	C8-N7	2.27	1.36	1.31
3	B	2501	ADP	C5-N7	-2.22	1.35	1.39
3	D	2501	ADP	C5-N7	-2.22	1.35	1.39
3	F	2501	ADP	C5-N7	-2.22	1.35	1.39
3	H	2501	ADP	C5-N7	-2.22	1.35	1.39
3	A	401	ADP	C4-N9	-2.08	1.33	1.37
3	C	401	ADP	C4-N9	-2.08	1.33	1.37
3	E	401	ADP	C4-N9	-2.08	1.33	1.37
3	G	401	ADP	C4-N9	-2.08	1.33	1.37
3	A	401	ADP	C8-N7	2.00	1.35	1.31
3	C	401	ADP	C8-N7	2.00	1.35	1.31
3	E	401	ADP	C8-N7	2.00	1.35	1.31
3	G	401	ADP	C8-N7	2.00	1.35	1.31

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	C5-C4-N3	-6.06	118.37	126.72
3	C	401	ADP	C5-C4-N3	-6.06	118.37	126.72
3	E	401	ADP	C5-C4-N3	-6.06	118.37	126.72
3	G	401	ADP	C5-C4-N3	-6.06	118.37	126.72
3	B	2502	ADP	C5-C4-N3	-5.83	118.70	126.72
3	D	2502	ADP	C5-C4-N3	-5.83	118.70	126.72
3	F	2502	ADP	C5-C4-N3	-5.83	118.70	126.72
3	H	2502	ADP	C5-C4-N3	-5.83	118.70	126.72
3	B	2501	ADP	C5-C4-N3	-5.75	118.80	126.72
3	D	2501	ADP	C5-C4-N3	-5.75	118.80	126.72
3	F	2501	ADP	C5-C4-N3	-5.75	118.80	126.72
3	H	2501	ADP	C5-C4-N3	-5.75	118.80	126.72
3	A	401	ADP	N3-C4-N9	4.97	135.62	127.17
3	C	401	ADP	N3-C4-N9	4.97	135.62	127.17
3	E	401	ADP	N3-C4-N9	4.97	135.62	127.17
3	G	401	ADP	N3-C4-N9	4.97	135.62	127.17
3	B	2502	ADP	N3-C4-N9	4.69	135.15	127.17
3	D	2502	ADP	N3-C4-N9	4.69	135.15	127.17
3	F	2502	ADP	N3-C4-N9	4.69	135.15	127.17
3	H	2502	ADP	N3-C4-N9	4.69	135.15	127.17
3	B	2501	ADP	N3-C4-N9	4.50	134.81	127.17
3	D	2501	ADP	N3-C4-N9	4.50	134.81	127.17
3	F	2501	ADP	N3-C4-N9	4.50	134.81	127.17
3	H	2501	ADP	N3-C4-N9	4.50	134.81	127.17
3	B	2501	ADP	C2-N3-C4	3.72	120.92	111.83
3	D	2501	ADP	C2-N3-C4	3.72	120.92	111.83
3	F	2501	ADP	C2-N3-C4	3.72	120.92	111.83
3	H	2501	ADP	C2-N3-C4	3.72	120.92	111.83
3	B	2502	ADP	C2-N3-C4	3.68	120.83	111.83
3	D	2502	ADP	C2-N3-C4	3.68	120.83	111.83
3	F	2502	ADP	C2-N3-C4	3.68	120.83	111.83
3	H	2502	ADP	C2-N3-C4	3.68	120.83	111.83
3	A	401	ADP	C2-N3-C4	3.63	120.71	111.83
3	C	401	ADP	C2-N3-C4	3.63	120.71	111.83
3	E	401	ADP	C2-N3-C4	3.63	120.71	111.83
3	G	401	ADP	C2-N3-C4	3.63	120.71	111.83
3	B	2501	ADP	C4-C5-N7	-3.39	106.71	110.58
3	D	2501	ADP	C4-C5-N7	-3.39	106.71	110.58
3	F	2501	ADP	C4-C5-N7	-3.39	106.71	110.58
3	H	2501	ADP	C4-C5-N7	-3.39	106.71	110.58
3	B	2502	ADP	C4-C5-N7	-3.32	106.79	110.58
3	D	2502	ADP	C4-C5-N7	-3.32	106.79	110.58
3	F	2502	ADP	C4-C5-N7	-3.32	106.79	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2502	ADP	C4-C5-N7	-3.32	106.79	110.58
3	B	2501	ADP	N3-C2-N1	-3.29	123.60	128.58
3	D	2501	ADP	N3-C2-N1	-3.29	123.60	128.58
3	F	2501	ADP	N3-C2-N1	-3.29	123.60	128.58
3	H	2501	ADP	N3-C2-N1	-3.29	123.60	128.58
3	B	2502	ADP	N3-C2-N1	-3.23	123.70	128.58
3	D	2502	ADP	N3-C2-N1	-3.23	123.70	128.58
3	F	2502	ADP	N3-C2-N1	-3.23	123.70	128.58
3	H	2502	ADP	N3-C2-N1	-3.23	123.70	128.58
3	A	401	ADP	N3-C2-N1	-3.05	123.96	128.58
3	C	401	ADP	N3-C2-N1	-3.05	123.96	128.58
3	E	401	ADP	N3-C2-N1	-3.05	123.96	128.58
3	G	401	ADP	N3-C2-N1	-3.05	123.96	128.58
3	A	401	ADP	C4-C5-N7	-2.92	107.25	110.58
3	C	401	ADP	C4-C5-N7	-2.92	107.25	110.58
3	E	401	ADP	C4-C5-N7	-2.92	107.25	110.58
3	G	401	ADP	C4-C5-N7	-2.92	107.25	110.58
3	A	401	ADP	C3'-C2'-C1'	2.74	106.64	101.46
3	C	401	ADP	C3'-C2'-C1'	2.74	106.64	101.46
3	E	401	ADP	C3'-C2'-C1'	2.74	106.64	101.46
3	G	401	ADP	C3'-C2'-C1'	2.74	106.64	101.46
3	B	2502	ADP	C4-N9-C8	2.67	108.54	105.74
3	D	2502	ADP	C4-N9-C8	2.67	108.54	105.74
3	F	2502	ADP	C4-N9-C8	2.67	108.54	105.74
3	H	2502	ADP	C4-N9-C8	2.67	108.54	105.74
3	B	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	D	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	F	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	H	2501	ADP	C4-N9-C8	2.62	108.49	105.74
3	B	2502	ADP	C5-N7-C8	2.48	107.35	103.45
3	D	2502	ADP	C5-N7-C8	2.48	107.35	103.45
3	F	2502	ADP	C5-N7-C8	2.48	107.35	103.45
3	H	2502	ADP	C5-N7-C8	2.48	107.35	103.45
3	B	2501	ADP	C5-N7-C8	2.43	107.27	103.45
3	D	2501	ADP	C5-N7-C8	2.43	107.27	103.45
3	F	2501	ADP	C5-N7-C8	2.43	107.27	103.45
3	H	2501	ADP	C5-N7-C8	2.43	107.27	103.45
3	A	401	ADP	C4-N9-C8	2.40	108.25	105.74
3	C	401	ADP	C4-N9-C8	2.40	108.25	105.74
3	E	401	ADP	C4-N9-C8	2.40	108.25	105.74
3	G	401	ADP	C4-N9-C8	2.40	108.25	105.74
3	B	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	F	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	H	2501	ADP	C3'-C2'-C1'	2.39	105.99	101.46
3	A	401	ADP	C5-N7-C8	2.18	106.88	103.45
3	C	401	ADP	C5-N7-C8	2.18	106.88	103.45
3	E	401	ADP	C5-N7-C8	2.18	106.88	103.45
3	G	401	ADP	C5-N7-C8	2.18	106.88	103.45
3	B	2501	ADP	C6-C5-N7	2.13	136.19	132.09
3	D	2501	ADP	C6-C5-N7	2.13	136.19	132.09
3	F	2501	ADP	C6-C5-N7	2.13	136.19	132.09
3	H	2501	ADP	C6-C5-N7	2.13	136.19	132.09
3	B	2502	ADP	C6-C5-N7	2.00	135.95	132.09
3	D	2502	ADP	C6-C5-N7	2.00	135.95	132.09
3	F	2502	ADP	C6-C5-N7	2.00	135.95	132.09
3	H	2502	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	C5'-O5'-PA-O3A
3	B	2502	ADP	C5'-O5'-PA-O3A
3	B	2502	ADP	O4'-C4'-C5'-O5'
3	C	401	ADP	C5'-O5'-PA-O3A
3	D	2502	ADP	C5'-O5'-PA-O3A
3	D	2502	ADP	O4'-C4'-C5'-O5'
3	E	401	ADP	C5'-O5'-PA-O3A
3	F	2502	ADP	C5'-O5'-PA-O3A
3	F	2502	ADP	O4'-C4'-C5'-O5'
3	G	401	ADP	C5'-O5'-PA-O3A
3	H	2502	ADP	C5'-O5'-PA-O3A
3	H	2502	ADP	O4'-C4'-C5'-O5'
3	B	2502	ADP	C3'-C4'-C5'-O5'
3	D	2502	ADP	C3'-C4'-C5'-O5'
3	F	2502	ADP	C3'-C4'-C5'-O5'
3	H	2502	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	O4'-C4'-C5'-O5'
3	C	401	ADP	O4'-C4'-C5'-O5'
3	E	401	ADP	O4'-C4'-C5'-O5'
3	G	401	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	C5'-O5'-PA-O1A
3	B	2502	ADP	C5'-O5'-PA-O2A

