Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 02:37 PM JST

PDB ID	:	9KGL / pdb_00009kgl
EMDB ID	:	EMD-62322
Title	:	Structure of KATP channel in complex with centipede toxin SpTx1
Authors	:	Chen, L.
Deposited on	:	2024-11-08
Resolution	:	2.88 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:

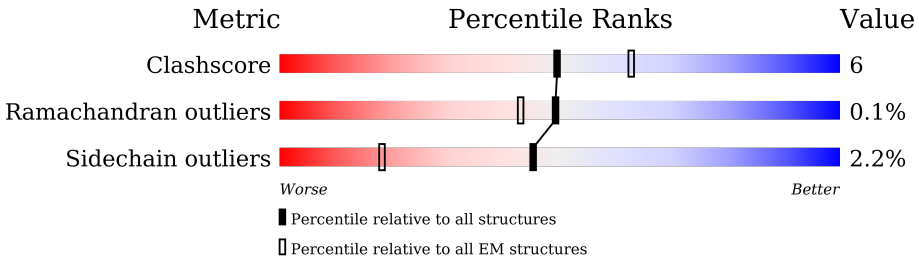
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

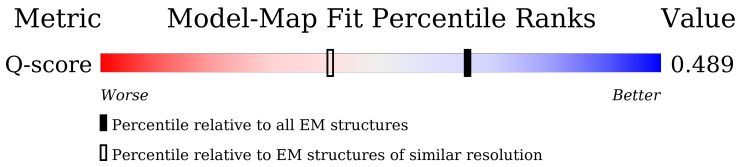
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.88 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.





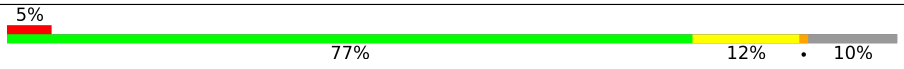
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

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 <=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	72% 12% • 16%
1	C	390	71% 12% • 16%
1	E	390	71% 12% • 16%
1	G	390	71% 12% • 16%

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Mol	Chain	Length	Quality of chain
2	B	1582	
2	D	1582	
2	F	1582	
2	H	1582	
3	I	56	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 55831 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	327	Total	C	N	O	S	0	0
			2560	1649	440	454	17		
1	C	327	Total	C	N	O	S	0	0
			2560	1649	440	454	17		
1	E	327	Total	C	N	O	S	0	0
			2559	1649	440	453	17		
1	G	327	Total	C	N	O	S	0	0
			2560	1649	440	454	17		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLU	LYS	variant	UNP Q14654
A	52	GLU	GLN	conflict	UNP Q14654
A	337	ILE	VAL	variant	UNP Q14654
C	23	GLU	LYS	variant	UNP Q14654
C	52	GLU	GLN	conflict	UNP Q14654
C	337	ILE	VAL	variant	UNP Q14654
E	23	GLU	LYS	variant	UNP Q14654
E	52	GLU	GLN	conflict	UNP Q14654
E	337	ILE	VAL	variant	UNP Q14654
G	23	GLU	LYS	variant	UNP Q14654
G	52	GLU	GLN	conflict	UNP Q14654
G	337	ILE	VAL	variant	UNP Q14654

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1429	Total	C	N	O	S	0	0
			11199	7293	1894	1953	59		
2	D	1429	Total	C	N	O	S	0	0
			11199	7293	1894	1953	59		
2	F	1429	Total	C	N	O	S	0	0
			11199	7293	1894	1953	59		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	1429	Total	C	N	O	S	0	0
			11199	7293	1894	1953	59		

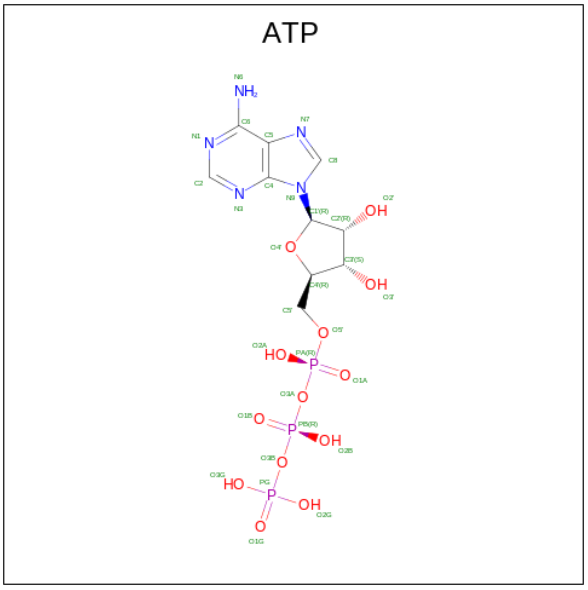
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	LYS	GLU	conflict	UNP A0A1U7R319
D	203	LYS	GLU	conflict	UNP A0A1U7R319
F	203	LYS	GLU	conflict	UNP A0A1U7R319
H	203	LYS	GLU	conflict	UNP A0A1U7R319

- Molecule 3 is a protein called SpTx1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	50	Total	C	N	O	S	0	0
			416	268	73	71	4		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



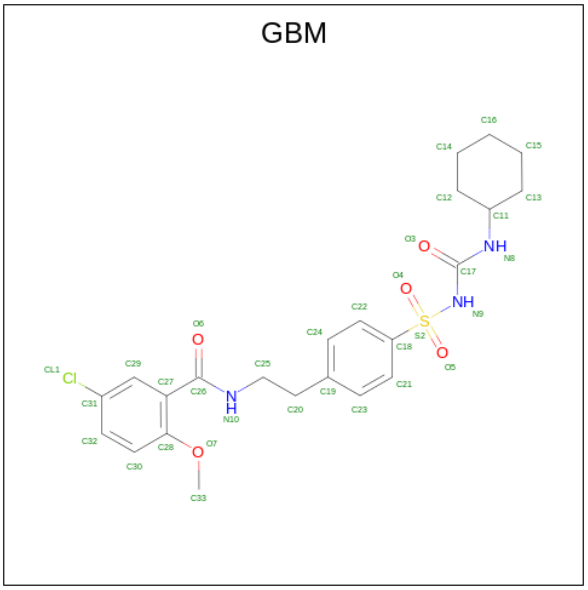
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 5 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (CCD ID: GBM) (formula: $C_{23}H_{28}ClN_3O_5S$).



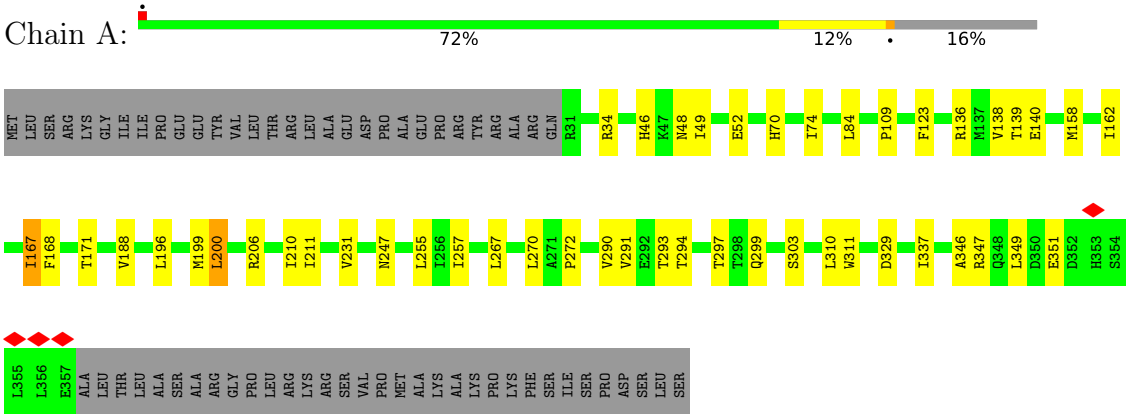
Mol	Chain	Residues	Atoms							AltConf
5	B	1	Total	C	Cl	N	O	S		0
			33	23	1	3	5	1		
5	D	1	Total	C	Cl	N	O	S		0
			33	23	1	3	5	1		
5	F	1	Total	C	Cl	N	O	S		0
			33	23	1	3	5	1		
5	H	1	Total	C	Cl	N	O	S		0
			33	23	1	3	5	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

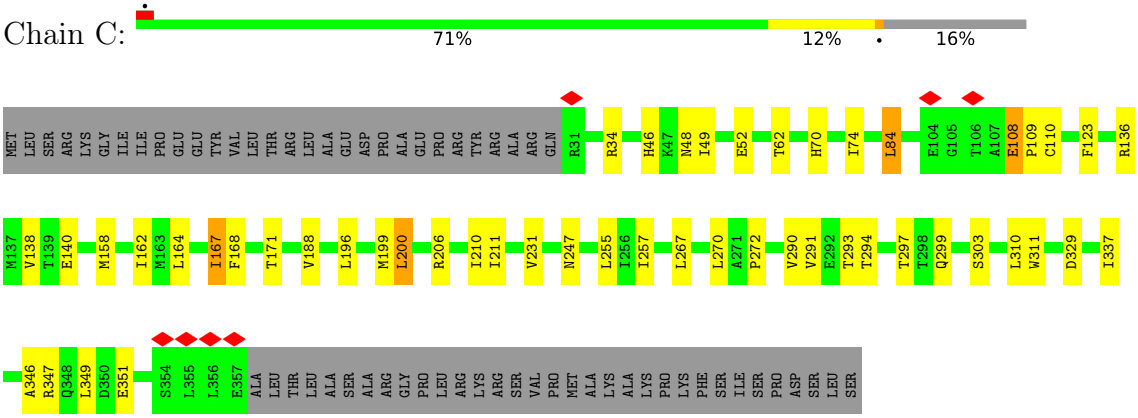
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain A:



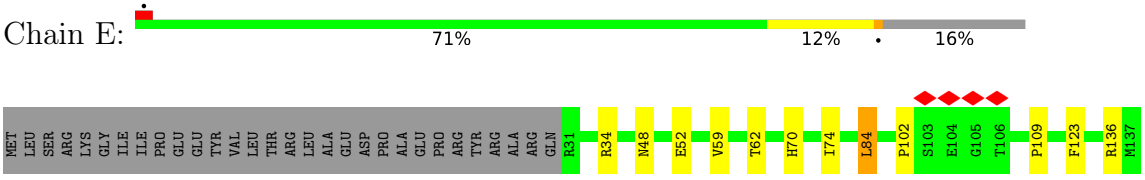
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

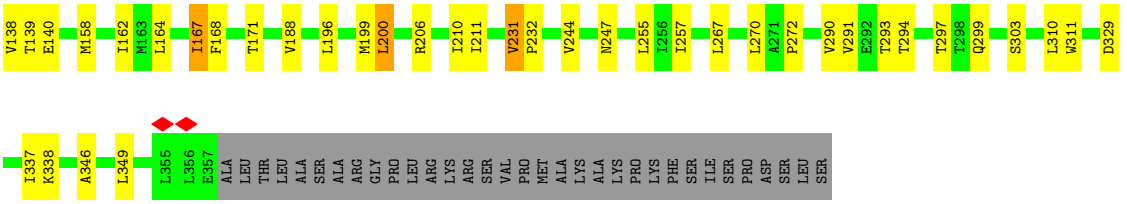
Chain C:



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

Chain E:

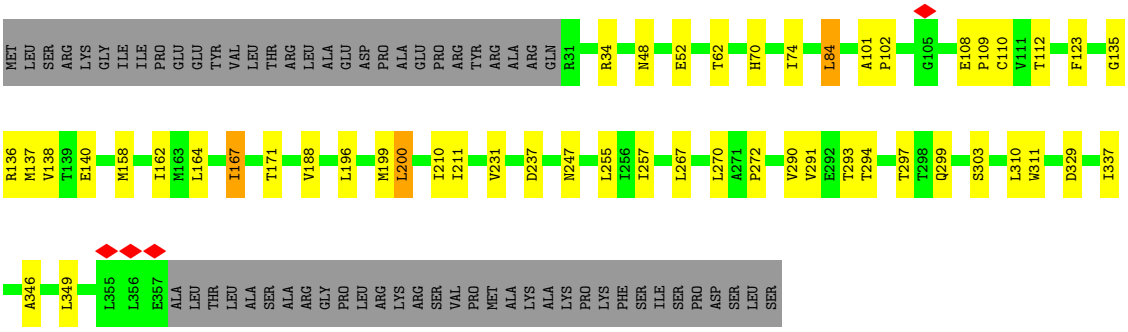




• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain G:

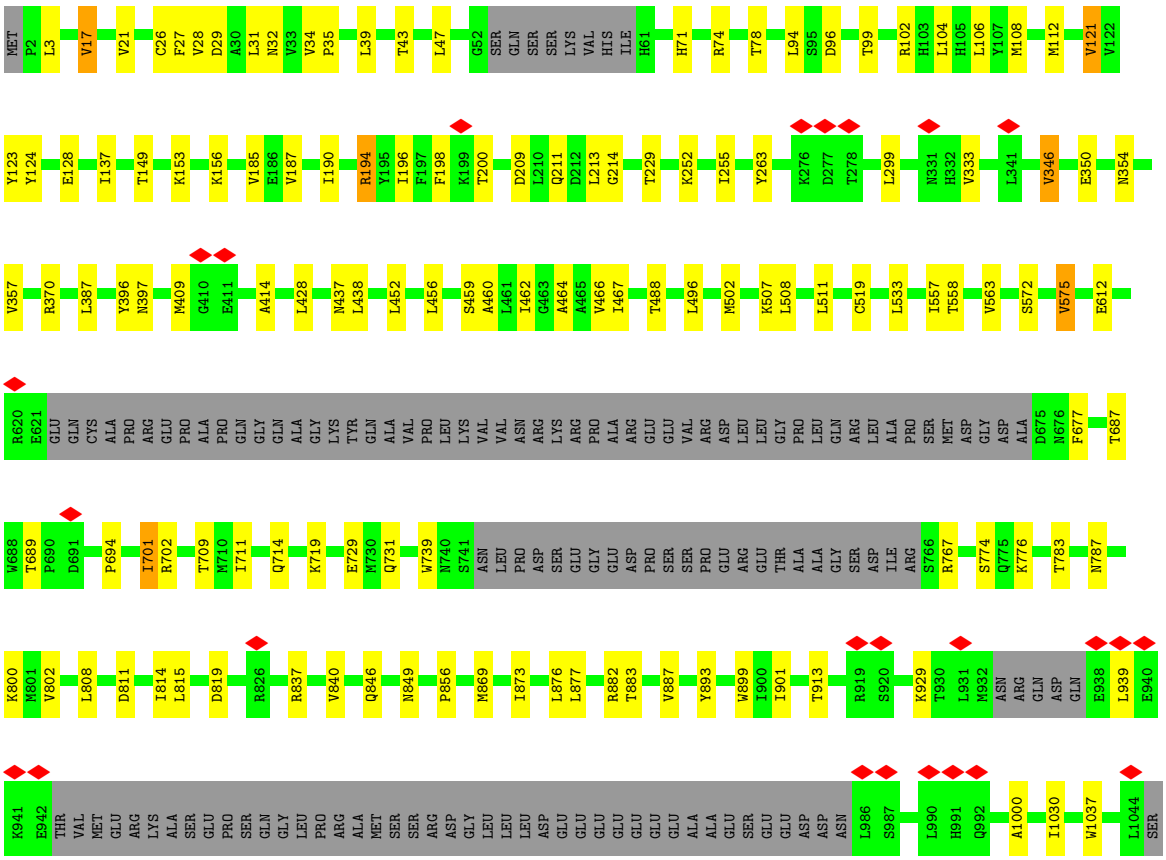


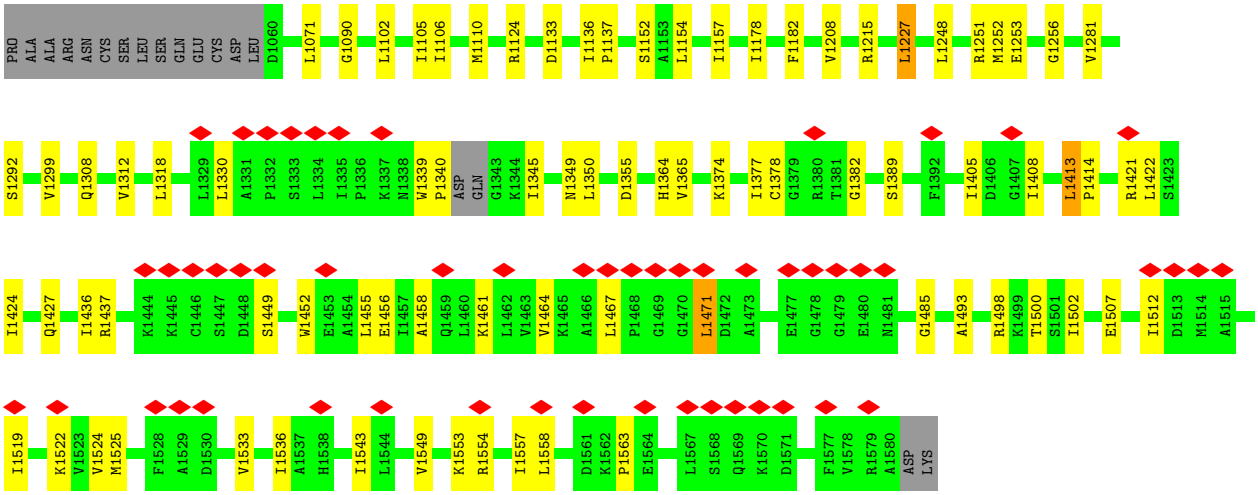


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain B:



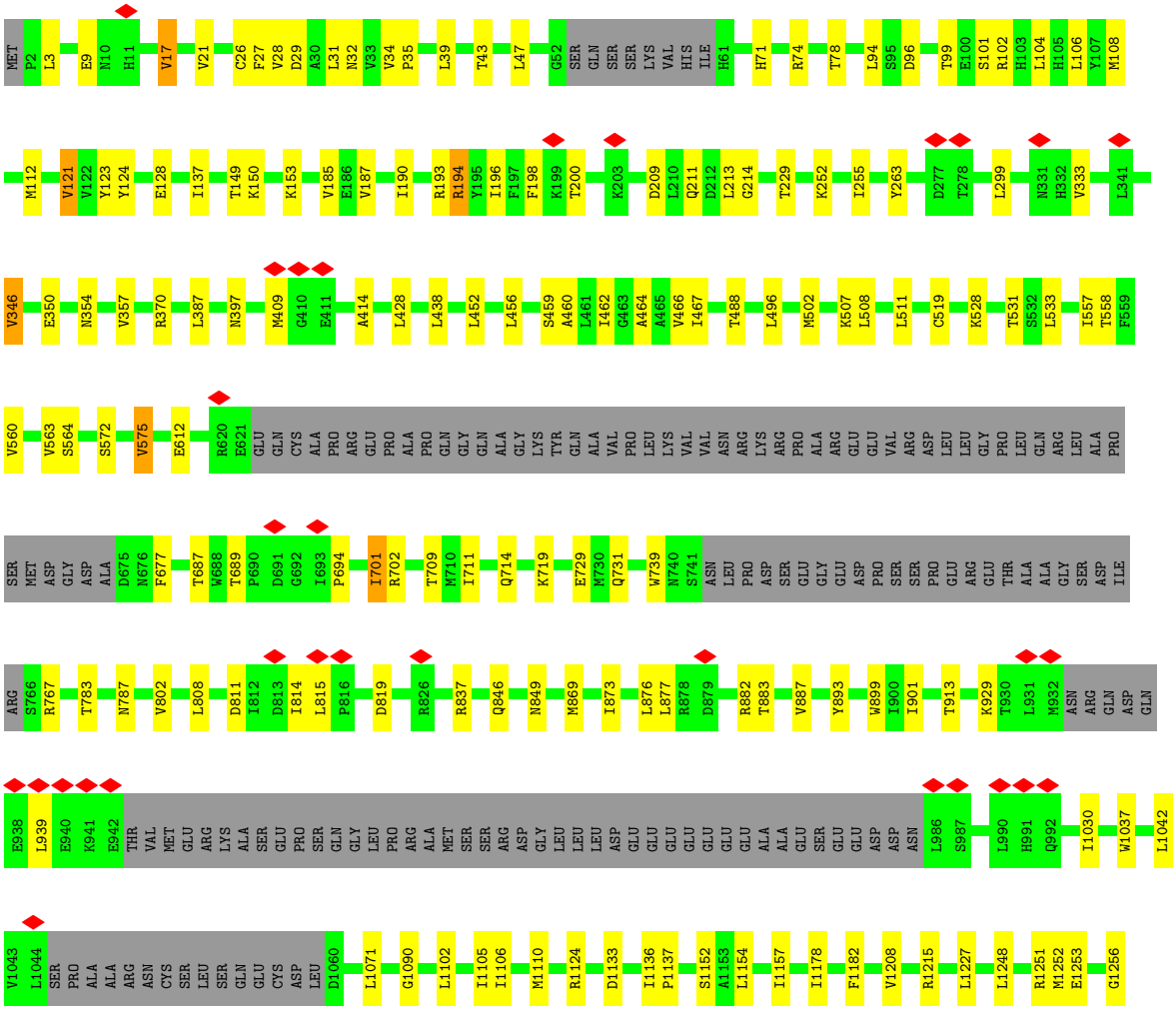


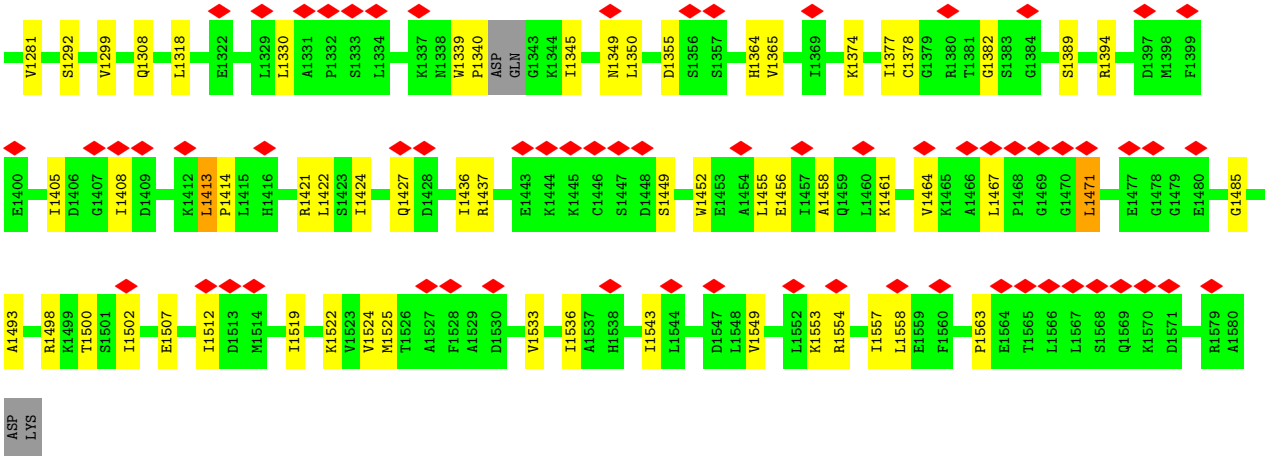


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain D:



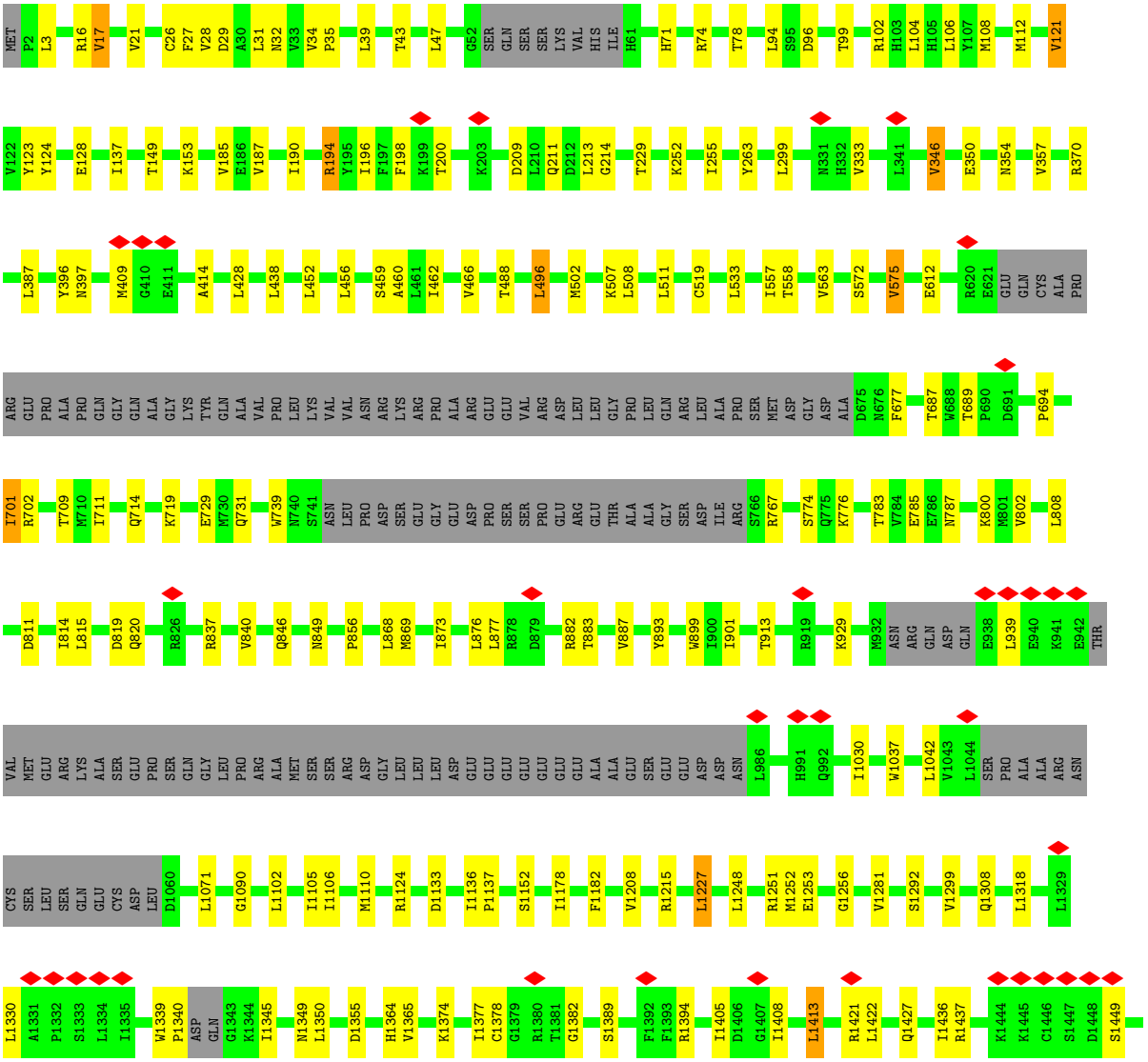


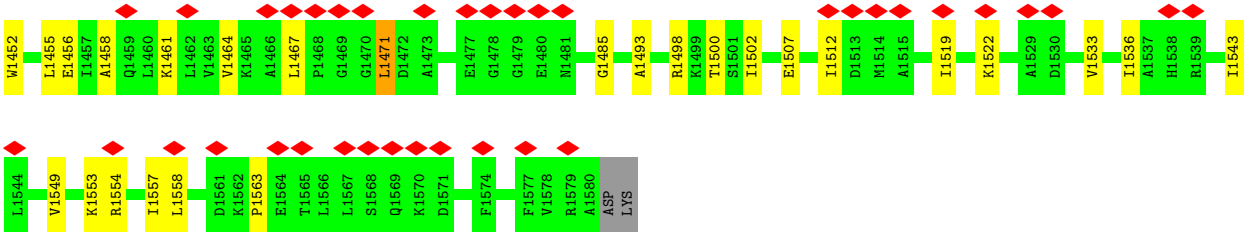


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain F:



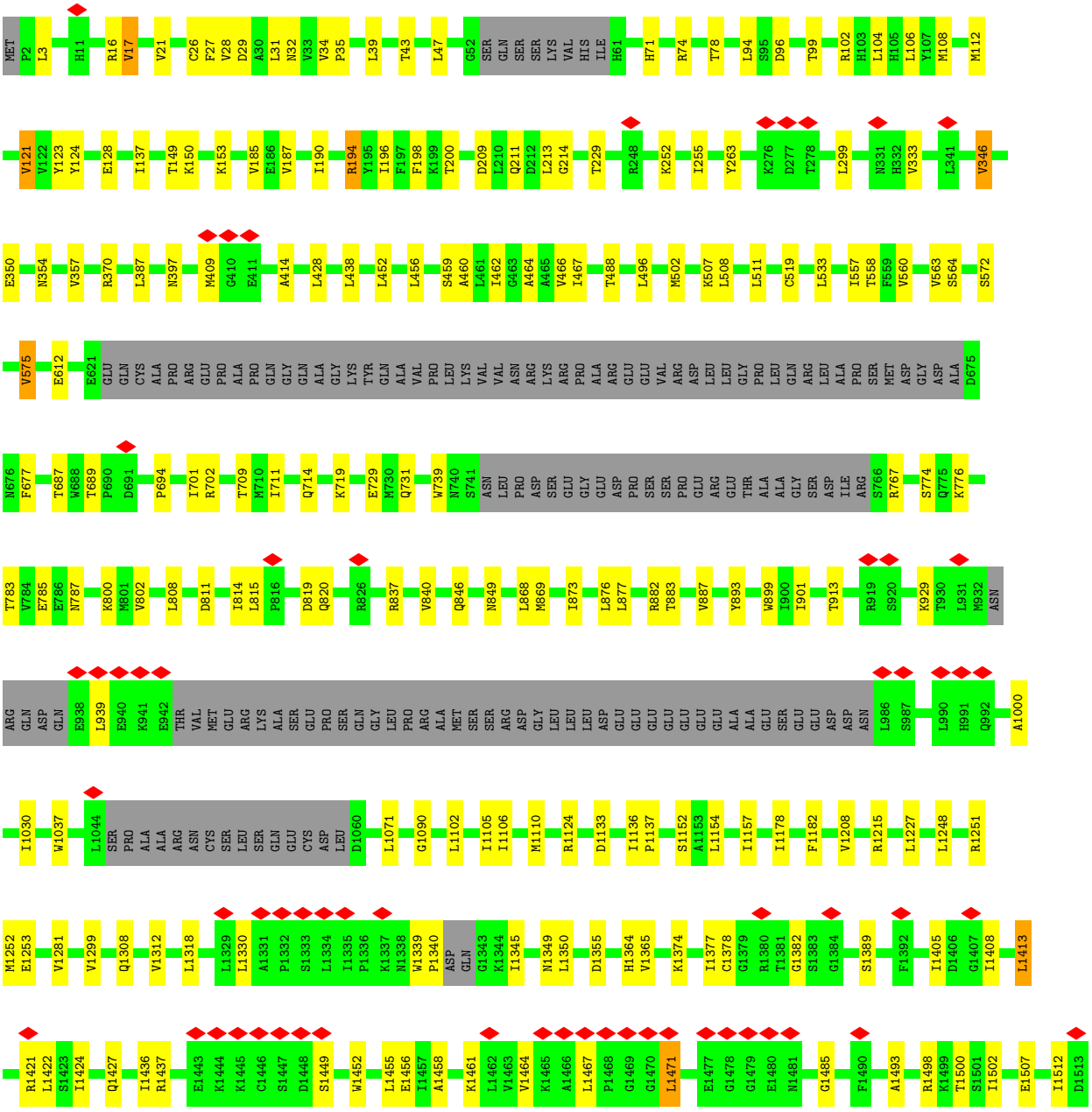


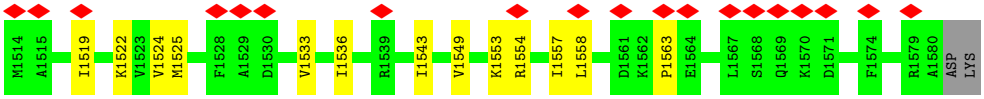


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

Chain H:







• Molecule 3: SpTx1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246583	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.588	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.075	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	338.944, 338.944, 338.944	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.324, 1.324, 1.324	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/2618	0.36	0/3558
1	C	0.22	0/2618	0.44	3/3558 (0.1%)
1	E	0.17	0/2617	0.37	0/3557
1	G	0.23	1/2618 (0.0%)	0.43	1/3558 (0.0%)
2	B	0.19	0/11437	0.38	0/15527
2	D	0.19	0/11437	0.38	0/15527
2	F	0.19	0/11437	0.38	0/15527
2	H	0.19	0/11437	0.38	0/15527
3	I	0.26	0/426	0.59	0/566
All	All	0.19	1/56645 (0.0%)	0.38	4/76905 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	101	ALA	C-N	5.84	1.47	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	110	CYS	N-CA-C	-7.16	103.40	111.14
1	C	110	CYS	N-CA-C	-6.70	103.91	111.14
1	C	108	GLU	CA-C-N	6.01	125.98	120.03
1	C	108	GLU	C-N-CA	6.01	125.98	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2591	29	0
1	C	2560	0	2591	33	0
1	E	2559	0	2588	35	0
1	G	2560	0	2591	44	0
2	B	11199	0	11498	131	0
2	D	11199	0	11498	130	0
2	F	11199	0	11498	133	0
2	H	11199	0	11498	131	0
3	I	416	0	415	24	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
5	B	33	0	28	1	0
5	D	33	0	28	0	0
5	F	33	0	28	0	0
5	H	33	0	28	0	0
All	All	55831	0	56976	644	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 6.

