



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 06:49 AM JST

PDB ID : 5YKF
EMDB ID : EMD-6832
Title : Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (3D class1 at 4.33A)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-10-14
Resolution : 4.33 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

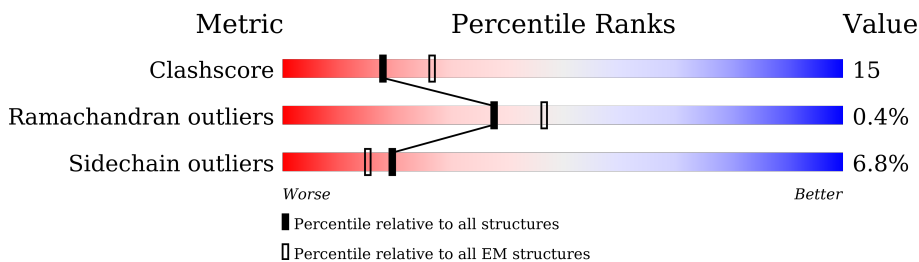
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.33 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	 50% 29% 17%
1	C	390	 50% 29% 17%
1	E	390	 50% 29% 17%
1	G	390	 51% 28% 17%
2	B	1582	 21% 59% 22% 17%
2	D	1582	 21% 59% 23% 17%
2	F	1582	 21% 59% 22% 17%
2	H	1582	 21% 59% 22% 17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 50988 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.

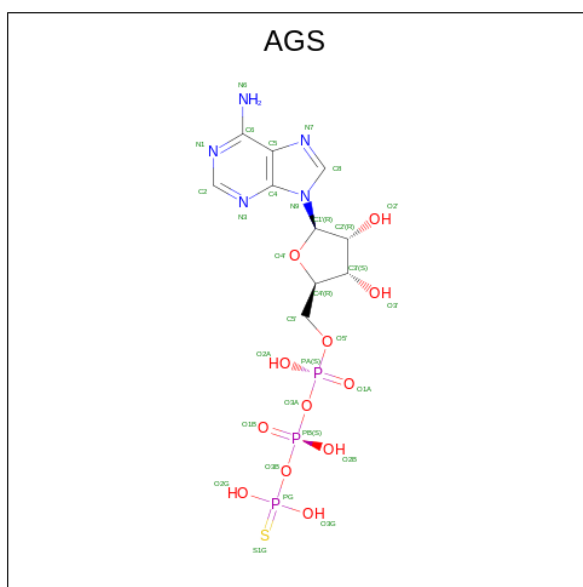
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

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

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

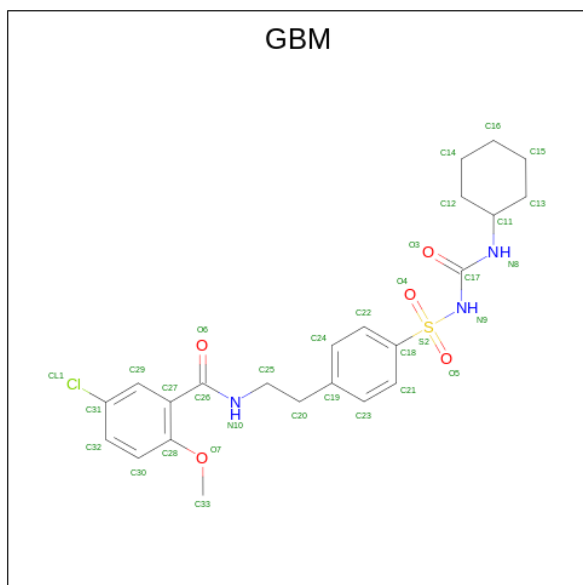
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1309	10189	6644	1724	1768	53	0	0
2	D	1309	10189	6644	1724	1768	53	0	0
2	F	1309	10189	6644	1724	1768	53	0	0
2	H	1309	10189	6644	1724	1768	53	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
3	A	1	Total 62	20	10	24	6	2	0
3	A	1	Total 62	20	10	24	6	2	0
3	B	1	Total 31	10	5	12	3	1	0
3	C	1	Total 31	10	5	12	3	1	0
3	D	1	Total 31	10	5	12	3	1	0
3	E	1	Total 31	10	5	12	3	1	0
3	F	1	Total 31	10	5	12	3	1	0
3	H	1	Total 31	10	5	12	3	1	0

- Molecule 4 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula: C₂₃H₂₈ClN₃O₅S).

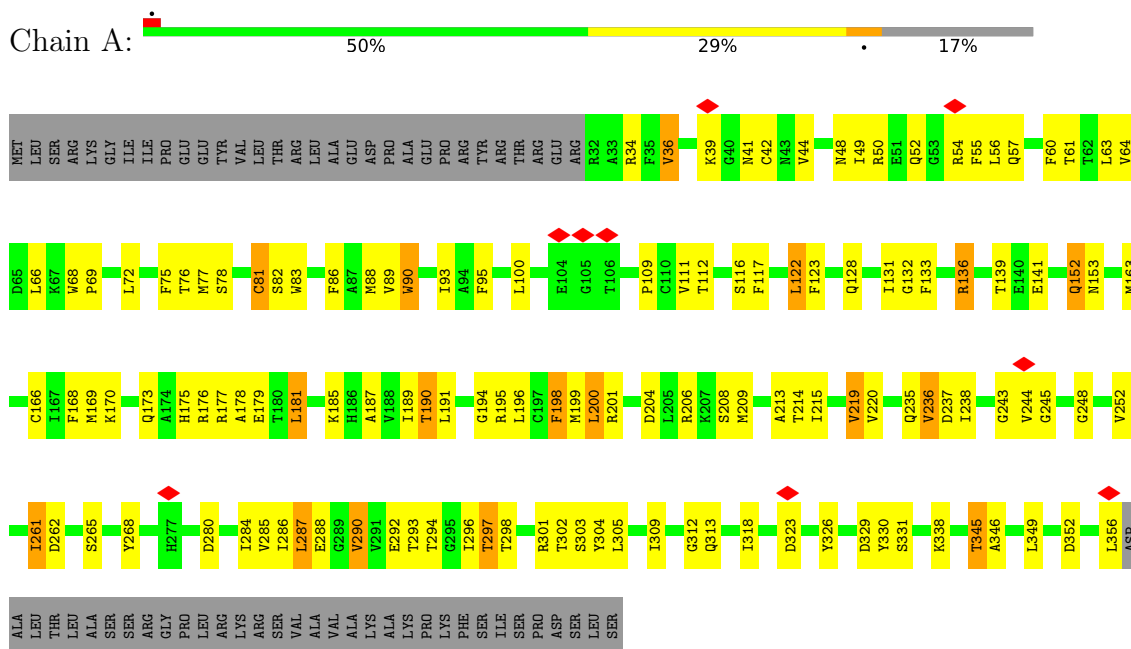


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	N	O		S
4	B	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	
4	D	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	
4	F	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	
4	H	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	

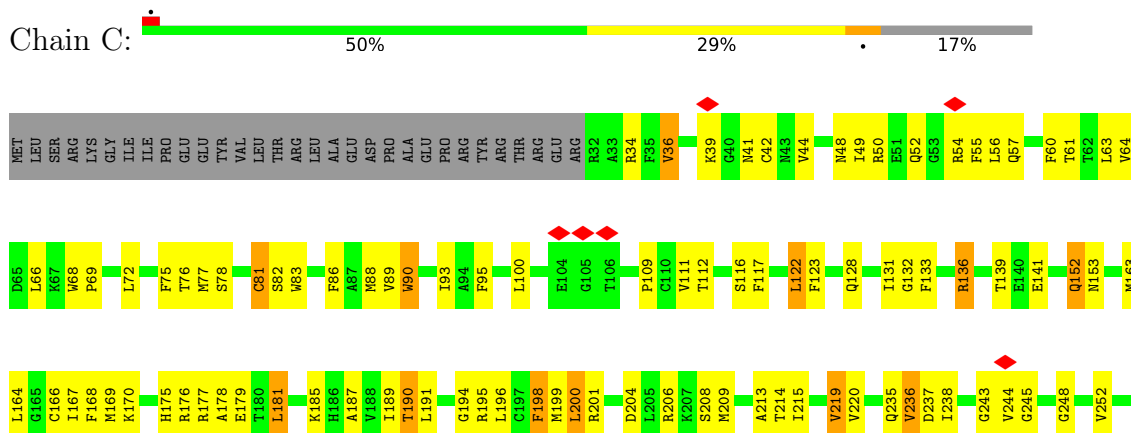
3 Residue-property plots [i](#)

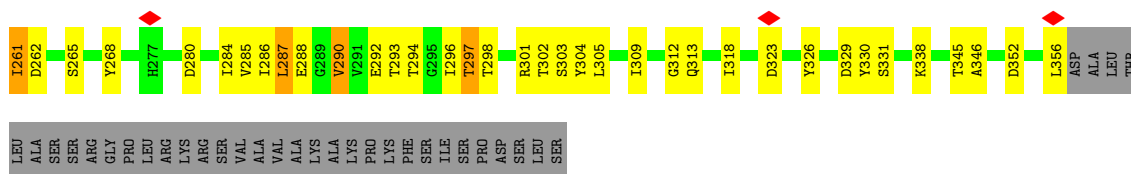
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



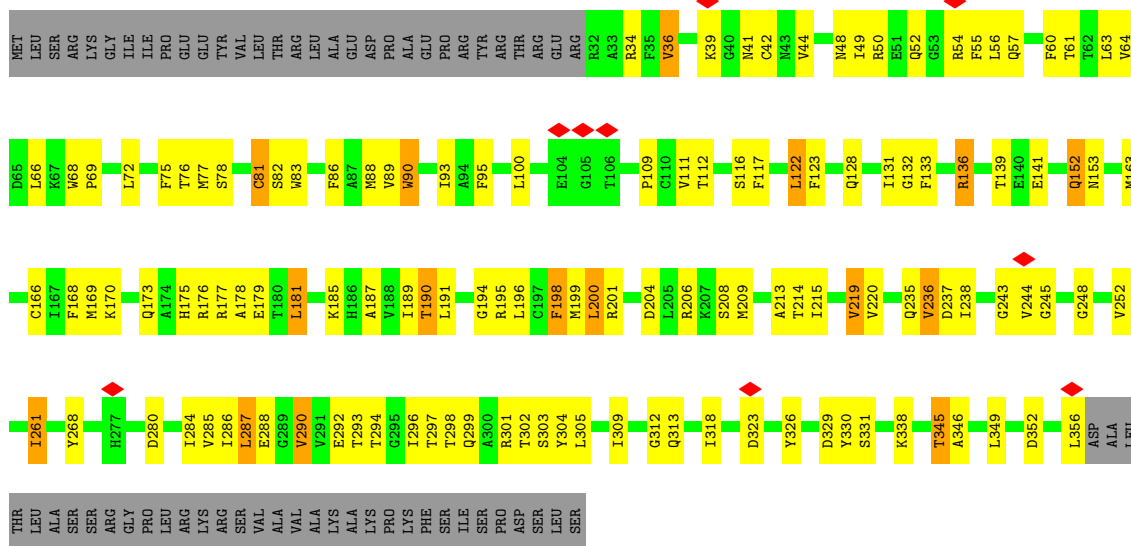
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11





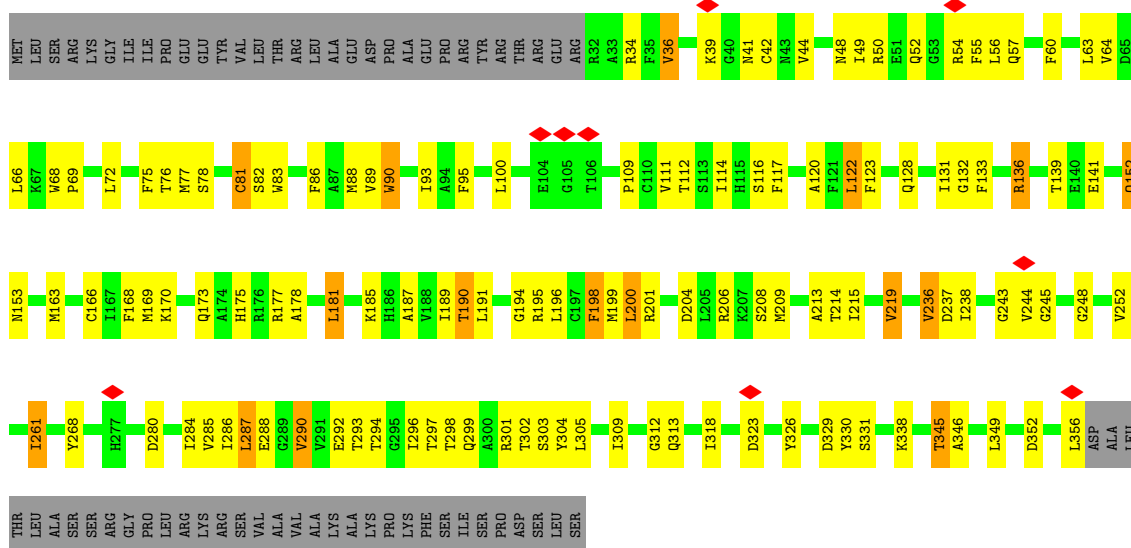
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E:

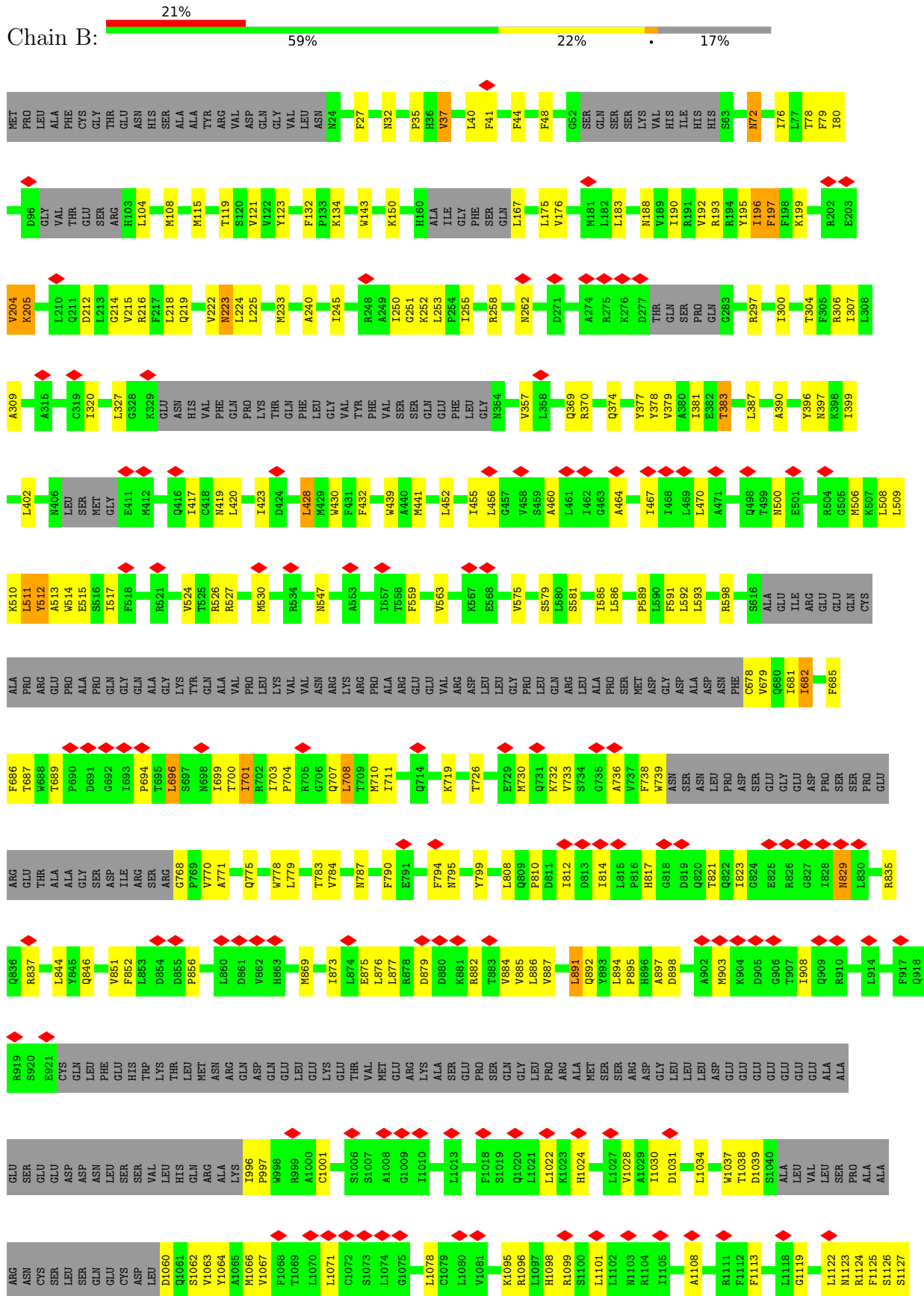


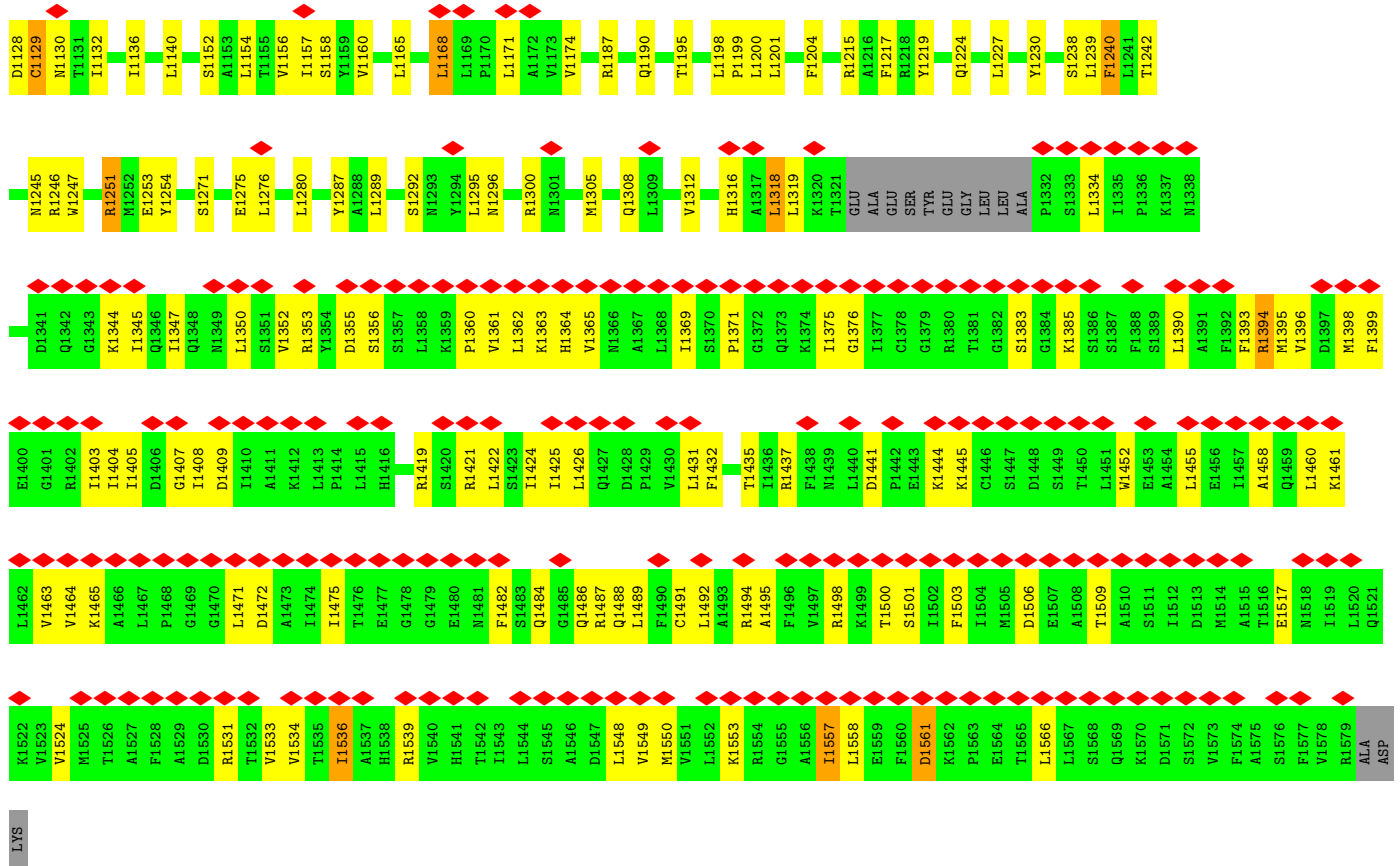
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain G:

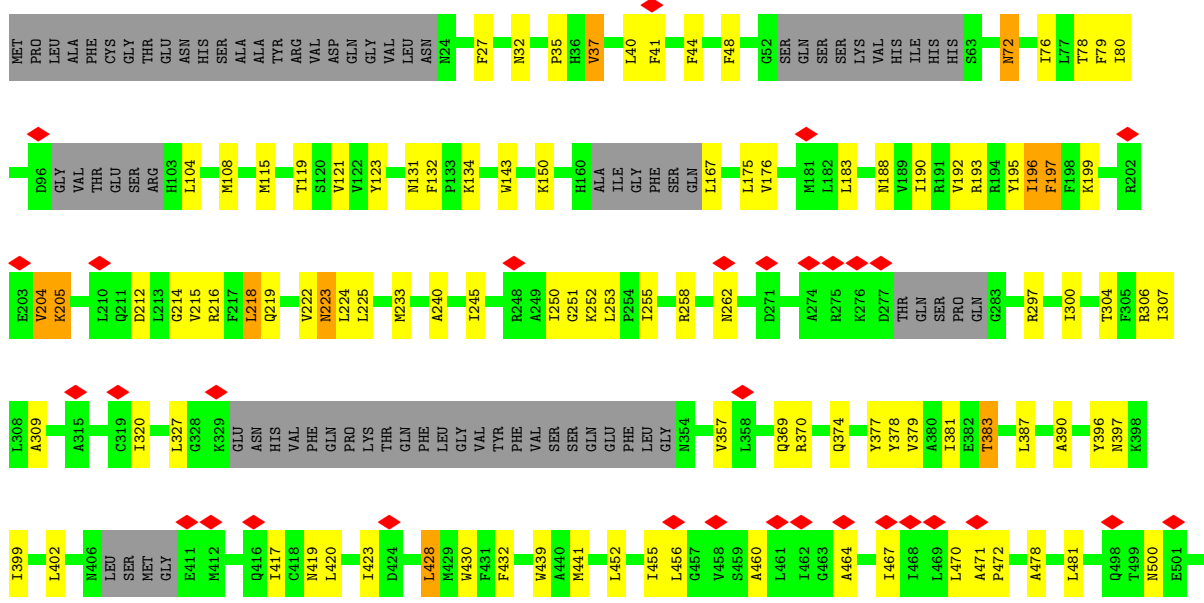


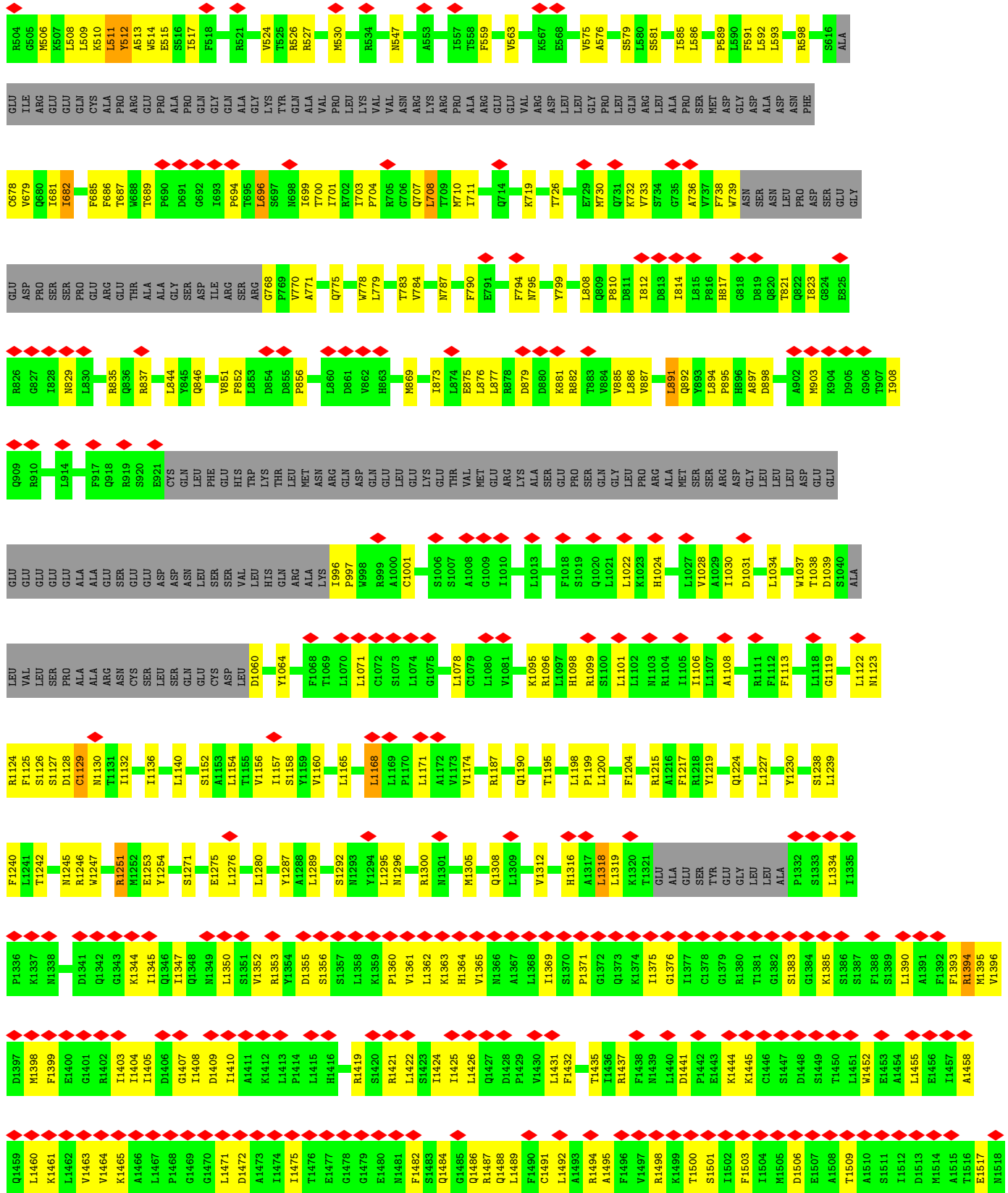
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

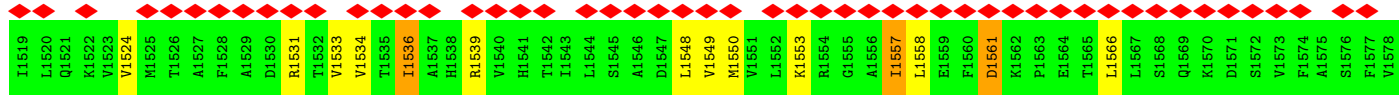




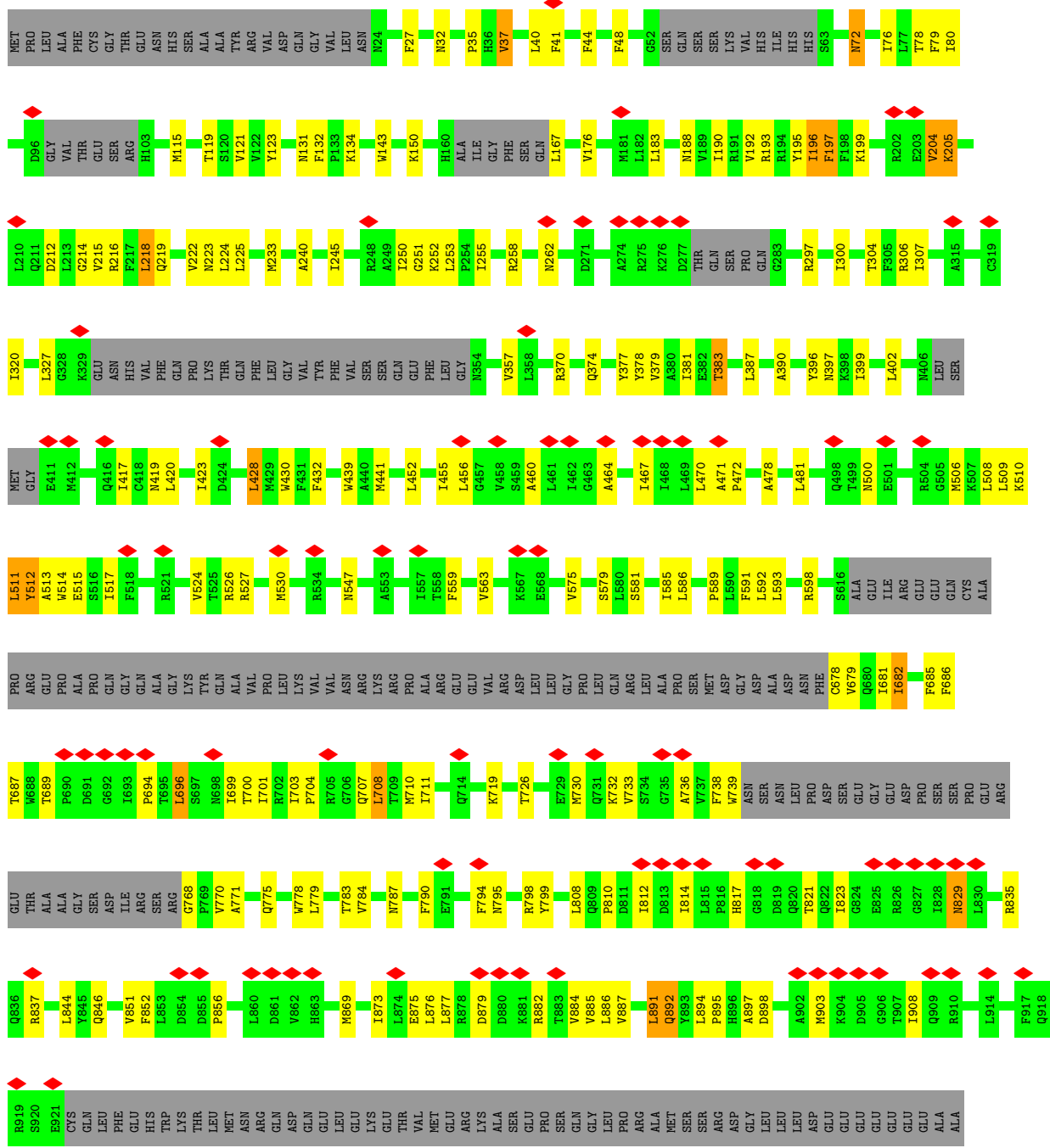
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