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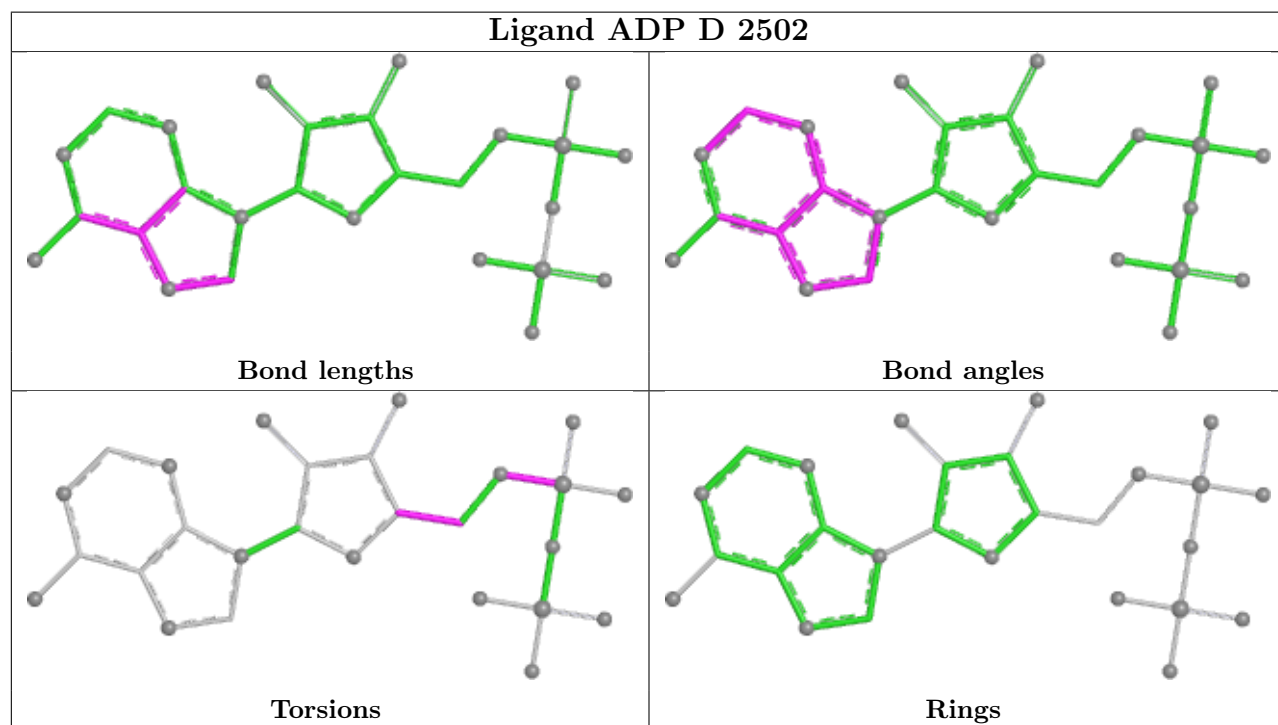
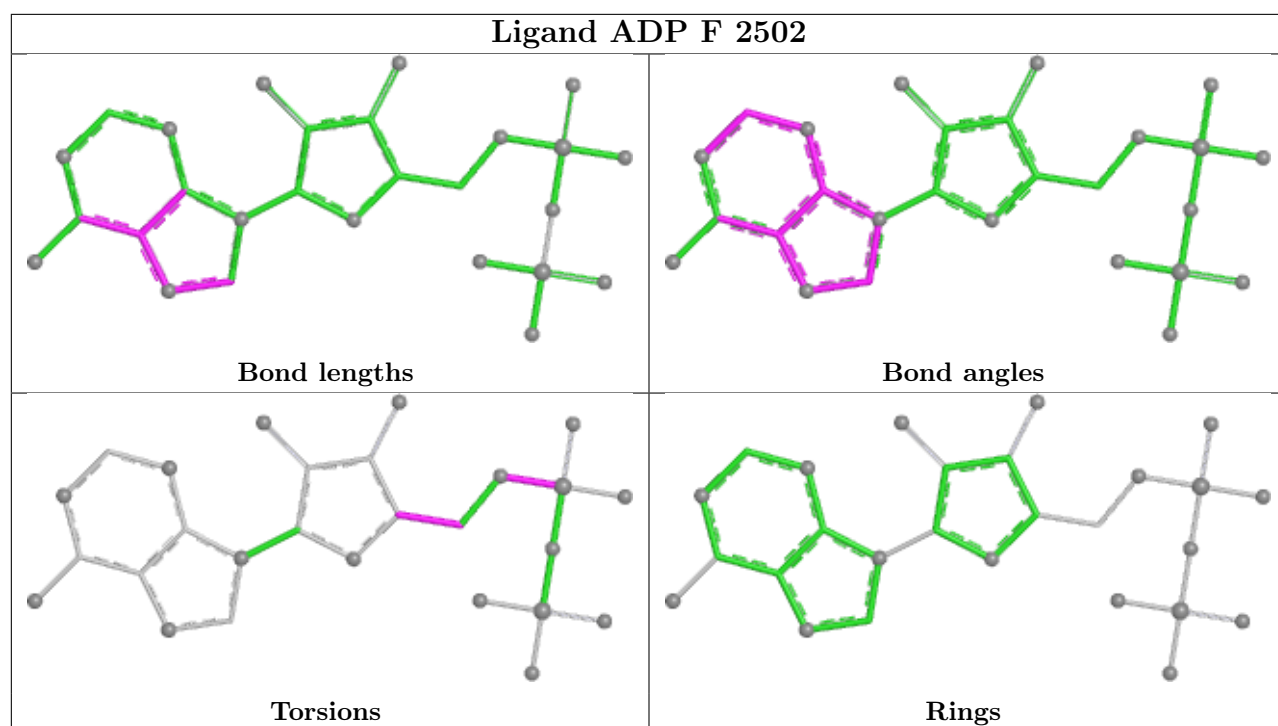
Mol	Chain	Res	Type	Atoms
3	C	401	ADP	C5'-O5'-PA-O1A
3	D	2502	ADP	C5'-O5'-PA-O2A
3	E	401	ADP	C5'-O5'-PA-O1A
3	F	2502	ADP	C5'-O5'-PA-O2A
3	G	401	ADP	C5'-O5'-PA-O1A
3	H	2502	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	C2'-C1'-N9-C8
3	C	401	ADP	C2'-C1'-N9-C8
3	E	401	ADP	C2'-C1'-N9-C8
3	G	401	ADP	C2'-C1'-N9-C8

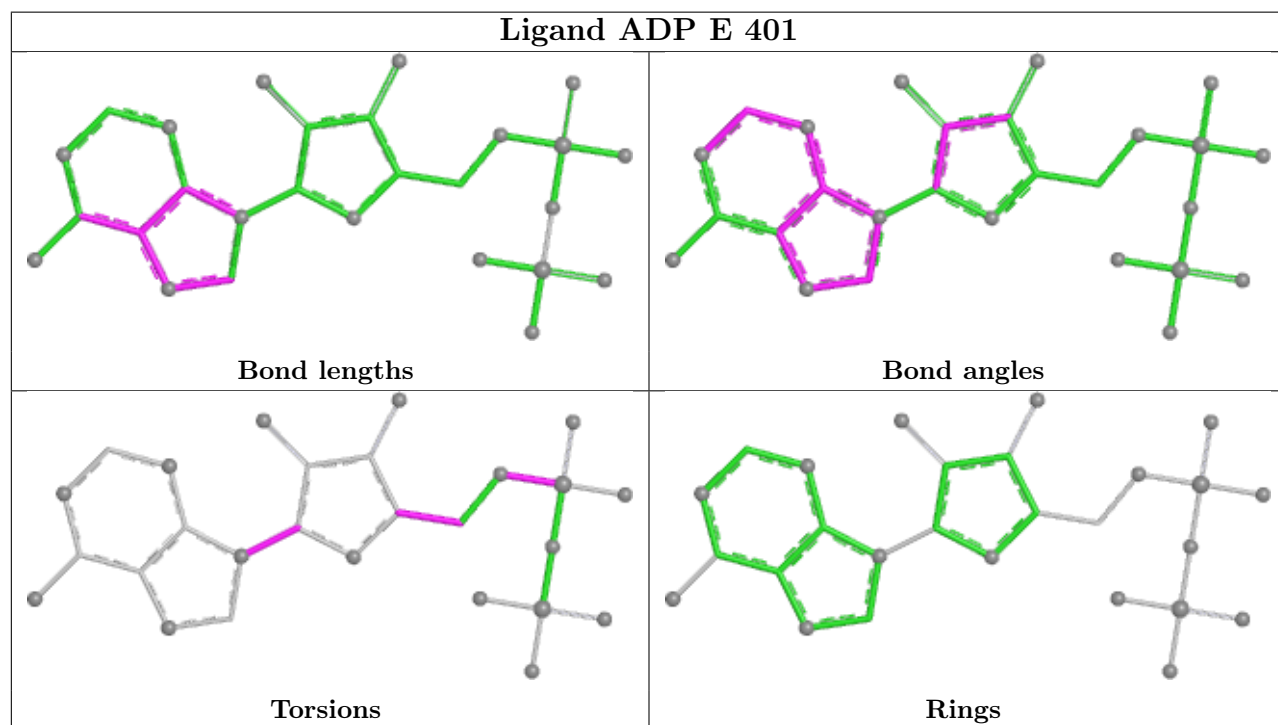
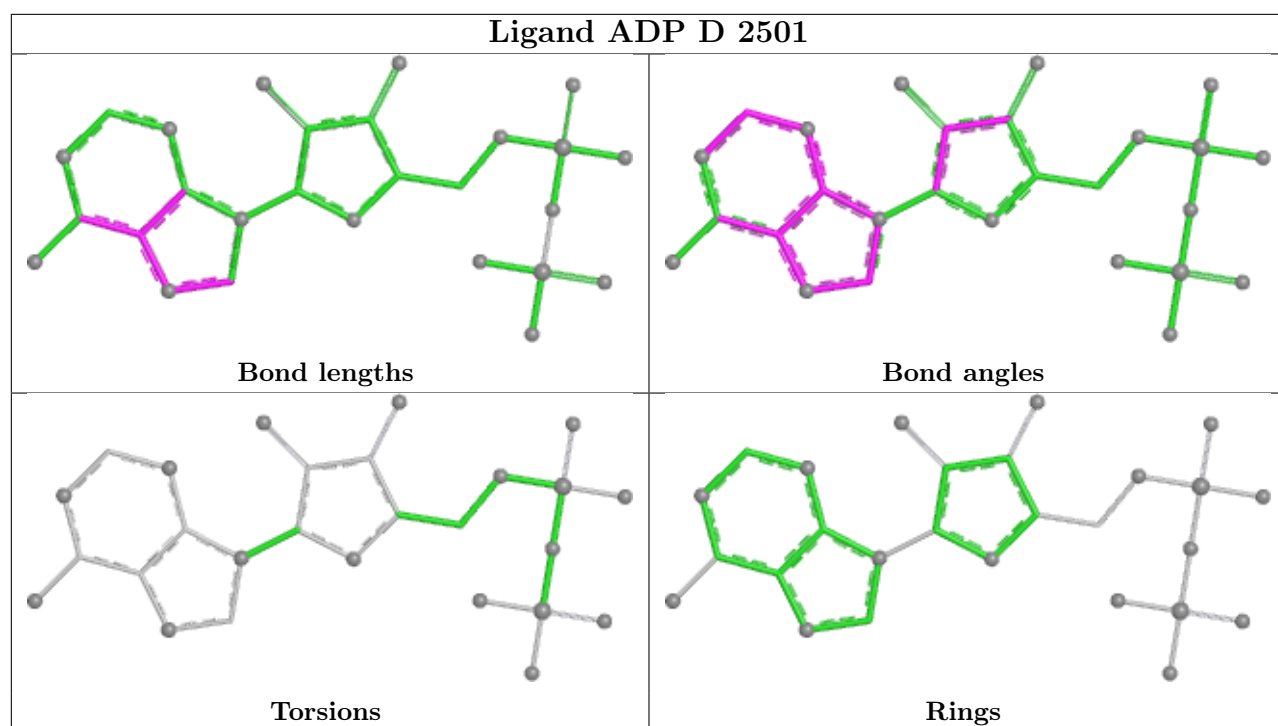
There are no ring outliers.