All (644) 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:B:1339:TRP:HB3	2:B:1421:ARG:HG2	1.32	1.11
2:D:1339:TRP:HB3	2:D:1421:ARG:HG2	1.32	1.09
2:F:1339:TRP:HB3	2:F:1421:ARG:HG2	1.32	1.06
2:H:1339:TRP:HB3	2:H:1421:ARG:HG2	1.32	1.05
1:G:112:THR:HG21	3:I:11:ARG:NH1	1.86	0.90
1:G:102:PRO:HG2	2:H:16:ARG:HH12	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1339:TRP:CG	2:B:1340:PRO:HD2	2.13	0.84
2:H:1339:TRP:CG	2:H:1340:PRO:HD2	2.12	0.84
2:D:1339:TRP:CG	2:D:1340:PRO:HD2	2.13	0.83
2:F:1339:TRP:CG	2:F:1340:PRO:HD2	2.13	0.83
2:B:1339:TRP:CZ3	2:B:1408:ILE:HD12	2.15	0.82
2:H:1339:TRP:CZ3	2:H:1408:ILE:HD12	2.15	0.81
2:D:1339:TRP:CZ3	2:D:1408:ILE:HD12	2.15	0.81
2:F:1339:TRP:CZ3	2:F:1408:ILE:HD12	2.15	0.81
1:E:102:PRO:HG2	2:F:16:ARG:HH12	1.47	0.77
1:G:102:PRO:HG2	2:H:16:ARG:NH1	2.00	0.76
2:F:1339:TRP:HH2	2:F:1408:ILE:HB	1.50	0.76
1:G:112:THR:HG21	3:I:11:ARG:CZ	2.15	0.75
2:B:1339:TRP:HH2	2:B:1408:ILE:HB	1.50	0.75
2:H:1339:TRP:HH2	2:H:1408:ILE:HB	1.50	0.74
2:D:1339:TRP:HH2	2:D:1408:ILE:HB	1.50	0.74
2:H:1339:TRP:CD2	2:H:1340:PRO:HD2	2.25	0.71
2:B:1339:TRP:CD2	2:B:1340:PRO:HD2	2.25	0.71
1:G:102:PRO:CG	2:H:16:ARG:HH12	2.02	0.71
2:D:1339:TRP:CD2	2:D:1340:PRO:HD2	2.25	0.70
2:F:1339:TRP:CD2	2:F:1340:PRO:HD2	2.25	0.70
2:B:1339:TRP:HZ3	2:B:1408:ILE:HD12	1.58	0.68
2:D:1339:TRP:HZ3	2:D:1408:ILE:HD12	1.58	0.68
1:G:137:MET:HE2	3:I:45:PHE:HE2	1.59	0.68
1:G:137:MET:CE	3:I:45:PHE:HE2	2.07	0.67
2:H:1339:TRP:HZ3	2:H:1408:ILE:HD12	1.58	0.67
2:F:1339:TRP:HZ3	2:F:1408:ILE:HD12	1.58	0.66
1:G:137:MET:CE	3:I:45:PHE:CE2	2.80	0.65
2:F:1339:TRP:CH2	2:F:1408:ILE:HD12	2.33	0.64
2:D:1339:TRP:CH2	2:D:1408:ILE:HD12	2.33	0.63
2:B:229:THR:O	2:B:1251:ARG:NH1	2.32	0.63
2:B:1339:TRP:CD1	2:B:1340:PRO:HD2	2.34	0.62
2:B:1339:TRP:CH2	2:B:1408:ILE:HD12	2.33	0.62
2:H:1339:TRP:CH2	2:H:1408:ILE:HD12	2.33	0.62
2:B:811:ASP:OD2	2:B:837:ARG:NH2	2.33	0.62
2:D:811:ASP:OD2	2:D:837:ARG:NH2	2.33	0.62
2:B:687:THR:HG22	2:B:694:PRO:HA	1.81	0.62
2:D:229:THR:O	2:D:1251:ARG:NH1	2.32	0.62
2:D:1339:TRP:CD1	2:D:1340:PRO:HD2	2.34	0.62
2:F:687:THR:HG22	2:F:694:PRO:HA	1.81	0.62
2:H:687:THR:HG22	2:H:694:PRO:HA	1.81	0.62
2:H:811:ASP:OD2	2:H:837:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1339:TRP:HB3	2:B:1421:ARG:CG	2.21	0.62
2:D:687:THR:HG22	2:D:694:PRO:HA	1.81	0.62
2:H:1339:TRP:CD1	2:H:1340:PRO:HD2	2.34	0.62
2:D:1339:TRP:HB3	2:D:1421:ARG:CG	2.21	0.62
2:F:1339:TRP:CD1	2:F:1340:PRO:HD2	2.34	0.62
1:E:329:ASP:OD1	1:G:48:ASN:ND2	2.33	0.61
2:F:811:ASP:OD2	2:F:837:ARG:NH2	2.33	0.61
2:H:229:THR:O	2:H:1251:ARG:NH1	2.32	0.61
2:F:229:THR:O	2:F:1251:ARG:NH1	2.32	0.61
2:H:1339:TRP:H	2:H:1421:ARG:NH1	2.00	0.59
2:D:1252:MET:HE3	2:D:1299:VAL:HG21	1.85	0.59
2:D:1377:ILE:HB	2:D:1536:ILE:HA	1.85	0.59
2:F:1252:MET:HE3	2:F:1299:VAL:HG21	1.85	0.59
3:I:4:ILE:HG22	3:I:52:TYR:O	2.01	0.58
1:C:329:ASP:OD1	1:E:48:ASN:ND2	2.36	0.58
2:D:1339:TRP:H	2:D:1421:ARG:NH1	2.00	0.58
2:F:1339:TRP:H	2:F:1421:ARG:NH1	2.00	0.58
2:H:1252:MET:HE3	2:H:1299:VAL:HG21	1.85	0.58
2:B:1252:MET:HE3	2:B:1299:VAL:HG21	1.85	0.58
2:B:1339:TRP:H	2:B:1421:ARG:NH1	2.00	0.58
2:F:1377:ILE:HB	2:F:1536:ILE:HA	1.85	0.58
2:H:1374:LYS:HG3	2:H:1533:VAL:HB	1.86	0.58
2:H:1377:ILE:HB	2:H:1536:ILE:HA	1.85	0.58
2:D:47:LEU:HD21	2:D:123:TYR:HA	1.86	0.58
1:E:102:PRO:HG2	2:F:16:ARG:NH1	2.16	0.58
2:B:1377:ILE:HB	2:B:1536:ILE:HA	1.85	0.58
2:D:1427:GLN:NE2	2:D:1507:GLU:OE1	2.37	0.58
2:H:47:LEU:HD21	2:H:123:TYR:HA	1.86	0.58
2:B:1427:GLN:NE2	2:B:1507:GLU:OE1	2.37	0.58
2:B:47:LEU:HD21	2:B:123:TYR:HA	1.86	0.58
2:F:47:LEU:HD21	2:F:123:TYR:HA	1.86	0.58
1:G:112:THR:CG2	3:I:11:ARG:CZ	2.81	0.58
2:H:1427:GLN:NE2	2:H:1507:GLU:OE1	2.37	0.58
2:F:1427:GLN:NE2	2:F:1507:GLU:OE1	2.37	0.57
2:F:1374:LYS:HG3	2:F:1533:VAL:HB	1.86	0.57
2:B:1374:LYS:HG3	2:B:1533:VAL:HB	1.86	0.57
2:D:1124:ARG:HG3	2:D:1318:LEU:HD22	1.87	0.57
1:C:108:GLU:HG2	1:C:109:PRO:HD2	1.87	0.57
2:D:370:ARG:HD3	2:D:1253:GLU:HB3	1.87	0.57
2:H:1124:ARG:HG3	2:H:1318:LEU:HD22	1.87	0.57
2:B:1124:ARG:HG3	2:B:1318:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:GLY:O	3:I:11:ARG:NH2	2.39	0.56
2:D:74:ARG:HB3	2:D:185:VAL:HG11	1.87	0.56
2:H:74:ARG:HB3	2:H:185:VAL:HG11	1.87	0.56
2:B:370:ARG:HD3	2:B:1253:GLU:HB3	1.87	0.56
2:F:1124:ARG:HG3	2:F:1318:LEU:HD22	1.87	0.56
2:H:687:THR:OG1	2:H:731:GLN:NE2	2.37	0.56
2:H:209:ASP:HB3	2:H:255:ILE:HG13	1.88	0.56
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.88	0.56
1:E:48:ASN:ND2	2:F:211:GLN:O	2.39	0.56
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.88	0.56
2:B:74:ARG:HB3	2:B:185:VAL:HG11	1.87	0.56
2:B:209:ASP:HB3	2:B:255:ILE:HG13	1.88	0.56
1:C:48:ASN:ND2	2:D:211:GLN:O	2.39	0.56
2:D:1374:LYS:HG3	2:D:1533:VAL:HB	1.86	0.56
2:F:74:ARG:HB3	2:F:185:VAL:HG11	1.87	0.56
2:B:711:ILE:HB	2:B:887:VAL:HG22	1.88	0.55
2:H:711:ILE:HB	2:H:887:VAL:HG22	1.88	0.55
2:D:711:ILE:HB	2:D:887:VAL:HG22	1.88	0.55
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.88	0.55
2:F:711:ILE:HB	2:F:887:VAL:HG22	1.88	0.55
1:A:48:ASN:ND2	1:G:329:ASP:OD1	2.38	0.55
2:D:209:ASP:HB3	2:D:255:ILE:HG13	1.88	0.55
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.88	0.55
2:H:1340:PRO:C	2:H:1500:THR:HG1	2.14	0.55
2:H:370:ARG:HD3	2:H:1253:GLU:HB3	1.87	0.55
2:H:1365:VAL:HG13	2:H:1557:ILE:HD11	1.88	0.55
1:A:48:ASN:ND2	2:B:211:GLN:O	2.39	0.55
1:C:108:GLU:CG	1:C:109:PRO:HD2	2.37	0.55
2:F:209:ASP:HB3	2:F:255:ILE:HG13	1.88	0.55
2:F:370:ARG:HD3	2:F:1253:GLU:HB3	1.87	0.55
2:H:1339:TRP:HB3	2:H:1421:ARG:CG	2.21	0.55
2:F:1365:VAL:HG13	2:F:1557:ILE:HD11	1.88	0.54
2:B:687:THR:OG1	2:B:731:GLN:NE2	2.37	0.54
1:G:48:ASN:ND2	2:H:211:GLN:O	2.39	0.54
2:B:1365:VAL:HG13	2:B:1557:ILE:HD11	1.89	0.54
2:D:687:THR:OG1	2:D:731:GLN:NE2	2.37	0.54
2:H:1339:TRP:CG	2:H:1340:PRO:CD	2.90	0.54
2:F:1340:PRO:C	2:F:1500:THR:HG1	2.15	0.54
2:F:214:GLY:O	2:F:252:LYS:N	2.39	0.54
2:H:711:ILE:HG12	2:H:901:ILE:HD12	1.88	0.54
2:D:1365:VAL:HG13	2:D:1557:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:711:ILE:HG12	2:F:901:ILE:HD12	1.88	0.54
2:B:711:ILE:HG12	2:B:901:ILE:HD12	1.88	0.54
1:A:167:ILE:O	1:A:171:THR:OG1	2.23	0.54
2:F:687:THR:OG1	2:F:731:GLN:NE2	2.37	0.54
2:F:1339:TRP:HB3	2:F:1421:ARG:CG	2.21	0.54
2:F:1339:TRP:CG	2:F:1340:PRO:CD	2.90	0.54
1:A:299:GLN:HE21	1:G:211:ILE:HG23	1.73	0.54
2:D:711:ILE:HG12	2:D:901:ILE:HD12	1.88	0.54
1:A:329:ASP:OD1	1:C:48:ASN:ND2	2.41	0.53
2:B:1464:VAL:HA	2:B:1467:LEU:HD12	1.91	0.53
2:H:1464:VAL:HA	2:H:1467:LEU:HD12	1.91	0.53
2:D:214:GLY:O	2:D:252:LYS:N	2.39	0.53
1:E:167:ILE:O	1:E:171:THR:OG1	2.23	0.53
2:F:1464:VAL:HA	2:F:1467:LEU:HD12	1.91	0.53
2:B:1339:TRP:CG	2:B:1340:PRO:CD	2.90	0.53
2:D:1464:VAL:HA	2:D:1467:LEU:HD12	1.91	0.53
1:A:211:ILE:HG23	1:C:299:GLN:HE21	1.74	0.53
2:H:26:CYS:HA	2:H:29:ASP:HB2	1.90	0.53
2:H:32:ASN:HD22	2:H:149:THR:HB	1.74	0.52
2:D:26:CYS:HA	2:D:29:ASP:HB2	1.90	0.52
2:B:26:CYS:HA	2:B:29:ASP:HB2	1.90	0.52
2:F:263:TYR:OH	2:F:397:ASN:ND2	2.43	0.52
1:G:112:THR:HG21	3:I:11:ARG:HH12	1.69	0.52
2:H:1340:PRO:O	2:H:1500:THR:OG1	2.27	0.52
3:I:4:ILE:HG23	3:I:6:LYS:NZ	2.24	0.52
1:C:211:ILE:HG23	1:E:299:GLN:HE21	1.75	0.52
2:F:26:CYS:HA	2:F:29:ASP:HB2	1.90	0.52
2:F:32:ASN:HD22	2:F:149:THR:HB	1.74	0.52
2:B:1340:PRO:C	2:B:1500:THR:HG1	2.17	0.52
2:D:1339:TRP:CG	2:D:1340:PRO:CD	2.90	0.52
2:D:1340:PRO:O	2:D:1500:THR:OG1	2.27	0.52
2:H:263:TYR:OH	2:H:397:ASN:ND2	2.43	0.52
1:E:211:ILE:HG23	1:G:299:GLN:HE21	1.75	0.51
2:B:783:THR:O	2:B:787:ASN:ND2	2.43	0.51
2:D:32:ASN:HD22	2:D:149:THR:HB	1.74	0.51
2:B:32:ASN:HD22	2:B:149:THR:HB	1.74	0.51
2:D:263:TYR:OH	2:D:397:ASN:ND2	2.43	0.51
2:F:783:THR:O	2:F:787:ASN:ND2	2.43	0.51
2:B:459:SER:OG	2:B:558:THR:O	2.29	0.51
2:B:1340:PRO:O	2:B:1500:THR:OG1	2.27	0.51
2:H:39:LEU:O	2:H:43:THR:OG1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:214:GLY:O	2:H:252:LYS:N	2.39	0.51
2:B:39:LEU:O	2:B:43:THR:OG1	2.24	0.51
2:B:462:ILE:HG22	2:B:557:ILE:HD12	1.93	0.51
2:D:849:ASN:O	2:D:883:THR:N	2.42	0.51
2:H:783:THR:O	2:H:787:ASN:ND2	2.43	0.51
2:B:346:VAL:HG23	2:B:350:GLU:HG3	1.93	0.51
2:F:459:SER:OG	2:F:558:THR:O	2.29	0.51
2:H:346:VAL:HG23	2:H:350:GLU:HG3	1.93	0.51
2:D:462:ILE:HG22	2:D:557:ILE:HD12	1.93	0.50
2:B:214:GLY:O	2:B:252:LYS:N	2.39	0.50
2:B:263:TYR:OH	2:B:397:ASN:ND2	2.43	0.50
2:F:1456:GLU:HB2	2:F:1461:LYS:HE2	1.93	0.50
2:H:462:ILE:HG22	2:H:557:ILE:HD12	1.93	0.50
2:B:99:THR:O	2:B:102:ARG:NH2	2.45	0.50
2:D:783:THR:O	2:D:787:ASN:ND2	2.43	0.50
2:D:1382:GLY:O	2:D:1554:ARG:NH1	2.45	0.50
2:F:563:VAL:HG21	2:F:1037:TRP:HZ2	1.75	0.50
2:F:1340:PRO:O	2:F:1500:THR:OG1	2.27	0.50
2:B:563:VAL:HG21	2:B:1037:TRP:HZ2	1.75	0.50
2:F:462:ILE:HG22	2:F:557:ILE:HD12	1.93	0.50
2:H:1456:GLU:HB2	2:H:1461:LYS:HE2	1.94	0.50
2:D:346:VAL:HG23	2:D:350:GLU:HG3	1.93	0.50
2:F:1382:GLY:O	2:F:1554:ARG:NH1	2.45	0.50
1:A:272:PRO:HG3	1:A:311:TRP:CE2	2.47	0.50
2:D:39:LEU:O	2:D:43:THR:OG1	2.24	0.50
2:F:1449:SER:HA	2:F:1452:TRP:HD1	1.77	0.50
2:F:99:THR:O	2:F:102:ARG:NH2	2.44	0.50
2:H:99:THR:O	2:H:102:ARG:NH2	2.44	0.50
1:A:140:GLU:OE2	1:G:136:ARG:NH2	2.45	0.49
2:D:563:VAL:HG21	2:D:1037:TRP:HZ2	1.75	0.49
1:G:102:PRO:CG	2:H:16:ARG:NH1	2.69	0.49
2:B:802:VAL:HG22	2:B:876:LEU:HD21	1.94	0.49
2:H:1449:SER:HA	2:H:1452:TRP:HD1	1.77	0.49
2:D:802:VAL:HG22	2:D:876:LEU:HD21	1.94	0.49
1:G:272:PRO:HG3	1:G:311:TRP:CE2	2.47	0.49
2:B:1382:GLY:O	2:B:1554:ARG:NH1	2.45	0.49
2:D:99:THR:O	2:D:102:ARG:NH2	2.44	0.49
1:E:272:PRO:HG3	1:E:311:TRP:CE2	2.47	0.49
2:F:39:LEU:O	2:F:43:THR:OG1	2.24	0.49
2:H:563:VAL:HG21	2:H:1037:TRP:HZ2	1.75	0.49
2:H:1382:GLY:O	2:H:1554:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1456:GLU:HB2	2:B:1461:LYS:HE2	1.93	0.49
2:B:1485:GLY:HA2	2:B:1512:ILE:HD12	1.95	0.49
2:D:1449:SER:HA	2:D:1452:TRP:HD1	1.77	0.49
2:F:346:VAL:HG23	2:F:350:GLU:HG3	1.93	0.49
2:F:456:LEU:HB3	2:F:460:ALA:HB2	1.95	0.49
2:H:1485:GLY:HA2	2:H:1512:ILE:HD12	1.95	0.49
2:D:1485:GLY:HA2	2:D:1512:ILE:HD12	1.95	0.49
2:H:71:HIS:ND1	2:H:128:GLU:OE2	2.46	0.49
2:H:1436:ILE:HB	2:H:1471:LEU:HD23	1.95	0.49
2:B:17:VAL:HG22	2:B:21:VAL:HA	1.95	0.49
2:B:71:HIS:ND1	2:B:128:GLU:OE2	2.46	0.49
1:C:272:PRO:HG3	1:C:311:TRP:CE2	2.47	0.49
2:D:71:HIS:ND1	2:D:128:GLU:OE2	2.46	0.49
2:D:456:LEU:HB3	2:D:460:ALA:HB2	1.95	0.49
2:D:1456:GLU:HB2	2:D:1461:LYS:HE2	1.93	0.49
2:F:32:ASN:OD1	2:F:153:LYS:HD2	2.13	0.49
2:F:572:SER:HB3	2:F:575:VAL:HG12	1.94	0.49
2:H:32:ASN:OD1	2:H:153:LYS:HD2	2.13	0.49
1:A:267:LEU:HD22	1:A:270:LEU:HD22	1.95	0.49
2:B:572:SER:HB3	2:B:575:VAL:HG12	1.95	0.49
2:B:729:GLU:OE1	2:B:1215:ARG:NH2	2.46	0.49
1:C:267:LEU:HD22	1:C:270:LEU:HD22	1.95	0.49
2:D:17:VAL:HG22	2:D:21:VAL:HA	1.95	0.49
2:D:459:SER:OG	2:D:558:THR:O	2.29	0.49
2:F:1349:ASN:OD1	2:F:1364:HIS:ND1	2.41	0.49
2:F:1485:GLY:HA2	2:F:1512:ILE:HD12	1.95	0.48
2:B:32:ASN:OD1	2:B:153:LYS:HD2	2.13	0.48
2:B:1449:SER:HA	2:B:1452:TRP:HD1	1.77	0.48
2:D:32:ASN:OD1	2:D:153:LYS:HD2	2.13	0.48
2:B:1345:ILE:HD11	2:B:1502:ILE:HD13	1.95	0.48
2:B:1436:ILE:HB	2:B:1471:LEU:HD23	1.95	0.48
2:D:572:SER:HB3	2:D:575:VAL:HG12	1.94	0.48
2:D:846:GLN:O	2:D:882:ARG:NH2	2.46	0.48
2:H:17:VAL:HG22	2:H:21:VAL:HA	1.95	0.48
2:H:1345:ILE:HD11	2:H:1502:ILE:HD13	1.95	0.48
1:E:267:LEU:HD22	1:E:270:LEU:HD22	1.95	0.48
2:F:846:GLN:O	2:F:882:ARG:NH2	2.47	0.48
2:H:459:SER:OG	2:H:558:THR:O	2.29	0.48
2:H:802:VAL:HG22	2:H:876:LEU:HD21	1.95	0.48
2:B:1178:ILE:HD13	2:B:1251:ARG:HB3	1.96	0.48
2:D:108:MET:HG2	2:D:112:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1437:ARG:HD2	2:H:1471:LEU:HD22	1.95	0.48
2:B:849:ASN:O	2:B:883:THR:N	2.42	0.48
2:F:17:VAL:HG22	2:F:21:VAL:HA	1.95	0.48
2:F:108:MET:HG2	2:F:112:MET:HE2	1.96	0.48
2:H:846:GLN:O	2:H:882:ARG:NH2	2.47	0.48
2:F:729:GLU:OE1	2:F:1215:ARG:NH2	2.46	0.48
2:F:802:VAL:HG22	2:F:876:LEU:HD21	1.94	0.48
2:F:1345:ILE:HD11	2:F:1502:ILE:HD13	1.95	0.48
1:G:267:LEU:HD22	1:G:270:LEU:HD22	1.95	0.48
2:H:456:LEU:HB3	2:H:460:ALA:HB2	1.95	0.48
2:B:846:GLN:O	2:B:882:ARG:NH2	2.47	0.48
1:C:167:ILE:O	1:C:171:THR:OG1	2.23	0.48
2:D:729:GLU:OE1	2:D:1215:ARG:NH2	2.46	0.48
2:D:1345:ILE:HD11	2:D:1502:ILE:HD13	1.95	0.48
2:D:1437:ARG:HD2	2:D:1471:LEU:HD22	1.95	0.48
2:F:1090:GLY:HA3	2:F:1137:PRO:HG3	1.96	0.48
1:G:167:ILE:O	1:G:171:THR:OG1	2.23	0.48
2:H:849:ASN:O	2:H:883:THR:N	2.42	0.48
2:H:1090:GLY:HA3	2:H:1137:PRO:HG3	1.96	0.48
2:B:456:LEU:HB3	2:B:460:ALA:HB2	1.95	0.48
2:D:1178:ILE:HD13	2:D:1251:ARG:HB3	1.96	0.48
2:D:1436:ILE:HB	2:D:1471:LEU:HD23	1.95	0.48
2:B:1090:GLY:HA3	2:B:1137:PRO:HG3	1.96	0.48
2:B:1339:TRP:CZ3	2:B:1408:ILE:CD1	2.95	0.47
1:E:136:ARG:NH2	1:G:140:GLU:OE2	2.46	0.47
1:G:108:GLU:HG3	1:G:109:PRO:HD2	1.95	0.47
2:H:572:SER:HB3	2:H:575:VAL:HG12	1.94	0.47
2:H:1178:ILE:HD13	2:H:1251:ARG:HB3	1.96	0.47
2:H:1519:ILE:HA	2:H:1522:LYS:HG2	1.96	0.47
2:B:108:MET:HG2	2:B:112:MET:HE2	1.96	0.47
2:B:1437:ARG:HD2	2:B:1471:LEU:HD22	1.95	0.47
2:D:869:MET:HE2	2:D:893:TYR:HB3	1.96	0.47
2:D:929:LYS:HG3	2:D:939:LEU:HD12	1.96	0.47
2:F:1178:ILE:HD13	2:F:1251:ARG:HB3	1.96	0.47
2:H:729:GLU:OE1	2:H:1215:ARG:NH2	2.46	0.47
2:H:869:MET:HE2	2:H:893:TYR:HB3	1.96	0.47
2:F:869:MET:HE2	2:F:893:TYR:HB3	1.97	0.47
2:B:869:MET:HE2	2:B:893:TYR:HB3	1.97	0.47
2:D:709:THR:HG23	2:D:899:TRP:HB3	1.97	0.47
2:D:1090:GLY:HA3	2:D:1137:PRO:HG3	1.96	0.47
2:D:1519:ILE:HA	2:D:1522:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:709:THR:HG23	2:F:899:TRP:HB3	1.97	0.47
2:F:1436:ILE:HB	2:F:1471:LEU:HD23	1.95	0.47
2:F:1519:ILE:HA	2:F:1522:LYS:HG2	1.96	0.47
1:G:135:GLY:HA2	3:I:46:PHE:CZ	2.49	0.47
2:H:108:MET:HG2	2:H:112:MET:HE2	1.96	0.47
2:F:1437:ARG:HD2	2:F:1471:LEU:HD22	1.95	0.47
2:B:1349:ASN:OD1	2:B:1364:HIS:ND1	2.41	0.47
2:D:687:THR:OG1	2:D:689:THR:O	2.23	0.47
2:H:929:LYS:HG3	2:H:939:LEU:HD12	1.96	0.47
2:B:1519:ILE:HA	2:B:1522:LYS:HG2	1.96	0.47
1:E:329:ASP:HB2	2:H:213:LEU:HD12	1.96	0.46
3:I:27:ALA:HA	3:I:31:THR:OG1	2.15	0.46
1:E:200:LEU:O	1:E:257:ILE:N	2.48	0.46
1:G:137:MET:HE1	3:I:45:PHE:CE2	2.49	0.46
2:B:929:LYS:HG3	2:B:939:LEU:HD12	1.96	0.46
1:C:34:ARG:HH21	1:C:303:SER:HB2	1.81	0.46
1:C:70:HIS:O	1:C:74:ILE:HG12	2.16	0.46
2:F:71:HIS:ND1	2:F:128:GLU:OE2	2.46	0.46
2:H:508:LEU:HA	2:H:511:LEU:HD12	1.98	0.46
1:C:200:LEU:O	1:C:257:ILE:N	2.48	0.46
2:D:3:LEU:HB3	2:D:104:LEU:HD11	1.98	0.46
1:E:34:ARG:HH21	1:E:303:SER:HB2	1.81	0.46
2:H:3:LEU:HB3	2:H:104:LEU:HD11	1.98	0.46
1:A:70:HIS:O	1:A:74:ILE:HG12	2.16	0.46
2:F:508:LEU:HA	2:F:511:LEU:HD12	1.98	0.46
2:F:929:LYS:HG3	2:F:939:LEU:HD12	1.96	0.46
2:B:709:THR:HG23	2:B:899:TRP:HB3	1.97	0.46
1:E:70:HIS:O	1:E:74:ILE:HG12	2.16	0.46
2:H:709:THR:HG23	2:H:899:TRP:HB3	1.96	0.46
1:G:34:ARG:HH21	1:G:303:SER:HB2	1.81	0.46
1:A:34:ARG:HH21	1:A:303:SER:HB2	1.81	0.46
1:C:329:ASP:HB2	2:F:213:LEU:HD12	1.97	0.46
3:I:42:LYS:O	3:I:48:CYS:HB2	2.15	0.46
1:G:247:ASN:OD1	1:G:247:ASN:N	2.50	0.45
2:D:354:ASN:HB3	2:D:357:VAL:HG22	1.98	0.45
3:I:8:LEU:HD12	3:I:9:PRO:HD2	1.97	0.45