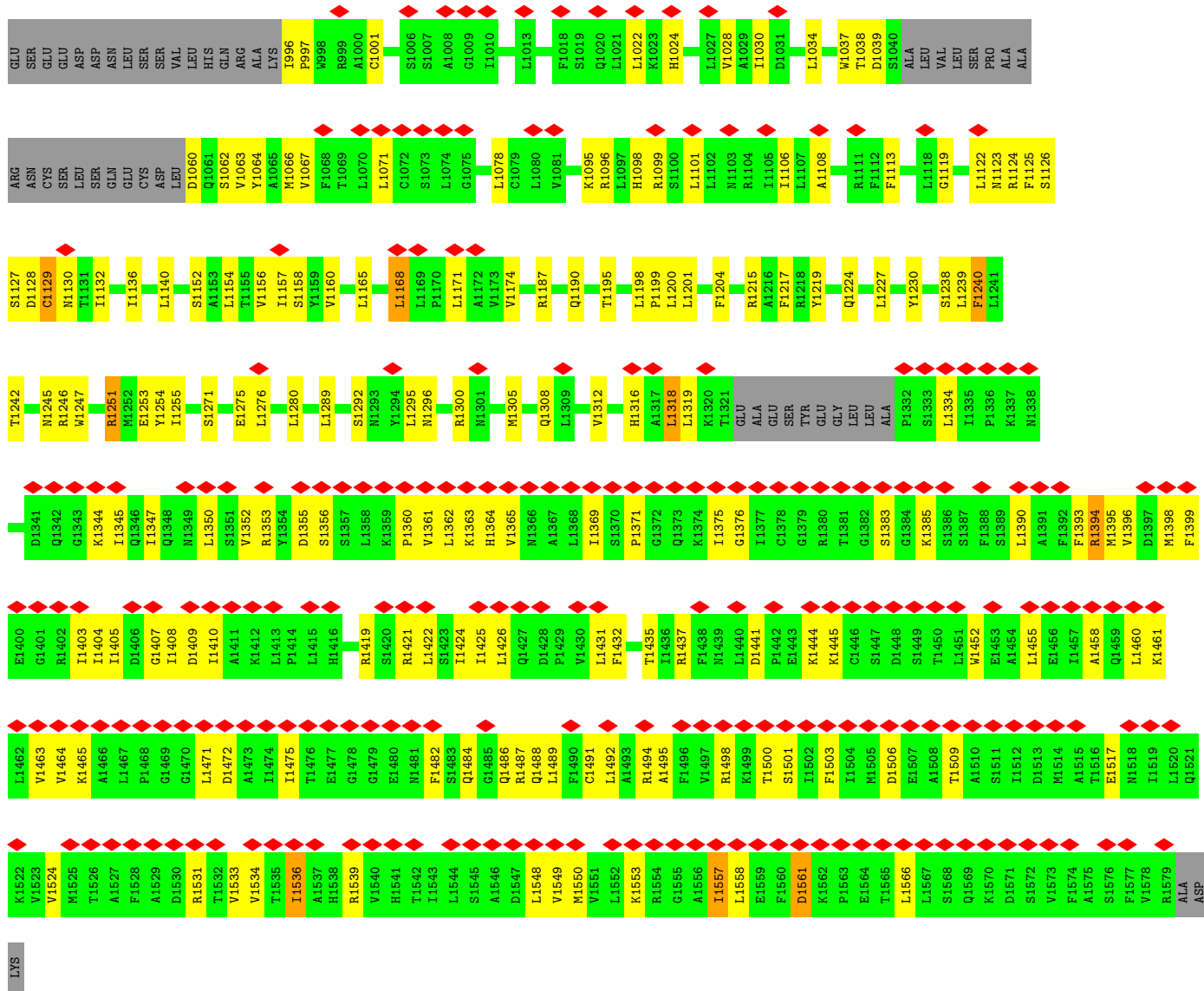




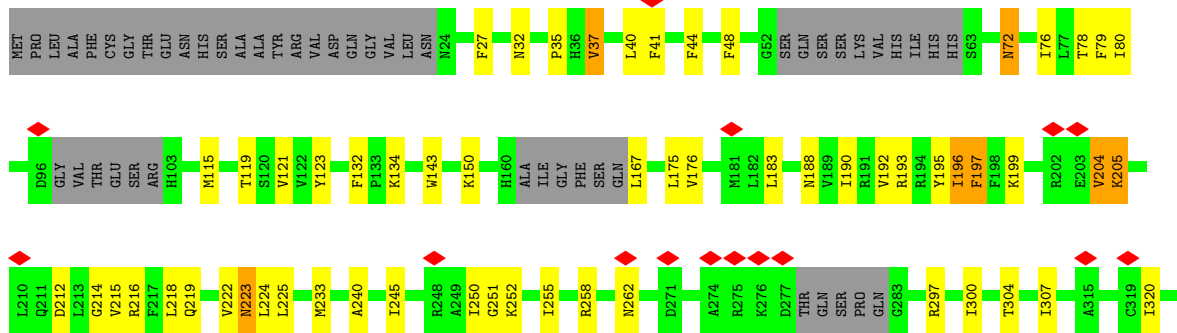


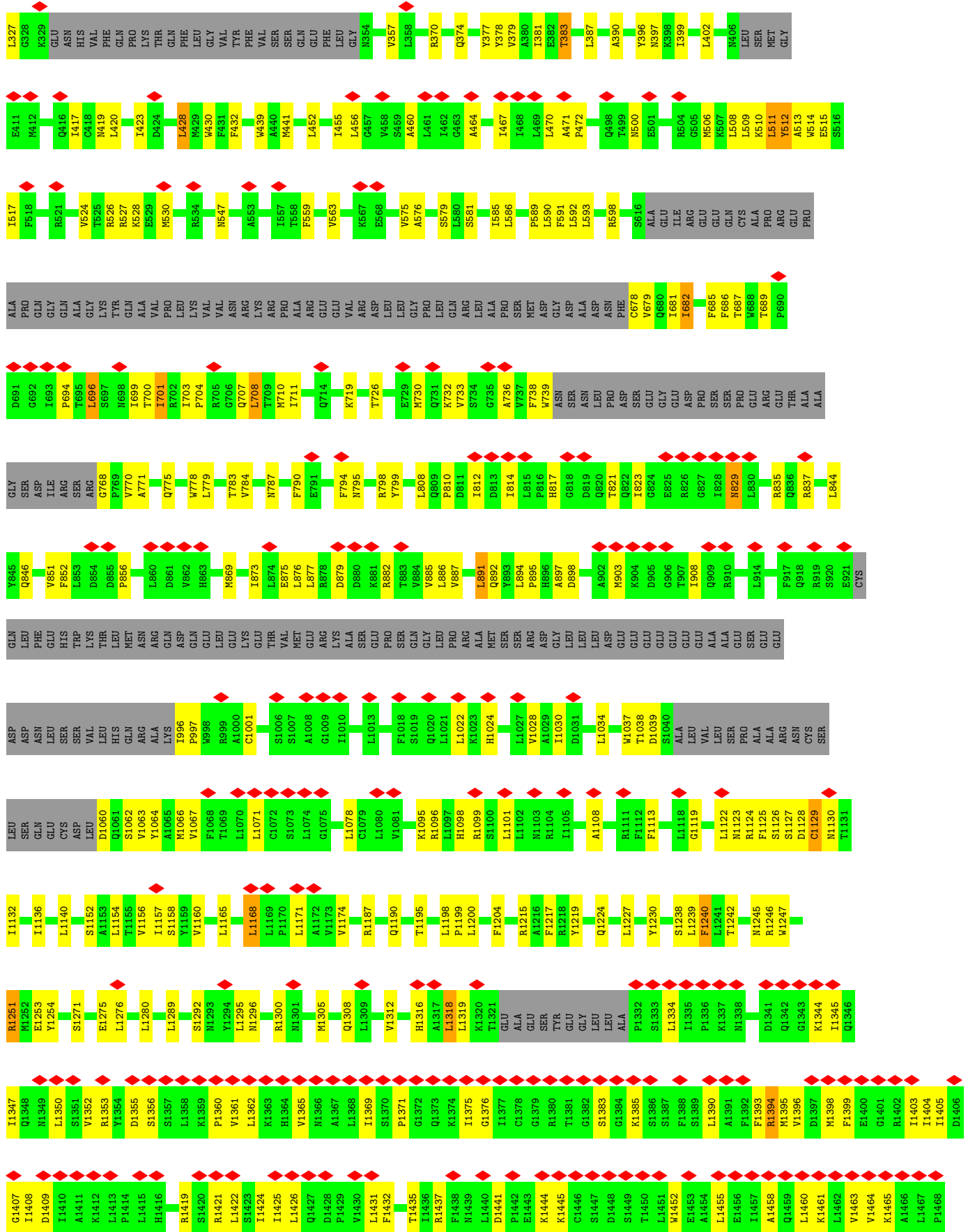
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





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





G1469	G1470	L1471	D1472	A1473	I1474	I1475	T1476	E1477	G1478	G1479	E1480	M1481	F1482	S1483	Q1484	Q1485	Q1486	R1487	Q1488	L1489	F1490	C1491	L1492	A1493	R1494	A1495	F1496	V1497	R1498	K1499	T1500	S1501	I1502	F1503	I1504	M1505	D1506	E1507	A1508	T1509	A1510	S1511	I1512	D1513	M1514	A1515	T1516	E1517	M1518	I1519	L1520	Q1521	K1522	V1523	V1524	M1525	T1526	A1527	F1528
A1529	D1530	R1531	T1532	V1533	V1534	T1535	I1536	A1537	H1538	R1539	V1540	H1541	T1542	I1543	L1544	S1545	A1546	D1547	L1548	V1549	M1550	V1551	L1552	K1553	R1554	G1555	A1556	I1557	L1558	E1559	F1560	D1561	K1562	P1563	E1564	T1565	L1566	L1567	S1568	Q1569	K1570	D1571	S1572	V1573	F1574	A1575	S1576	F1577	V1578	R1579	ALA	ASP	LYS						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27322	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	0.088	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\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 (\AA)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/2518	0.55	0/3430
1	C	0.38	0/2518	0.55	0/3430
1	E	0.38	0/2518	0.55	0/3430
1	G	0.38	0/2518	0.55	0/3430
2	B	0.28	0/10394	0.45	0/14113
2	D	0.28	0/10394	0.45	0/14113
2	F	0.28	0/10394	0.45	0/14113
2	H	0.28	0/10394	0.45	0/14113
All	All	0.30	0/51648	0.47	0/70172

There are no bond length outliers.

There are no bond angle outliers.