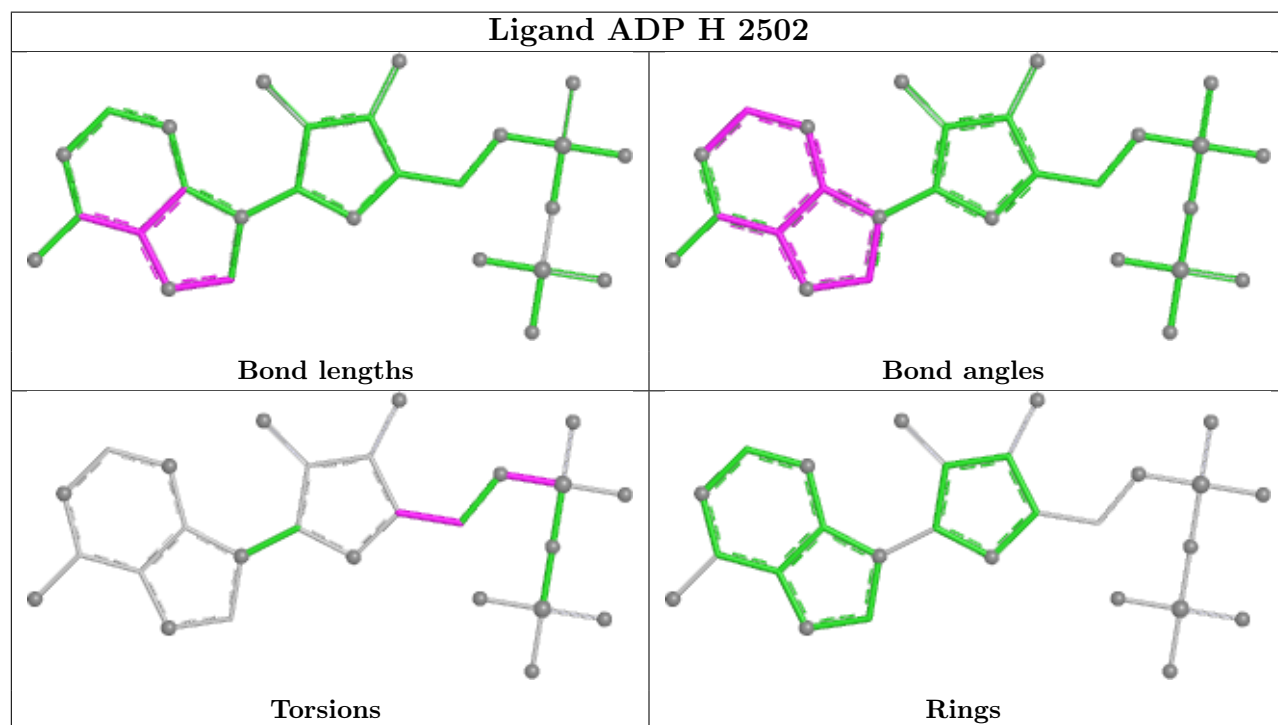
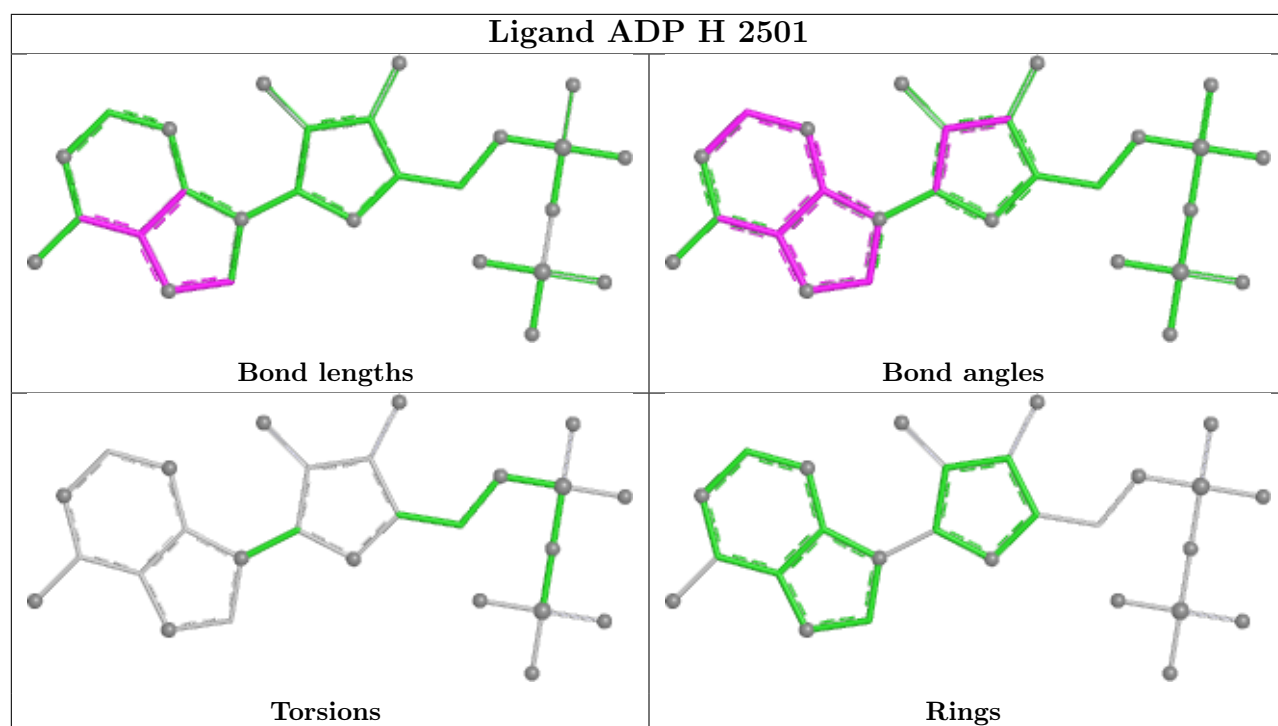
12 monomers are involved in 55 short contacts:

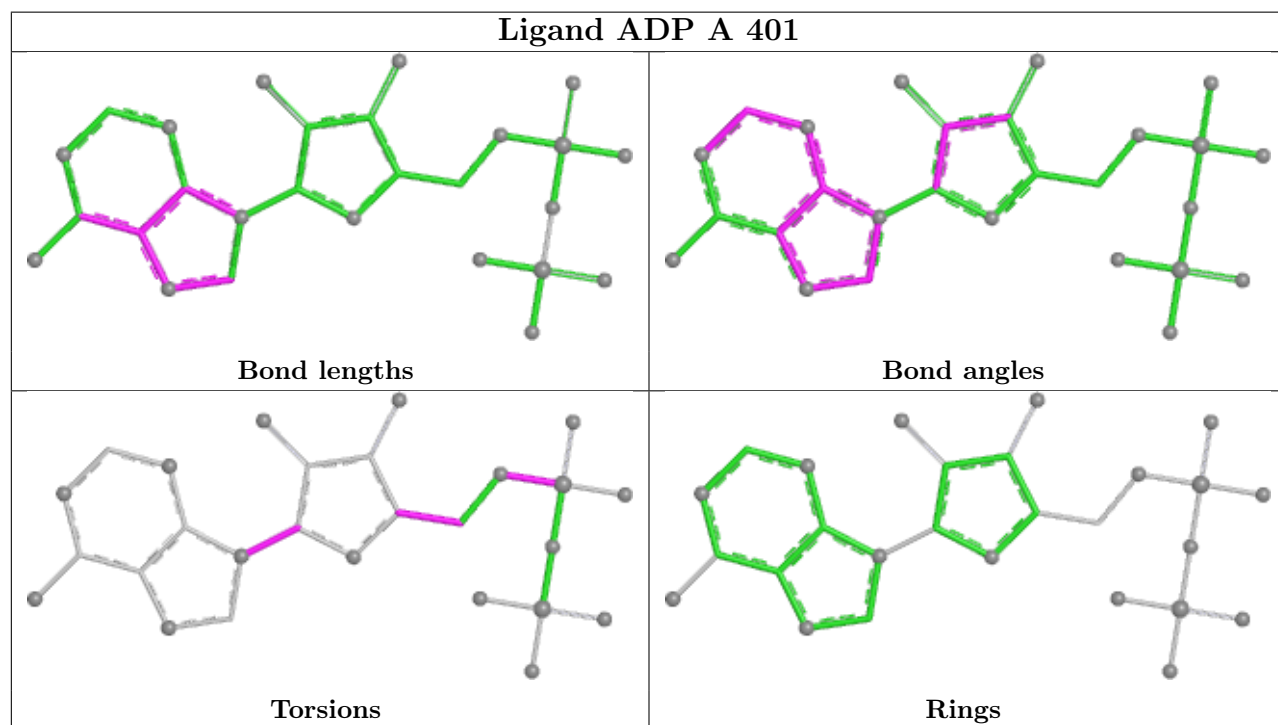
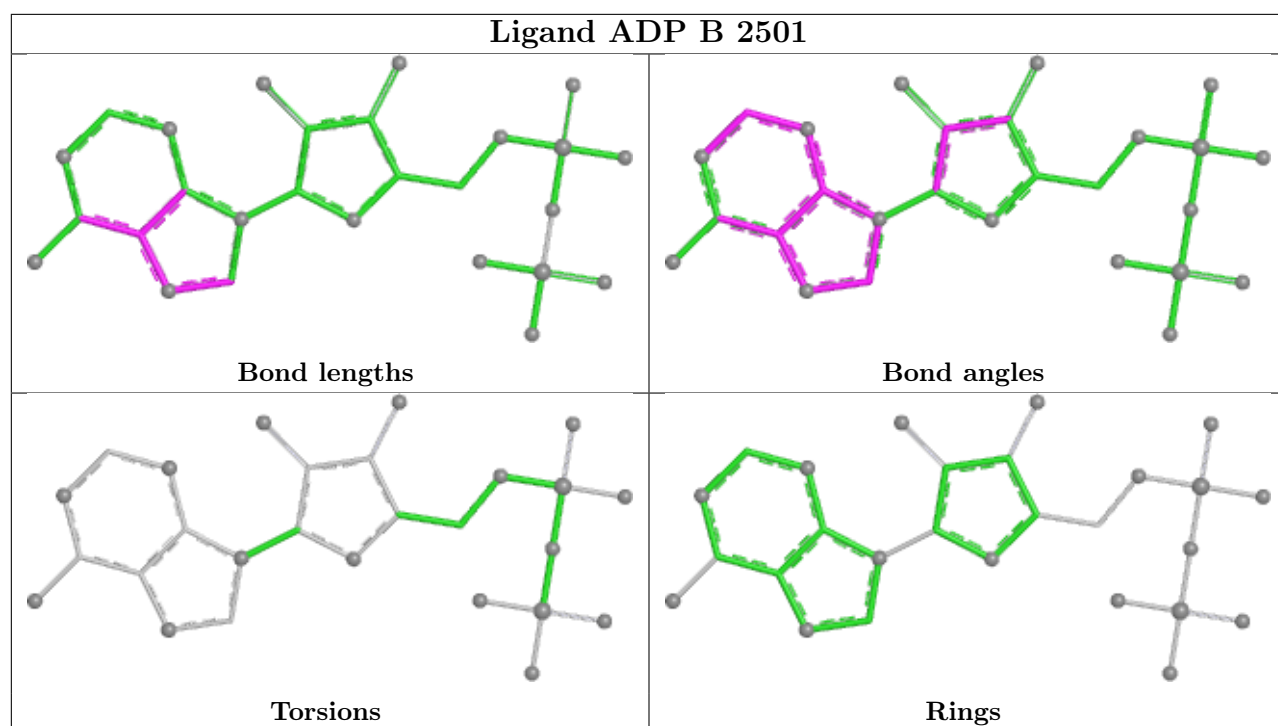
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2502	ADP	2	0
3	D	2502	ADP	3	0
3	D	2501	ADP	1	0
3	E	401	ADP	9	0
3	H	2501	ADP	2	0
3	H	2502	ADP	3	0
3	B	2501	ADP	2	0
3	A	401	ADP	10	0
3	B	2502	ADP	3	0
3	F	2501	ADP	2	0
3	G	401	ADP	9	0
3	C	401	ADP	9	0