2:B:213:LEU:HD23	2:B:213:LEU:HA	1.86	0.45
2:B:714:GLN:O	2:B:719:LYS:NZ	2.50	0.45
2:F:74:ARG:HD3	2:F:124:TYR:CZ	2.52	0.45
1:G:70:HIS:O	1:G:74:ILE:HG12	2.16	0.45
2:H:1507:GLU:N	2:H:1536:ILE:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:24:GLN:NE2	3:I:25:ASP:OD1	2.49	0.45
1:A:247:ASN:OD1	1:A:247:ASN:N	2.49	0.45
2:B:354:ASN:HB3	2:B:357:VAL:HG22	1.98	0.45
2:D:137:ILE:HD11	2:D:196:ILE:HG21	1.99	0.45
2:B:508:LEU:HA	2:B:511:LEU:HD12	1.98	0.45
2:B:687:THR:OG1	2:B:689:THR:O	2.23	0.45
1:C:247:ASN:OD1	1:C:247:ASN:N	2.49	0.45
2:D:508:LEU:HA	2:D:511:LEU:HD12	1.98	0.45
2:B:1339:TRP:HH2	2:B:1408:ILE:CB	2.25	0.45
2:D:34:VAL:HB	2:D:35:PRO:CD	2.47	0.45
2:D:1389:SER:HB3	2:D:1536:ILE:HD13	1.99	0.45
2:F:1339:TRP:CH2	2:F:1408:ILE:HB	2.41	0.45
2:F:34:VAL:HB	2:F:35:PRO:CD	2.47	0.45
2:F:849:ASN:O	2:F:883:THR:N	2.42	0.45
2:H:74:ARG:HD3	2:H:124:TYR:CZ	2.52	0.45
2:H:560:VAL:O	2:H:564:SER:OG	2.34	0.45
1:A:109:PRO:O	1:A:139:THR:OG1	2.34	0.45
2:B:34:VAL:HB	2:B:35:PRO:CD	2.47	0.45
2:D:74:ARG:HD3	2:D:124:TYR:CZ	2.52	0.45
2:D:488:THR:HG21	2:D:533:LEU:HD13	1.99	0.45
2:D:1349:ASN:OD1	2:D:1364:HIS:ND1	2.41	0.45
2:F:3:LEU:HB3	2:F:104:LEU:HD11	1.98	0.45
1:E:247:ASN:OD1	1:E:247:ASN:N	2.49	0.45
2:H:714:GLN:O	2:H:719:LYS:NZ	2.50	0.45
2:B:3:LEU:HB3	2:B:104:LEU:HD11	1.98	0.44
2:B:488:THR:HG21	2:B:533:LEU:HD13	1.99	0.44
2:D:1553:LYS:HE2	2:D:1558:LEU:HD11	2.00	0.44
1:E:109:PRO:O	1:E:139:THR:OG1	2.35	0.44
1:A:200:LEU:O	1:A:257:ILE:N	2.48	0.44
2:B:1345:ILE:HG12	2:B:1405:ILE:HG12	1.99	0.44
2:D:1105:ILE:HD11	2:D:1318:LEU:HG	2.00	0.44
2:H:354:ASN:HB3	2:H:357:VAL:HG22	1.98	0.44
2:B:701:ILE:HD13	2:B:701:ILE:HA	1.78	0.44
2:B:774:SER:OG	2:B:776:LYS:O	2.33	0.44
2:D:1339:TRP:CH2	2:D:1408:ILE:HB	2.41	0.44
1:E:196:LEU:HD22	1:E:346:ALA:HB2	1.99	0.44
2:F:774:SER:OG	2:F:776:LYS:O	2.33	0.44
2:H:1422:LEU:O	2:H:1498:ARG:NH2	2.50	0.44
2:B:1553:LYS:HE2	2:B:1558:LEU:HD11	2.00	0.44
1:C:196:LEU:HD22	1:C:346:ALA:HB2	1.99	0.44
2:D:96:ASP:HB3	2:D:106:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:ARG:HH22	1:G:62:THR:HG22	1.82	0.44
2:F:1105:ILE:HD11	2:F:1318:LEU:HG	2.00	0.44
2:F:1553:LYS:HE2	2:F:1558:LEU:HD11	1.99	0.44
2:H:137:ILE:HD11	2:H:196:ILE:HG21	1.99	0.44
2:B:74:ARG:HD3	2:B:124:TYR:CZ	2.52	0.44
1:C:123:PHE:HZ	1:C:138:VAL:HG23	1.82	0.44
2:F:714:GLN:O	2:F:719:LYS:NZ	2.50	0.44
2:F:1378:CYS:HB3	2:F:1543:ILE:HD11	2.00	0.44
2:H:1389:SER:HB3	2:H:1536:ILE:HD13	1.99	0.44
1:A:196:LEU:HD22	1:A:346:ALA:HB2	1.99	0.44
2:D:9:GLU:OE2	2:D:101:SER:OG	2.33	0.44
2:D:1378:CYS:HB3	2:D:1543:ILE:HD11	2.00	0.44
2:F:354:ASN:HB3	2:F:357:VAL:HG22	1.98	0.44
2:F:1339:TRP:HH2	2:F:1408:ILE:CB	2.25	0.44
2:B:1422:LEU:O	2:B:1498:ARG:NH2	2.50	0.44
2:F:1345:ILE:HG12	2:F:1405:ILE:HG12	1.99	0.44
1:G:123:PHE:HZ	1:G:138:VAL:HG23	1.82	0.44
1:A:123:PHE:HZ	1:A:138:VAL:HG23	1.82	0.44
1:A:188:VAL:HG12	1:A:310:LEU:HB2	2.00	0.44
2:B:1339:TRP:CH2	2:B:1408:ILE:HB	2.41	0.44
2:F:137:ILE:HD11	2:F:196:ILE:HG21	1.99	0.44
2:H:34:VAL:HB	2:H:35:PRO:CD	2.47	0.44
2:H:1553:LYS:HE2	2:H:1558:LEU:HD11	1.99	0.44
2:B:137:ILE:HD11	2:B:196:ILE:HG21	1.99	0.44
2:B:1389:SER:HB3	2:B:1536:ILE:HD13	1.99	0.44
1:E:188:VAL:HG12	1:E:310:LEU:HB2	2.00	0.44
1:G:158:MET:HE3	1:G:162:ILE:HG12	2.00	0.44
3:I:21:GLU:O	3:I:24:GLN:NE2	2.50	0.44
2:D:714:GLN:O	2:D:719:LYS:NZ	2.50	0.43
2:D:1339:TRP:CZ3	2:D:1408:ILE:CD1	2.95	0.43
2:F:1389:SER:HB3	2:F:1536:ILE:HD13	1.99	0.43
1:G:188:VAL:HG12	1:G:310:LEU:HB2	2.00	0.43
2:H:96:ASP:HB3	2:H:106:LEU:HD12	2.00	0.43
2:B:96:ASP:HB3	2:B:106:LEU:HD12	2.00	0.43
1:C:84:LEU:HD13	1:C:84:LEU:HA	1.91	0.43
1:C:188:VAL:HG12	1:C:310:LEU:HB2	2.00	0.43
1:E:158:MET:HE3	1:E:162:ILE:HG12	2.00	0.43
2:F:687:THR:OG1	2:F:689:THR:O	2.23	0.43
2:H:800:LYS:HD3	2:H:800:LYS:HA	1.83	0.43
1:A:158:MET:HE3	1:A:162:ILE:HG12	2.00	0.43
2:B:533:LEU:HD21	2:B:1133:ASP:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:LEU:HD22	1:G:346:ALA:HB2	1.99	0.43
2:H:502:MET:HE1	2:H:1102:LEU:HD11	2.01	0.43
2:H:1105:ILE:HD11	2:H:1318:LEU:HG	1.99	0.43
2:H:1350:LEU:N	2:H:1365:VAL:O	2.46	0.43
2:H:1345:ILE:HG12	2:H:1405:ILE:HG12	1.99	0.43
1:A:168:PHE:HZ	1:C:164:LEU:HD23	1.84	0.43
2:D:213:LEU:HD23	2:D:213:LEU:HA	1.86	0.43
2:D:1345:ILE:HG12	2:D:1405:ILE:HG12	1.99	0.43
2:F:96:ASP:HB3	2:F:106:LEU:HD12	2.00	0.43
2:F:701:ILE:HD13	2:F:701:ILE:HA	1.78	0.43
2:F:1182:PHE:CE2	2:F:1248:LEU:HD22	2.54	0.43
2:F:1437:ARG:HH11	2:F:1471:LEU:HD22	1.84	0.43
2:H:533:LEU:HD21	2:H:1133:ASP:HB3	2.01	0.43
2:B:187:VAL:HA	2:B:190:ILE:HD12	2.01	0.43
2:D:194:ARG:HB3	2:D:198:PHE:HB2	2.01	0.43
2:F:507:LYS:HB2	2:F:1110:MET:HE2	2.01	0.43
2:H:187:VAL:HA	2:H:190:ILE:HD12	2.01	0.43
2:H:1437:ARG:HH11	2:H:1471:LEU:HD22	1.84	0.43
2:B:1437:ARG:HH11	2:B:1471:LEU:HD22	1.84	0.43
2:D:1437:ARG:HH11	2:D:1471:LEU:HD22	1.84	0.43
1:E:123:PHE:HZ	1:E:138:VAL:HG23	1.82	0.43
2:H:213:LEU:HD23	2:H:213:LEU:HA	1.86	0.43
2:H:488:THR:HG21	2:H:533:LEU:HD13	1.99	0.43
2:H:1182:PHE:CE2	2:H:1248:LEU:HD22	2.54	0.43
2:H:1458:ALA:HB2	2:H:1493:ALA:HB2	2.00	0.43
3:I:21:GLU:O	3:I:24:GLN:HG3	2.18	0.43
1:A:329:ASP:HB2	2:D:213:LEU:HD12	2.00	0.43
2:D:739:TRP:CE2	2:D:767:ARG:HG3	2.54	0.43
2:D:1422:LEU:O	2:D:1498:ARG:NH2	2.50	0.43
1:E:244:VAL:HG13	1:G:237:ASP:HB3	2.01	0.43
1:E:290:VAL:HA	1:E:297:THR:HA	2.01	0.43
2:F:387:LEU:HD21	2:F:428:LEU:HG	2.01	0.43
2:F:488:THR:HG21	2:F:533:LEU:HD13	1.99	0.43
2:F:1339:TRP:CZ3	2:F:1408:ILE:CD1	2.95	0.43
1:G:112:THR:CG2	3:I:11:ARG:NH2	2.82	0.43
2:H:414:ALA:HA	2:H:1208:VAL:HG11	2.01	0.43
2:B:1030:ILE:HG12	2:B:1071:LEU:HB3	2.01	0.43
2:B:1105:ILE:HD13	2:B:1105:ILE:HA	1.87	0.43
2:D:187:VAL:HA	2:D:190:ILE:HD12	2.01	0.43
2:F:194:ARG:HB3	2:F:198:PHE:HB2	2.01	0.43
2:H:739:TRP:CE2	2:H:767:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ARG:HB3	2:B:198:PHE:HB2	2.01	0.43
2:B:502:MET:HE1	2:B:1102:LEU:HD11	2.01	0.43
2:B:1105:ILE:HD11	2:B:1318:LEU:HG	2.00	0.43
2:D:1182:PHE:CE2	2:D:1248:LEU:HD22	2.54	0.43
2:D:1458:ALA:HB2	2:D:1493:ALA:HB2	2.00	0.43
2:F:414:ALA:HA	2:F:1208:VAL:HG11	2.01	0.43
2:F:502:MET:HE1	2:F:1102:LEU:HD11	2.01	0.43
2:F:739:TRP:CE2	2:F:767:ARG:HG3	2.54	0.43
2:H:1330:LEU:HD23	2:H:1413:LEU:HD12	2.01	0.43
1:A:188:VAL:HG23	1:A:199:MET:HB2	2.01	0.42
2:B:1452:TRP:HE3	2:B:1461:LYS:HZ2	1.67	0.42
1:C:158:MET:HE3	1:C:162:ILE:HG12	2.00	0.42
1:C:168:PHE:HZ	1:E:164:LEU:HD23	1.84	0.42
2:D:1339:TRP:HH2	2:D:1408:ILE:CB	2.25	0.42
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	2.01	0.42
1:E:188:VAL:HG23	1:E:199:MET:HB2	2.01	0.42
1:G:293:THR:OG1	1:G:294:THR:N	2.52	0.42
2:H:194:ARG:HB3	2:H:198:PHE:HB2	2.01	0.42
2:H:1378:CYS:HB3	2:H:1543:ILE:HD11	2.00	0.42
2:B:1182:PHE:CE2	2:B:1248:LEU:HD22	2.54	0.42
2:B:1458:ALA:HB2	2:B:1493:ALA:HB2	2.00	0.42
1:E:231:VAL:HA	1:E:232:PRO:HD3	1.89	0.42
1:E:291:VAL:HG12	1:E:293:THR:H	1.84	0.42
2:F:94:LEU:HD22	2:F:346:VAL:HG21	2.01	0.42
2:F:1030:ILE:HG12	2:F:1071:LEU:HB3	2.01	0.42
2:F:1458:ALA:HB2	2:F:1493:ALA:HB2	2.00	0.42
2:F:1507:GLU:N	2:F:1536:ILE:O	2.49	0.42
1:G:188:VAL:HG23	1:G:199:MET:HB2	2.01	0.42
2:H:94:LEU:HD22	2:H:346:VAL:HG21	2.01	0.42
2:H:1350:LEU:O	2:H:1365:VAL:N	2.44	0.42
3:I:31:THR:HB	3:I:37:LYS:HE3	2.02	0.42
1:A:290:VAL:HA	1:A:297:THR:HA	2.01	0.42
2:B:414:ALA:HA	2:B:1208:VAL:HG11	2.01	0.42
2:B:739:TRP:CE2	2:B:767:ARG:HG3	2.54	0.42
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	2.01	0.42
2:B:1378:CYS:HB3	2:B:1543:ILE:HD11	2.00	0.42
2:F:533:LEU:HD21	2:F:1133:ASP:HB3	2.01	0.42
2:F:1350:LEU:N	2:F:1365:VAL:O	2.46	0.42
2:H:1339:TRP:HH2	2:H:1408:ILE:CB	2.25	0.42
2:B:213:LEU:HD12	1:G:329:ASP:HB2	2.01	0.42
2:B:1507:GLU:N	2:B:1536:ILE:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HH22	1:E:62:THR:HG22	1.84	0.42
1:C:291:VAL:HG12	1:C:293:THR:H	1.84	0.42
2:D:507:LYS:HB2	2:D:1110:MET:HE2	2.00	0.42
2:D:533:LEU:HD21	2:D:1133:ASP:HB3	2.01	0.42
1:E:84:LEU:HD13	1:E:84:LEU:HA	1.91	0.42
2:F:1105:ILE:HD13	2:F:1105:ILE:HA	1.87	0.42
1:G:290:VAL:HA	1:G:297:THR:HA	2.01	0.42
1:G:291:VAL:HG12	1:G:293:THR:H	1.84	0.42
2:H:774:SER:OG	2:H:776:LYS:O	2.33	0.42
2:H:1030:ILE:HG12	2:H:1071:LEU:HB3	2.01	0.42
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	2.01	0.42
1:A:206:ARG:HH22	1:C:62:THR:HG22	1.85	0.42
2:B:1330:LEU:HD23	2:B:1413:LEU:HD12	2.01	0.42
1:C:290:VAL:HA	1:C:297:THR:HA	2.00	0.42
2:D:387:LEU:HD21	2:D:428:LEU:HG	2.01	0.42
2:D:1030:ILE:HG12	2:D:1071:LEU:HB3	2.01	0.42
2:D:1507:GLU:N	2:D:1536:ILE:O	2.49	0.42
1:E:168:PHE:HZ	1:G:164:LEU:HD23	1.83	0.42
2:F:187:VAL:HA	2:F:190:ILE:HD12	2.01	0.42
2:F:1452:TRP:HE3	2:F:1461:LYS:HZ2	1.67	0.42
1:A:291:VAL:HG12	1:A:293:THR:H	1.84	0.42
2:B:1524:VAL:HG12	2:B:1525:MET:HE2	2.02	0.42
1:E:293:THR:OG1	1:E:294:THR:N	2.52	0.42
2:F:1330:LEU:HD23	2:F:1413:LEU:HD12	2.01	0.42
3:I:4:ILE:HG23	3:I:6:LYS:HZ3	1.85	0.42
1:A:293:THR:OG1	1:A:294:THR:N	2.52	0.42
2:B:27:PHE:O	2:B:31:LEU:HG	2.20	0.42
2:D:560:VAL:O	2:D:564:SER:OG	2.34	0.42
2:H:1339:TRP:CZ3	2:H:1408:ILE:CD1	2.95	0.42
2:B:156:LYS:HD3	2:B:156:LYS:HA	1.87	0.42
1:C:188:VAL:HG23	1:C:199:MET:HB2	2.01	0.42
1:C:293:THR:OG1	1:C:294:THR:N	2.52	0.42
2:D:414:ALA:HA	2:D:1208:VAL:HG11	2.01	0.42
2:D:502:MET:HE1	2:D:1102:LEU:HD11	2.01	0.42
3:I:20:SER:O	3:I:23:VAL:HG22	2.20	0.42
2:F:507:LYS:HE3	2:F:1110:MET:HE2	2.02	0.42
2:F:1339:TRP:CE2	2:F:1340:PRO:HD2	2.55	0.42
1:G:112:THR:HG21	3:I:11:ARG:NH2	2.34	0.42
2:H:387:LEU:HD21	2:H:428:LEU:HG	2.01	0.42
2:H:507:LYS:HE3	2:H:1110:MET:HE2	2.02	0.42
2:B:1154:LEU:HD23	2:B:1157:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1421:ARG:HA	2:B:1421:ARG:HD3	1.82	0.42
2:D:1339:TRP:CE2	2:D:1340:PRO:HD2	2.55	0.42
2:D:1452:TRP:HE3	2:D:1461:LYS:HZ2	1.67	0.42
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	2.01	0.42
1:G:200:LEU:O	1:G:257:ILE:N	2.48	0.42
1:A:290:VAL:HG21	1:C:297:THR:HB	2.01	0.41
2:B:387:LEU:HD21	2:B:428:LEU:HG	2.01	0.41
2:B:507:LYS:HB2	2:B:1110:MET:HE2	2.00	0.41
2:B:1136:ILE:HG12	2:B:1308:GLN:HB3	2.02	0.41
2:D:27:PHE:O	2:D:31:LEU:HG	2.20	0.41
2:D:193:ARG:HE	2:D:193:ARG:HB3	1.73	0.41
1:E:59:VAL:O	1:E:62:THR:OG1	2.33	0.41
2:F:1042:LEU:HD23	2:F:1042:LEU:HA	1.93	0.41
2:F:1350:LEU:O	2:F:1365:VAL:N	2.44	0.41
2:H:27:PHE:O	2:H:31:LEU:HG	2.20	0.41
2:H:507:LYS:HB2	2:H:1110:MET:HE2	2.00	0.41
2:H:1524:VAL:HG12	2:H:1525:MET:HE2	2.02	0.41
2:D:452:LEU:HB3	2:D:460:ALA:HB1	2.02	0.41
2:D:1330:LEU:HD23	2:D:1413:LEU:HD12	2.01	0.41
2:D:1524:VAL:HG12	2:D:1525:MET:HE2	2.02	0.41
2:F:1421:ARG:HD3	2:F:1421:ARG:HA	1.82	0.41
2:D:808:LEU:HD23	2:D:837:ARG:HH21	1.85	0.41
2:F:1256:GLY:HA3	2:F:1292:SER:HB3	2.02	0.41
2:F:1422:LEU:O	2:F:1498:ARG:NH2	2.50	0.41
2:H:78:THR:HG21	2:H:121:VAL:HG23	2.02	0.41
2:H:452:LEU:HB3	2:H:460:ALA:HB1	2.02	0.41
2:H:808:LEU:HD23	2:H:837:ARG:HH21	1.85	0.41
2:H:1136:ILE:HG12	2:H:1308:GLN:HB3	2.02	0.41
2:B:464:ALA:HA	2:B:467:ILE:HG22	2.03	0.41
2:B:800:LYS:HA	2:B:800:LYS:HD3	1.83	0.41
2:B:94:LEU:HD22	2:B:346:VAL:HG21	2.01	0.41
2:B:437:ASN:ND2	5:B:2001:GBM:O6	2.42	0.41
2:B:808:LEU:HD23	2:B:837:ARG:HH21	1.85	0.41
2:D:78:THR:HG21	2:D:121:VAL:HG23	2.02	0.41
2:D:94:LEU:HD22	2:D:346:VAL:HG21	2.01	0.41
2:D:1042:LEU:HD23	2:D:1042:LEU:HA	1.93	0.41
2:D:1154:LEU:HD23	2:D:1157:ILE:HD11	2.02	0.41
2:D:1421:ARG:HA	2:D:1421:ARG:HD3	1.82	0.41
2:F:519:CYS:SG	2:F:1106:ILE:HG13	2.61	0.41
1:G:84:LEU:HD13	1:G:84:LEU:HA	1.91	0.41
3:I:26:CYS:HB3	3:I:38:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:519:CYS:SG	2:B:1106:ILE:HG13	2.61	0.41
1:C:136:ARG:NH2	1:E:140:GLU:OE2	2.53	0.41
2:F:27:PHE:O	2:F:31:LEU:HG	2.20	0.41
2:H:511:LEU:HD22	2:H:1424:ILE:HG21	2.02	0.41
2:H:519:CYS:SG	2:H:1106:ILE:HG13	2.61	0.41
2:B:1256:GLY:HA3	2:B:1292:SER:HB3	2.02	0.41
2:H:1349:ASN:OD1	2:H:1364:HIS:ND1	2.41	0.41
2:H:1421:ARG:HA	2:H:1421:ARG:HD3	1.81	0.41
2:B:507:LYS:HE3	2:B:1110:MET:HE2	2.02	0.41
2:B:511:LEU:HD22	2:B:1424:ILE:HG21	2.02	0.41
2:D:507:LYS:HE3	2:D:1110:MET:HE2	2.02	0.41
2:D:528:LYS:O	2:D:531:THR:OG1	2.33	0.41
2:D:1394:ARG:NH1	2:D:1413:LEU:O	2.54	0.41
2:F:396:TYR:CD1	2:F:1227:LEU:HD13	2.56	0.41
2:F:840:VAL:HG21	2:F:856:PRO:HB3	2.03	0.41
2:F:1136:ILE:HG12	2:F:1308:GLN:HB3	2.02	0.41
2:H:150:LYS:HA	2:H:150:LYS:HD3	1.91	0.41
1:A:347:ARG:O	1:A:351:GLU:HG2	2.21	0.41
2:B:1339:TRP:CE2	2:B:1340:PRO:HD2	2.55	0.41
2:D:519:CYS:SG	2:D:1106:ILE:HG13	2.61	0.41
2:D:1136:ILE:HG12	2:D:1308:GLN:HB3	2.02	0.41
2:F:785:GLU:OE1	2:F:820:GLN:NE2	2.54	0.41
2:B:396:TYR:CD1	2:B:1227:LEU:HD13	2.56	0.41
2:B:452:LEU:HB3	2:B:460:ALA:HB1	2.02	0.41
2:B:1413:LEU:HG	2:B:1414:PRO:HD2	2.03	0.41
2:F:452:LEU:HB3	2:F:460:ALA:HB1	2.02	0.41
2:F:496:LEU:HD13	2:F:496:LEU:HA	1.95	0.41
2:F:677:PHE:CD1	2:F:702:ARG:HG2	2.56	0.41
2:F:840:VAL:HG11	2:F:868:LEU:HD21	2.03	0.41
2:H:1339:TRP:CH2	2:H:1408:ILE:HB	2.41	0.41
2:B:78:THR:HG21	2:B:121:VAL:HG23	2.02	0.40
2:B:840:VAL:HG21	2:B:856:PRO:HB3	2.03	0.40
1:C:347:ARG:O	1:C:351:GLU:HG2	2.21	0.40
2:D:150:LYS:HD3	2:D:150:LYS:HA	1.91	0.40
2:D:464:ALA:HA	2:D:467:ILE:HG22	2.03	0.40
2:D:701:ILE:HA	2:D:701:ILE:HD13	1.78	0.40
2:D:1377:ILE:HB	2:D:1536:ILE:HG13	2.04	0.40
2:F:800:LYS:HA	2:F:800:LYS:HD3	1.83	0.40
2:F:808:LEU:HD23	2:F:837:ARG:HH21	1.85	0.40
2:F:1394:ARG:NH1	2:F:1413:LEU:O	2.54	0.40
2:H:464:ALA:HA	2:H:467:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:677:PHE:CD1	2:H:702:ARG:HG2	2.56	0.40
2:H:785:GLU:OE1	2:H:820:GLN:NE2	2.54	0.40
2:H:840:VAL:HG11	2:H:868:LEU:HD21	2.03	0.40
2:H:1549:VAL:HG23	2:H:1563:PRO:HG3	2.03	0.40
2:B:677:PHE:CD1	2:B:702:ARG:HG2	2.56	0.40
1:C:46:HIS:HB3	1:C:49:ILE:HD11	2.03	0.40
2:D:677:PHE:CD1	2:D:702:ARG:HG2	2.56	0.40
2:D:1413:LEU:HG	2:D:1414:PRO:HD2	2.03	0.40
2:F:1549:VAL:HG23	2:F:1563:PRO:HG3	2.03	0.40
1:A:136:ARG:NH2	1:C:140:GLU:OE2	2.55	0.40
2:B:1549:VAL:HG23	2:B:1563:PRO:HG3	2.04	0.40
2:F:209:ASP:OD1	2:F:209:ASP:N	2.55	0.40
2:H:1154:LEU:HD23	2:H:1157:ILE:HD11	2.02	0.40
1:A:46:HIS:HB3	1:A:49:ILE:HD11	2.03	0.40
2:D:511:LEU:HD22	2:D:1424:ILE:HG21	2.02	0.40
2:D:1256:GLY:HA3	2:D:1292:SER:HB3	2.02	0.40
2:D:1549:VAL:HG23	2:D:1563:PRO:HG3	2.03	0.40
2:H:687:THR:OG1	2:H:689:THR:O	2.23	0.40
2:H:1000:ALA:HB1	2:H:1312:VAL:HG13	2.03	0.40
2:B:1000:ALA:HB1	2:B:1312:VAL:HG13	2.04	0.40
1:E:338:LYS:HE3	1:E:338:LYS:HB2	1.90	0.40
2:F:78:THR:HG21	2:F:121:VAL:HG23	2.02	0.40
2:F:1377:ILE:HB	2:F:1536:ILE:HG13	2.03	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	325/390 (83%)	314 (97%)	11 (3%)	0	100	100
1	C	325/390 (83%)	313 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	325/390 (83%)	313 (96%)	12 (4%)	0	100	100
1	G	325/390 (83%)	313 (96%)	12 (4%)	0	100	100
2	B	1413/1582 (89%)	1383 (98%)	28 (2%)	2 (0%)	48	74
2	D	1413/1582 (89%)	1384 (98%)	27 (2%)	2 (0%)	48	74
2	F	1413/1582 (89%)	1383 (98%)	28 (2%)	2 (0%)	48	74
2	H	1413/1582 (89%)	1383 (98%)	28 (2%)	2 (0%)	48	74
3	I	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
All	All	7000/7944 (88%)	6833 (98%)	159 (2%)	8 (0%)	49	74