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	2463	0	2451	106	0
1	C	2463	0	2451	104	0
1	E	2463	0	2451	105	0
1	G	2463	0	2451	104	0
2	B	10189	0	10510	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10189	0	10510	290	0
2	F	10189	0	10510	291	0
2	H	10189	0	10510	288	0
3	A	62	0	24	10	0
3	B	31	0	12	2	0
3	C	31	0	12	5	0
3	D	31	0	12	2	0
3	E	31	0	12	5	0
3	F	31	0	12	2	0
3	H	31	0	12	2	0
4	B	33	0	28	4	0
4	D	33	0	28	4	0
4	F	33	0	28	3	0
4	H	33	0	28	3	0
All	All	50988	0	52052	1537	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 (1537) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:LEU:HD12	1:G:201:ARG:N	1.51	1.25
1:A:200:LEU:HD12	1:A:201:ARG:N	1.51	1.25
1:C:200:LEU:HD12	1:C:201:ARG:N	1.51	1.22
1:E:200:LEU:HD12	1:E:201:ARG:N	1.51	1.22
1:A:200:LEU:CD1	1:A:201:ARG:N	2.05	1.20
1:E:200:LEU:CD1	1:E:201:ARG:N	2.05	1.19
2:F:1350:LEU:HD11	2:F:1403:ILE:HD11	1.20	1.19
1:G:200:LEU:CD1	1:G:201:ARG:N	2.05	1.19
1:C:200:LEU:CD1	1:C:201:ARG:N	2.05	1.19
2:D:1350:LEU:HD11	2:D:1403:ILE:HD11	1.20	1.17
2:H:1350:LEU:HD11	2:H:1403:ILE:HD11	1.20	1.15
2:B:1350:LEU:HD11	2:B:1403:ILE:HD11	1.20	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	1.13
2:D:190:ILE:HG13	2:D:195:TYR:CB	1.79	1.12
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
2:D:512:TYR:CB	2:D:1498:ARG:HH12	1.65	1.10
2:B:512:TYR:CB	2:B:1498:ARG:HH12	1.65	1.09
2:H:1350:LEU:HD13	2:H:1403:ILE:HG12	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:512:TYR:CB	2:F:1498:ARG:HH12	1.65	1.09
2:D:512:TYR:HB3	2:D:1498:ARG:NH1	1.67	1.09
2:H:512:TYR:HB3	2:H:1498:ARG:NH1	1.67	1.09
2:H:512:TYR:CB	2:H:1498:ARG:HH12	1.65	1.08
2:D:1350:LEU:HD13	2:D:1403:ILE:HG12	1.35	1.08
2:F:1350:LEU:HD13	2:F:1403:ILE:HG12	1.35	1.08
1:G:198:PHE:HD1	1:G:199:MET:N	1.52	1.08
1:A:198:PHE:HD1	1:A:199:MET:N	1.52	1.08
2:B:512:TYR:HB3	2:B:1498:ARG:NH1	1.67	1.08
1:E:198:PHE:HD1	1:E:199:MET:N	1.52	1.07
1:C:198:PHE:HD1	1:C:199:MET:N	1.52	1.07
2:D:1125:PHE:HA	2:D:1129:CYS:SG	1.95	1.07
1:A:198:PHE:HD1	1:A:198:PHE:C	1.56	1.07
2:B:1350:LEU:HD13	2:B:1403:ILE:HG12	1.35	1.06
2:F:512:TYR:HB3	2:F:1498:ARG:NH1	1.67	1.06
2:F:1125:PHE:HA	2:F:1129:CYS:SG	1.95	1.06
1:C:198:PHE:HD1	1:C:198:PHE:C	1.56	1.06
2:B:1350:LEU:HD13	2:B:1403:ILE:CG1	1.85	1.06
2:B:1125:PHE:HA	2:B:1129:CYS:SG	1.95	1.05
2:H:1125:PHE:HA	2:H:1129:CYS:SG	1.95	1.05
2:H:1350:LEU:HD13	2:H:1403:ILE:CG1	1.85	1.05
2:D:1350:LEU:HD13	2:D:1403:ILE:CG1	1.85	1.05
1:E:198:PHE:HD1	1:E:198:PHE:C	1.56	1.04
2:F:1350:LEU:HD13	2:F:1403:ILE:CG1	1.85	1.04
1:G:198:PHE:HD1	1:G:198:PHE:C	1.56	1.04
2:H:1124:ARG:HD2	2:H:1318:LEU:HD12	1.41	1.03
2:B:1494:ARG:O	2:B:1498:ARG:HG3	1.59	1.02
2:F:1494:ARG:O	2:F:1498:ARG:HG3	1.59	1.01
1:E:200:LEU:HD13	1:E:201:ARG:H	1.26	1.01
2:F:1124:ARG:HD2	2:F:1318:LEU:HD12	1.41	1.01
2:B:1124:ARG:HD2	2:B:1318:LEU:HD12	1.41	1.01
2:D:1494:ARG:O	2:D:1498:ARG:HG3	1.59	1.01
2:H:1494:ARG:O	2:H:1498:ARG:HG3	1.59	1.00
1:G:200:LEU:HD13	1:G:201:ARG:H	1.26	1.00
2:D:1124:ARG:HD2	2:D:1318:LEU:HD12	1.41	0.99
2:D:1350:LEU:CD1	2:D:1403:ILE:HD11	1.92	0.99
1:C:200:LEU:HD13	1:C:201:ARG:H	1.26	0.99
2:B:1350:LEU:CD1	2:B:1403:ILE:HD11	1.92	0.99
2:F:1350:LEU:CD1	2:F:1403:ILE:HD11	1.92	0.99
1:G:198:PHE:C	1:G:198:PHE:CD1	2.30	0.98
2:H:1350:LEU:CD1	2:H:1403:ILE:HD11	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PHE:C	1:C:198:PHE:CD1	2.30	0.98
1:E:198:PHE:C	1:E:198:PHE:CD1	2.30	0.96
2:H:190:ILE:CG1	2:H:195:TYR:CB	2.44	0.96
2:B:512:TYR:CB	2:B:1498:ARG:NH1	2.27	0.96
1:A:200:LEU:HD13	1:A:201:ARG:H	1.26	0.96
2:D:190:ILE:CG1	2:D:195:TYR:CB	2.44	0.96
2:B:190:ILE:CG1	2:B:195:TYR:CB	2.44	0.95
2:F:190:ILE:CG1	2:F:195:TYR:CB	2.44	0.95
2:D:512:TYR:CB	2:D:1498:ARG:NH1	2.27	0.94
2:H:512:TYR:CB	2:H:1498:ARG:NH1	2.27	0.94
1:A:198:PHE:C	1:A:198:PHE:CD1	2.30	0.93
2:B:500:ASN:OD1	2:B:1122:LEU:HD21	1.70	0.92
2:F:512:TYR:CB	2:F:1498:ARG:NH1	2.27	0.92
2:B:1350:LEU:HD11	2:B:1403:ILE:CD1	2.00	0.92
2:D:500:ASN:OD1	2:D:1122:LEU:HD21	1.70	0.92
2:D:1350:LEU:HD11	2:D:1403:ILE:CD1	2.00	0.92
2:H:500:ASN:OD1	2:H:1122:LEU:HD21	1.70	0.91
3:A:402:AGS:O1B	1:C:185:LYS:HD2	1.71	0.91
3:E:401:AGS:O1B	1:G:185:LYS:HD2	1.71	0.91
2:F:500:ASN:OD1	2:F:1122:LEU:HD21	1.70	0.91
3:C:401:AGS:O1B	1:E:185:LYS:HD2	1.71	0.90
1:A:185:LYS:HD2	3:A:401:AGS:O1B	1.71	0.90
2:F:1350:LEU:HD11	2:F:1403:ILE:CD1	2.00	0.90
2:B:72:ASN:HB3	2:B:224:LEU:CD1	2.02	0.89
2:D:512:TYR:HB3	2:D:1498:ARG:CZ	2.03	0.89
2:D:72:ASN:HB3	2:D:224:LEU:CD1	2.02	0.89
2:H:72:ASN:HB3	2:H:224:LEU:CD1	2.02	0.89
1:A:200:LEU:HD12	1:A:200:LEU:C	1.93	0.89
2:H:1350:LEU:HD11	2:H:1403:ILE:CD1	2.00	0.89
2:F:72:ASN:HB3	2:F:224:LEU:CD1	2.02	0.88
1:E:200:LEU:HD12	1:E:200:LEU:C	1.93	0.88
2:F:512:TYR:HB3	2:F:1498:ARG:CZ	2.03	0.88
2:B:512:TYR:HB3	2:B:1498:ARG:CZ	2.03	0.88
1:C:200:LEU:HD12	1:C:200:LEU:C	1.93	0.88
1:G:200:LEU:HD12	1:G:200:LEU:C	1.93	0.88
2:H:512:TYR:HB3	2:H:1498:ARG:CZ	2.03	0.88
2:H:1350:LEU:CD1	2:H:1403:ILE:CG1	2.52	0.87
2:F:1350:LEU:CD1	2:F:1403:ILE:CG1	2.52	0.87
2:B:512:TYR:CB	2:B:1498:ARG:HH22	1.87	0.87
2:F:512:TYR:CB	2:F:1498:ARG:HH22	1.87	0.87
2:D:512:TYR:CB	2:D:1498:ARG:HH22	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1350:LEU:CD1	2:B:1403:ILE:CG1	2.52	0.86
3:C:401:AGS:O1B	1:E:185:LYS:CD	2.24	0.86
1:A:185:LYS:CD	3:A:401:AGS:O1B	2.24	0.86
1:G:198:PHE:CD1	1:G:199:MET:N	2.43	0.86
2:H:512:TYR:CB	2:H:1498:ARG:HH22	1.87	0.86
3:A:402:AGS:O1B	1:C:185:LYS:CD	2.24	0.86
2:D:1350:LEU:CD1	2:D:1403:ILE:CG1	2.52	0.85
3:E:401:AGS:O1B	1:G:185:LYS:CD	2.24	0.85
1:C:200:LEU:HD13	1:C:201:ARG:N	1.86	0.85
1:C:200:LEU:CD1	1:C:201:ARG:H	1.78	0.84
1:E:198:PHE:CD1	1:E:199:MET:N	2.43	0.84
1:A:200:LEU:HD13	1:A:201:ARG:N	1.86	0.84
1:E:200:LEU:CD1	1:E:201:ARG:H	1.78	0.84
1:A:198:PHE:CD1	1:A:199:MET:N	2.43	0.83
2:D:1350:LEU:CD1	2:D:1403:ILE:CD1	2.57	0.83
1:A:200:LEU:CD1	1:A:201:ARG:H	1.78	0.82
2:B:512:TYR:HB2	2:B:1498:ARG:HH12	1.42	0.82
2:B:1350:LEU:CD1	2:B:1403:ILE:CD1	2.57	0.82
1:G:200:LEU:CD1	1:G:201:ARG:H	1.78	0.82
2:D:512:TYR:HB2	2:D:1498:ARG:HH12	1.42	0.81
2:F:512:TYR:HB2	2:F:1498:ARG:HH12	1.42	0.81
2:H:512:TYR:HB2	2:H:1498:ARG:HH12	1.42	0.81
2:F:1350:LEU:CD1	2:F:1403:ILE:CD1	2.57	0.81
2:B:512:TYR:CB	2:B:1498:ARG:NH2	2.44	0.81
2:D:512:TYR:CB	2:D:1498:ARG:NH2	2.44	0.81
2:F:512:TYR:CB	2:F:1498:ARG:NH2	2.44	0.81
2:F:512:TYR:CD2	2:F:1498:ARG:NH2	2.49	0.81
2:F:1101:LEU:HD23	2:F:1125:PHE:CE1	2.16	0.81
2:H:1101:LEU:HD23	2:H:1125:PHE:CE1	2.16	0.81
2:B:512:TYR:CD2	2:B:1498:ARG:NH2	2.49	0.81
2:D:512:TYR:CD2	2:D:1498:ARG:NH2	2.49	0.81
2:H:512:TYR:CB	2:H:1498:ARG:NH2	2.44	0.81
1:C:198:PHE:CD1	1:C:199:MET:N	2.43	0.81
2:D:1101:LEU:HD23	2:D:1125:PHE:CE1	2.16	0.80
2:B:1101:LEU:HD23	2:B:1125:PHE:CE1	2.16	0.80
2:H:512:TYR:CD2	2:H:1498:ARG:NH2	2.49	0.80
2:H:1350:LEU:CD1	2:H:1403:ILE:CD1	2.57	0.80
2:B:1037:TRP:CD1	2:B:1064:TYR:HB3	2.19	0.78
2:F:1037:TRP:CD1	2:F:1064:TYR:HB3	2.19	0.78
2:H:204:VAL:O	2:H:205:LYS:HB3	1.83	0.78
1:A:219:VAL:HG13	1:A:236:VAL:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:VAL:HG13	1:G:236:VAL:HG23	1.65	0.78
2:H:1037:TRP:CD1	2:H:1064:TYR:HB3	2.19	0.78
1:C:219:VAL:HG13	1:C:236:VAL:HG23	1.65	0.77
2:D:1037:TRP:CD1	2:D:1064:TYR:HB3	2.19	0.77
1:E:219:VAL:HG13	1:E:236:VAL:HG23	1.65	0.77
2:B:1132:ILE:HD11	2:B:1312:VAL:HG22	1.67	0.77
2:B:204:VAL:O	2:B:205:LYS:HB3	1.83	0.77
2:B:1124:ARG:CD	2:B:1318:LEU:HD12	2.15	0.77
2:D:1124:ARG:CD	2:D:1318:LEU:HD12	2.15	0.77
2:F:1124:ARG:CD	2:F:1318:LEU:HD12	2.15	0.77
2:D:204:VAL:O	2:D:205:LYS:HB3	1.83	0.77
2:D:1132:ILE:HD11	2:D:1312:VAL:HG22	1.67	0.77
2:F:196:ILE:O	2:F:197:PHE:O	2.03	0.76
2:H:1124:ARG:CD	2:H:1318:LEU:HD12	2.15	0.76
2:B:196:ILE:O	2:B:197:PHE:O	2.03	0.76
2:D:196:ILE:O	2:D:197:PHE:O	2.03	0.75
2:F:204:VAL:O	2:F:205:LYS:HB3	1.83	0.75
2:F:1132:ILE:HD11	2:F:1312:VAL:HG22	1.67	0.75
2:H:196:ILE:O	2:H:197:PHE:O	2.03	0.75
2:H:1132:ILE:HD11	2:H:1312:VAL:HG22	1.67	0.75
2:D:72:ASN:HB3	2:D:224:LEU:HD13	1.69	0.75
2:F:72:ASN:HB3	2:F:224:LEU:HD13	1.69	0.74
2:B:72:ASN:HB3	2:B:224:LEU:HD13	1.69	0.74
2:D:1125:PHE:CA	2:D:1129:CYS:SG	2.76	0.74
2:H:72:ASN:HB3	2:H:224:LEU:HD13	1.69	0.73
2:H:456:LEU:HB2	2:H:460:ALA:HB2	1.70	0.73
2:H:1125:PHE:CA	2:H:1129:CYS:SG	2.76	0.73
2:F:456:LEU:HB2	2:F:460:ALA:HB2	1.70	0.73
2:B:456:LEU:HB2	2:B:460:ALA:HB2	1.70	0.73
2:D:456:LEU:HB2	2:D:460:ALA:HB2	1.70	0.73
1:A:36:VAL:HG12	1:A:42:CYS:HA	1.71	0.73
2:B:512:TYR:CB	2:B:1498:ARG:CZ	2.67	0.72
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.71	0.72
2:F:1125:PHE:CA	2:F:1129:CYS:SG	2.76	0.72
2:D:79:PHE:HZ	2:D:225:LEU:HD12	1.55	0.72
1:E:213:ALA:HA	1:E:288:GLU:O	1.90	0.72
2:F:72:ASN:HA	2:F:224:LEU:HD13	1.72	0.72
2:H:72:ASN:HA	2:H:224:LEU:HD13	1.72	0.72
2:B:79:PHE:HZ	2:B:225:LEU:HD12	1.55	0.72
2:B:1125:PHE:CA	2:B:1129:CYS:SG	2.76	0.72
2:B:1441:ASP:OD2	2:B:1444:LYS:HA	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:ALA:HA	1:G:288:GLU:O	1.90	0.72
2:B:1422:LEU:C	2:B:1500:THR:HG21	2.10	0.71
2:B:72:ASN:HA	2:B:224:LEU:HD13	1.72	0.71
2:F:1422:LEU:C	2:F:1500:THR:HG21	2.10	0.71
2:H:1422:LEU:C	2:H:1500:THR:HG21	2.10	0.71
2:H:216:ARG:HD2	2:H:250:ILE:C	2.11	0.71
1:C:54:ARG:HA	1:C:57:GLN:HB2	1.73	0.71
1:A:54:ARG:HA	1:A:57:GLN:HB2	1.73	0.71
1:C:213:ALA:HA	1:C:288:GLU:O	1.90	0.71
2:D:72:ASN:HA	2:D:224:LEU:HD13	1.72	0.71
1:E:36:VAL:HG12	1:E:42:CYS:HA	1.71	0.71
2:D:216:ARG:HD2	2:D:250:ILE:C	2.11	0.71
2:F:79:PHE:HZ	2:F:225:LEU:HD12	1.55	0.71
2:F:1441:ASP:OD2	2:F:1444:LYS:HA	1.90	0.71
1:G:36:VAL:HG12	1:G:42:CYS:HA	1.71	0.71
2:D:1441:ASP:OD2	2:D:1444:LYS:HA	1.90	0.71
2:H:512:TYR:CB	2:H:1498:ARG:CZ	2.67	0.71
2:H:1441:ASP:OD2	2:H:1444:LYS:HA	1.90	0.71
2:H:79:PHE:HZ	2:H:225:LEU:HD12	1.55	0.71
2:B:216:ARG:HD2	2:B:250:ILE:C	2.11	0.70
2:D:1422:LEU:C	2:D:1500:THR:HG21	2.10	0.70
2:B:1124:ARG:HD2	2:B:1318:LEU:CD1	2.21	0.70
2:D:204:VAL:O	2:D:205:LYS:CB	2.40	0.70
2:H:204:VAL:O	2:H:205:LYS:CB	2.40	0.70
1:A:213:ALA:HA	1:A:288:GLU:O	1.90	0.70
2:F:216:ARG:HD2	2:F:250:ILE:C	2.11	0.70
2:F:1124:ARG:HD2	2:F:1318:LEU:CD1	2.21	0.70
1:E:54:ARG:HA	1:E:57:GLN:HB2	1.73	0.70
1:G:54:ARG:HA	1:G:57:GLN:HB2	1.73	0.70
2:F:1125:PHE:O	2:F:1129:CYS:SG	2.50	0.70
2:D:512:TYR:CB	2:D:1498:ARG:CZ	2.67	0.69
2:D:1125:PHE:O	2:D:1129:CYS:SG	2.50	0.69
2:H:72:ASN:CB	2:H:224:LEU:CD1	2.70	0.69
1:G:200:LEU:CD1	1:G:201:ARG:O	2.41	0.69
2:H:1124:ARG:HD2	2:H:1318:LEU:CD1	2.21	0.69
2:F:72:ASN:CB	2:F:224:LEU:CD1	2.70	0.69
2:B:72:ASN:CB	2:B:224:LEU:HD13	2.23	0.69
2:D:72:ASN:CB	2:D:224:LEU:CD1	2.70	0.69
1:E:200:LEU:CD1	1:E:201:ARG:O	2.41	0.69
2:H:1125:PHE:O	2:H:1129:CYS:SG	2.50	0.69
2:B:1125:PHE:O	2:B:1129:CYS:SG	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASN:CB	2:D:224:LEU:HD13	2.23	0.69
1:E:243:GLY:O	1:E:245:GLY:N	2.26	0.69
1:A:243:GLY:O	1:A:245:GLY:N	2.26	0.69
2:B:204:VAL:O	2:B:205:LYS:CB	2.40	0.69
1:E:95:PHE:HD1	1:E:100:LEU:HD23	1.58	0.68
2:F:1509:THR:HG23	2:F:1517:GLU:HG2	1.75	0.68
1:G:200:LEU:HD13	1:G:201:ARG:N	1.86	0.68
2:B:72:ASN:CB	2:B:224:LEU:CD1	2.70	0.68
2:F:72:ASN:CB	2:F:224:LEU:HD13	2.23	0.68
1:A:200:LEU:CD1	1:A:201:ARG:O	2.41	0.68
2:F:512:TYR:CB	2:F:1498:ARG:CZ	2.67	0.68
2:F:1421:ARG:HG3	2:F:1422:LEU:HG	1.76	0.68
2:H:72:ASN:CB	2:H:224:LEU:HD13	2.23	0.68
2:B:1353:ARG:HH11	2:B:1398:MET:HE3	1.59	0.68
1:C:200:LEU:CD1	1:C:201:ARG:O	2.41	0.68
1:C:243:GLY:O	1:C:245:GLY:N	2.26	0.68
2:D:687:THR:HB	2:D:694:PRO:HA	1.75	0.68
1:E:194:GLY:O	1:E:195:ARG:HD2	1.94	0.68
2:H:687:THR:HB	2:H:694:PRO:HA	1.75	0.68
2:B:1345:ILE:HD11	2:B:1369:ILE:HD12	1.76	0.68
2:B:1421:ARG:HG3	2:B:1422:LEU:HG	1.76	0.68
1:C:95:PHE:HD1	1:C:100:LEU:HD23	1.58	0.68
2:D:1421:ARG:HG3	2:D:1422:LEU:HG	1.76	0.68
3:A:401:AGS:O2A	3:A:401:AGS:H8	1.94	0.68
2:B:512:TYR:CG	2:B:1498:ARG:NH2	2.62	0.68
2:F:1165:LEU:HA	2:F:1168:LEU:HD23	1.76	0.68
2:B:530:MET:HG3	2:B:1095:LYS:HE2	1.76	0.68
2:D:1165:LEU:HA	2:D:1168:LEU:HD23	1.76	0.68
2:H:1353:ARG:HH11	2:H:1398:MET:HE3	1.59	0.68
2:H:1421:ARG:HG3	2:H:1422:LEU:HG	1.76	0.68
2:H:1509:THR:HG23	2:H:1517:GLU:HG2	1.75	0.68
1:A:200:LEU:HD21	1:A:304:TYR:CZ	2.28	0.67
3:A:402:AGS:H8	3:A:402:AGS:O2A	1.94	0.67
1:C:200:LEU:HD21	1:C:304:TYR:CZ	2.28	0.67
2:D:512:TYR:CG	2:D:1498:ARG:NH2	2.62	0.67
2:D:530:MET:HG3	2:D:1095:LYS:HE2	1.76	0.67
2:D:1126:SER:O	2:D:1130:ASN:ND2	2.28	0.67
2:D:1353:ARG:HH11	2:D:1398:MET:HE3	1.59	0.67
2:F:530:MET:HG3	2:F:1095:LYS:HE2	1.76	0.67
2:H:1101:LEU:HG	2:H:1125:PHE:CZ	2.29	0.67
2:H:1165:LEU:HA	2:H:1168:LEU:HD23	1.76	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	1.94	0.67
2:H:1126:SER:O	2:H:1130:ASN:ND2	2.28	0.67
1:A:194:GLY:O	1:A:195:ARG:HD2	1.94	0.67
2:B:687:THR:HB	2:B:694:PRO:HA	1.75	0.67
2:F:1353:ARG:HH11	2:F:1398:MET:HE3	1.59	0.67
1:G:243:GLY:O	1:G:245:GLY:N	2.26	0.67
2:B:1509:THR:HG23	2:B:1517:GLU:HG2	1.75	0.67
3:C:401:AGS:O2A	3:C:401:AGS:H8	1.94	0.67
2:D:1101:LEU:HG	2:D:1125:PHE:CZ	2.29	0.67
2:D:1345:ILE:HD11	2:D:1369:ILE:HD12	1.76	0.67
1:G:200:LEU:HD21	1:G:304:TYR:CZ	2.28	0.67
1:E:200:LEU:HD21	1:E:304:TYR:CZ	2.28	0.67
2:H:530:MET:HG3	2:H:1095:LYS:HE2	1.76	0.67
2:H:1345:ILE:HD11	2:H:1369:ILE:HD12	1.76	0.67
2:B:1165:LEU:HA	2:B:1168:LEU:HD23	1.76	0.67
1:G:95:PHE:HD1	1:G:100:LEU:HD23	1.58	0.67
2:B:1101:LEU:HG	2:B:1125:PHE:CZ	2.29	0.67
2:F:1101:LEU:HG	2:F:1125:PHE:CZ	2.29	0.67
2:F:1126:SER:O	2:F:1130:ASN:ND2	2.28	0.67
1:A:95:PHE:HD1	1:A:100:LEU:HD23	1.58	0.67
2:D:1509:THR:HG23	2:D:1517:GLU:HG2	1.75	0.67
1:E:200:LEU:HD13	1:E:201:ARG:N	1.86	0.67
2:F:1441:ASP:OD2	2:F:1444:LYS:CA	2.43	0.67
1:G:194:GLY:O	1:G:195:ARG:HD2	1.94	0.67
2:H:1441:ASP:OD2	2:H:1444:LYS:CA	2.43	0.67
3:E:401:AGS:O2A	3:E:401:AGS:H8	1.94	0.67
2:B:512:TYR:HB2	2:B:1498:ARG:HH22	1.60	0.66
2:B:1126:SER:O	2:B:1130:ASN:ND2	2.28	0.66
2:F:204:VAL:O	2:F:205:LYS:CB	2.40	0.66
2:F:1345:ILE:HD11	2:F:1369:ILE:HD12	1.76	0.66
2:D:1441:ASP:OD2	2:D:1444:LYS:CA	2.43	0.66
2:F:687:THR:HB	2:F:694:PRO:HA	1.75	0.66
2:D:1136:ILE:HD11	2:D:1308:GLN:HB3	1.77	0.66
2:H:512:TYR:HB2	2:H:1498:ARG:HH22	1.60	0.66
2:B:1441:ASP:OD2	2:B:1444:LYS:CA	2.43	0.66
2:D:1122:LEU:HD12	2:D:1122:LEU:O	1.96	0.66
2:B:1122:LEU:HD12	2:B:1122:LEU:O	1.96	0.66
2:B:1136:ILE:HD11	2:B:1308:GLN:HB3	1.77	0.66
2:H:1136:ILE:HD11	2:H:1308:GLN:HB3	1.77	0.65
2:F:1122:LEU:HD12	2:F:1122:LEU:O	1.96	0.65
2:D:512:TYR:HB2	2:D:1498:ARG:HH22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1404:ILE:HG23	2:F:1408:ILE:N	2.11	0.65
2:D:1404:ILE:HG23	2:D:1408:ILE:N	2.11	0.65
2:F:1136:ILE:HD11	2:F:1308:GLN:HB3	1.77	0.65
2:F:1491:CYS:HA	2:F:1494:ARG:HD2	1.79	0.65
2:H:1122:LEU:O	2:H:1122:LEU:HD12	1.96	0.65
2:H:1404:ILE:HG23	2:H:1408:ILE:N	2.11	0.65
2:H:1352:VAL:HA	2:H:1399:PHE:HA	1.79	0.65
1:C:177:ARG:NH1	1:C:208:SER:OG	2.30	0.65
2:D:72:ASN:HB3	2:D:224:LEU:HD11	1.79	0.65
2:H:1503:PHE:HB2	2:H:1533:VAL:HG22	1.79	0.65
1:A:177:ARG:NH1	1:A:208:SER:OG	2.30	0.64
2:B:1503:PHE:HB2	2:B:1533:VAL:HG22	1.79	0.64
1:E:200:LEU:HD21	1:E:304:TYR:OH	1.98	0.64
2:F:512:TYR:HB2	2:F:1498:ARG:HH22	1.60	0.64
1:G:177:ARG:NH1	1:G:208:SER:OG	2.30	0.64
2:H:1491:CYS:HA	2:H:1494:ARG:HD2	1.79	0.64
3:C:401:AGS:O1B	1:E:185:LYS:HD3	1.97	0.64
2:D:1352:VAL:HA	2:D:1399:PHE:HA	1.79	0.64
2:B:1404:ILE:HG23	2:B:1408:ILE:N	2.11	0.64
2:F:72:ASN:HB3	2:F:224:LEU:HD11	1.79	0.64
1:A:200:LEU:HD21	1:A:304:TYR:OH	1.98	0.64
2:B:1352:VAL:HA	2:B:1399:PHE:HA	1.79	0.64
1:C:200:LEU:HD21	1:C:304:TYR:OH	1.98	0.64
1:E:177:ARG:NH1	1:E:208:SER:OG	2.30	0.64
2:H:846:GLN:O	2:H:882:ARG:NH1	2.31	0.64
2:F:1352:VAL:HA	2:F:1399:PHE:HA	1.79	0.64
2:B:846:GLN:O	2:B:882:ARG:NH1	2.31	0.64
2:F:452:LEU:HD11	2:F:464:ALA:HB2	1.80	0.64
2:H:262:ASN:HB3	2:H:390:ALA:HB2	1.80	0.64
2:D:1491:CYS:HA	2:D:1494:ARG:HD2	1.79	0.64
2:F:262:ASN:HB3	2:F:390:ALA:HB2	1.80	0.64
2:H:452:LEU:HD11	2:H:464:ALA:HB2	1.80	0.64
2:H:530:MET:CE	2:H:1095:LYS:HG2	2.28	0.64
2:B:530:MET:CE	2:B:1095:LYS:HG2	2.28	0.64
2:B:72:ASN:HB3	2:B:224:LEU:HD11	1.79	0.64
2:D:530:MET:CE	2:D:1095:LYS:HG2	2.28	0.64
2:F:530:MET:CE	2:F:1095:LYS:HG2	2.28	0.63
2:B:1491:CYS:HA	2:B:1494:ARG:HD2	1.79	0.63
2:F:1503:PHE:HB2	2:F:1533:VAL:HG22	1.79	0.63
2:H:190:ILE:CB	2:H:195:TYR:CB	2.76	0.63
2:D:1503:PHE:HB2	2:D:1533:VAL:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD12	1:E:201:ARG:CA	2.29	0.63
2:F:190:ILE:CB	2:F:195:TYR:CB	2.76	0.63
2:F:846:GLN:O	2:F:882:ARG:NH1	2.31	0.63
1:G:200:LEU:HD21	1:G:304:TYR:OH	1.98	0.63
2:D:846:GLN:O	2:D:882:ARG:NH1	2.31	0.63
2:D:1124:ARG:HD2	2:D:1318:LEU:CD1	2.21	0.62
1:E:132:GLY:HA3	1:G:131:ILE:O	1.99	0.62
1:A:185:LYS:HD3	3:A:401:AGS:O1B	1.97	0.62
2:F:387:LEU:HD21	2:F:428:LEU:HD22	1.81	0.62
2:H:72:ASN:HB3	2:H:224:LEU:HD11	1.79	0.62
2:B:190:ILE:CB	2:B:195:TYR:CB	2.76	0.62
2:B:452:LEU:HD11	2:B:464:ALA:HB2	1.80	0.62
2:B:771:ALA:HB3	2:B:851:VAL:HG12	1.82	0.62
2:H:1125:PHE:C	2:H:1129:CYS:HG	2.01	0.62
1:A:132:GLY:HA3	1:C:131:ILE:O	1.99	0.62
1:G:109:PRO:HG2	1:G:112:THR:HA	1.82	0.62
2:H:387:LEU:HD21	2:H:428:LEU:HD22	1.81	0.62
2:H:771:ALA:HB3	2:H:851:VAL:HG12	1.82	0.62
2:B:262:ASN:HB3	2:B:390:ALA:HB2	1.80	0.62
2:D:262:ASN:HB3	2:D:390:ALA:HB2	1.80	0.62
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.82	0.62
2:B:1198:LEU:HB3	2:B:1199:PRO:HD3	1.82	0.62
1:C:109:PRO:HG2	1:C:112:THR:HA	1.82	0.62
2:D:216:ARG:HB2	2:D:251:GLY:HA3	1.82	0.62
2:D:452:LEU:HD11	2:D:464:ALA:HB2	1.80	0.62
2:D:783:THR:O	2:D:787:ASN:ND2	2.31	0.62
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.82	0.62
1:A:109:PRO:HG2	1:A:112:THR:HA	1.82	0.62
1:A:131:ILE:O	1:G:132:GLY:HA3	1.99	0.62
2:D:190:ILE:CB	2:D:195:TYR:CB	2.76	0.62
2:D:530:MET:HE2	2:D:1095:LYS:HG2	1.80	0.62
1:A:200:LEU:HD12	1:A:201:ARG:CA	2.29	0.62
2:B:682:ILE:HG23	2:B:736:ALA:HB3	1.82	0.62
2:D:1404:ILE:CG2	2:D:1405:ILE:N	2.63	0.62
3:E:401:AGS:O1B	1:G:185:LYS:HD3	1.97	0.62
2:F:1101:LEU:CD2	2:F:1125:PHE:CE1	2.83	0.62
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.82	0.62
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.82	0.62
2:F:1404:ILE:HG23	2:F:1408:ILE:H	1.64	0.62
2:B:530:MET:HE2	2:B:1095:LYS:HG2	1.82	0.62
2:D:1245:ASN:OD1	2:D:1300:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1404:ILE:CG2	2:B:1405:ILE:N	2.63	0.61
1:C:54:ARG:O	1:E:206:ARG:NH2	2.33	0.61
2:D:1198:LEU:HB3	2:D:1199:PRO:HD3	1.82	0.61
1:E:109:PRO:HG2	1:E:112:THR:HA	1.82	0.61
2:F:216:ARG:HB2	2:F:251:GLY:HA3	1.82	0.61
2:H:399:ILE:HD11	2:H:417:ILE:HD13	1.82	0.61
1:A:206:ARG:NH2	1:G:54:ARG:O	2.33	0.61
1:C:132:GLY:HA3	1:E:131:ILE:O	1.99	0.61
2:D:686:PHE:HB2	2:D:732:LYS:HA	1.82	0.61
2:H:1404:ILE:HG23	2:H:1408:ILE:H	1.64	0.61
2:B:1506:ASP:HA	2:B:1536:ILE:HG13	1.83	0.61
2:D:682:ILE:HG23	2:D:736:ALA:HB3	1.82	0.61
2:D:1101:LEU:CD2	2:D:1125:PHE:CE1	2.83	0.61
2:F:1198:LEU:HB3	2:F:1199:PRO:HD3	1.82	0.61
2:F:1347:ILE:CG2	2:F:1403:ILE:HG12	2.30	0.61
1:G:200:LEU:HD12	1:G:201:ARG:CA	2.29	0.61
2:H:1198:LEU:HB3	2:H:1199:PRO:HD3	1.82	0.61
2:H:1404:ILE:CG2	2:H:1405:ILE:N	2.63	0.61
1:C:83:TRP:CD1	1:C:128:GLN:HG2	2.36	0.61
2:F:771:ALA:HB3	2:F:851:VAL:HG12	1.82	0.61
2:H:1245:ASN:OD1	2:H:1300:ARG:NH2	2.33	0.61
1:A:83:TRP:CD1	1:A:128:GLN:HG2	2.36	0.61
3:A:402:AGS:O1B	1:C:185:LYS:HD3	1.97	0.61
2:D:1347:ILE:CG2	2:D:1403:ILE:HG12	2.30	0.61
2:H:1101:LEU:CD2	2:H:1125:PHE:CE1	2.83	0.61
2:B:686:PHE:HB2	2:B:732:LYS:HA	1.82	0.61
2:B:1157:ILE:HD11	2:B:1168:LEU:HD22	1.82	0.61
2:D:387:LEU:HD21	2:D:428:LEU:HD22	1.81	0.61
2:D:771:ALA:HB3	2:D:851:VAL:HG12	1.82	0.61
2:F:399:ILE:HD11	2:F:417:ILE:HD13	1.82	0.61
2:F:1245:ASN:OD1	2:F:1300:ARG:NH2	2.33	0.61
2:F:1404:ILE:CG2	2:F:1405:ILE:N	2.63	0.61
2:H:216:ARG:HB2	2:H:251:GLY:HA3	1.82	0.61
2:H:1506:ASP:HA	2:H:1536:ILE:HG13	1.83	0.61
2:B:1245:ASN:OD1	2:B:1300:ARG:NH2	2.33	0.61
2:B:1347:ILE:CG2	2:B:1403:ILE:HG12	2.30	0.61
2:D:1404:ILE:HG23	2:D:1408:ILE:H	1.64	0.61
1:E:54:ARG:O	1:G:206:ARG:NH2	2.33	0.61
2:H:547:ASN:HA	2:H:591:PHE:HZ	1.66	0.61
2:B:387:LEU:HD21	2:B:428:LEU:HD22	1.81	0.61
2:D:547:ASN:HA	2:D:591:PHE:HZ	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1347:ILE:HG23	2:D:1403:ILE:HG23	1.83	0.61
2:F:686:PHE:HB2	2:F:732:LYS:HA	1.82	0.61
2:D:72:ASN:CA	2:D:224:LEU:HD13	2.31	0.61
1:E:83:TRP:CD1	1:E:128:GLN:HG2	2.36	0.61
2:H:1347:ILE:CG2	2:H:1403:ILE:HG12	2.30	0.61
1:A:54:ARG:O	1:C:206:ARG:NH2	2.33	0.60
2:B:1404:ILE:HG23	2:B:1408:ILE:H	1.64	0.60
2:F:547:ASN:HA	2:F:591:PHE:HZ	1.66	0.60
2:F:1157:ILE:HD11	2:F:1168:LEU:HD22	1.82	0.60
1:G:83:TRP:CD1	1:G:128:GLN:HG2	2.36	0.60
2:H:783:THR:O	2:H:787:ASN:ND2	2.31	0.60
2:B:1096:ARG:HG2	2:B:1099:ARG:HH12	1.66	0.60
2:B:1101:LEU:CD2	2:B:1125:PHE:CE1	2.83	0.60
2:F:1347:ILE:HG23	2:F:1403:ILE:HG23	1.83	0.60
2:H:682:ILE:HG23	2:H:736:ALA:HB3	1.82	0.60
2:H:1157:ILE:HD11	2:H:1168:LEU:HD22	1.82	0.60
2:D:563:VAL:HG21	2:D:1037:TRP:HH2	1.67	0.60
2:H:1347:ILE:HG23	2:H:1403:ILE:HG23	1.83	0.60
2:B:1347:ILE:HG23	2:B:1403:ILE:HG23	1.83	0.60
2:F:1506:ASP:HA	2:F:1536:ILE:HG13	1.83	0.60
2:H:563:VAL:HG21	2:H:1037:TRP:HH2	1.67	0.60
2:H:686:PHE:HB2	2:H:732:LYS:HA	1.82	0.60
2:B:72:ASN:CA	2:B:224:LEU:HD13	2.31	0.60
1:C:200:LEU:HD12	1:C:201:ARG:CA	2.29	0.60
2:D:190:ILE:HB	2:D:195:TYR:CB	2.32	0.60
1:E:200:LEU:HD11	1:E:201:ARG:O	2.02	0.60
2:B:377:TYR:O	2:B:381:ILE:HG12	2.02	0.60
2:B:547:ASN:HA	2:B:591:PHE:HZ	1.66	0.60
2:F:682:ILE:HG23	2:F:736:ALA:HB3	1.82	0.60
2:B:190:ILE:HB	2:B:195:TYR:CB	2.32	0.60
2:B:216:ARG:HB2	2:B:251:GLY:HA3	1.82	0.60
2:B:399:ILE:HD11	2:B:417:ILE:HD13	1.82	0.60
2:B:563:VAL:HG21	2:B:1037:TRP:HH2	1.67	0.60
2:D:377:TYR:O	2:D:381:ILE:HG12	2.02	0.60
2:D:1157:ILE:HD11	2:D:1168:LEU:HD22	1.82	0.60
2:F:1096:ARG:HG2	2:F:1099:ARG:HH12	1.66	0.60
2:D:399:ILE:HD11	2:D:417:ILE:HD13	1.82	0.60
2:F:72:ASN:CA	2:F:224:LEU:HD13	2.31	0.60
2:H:190:ILE:HB	2:H:195:TYR:CB	2.32	0.60
2:F:783:THR:O	2:F:787:ASN:ND2	2.31	0.59
2:H:1096:ARG:HG2	2:H:1099:ARG:HH12	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:783:THR:O	2:B:787:ASN:ND2	2.31	0.59
1:C:200:LEU:HD11	1:C:201:ARG:O	2.02	0.59
2:F:377:TYR:O	2:F:381:ILE:HG12	2.02	0.59
2:F:563:VAL:HG21	2:F:1037:TRP:HH2	1.67	0.59
1:G:200:LEU:HD11	1:G:201:ARG:O	2.02	0.59
2:B:1125:PHE:HA	2:B:1129:CYS:HG	1.66	0.59
1:A:200:LEU:HD12	1:A:201:ARG:O	2.02	0.59
2:D:1506:ASP:HA	2:D:1536:ILE:HG13	1.83	0.59
2:F:190:ILE:HB	2:F:195:TYR:CB	2.32	0.59
2:F:1344:LYS:HB2	2:F:1371:PRO:HG3	1.83	0.59
2:H:1344:LYS:HB2	2:H:1371:PRO:HG3	1.83	0.59
1:E:200:LEU:CD1	1:E:200:LEU:C	2.50	0.59
2:D:216:ARG:HB2	2:D:251:GLY:CA	2.33	0.59
2:H:72:ASN:CA	2:H:224:LEU:HD13	2.31	0.59
2:B:510:LYS:O	2:B:1419:ARG:NH1	2.36	0.59
2:B:1125:PHE:C	2:B:1129:CYS:HG	2.06	0.59
2:D:1352:VAL:HG13	2:D:1361:VAL:HB	1.84	0.59
2:B:1124:ARG:HA	2:B:1128:ASP:OD2	2.03	0.59
2:D:1344:LYS:HB2	2:D:1371:PRO:HG3	1.83	0.59
2:F:216:ARG:HB2	2:F:251:GLY:CA	2.33	0.59
1:G:200:LEU:HD12	1:G:201:ARG:O	2.02	0.59
2:H:1362:LEU:HD13	2:H:1365:VAL:HG21	1.85	0.59
2:B:1501:SER:HA	2:B:1531:ARG:HD3	1.85	0.59
2:D:510:LYS:O	2:D:1419:ARG:NH1	2.36	0.59
2:D:1096:ARG:HG2	2:D:1099:ARG:HH12	1.66	0.59
2:F:510:LYS:O	2:F:1419:ARG:NH1	2.36	0.59
2:H:216:ARG:HB2	2:H:251:GLY:CA	2.33	0.59
2:B:399:ILE:HA	2:B:402:LEU:HD23	1.85	0.58
1:C:34:ARG:HG2	1:C:305:LEU:HD21	1.85	0.58
1:G:34:ARG:HG2	1:G:305:LEU:HD21	1.85	0.58
2:H:377:TYR:O	2:H:381:ILE:HG12	2.02	0.58
1:A:34:ARG:HG2	1:A:305:LEU:HD21	1.85	0.58
2:B:304:THR:HA	2:B:307:ILE:HG22	1.85	0.58
2:B:1345:ILE:HG12	2:B:1369:ILE:HB	1.86	0.58
2:F:304:THR:HA	2:F:307:ILE:HG22	1.85	0.58
2:F:1124:ARG:HA	2:F:1128:ASP:OD2	2.03	0.58
2:F:1271:SER:HA	2:F:1275:GLU:HB3	1.85	0.58
2:F:1352:VAL:HG13	2:F:1361:VAL:HB	1.84	0.58