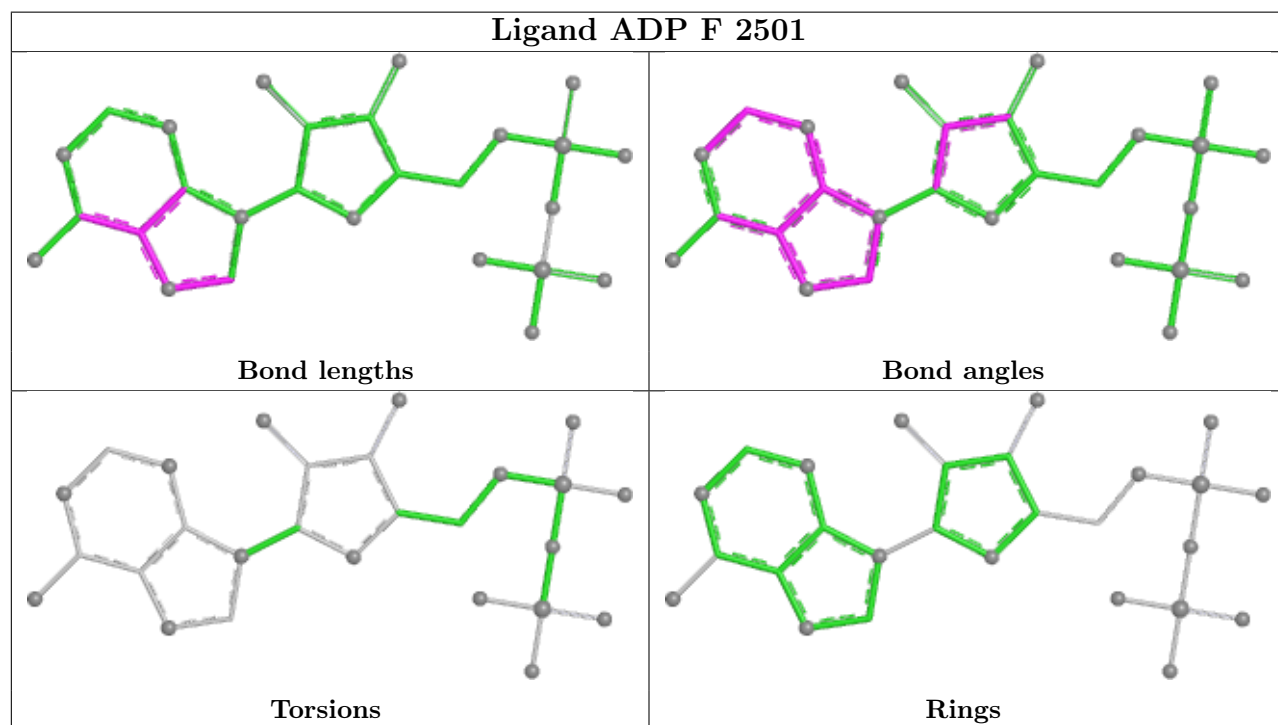
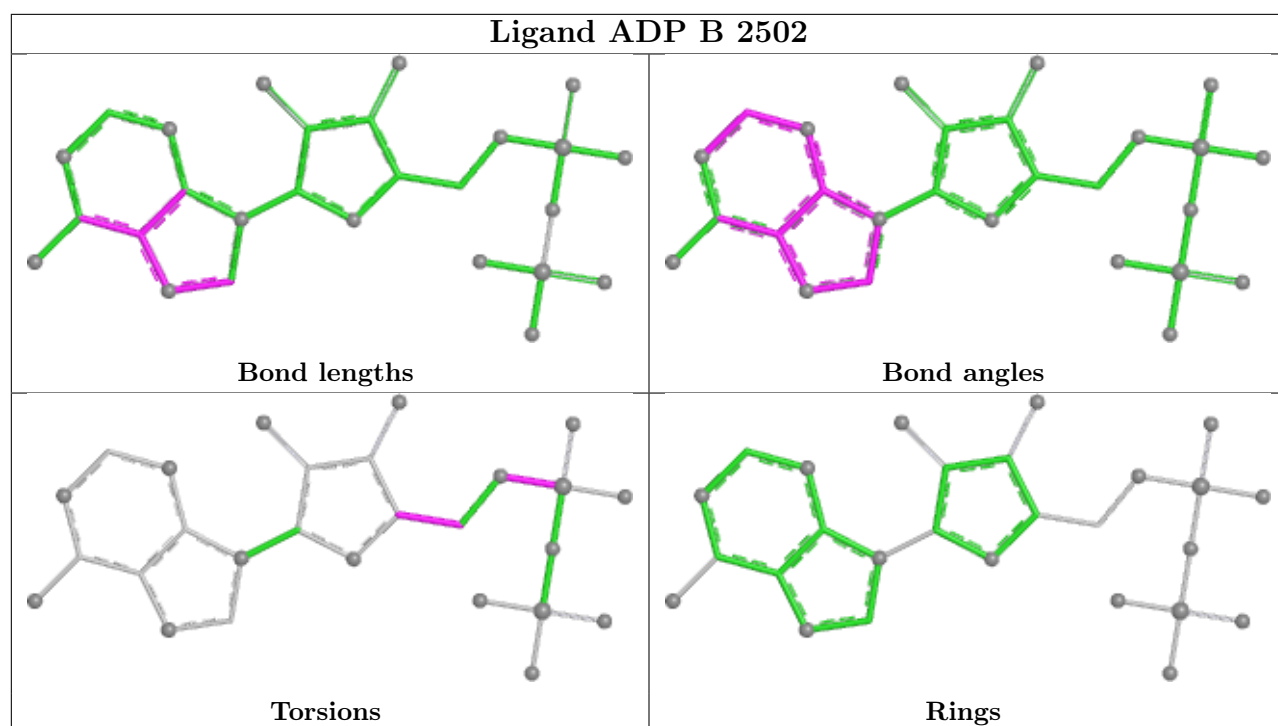
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