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	819	ASP
2	D	819	ASP
2	F	819	ASP
2	H	819	ASP
2	B	815	LEU
2	D	815	LEU
2	F	815	LEU
2	H	815	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/336 (84%)	272 (97%)	9 (3%)	34	65
1	C	281/336 (84%)	272 (97%)	9 (3%)	34	65
1	E	280/336 (83%)	271 (97%)	9 (3%)	34	65
1	G	281/336 (84%)	272 (97%)	9 (3%)	34	65
2	B	1215/1371 (89%)	1191 (98%)	24 (2%)	48	76
2	D	1215/1371 (89%)	1191 (98%)	24 (2%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	1215/1371 (89%)	1191 (98%)	24 (2%)	48 76
2	H	1215/1371 (89%)	1191 (98%)	24 (2%)	48 76
3	I	46/50 (92%)	46 (100%)	0	100 100
All	All	6029/6878 (88%)	5897 (98%)	132 (2%)	45 75

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	84	LEU
1	A	167	ILE
1	A	200	LEU
1	A	210	ILE
1	A	231	VAL
1	A	255	LEU
1	A	337	ILE
1	A	349	LEU
2	B	17	VAL
2	B	28	VAL
2	B	121	VAL
2	B	194	ARG
2	B	200	THR
2	B	299	LEU
2	B	333	VAL
2	B	346	VAL
2	B	409	MET
2	B	438	LEU
2	B	466	VAL
2	B	496	LEU
2	B	575	VAL
2	B	612	GLU
2	B	701	ILE
2	B	814	ILE
2	B	913	THR
2	B	1152	SER
2	B	1227	LEU
2	B	1281	VAL
2	B	1355	ASP
2	B	1413	LEU
2	B	1455	LEU
2	B	1471	LEU

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Mol	Chain	Res	Type
1	C	52	GLU
1	C	84	LEU
1	C	167	ILE
1	C	200	LEU
1	C	210	ILE
1	C	231	VAL
1	C	255	LEU
1	C	337	ILE
1	C	349	LEU
2	D	17	VAL
2	D	28	VAL
2	D	121	VAL
2	D	194	ARG
2	D	200	THR
2	D	299	LEU
2	D	333	VAL
2	D	346	VAL
2	D	409	MET
2	D	438	LEU
2	D	466	VAL
2	D	496	LEU
2	D	575	VAL
2	D	612	GLU
2	D	701	ILE
2	D	814	ILE
2	D	913	THR
2	D	1152	SER
2	D	1227	LEU
2	D	1281	VAL
2	D	1355	ASP
2	D	1413	LEU
2	D	1455	LEU
2	D	1471	LEU
1	E	52	GLU
1	E	84	LEU
1	E	167	ILE
1	E	200	LEU
1	E	210	ILE
1	E	231	VAL
1	E	255	LEU
1	E	337	ILE
1	E	349	LEU

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Mol	Chain	Res	Type
2	F	17	VAL
2	F	28	VAL
2	F	121	VAL
2	F	194	ARG
2	F	200	THR
2	F	299	LEU
2	F	333	VAL
2	F	346	VAL
2	F	409	MET
2	F	438	LEU
2	F	466	VAL
2	F	496	LEU
2	F	575	VAL
2	F	612	GLU
2	F	701	ILE
2	F	814	ILE
2	F	913	THR
2	F	1152	SER
2	F	1227	LEU
2	F	1281	VAL
2	F	1355	ASP
2	F	1413	LEU
2	F	1455	LEU
2	F	1471	LEU
1	G	52	GLU
1	G	84	LEU
1	G	167	ILE
1	G	200	LEU
1	G	210	ILE
1	G	231	VAL
1	G	255	LEU
1	G	337	ILE
1	G	349	LEU
2	H	17	VAL
2	H	28	VAL
2	H	121	VAL
2	H	194	ARG
2	H	200	THR
2	H	299	LEU
2	H	333	VAL
2	H	346	VAL
2	H	409	MET

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Mol	Chain	Res	Type
2	H	438	LEU
2	H	466	VAL
2	H	496	LEU
2	H	575	VAL
2	H	612	GLU
2	H	701	ILE
2	H	814	ILE
2	H	913	THR
2	H	1152	SER
2	H	1227	LEU
2	H	1281	VAL
2	H	1355	ASP
2	H	1413	LEU
2	H	1455	LEU
2	H	1471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	48	ASN
1	A	173	GLN
1	A	299	GLN
2	B	32	ASN
2	B	273	GLN
2	B	397	ASN
2	B	474	GLN
2	B	500	ASN
2	B	584	HIS
2	B	707	GLN
2	B	795	ASN
2	B	809	GLN
2	B	1061	GLN
2	B	1484	GLN
2	B	1488	GLN
1	C	41	ASN
1	C	48	ASN
1	C	173	GLN
1	C	299	GLN
2	D	32	ASN
2	D	273	GLN
2	D	397	ASN

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Mol	Chain	Res	Type
2	D	474	GLN
2	D	500	ASN
2	D	584	HIS
2	D	707	GLN
2	D	781	ASN
2	D	795	ASN
2	D	809	GLN
2	D	1061	GLN
2	D	1484	GLN
2	D	1488	GLN
1	E	41	ASN
1	E	48	ASN
1	E	173	GLN
1	E	299	GLN
2	F	32	ASN
2	F	273	GLN
2	F	397	ASN
2	F	474	GLN
2	F	500	ASN
2	F	584	HIS
2	F	707	GLN
2	F	795	ASN
2	F	809	GLN
2	F	1061	GLN
2	F	1484	GLN
2	F	1488	GLN
1	G	41	ASN
1	G	48	ASN
1	G	173	GLN
1	G	299	GLN
2	H	32	ASN
2	H	273	GLN
2	H	397	ASN
2	H	474	GLN
2	H	500	ASN
2	H	584	HIS
2	H	707	GLN
2	H	795	ASN
2	H	809	GLN
2	H	1061	GLN
2	H	1484	GLN
2	H	1488	GLN

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Mol	Chain	Res	Type
3	I	24	GLN

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)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GBM	D	2001	-	35,35,35	2.11	4 (11%)	48,48,48	1.66	5 (10%)
4	ATP	G	401	-	29,33,33	0.26	0	44,52,52	0.46	1 (2%)
5	GBM	B	2001	-	35,35,35	2.11	4 (11%)	48,48,48	1.65	5 (10%)
4	ATP	E	401	-	29,33,33	0.26	0	44,52,52	0.46	1 (2%)
4	ATP	D	2002	-	29,33,33	0.27	0	44,52,52	0.47	1 (2%)
4	ATP	F	2002	-	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
4	ATP	A	401	-	29,33,33	0.26	0	44,52,52	0.46	1 (2%)
4	ATP	C	401	-	29,33,33	0.26	0	44,52,52	0.46	1 (2%)
4	ATP	H	2002	-	29,33,33	0.27	0	44,52,52	0.47	1 (2%)
4	ATP	B	2002	-	29,33,33	0.27	0	44,52,52	0.47	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GBM	H	2001	-	35,35,35	2.11	4 (11%)	48,48,48	1.65	5 (10%)
5	GBM	F	2001	-	35,35,35	2.12	4 (11%)	48,48,48	1.66	5 (10%)

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
5	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
4	ATP	G	401	-	-	4/22/38/38	0/3/3/3
5	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
4	ATP	E	401	-	-	4/22/38/38	0/3/3/3
4	ATP	D	2002	-	-	5/22/38/38	0/3/3/3
4	ATP	F	2002	-	-	5/22/38/38	0/3/3/3
4	ATP	A	401	-	-	4/22/38/38	0/3/3/3
4	ATP	C	401	-	-	4/22/38/38	0/3/3/3
4	ATP	H	2002	-	-	5/22/38/38	0/3/3/3
4	ATP	B	2002	-	-	5/22/38/38	0/3/3/3
5	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
5	GBM	F	2001	-	-	8/27/35/35	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2001	GBM	C18-S2	-10.69	1.59	1.76
5	B	2001	GBM	C18-S2	-10.67	1.60	1.76
5	H	2001	GBM	C18-S2	-10.65	1.60	1.76
5	D	2001	GBM	C18-S2	-10.64	1.60	1.76
5	B	2001	GBM	C27-C28	4.39	1.48	1.40
5	D	2001	GBM	C27-C28	4.38	1.48	1.40
5	F	2001	GBM	C27-C28	4.37	1.48	1.40
5	H	2001	GBM	C27-C28	4.34	1.48	1.40
5	F	2001	GBM	C17-N9	-2.65	1.33	1.39
5	D	2001	GBM	C17-N9	-2.64	1.33	1.39
5	H	2001	GBM	C17-N9	-2.61	1.33	1.39
5	B	2001	GBM	C17-N9	-2.57	1.33	1.39
5	B	2001	GBM	C31-CL1	2.55	1.80	1.74
5	D	2001	GBM	C31-CL1	2.53	1.80	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2001	GBM	C31-CL1	2.52	1.80	1.74
5	H	2001	GBM	C31-CL1	2.51	1.80	1.74

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	2001	GBM	O5-S2-O4	-8.74	108.80	119.55
5	B	2001	GBM	O5-S2-O4	-8.72	108.83	119.55
5	D	2001	GBM	O5-S2-O4	-8.70	108.85	119.55
5	H	2001	GBM	O5-S2-O4	-8.70	108.85	119.55
5	D	2001	GBM	C28-C27-C26	-3.01	120.67	126.16
5	F	2001	GBM	C28-C27-C26	-2.99	120.71	126.16
5	B	2001	GBM	C28-C27-C26	-2.98	120.72	126.16
5	H	2001	GBM	C28-C27-C26	-2.97	120.74	126.16
5	H	2001	GBM	C18-S2-N9	2.80	110.21	105.97
5	B	2001	GBM	C18-S2-N9	2.79	110.20	105.97
5	F	2001	GBM	C18-S2-N9	2.79	110.20	105.97
5	D	2001	GBM	C18-S2-N9	2.77	110.17	105.97
5	D	2001	GBM	O7-C28-C27	2.54	120.24	116.55
5	F	2001	GBM	O7-C28-C27	2.51	120.20	116.55
5	H	2001	GBM	O7-C28-C27	2.50	120.18	116.55
5	B	2001	GBM	O7-C28-C27	2.46	120.13	116.55
5	D	2001	GBM	C33-O7-C28	2.34	121.06	117.53
5	F	2001	GBM	C33-O7-C28	2.32	121.04	117.53
5	H	2001	GBM	C33-O7-C28	2.32	121.02	117.53
5	B	2001	GBM	C33-O7-C28	2.28	120.96	117.53
4	E	401	ATP	PB-O3B-PG	2.10	140.04	132.83
4	G	401	ATP	PB-O3B-PG	2.10	140.04	132.83
4	A	401	ATP	PB-O3B-PG	2.10	140.03	132.83
4	C	401	ATP	PB-O3B-PG	2.09	139.99	132.83
4	D	2002	ATP	PB-O3B-PG	2.08	139.96	132.83
4	H	2002	ATP	PB-O3B-PG	2.06	139.91	132.83
4	F	2002	ATP	PB-O3B-PG	2.06	139.89	132.83
4	B	2002	ATP	PB-O3B-PG	2.05	139.86	132.83

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	C5'-O5'-PA-O1A
4	A	401	ATP	C5'-O5'-PA-O2A
4	A	401	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	C	401	ATP	C5'-O5'-PA-O1A
4	C	401	ATP	C5'-O5'-PA-O2A
4	C	401	ATP	C5'-O5'-PA-O3A
4	E	401	ATP	C5'-O5'-PA-O1A
4	E	401	ATP	C5'-O5'-PA-O2A
4	E	401	ATP	C5'-O5'-PA-O3A
4	G	401	ATP	C5'-O5'-PA-O1A
4	G	401	ATP	C5'-O5'-PA-O2A
4	G	401	ATP	C5'-O5'-PA-O3A
5	B	2001	GBM	C21-C18-S2-O5
5	D	2001	GBM	C21-C18-S2-O5
5	F	2001	GBM	C21-C18-S2-O5
5	H	2001	GBM	C21-C18-S2-O5
5	D	2001	GBM	C22-C18-S2-O5
5	F	2001	GBM	C22-C18-S2-O5
5	B	2001	GBM	C22-C18-S2-O5
5	H	2001	GBM	C22-C18-S2-O5
5	B	2001	GBM	C24-C19-C20-C25
5	D	2001	GBM	C24-C19-C20-C25
5	F	2001	GBM	C24-C19-C20-C25
5	H	2001	GBM	C24-C19-C20-C25
5	B	2001	GBM	C23-C19-C20-C25
5	D	2001	GBM	C23-C19-C20-C25
5	F	2001	GBM	C23-C19-C20-C25
5	H	2001	GBM	C23-C19-C20-C25
5	B	2001	GBM	C21-C18-S2-N9
5	H	2001	GBM	C21-C18-S2-N9
5	F	2001	GBM	C21-C18-S2-N9
5	D	2001	GBM	C21-C18-S2-N9
5	D	2001	GBM	C22-C18-S2-N9
5	B	2001	GBM	C22-C18-S2-N9
5	F	2001	GBM	C22-C18-S2-N9
5	H	2001	GBM	C22-C18-S2-N9
4	B	2002	ATP	PB-O3B-PG-O1G
4	D	2002	ATP	PB-O3B-PG-O1G
4	F	2002	ATP	PB-O3B-PG-O1G
4	H	2002	ATP	PB-O3B-PG-O1G
4	A	401	ATP	PB-O3A-PA-O1A
4	C	401	ATP	PB-O3A-PA-O1A
4	E	401	ATP	PB-O3A-PA-O1A
4	G	401	ATP	PB-O3A-PA-O1A
5	B	2001	GBM	O6-C26-N10-C25

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Mol	Chain	Res	Type	Atoms
5	H	2001	GBM	O6-C26-N10-C25
5	F	2001	GBM	O6-C26-N10-C25
5	D	2001	GBM	O6-C26-N10-C25
4	B	2002	ATP	PB-O3B-PG-O2G
4	B	2002	ATP	PB-O3B-PG-O3G
4	D	2002	ATP	PB-O3B-PG-O2G
4	D	2002	ATP	PB-O3B-PG-O3G
4	F	2002	ATP	PB-O3B-PG-O2G
4	F	2002	ATP	PB-O3B-PG-O3G
4	H	2002	ATP	PB-O3B-PG-O2G
4	H	2002	ATP	PB-O3B-PG-O3G
5	H	2001	GBM	C27-C26-N10-C25
5	B	2001	GBM	C27-C26-N10-C25
5	D	2001	GBM	C27-C26-N10-C25
5	F	2001	GBM	C27-C26-N10-C25
4	B	2002	ATP	PG-O3B-PB-O1B
4	B	2002	ATP	PG-O3B-PB-O2B
4	D	2002	ATP	PG-O3B-PB-O1B
4	D	2002	ATP	PG-O3B-PB-O2B
4	F	2002	ATP	PG-O3B-PB-O1B
4	F	2002	ATP	PG-O3B-PB-O2B
4	H	2002	ATP	PG-O3B-PB-O1B
4	H	2002	ATP	PG-O3B-PB-O2B

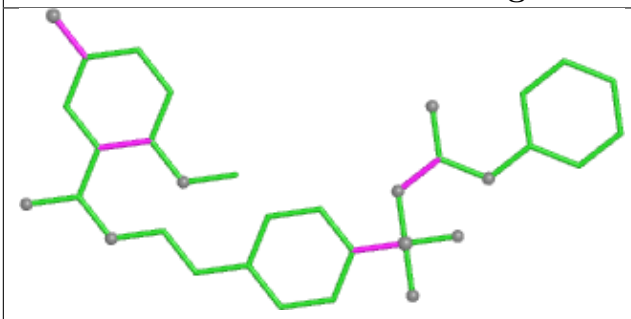
There are no ring outliers.