2:H:510:LYS:O	2:H:1419:ARG:NH1	2.36	0.58
2:H:1125:PHE:HA	2:H:1129:CYS:HG	1.66	0.58
1:E:34:ARG:HG2	1:E:305:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:686:PHE:HD1	2:H:733:VAL:HG23	1.69	0.58
2:B:1344:LYS:HB2	2:B:1371:PRO:HG3	1.83	0.58
1:E:200:LEU:HD12	1:E:201:ARG:O	2.02	0.58
1:G:209:MET:HB2	1:G:292:GLU:OE2	2.04	0.58
2:B:686:PHE:HD1	2:B:733:VAL:HG23	1.69	0.58
2:B:1352:VAL:HG13	2:B:1361:VAL:HB	1.84	0.58
1:C:209:MET:HB2	1:C:292:GLU:OE2	2.04	0.58
2:D:304:THR:HA	2:D:307:ILE:HG22	1.85	0.58
2:D:1271:SER:HA	2:D:1275:GLU:HB3	1.85	0.58
2:H:399:ILE:HA	2:H:402:LEU:HD23	1.85	0.58
2:H:1390:LEU:HB3	2:H:1395:MET:HB2	1.86	0.58
1:A:312:GLY:O	1:A:313:GLN:NE2	2.37	0.58
2:D:399:ILE:HA	2:D:402:LEU:HD23	1.85	0.58
2:D:1334:LEU:HD13	2:D:1408:ILE:HG12	1.86	0.58
1:C:312:GLY:O	1:C:313:GLN:NE2	2.37	0.58
2:F:530:MET:HE2	2:F:1095:LYS:HG2	1.85	0.58
1:C:200:LEU:HD12	1:C:201:ARG:O	2.02	0.58
2:H:1124:ARG:HA	2:H:1128:ASP:OD2	2.03	0.58
1:A:209:MET:HB2	1:A:292:GLU:OE2	2.04	0.58
2:D:1124:ARG:HA	2:D:1128:ASP:OD2	2.03	0.58
2:D:1362:LEU:HD13	2:D:1365:VAL:HG21	1.85	0.58
2:F:1362:LEU:HD13	2:F:1365:VAL:HG21	1.85	0.58
1:G:312:GLY:O	1:G:313:GLN:NE2	2.37	0.58
2:H:1125:PHE:CA	2:H:1129:CYS:HG	2.16	0.58
2:H:1345:ILE:HG12	2:H:1369:ILE:HB	1.86	0.58
2:B:216:ARG:HB2	2:B:251:GLY:CA	2.33	0.58
1:E:312:GLY:O	1:E:313:GLN:NE2	2.37	0.58
2:H:304:THR:HA	2:H:307:ILE:HG22	1.85	0.58
1:A:200:LEU:HD11	1:A:201:ARG:O	2.02	0.57
2:B:1362:LEU:HD13	2:B:1365:VAL:HG21	1.85	0.57
2:D:1501:SER:HA	2:D:1531:ARG:HD3	1.85	0.57
2:F:1393:PHE:CZ	2:F:1422:LEU:HB2	2.39	0.57
2:H:1352:VAL:HG13	2:H:1361:VAL:HB	1.84	0.57
2:H:1548:LEU:HG	2:H:1561:ASP:HA	1.86	0.57
1:A:214:THR:HA	1:A:248:GLY:HA2	1.87	0.57
2:B:1119:GLY:O	2:B:1123:ASN:HB2	2.04	0.57
1:E:209:MET:HB2	1:E:292:GLU:OE2	2.04	0.57
2:F:1334:LEU:HD13	2:F:1408:ILE:HG12	1.86	0.57
1:G:352:ASP:O	1:G:356:LEU:N	2.38	0.57
2:H:512:TYR:CG	2:H:1498:ARG:NH2	2.62	0.57
2:H:1119:GLY:O	2:H:1123:ASN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1501:SER:HA	2:H:1531:ARG:HD3	1.85	0.57
2:D:1393:PHE:CZ	2:D:1422:LEU:HB2	2.39	0.57
1:E:352:ASP:O	1:E:356:LEU:N	2.38	0.57
2:F:1345:ILE:HG12	2:F:1369:ILE:HB	1.86	0.57
2:H:1334:LEU:HD13	2:H:1408:ILE:HG12	1.86	0.57
2:B:1334:LEU:HD13	2:B:1408:ILE:HG12	1.86	0.57
1:C:352:ASP:O	1:C:356:LEU:N	2.38	0.57
2:D:512:TYR:HB3	2:D:1498:ARG:NH2	2.16	0.57
2:F:686:PHE:HD1	2:F:733:VAL:HG23	1.69	0.57
2:F:1119:GLY:O	2:F:1123:ASN:HB2	2.04	0.57
2:B:1271:SER:HA	2:B:1275:GLU:HB3	1.85	0.57
2:B:1390:LEU:HB3	2:B:1395:MET:HB2	1.86	0.57
2:B:1393:PHE:CZ	2:B:1422:LEU:HB2	2.39	0.57
1:C:214:THR:HA	1:C:248:GLY:HA2	1.87	0.57
2:D:1125:PHE:HA	2:D:1129:CYS:HG	1.66	0.57
2:F:399:ILE:HA	2:F:402:LEU:HD23	1.85	0.57
2:F:512:TYR:CG	2:F:1498:ARG:NH2	2.62	0.57
2:F:1548:LEU:HG	2:F:1561:ASP:HA	1.86	0.57
2:H:1422:LEU:O	2:H:1500:THR:HG21	2.05	0.57
2:F:1501:SER:HA	2:F:1531:ARG:HD3	1.85	0.57
1:A:352:ASP:O	1:A:356:LEU:N	2.38	0.57
2:F:1390:LEU:HB3	2:F:1395:MET:HB2	1.86	0.57
2:H:1393:PHE:CZ	2:H:1422:LEU:HB2	2.39	0.57
2:D:1119:GLY:O	2:D:1123:ASN:HB2	2.04	0.57
2:B:1125:PHE:CA	2:B:1129:CYS:HG	2.18	0.57
2:D:686:PHE:HD1	2:D:733:VAL:HG23	1.69	0.57
2:H:512:TYR:HB3	2:H:1498:ARG:NH2	2.16	0.57
2:D:1345:ILE:HG12	2:D:1369:ILE:HB	1.86	0.57
2:F:844:LEU:HD21	2:F:876:LEU:HD23	1.87	0.57
2:F:1422:LEU:O	2:F:1500:THR:HG21	2.05	0.57
1:G:214:THR:HA	1:G:248:GLY:HA2	1.87	0.56
2:H:844:LEU:HD21	2:H:876:LEU:HD23	1.87	0.56
1:C:122:LEU:HD22	1:C:136:ARG:HH12	1.71	0.56
1:G:122:LEU:HD22	1:G:136:ARG:HH12	1.71	0.56
1:A:122:LEU:HD22	1:A:136:ARG:HH12	1.71	0.56
2:B:1422:LEU:O	2:B:1500:THR:HG21	2.05	0.56
1:C:139:THR:HG23	1:C:141:GLU:H	1.70	0.56
2:D:215:VAL:HG13	2:D:252:LYS:O	2.06	0.56
1:E:139:THR:HG23	1:E:141:GLU:H	1.70	0.56
2:F:215:VAL:HG13	2:F:252:LYS:O	2.06	0.56
2:H:1271:SER:HA	2:H:1275:GLU:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LEU:HD22	1:E:136:ARG:HH12	1.71	0.56
1:E:169:MET:HB2	1:G:168:PHE:HE1	1.71	0.56
1:A:168:PHE:HE1	1:G:169:MET:HB2	1.71	0.56
2:B:215:VAL:HG13	2:B:252:LYS:O	2.06	0.56
2:D:1390:LEU:HB3	2:D:1395:MET:HB2	1.86	0.56
2:B:512:TYR:HB2	2:B:1498:ARG:NH1	2.11	0.56
2:B:1344:LYS:HA	2:B:1369:ILE:O	2.06	0.56
2:B:1548:LEU:HG	2:B:1561:ASP:HA	1.86	0.56
1:E:214:THR:HA	1:E:248:GLY:HA2	1.87	0.56
2:D:1422:LEU:O	2:D:1500:THR:HG21	2.05	0.56
2:H:559:PHE:HE2	2:H:1034:LEU:HD11	1.71	0.56
2:B:1251:ARG:HH11	2:B:1251:ARG:HB2	1.71	0.56
2:D:1251:ARG:HB2	2:D:1251:ARG:HH11	1.71	0.56
2:D:1548:LEU:HG	2:D:1561:ASP:HA	1.86	0.56
1:E:44:VAL:HG22	1:G:326:TYR:HB2	1.88	0.56
2:F:1344:LYS:HA	2:F:1369:ILE:O	2.06	0.56
2:F:1158:SER:HB2	2:F:1165:LEU:HD12	1.88	0.55
2:H:1495:ALA:HB1	2:H:1503:PHE:HE2	1.72	0.55
1:A:44:VAL:HG22	1:C:326:TYR:HB2	1.88	0.55
2:B:844:LEU:HD21	2:B:876:LEU:HD23	1.87	0.55
2:D:844:LEU:HD21	2:D:876:LEU:HD23	1.87	0.55
2:F:1125:PHE:HA	2:F:1129:CYS:HG	1.66	0.55
2:B:1495:ALA:HB1	2:B:1503:PHE:HE2	1.72	0.55
2:H:1251:ARG:HH11	2:H:1251:ARG:HB2	1.71	0.55
1:A:169:MET:HB2	1:C:168:PHE:HE1	1.71	0.55
2:D:467:ILE:HD12	2:D:586:LEU:HD22	1.88	0.55
2:D:681:ILE:O	2:D:700:THR:HA	2.07	0.55
2:F:512:TYR:HB3	2:F:1498:ARG:NH2	2.16	0.55
1:G:63:LEU:HA	1:G:66:LEU:HG	1.89	0.55
2:H:215:VAL:HG13	2:H:252:LYS:O	2.06	0.55
2:H:530:MET:HE2	2:H:1095:LYS:HG2	1.88	0.55
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.88	0.55
1:A:326:TYR:HB2	1:G:44:VAL:HG22	1.88	0.55
2:B:467:ILE:HD12	2:B:586:LEU:HD22	1.88	0.55
1:C:169:MET:HB2	1:E:168:PHE:HE1	1.71	0.55
2:D:1495:ALA:HB1	2:D:1503:PHE:HE2	1.72	0.55
2:F:1125:PHE:CA	2:F:1129:CYS:HG	2.19	0.55
2:F:1251:ARG:HB2	2:F:1251:ARG:HH11	1.71	0.55
2:F:1125:PHE:C	2:F:1129:CYS:HG	2.10	0.55
1:A:63:LEU:HA	1:A:66:LEU:HG	1.89	0.55
2:B:559:PHE:HE2	2:B:1034:LEU:HD11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:514:TRP:CZ2	2:F:1498:ARG:NH2	2.75	0.55
1:A:139:THR:HG23	1:A:141:GLU:H	1.70	0.55
2:B:681:ILE:O	2:B:700:THR:HA	2.07	0.55
2:D:514:TRP:CZ2	2:D:1498:ARG:NH2	2.75	0.55
2:D:1158:SER:HB2	2:D:1165:LEU:HD12	1.88	0.55
2:D:1344:LYS:HA	2:D:1369:ILE:O	2.06	0.55
2:F:699:ILE:HG23	2:F:908:ILE:HD11	1.88	0.55
2:F:1495:ALA:HB1	2:F:1503:PHE:HE2	1.72	0.55
2:H:1344:LYS:HA	2:H:1369:ILE:O	2.06	0.55
2:B:699:ILE:HG23	2:B:908:ILE:HD11	1.88	0.55
2:D:1125:PHE:C	2:D:1129:CYS:HG	2.10	0.55
1:G:139:THR:HG23	1:G:141:GLU:H	1.70	0.55
2:F:1435:THR:HB	2:F:1472:ASP:HA	1.88	0.55
2:H:1347:ILE:HG21	2:H:1350:LEU:HD22	1.89	0.55
1:C:44:VAL:HG22	1:E:326:TYR:HB2	1.88	0.54
1:C:39:LYS:HE2	1:C:41:ASN:HB2	1.89	0.54
1:E:63:LEU:HA	1:E:66:LEU:HG	1.89	0.54
2:H:514:TRP:CZ2	2:H:1498:ARG:NH2	2.75	0.54
2:F:1347:ILE:HG21	2:F:1350:LEU:HD22	1.89	0.54
2:B:514:TRP:CZ2	2:B:1498:ARG:NH2	2.75	0.54
2:D:1353:ARG:HG2	2:D:1360:PRO:HA	1.90	0.54
2:H:1158:SER:HB2	2:H:1165:LEU:HD12	1.88	0.54
2:H:1292:SER:HA	2:H:1295:LEU:HD12	1.90	0.54
2:B:707:GLN:HG3	2:B:898:ASP:HB2	1.90	0.54
2:F:1461:LYS:HE2	2:F:1465:LYS:HE2	1.89	0.54
2:B:1292:SER:HA	2:B:1295:LEU:HD12	1.90	0.54
1:G:39:LYS:HE2	1:G:41:ASN:HB2	1.89	0.54
2:D:686:PHE:CD2	2:D:730:MET:HB3	2.43	0.54
2:F:467:ILE:HD12	2:F:586:LEU:HD22	1.88	0.54
2:H:512:TYR:HB2	2:H:1498:ARG:NH1	2.11	0.54
2:H:686:PHE:CD2	2:H:730:MET:HB3	2.43	0.54
2:B:1158:SER:HB2	2:B:1165:LEU:HD12	1.88	0.54
2:B:1347:ILE:HG21	2:B:1350:LEU:HD22	1.89	0.54
2:F:559:PHE:HE2	2:F:1034:LEU:HD11	1.71	0.54
2:F:686:PHE:CD2	2:F:730:MET:HB3	2.43	0.54
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	1.90	0.54
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	1.90	0.54
2:H:1435:THR:HB	2:H:1472:ASP:HA	1.88	0.54
2:B:397:ASN:OD1	2:B:1224:GLN:NE2	2.41	0.54
1:C:63:LEU:HA	1:C:66:LEU:HG	1.89	0.54
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.89	0.54
2:F:1353:ARG:HG2	2:F:1360:PRO:HA	1.90	0.54
2:D:1125:PHE:CA	2:D:1129:CYS:HG	2.19	0.54
2:D:1347:ILE:HG23	2:D:1403:ILE:HG12	1.90	0.54
2:F:707:GLN:HG3	2:F:898:ASP:HB2	1.90	0.54
2:B:1353:ARG:HG2	2:B:1360:PRO:HA	1.90	0.53
2:B:1435:THR:HB	2:B:1472:ASP:HA	1.88	0.53
2:D:1435:THR:HB	2:D:1472:ASP:HA	1.88	0.53
2:F:681:ILE:O	2:F:700:THR:HA	2.07	0.53
1:A:39:LYS:HE2	1:A:41:ASN:HB2	1.89	0.53
2:D:1292:SER:HA	2:D:1295:LEU:HD12	1.90	0.53
2:H:467:ILE:HD12	2:H:586:LEU:HD22	1.88	0.53
2:B:686:PHE:CD2	2:B:730:MET:HB3	2.43	0.53
2:B:1347:ILE:HG23	2:B:1403:ILE:HG12	1.90	0.53
2:D:397:ASN:OD1	2:D:1224:GLN:NE2	2.41	0.53
2:F:589:PRO:HA	2:F:592:LEU:HD12	1.90	0.53
2:H:681:ILE:O	2:H:700:THR:HA	2.07	0.53
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	1.90	0.53
1:E:39:LYS:HE2	1:E:41:ASN:HB2	1.89	0.53
2:D:524:VAL:HG22	2:D:527:ARG:HH12	1.74	0.53
2:D:707:GLN:HG3	2:D:898:ASP:HB2	1.90	0.53
2:F:1345:ILE:HG22	2:F:1405:ILE:HA	1.91	0.53
2:D:1160:VAL:HG13	2:D:1280:LEU:HB3	1.91	0.53
2:D:1345:ILE:HG22	2:D:1405:ILE:HA	1.91	0.53
2:D:1347:ILE:HG21	2:D:1350:LEU:HD22	1.89	0.53
2:F:1292:SER:HA	2:F:1295:LEU:HD12	1.90	0.53
2:H:397:ASN:OD1	2:H:1224:GLN:NE2	2.41	0.53
2:H:1160:VAL:HG13	2:H:1280:LEU:HB3	1.91	0.53
2:B:456:LEU:HD11	2:B:579:SER:HB3	1.91	0.53
2:B:524:VAL:HG22	2:B:527:ARG:HH12	1.74	0.53
2:B:589:PRO:HA	2:B:592:LEU:HD12	1.90	0.53
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.89	0.53
2:F:397:ASN:OD1	2:F:1224:GLN:NE2	2.41	0.53
1:G:198:PHE:CE1	1:G:200:LEU:HB2	2.44	0.53
2:H:1461:LYS:HE2	2:H:1465:LYS:HE2	1.89	0.53
2:H:1463:VAL:HG21	2:H:1486:GLN:HE22	1.74	0.53
2:B:419:ASN:O	2:B:423:ILE:HG13	2.09	0.53
2:D:559:PHE:HE2	2:D:1034:LEU:HD11	1.71	0.53
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	1.90	0.53
2:F:1160:VAL:HG13	2:F:1280:LEU:HB3	1.91	0.53
2:H:1246:ARG:HH11	2:H:1246:ARG:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1345:ILE:HG22	2:H:1405:ILE:HA	1.91	0.53
1:A:198:PHE:CE1	1:A:200:LEU:HB2	2.44	0.53
2:F:419:ASN:O	2:F:423:ILE:HG13	2.09	0.53
2:F:524:VAL:HG22	2:F:527:ARG:HH12	1.74	0.53
2:B:1246:ARG:HA	2:B:1246:ARG:HH11	1.74	0.52
2:B:1345:ILE:HG22	2:B:1405:ILE:HA	1.91	0.52
2:D:685:PHE:HD2	2:D:733:VAL:HB	1.75	0.52
2:F:1463:VAL:HG21	2:F:1486:GLN:HE22	1.74	0.52
2:H:456:LEU:HD11	2:H:579:SER:HB3	1.91	0.52
1:C:81:CYS:SG	2:D:41:PHE:HB3	2.49	0.52
2:D:686:PHE:H	2:D:696:LEU:HB3	1.74	0.52
2:D:1246:ARG:HA	2:D:1246:ARG:HH11	1.74	0.52
2:D:1484:GLN:OE1	2:D:1487:ARG:NH2	2.43	0.52
1:E:81:CYS:SG	2:F:41:PHE:HB3	2.49	0.52
2:F:686:PHE:H	2:F:696:LEU:HB3	1.74	0.52
2:F:1484:GLN:OE1	2:F:1487:ARG:NH2	2.43	0.52
2:H:686:PHE:H	2:H:696:LEU:HB3	1.74	0.52
2:H:1353:ARG:HG2	2:H:1360:PRO:HA	1.90	0.52
2:F:1246:ARG:HA	2:F:1246:ARG:HH11	1.74	0.52
2:H:524:VAL:HG22	2:H:527:ARG:HH12	1.74	0.52
2:F:456:LEU:HD11	2:F:579:SER:HB3	1.91	0.52
2:F:1347:ILE:HG23	2:F:1403:ILE:HG12	1.90	0.52
2:H:419:ASN:O	2:H:423:ILE:HG13	2.09	0.52
2:B:686:PHE:H	2:B:696:LEU:HB3	1.74	0.52
2:B:1160:VAL:HG13	2:B:1280:LEU:HB3	1.91	0.52
1:G:81:CYS:SG	2:H:41:PHE:HB3	2.49	0.52
1:A:81:CYS:SG	2:B:41:PHE:HB3	2.49	0.52
1:A:190:THR:HG22	1:A:191:LEU:H	1.75	0.52
1:C:190:THR:HG22	1:C:191:LEU:H	1.75	0.52
2:D:808:LEU:HD13	2:D:837:ARG:HE	1.75	0.52
2:F:685:PHE:HD2	2:F:733:VAL:HB	1.75	0.52
2:H:685:PHE:HD2	2:H:733:VAL:HB	1.75	0.52
2:H:1347:ILE:HG23	2:H:1403:ILE:HG12	1.90	0.52
1:G:190:THR:HG22	1:G:191:LEU:H	1.75	0.52
1:E:198:PHE:CE1	1:E:200:LEU:HB2	2.44	0.52
2:H:707:GLN:HG3	2:H:898:ASP:HB2	1.90	0.52
2:B:1217:PHE:HB3	2:B:1219:TYR:HD2	1.75	0.52
2:D:419:ASN:O	2:D:423:ILE:HG13	2.09	0.52
2:D:1404:ILE:HG12	2:D:1409:ASP:HB3	1.92	0.52
2:D:1463:VAL:HG21	2:D:1486:GLN:HE22	1.74	0.52
2:H:589:PRO:HA	2:H:592:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:MET:HG2	2:B:593:LEU:HD12	1.92	0.52
1:C:198:PHE:CE1	1:C:200:LEU:HB2	2.44	0.52
2:F:808:LEU:HD13	2:F:837:ARG:HE	1.75	0.52
2:H:808:LEU:HD13	2:H:837:ARG:HE	1.75	0.52
2:B:1484:GLN:OE1	2:B:1487:ARG:NH2	2.43	0.51
2:D:589:PRO:HA	2:D:592:LEU:HD12	1.90	0.51
2:B:1404:ILE:HG12	2:B:1409:ASP:HB3	1.92	0.51
2:B:1463:VAL:HG21	2:B:1486:GLN:HE22	1.74	0.51
2:H:1217:PHE:HB3	2:H:1219:TYR:HD2	1.75	0.51
2:D:441:MET:HG2	2:D:593:LEU:HD12	1.92	0.51
2:B:143:TRP:HB3	2:B:183:LEU:HG	1.92	0.51
2:D:456:LEU:HD11	2:D:579:SER:HB3	1.91	0.51
2:F:143:TRP:HB3	2:F:183:LEU:HG	1.92	0.51
2:B:685:PHE:HD2	2:B:733:VAL:HB	1.75	0.51
2:B:1022:LEU:HB3	2:B:1078:LEU:HD21	1.93	0.51
1:C:72:LEU:O	1:C:76:THR:HG22	2.11	0.51
2:D:1217:PHE:HB3	2:D:1219:TYR:HD2	1.75	0.51
1:A:72:LEU:O	1:A:76:THR:HG22	2.11	0.51
2:F:1404:ILE:HG12	2:F:1409:ASP:HB3	1.92	0.51
2:H:143:TRP:HB3	2:H:183:LEU:HG	1.92	0.51
2:B:808:LEU:HD13	2:B:837:ARG:HE	1.75	0.51
1:G:72:LEU:O	1:G:76:THR:HG22	2.11	0.51
1:A:175:HIS:O	1:A:178:ALA:N	2.44	0.51
2:D:143:TRP:HB3	2:D:183:LEU:HG	1.92	0.51
2:D:1404:ILE:HG22	2:D:1405:ILE:N	2.26	0.51
1:G:175:HIS:O	1:G:178:ALA:N	2.44	0.51
2:H:441:MET:HG2	2:H:593:LEU:HD12	1.92	0.51
2:B:76:ILE:O	2:B:80:ILE:HG13	2.11	0.51
2:D:76:ILE:O	2:D:80:ILE:HG13	2.11	0.51
1:E:190:THR:HG22	1:E:191:LEU:H	1.75	0.51
1:E:200:LEU:HD12	1:E:201:ARG:C	2.32	0.51
1:G:200:LEU:CD2	1:G:304:TYR:CZ	2.94	0.51
2:H:1484:GLN:OE1	2:H:1487:ARG:NH2	2.43	0.51
1:G:200:LEU:HD12	1:G:201:ARG:C	2.32	0.50
1:A:200:LEU:HD12	1:A:201:ARG:C	2.32	0.50
2:B:1127:SER:O	2:B:1128:ASP:C	2.50	0.50
2:B:1350:LEU:CD1	2:B:1403:ILE:HG13	2.39	0.50
2:B:1455:LEU:HD13	2:B:1464:VAL:HG21	1.94	0.50
1:E:175:HIS:O	1:E:178:ALA:N	2.44	0.50
2:F:370:ARG:HB3	2:F:1253:GLU:HG2	1.94	0.50
2:F:1022:LEU:HB3	2:F:1078:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1455:LEU:HD13	2:F:1464:VAL:HG21	1.94	0.50
2:H:76:ILE:O	2:H:80:ILE:HG13	2.11	0.50
2:H:1127:SER:O	2:H:1128:ASP:C	2.50	0.50
1:C:90:TRP:HZ3	1:C:152:GLN:HE21	1.59	0.50
2:D:784:VAL:HG22	2:D:823:ILE:HD11	1.94	0.50
2:D:370:ARG:HB3	2:D:1253:GLU:HG2	1.94	0.50
2:F:784:VAL:HG22	2:F:823:ILE:HD11	1.94	0.50
2:F:1217:PHE:HB3	2:F:1219:TYR:HD2	1.75	0.50
2:F:1385:LYS:HB2	2:F:1536:ILE:HG21	1.94	0.50
2:H:1404:ILE:HG12	2:H:1409:ASP:HB3	1.92	0.50
2:D:513:ALA:HB2	2:D:1419:ARG:HG3	1.94	0.50
2:F:76:ILE:O	2:F:80:ILE:HG13	2.11	0.50
2:F:513:ALA:HB2	2:F:1419:ARG:HG3	1.94	0.50
2:H:1022:LEU:HB3	2:H:1078:LEU:HD21	1.93	0.50
2:H:1385:LYS:HB2	2:H:1536:ILE:HG21	1.94	0.50
2:B:233:MET:HB2	2:B:1247:TRP:CD1	2.47	0.50
2:F:441:MET:HG2	2:F:593:LEU:HD12	1.92	0.50
2:F:869:MET:HA	2:F:873:ILE:HD12	1.94	0.50
2:H:513:ALA:HB2	2:H:1419:ARG:HG3	1.94	0.50
2:H:1404:ILE:HG22	2:H:1405:ILE:N	2.26	0.50
1:A:90:TRP:HZ3	1:A:152:GLN:HE21	1.59	0.50
1:C:175:HIS:O	1:C:178:ALA:N	2.44	0.50
2:B:508:LEU:HD12	2:B:1426:LEU:HD23	1.94	0.50
2:B:784:VAL:HG22	2:B:823:ILE:HD11	1.94	0.50
1:C:200:LEU:CD2	1:C:304:TYR:CZ	2.94	0.50
2:H:784:VAL:HG22	2:H:823:ILE:HD11	1.94	0.50
3:H:2002:AGS:O2A	3:H:2002:AGS:S1G	2.70	0.50
2:B:223:ASN:OD1	2:B:223:ASN:N	2.41	0.50
2:B:1404:ILE:HG22	2:B:1405:ILE:N	2.26	0.50
2:D:512:TYR:HB2	2:D:1498:ARG:NH1	2.11	0.50
2:D:1022:LEU:HB3	2:D:1078:LEU:HD21	1.93	0.50
2:F:1404:ILE:HG22	2:F:1405:ILE:N	2.26	0.50
2:H:1455:LEU:HD13	2:H:1464:VAL:HG21	1.94	0.50
2:B:513:ALA:HB2	2:B:1419:ARG:HG3	1.94	0.49
2:D:233:MET:HB2	2:D:1247:TRP:CD1	2.47	0.49
2:D:869:MET:HA	2:D:873:ILE:HD12	1.94	0.49
2:D:1385:LYS:HB2	2:D:1536:ILE:HG21	1.94	0.49
2:D:1455:LEU:HD13	2:D:1464:VAL:HG21	1.94	0.49
2:F:512:TYR:HB2	2:F:1498:ARG:NH2	2.24	0.49
2:B:1385:LYS:HB2	2:B:1536:ILE:HG21	1.94	0.49
1:C:200:LEU:HD12	1:C:201:ARG:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:LEU:O	1:E:76:THR:HG22	2.11	0.49
1:E:200:LEU:CD2	1:E:304:TYR:CZ	2.94	0.49
2:F:563:VAL:HG21	2:F:1037:TRP:CH2	2.47	0.49
2:H:370:ARG:HB3	2:H:1253:GLU:HG2	1.94	0.49
1:A:200:LEU:CD2	1:A:304:TYR:CZ	2.94	0.49
3:D:2002:AGS:O2A	3:D:2002:AGS:S1G	2.70	0.49
2:F:233:MET:HB2	2:F:1247:TRP:CD1	2.47	0.49
2:H:508:LEU:HD12	2:H:1426:LEU:HD23	1.94	0.49
2:B:370:ARG:HB3	2:B:1253:GLU:HG2	1.94	0.49
2:B:869:MET:HA	2:B:873:ILE:HD12	1.94	0.49
2:D:1350:LEU:CD1	2:D:1403:ILE:HG13	2.39	0.49
2:F:1024:HIS:O	2:F:1028:VAL:HG12	2.13	0.49
2:H:1132:ILE:CD1	2:H:1312:VAL:HG22	2.41	0.49
2:F:1140:LEU:HB2	2:F:1305:MET:HE1	1.95	0.49
3:F:2002:AGS:O2A	3:F:2002:AGS:S1G	2.70	0.49
2:H:255:ILE:HA	2:H:258:ARG:HE	1.77	0.49
2:H:1024:HIS:O	2:H:1028:VAL:HG12	2.13	0.49
3:B:2002:AGS:O2A	3:B:2002:AGS:S1G	2.70	0.49
2:F:711:ILE:HB	2:F:887:VAL:HG13	1.95	0.49
2:F:1127:SER:O	2:F:1128:ASP:C	2.50	0.49
2:D:563:VAL:HG21	2:D:1037:TRP:CH2	2.47	0.49
2:D:711:ILE:HB	2:D:887:VAL:HG13	1.95	0.49
2:D:1127:SER:O	2:D:1128:ASP:C	2.50	0.49
2:F:1350:LEU:CD1	2:F:1403:ILE:HG13	2.39	0.49
2:B:1132:ILE:CD1	2:B:1312:VAL:HG22	2.41	0.49
2:D:1024:HIS:O	2:D:1028:VAL:HG12	2.13	0.49
1:E:90:TRP:HZ3	1:E:152:GLN:HE21	1.59	0.49
2:F:255:ILE:HA	2:F:258:ARG:HE	1.77	0.49
1:G:290:VAL:HG23	1:G:296:ILE:O	2.13	0.49
2:H:530:MET:HE3	2:H:1095:LYS:CG	2.43	0.49
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.95	0.49
1:E:68:TRP:CE2	1:E:170:LYS:HE2	2.48	0.49
1:E:290:VAL:HG23	1:E:296:ILE:O	2.13	0.49
2:F:512:TYR:HB2	2:F:1498:ARG:NH1	2.11	0.49
1:C:68:TRP:CE2	1:C:170:LYS:HE2	2.48	0.49
2:H:233:MET:HB2	2:H:1247:TRP:CD1	2.47	0.49
2:D:508:LEU:HD12	2:D:1426:LEU:HD23	1.94	0.48
2:D:1171:LEU:O	2:D:1174:VAL:HB	2.13	0.48
1:E:60:PHE:O	1:E:64:VAL:HG13	2.13	0.48
1:G:90:TRP:HZ3	1:G:152:GLN:HE21	1.59	0.48
2:H:1171:LEU:O	2:H:1174:VAL:HB	2.13	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
2:B:1495:ALA:HB1	2:B:1503:PHE:CE2	2.48	0.48
2:D:32:ASN:O	2:D:35:PRO:HD2	2.14	0.48
2:F:1132:ILE:CD1	2:F:1312:VAL:HG22	2.41	0.48
2:H:711:ILE:HB	2:H:887:VAL:HG13	1.95	0.48
2:H:1495:ALA:HB1	2:H:1503:PHE:CE2	2.48	0.48
1:A:68:TRP:CE2	1:A:170:LYS:HE2	2.48	0.48
1:C:280:ASP:N	1:C:280:ASP:OD1	2.47	0.48
2:D:1561:ASP:OD1	2:D:1561:ASP:N	2.46	0.48
1:A:56:LEU:HB2	2:B:132:PHE:CZ	2.49	0.48
2:B:563:VAL:HG21	2:B:1037:TRP:CH2	2.47	0.48
1:E:280:ASP:OD1	1:E:280:ASP:N	2.47	0.48
1:G:60:PHE:O	1:G:64:VAL:HG13	2.13	0.48
1:G:123:PHE:HD2	1:G:136:ARG:HG3	1.78	0.48
2:H:869:MET:HA	2:H:873:ILE:HD12	1.94	0.48
2:H:1030:ILE:HA	2:H:1071:LEU:HD13	1.96	0.48
2:B:32:ASN:O	2:B:35:PRO:HD2	2.14	0.48
2:B:455:ILE:HG22	2:B:575:VAL:HG13	1.96	0.48
1:C:60:PHE:O	1:C:64:VAL:HG13	2.13	0.48
2:F:32:ASN:O	2:F:35:PRO:HD2	2.14	0.48
2:F:1171:LEU:O	2:F:1174:VAL:HB	2.13	0.48
1:A:290:VAL:HG23	1:A:296:ILE:O	2.13	0.48
2:B:1404:ILE:HG21	2:B:1407:GLY:CA	2.44	0.48
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.95	0.48
2:D:320:ILE:HD11	2:D:1289:LEU:HD13	1.95	0.48
2:F:1404:ILE:HG21	2:F:1407:GLY:CA	2.44	0.48
1:G:280:ASP:OD1	1:G:280:ASP:N	2.47	0.48
1:C:56:LEU:HB2	2:D:132:PHE:CZ	2.49	0.48
1:C:95:PHE:CD1	1:C:100:LEU:HD23	2.45	0.48
1:C:290:VAL:HG23	1:C:296:ILE:O	2.13	0.48
2:D:1125:PHE:C	2:D:1129:CYS:SG	2.92	0.48
2:D:1495:ALA:HB1	2:D:1503:PHE:CE2	2.48	0.48
1:E:56:LEU:HB2	2:F:132:PHE:CZ	2.49	0.48
2:F:508:LEU:HD12	2:F:1426:LEU:HD23	1.94	0.48
2:F:559:PHE:CE2	2:F:1034:LEU:HD11	2.49	0.48
2:F:1030:ILE:HA	2:F:1071:LEU:HD13	1.96	0.48
2:H:1431:LEU:HD23	2:H:1494:ARG:HH21	1.79	0.48
1:A:280:ASP:OD1	1:A:280:ASP:N	2.47	0.48
2:B:1024:HIS:O	2:B:1028:VAL:HG12	2.13	0.48
1:E:198:PHE:HE1	1:E:200:LEU:HB2	1.79	0.48
2:F:455:ILE:HG22	2:F:575:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1125:PHE:C	2:F:1129:CYS:SG	2.92	0.48
2:H:563:VAL:HG21	2:H:1037:TRP:CH2	2.47	0.48
2:H:1140:LEU:HB2	2:H:1305:MET:HE1	1.95	0.48
2:B:1171:LEU:O	2:B:1174:VAL:HB	2.13	0.48
2:F:829:ASN:OD1	2:F:829:ASN:N	2.36	0.48
2:F:1495:ALA:HB1	2:F:1503:PHE:CE2	2.48	0.48
2:F:1561:ASP:OD1	2:F:1561:ASP:N	2.46	0.48
1:G:68:TRP:CE2	1:G:170:LYS:HE2	2.48	0.48
1:G:90:TRP:HA	1:G:93:ILE:HG22	1.95	0.48
1:A:60:PHE:O	1:A:64:VAL:HG13	2.13	0.47
2:B:255:ILE:HA	2:B:258:ARG:HE	1.77	0.47
1:C:49:ILE:HG21	1:C:55:PHE:HZ	1.79	0.47
1:C:123:PHE:HD2	1:C:136:ARG:HG3	1.78	0.47
2:D:779:LEU:HD11	2:D:835:ARG:HG2	1.95	0.47
1:E:90:TRP:HA	1:E:93:ILE:HG22	1.95	0.47
2:F:1431:LEU:HD23	2:F:1494:ARG:HH21	1.79	0.47
1:G:56:LEU:HB2	2:H:132:PHE:CZ	2.49	0.47
2:H:779:LEU:HD11	2:H:835:ARG:HG2	1.95	0.47
2:H:1404:ILE:HG21	2:H:1407:GLY:CA	2.44	0.47
1:A:49:ILE:HG21	1:A:55:PHE:HZ	1.79	0.47
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.95	0.47
2:B:1553:LYS:HE3	2:B:1558:LEU:HB2	1.96	0.47
2:D:1404:ILE:HG21	2:D:1407:GLY:CA	2.44	0.47
2:F:779:LEU:HD11	2:F:835:ARG:HG2	1.95	0.47
2:D:131:ASN:OD1	2:D:131:ASN:N	2.43	0.47
2:F:775:GLN:OE1	3:F:2002:AGS:S1G	2.73	0.47
2:B:779:LEU:HD11	2:B:835:ARG:HG2	1.95	0.47
2:B:1030:ILE:HA	2:B:1071:LEU:HD13	1.96	0.47
2:B:1140:LEU:HB2	2:B:1305:MET:HE1	1.96	0.47
2:B:1431:LEU:HD23	2:B:1494:ARG:HH21	1.79	0.47
2:D:255:ILE:HA	2:D:258:ARG:HE	1.77	0.47
2:D:775:GLN:OE1	3:D:2002:AGS:S1G	2.73	0.47
2:F:1553:LYS:HE3	2:F:1558:LEU:HB2	1.96	0.47
1:G:189:ILE:HA	1:G:198:PHE:HA	1.96	0.47
2:H:1553:LYS:HE3	2:H:1558:LEU:HB2	1.96	0.47
2:H:1561:ASP:OD1	2:H:1561:ASP:N	2.46	0.47
1:A:345:THR:O	1:A:349:LEU:N	2.40	0.47
2:B:320:ILE:HD11	2:B:1289:LEU:HD13	1.95	0.47
1:C:48:ASN:ND2	1:E:331:SER:OG	2.48	0.47
2:D:396:TYR:HE2	2:D:1224:GLN:HG3	1.80	0.47
2:D:1553:LYS:HE3	2:D:1558:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:559:PHE:CE2	2:H:1034:LEU:HD11	2.49	0.47
1:A:331:SER:OG	1:G:48:ASN:ND2	2.48	0.47
2:B:396:TYR:HE2	2:B:1224:GLN:HG3	1.80	0.47
2:B:559:PHE:CE2	2:B:1034:LEU:HD11	2.49	0.47
2:B:775:GLN:OE1	3:B:2002:AGS:S1G	2.73	0.47
2:B:1125:PHE:C	2:B:1129:CYS:SG	2.92	0.47
1:C:198:PHE:HE1	1:C:200:LEU:HB2	1.79	0.47
1:E:48:ASN:ND2	1:G:331:SER:OG	2.48	0.47
2:F:506:MET:SD	2:F:1113:PHE:HB3	2.55	0.47
2:H:1350:LEU:CD1	2:H:1403:ILE:HG13	2.39	0.47
1:A:48:ASN:ND2	1:C:331:SER:OG	2.48	0.47
1:C:189:ILE:HA	1:C:198:PHE:HA	1.96	0.47
2:D:506:MET:SD	2:D:1113:PHE:HB3	2.55	0.47
2:D:1030:ILE:HA	2:D:1071:LEU:HD13	1.96	0.47
2:D:1140:LEU:HB2	2:D:1305:MET:HE1	1.96	0.47
1:E:123:PHE:HD2	1:E:136:ARG:HG3	1.78	0.47
2:F:320:ILE:HD11	2:F:1289:LEU:HD13	1.95	0.47
2:F:1441:ASP:OD2	2:F:1444:LYS:C	2.53	0.47
2:H:455:ILE:HG22	2:H:575:VAL:HG13	1.96	0.47
2:H:775:GLN:OE1	3:H:2002:AGS:S1G	2.73	0.47
2:B:1441:ASP:OD2	2:B:1444:LYS:C	2.53	0.47
2:B:1561:ASP:N	2:B:1561:ASP:OD1	2.46	0.47
2:D:559:PHE:CE2	2:D:1034:LEU:HD11	2.49	0.47
1:E:49:ILE:HG21	1:E:55:PHE:HZ	1.79	0.47
1:G:198:PHE:HE1	1:G:200:LEU:HB2	1.79	0.47
2:H:32:ASN:O	2:H:35:PRO:HD2	2.14	0.47
2:H:240:ALA:HB1	2:H:245:ILE:HD11	1.97	0.47
2:H:829:ASN:OD1	2:H:829:ASN:N	2.36	0.47
2:B:1187:ARG:O	2:B:1190:GLN:HB3	2.15	0.47
2:B:1458:ALA:O	2:B:1489:LEU:HG	2.15	0.47
2:F:396:TYR:HE2	2:F:1224:GLN:HG3	1.80	0.47
2:H:320:ILE:HD11	2:H:1289:LEU:HD13	1.95	0.47
2:H:506:MET:SD	2:H:1113:PHE:HB3	2.55	0.47
2:H:846:GLN:HG3	2:H:1217:PHE:HE2	1.80	0.47
2:D:679:VAL:HB	2:D:703:ILE:HB	1.97	0.46
2:H:1441:ASP:OD2	2:H:1444:LYS:C	2.53	0.46
2:B:240:ALA:HB1	2:B:245:ILE:HD11	1.97	0.46
2:B:506:MET:SD	2:B:1113:PHE:HB3	2.55	0.46
2:D:240:ALA:HB1	2:D:245:ILE:HD11	1.97	0.46
2:D:455:ILE:HG22	2:D:575:VAL:HG13	1.96	0.46
2:F:679:VAL:HB	2:F:703:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ILE:HG21	1:G:55:PHE:HZ	1.79	0.46
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.97	0.46
2:H:1458:ALA:O	2:H:1489:LEU:HG	2.15	0.46
2:B:846:GLN:HG3	2:B:1217:PHE:HE2	1.80	0.46
2:D:846:GLN:HG3	2:D:1217:PHE:HE2	1.80	0.46
2:D:1431:LEU:HD23	2:D:1494:ARG:HH21	1.79	0.46
2:F:846:GLN:HG3	2:F:1217:PHE:HE2	1.80	0.46
2:D:1458:ALA:O	2:D:1489:LEU:HG	2.15	0.46
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.97	0.46
2:F:530:MET:HE3	2:F:1095:LYS:CG	2.46	0.46
1:A:198:PHE:HE1	1:A:200:LEU:HB2	1.79	0.46
2:B:1034:LEU:O	2:B:1038:THR:HG23	2.16	0.46
2:D:1246:ARG:HA	2:D:1246:ARG:HD3	1.71	0.46
2:D:1441:ASP:OD2	2:D:1444:LYS:C	2.53	0.46
1:E:189:ILE:HA	1:E:198:PHE:HA	1.96	0.46
2:F:240:ALA:HB1	2:F:245:ILE:HD11	1.97	0.46
2:H:1187:ARG:O	2:H:1190:GLN:HB3	2.15	0.46
1:A:189:ILE:HA	1:A:198:PHE:HA	1.96	0.46
2:D:223:ASN:OD1	2:D:223:ASN:N	2.41	0.46
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.97	0.46
2:D:190:ILE:CD1	2:D:195:TYR:CB	2.94	0.46
2:H:396:TYR:HE2	2:H:1224:GLN:HG3	1.80	0.46
2:H:1034:LEU:O	2:H:1038:THR:HG23	2.16	0.46