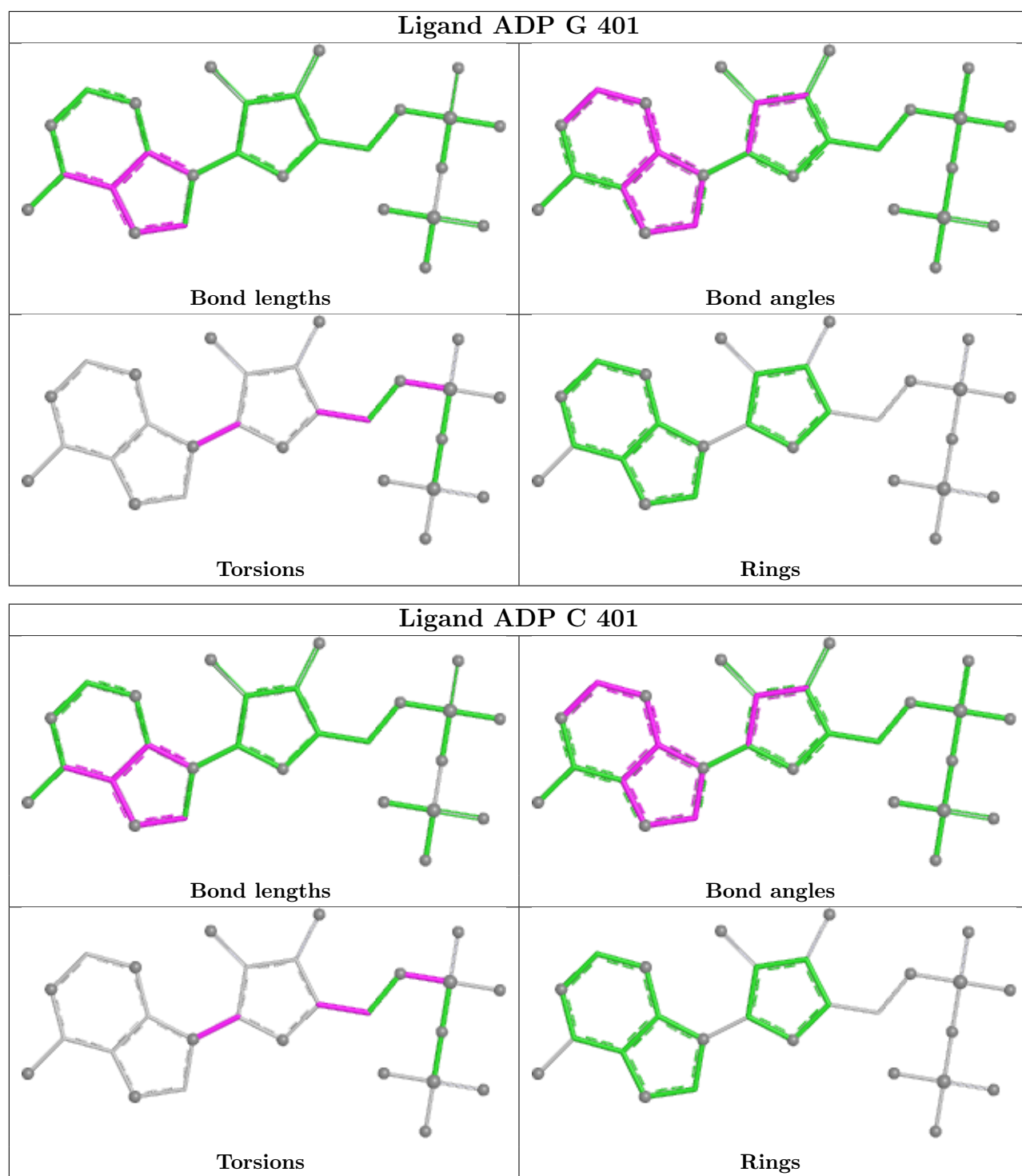












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

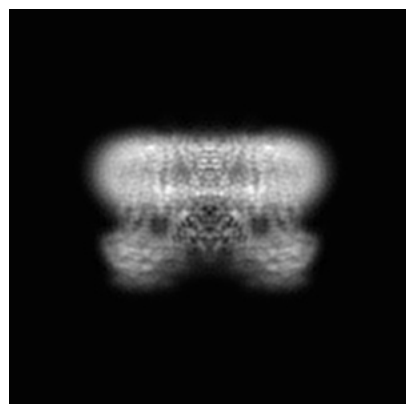
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6852. These allow visual inspection of the internal detail of the map and identification of artifacts.

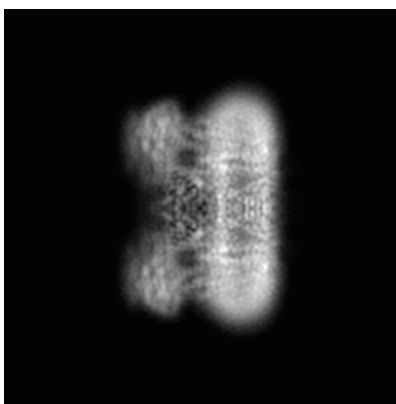
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

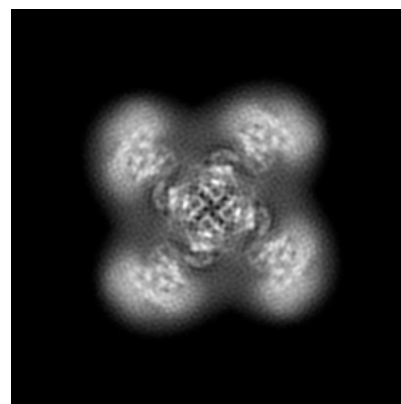
6.1.1 Primary map



X

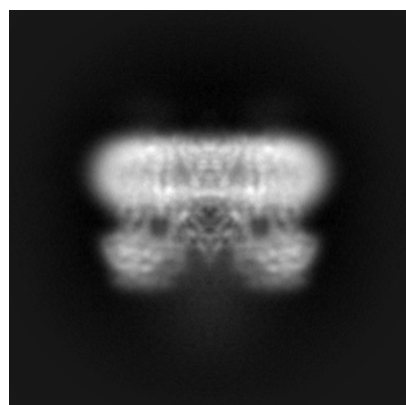


Y

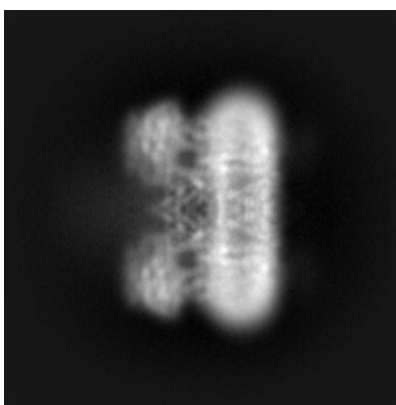


Z

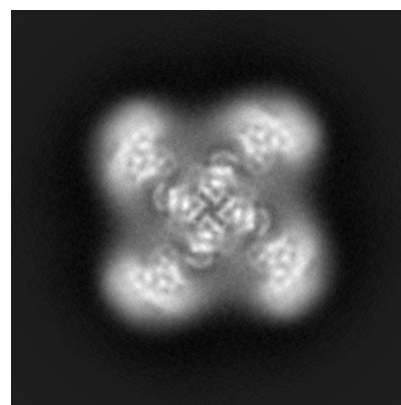
6.1.2 Raw map



X



Y

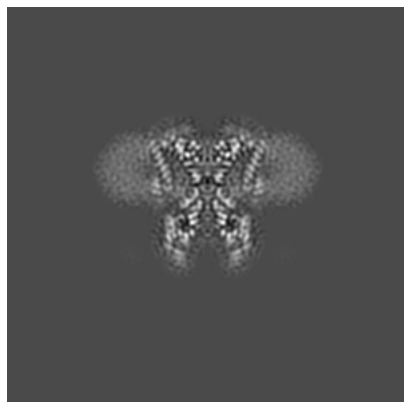


Z

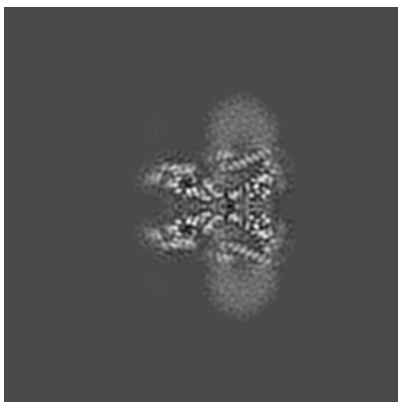
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

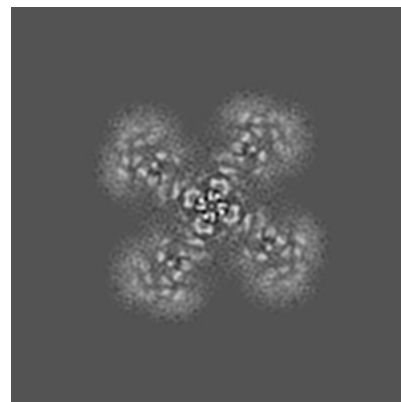
6.2.1 Primary map



X Index: 156

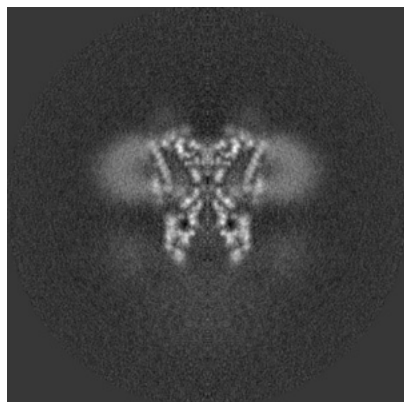


Y Index: 156

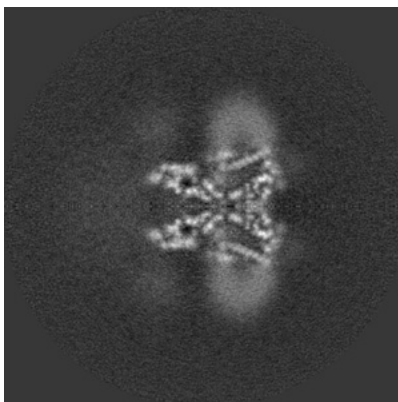


Z Index: 156

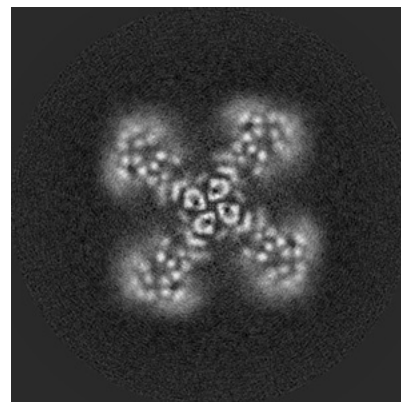
6.2.2 Raw map



X Index: 156



Y Index: 156

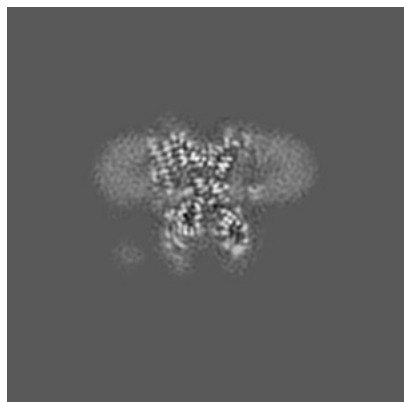


Z Index: 156

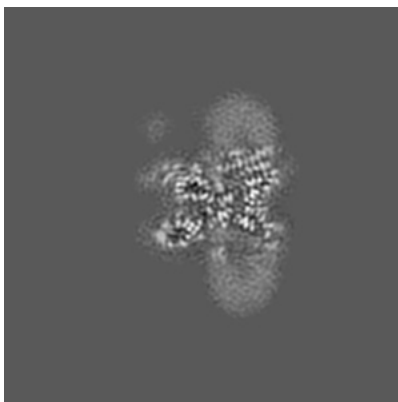
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