1 monomer is involved in 1 short contact:

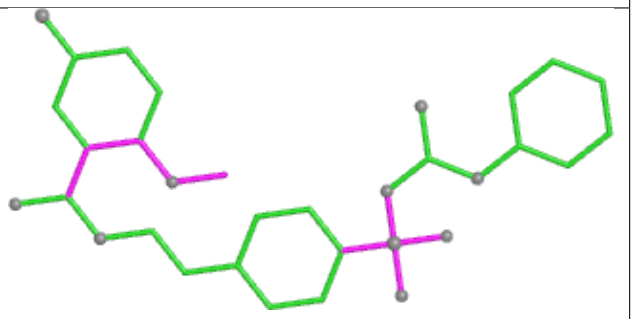
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	GBM	1	0

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

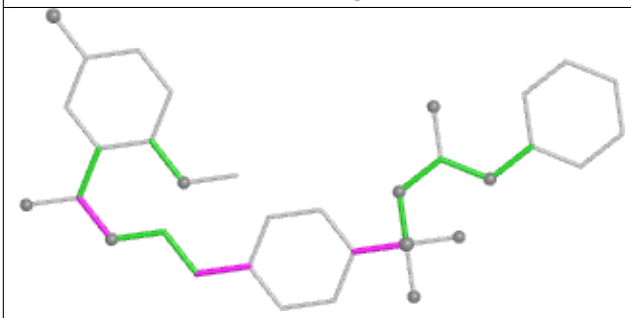
Ligand GBM D 2001



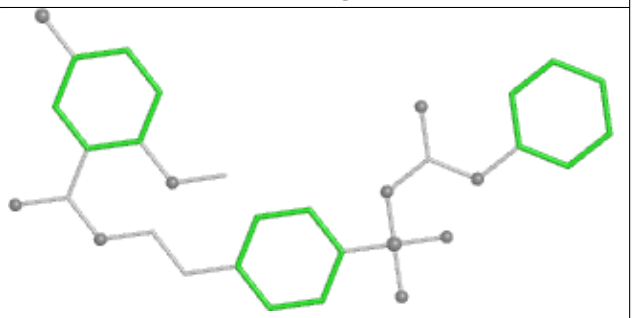
Bond lengths



Bond angles

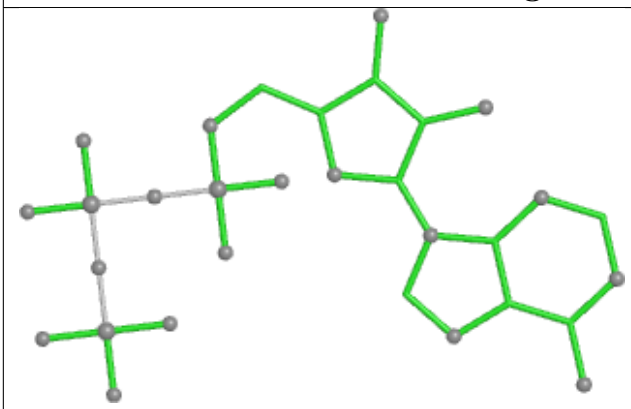


Torsions

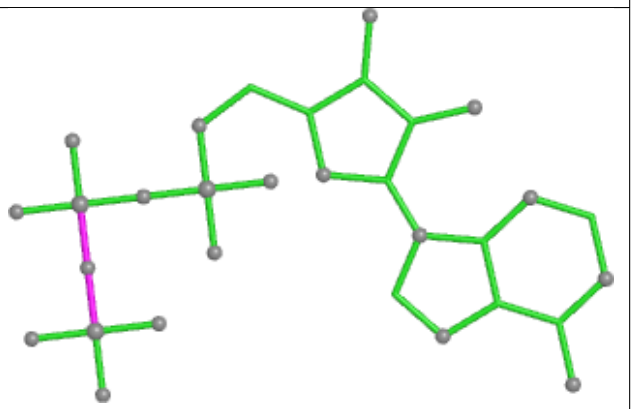


Rings

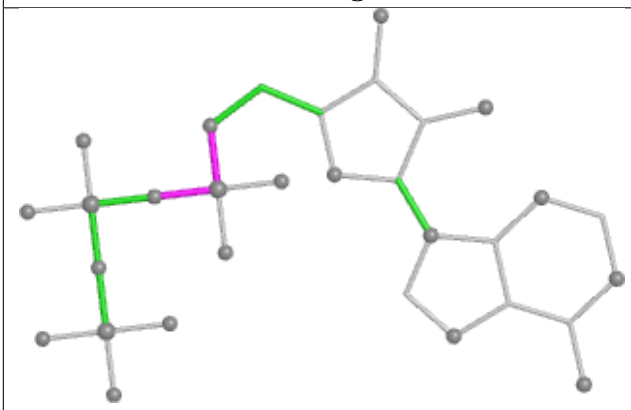
Ligand ATP G 401



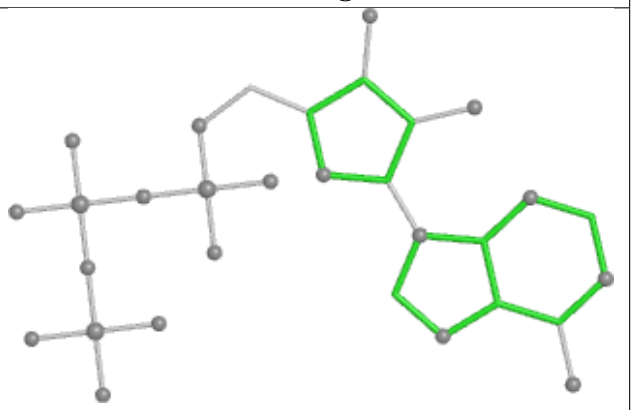
Bond lengths



Bond angles

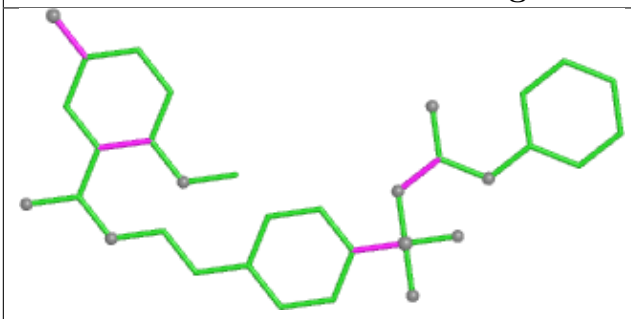


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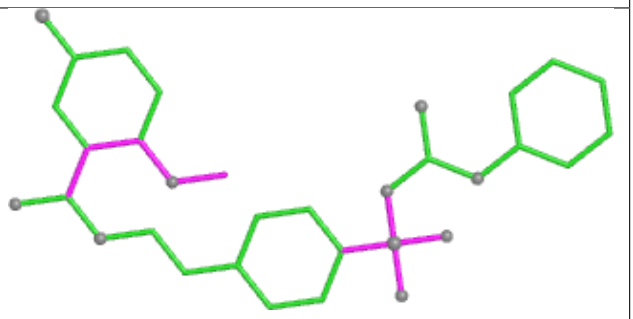


Rings

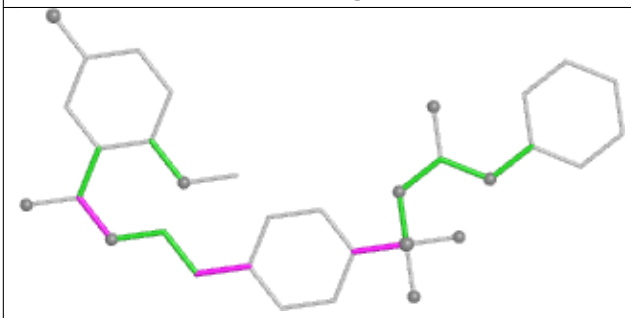
Ligand GBM B 2001



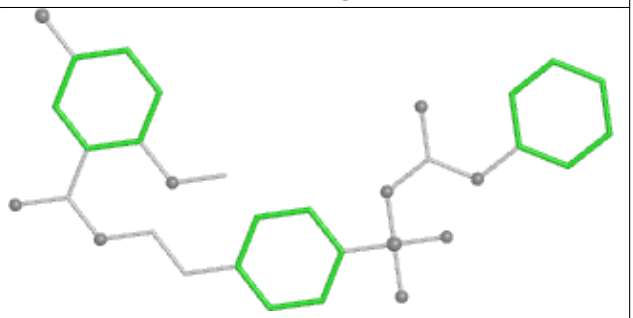
Bond lengths



Bond angles

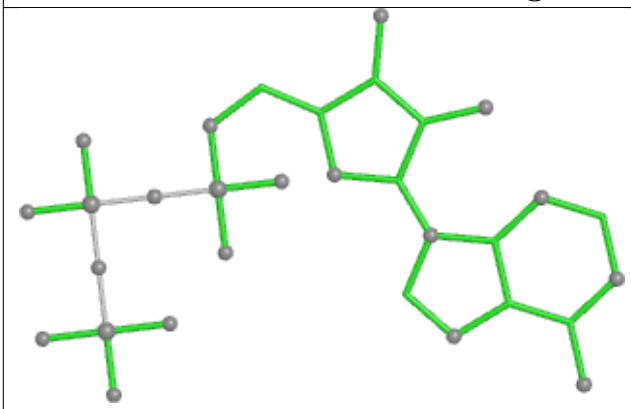


Torsions

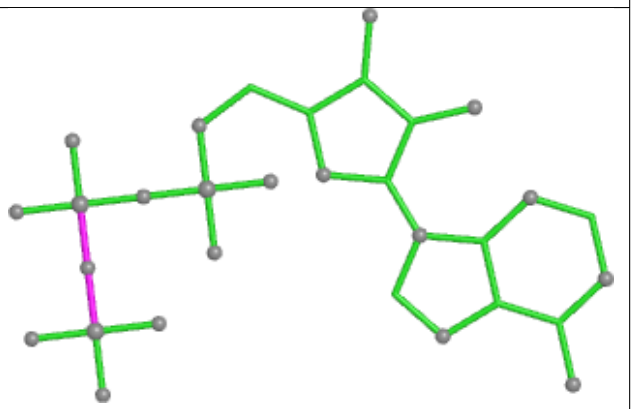


Rings

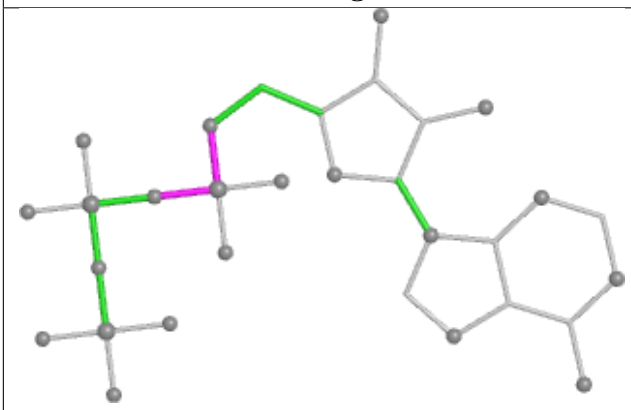
Ligand ATP E 401



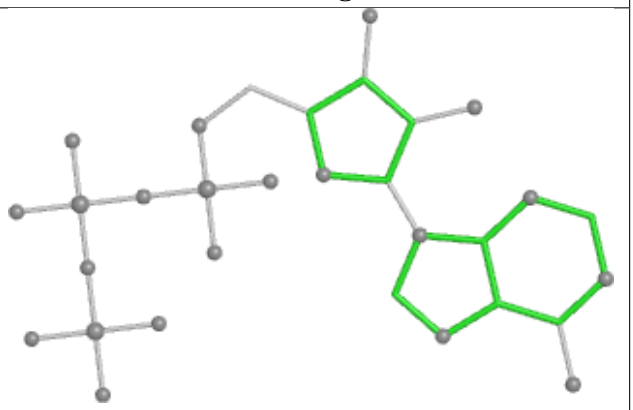
Bond lengths



Bond angles

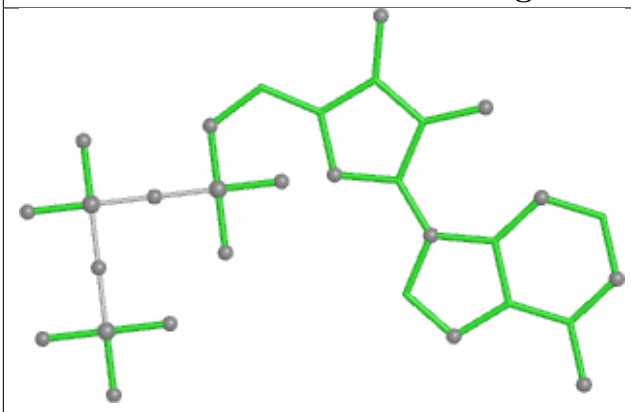


Torsions

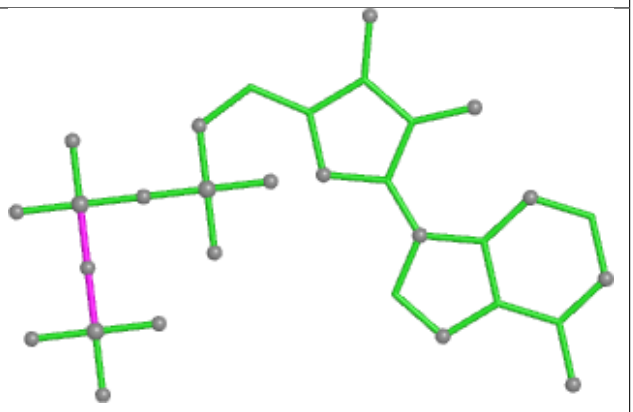


Rings

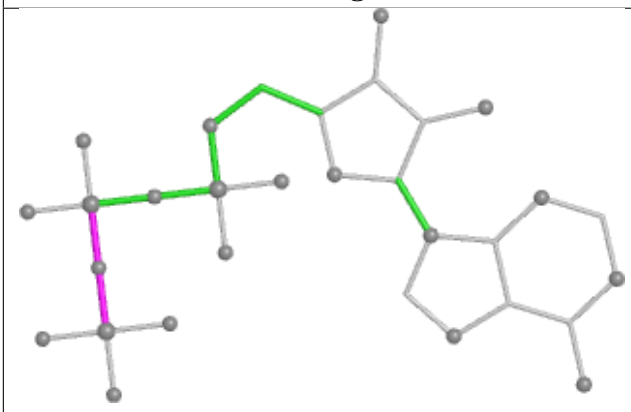
Ligand ATP D 2002



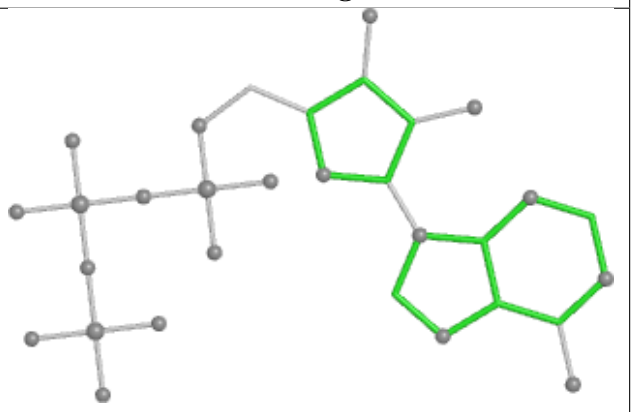
Bond lengths



Bond angles

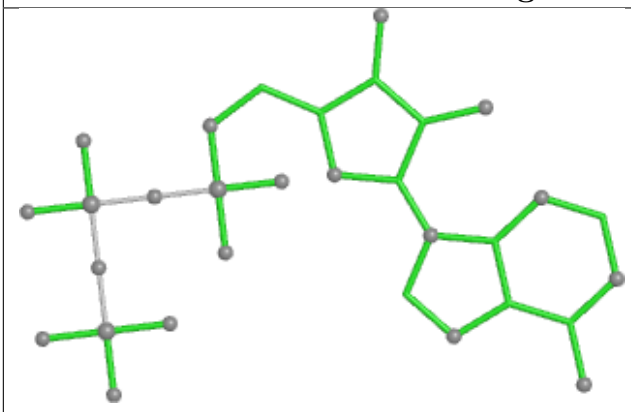


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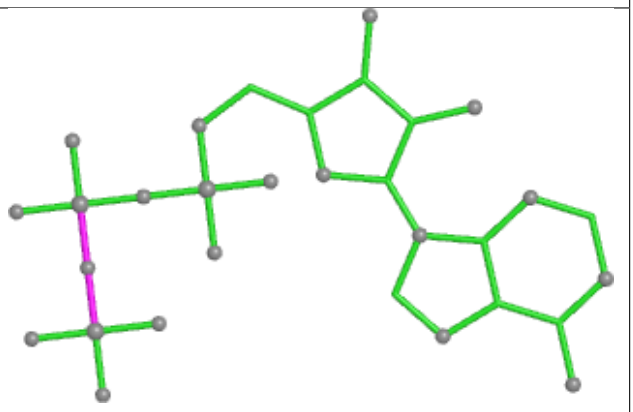


Rings

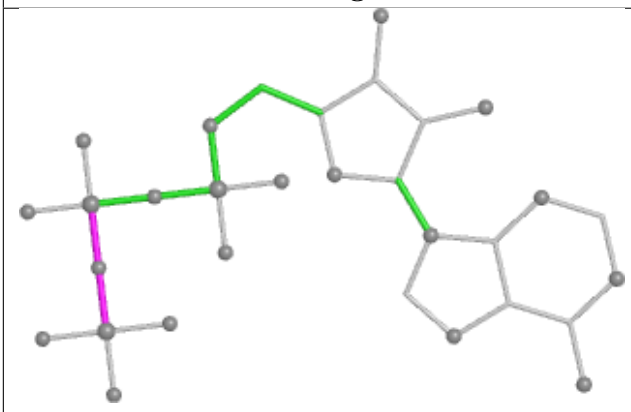
Ligand ATP F 2002



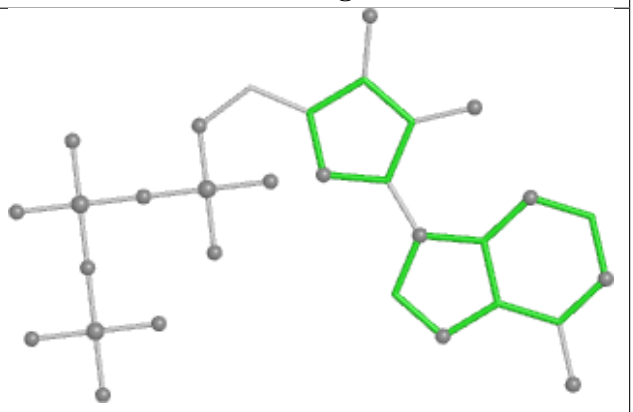
Bond lengths



Bond angles

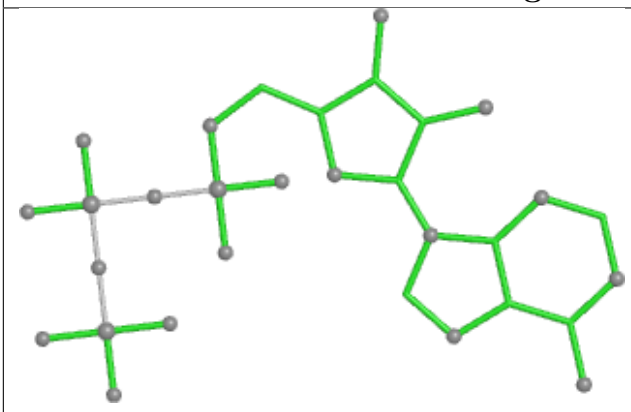


Torsions

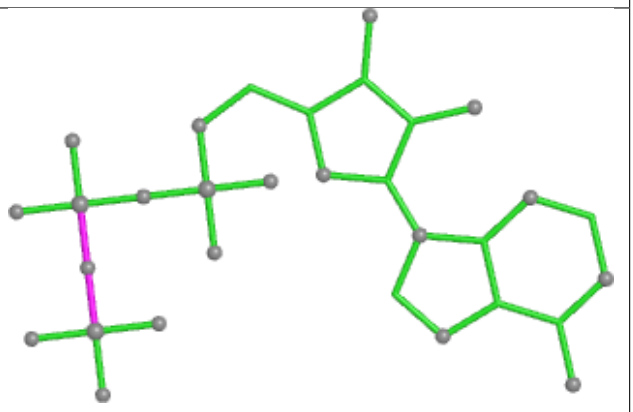


Rings

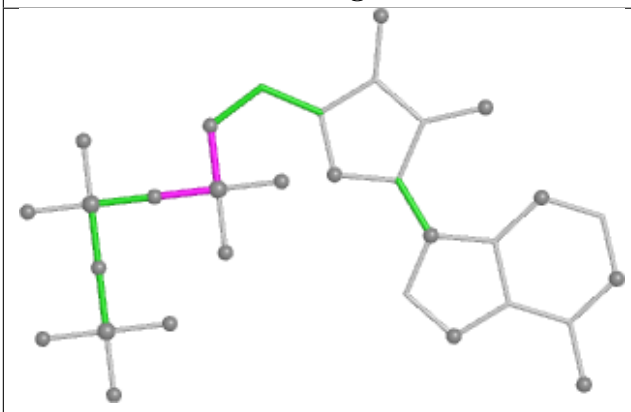
Ligand ATP A 401



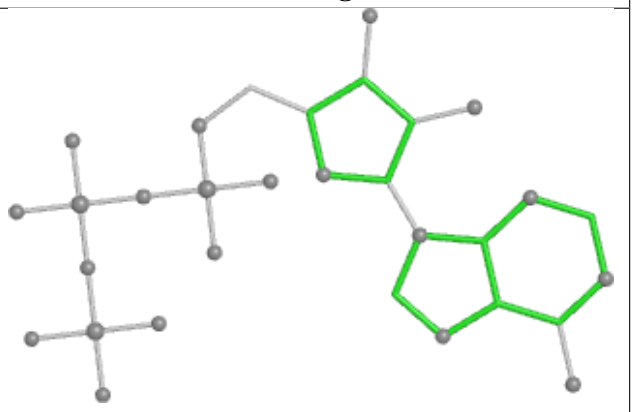
Bond lengths



Bond angles

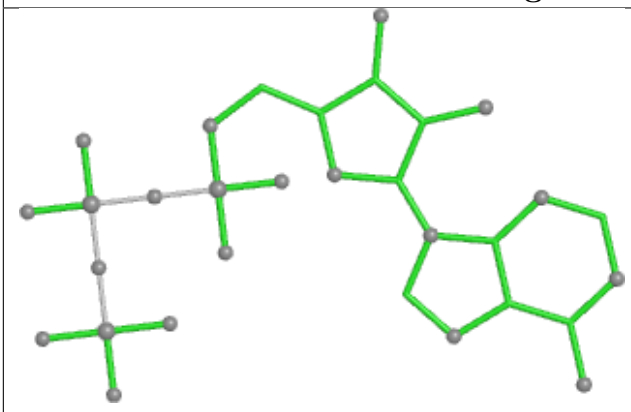


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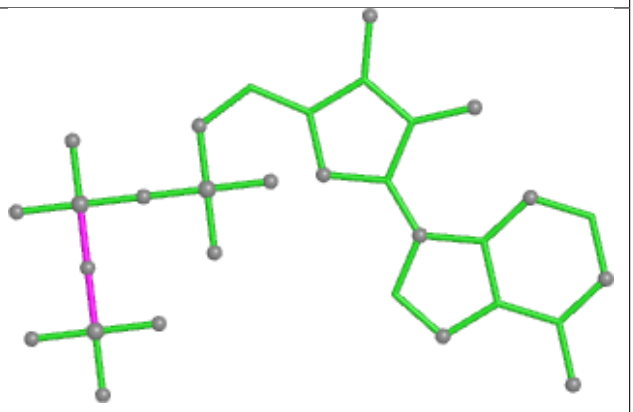