2:B:1404:ILE:HG23	2:B:1408:ILE:O	2.16	0.46
2:D:1246:ARG:NH2	4:D:2001:GBM:H18	2.31	0.46
2:D:1376:GLY:O	2:D:1549:VAL:HA	2.16	0.46
2:F:1404:ILE:HG23	2:F:1408:ILE:O	2.16	0.46
2:F:1458:ALA:O	2:F:1489:LEU:HG	2.15	0.46
2:D:808:LEU:HG	2:D:812:ILE:HG12	1.98	0.46
2:D:1375:ILE:HB	2:D:1534:VAL:HG22	1.98	0.46
2:F:808:LEU:HG	2:F:812:ILE:HG12	1.98	0.46
2:F:996:ILE:HD12	2:F:997:PRO:HD2	1.98	0.46
2:F:1187:ARG:O	2:F:1190:GLN:HB3	2.15	0.46
2:F:1246:ARG:NH2	4:F:2001:GBM:H18	2.31	0.46
1:A:95:PHE:HE2	2:B:27:PHE:HB2	1.81	0.45
2:B:190:ILE:CD1	2:B:195:TYR:CB	2.94	0.45
2:D:1404:ILE:HG23	2:D:1408:ILE:O	2.16	0.45
2:F:1034:LEU:O	2:F:1038:THR:HG23	2.16	0.45
2:H:1375:ILE:HB	2:H:1534:VAL:HG22	1.98	0.45
2:H:1404:ILE:HG23	2:H:1408:ILE:O	2.16	0.45
1:A:261:ILE:H	1:A:261:ILE:HG13	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:739:TRP:HE1	2:B:768:GLY:N	2.15	0.45
2:B:1246:ARG:NH2	4:B:2001:GBM:H18	2.31	0.45
2:B:1375:ILE:HB	2:B:1534:VAL:HG22	1.98	0.45
4:B:2001:GBM:H20	4:B:2001:GBM:H22	1.75	0.45
2:D:1132:ILE:CD1	2:D:1312:VAL:HG22	2.41	0.45
2:F:196:ILE:C	2:F:197:PHE:O	2.55	0.45
2:H:590:LEU:HD23	2:H:590:LEU:HA	1.83	0.45
2:D:996:ILE:HD12	2:D:997:PRO:HD2	1.98	0.45
2:D:1187:ARG:O	2:D:1190:GLN:HB3	2.15	0.45
2:F:678:CYS:HB3	2:F:704:PRO:HA	1.99	0.45
2:F:1375:ILE:HB	2:F:1534:VAL:HG22	1.98	0.45
2:F:1376:GLY:O	2:F:1549:VAL:HA	2.16	0.45
1:G:95:PHE:HE2	2:H:27:PHE:HB2	1.81	0.45
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.71	0.45
2:B:512:TYR:HB3	2:B:1498:ARG:NH2	2.16	0.45
2:D:739:TRP:HE1	2:D:768:GLY:N	2.15	0.45
2:D:1034:LEU:O	2:D:1038:THR:HG23	2.16	0.45
2:H:996:ILE:HD12	2:H:997:PRO:HD2	1.98	0.45
2:B:679:VAL:HB	2:B:703:ILE:HB	1.97	0.45
2:B:808:LEU:HG	2:B:812:ILE:HG12	1.98	0.45
2:D:678:CYS:HB3	2:D:704:PRO:HA	1.99	0.45
2:F:37:VAL:HG13	2:F:41:PHE:CE2	2.52	0.45
2:F:875:GLU:O	2:F:879:ASP:HB2	2.17	0.45
2:H:679:VAL:HB	2:H:703:ILE:HB	1.97	0.45
2:F:131:ASN:OD1	2:F:131:ASN:N	2.43	0.45
2:F:190:ILE:CD1	2:F:195:TYR:CB	2.94	0.45
1:G:196:LEU:CB	1:G:261:ILE:HD11	2.47	0.45
2:B:996:ILE:HD12	2:B:997:PRO:HD2	1.98	0.45
2:B:1039:ASP:OD1	2:B:1039:ASP:N	2.50	0.45
1:C:116:SER:OG	1:C:117:PHE:N	2.50	0.45
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.97	0.45
2:D:196:ILE:C	2:D:197:PHE:O	2.55	0.45
2:D:875:GLU:O	2:D:879:ASP:HB2	2.17	0.45
1:E:95:PHE:HE2	2:F:27:PHE:HB2	1.81	0.45
2:F:892:GLN:H	2:F:892:GLN:HG3	1.46	0.45
2:F:1369:ILE:HD13	2:F:1375:ILE:HG13	1.99	0.45
1:G:116:SER:OG	1:G:117:PHE:N	2.50	0.45
2:H:739:TRP:HE1	2:H:768:GLY:N	2.15	0.45
2:H:1125:PHE:C	2:H:1129:CYS:SG	2.92	0.45
2:B:678:CYS:HB3	2:B:704:PRO:HA	1.99	0.45
2:B:1376:GLY:O	2:B:1549:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:SER:OG	1:E:117:PHE:N	2.50	0.45
2:H:379:VAL:O	2:H:383:THR:OG1	2.35	0.45
2:H:808:LEU:HG	2:H:812:ILE:HG12	1.98	0.45
2:H:891:LEU:H	2:H:891:LEU:HD23	1.81	0.45
2:H:1246:ARG:NH2	4:H:2001:GBM:H18	2.31	0.45
2:H:1376:GLY:O	2:H:1549:VAL:HA	2.16	0.45
2:B:1246:ARG:HH21	4:B:2001:GBM:H18	1.82	0.45
2:H:856:PRO:HD2	2:H:886:LEU:HD21	1.99	0.45
1:A:116:SER:OG	1:A:117:PHE:N	2.50	0.45
1:C:196:LEU:CB	1:C:261:ILE:HD11	2.47	0.45
2:D:37:VAL:HG13	2:D:41:PHE:CE2	2.52	0.45
2:D:1369:ILE:HD13	2:D:1375:ILE:HG13	1.99	0.45
2:F:216:ARG:HD2	2:F:251:GLY:N	2.32	0.45
2:F:379:VAL:O	2:F:383:THR:OG1	2.35	0.45
2:F:581:SER:O	2:F:585:ILE:HG12	2.17	0.45
2:F:739:TRP:HE1	2:F:768:GLY:N	2.15	0.45
2:F:891:LEU:H	2:F:891:LEU:HD23	1.81	0.45
2:H:223:ASN:OD1	2:H:223:ASN:N	2.41	0.45
2:H:1355:ASP:OD1	2:H:1356:SER:N	2.50	0.45
2:B:379:VAL:O	2:B:383:THR:OG1	2.35	0.44
2:B:875:GLU:O	2:B:879:ASP:HB2	2.17	0.44
2:B:1460:LEU:HD13	2:B:1489:LEU:HD23	1.99	0.44
2:D:1246:ARG:HH21	4:D:2001:GBM:H18	1.82	0.44
1:G:170:LYS:O	1:G:173:GLN:N	2.48	0.44
2:H:196:ILE:C	2:H:197:PHE:O	2.55	0.44
2:H:1369:ILE:HD13	2:H:1375:ILE:HG13	1.99	0.44
1:A:170:LYS:O	1:A:173:GLN:N	2.48	0.44
1:A:196:LEU:CB	1:A:261:ILE:HD11	2.47	0.44
2:B:512:TYR:HB2	2:B:1498:ARG:NH2	2.24	0.44
2:B:581:SER:O	2:B:585:ILE:HG12	2.17	0.44
1:C:261:ILE:H	1:C:261:ILE:HG13	1.54	0.44
1:E:196:LEU:CB	1:E:261:ILE:HD11	2.47	0.44
2:H:810:PRO:O	2:H:814:ILE:HG13	2.17	0.44
2:H:875:GLU:O	2:H:879:ASP:HB2	2.17	0.44
1:A:95:PHE:CD1	1:A:100:LEU:HD23	2.45	0.44
1:A:330:TYR:HB2	1:G:48:ASN:O	2.18	0.44
2:B:790:PHE:HB3	2:B:846:GLN:HE21	1.83	0.44
2:B:856:PRO:HD2	2:B:886:LEU:HD21	1.99	0.44
2:D:402:LEU:O	2:D:1215:ARG:NH1	2.50	0.44
2:D:790:PHE:HB3	2:D:846:GLN:HE21	1.83	0.44
2:D:1460:LEU:HD13	2:D:1489:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PHE:CD1	1:E:100:LEU:HD23	2.45	0.44
1:G:345:THR:O	1:G:349:LEU:N	2.40	0.44
2:H:581:SER:O	2:H:585:ILE:HG12	2.17	0.44
2:B:37:VAL:HG13	2:B:41:PHE:CE2	2.52	0.44
2:B:509:LEU:HD11	2:B:515:GLU:HA	2.00	0.44
2:B:511:LEU:HG	2:B:1424:ILE:HG21	1.98	0.44
2:D:216:ARG:HD2	2:D:251:GLY:N	2.32	0.44
1:E:313:GLN:HE22	1:E:338:LYS:HD2	1.83	0.44
2:F:218:LEU:H	2:F:218:LEU:HG	1.70	0.44
2:F:511:LEU:HG	2:F:1424:ILE:HG21	1.98	0.44
2:H:509:LEU:HD11	2:H:515:GLU:HA	2.00	0.44
2:H:678:CYS:HB3	2:H:704:PRO:HA	1.99	0.44
2:H:790:PHE:HB3	2:H:846:GLN:HE21	1.83	0.44
2:D:511:LEU:HG	2:D:1424:ILE:HG21	1.98	0.44
2:D:810:PRO:O	2:D:814:ILE:HG13	2.17	0.44
1:E:215:ILE:HD13	1:E:215:ILE:HA	1.83	0.44
1:E:345:THR:O	1:E:349:LEU:N	2.40	0.44
2:F:894:LEU:HB2	2:F:895:PRO:HD3	1.99	0.44
2:B:196:ILE:C	2:B:197:PHE:O	2.55	0.44
1:C:313:GLN:HE22	1:C:338:LYS:HD2	1.83	0.44
2:D:253:LEU:HD12	2:D:253:LEU:HA	1.86	0.44
2:F:790:PHE:HB3	2:F:846:GLN:HE21	1.83	0.44
2:F:856:PRO:HD2	2:F:886:LEU:HD21	1.99	0.44
2:F:1039:ASP:N	2:F:1039:ASP:OD1	2.50	0.44
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.52	0.44
2:H:530:MET:CE	2:H:1095:LYS:CG	2.96	0.44
2:B:1154:LEU:HD22	2:B:1168:LEU:HD13	2.00	0.44
2:B:1375:ILE:HD12	2:B:1548:LEU:HB2	2.00	0.44
1:C:68:TRP:N	1:C:69:PRO:HD2	2.33	0.44
1:A:68:TRP:N	1:A:69:PRO:HD2	2.33	0.44
1:C:95:PHE:HE2	2:D:27:PHE:HB2	1.81	0.44
2:D:297:ARG:O	2:D:300:ILE:HG13	2.18	0.44
2:D:379:VAL:O	2:D:383:THR:OG1	2.35	0.44
2:H:511:LEU:HG	2:H:1424:ILE:HG21	1.98	0.44
1:A:215:ILE:HD13	1:A:215:ILE:HA	1.83	0.44
2:B:530:MET:CE	2:B:1095:LYS:CG	2.96	0.44
2:B:891:LEU:HD23	2:B:891:LEU:H	1.81	0.44
2:D:581:SER:O	2:D:585:ILE:HG12	2.17	0.44
2:D:891:LEU:HD23	2:D:891:LEU:H	1.81	0.44
1:E:268:TYR:O	1:E:346:ALA:HB3	2.18	0.44
2:F:297:ARG:O	2:F:300:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1246:ARG:HH21	4:F:2001:GBM:H18	1.82	0.44
1:G:313:GLN:HE22	1:G:338:LYS:HD2	1.83	0.44
2:H:681:ILE:HD11	2:H:726:THR:HG22	1.99	0.44
2:B:297:ARG:O	2:B:300:ILE:HG13	2.18	0.43
2:B:306:ARG:NH2	4:B:2001:GBM:CL1	2.72	0.43
2:B:1369:ILE:HD13	2:B:1375:ILE:HG13	1.99	0.43
1:C:48:ASN:O	1:E:330:TYR:HB2	2.18	0.43
2:D:681:ILE:HD11	2:D:726:THR:HG22	1.99	0.43
2:F:509:LEU:HD11	2:F:515:GLU:HA	2.00	0.43
1:G:268:TYR:O	1:G:346:ALA:HB3	2.18	0.43
2:H:1393:PHE:O	2:H:1394:ARG:HG3	2.18	0.43
1:A:268:TYR:O	1:A:346:ALA:HB3	2.18	0.43
1:A:284:ILE:HA	1:A:302:THR:O	2.19	0.43
2:B:1393:PHE:O	2:B:1394:ARG:HG3	2.18	0.43
1:C:284:ILE:HA	1:C:302:THR:O	2.19	0.43
1:E:77:MET:HG3	2:F:48:PHE:HE2	1.83	0.43
2:H:40:LEU:O	2:H:44:PHE:HD2	2.01	0.43
2:H:512:TYR:HB2	2:H:1498:ARG:NH2	2.24	0.43
2:H:1460:LEU:HD13	2:H:1489:LEU:HD23	1.99	0.43
1:A:48:ASN:O	1:C:330:TYR:HB2	2.18	0.43
1:A:262:ASP:OD1	1:A:265:SER:OG	2.32	0.43
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.99	0.43
1:C:176:ARG:O	1:C:179:GLU:N	2.51	0.43
1:E:48:ASN:O	1:G:330:TYR:HB2	2.18	0.43
1:E:284:ILE:HA	1:E:302:THR:O	2.19	0.43
2:F:1201:LEU:HD23	2:F:1201:LEU:HA	1.84	0.43
2:F:1393:PHE:O	2:F:1394:ARG:HG3	2.18	0.43
2:F:1460:LEU:HD13	2:F:1489:LEU:HD23	1.99	0.43
2:H:190:ILE:CD1	2:H:195:TYR:CB	2.94	0.43
2:B:1246:ARG:HA	2:B:1246:ARG:HD3	1.71	0.43
2:F:681:ILE:HD11	2:F:726:THR:HG22	1.99	0.43
2:F:810:PRO:O	2:F:814:ILE:HG13	2.17	0.43
1:A:77:MET:HG3	2:B:48:PHE:HE2	1.83	0.43
2:B:894:LEU:HB2	2:B:895:PRO:HD3	1.99	0.43
2:D:509:LEU:HD11	2:D:515:GLU:HA	2.00	0.43
2:D:856:PRO:HD2	2:D:886:LEU:HD21	1.99	0.43
1:G:261:ILE:H	1:G:261:ILE:HG13	1.54	0.43
1:G:284:ILE:HA	1:G:302:THR:O	2.19	0.43
2:H:216:ARG:HD2	2:H:251:GLY:N	2.32	0.43
1:A:326:TYR:O	1:G:44:VAL:HG13	2.19	0.43
1:C:196:LEU:HB2	1:C:261:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:LEU:O	2:D:44:PHE:HD2	2.01	0.43
2:D:396:TYR:CE2	2:D:1224:GLN:HG3	2.54	0.43
2:F:686:PHE:CE2	2:F:730:MET:HB3	2.54	0.43
2:F:1154:LEU:HD22	2:F:1168:LEU:HD13	2.00	0.43
1:G:77:MET:HG3	2:H:48:PHE:HE2	1.83	0.43
2:H:297:ARG:O	2:H:300:ILE:HG13	2.18	0.43
2:H:812:ILE:HD13	2:H:812:ILE:HA	1.84	0.43
2:H:1375:ILE:HD12	2:H:1548:LEU:HB2	2.00	0.43
2:B:530:MET:HE3	2:B:1095:LYS:CG	2.49	0.43
2:B:1031:ASP:OD2	2:B:1287:TYR:OH	2.25	0.43
2:B:1240:PHE:HD1	2:B:1240:PHE:HA	1.67	0.43
2:D:512:TYR:HB2	2:D:1498:ARG:NH2	2.24	0.43
2:D:894:LEU:HB2	2:D:895:PRO:HD3	1.99	0.43
2:D:1154:LEU:HD22	2:D:1168:LEU:HD13	2.00	0.43
1:E:68:TRP:N	1:E:69:PRO:HD2	2.33	0.43
1:E:196:LEU:HB2	1:E:261:ILE:HD11	2.01	0.43
2:F:530:MET:CE	2:F:1095:LYS:CG	2.96	0.43
2:F:1347:ILE:HG22	2:F:1350:LEU:HB2	2.01	0.43
1:G:49:ILE:HG21	1:G:55:PHE:CZ	2.54	0.43
2:H:894:LEU:HB2	2:H:895:PRO:HD3	1.99	0.43
4:H:2001:GBM:H20	4:H:2001:GBM:H22	1.75	0.43
1:A:313:GLN:HE22	1:A:338:LYS:HD2	1.83	0.43
2:B:40:LEU:O	2:B:44:PHE:HD2	2.01	0.43
2:D:1355:ASP:OD1	2:D:1356:SER:N	2.50	0.43
2:D:1375:ILE:HD12	2:D:1548:LEU:HB2	2.00	0.43
4:D:2001:GBM:H20	4:D:2001:GBM:H22	1.75	0.43
2:F:1355:ASP:OD1	2:F:1356:SER:N	2.50	0.43
2:H:44:PHE:HD1	2:H:48:PHE:CE2	2.37	0.43
1:A:56:LEU:HB2	2:B:132:PHE:HZ	1.84	0.43
2:B:216:ARG:HD2	2:B:251:GLY:N	2.32	0.43
2:B:396:TYR:CE2	2:B:1224:GLN:HG3	2.54	0.43
2:B:511:LEU:HD13	2:B:511:LEU:HA	1.85	0.43
2:B:511:LEU:HD23	2:B:1426:LEU:HD21	2.01	0.43
2:B:810:PRO:O	2:B:814:ILE:HG13	2.17	0.43
1:C:268:TYR:O	1:C:346:ALA:HB3	2.18	0.43
2:D:1124:ARG:O	2:D:1128:ASP:HB2	2.19	0.43
1:G:187:ALA:O	1:G:309:ILE:HG13	2.19	0.43
2:H:1039:ASP:OD1	2:H:1039:ASP:N	2.50	0.43
1:A:297:THR:O	1:A:297:THR:OG1	2.37	0.43
2:B:686:PHE:CE2	2:B:730:MET:HB3	2.54	0.43
2:B:1124:ARG:O	2:B:1128:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:MET:HG3	2:D:48:PHE:HE2	1.83	0.43
2:D:1475:ILE:HD12	2:D:1482:PHE:HE2	1.84	0.43
1:G:56:LEU:HB2	2:H:132:PHE:HZ	1.84	0.43
1:G:95:PHE:CD1	1:G:100:LEU:HD23	2.45	0.43
2:H:528:LYS:HB3	2:H:528:LYS:HE3	1.84	0.43
2:H:1124:ARG:O	2:H:1128:ASP:HB2	2.19	0.43
2:H:1246:ARG:HH21	4:H:2001:GBM:H18	1.82	0.43
2:H:1347:ILE:HG22	2:H:1350:LEU:HB2	2.01	0.43
2:B:78:THR:HG21	2:B:121:VAL:HG23	2.01	0.42
2:B:1200:LEU:HD13	2:B:1230:TYR:HB3	2.01	0.42
1:E:49:ILE:HG21	1:E:55:PHE:CZ	2.54	0.42
2:F:40:LEU:O	2:F:44:PHE:HD2	2.01	0.42
1:G:68:TRP:N	1:G:69:PRO:HD2	2.33	0.42
1:A:187:ALA:O	1:A:309:ILE:HG13	2.19	0.42
1:C:237:ASP:HB3	1:E:243:GLY:HA3	2.02	0.42
2:D:218:LEU:H	2:D:218:LEU:HG	1.70	0.42
2:D:530:MET:CE	2:D:1095:LYS:CG	2.96	0.42
1:E:44:VAL:HG13	1:G:326:TYR:O	2.19	0.42
1:E:187:ALA:O	1:E:309:ILE:HG13	2.19	0.42
1:E:261:ILE:H	1:E:261:ILE:HG13	1.54	0.42
2:F:150:LYS:HB3	2:F:176:VAL:HG22	2.01	0.42
2:F:306:ARG:NH2	4:F:2001:GBM:CL1	2.72	0.42
2:F:396:TYR:CE2	2:F:1224:GLN:HG3	2.54	0.42
2:F:1240:PHE:HD1	2:F:1240:PHE:HA	1.67	0.42
2:H:78:THR:HG21	2:H:121:VAL:HG23	2.01	0.42
2:H:1475:ILE:HD12	2:H:1482:PHE:HE2	1.84	0.42
1:A:77:MET:HG3	2:B:48:PHE:CE2	2.55	0.42
1:A:136:ARG:H	1:A:136:ARG:HG2	1.71	0.42
1:A:196:LEU:HB2	1:A:261:ILE:HD11	2.01	0.42
2:B:514:TRP:HA	2:B:517:ILE:HD13	2.01	0.42
1:C:49:ILE:HG21	1:C:55:PHE:CZ	2.54	0.42
2:D:78:THR:HG21	2:D:121:VAL:HG23	2.01	0.42
2:D:150:LYS:HB3	2:D:176:VAL:HG22	2.01	0.42
2:D:1200:LEU:HD13	2:D:1230:TYR:HB3	2.01	0.42
2:D:1393:PHE:O	2:D:1394:ARG:HG3	2.18	0.42
2:F:402:LEU:O	2:F:1215:ARG:NH1	2.50	0.42
2:H:511:LEU:HD23	2:H:1426:LEU:HD21	2.01	0.42
1:A:50:ARG:HD3	3:A:402:AGS:N7	2.35	0.42
2:B:1452:TRP:CE3	2:B:1461:LYS:HE3	2.55	0.42
2:D:1108:ALA:HB3	2:D:1113:PHE:CE2	2.55	0.42
2:D:1365:VAL:HG22	2:D:1557:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ARG:HD3	3:E:401:AGS:N7	2.35	0.42
2:H:1154:LEU:HD22	2:H:1168:LEU:HD13	2.00	0.42
1:A:237:ASP:HB3	1:C:243:GLY:HA3	2.02	0.42
2:B:44:PHE:HD1	2:B:48:PHE:CE2	2.37	0.42
2:B:1437:ARG:HG3	2:B:1471:LEU:O	2.20	0.42
2:F:1108:ALA:HB3	2:F:1113:PHE:CE2	2.55	0.42
2:F:1365:VAL:HG22	2:F:1557:ILE:HG13	2.01	0.42
2:H:402:LEU:O	2:H:1215:ARG:NH1	2.50	0.42
2:H:708:LEU:HB3	2:H:897:ALA:HA	2.02	0.42
2:B:175:LEU:HA	2:B:175:LEU:HD23	1.81	0.42
1:C:77:MET:HG3	2:D:48:PHE:CE2	2.55	0.42
2:F:1375:ILE:HD12	2:F:1548:LEU:HB2	2.00	0.42
1:G:196:LEU:HB2	1:G:261:ILE:HD11	2.01	0.42
2:H:719:LYS:HB3	2:H:887:VAL:HG11	2.01	0.42
2:H:1108:ALA:HB3	2:H:1113:PHE:CE2	2.55	0.42
1:A:181:LEU:HD23	1:A:287:LEU:HD21	2.02	0.42
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.20	0.42
2:B:719:LYS:HB3	2:B:887:VAL:HG11	2.01	0.42
2:B:1347:ILE:HG22	2:B:1350:LEU:HB2	2.01	0.42
1:C:187:ALA:O	1:C:309:ILE:HG13	2.19	0.42
2:D:514:TRP:HA	2:D:517:ILE:HD13	2.01	0.42
2:D:686:PHE:CE2	2:D:730:MET:HB3	2.54	0.42
1:E:77:MET:HG3	2:F:48:PHE:CE2	2.55	0.42
2:F:44:PHE:HD1	2:F:48:PHE:CE2	2.37	0.42
2:F:78:THR:HG21	2:F:121:VAL:HG23	2.01	0.42
2:F:1200:LEU:HD13	2:F:1230:TYR:HB3	2.01	0.42
1:G:77:MET:HG3	2:H:48:PHE:CE2	2.55	0.42
1:G:181:LEU:HD23	1:G:287:LEU:HD21	2.02	0.42
1:A:44:VAL:HG13	1:C:326:TYR:O	2.19	0.42
1:A:49:ILE:HG21	1:A:55:PHE:CZ	2.54	0.42
1:A:176:ARG:O	1:A:179:GLU:N	2.51	0.42
3:A:401:AGS:N7	1:G:50:ARG:HD3	2.35	0.42
2:B:1201:LEU:HD23	2:B:1201:LEU:HA	1.84	0.42
2:D:1031:ASP:OD2	2:D:1287:TYR:OH	2.25	0.42
2:F:708:LEU:HB3	2:F:897:ALA:HA	2.02	0.42
2:F:1124:ARG:O	2:F:1128:ASP:HB2	2.19	0.42
2:H:686:PHE:CE2	2:H:730:MET:HB3	2.54	0.42
2:H:1132:ILE:HA	2:H:1136:ILE:HD13	2.02	0.42
2:H:1200:LEU:HD13	2:H:1230:TYR:HB3	2.01	0.42
2:H:1316:HIS:HA	2:H:1319:LEU:HD12	2.02	0.42
1:A:243:GLY:HA3	1:G:237:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD12	1:A:329:ASP:O	2.20	0.42
2:B:188:ASN:O	2:B:192:VAL:HG23	2.20	0.42
2:B:1127:SER:O	2:B:1130:ASN:N	2.53	0.42
1:C:220:VAL:HG12	1:C:235:GLN:HG2	2.02	0.42
1:C:297:THR:O	1:C:297:THR:OG1	2.37	0.42
1:C:318:ILE:HD12	1:C:329:ASP:O	2.20	0.42
2:D:44:PHE:HD1	2:D:48:PHE:CE2	2.37	0.42
2:D:1039:ASP:OD1	2:D:1039:ASP:N	2.50	0.42
2:D:1347:ILE:HG22	2:D:1350:LEU:HB2	2.01	0.42
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.20	0.42
2:F:852:PHE:CD1	2:F:885:VAL:HB	2.55	0.42
2:H:150:LYS:HB3	2:H:176:VAL:HG22	2.01	0.42
1:C:50:ARG:HD3	3:C:401:AGS:N7	2.35	0.42
1:C:56:LEU:HB2	2:D:132:PHE:HZ	1.84	0.42
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.20	0.42
2:F:1132:ILE:HA	2:F:1136:ILE:HD13	2.02	0.42
2:F:1316:HIS:HA	2:F:1319:LEU:HD12	2.02	0.42
2:F:1475:ILE:HD12	2:F:1482:PHE:HE2	1.84	0.42
2:H:396:TYR:CE2	2:H:1224:GLN:HG3	2.54	0.42
2:H:514:TRP:HA	2:H:517:ILE:HD13	2.01	0.42
2:H:1437:ARG:HG3	2:H:1471:LEU:O	2.20	0.42
2:H:1441:ASP:OD2	2:H:1445:LYS:N	2.53	0.42
2:D:1441:ASP:OD2	2:D:1445:LYS:N	2.53	0.41
1:E:181:LEU:HD23	1:E:287:LEU:HD21	2.02	0.41
1:E:338:LYS:HB3	1:E:338:LYS:HE3	1.76	0.41
2:F:511:LEU:HD23	2:F:1426:LEU:HD21	2.01	0.41
2:H:817:HIS:O	2:H:821:THR:OG1	2.38	0.41
2:H:1240:PHE:HD1	2:H:1240:PHE:HA	1.67	0.41
2:B:817:HIS:O	2:B:821:THR:OG1	2.38	0.41
2:B:1365:VAL:HG22	2:B:1557:ILE:HG13	2.01	0.41
1:C:44:VAL:HG13	1:E:326:TYR:O	2.19	0.41
1:E:318:ILE:HD12	1:E:329:ASP:O	2.20	0.41
2:F:40:LEU:HD11	2:F:115:MET:HB2	2.03	0.41
2:F:526:ARG:NH1	2:F:1098:HIS:ND1	2.68	0.41
2:H:710:MET:HG2	2:H:897:ALA:HB2	2.02	0.41
2:H:1404:ILE:HG21	2:H:1407:GLY:HA2	2.03	0.41
2:H:1452:TRP:CE3	2:H:1461:LYS:HE3	2.55	0.41
1:A:36:VAL:HG23	1:A:303:SER:OG	2.21	0.41
1:A:75:PHE:HB3	1:A:163:MET:SD	2.61	0.41
2:B:710:MET:HG2	2:B:897:ALA:HB2	2.02	0.41
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1475:ILE:HD12	2:B:1482:PHE:HE2	1.84	0.41
2:D:188:ASN:O	2:D:192:VAL:HG23	2.20	0.41
2:D:511:LEU:HD23	2:D:1426:LEU:HD21	2.01	0.41
2:D:1060:ASP:N	2:D:1060:ASP:OD1	2.53	0.41
2:D:1127:SER:O	2:D:1130:ASN:N	2.53	0.41
2:D:1132:ILE:HA	2:D:1136:ILE:HD13	2.02	0.41
2:D:1437:ARG:HG3	2:D:1471:LEU:O	2.20	0.41
1:E:56:LEU:HB2	2:F:132:PHE:HZ	1.84	0.41
1:E:195:ARG:HH11	1:E:195:ARG:HG3	1.85	0.41
2:F:1441:ASP:OD2	2:F:1445:LYS:N	2.53	0.41
1:G:195:ARG:HG3	1:G:195:ARG:HH11	1.85	0.41
1:G:318:ILE:HD12	1:G:329:ASP:O	2.20	0.41
2:H:175:LEU:HA	2:H:175:LEU:HD23	1.81	0.41
2:H:1239:LEU:O	2:H:1242:THR:HG22	2.21	0.41
2:B:877:LEU:HB3	2:B:884:VAL:HG21	2.02	0.41
2:B:1108:ALA:HB3	2:B:1113:PHE:CE2	2.55	0.41
1:C:75:PHE:HB3	1:C:163:MET:SD	2.61	0.41
2:F:216:ARG:HB2	2:F:251:GLY:N	2.36	0.41
2:F:812:ILE:HD13	2:F:812:ILE:HA	1.84	0.41
2:F:1239:LEU:O	2:F:1242:THR:HG22	2.21	0.41
2:F:1452:TRP:CE3	2:F:1461:LYS:HE3	2.55	0.41
1:G:36:VAL:HG23	1:G:303:SER:OG	2.21	0.41
1:G:215:ILE:HD13	1:G:215:ILE:HA	1.83	0.41
2:H:852:PHE:CD1	2:H:885:VAL:HB	2.55	0.41
2:H:1127:SER:O	2:H:1130:ASN:N	2.53	0.41
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.85	0.41
1:A:220:VAL:HG12	1:A:235:GLN:HG2	2.02	0.41
2:B:150:LYS:HB3	2:B:176:VAL:HG22	2.01	0.41
2:B:1355:ASP:OD1	2:B:1356:SER:N	2.50	0.41
2:B:1441:ASP:OD2	2:B:1445:LYS:N	2.53	0.41
2:D:216:ARG:HB2	2:D:251:GLY:N	2.36	0.41
2:D:719:LYS:HB3	2:D:887:VAL:HG11	2.01	0.41
1:E:75:PHE:HB3	1:E:163:MET:SD	2.61	0.41
1:E:237:ASP:HB3	1:G:243:GLY:HA3	2.02	0.41
1:G:136:ARG:H	1:G:136:ARG:HG2	1.71	0.41
2:H:188:ASN:O	2:H:192:VAL:HG23	2.20	0.41
2:D:526:ARG:NH1	2:D:1098:HIS:ND1	2.68	0.41
2:D:710:MET:HG2	2:D:897:ALA:HB2	2.02	0.41
2:D:852:PHE:CD1	2:D:885:VAL:HB	2.55	0.41
2:D:1452:TRP:CE3	2:D:1461:LYS:HE3	2.55	0.41
2:F:710:MET:HG2	2:F:897:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:877:LEU:HB3	2:F:884:VAL:HG21	2.02	0.41
2:F:1437:ARG:HG3	2:F:1471:LEU:O	2.20	0.41
2:H:40:LEU:HD11	2:H:115:MET:HB2	2.03	0.41
2:H:216:ARG:HB2	2:H:251:GLY:N	2.36	0.41
2:H:1060:ASP:OD1	2:H:1060:ASP:N	2.53	0.41
2:H:1425:ILE:HD13	2:H:1492:LEU:HD12	2.02	0.41
1:A:286:ILE:HG23	1:A:301:ARG:HG2	2.03	0.41
2:B:708:LEU:HB3	2:B:897:ALA:HA	2.02	0.41
2:B:903:MET:SD	2:B:908:ILE:HG12	2.60	0.41
1:C:136:ARG:H	1:C:136:ARG:HG2	1.71	0.41
1:C:181:LEU:HD23	1:C:287:LEU:HD21	2.02	0.41
2:D:1394:ARG:HG2	2:D:1410:ILE:HG21	2.03	0.41
2:D:1425:ILE:HD13	2:D:1492:LEU:HD12	2.02	0.41
1:E:220:VAL:HG12	1:E:235:GLN:HG2	2.02	0.41
2:F:253:LEU:HD12	2:F:253:LEU:HA	1.86	0.41
1:G:50:ARG:HE	1:G:50:ARG:HB3	1.64	0.41
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.20	0.41
2:B:812:ILE:HD13	2:B:812:ILE:HA	1.84	0.41
2:B:1062:SER:O	2:B:1066:MET:HG2	2.21	0.41
2:B:1132:ILE:HA	2:B:1136:ILE:HD13	2.02	0.41
2:B:1404:ILE:HG21	2:B:1407:GLY:HA2	2.03	0.41
1:C:86:PHE:HA	1:C:89:VAL:HG12	2.03	0.41
1:C:195:ARG:HH11	1:C:195:ARG:HG3	1.85	0.41
1:C:262:ASP:OD1	1:C:265:SER:OG	2.32	0.41
1:C:286:ILE:HG23	1:C:301:ARG:HG2	2.03	0.41
2:D:530:MET:HE3	2:D:1095:LYS:CG	2.50	0.41
1:E:36:VAL:HG23	1:E:303:SER:OG	2.21	0.41
2:F:188:ASN:O	2:F:192:VAL:HG23	2.20	0.41
2:F:719:LYS:HB3	2:F:887:VAL:HG11	2.01	0.41
1:G:75:PHE:HB3	1:G:163:MET:SD	2.61	0.41
1:G:299:GLN:HE21	1:G:301:ARG:HD3	1.86	0.41
2:H:526:ARG:NH1	2:H:1098:HIS:ND1	2.68	0.41
2:H:1152:SER:O	2:H:1156:VAL:HG23	2.21	0.41
2:B:40:LEU:HD11	2:B:115:MET:HB2	2.03	0.41
2:B:72:ASN:OD1	2:B:72:ASN:N	2.54	0.41
2:B:216:ARG:HB2	2:B:251:GLY:N	2.36	0.41
2:B:253:LEU:HD12	2:B:253:LEU:HA	1.86	0.41
2:B:309:ALA:O	2:B:369:GLN:HG3	2.21	0.41
2:B:1239:LEU:O	2:B:1242:THR:HG22	2.21	0.41
2:D:306:ARG:NH2	4:D:2001:GBM:CL1	2.72	0.41
2:D:708:LEU:HB3	2:D:897:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:795:ASN:O	2:D:799:TYR:HB3	2.21	0.41
1:E:86:PHE:HA	1:E:89:VAL:HG12	2.03	0.41
1:E:299:GLN:HE21	1:E:301:ARG:HD3	1.86	0.41
2:F:795:ASN:HB3	2:F:798:ARG:HB3	2.03	0.41
2:F:795:ASN:O	2:F:799:TYR:HB3	2.21	0.41
2:F:1060:ASP:N	2:F:1060:ASP:OD1	2.53	0.41
2:F:1127:SER:O	2:F:1130:ASN:N	2.53	0.41
2:F:1152:SER:O	2:F:1156:VAL:HG23	2.21	0.41
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.71	0.41
2:F:1404:ILE:HG21	2:F:1407:GLY:HA2	2.03	0.41
2:H:471:ALA:HB3	2:H:472:PRO:HD3	2.03	0.41
2:H:576:ALA:O	2:H:579:SER:OG	2.33	0.41
2:H:903:MET:SD	2:H:908:ILE:HG12	2.60	0.41
2:H:1062:SER:O	2:H:1066:MET:HG2	2.21	0.41
2:B:795:ASN:O	2:B:799:TYR:HB3	2.21	0.41
2:B:852:PHE:CD1	2:B:885:VAL:HB	2.55	0.41
2:D:72:ASN:OD1	2:D:72:ASN:N	2.54	0.41
2:D:881:LYS:HA	2:D:881:LYS:HD3	1.89	0.41
2:D:903:MET:SD	2:D:908:ILE:HG12	2.60	0.41
2:D:1239:LEU:O	2:D:1242:THR:HG22	2.21	0.41
1:E:61:THR:HA	1:E:64:VAL:HG22	2.02	0.41
2:F:514:TRP:HA	2:F:517:ILE:HD13	2.01	0.41
2:F:1394:ARG:HG2	2:F:1410:ILE:HG21	2.03	0.41
2:H:795:ASN:O	2:H:799:TYR:HB3	2.21	0.41
2:H:1063:VAL:O	2:H:1067:VAL:HG23	2.21	0.41
2:B:512:TYR:HD2	2:B:1498:ARG:NH2	2.14	0.40
2:B:1060:ASP:OD1	2:B:1060:ASP:N	2.53	0.40
1:C:61:THR:HA	1:C:64:VAL:HG22	2.02	0.40
2:F:478:ALA:O	2:F:481:LEU:HB3	2.21	0.40
2:F:1062:SER:O	2:F:1066:MET:HG2	2.21	0.40
2:H:681:ILE:HB	2:H:701:ILE:HG23	2.03	0.40
2:H:1365:VAL:HG22	2:H:1557:ILE:HG13	2.01	0.40
2:H:1405:ILE:HD13	2:H:1422:LEU:HD21	2.03	0.40
1:A:61:THR:HA	1:A:64:VAL:HG22	2.02	0.40
1:C:215:ILE:HA	1:C:215:ILE:HD13	1.83	0.40
2:D:40:LEU:HD11	2:D:115:MET:HB2	2.03	0.40
2:D:471:ALA:HB3	2:D:472:PRO:HD3	2.03	0.40
2:F:817:HIS:O	2:F:821:THR:OG1	2.38	0.40
2:F:903:MET:SD	2:F:908:ILE:HG12	2.60	0.40
2:F:1106:ILE:HD13	2:F:1106:ILE:HA	1.78	0.40
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LYS:O	1:G:173:GLN:HG2	2.22	0.40
2:H:699:ILE:HG12	2:H:908:ILE:HG13	2.03	0.40
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.86	0.40
1:A:86:PHE:HA	1:A:89:VAL:HG12	2.03	0.40
2:B:526:ARG:NH1	2:B:1098:HIS:ND1	2.68	0.40
2:B:681:ILE:HB	2:B:701:ILE:HG23	2.03	0.40
2:B:1363:LYS:HE3	2:B:1364:HIS:CE1	2.57	0.40
2:B:1405:ILE:HD13	2:B:1422:LEU:HD21	2.03	0.40
2:D:175:LEU:HD23	2:D:175:LEU:HA	1.81	0.40
2:D:196:ILE:O	2:D:197:PHE:C	2.60	0.40
2:D:817:HIS:O	2:D:821:THR:OG1	2.38	0.40
2:D:1106:ILE:HA	2:D:1106:ILE:HD13	1.78	0.40
2:D:1363:LYS:HE3	2:D:1364:HIS:CE1	2.57	0.40
2:D:1404:ILE:HG21	2:D:1407:GLY:HA2	2.03	0.40
1:E:286:ILE:HG23	1:E:301:ARG:HG2	2.03	0.40
2:F:471:ALA:HB3	2:F:472:PRO:HD3	2.03	0.40
2:F:1255:ILE:HD13	2:F:1255:ILE:HA	1.91	0.40
2:F:1363:LYS:HE3	2:F:1364:HIS:CE1	2.57	0.40
2:H:196:ILE:O	2:H:197:PHE:C	2.60	0.40
2:B:370:ARG:HG3	2:B:1253:GLU:CD	2.42	0.40
2:B:1063:VAL:O	2:B:1067:VAL:HG23	2.21	0.40
2:B:1152:SER:O	2:B:1156:VAL:HG23	2.21	0.40
2:B:1316:HIS:HA	2:B:1319:LEU:HD12	2.02	0.40
2:B:1404:ILE:CG2	2:B:1408:ILE:N	2.84	0.40
2:D:576:ALA:O	2:D:579:SER:OG	2.33	0.40
2:D:1152:SER:O	2:D:1156:VAL:HG23	2.21	0.40
2:D:1316:HIS:HA	2:D:1319:LEU:HD12	2.02	0.40
1:E:170:LYS:O	1:E:173:GLN:HG2	2.22	0.40
2:F:1063:VAL:O	2:F:1067:VAL:HG23	2.21	0.40
1:G:86:PHE:HA	1:G:89:VAL:HG12	2.03	0.40
1:G:114:ILE:HD11	1:G:120:ALA:HA	2.04	0.40
1:G:286:ILE:HG23	1:G:301:ARG:HG2	2.03	0.40
2:H:795:ASN:HB3	2:H:798:ARG:HB3	2.03	0.40
2:B:104:LEU:O	2:B:108:MET:HG2	2.22	0.40
2:B:402:LEU:O	2:B:1215:ARG:NH1	2.50	0.40
2:B:829:ASN:OD1	2:B:829:ASN:N	2.36	0.40
1:C:36:VAL:HG23	1:C:303:SER:OG	2.21	0.40
1:C:164:LEU:O	1:C:167:ILE:HG13	2.22	0.40
2:D:104:LEU:O	2:D:108:MET:HG2	2.22	0.40
2:D:309:ALA:O	2:D:369:GLN:HG3	2.21	0.40
2:D:478:ALA:O	2:D:481:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ARG:O	1:E:179:GLU:N	2.51	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%)	304 (94%)	18 (6%)	1 (0%)	41	76
1	C	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	41	76
1	E	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	41	76
1	G	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	41	76
2	B	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	29	68
2	D	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	29	68
2	F	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	29	68
2	H	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	29	68
All	All	6432/7888 (82%)	6120 (95%)	284 (4%)	28 (0%)	38	72