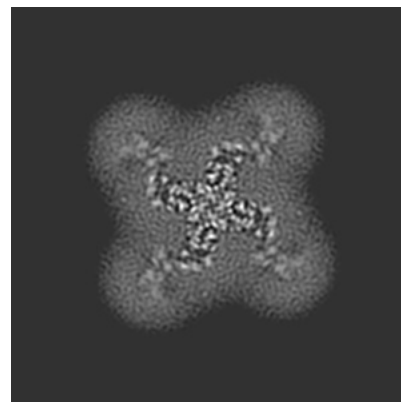
6.3.1 Primary map



X Index: 152

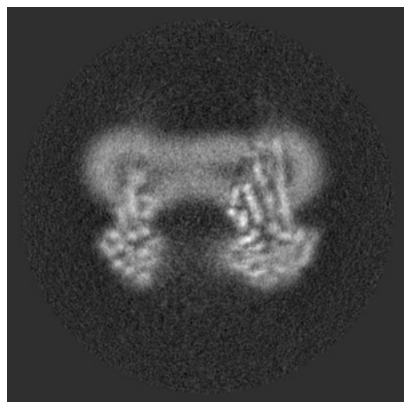


Y Index: 152

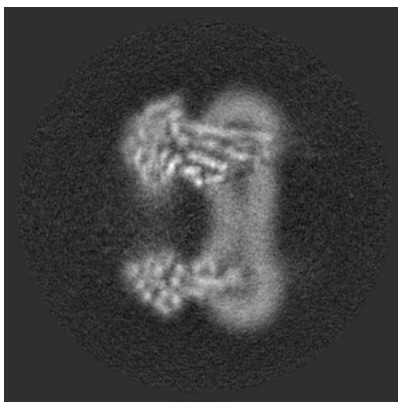


Z Index: 203

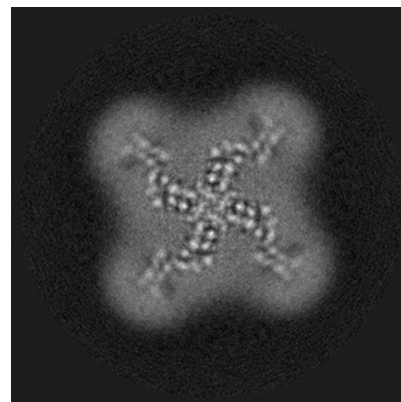
6.3.2 Raw map



X Index: 97



Y Index: 215

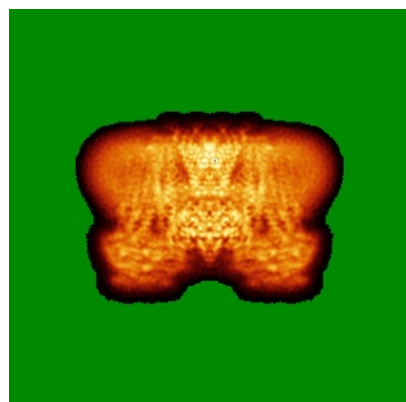


Z Index: 202

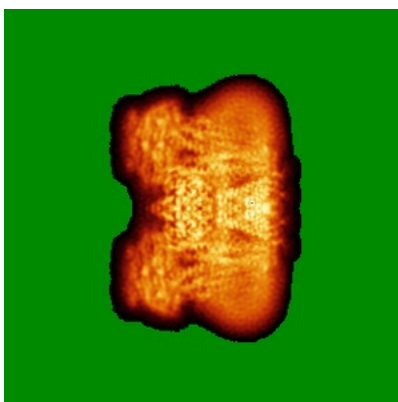
The images above show the largest variance slices of the map in three orthogonal directions.

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

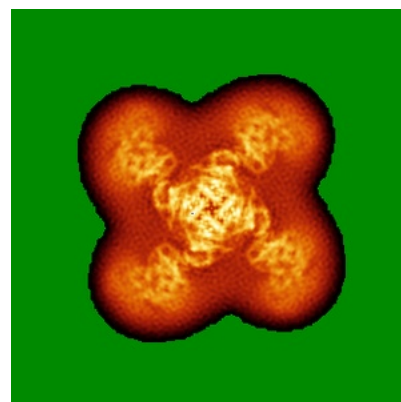
6.4.1 Primary map



X

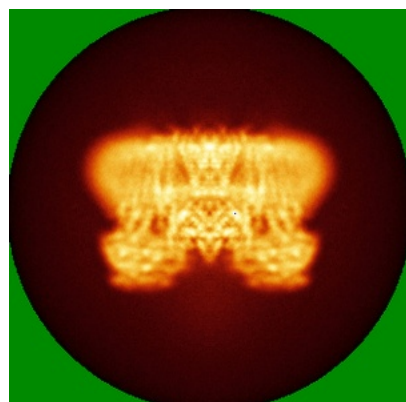


Y

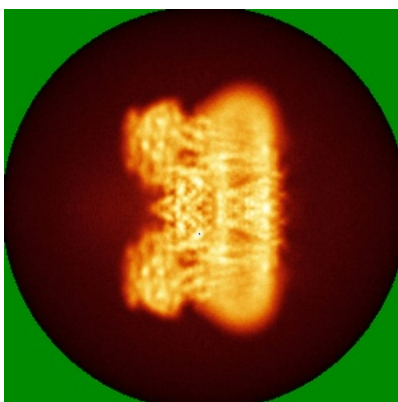


Z

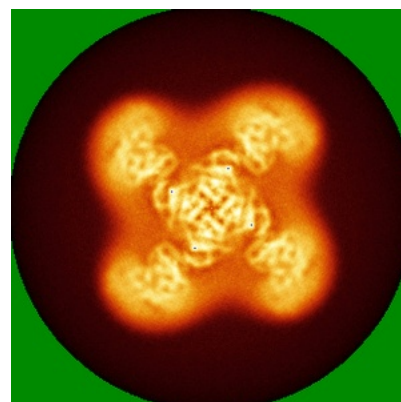
6.4.2 Raw map



X



Y

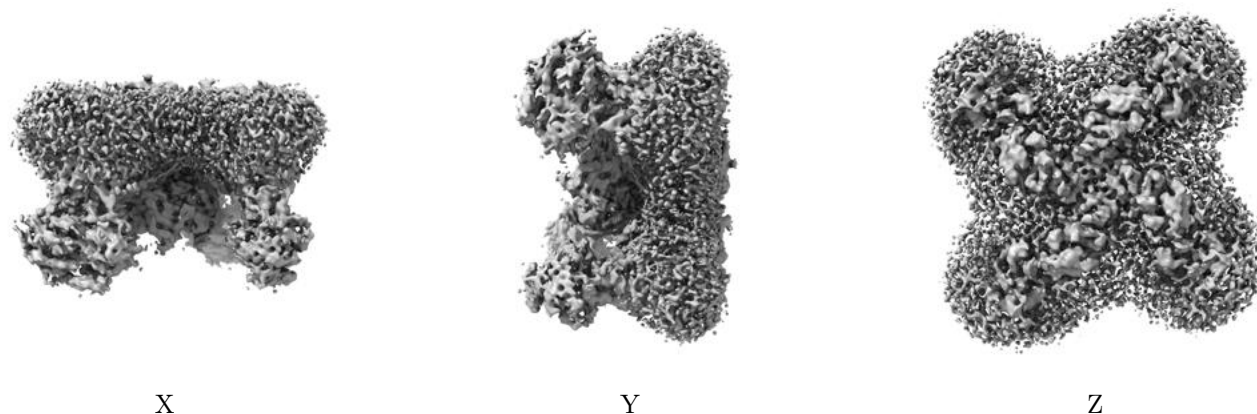


Z

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

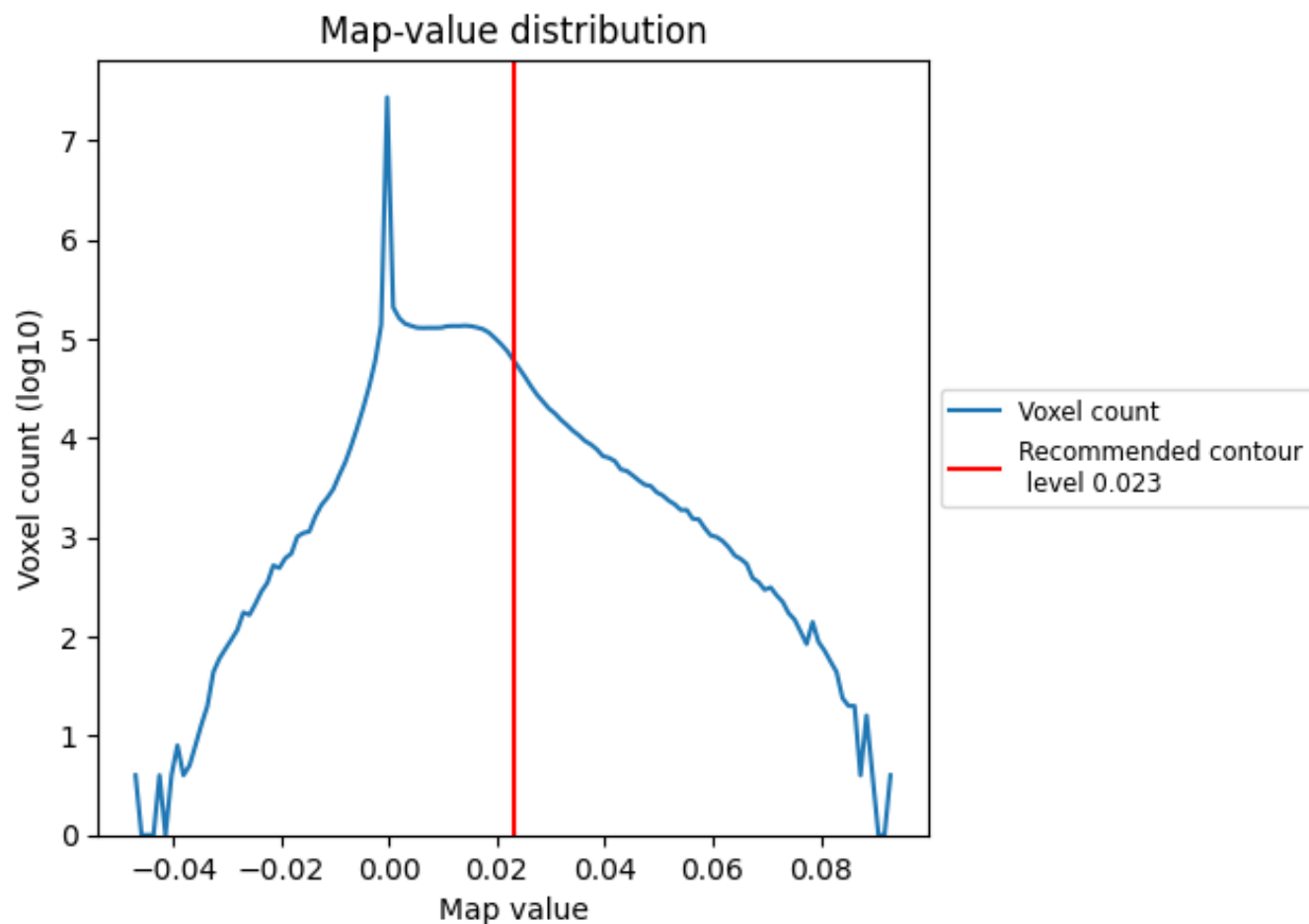
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