Rings

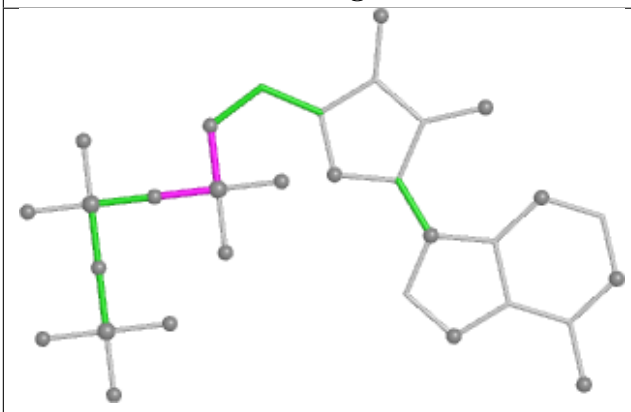
Ligand ATP C 401



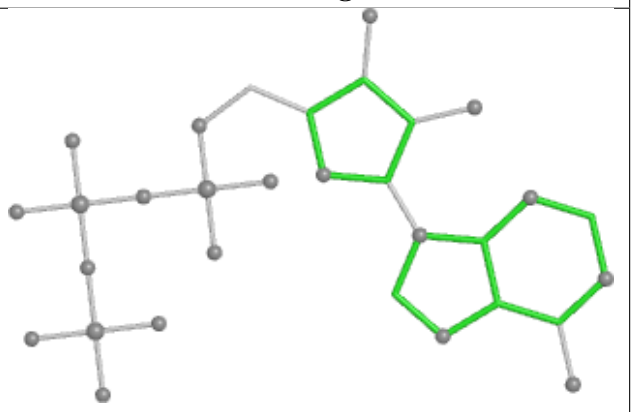
Bond lengths



Bond angles

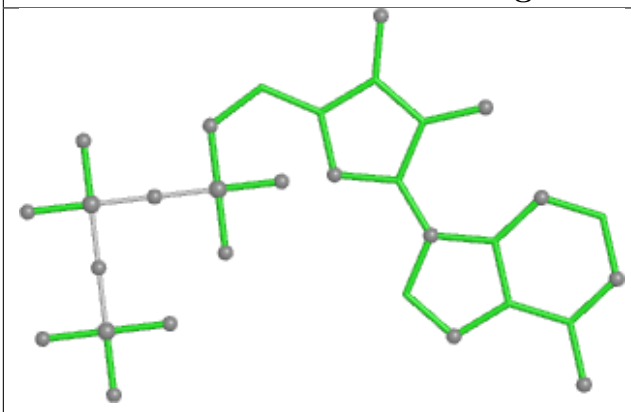


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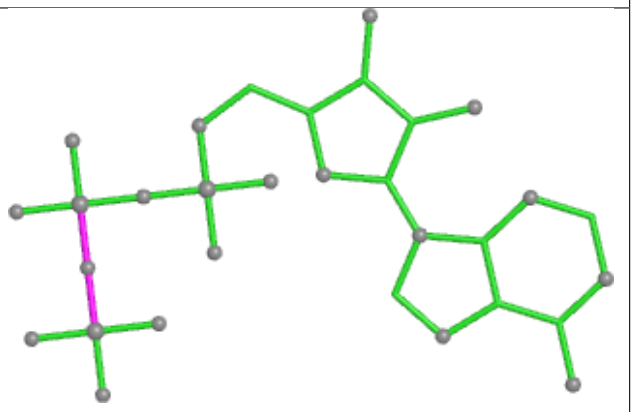


Rings

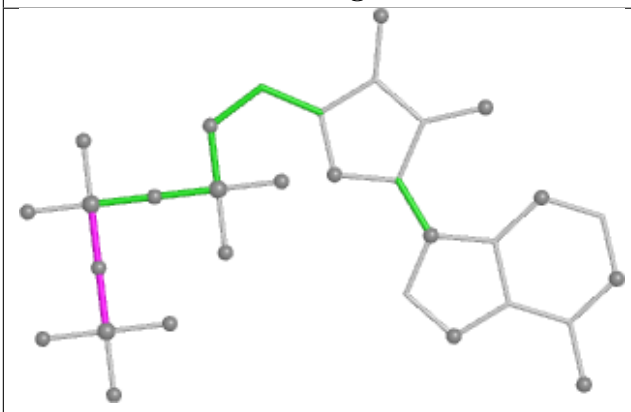
Ligand ATP H 2002



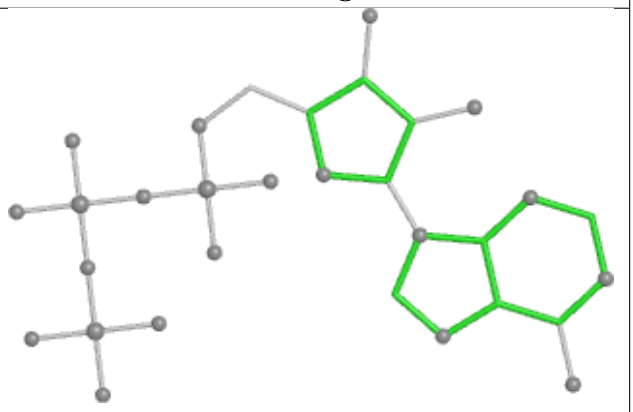
Bond lengths



Bond angles

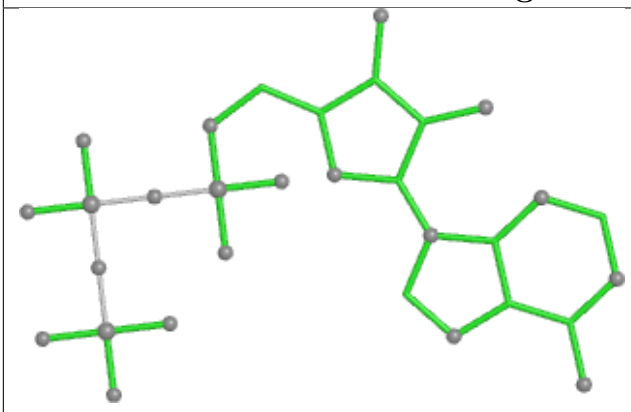


Torsions

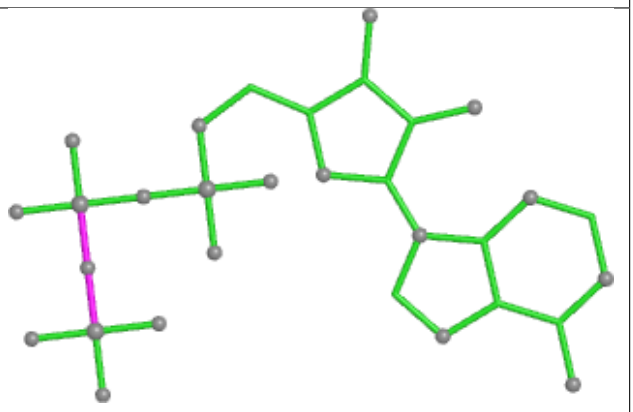


Rings

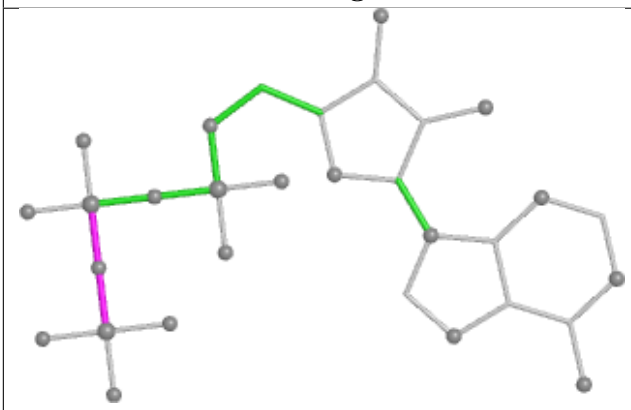
Ligand ATP B 2002



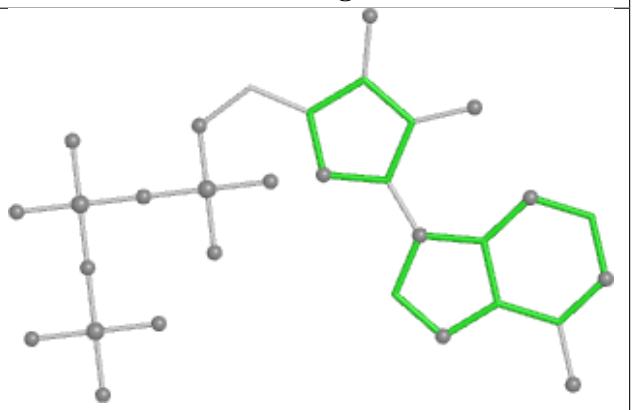
Bond lengths



Bond angles

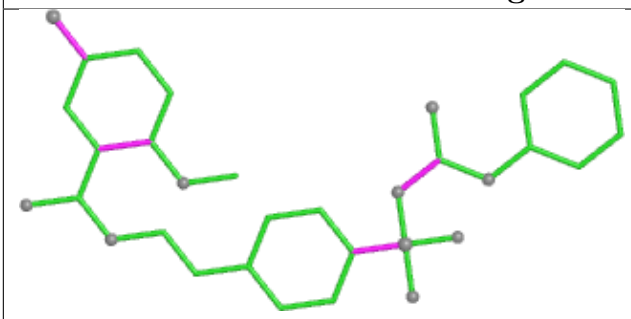


Torsions

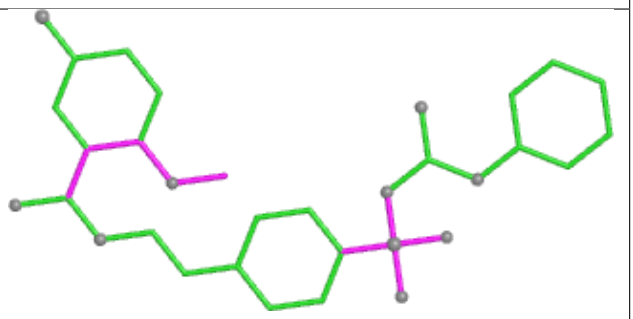


Rings

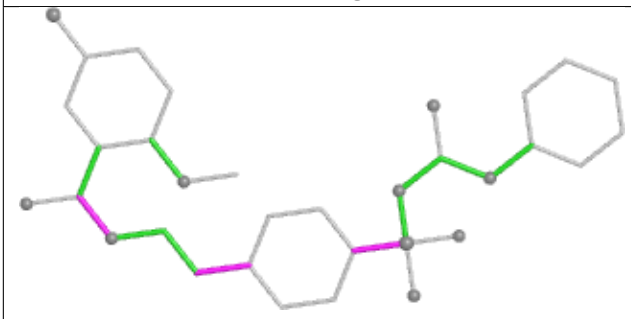
Ligand GBM H 2001



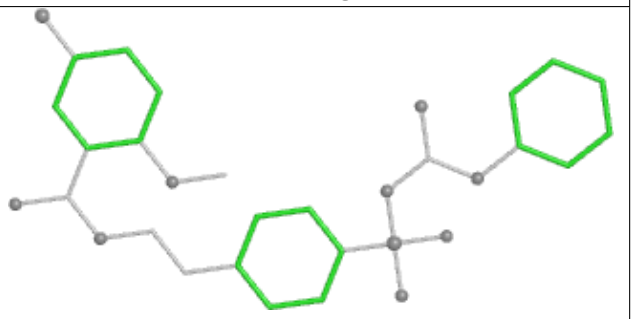
Bond lengths



Bond angles

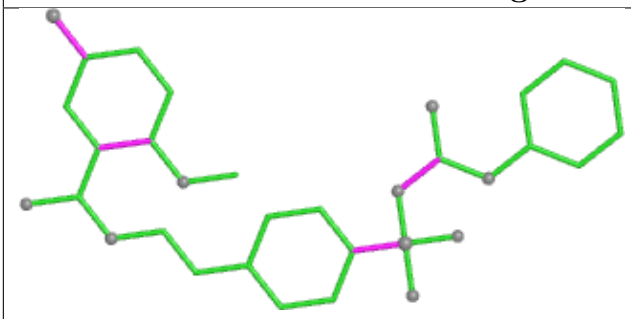


Torsions

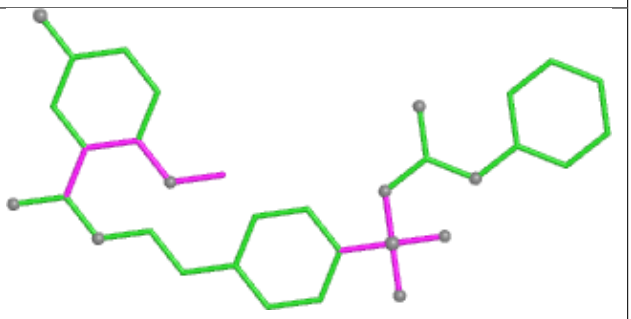


Rings

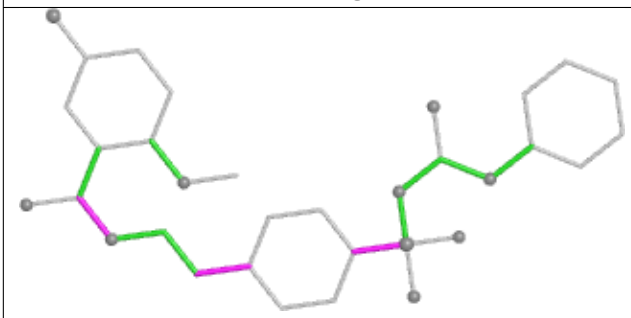
Ligand GBM F 2001



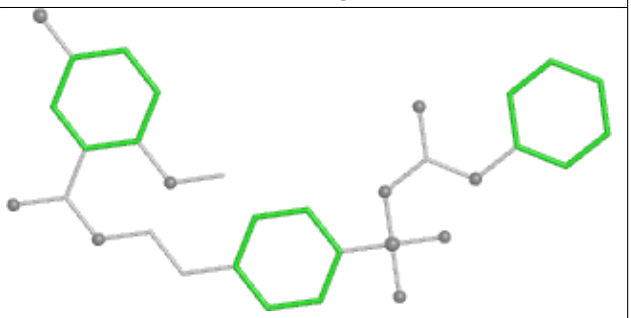
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

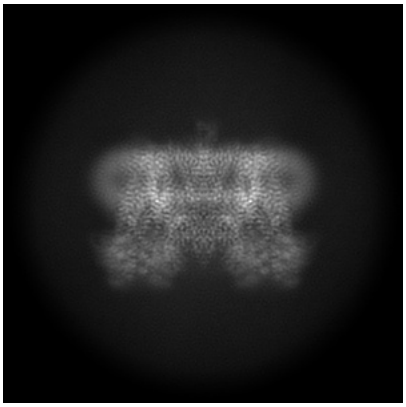
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62322. These allow visual inspection of the internal detail of the map and identification of artifacts.

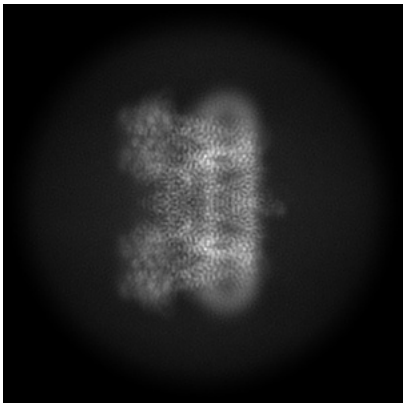
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

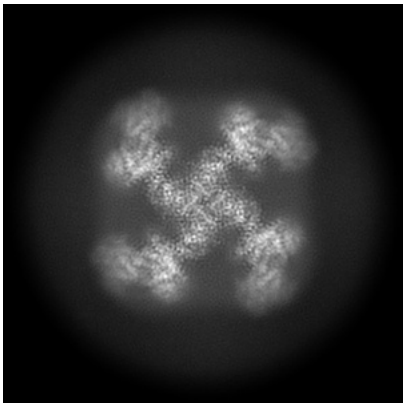
6.1.1 Primary map



X



Y

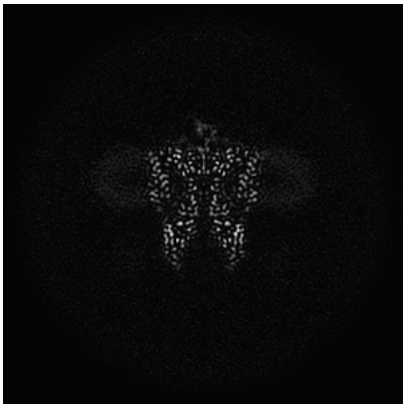


Z

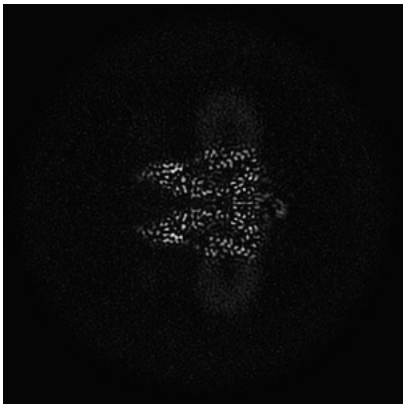
The images above show the map projected in three orthogonal directions.

6.2 Central slices

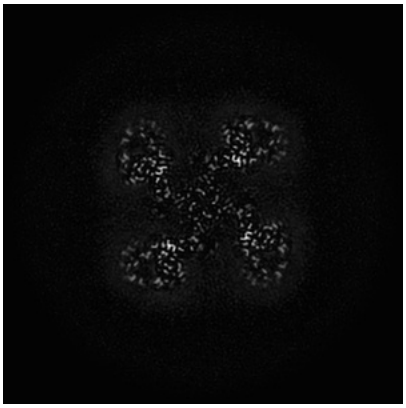
6.2.1 Primary map



X Index: 128



Y Index: 128

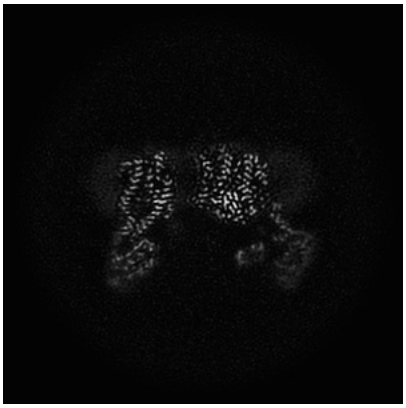


Z Index: 128

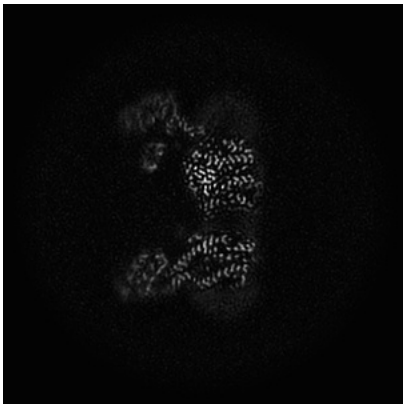
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

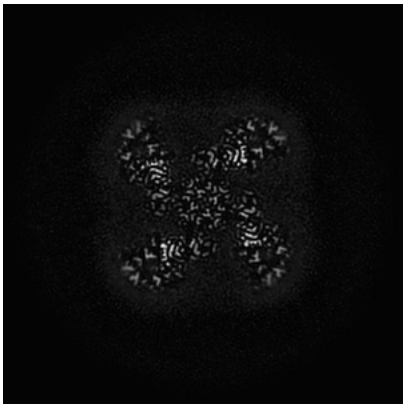
6.3.1 Primary map



X Index: 98



Y Index: 158

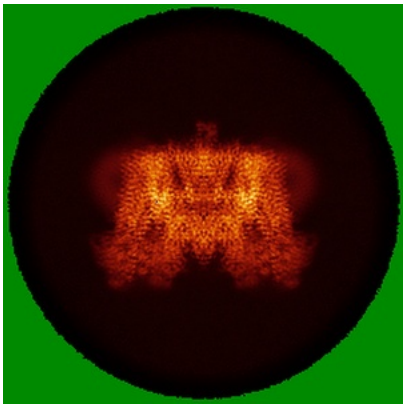


Z Index: 131

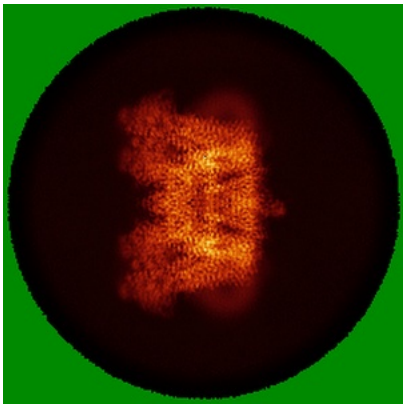
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