All (28) 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
2	F	199	LYS
2	H	197	PHE
2	H	199	LYS
1	A	244	VAL

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Mol	Chain	Res	Type
2	B	214	GLY
1	C	244	VAL
2	D	214	GLY
1	E	244	VAL
2	F	214	GLY
1	G	244	VAL
2	H	214	GLY
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 [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	258/339 (76%)	226 (88%)	32 (12%)	4	22
1	C	258/339 (76%)	226 (88%)	32 (12%)	4	22
1	E	258/339 (76%)	226 (88%)	32 (12%)	4	22
1	G	258/339 (76%)	226 (88%)	32 (12%)	4	22
2	B	1102/1371 (80%)	1041 (94%)	61 (6%)	21	49
2	D	1102/1371 (80%)	1041 (94%)	61 (6%)	21	49
2	F	1102/1371 (80%)	1041 (94%)	61 (6%)	21	49
2	H	1102/1371 (80%)	1041 (94%)	61 (6%)	21	49
All	All	5440/6840 (80%)	5068 (93%)	372 (7%)	19	43

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	52	GLN
1	A	78	SER
1	A	81	CYS
1	A	82	SER
1	A	88	MET
1	A	90	TRP
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	190	THR
1	A	198	PHE
1	A	200	LEU
1	A	204	ASP
1	A	219	VAL
1	A	236	VAL
1	A	238	ILE
1	A	252	VAL
1	A	261	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
1	A	323	ASP
1	A	345	THR
2	B	37	VAL
2	B	72	ASN
2	B	119	THR
2	B	123	TYR
2	B	134	LYS
2	B	167	LEU
2	B	193	ARG
2	B	204	VAL
2	B	218	LEU
2	B	222	VAL

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Mol	Chain	Res	Type
2	B	223	ASN
2	B	327	LEU
2	B	357	VAL
2	B	374	GLN
2	B	383	THR
2	B	420	LEU
2	B	428	LEU
2	B	430	TRP
2	B	432	PHE
2	B	439	TRP
2	B	470	LEU
2	B	511	LEU
2	B	512	TYR
2	B	598	ARG
2	B	682	ILE
2	B	689	THR
2	B	696	LEU
2	B	701	ILE
2	B	708	LEU
2	B	738	PHE
2	B	770	VAL
2	B	778	TRP
2	B	794	PHE
2	B	829	ASN
2	B	891	LEU
2	B	892	GLN
2	B	1001	CYS
2	B	1129	CYS
2	B	1168	LEU
2	B	1195	THR
2	B	1204	PHE
2	B	1227	LEU
2	B	1238	SER
2	B	1240	PHE
2	B	1251	ARG
2	B	1254	TYR
2	B	1276	LEU
2	B	1296	ASN
2	B	1318	LEU
2	B	1383	SER
2	B	1394	ARG
2	B	1396	VAL

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Mol	Chain	Res	Type
2	B	1432	PHE
2	B	1488	GLN
2	B	1524	VAL
2	B	1536	ILE
2	B	1539	ARG
2	B	1550	MET
2	B	1557	ILE
2	B	1561	ASP
2	B	1566	LEU
1	C	36	VAL
1	C	52	GLN
1	C	78	SER
1	C	81	CYS
1	C	82	SER
1	C	88	MET
1	C	90	TRP
1	C	111	VAL
1	C	122	LEU
1	C	133	PHE
1	C	136	ARG
1	C	152	GLN
1	C	153	ASN
1	C	166	CYS
1	C	181	LEU
1	C	190	THR
1	C	198	PHE
1	C	200	LEU
1	C	204	ASP
1	C	219	VAL
1	C	236	VAL
1	C	238	ILE
1	C	252	VAL
1	C	261	ILE
1	C	287	LEU
1	C	290	VAL
1	C	293	THR
1	C	294	THR
1	C	297	THR
1	C	298	THR
1	C	323	ASP
1	C	345	THR
2	D	37	VAL

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Mol	Chain	Res	Type
2	D	72	ASN
2	D	119	THR
2	D	123	TYR
2	D	134	LYS
2	D	167	LEU
2	D	193	ARG
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	223	ASN
2	D	327	LEU
2	D	357	VAL
2	D	374	GLN
2	D	383	THR
2	D	420	LEU
2	D	428	LEU
2	D	430	TRP
2	D	432	PHE
2	D	439	TRP
2	D	470	LEU
2	D	511	LEU
2	D	512	TYR
2	D	598	ARG
2	D	682	ILE
2	D	689	THR
2	D	696	LEU
2	D	701	ILE
2	D	708	LEU
2	D	738	PHE
2	D	770	VAL
2	D	778	TRP
2	D	794	PHE
2	D	829	ASN
2	D	891	LEU
2	D	892	GLN
2	D	1001	CYS
2	D	1129	CYS
2	D	1168	LEU
2	D	1195	THR
2	D	1204	PHE
2	D	1227	LEU
2	D	1238	SER

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Mol	Chain	Res	Type
2	D	1240	PHE
2	D	1251	ARG
2	D	1254	TYR
2	D	1276	LEU
2	D	1296	ASN
2	D	1318	LEU
2	D	1383	SER
2	D	1394	ARG
2	D	1396	VAL
2	D	1432	PHE
2	D	1488	GLN
2	D	1524	VAL
2	D	1536	ILE
2	D	1539	ARG
2	D	1550	MET
2	D	1557	ILE
2	D	1561	ASP
2	D	1566	LEU
1	E	36	VAL
1	E	52	GLN
1	E	78	SER
1	E	81	CYS
1	E	82	SER
1	E	88	MET
1	E	90	TRP
1	E	111	VAL
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	190	THR
1	E	198	PHE
1	E	200	LEU
1	E	204	ASP
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	252	VAL
1	E	261	ILE

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Mol	Chain	Res	Type
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	123	TYR
2	F	134	LYS
2	F	167	LEU
2	F	193	ARG
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	223	ASN
2	F	327	LEU
2	F	357	VAL
2	F	374	GLN
2	F	383	THR
2	F	420	LEU
2	F	428	LEU
2	F	430	TRP
2	F	432	PHE
2	F	439	TRP
2	F	470	LEU
2	F	511	LEU
2	F	512	TYR
2	F	598	ARG
2	F	682	ILE
2	F	689	THR
2	F	696	LEU
2	F	701	ILE
2	F	708	LEU
2	F	738	PHE
2	F	770	VAL
2	F	778	TRP
2	F	794	PHE
2	F	829	ASN

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Mol	Chain	Res	Type
2	F	891	LEU
2	F	892	GLN
2	F	1001	CYS
2	F	1129	CYS
2	F	1168	LEU
2	F	1195	THR
2	F	1204	PHE
2	F	1227	LEU
2	F	1238	SER
2	F	1240	PHE
2	F	1251	ARG
2	F	1254	TYR
2	F	1276	LEU
2	F	1296	ASN
2	F	1318	LEU
2	F	1383	SER
2	F	1394	ARG
2	F	1396	VAL
2	F	1432	PHE
2	F	1488	GLN
2	F	1524	VAL
2	F	1536	ILE
2	F	1539	ARG
2	F	1550	MET
2	F	1557	ILE
2	F	1561	ASP
2	F	1566	LEU
1	G	36	VAL
1	G	52	GLN
1	G	78	SER
1	G	81	CYS
1	G	82	SER
1	G	88	MET
1	G	90	TRP
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

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Mol	Chain	Res	Type
1	G	190	THR
1	G	198	PHE
1	G	200	LEU
1	G	204	ASP
1	G	219	VAL
1	G	236	VAL
1	G	238	ILE
1	G	252	VAL
1	G	261	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	123	TYR
2	H	134	LYS
2	H	167	LEU
2	H	193	ARG
2	H	204	VAL
2	H	218	LEU
2	H	222	VAL
2	H	223	ASN
2	H	327	LEU
2	H	357	VAL
2	H	374	GLN
2	H	383	THR
2	H	420	LEU
2	H	428	LEU
2	H	430	TRP
2	H	432	PHE
2	H	439	TRP
2	H	470	LEU
2	H	511	LEU
2	H	512	TYR
2	H	598	ARG
2	H	682	ILE

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Mol	Chain	Res	Type
2	H	689	THR
2	H	696	LEU
2	H	701	ILE
2	H	708	LEU
2	H	738	PHE
2	H	770	VAL
2	H	778	TRP
2	H	794	PHE
2	H	829	ASN
2	H	891	LEU
2	H	892	GLN
2	H	1001	CYS
2	H	1129	CYS
2	H	1168	LEU
2	H	1195	THR
2	H	1204	PHE
2	H	1227	LEU
2	H	1238	SER
2	H	1240	PHE
2	H	1251	ARG
2	H	1254	TYR
2	H	1276	LEU
2	H	1296	ASN
2	H	1318	LEU
2	H	1383	SER
2	H	1394	ARG
2	H	1396	VAL
2	H	1432	PHE
2	H	1488	GLN
2	H	1524	VAL
2	H	1536	ILE
2	H	1539	ARG
2	H	1550	MET
2	H	1557	ILE
2	H	1561	ASP
2	H	1566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	48	ASN

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	152	GLN
1	A	173	GLN
1	A	259	HIS
1	A	299	GLN
2	B	485	GLN
2	B	1135	HIS
1	C	46	HIS
1	C	48	ASN
1	C	128	GLN
1	C	152	GLN
1	C	173	GLN
1	C	259	HIS
1	C	299	GLN
2	D	1135	HIS
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	152	GLN
1	E	173	GLN
1	E	259	HIS
1	E	299	GLN
2	F	1135	HIS
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN
1	G	152	GLN
1	G	173	GLN
1	G	259	HIS
1	G	299	GLN
2	H	485	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 monosaccharides 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
4	GBM	D	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	A	402	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
3	AGS	F	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
4	GBM	F	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
4	GBM	H	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	E	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
3	AGS	H	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
3	AGS	A	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
4	GBM	B	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	D	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
3	AGS	B	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
3	AGS	C	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)

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
4	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	A	402	-	-	5/17/38/38	0/3/3/3
3	AGS	F	2002	-	-	2/17/38/38	0/3/3/3
4	GBM	F	2001	-	-	8/27/35/35	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	E	401	-	-	5/17/38/38	0/3/3/3
3	AGS	H	2002	-	-	2/17/38/38	0/3/3/3
3	AGS	A	401	-	-	5/17/38/38	0/3/3/3
4	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	D	2002	-	-	2/17/38/38	0/3/3/3
3	AGS	B	2002	-	-	2/17/38/38	0/3/3/3
3	AGS	C	401	-	-	5/17/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AGS	PG-S1G	10.12	2.12	1.90
3	A	402	AGS	PG-S1G	10.12	2.12	1.90
3	C	401	AGS	PG-S1G	10.12	2.12	1.90
3	E	401	AGS	PG-S1G	10.12	2.12	1.90
4	B	2001	GBM	C18-S2	-10.08	1.60	1.76
4	D	2001	GBM	C18-S2	-10.08	1.60	1.76
4	F	2001	GBM	C18-S2	-10.08	1.60	1.76
4	H	2001	GBM	C18-S2	-10.08	1.60	1.76
3	B	2002	AGS	PG-S1G	7.96	2.08	1.90
3	D	2002	AGS	PG-S1G	7.96	2.08	1.90
3	F	2002	AGS	PG-S1G	7.96	2.08	1.90
3	H	2002	AGS	PG-S1G	7.96	2.08	1.90
4	B	2001	GBM	C27-C28	4.65	1.49	1.40
4	D	2001	GBM	C27-C28	4.65	1.49	1.40
4	F	2001	GBM	C27-C28	4.65	1.49	1.40
4	H	2001	GBM	C27-C28	4.65	1.49	1.40
3	A	401	AGS	PG-O2G	3.23	1.65	1.54
3	A	402	AGS	PG-O2G	3.23	1.65	1.54
3	C	401	AGS	PG-O2G	3.23	1.65	1.54
3	E	401	AGS	PG-O2G	3.23	1.65	1.54
4	B	2001	GBM	C31-CL1	2.56	1.80	1.74
4	D	2001	GBM	C31-CL1	2.56	1.80	1.74
4	F	2001	GBM	C31-CL1	2.56	1.80	1.74
4	H	2001	GBM	C31-CL1	2.56	1.80	1.74
3	B	2002	AGS	C5-C4	2.47	1.47	1.40
3	D	2002	AGS	C5-C4	2.47	1.47	1.40
3	F	2002	AGS	C5-C4	2.47	1.47	1.40
3	H	2002	AGS	C5-C4	2.47	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AGS	C5-C4	2.35	1.47	1.40
3	A	402	AGS	C5-C4	2.35	1.47	1.40
3	C	401	AGS	C5-C4	2.35	1.47	1.40
3	E	401	AGS	C5-C4	2.35	1.47	1.40
4	B	2001	GBM	C17-N9	-2.22	1.34	1.39
4	D	2001	GBM	C17-N9	-2.22	1.34	1.39
4	F	2001	GBM	C17-N9	-2.22	1.34	1.39
4	H	2001	GBM	C17-N9	-2.22	1.34	1.39
3	B	2002	AGS	PG-O2G	2.02	1.61	1.54
3	D	2002	AGS	PG-O2G	2.02	1.61	1.54
3	F	2002	AGS	PG-O2G	2.02	1.61	1.54
3	H	2002	AGS	PG-O2G	2.02	1.61	1.54
3	B	2002	AGS	PG-O3G	-2.00	1.48	1.54
3	D	2002	AGS	PG-O3G	-2.00	1.48	1.54
3	F	2002	AGS	PG-O3G	-2.00	1.48	1.54
3	H	2002	AGS	PG-O3G	-2.00	1.48	1.54

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	D	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	F	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	H	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	B	2001	GBM	O7-C28-C27	3.75	122.01	116.55
4	D	2001	GBM	O7-C28-C27	3.75	122.01	116.55
4	F	2001	GBM	O7-C28-C27	3.75	122.01	116.55
4	H	2001	GBM	O7-C28-C27	3.75	122.01	116.55
3	A	401	AGS	C3'-C2'-C1'	3.59	106.38	100.98
3	A	402	AGS	C3'-C2'-C1'	3.59	106.38	100.98
3	C	401	AGS	C3'-C2'-C1'	3.59	106.38	100.98
3	E	401	AGS	C3'-C2'-C1'	3.59	106.38	100.98
3	B	2002	AGS	C3'-C2'-C1'	3.42	106.12	100.98
3	D	2002	AGS	C3'-C2'-C1'	3.42	106.12	100.98
3	F	2002	AGS	C3'-C2'-C1'	3.42	106.12	100.98
3	H	2002	AGS	C3'-C2'-C1'	3.42	106.12	100.98
4	B	2001	GBM	C18-S2-N9	3.25	110.89	105.97
4	D	2001	GBM	C18-S2-N9	3.25	110.89	105.97
4	F	2001	GBM	C18-S2-N9	3.25	110.89	105.97
4	H	2001	GBM	C18-S2-N9	3.25	110.89	105.97
3	B	2002	AGS	PA-O3A-PB	-3.23	121.74	132.83
3	D	2002	AGS	PA-O3A-PB	-3.23	121.74	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2002	AGS	PA-O3A-PB	-3.23	121.74	132.83
3	H	2002	AGS	PA-O3A-PB	-3.23	121.74	132.83
3	B	2002	AGS	N3-C2-N1	-3.19	123.70	128.68
3	D	2002	AGS	N3-C2-N1	-3.19	123.70	128.68
3	F	2002	AGS	N3-C2-N1	-3.19	123.70	128.68
3	H	2002	AGS	N3-C2-N1	-3.19	123.70	128.68
3	A	401	AGS	N3-C2-N1	-2.94	124.08	128.68
3	A	402	AGS	N3-C2-N1	-2.94	124.08	128.68
3	C	401	AGS	N3-C2-N1	-2.94	124.08	128.68
3	E	401	AGS	N3-C2-N1	-2.94	124.08	128.68
4	B	2001	GBM	O7-C28-C30	-2.90	119.40	124.37
4	D	2001	GBM	O7-C28-C30	-2.90	119.40	124.37
4	F	2001	GBM	O7-C28-C30	-2.90	119.40	124.37
4	H	2001	GBM	O7-C28-C30	-2.90	119.40	124.37
3	A	401	AGS	PA-O3A-PB	-2.86	123.02	132.83
3	A	402	AGS	PA-O3A-PB	-2.86	123.02	132.83
3	C	401	AGS	PA-O3A-PB	-2.86	123.02	132.83
3	E	401	AGS	PA-O3A-PB	-2.86	123.02	132.83
3	A	401	AGS	O3G-PG-O3B	2.69	113.63	104.64
3	A	402	AGS	O3G-PG-O3B	2.69	113.63	104.64
3	C	401	AGS	O3G-PG-O3B	2.69	113.63	104.64
3	E	401	AGS	O3G-PG-O3B	2.69	113.63	104.64
3	B	2002	AGS	C4-C5-N7	-2.58	106.71	109.40
3	D	2002	AGS	C4-C5-N7	-2.58	106.71	109.40
3	F	2002	AGS	C4-C5-N7	-2.58	106.71	109.40
3	H	2002	AGS	C4-C5-N7	-2.58	106.71	109.40
4	B	2001	GBM	C25-C20-C19	-2.25	107.66	112.87
4	D	2001	GBM	C25-C20-C19	-2.25	107.66	112.87
4	F	2001	GBM	C25-C20-C19	-2.25	107.66	112.87
4	H	2001	GBM	C25-C20-C19	-2.25	107.66	112.87
3	A	401	AGS	O2B-PB-O1B	-2.23	101.20	112.24
3	A	402	AGS	O2B-PB-O1B	-2.23	101.20	112.24
3	C	401	AGS	O2B-PB-O1B	-2.23	101.20	112.24
3	E	401	AGS	O2B-PB-O1B	-2.23	101.20	112.24
3	A	401	AGS	C4-C5-N7	-2.07	107.24	109.40
3	A	402	AGS	C4-C5-N7	-2.07	107.24	109.40
3	C	401	AGS	C4-C5-N7	-2.07	107.24	109.40
3	E	401	AGS	C4-C5-N7	-2.07	107.24	109.40
4	B	2001	GBM	C28-C27-C26	-2.06	122.40	126.16
4	D	2001	GBM	C28-C27-C26	-2.06	122.40	126.16
4	F	2001	GBM	C28-C27-C26	-2.06	122.40	126.16
4	H	2001	GBM	C28-C27-C26	-2.06	122.40	126.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	GBM	C33-O7-C28	2.04	120.61	117.53
4	D	2001	GBM	C33-O7-C28	2.04	120.61	117.53
4	F	2001	GBM	C33-O7-C28	2.04	120.61	117.53
4	H	2001	GBM	C33-O7-C28	2.04	120.61	117.53
3	A	401	AGS	C2-N1-C6	2.01	122.19	118.75
3	A	402	AGS	C2-N1-C6	2.01	122.19	118.75
3	C	401	AGS	C2-N1-C6	2.01	122.19	118.75
3	E	401	AGS	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	AGS	PB-O3B-PG-O2G
3	B	2002	AGS	PB-O3B-PG-O3G
3	D	2002	AGS	PB-O3B-PG-O2G
3	D	2002	AGS	PB-O3B-PG-O3G
3	F	2002	AGS	PB-O3B-PG-O2G
3	F	2002	AGS	PB-O3B-PG-O3G
3	H	2002	AGS	PB-O3B-PG-O2G
3	H	2002	AGS	PB-O3B-PG-O3G
4	B	2001	GBM	C27-C26-N10-C25
4	D	2001	GBM	C27-C26-N10-C25
4	F	2001	GBM	C27-C26-N10-C25
4	H	2001	GBM	C27-C26-N10-C25
4	B	2001	GBM	O6-C26-N10-C25
4	D	2001	GBM	O6-C26-N10-C25
4	F	2001	GBM	O6-C26-N10-C25
4	H	2001	GBM	O6-C26-N10-C25
4	B	2001	GBM	O3-C17-N8-C11
4	D	2001	GBM	O3-C17-N8-C11
4	F	2001	GBM	O3-C17-N8-C11
4	H	2001	GBM	O3-C17-N8-C11
3	A	401	AGS	O4'-C4'-C5'-O5'
3	A	402	AGS	O4'-C4'-C5'-O5'
3	C	401	AGS	O4'-C4'-C5'-O5'
3	E	401	AGS	O4'-C4'-C5'-O5'
4	B	2001	GBM	C30-C28-O7-C33
4	D	2001	GBM	C30-C28-O7-C33
4	F	2001	GBM	C30-C28-O7-C33
4	H	2001	GBM	C30-C28-O7-C33
4	B	2001	GBM	C27-C28-O7-C33

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Mol	Chain	Res	Type	Atoms
4	D	2001	GBM	C27-C28-O7-C33
4	F	2001	GBM	C27-C28-O7-C33
4	H	2001	GBM	C27-C28-O7-C33
4	B	2001	GBM	N9-C17-N8-C11
4	D	2001	GBM	N9-C17-N8-C11
4	F	2001	GBM	N9-C17-N8-C11
4	H	2001	GBM	N9-C17-N8-C11
4	B	2001	GBM	C24-C19-C20-C25
4	D	2001	GBM	C24-C19-C20-C25
4	F	2001	GBM	C24-C19-C20-C25
4	H	2001	GBM	C24-C19-C20-C25
3	A	401	AGS	PG-O3B-PB-O2B
3	A	402	AGS	PG-O3B-PB-O2B
3	C	401	AGS	PG-O3B-PB-O2B
3	E	401	AGS	PG-O3B-PB-O2B
4	B	2001	GBM	C23-C19-C20-C25
4	D	2001	GBM	C23-C19-C20-C25
4	F	2001	GBM	C23-C19-C20-C25
4	H	2001	GBM	C23-C19-C20-C25
3	A	401	AGS	PB-O3A-PA-O1A
3	A	402	AGS	PB-O3A-PA-O1A
3	C	401	AGS	PB-O3A-PA-O1A
3	E	401	AGS	PB-O3A-PA-O1A
3	A	401	AGS	PG-O3B-PB-O1B
3	A	402	AGS	PG-O3B-PB-O1B
3	C	401	AGS	PG-O3B-PB-O1B
3	E	401	AGS	PG-O3B-PB-O1B
3	A	401	AGS	PB-O3A-PA-O2A
3	A	402	AGS	PB-O3A-PA-O2A
3	C	401	AGS	PB-O3A-PA-O2A
3	E	401	AGS	PB-O3A-PA-O2A

There are no ring outliers.

12 monomers are involved in 42 short contacts:

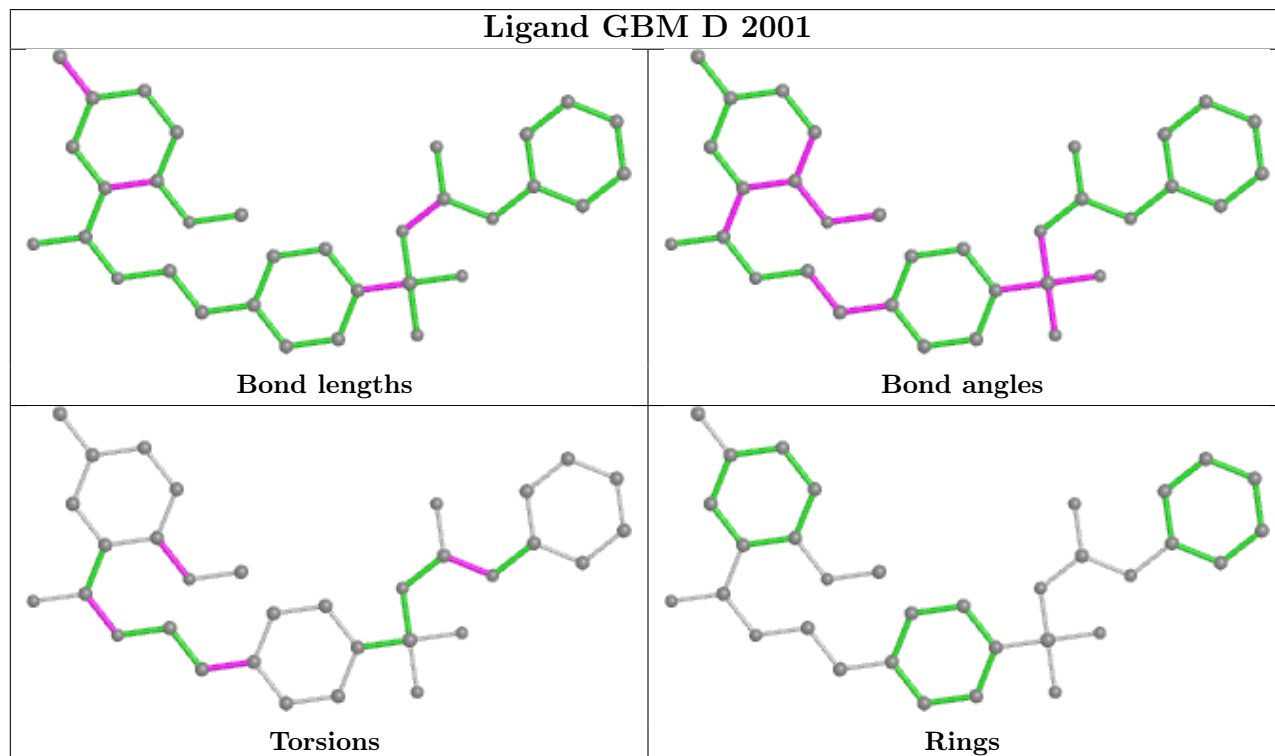
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2001	GBM	4	0
3	A	402	AGS	5	0
3	F	2002	AGS	2	0
4	F	2001	GBM	3	0
4	H	2001	GBM	3	0
3	E	401	AGS	5	0

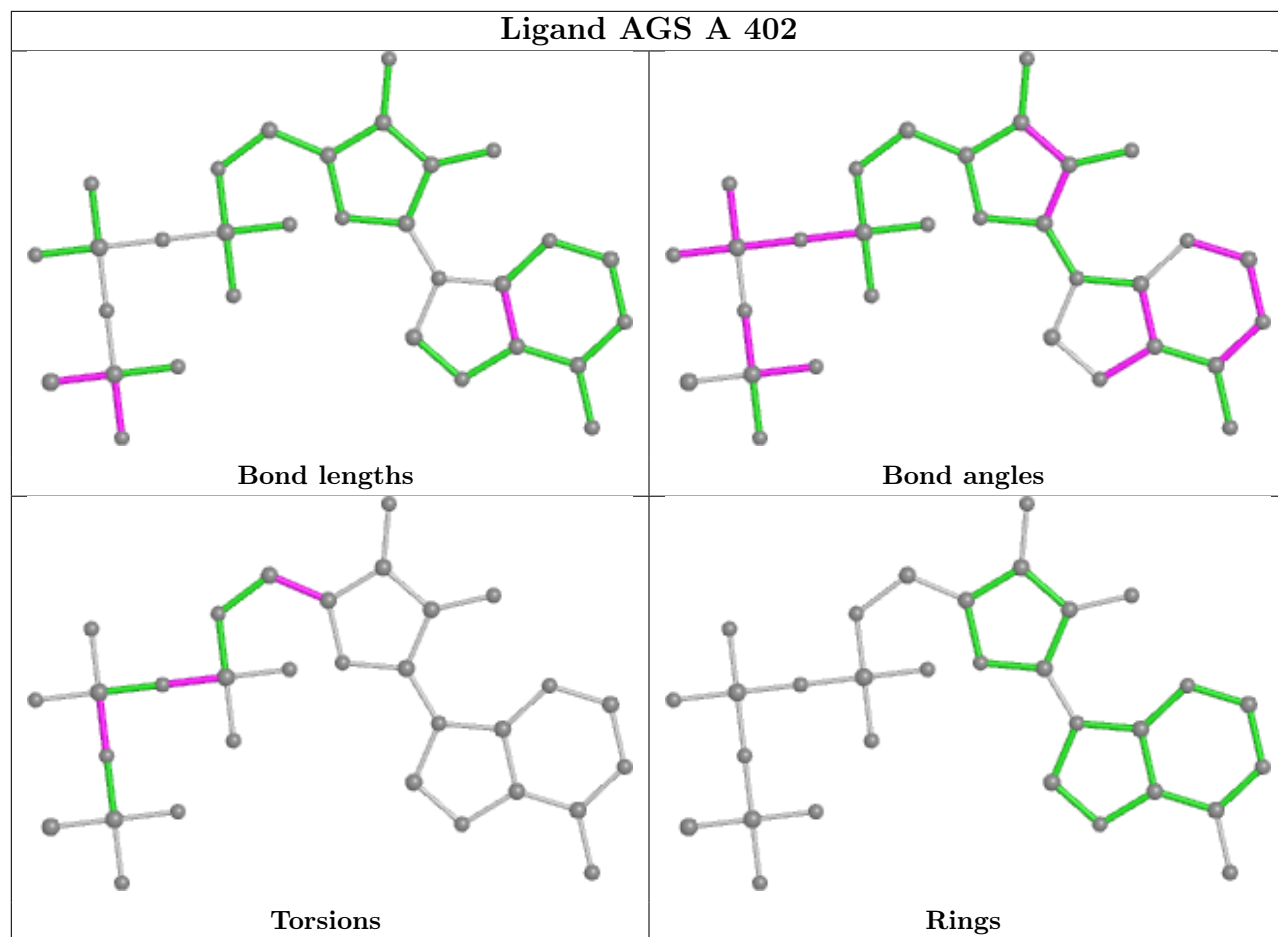
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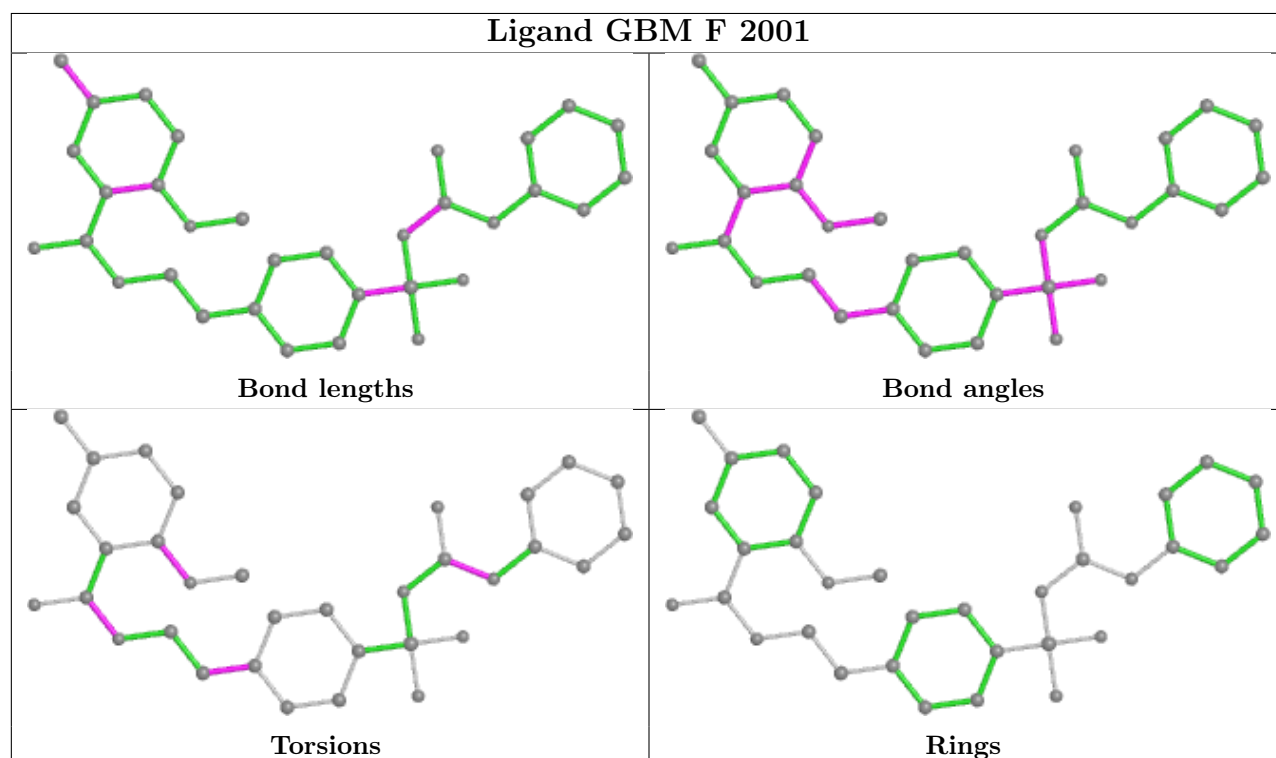
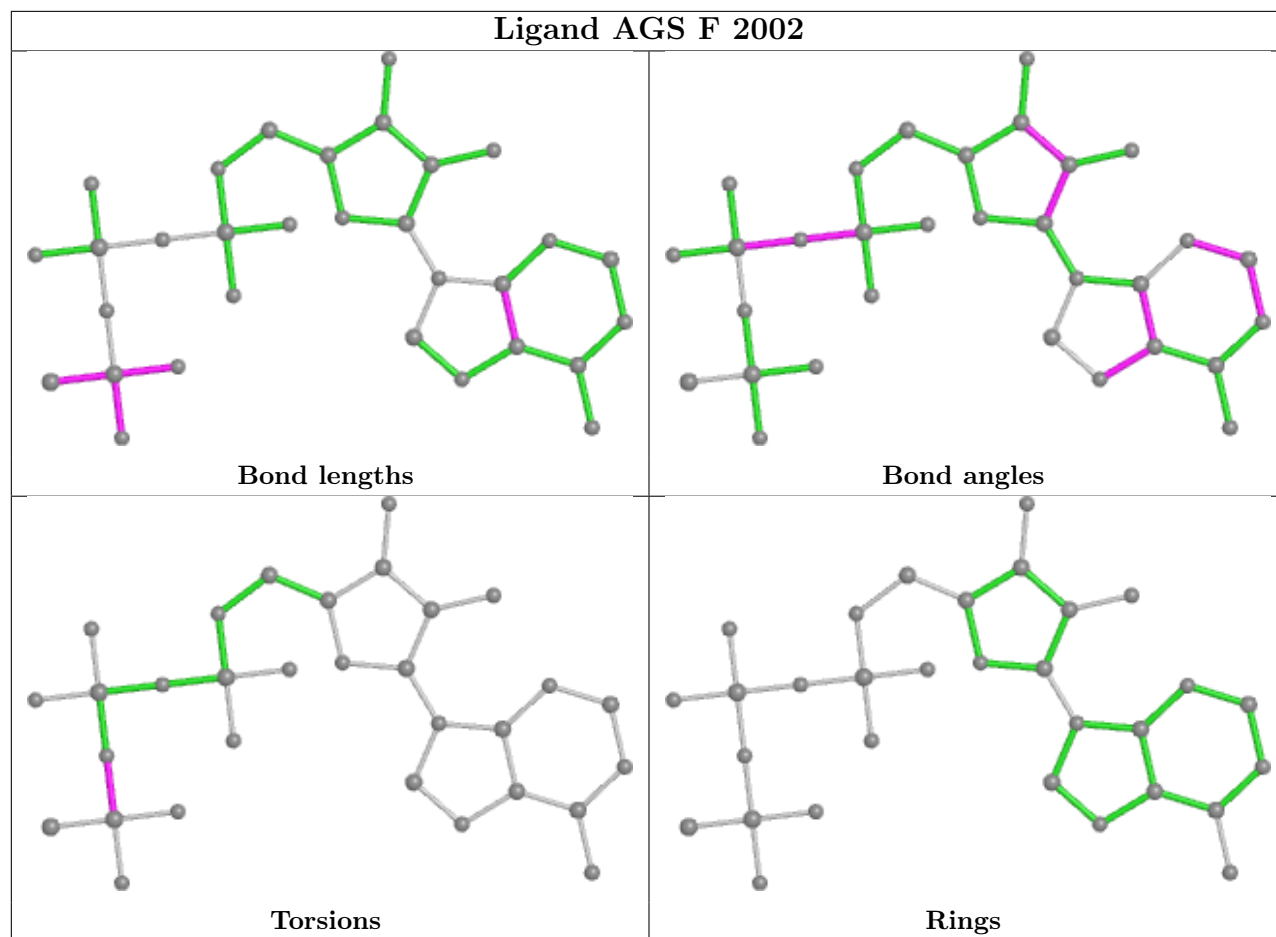
Continued from previous page...