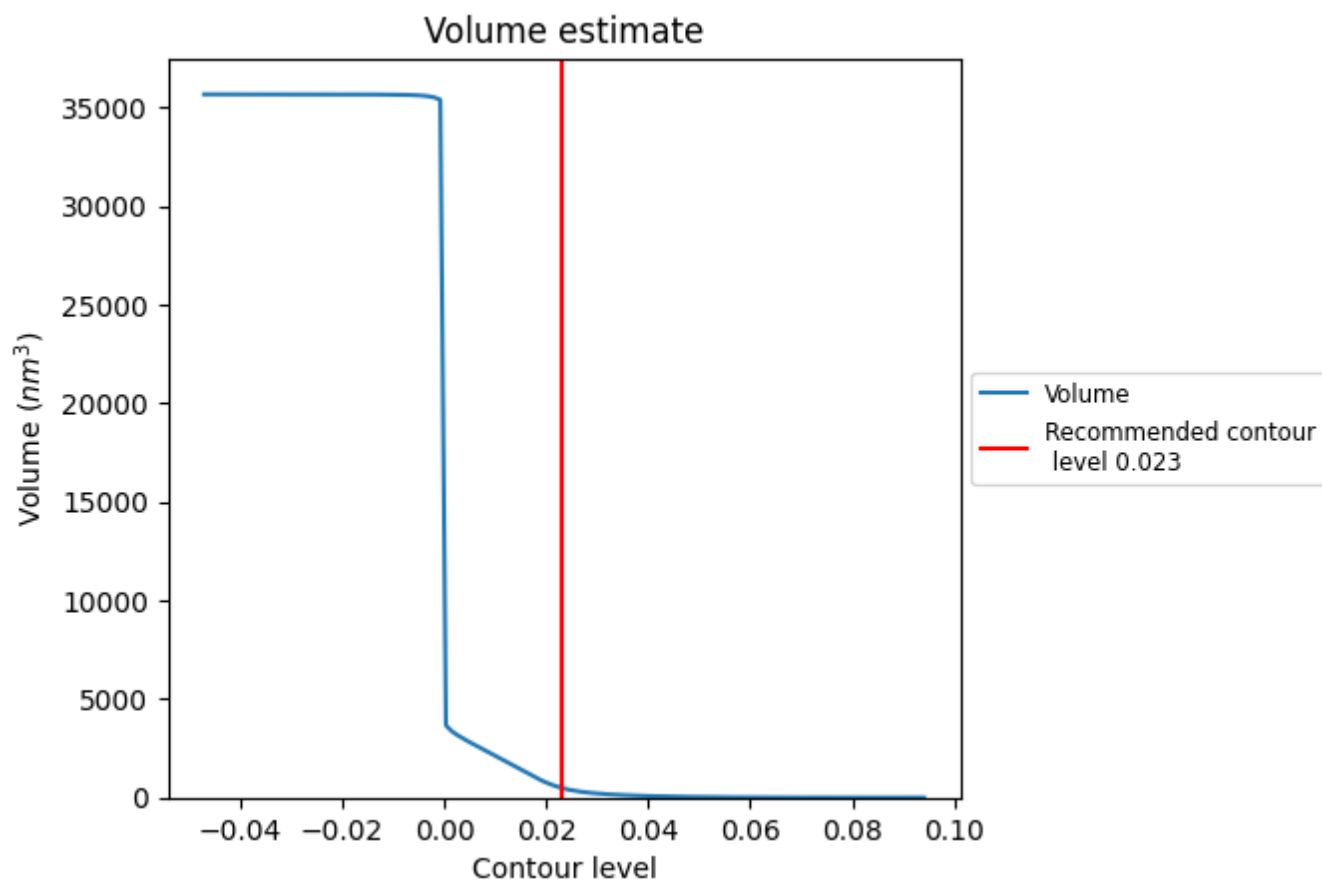
This section contains the results of statistical analysis of the map.

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.

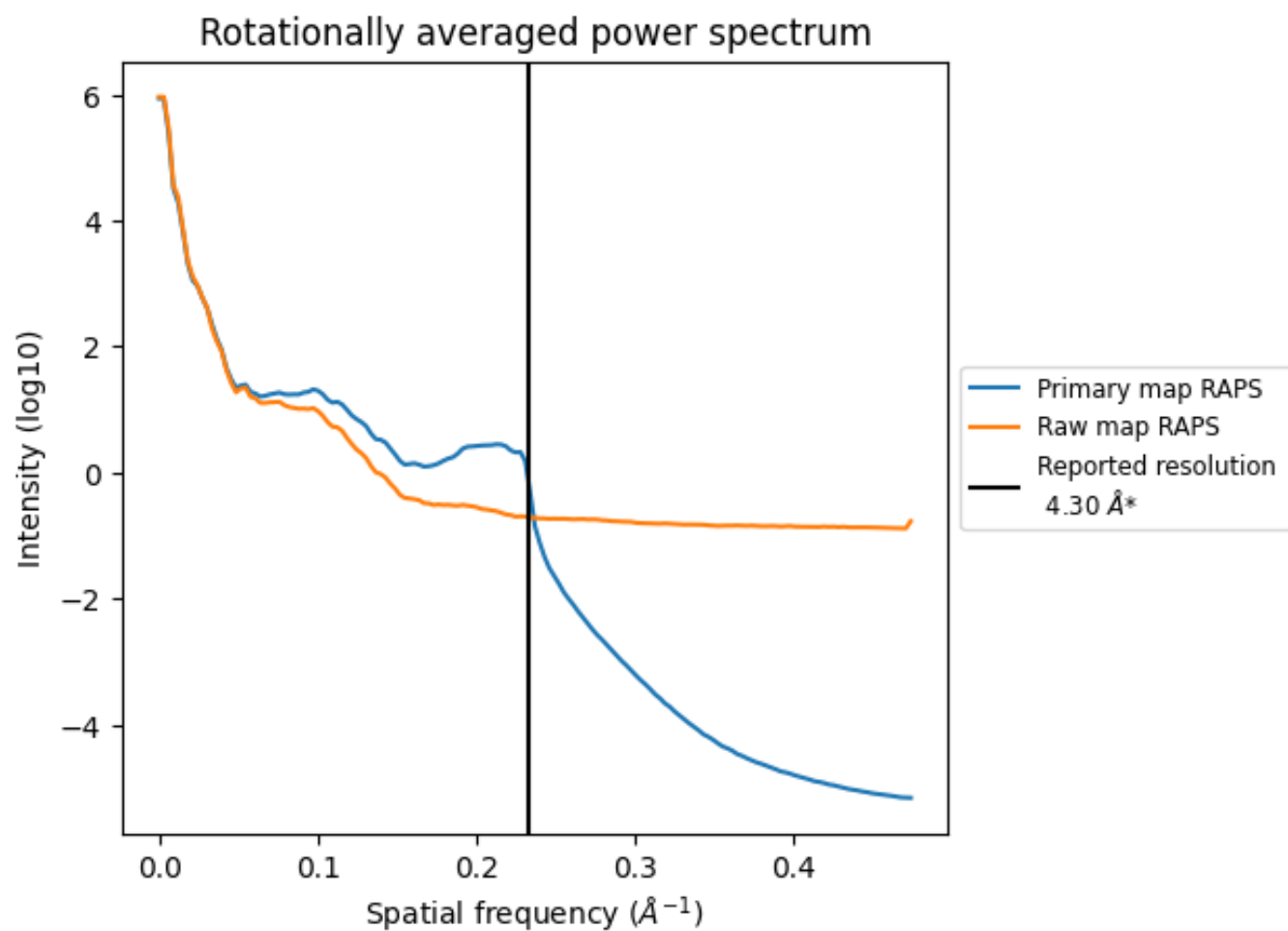
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 ⓘ

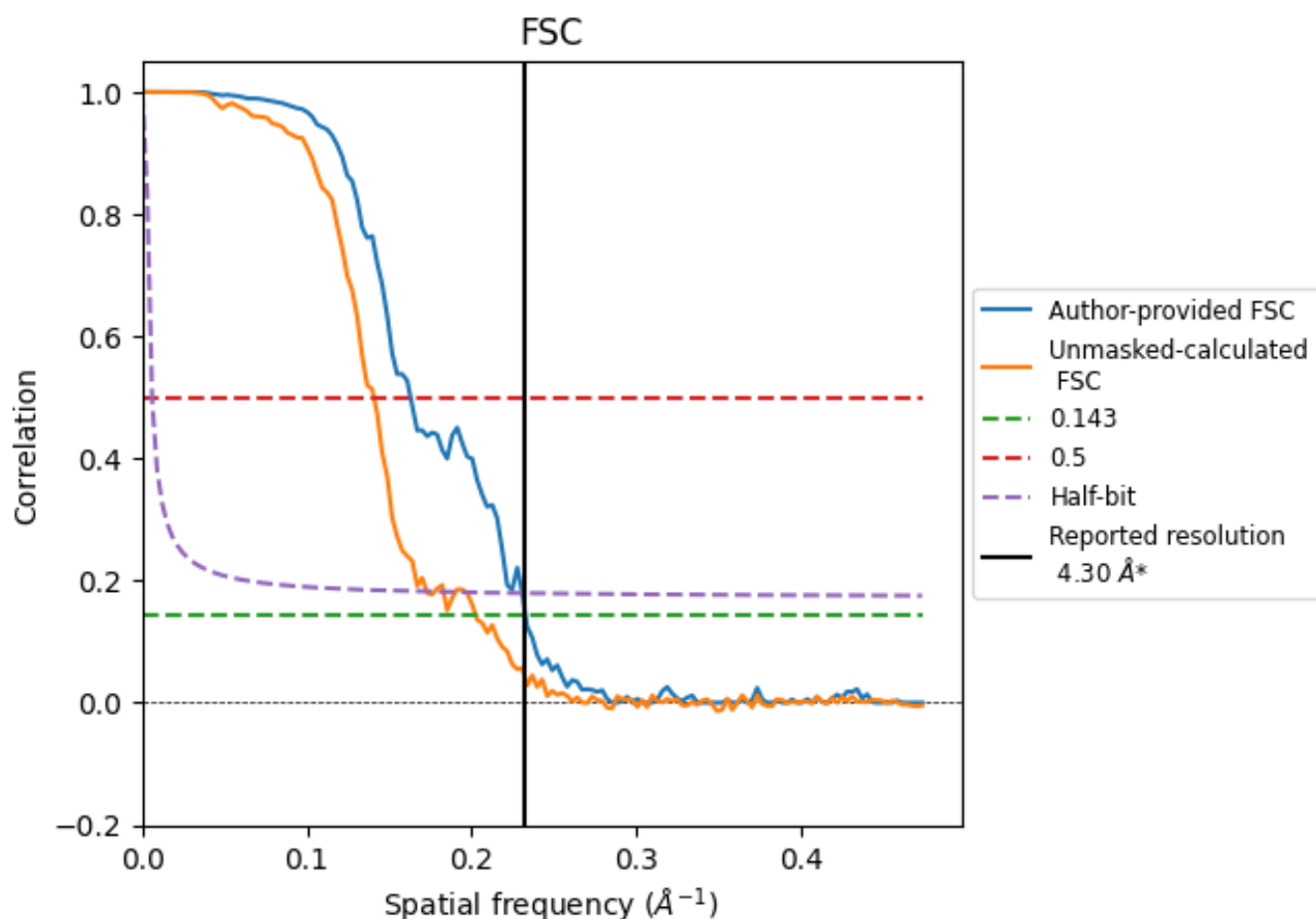


*Reported resolution corresponds to spatial frequency of 0.233 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.233 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