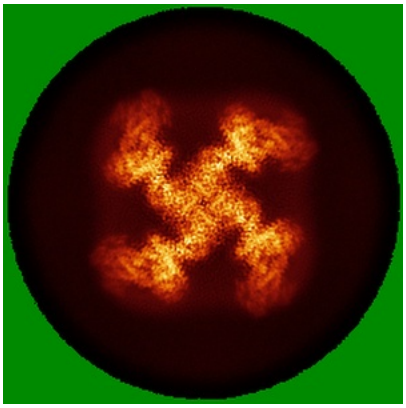
6.4.1 Primary map



X



Y

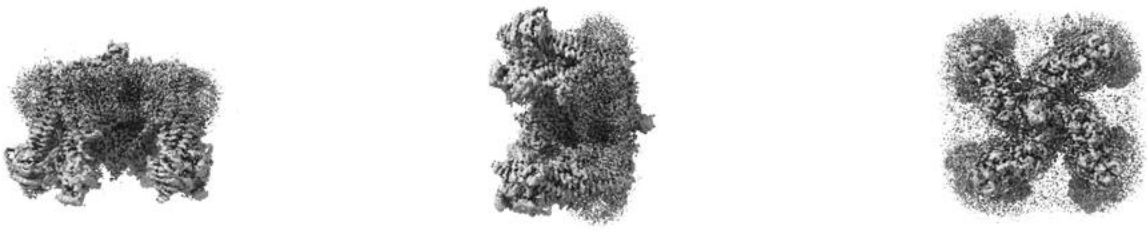


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

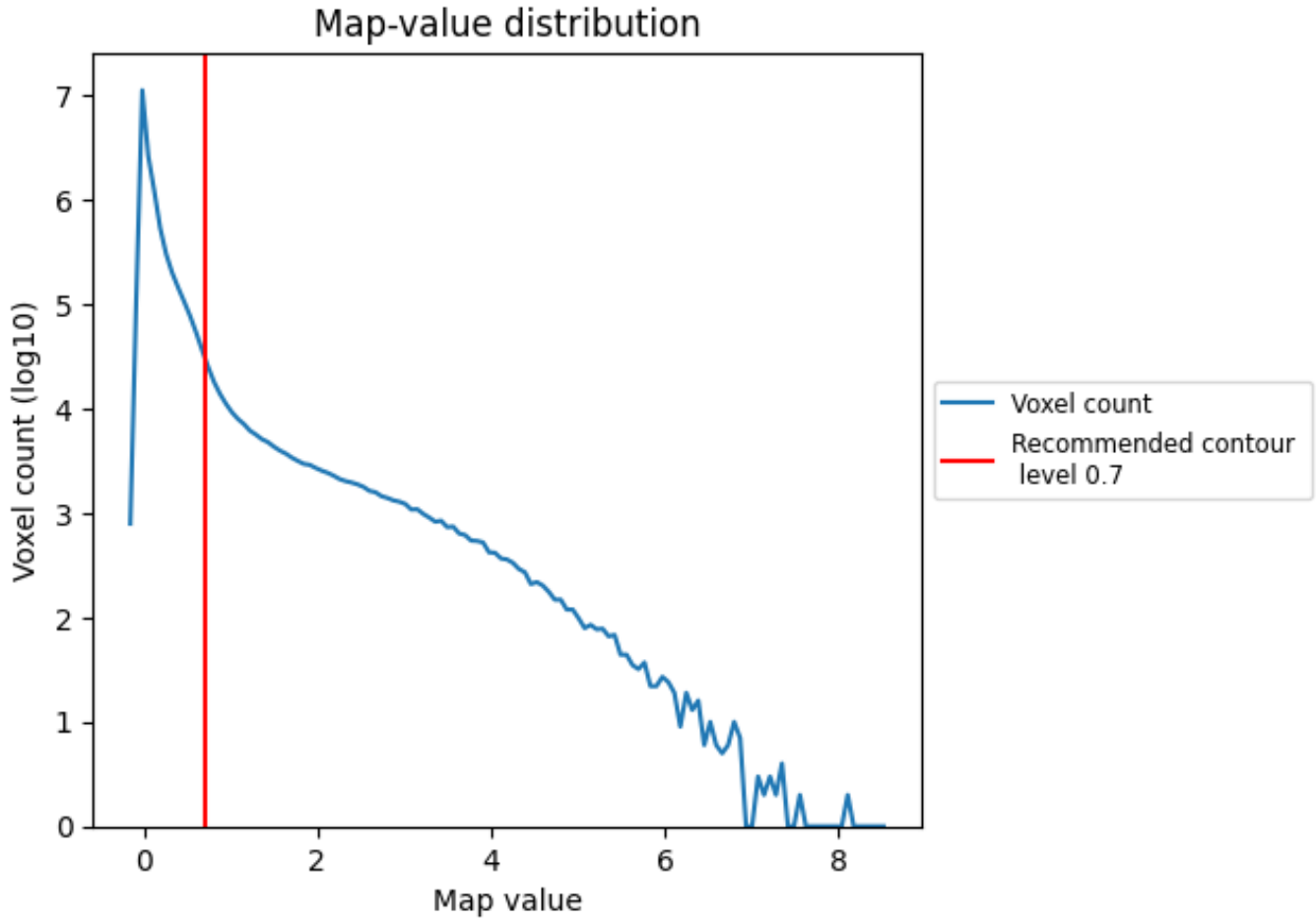
6.6 Mask visualisation (i)

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

7 Map analysis

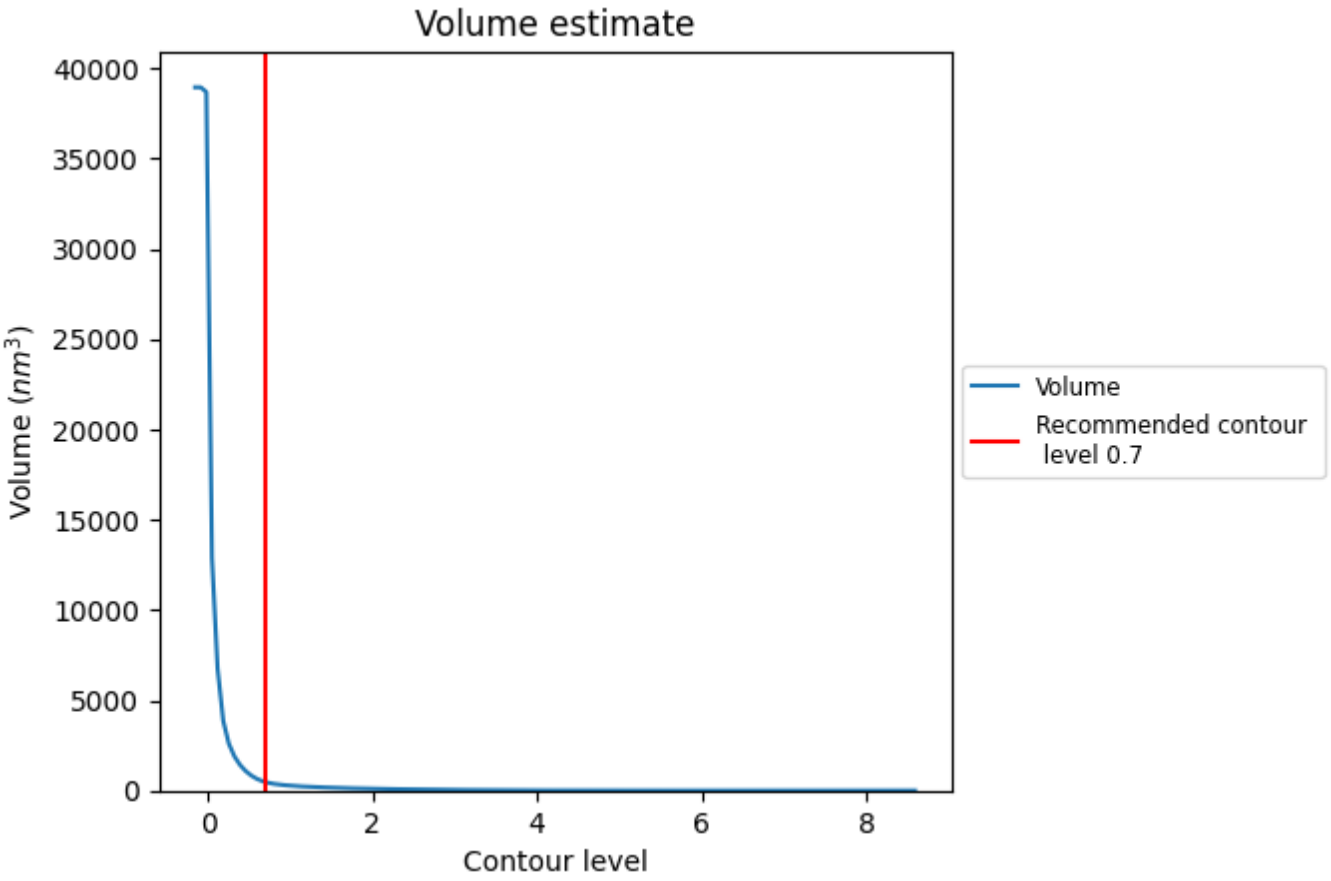
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

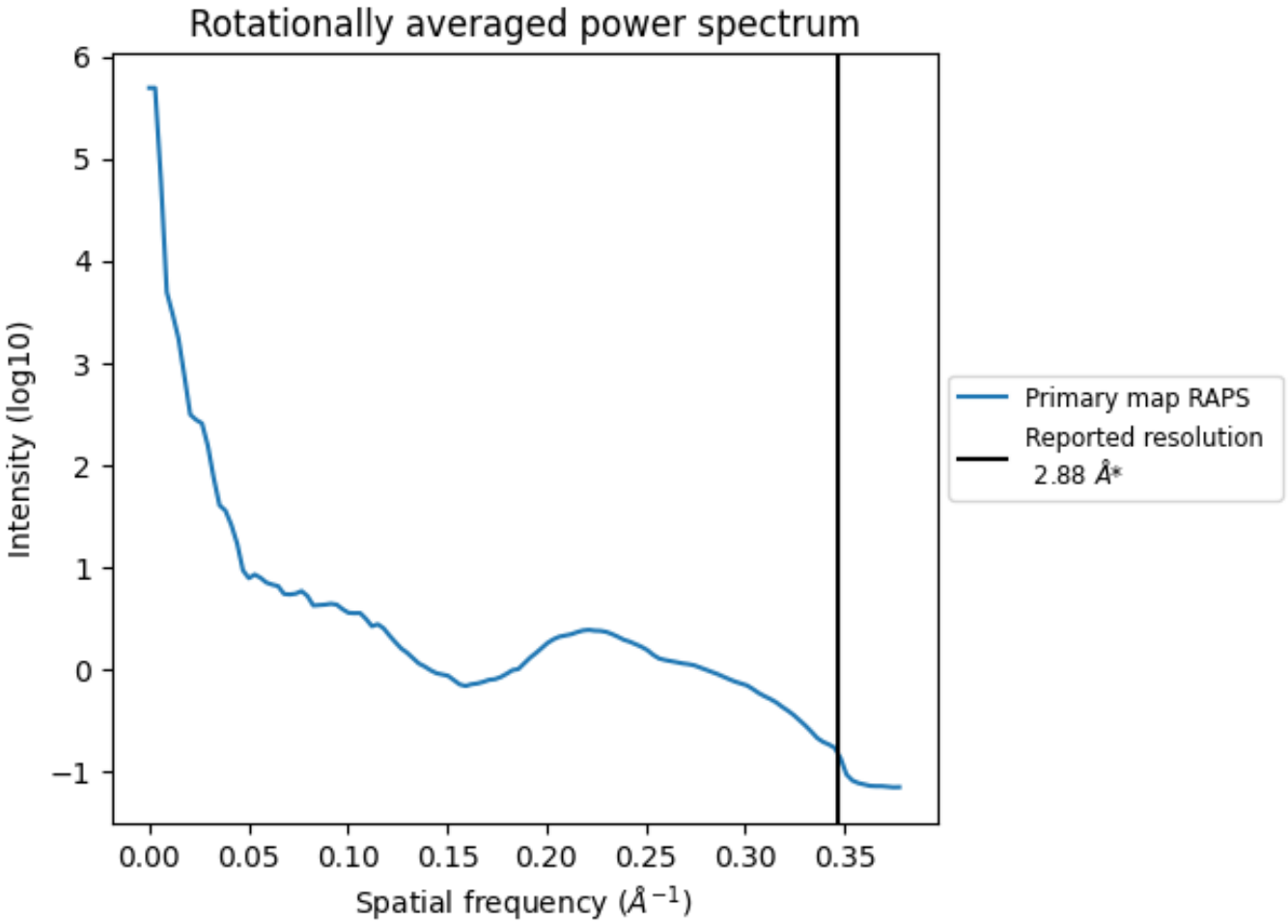
7.2 Volume estimate



The volume at the recommended contour level is 477 nm^3; this corresponds to an approximate mass of 431 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 (i)



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

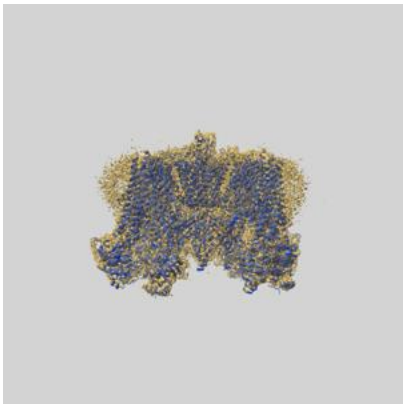
8 Fourier-Shell correlation

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

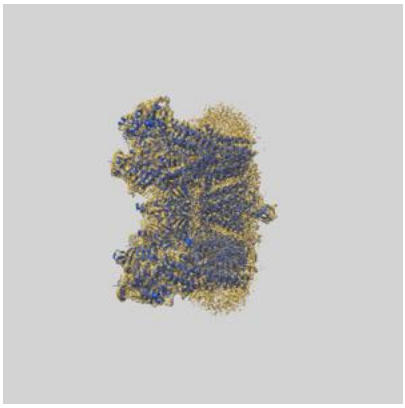
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62322 and PDB model 9KGL. Per-residue inclusion information can be found in section 3 on page 7.

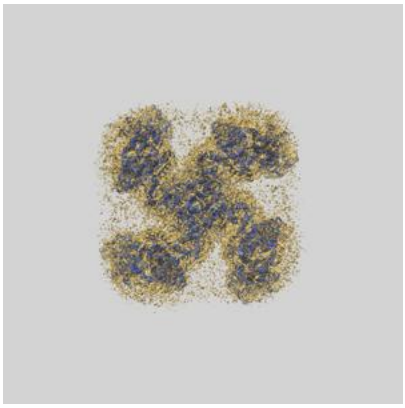
9.1 Map-model overlay



X



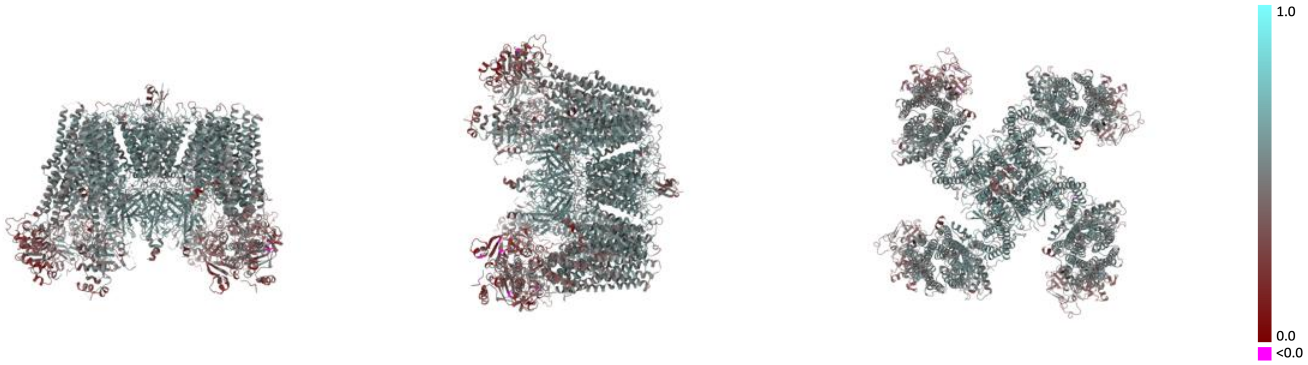
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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.

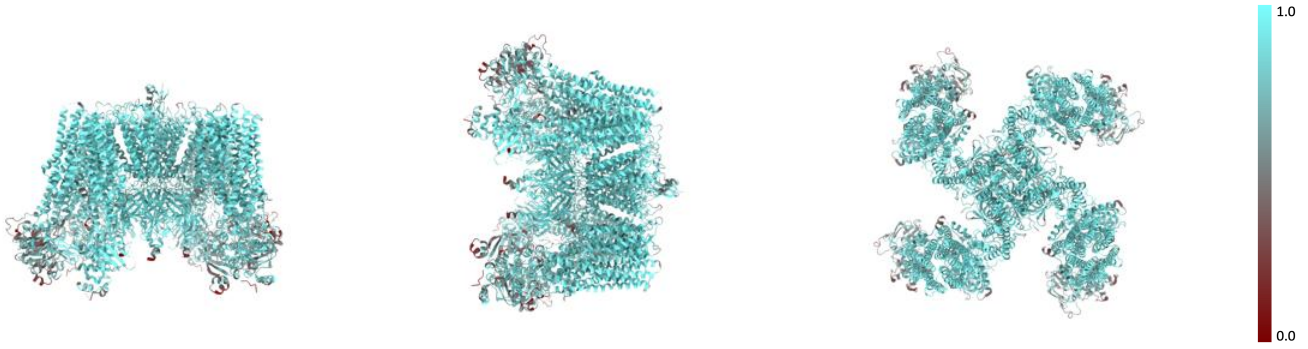
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

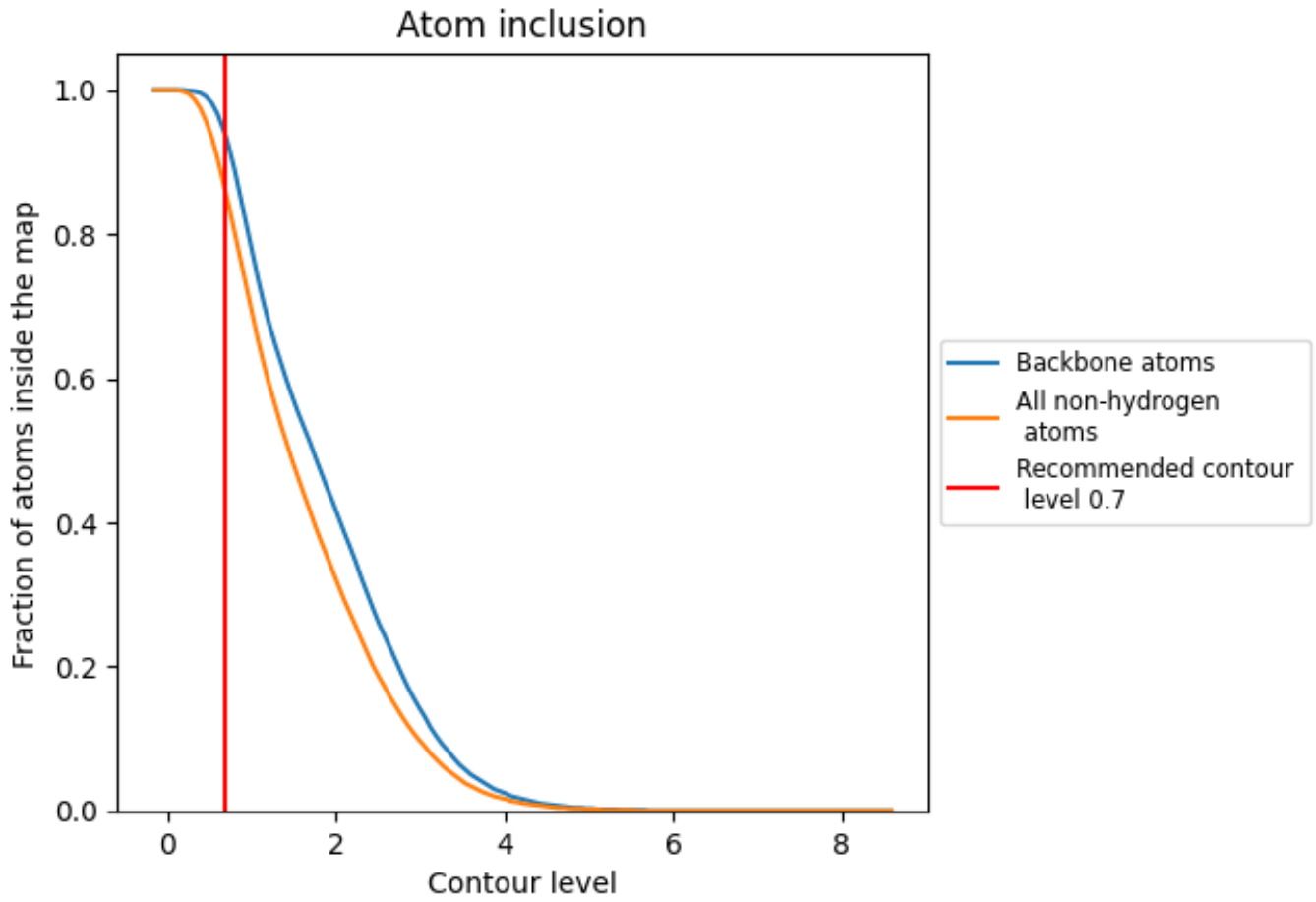
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.4890
A	0.9350	0.5740
B	0.8480	0.4830
C	0.9250	0.5660
D	0.8220	0.4470
E	0.9270	0.5650
F	0.8480	0.4800
G	0.9260	0.5670
H	0.8410	0.4770
I	0.7940	0.4140