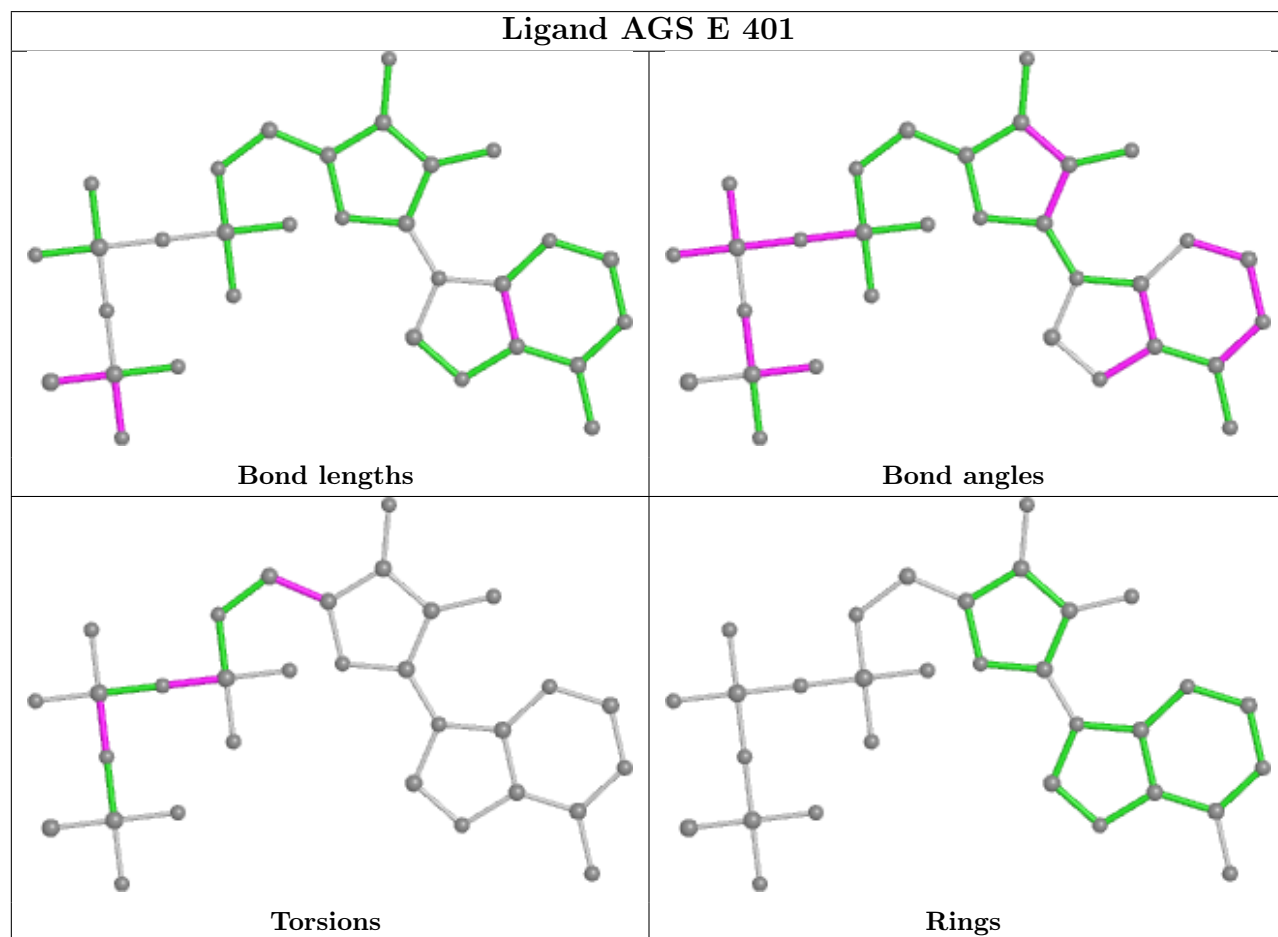
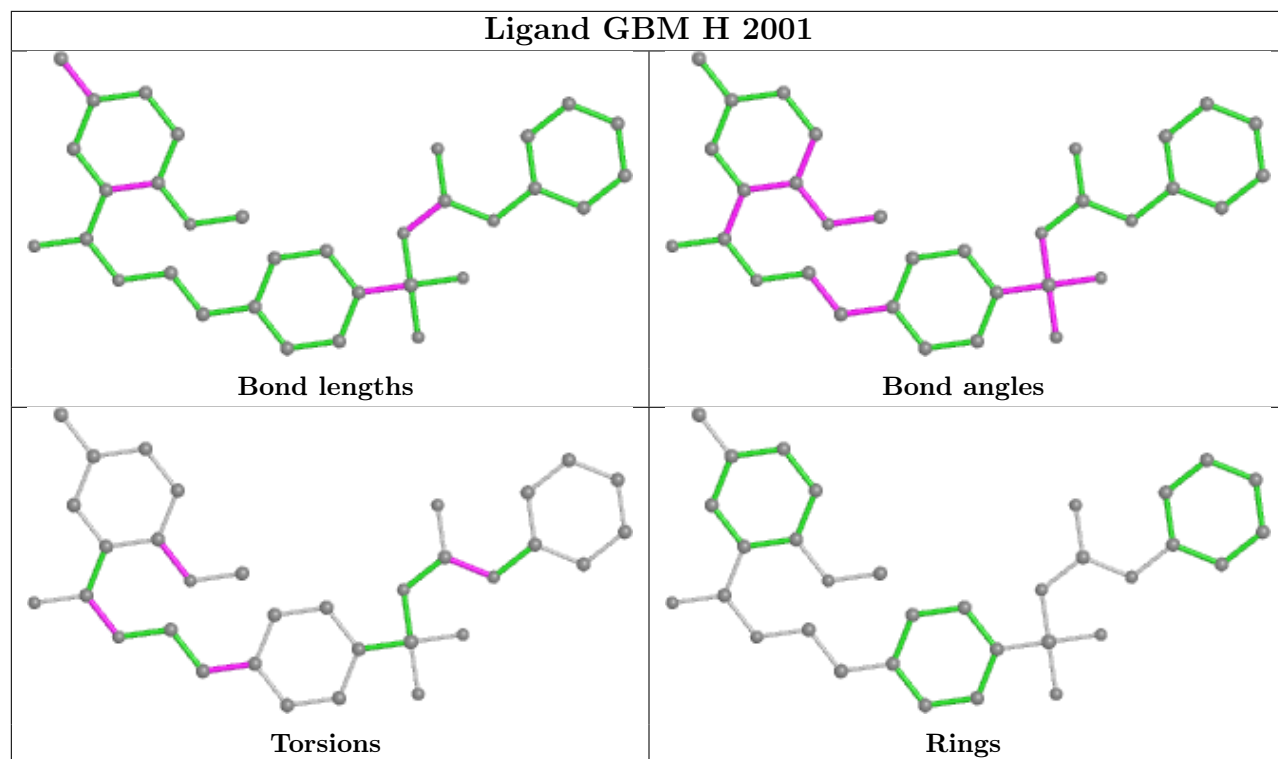
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2002	AGS	2	0
3	A	401	AGS	5	0
4	B	2001	GBM	4	0
3	D	2002	AGS	2	0
3	B	2002	AGS	2	0
3	C	401	AGS	5	0

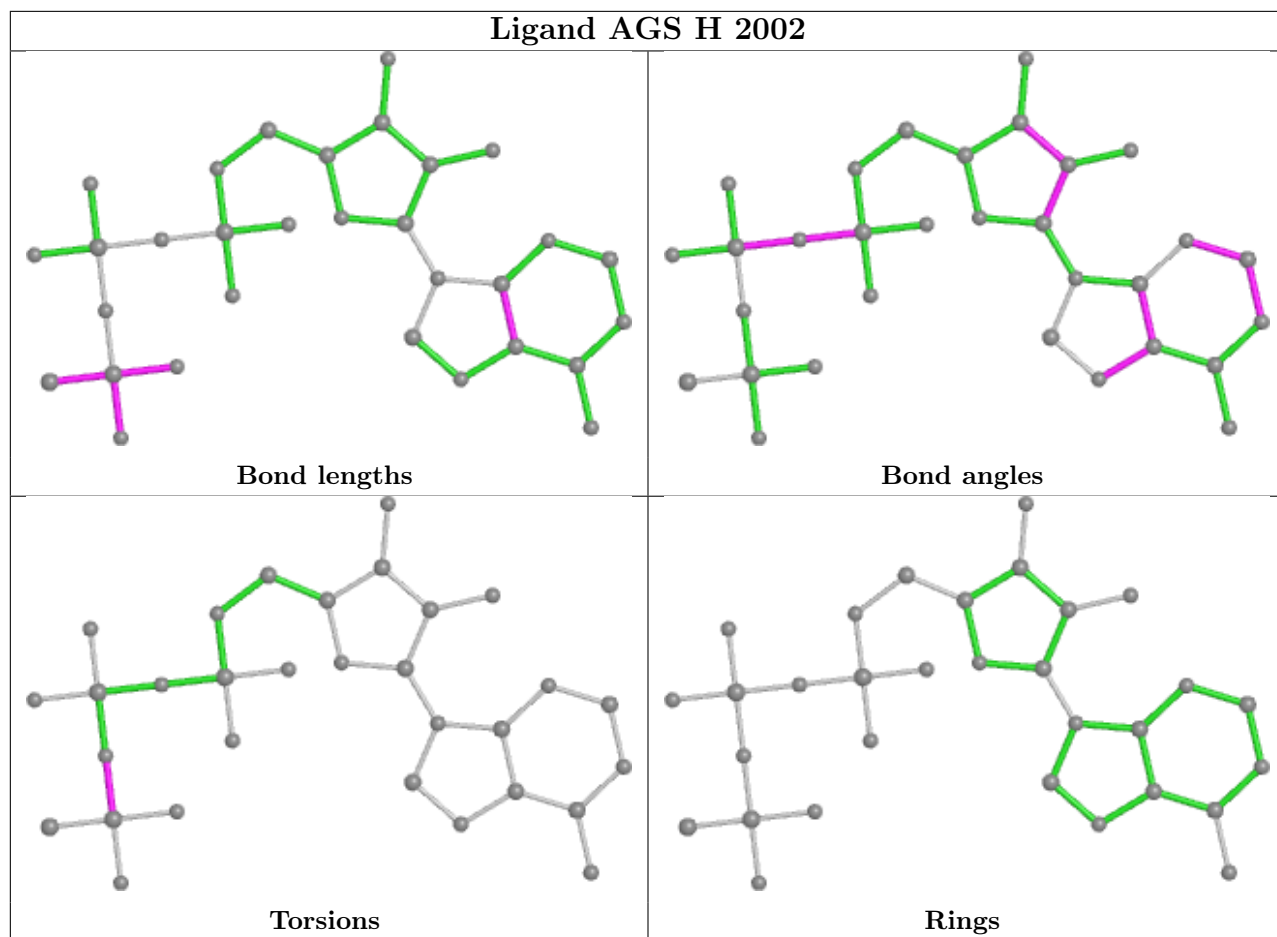
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

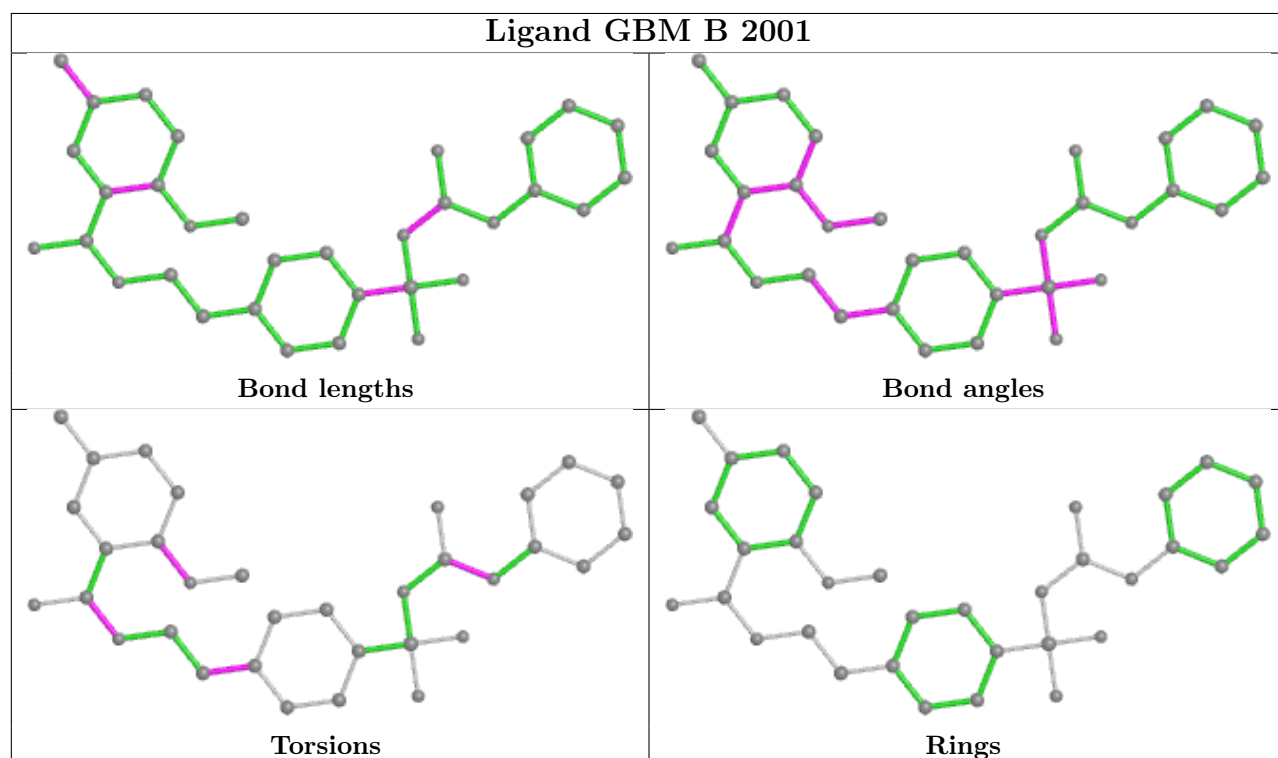
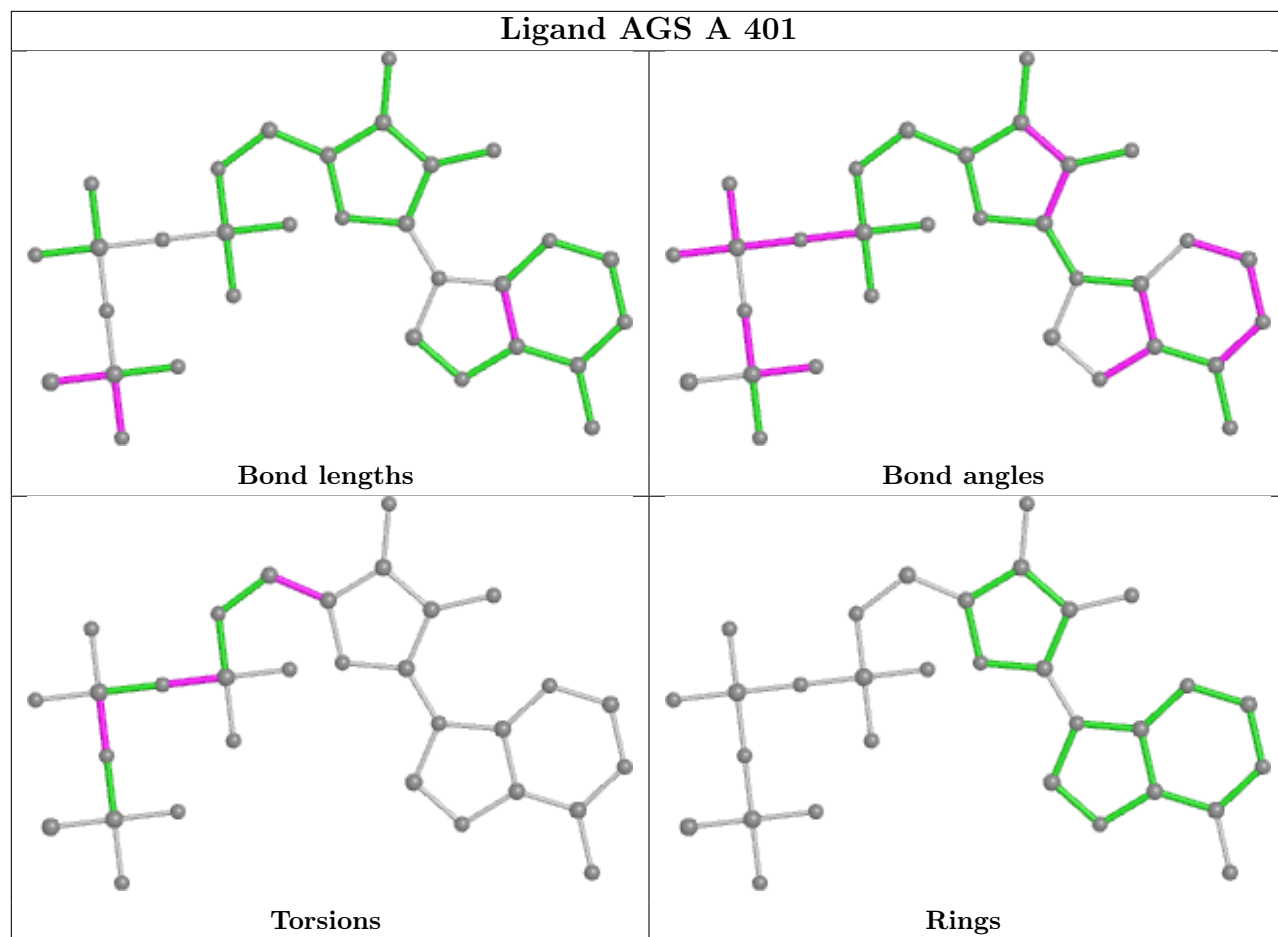


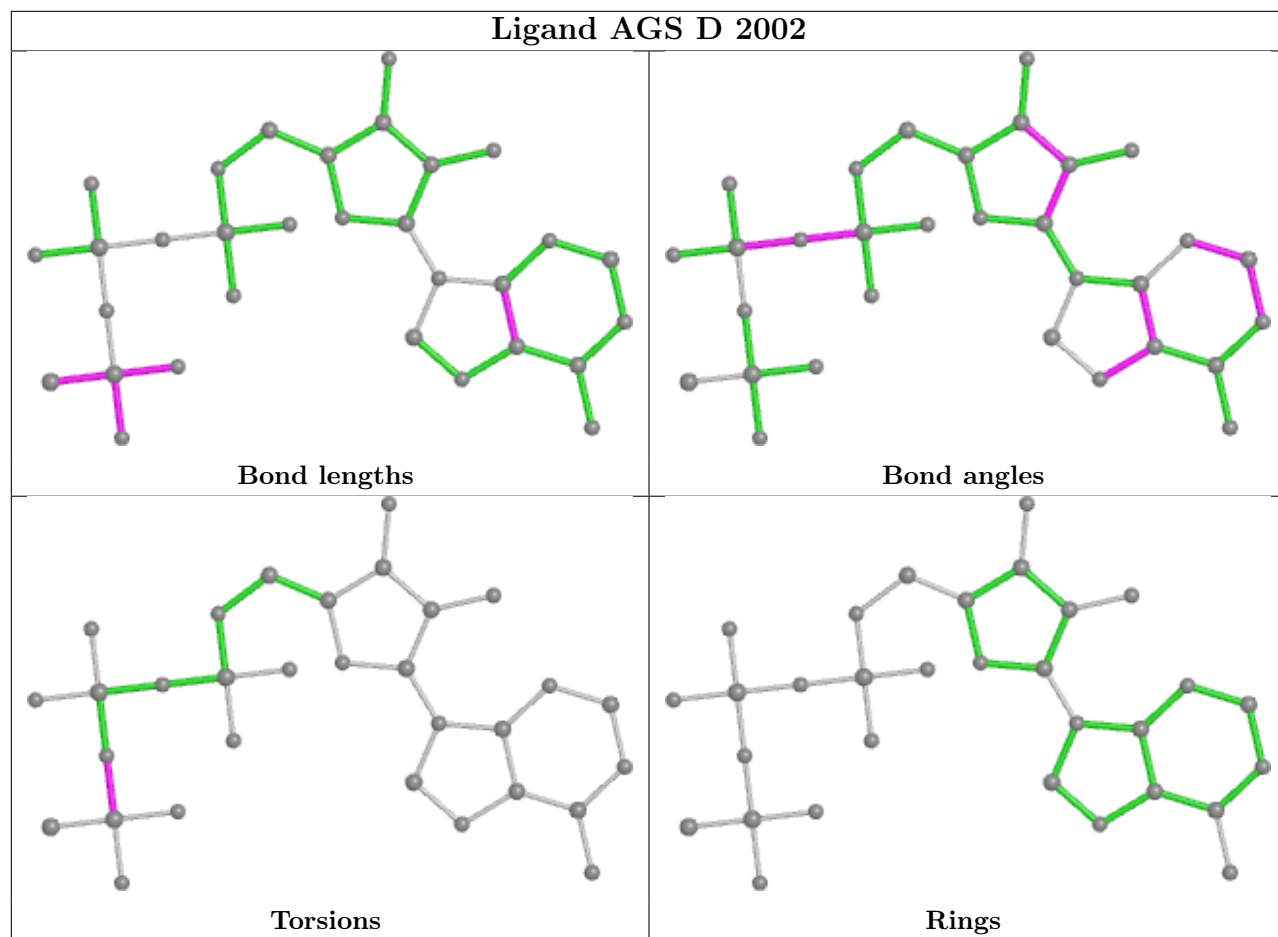


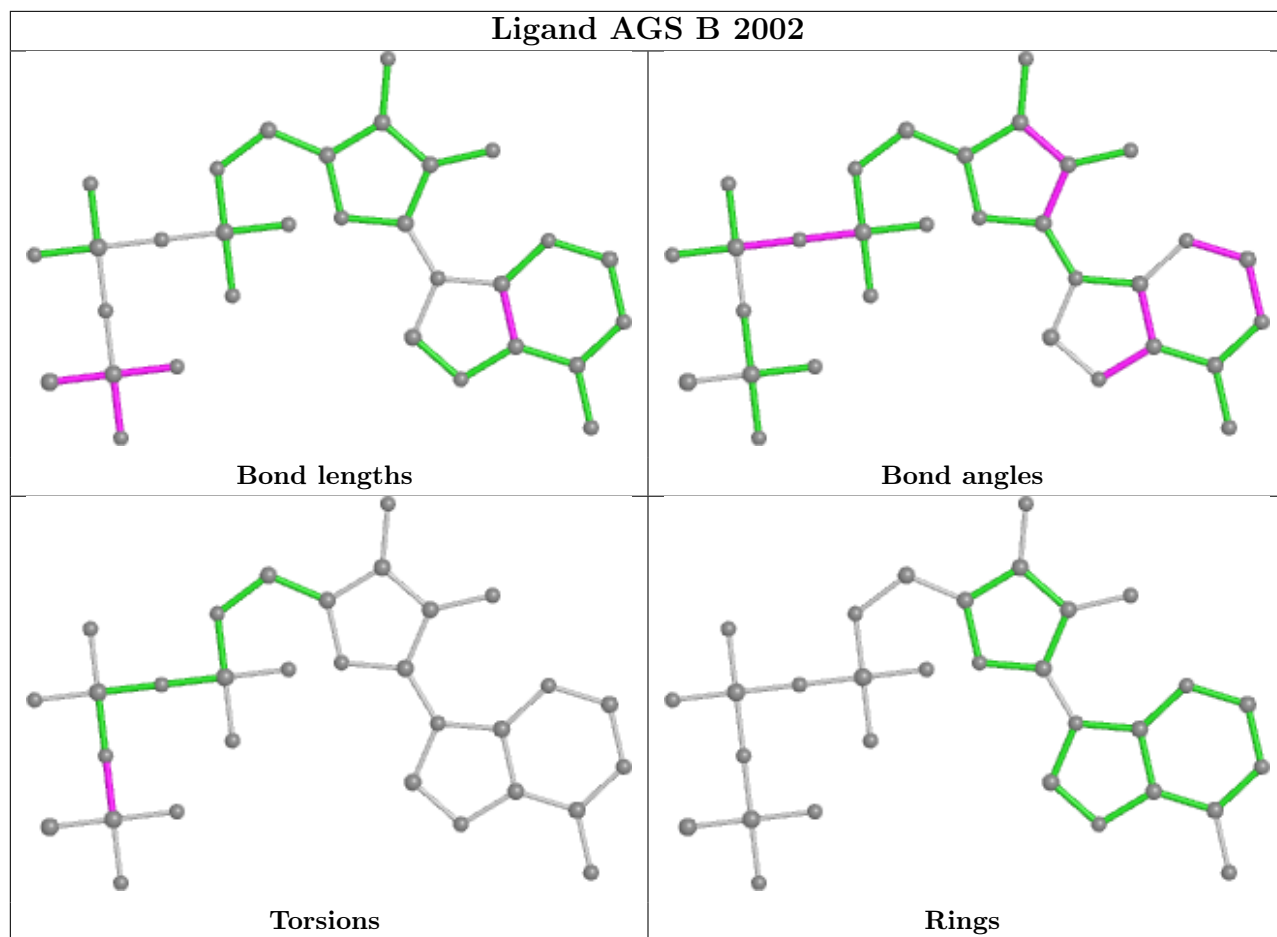


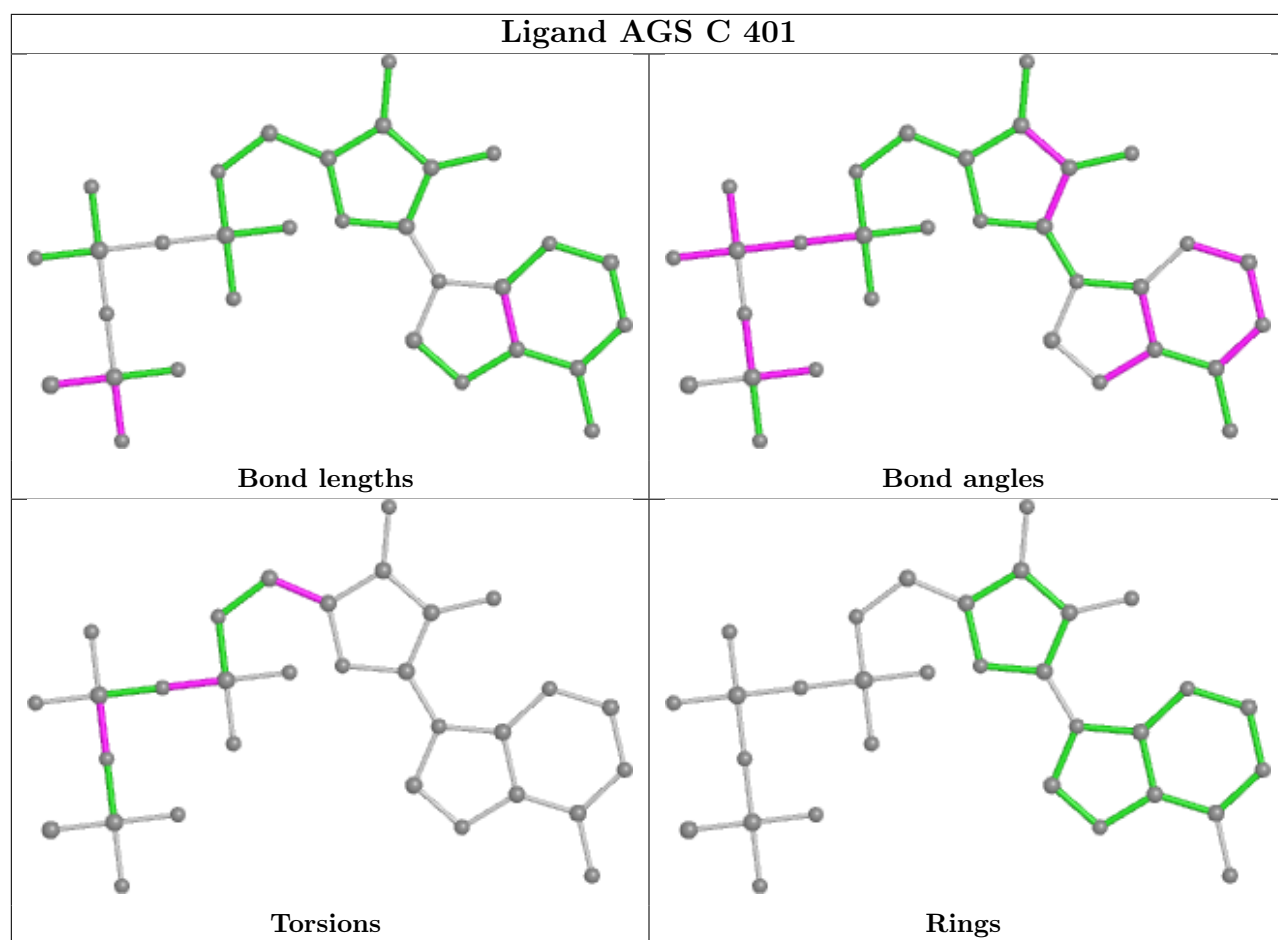












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

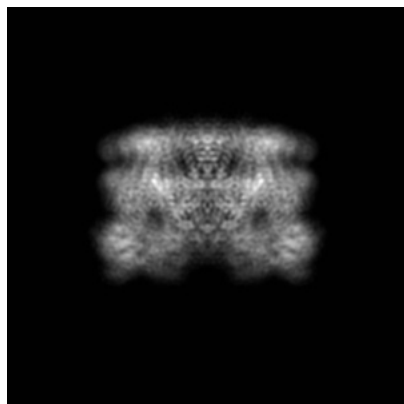
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6832. These allow visual inspection of the internal detail of the map and identification of artifacts.