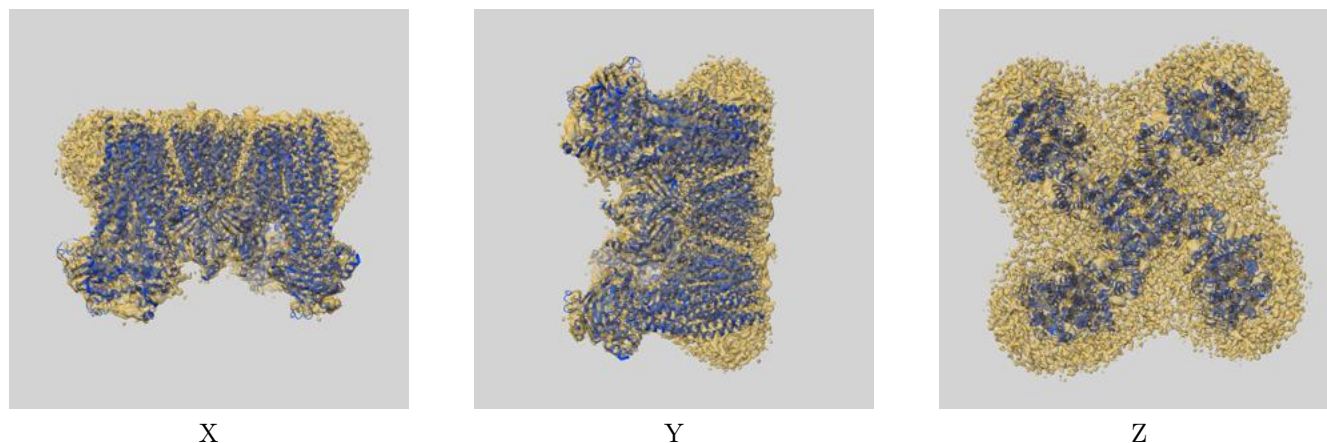
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.29	6.13	4.33
Unmasked-calculated*	4.93	7.10	5.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.93 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

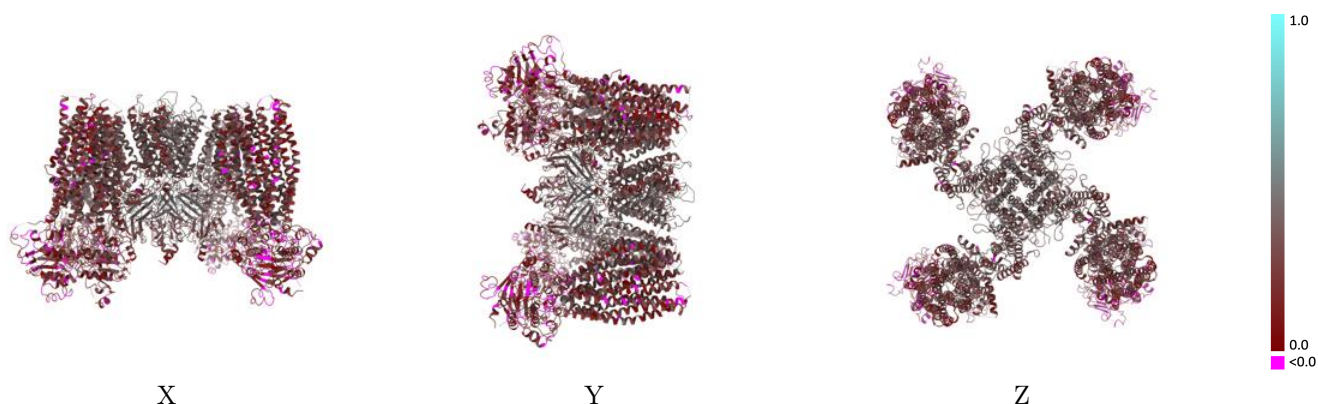
This section contains information regarding the fit between EMDB map EMD-6852 and PDB model 5YWC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



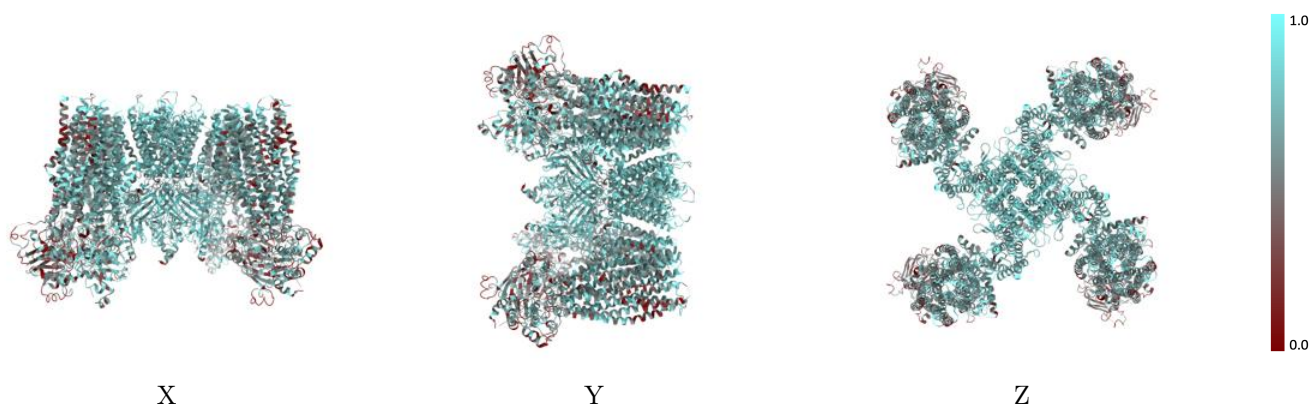
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



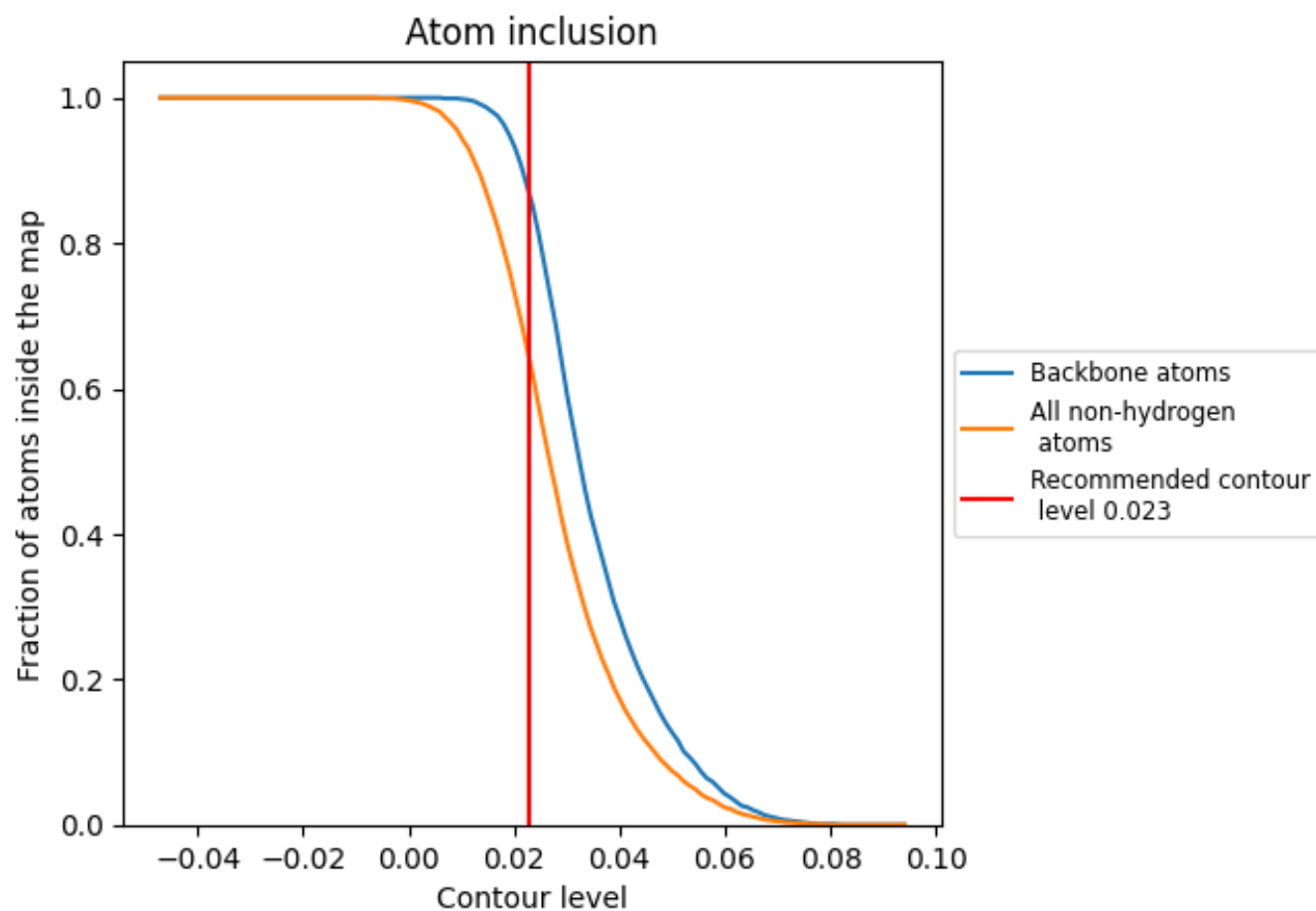
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6370	0.2590
A	0.7920	0.3680
B	0.5990	0.2330
C	0.7920	0.3680
D	0.5990	0.2320
E	0.7930	0.3670
F	0.5990	0.2330
G	0.7920	0.3650
H	0.5990	0.2330

1.0

0.0

<0.0