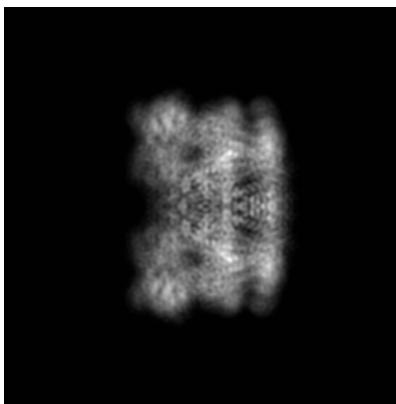
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

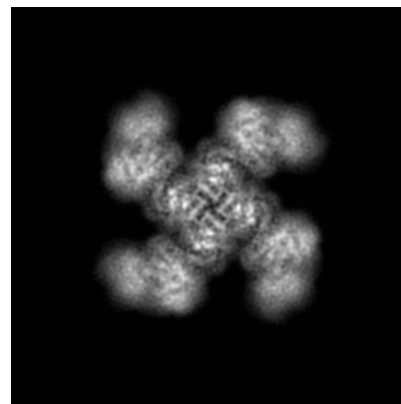
6.1.1 Primary map



X

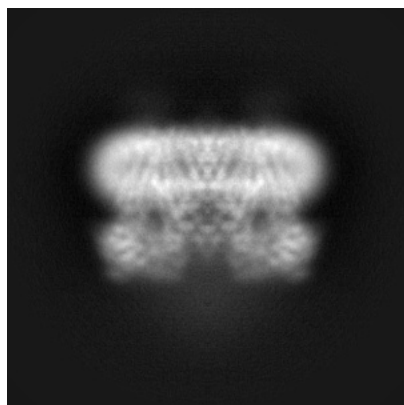


Y

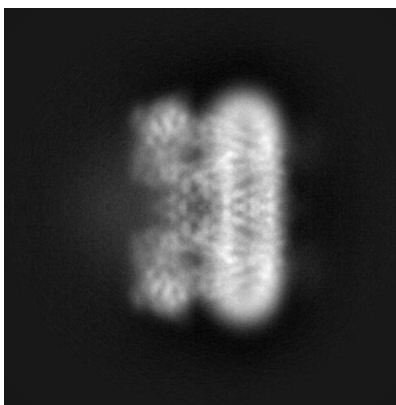


Z

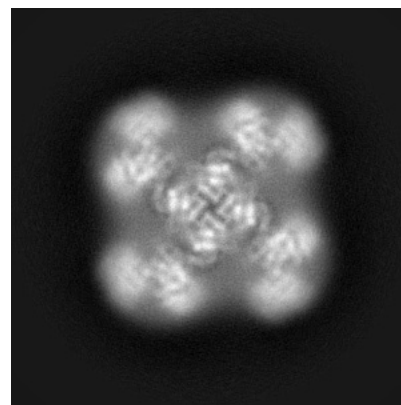
6.1.2 Raw map



X



Y

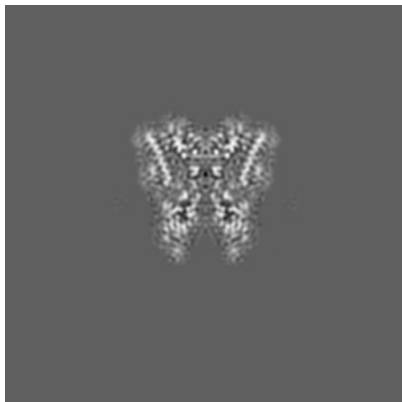


Z

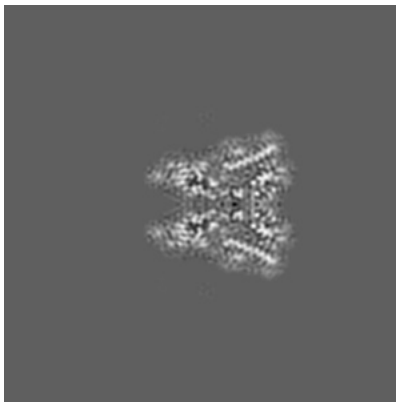
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

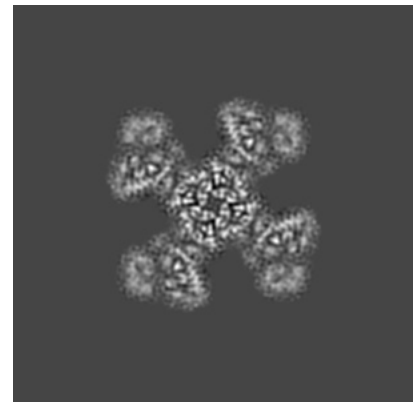
6.2.1 Primary map



X Index: 156

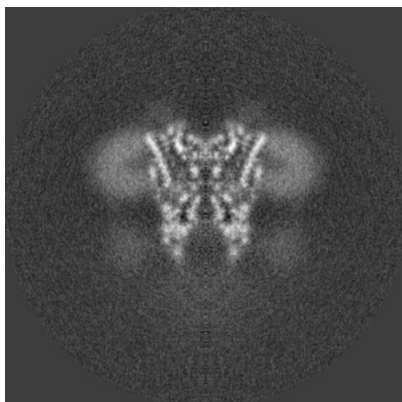


Y Index: 156

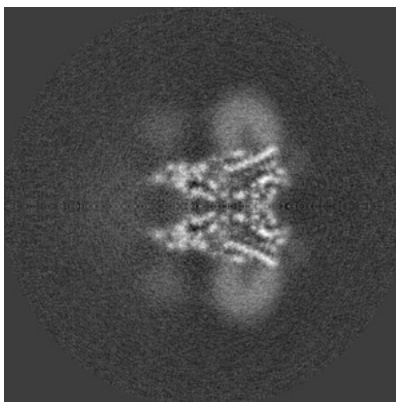


Z Index: 156

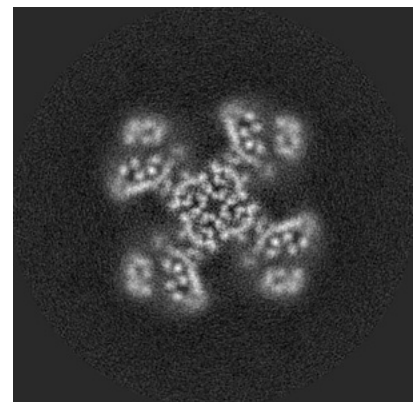
6.2.2 Raw map



X Index: 156



Y Index: 156

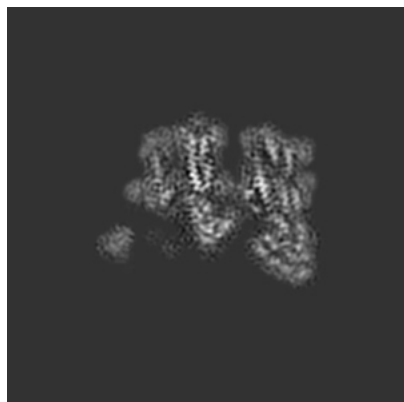


Z Index: 156

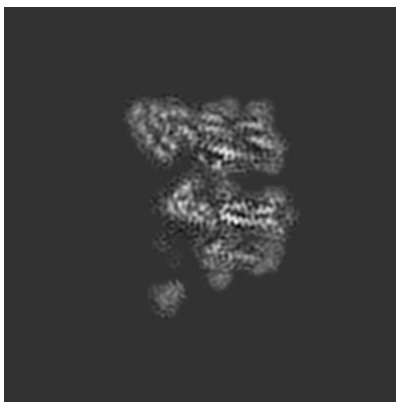
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

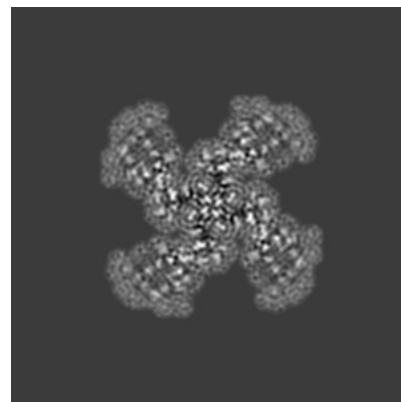
6.3.1 Primary map



X Index: 187

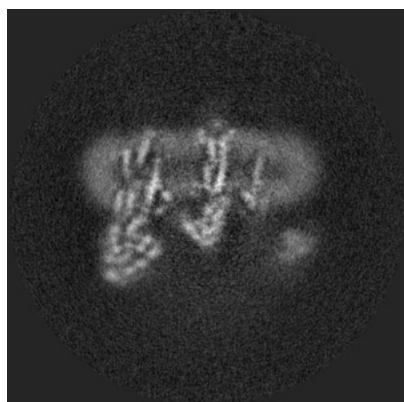


Y Index: 125

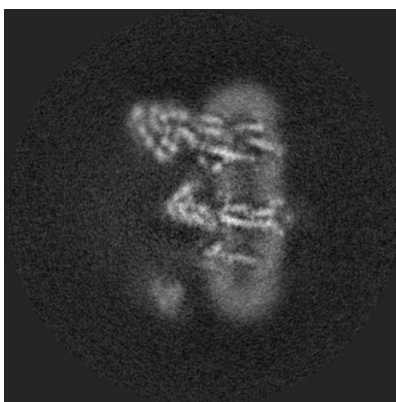


Z Index: 175

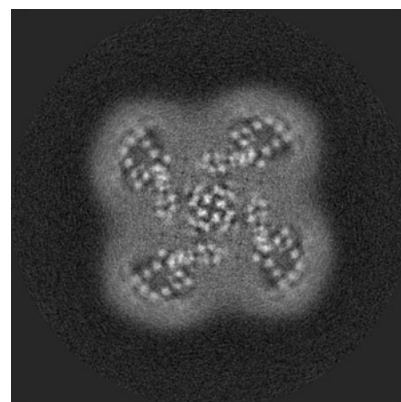
6.3.2 Raw map



X Index: 125



Y Index: 125

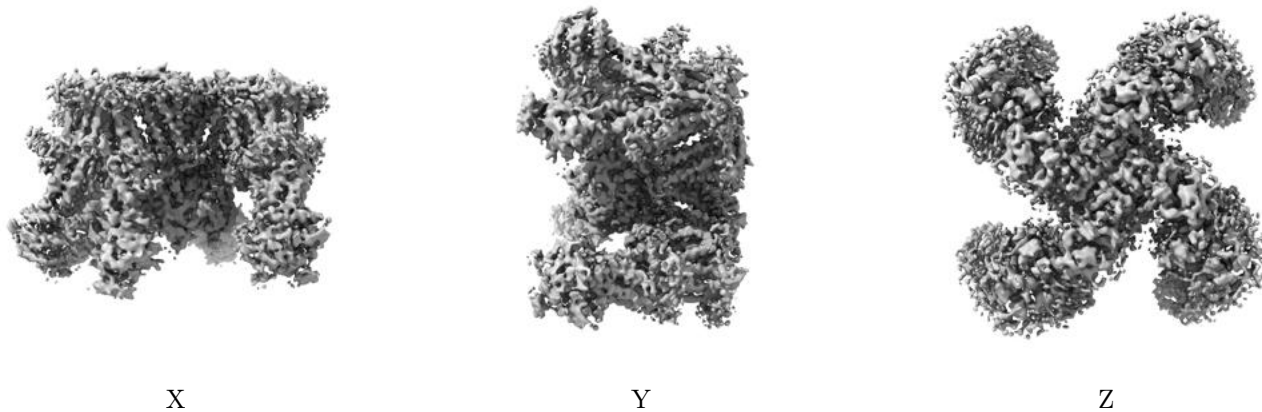


Z Index: 173

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

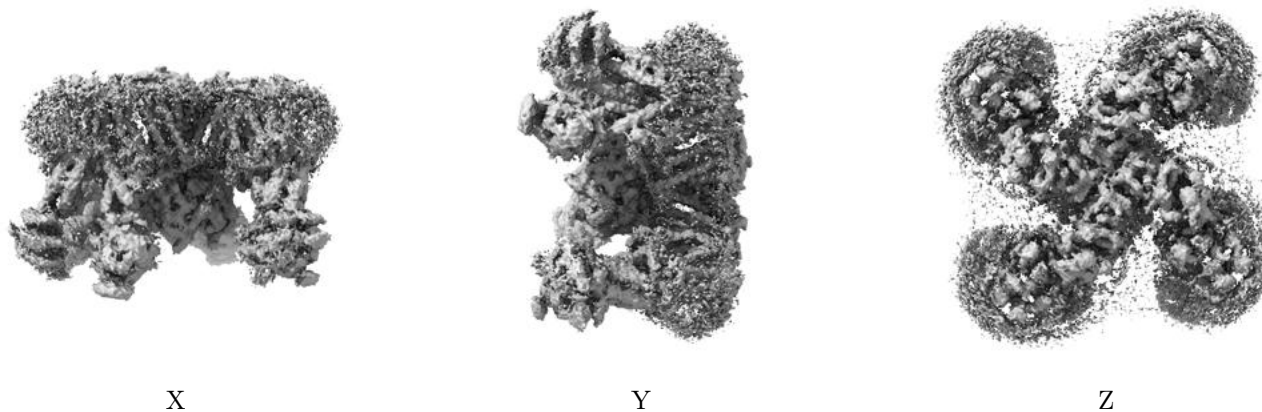
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

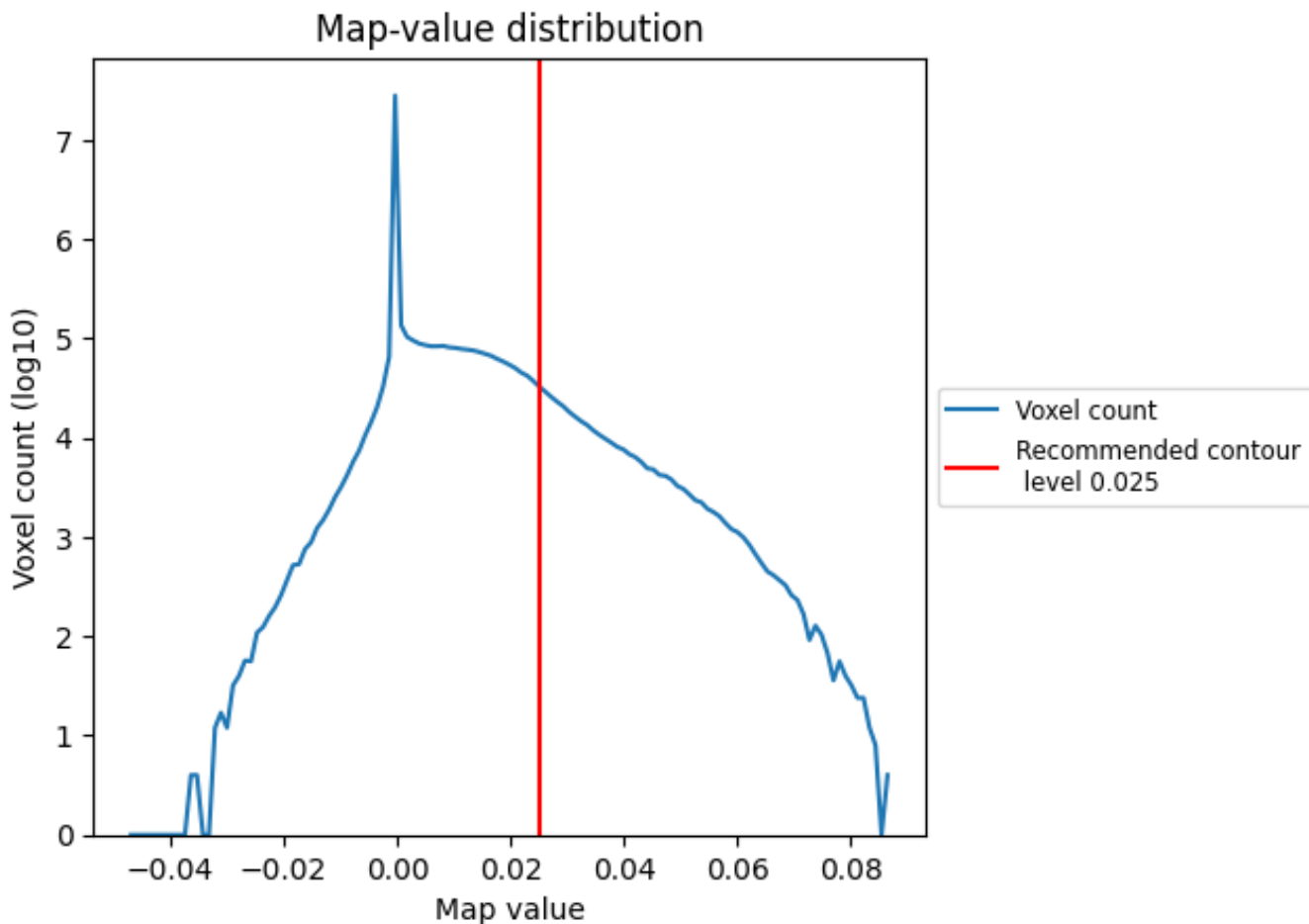
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

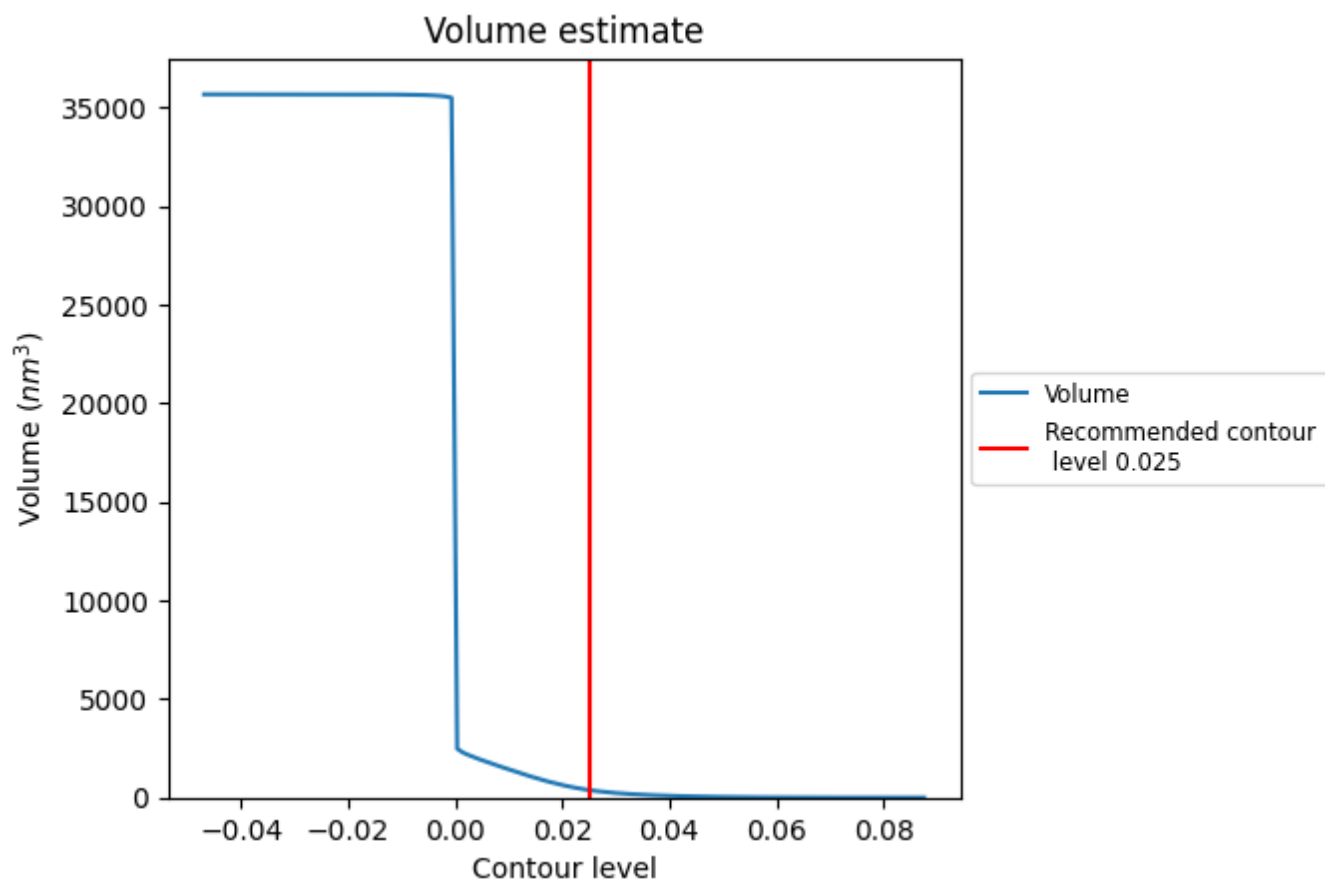
This section contains the results of statistical analysis of the map.

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.

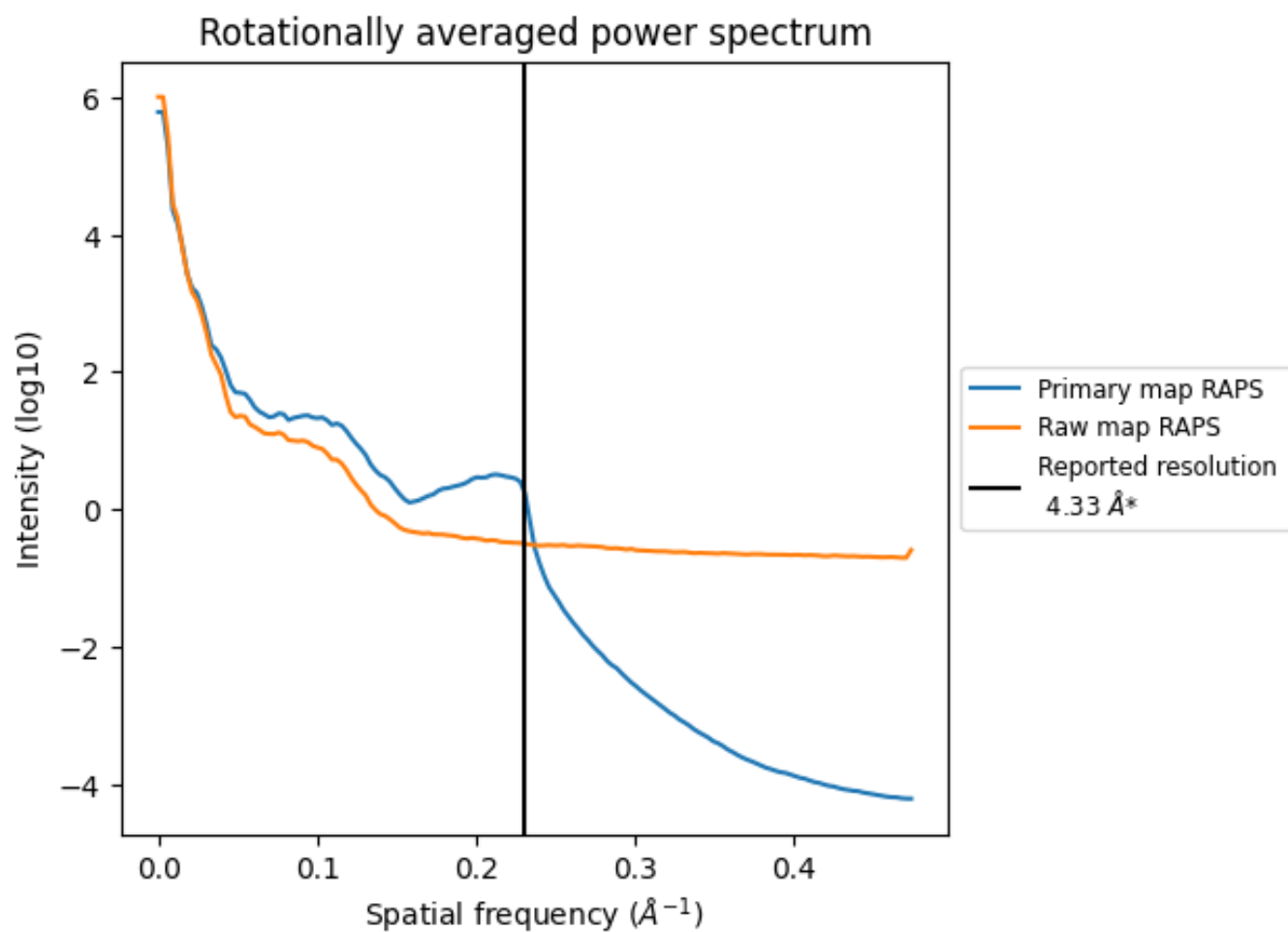
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm^3 ; this corresponds to an approximate mass of 345 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

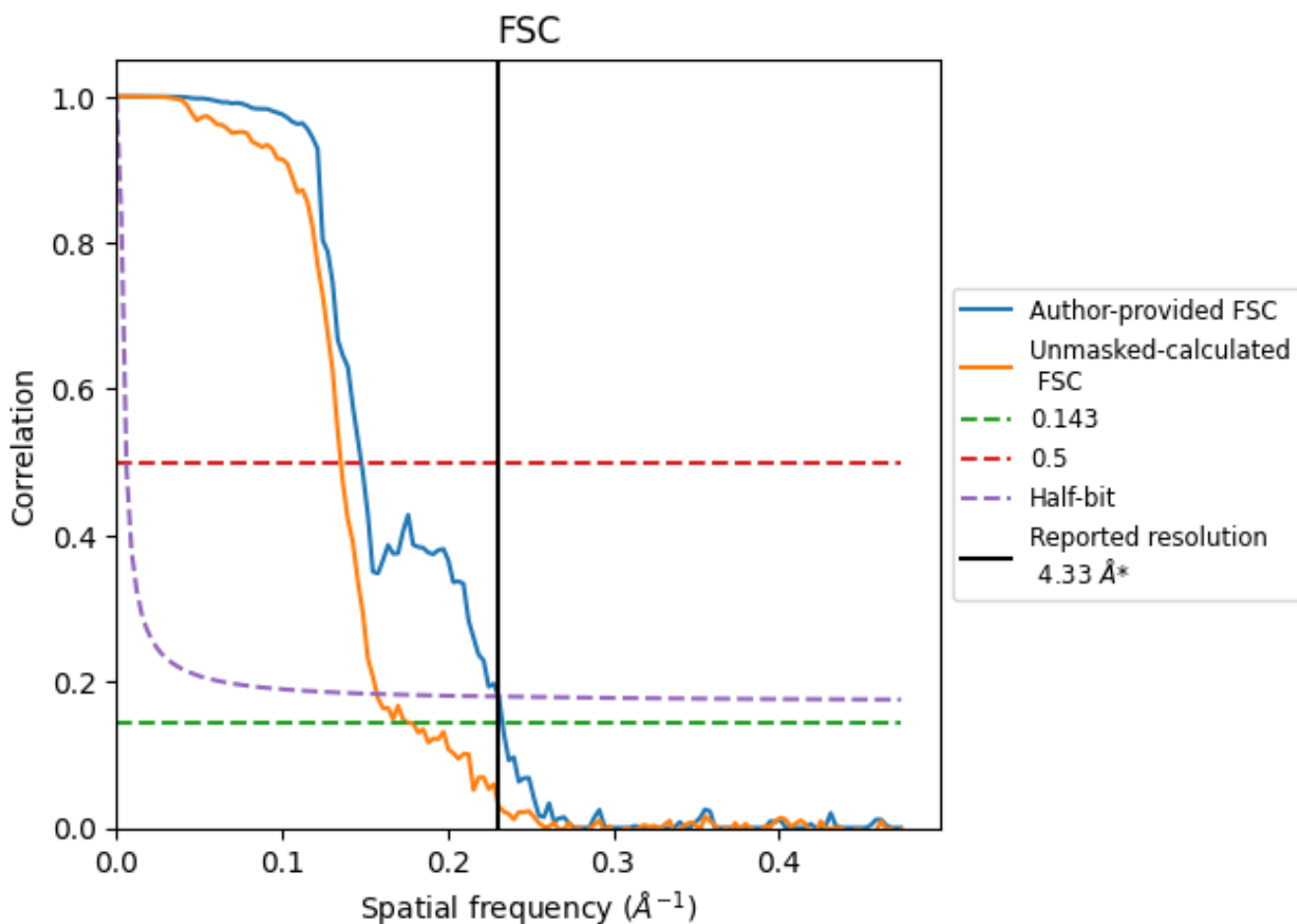


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

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 0.231\AA^{-1}

8.2 Resolution estimates [i](#)

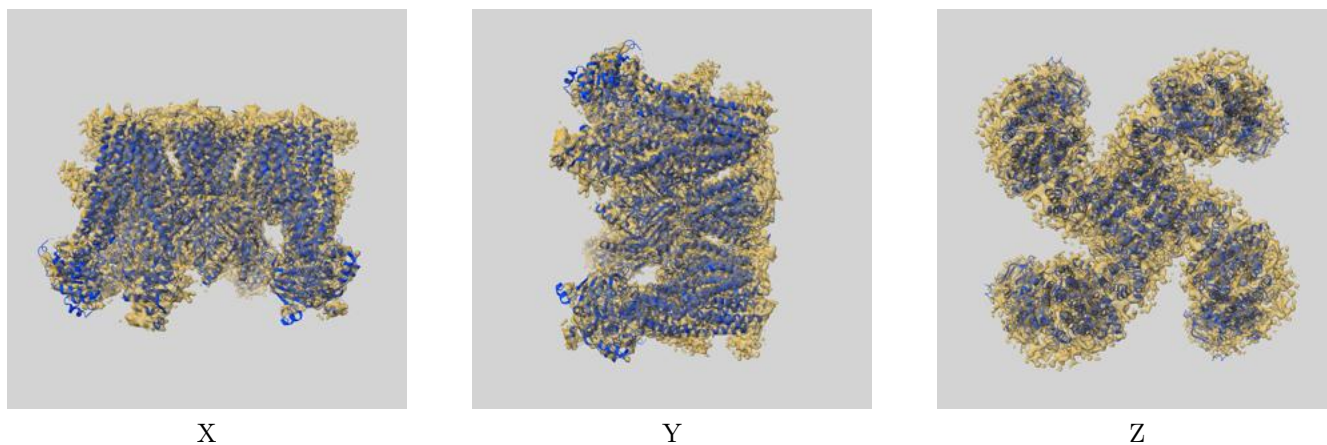
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.29	6.77	4.33
Unmasked-calculated*	5.58	7.38	6.35

*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 5.58 differs from the reported value 4.33 by more than 10 %

9 Map-model fit [i](#)

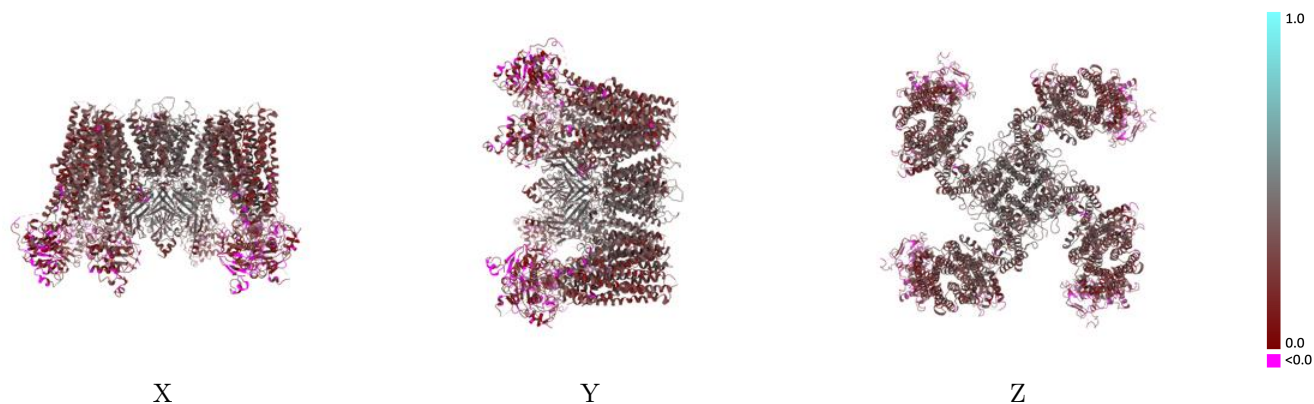
This section contains information regarding the fit between EMDB map EMD-6832 and PDB model 5YKF. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



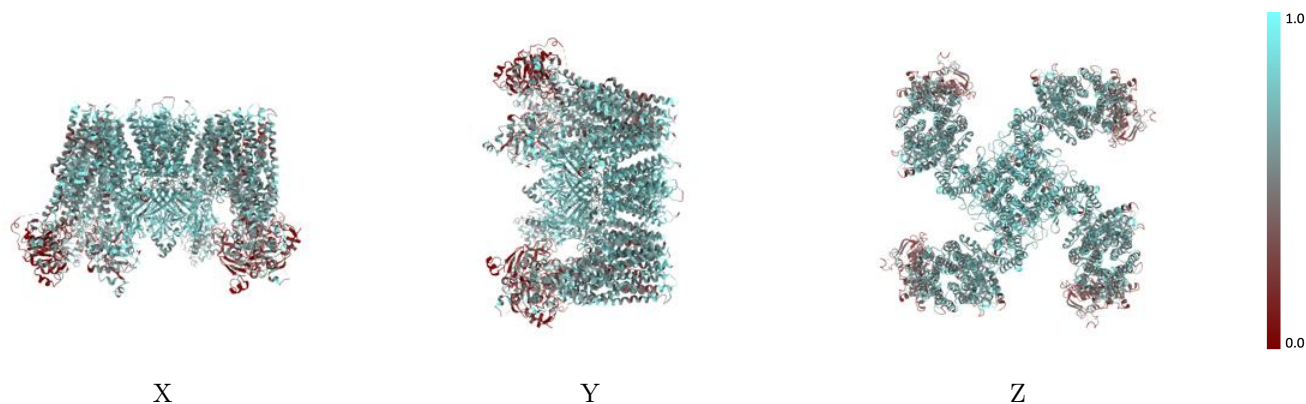
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



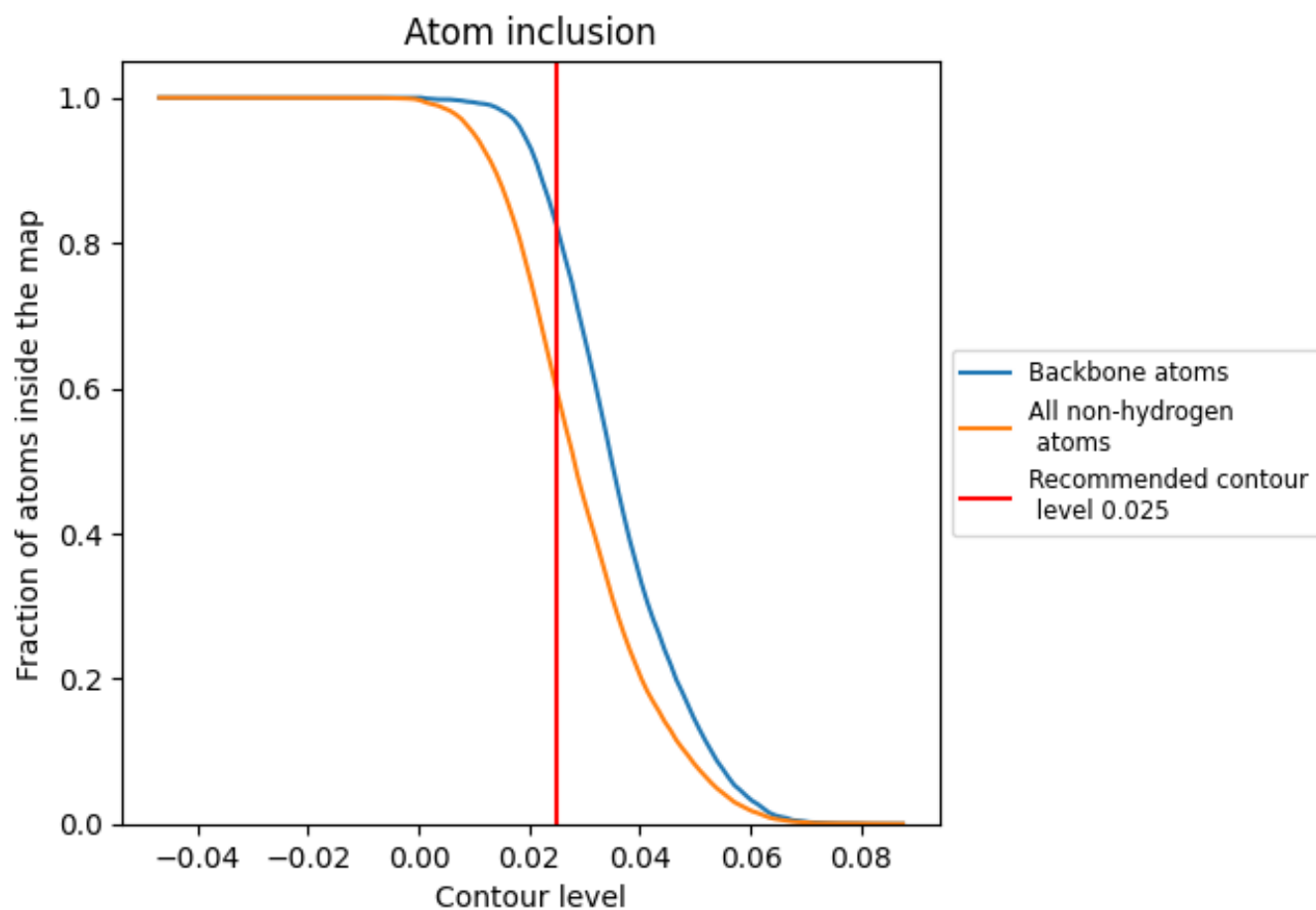
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 59% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5949	 0.2740
A	 0.7658	 0.3990
B	 0.5539	 0.2420
C	 0.7637	 0.3970
D	 0.5538	 0.2430
E	 0.7637	 0.3990
F	 0.5537	 0.2440
G	 0.7615	 0.4000
H	 0.5538	 0.2430

