



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:19 AM UTC

PDB ID : 5YKF / pdb_00005ykf
EMDB ID : EMD-6832
Title : Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (3D class1 at 4.33Å)
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

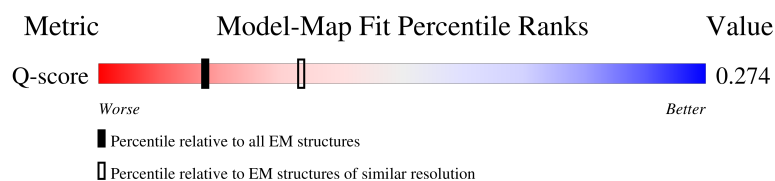
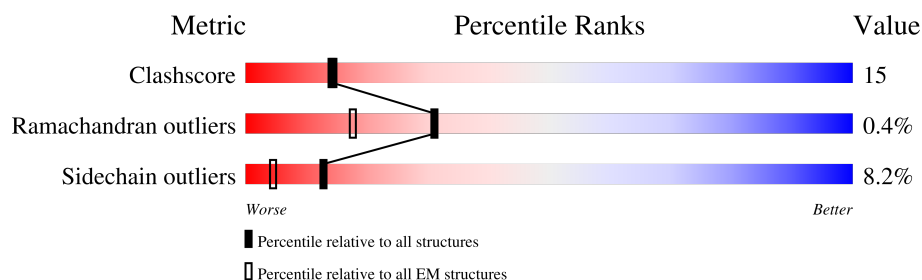
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.33 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3854 (3.83 - 4.83)

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	
1	C	390	
1	E	390	
1	G	390	

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Mol	Chain	Length	Quality of chain
2	B	1582	21% 58% 22% • 17%
2	D	1582	21% 58% 22% • 17%
2	F	1582	21% 58% 22% • 17%
2	H	1582	21% 59% 22% • 17%

2 Entry composition

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.

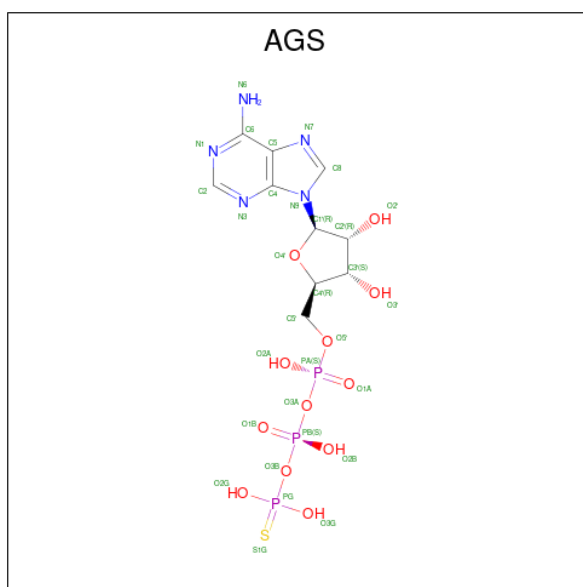
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

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

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

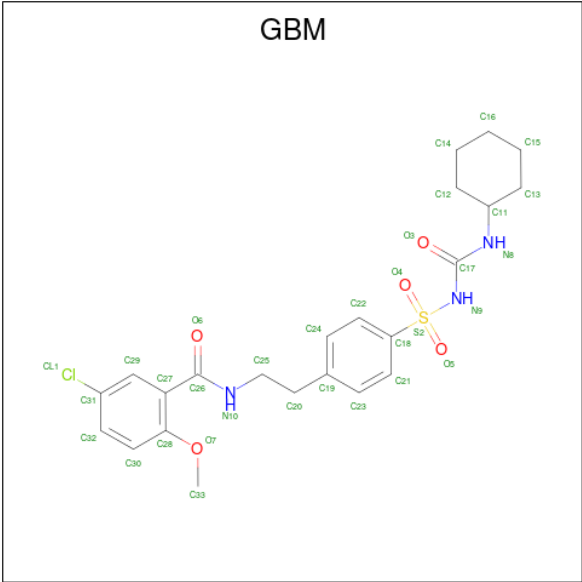
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	D	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	F	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	H	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

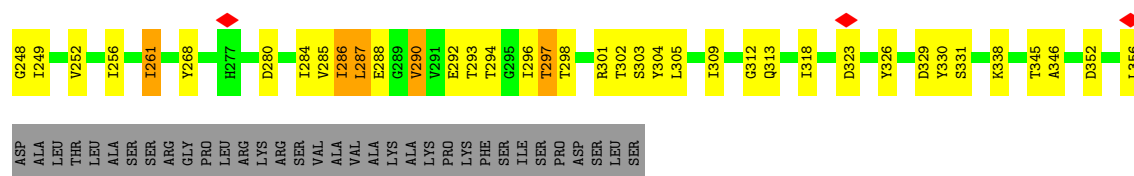


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	F	1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

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

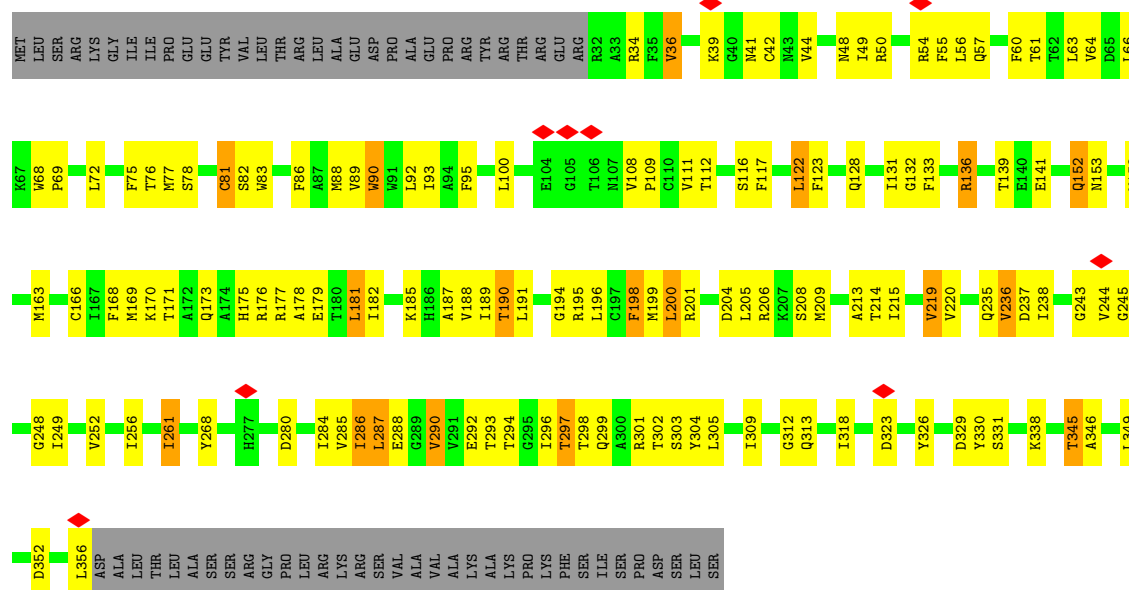


Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	D	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	F	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	H	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0



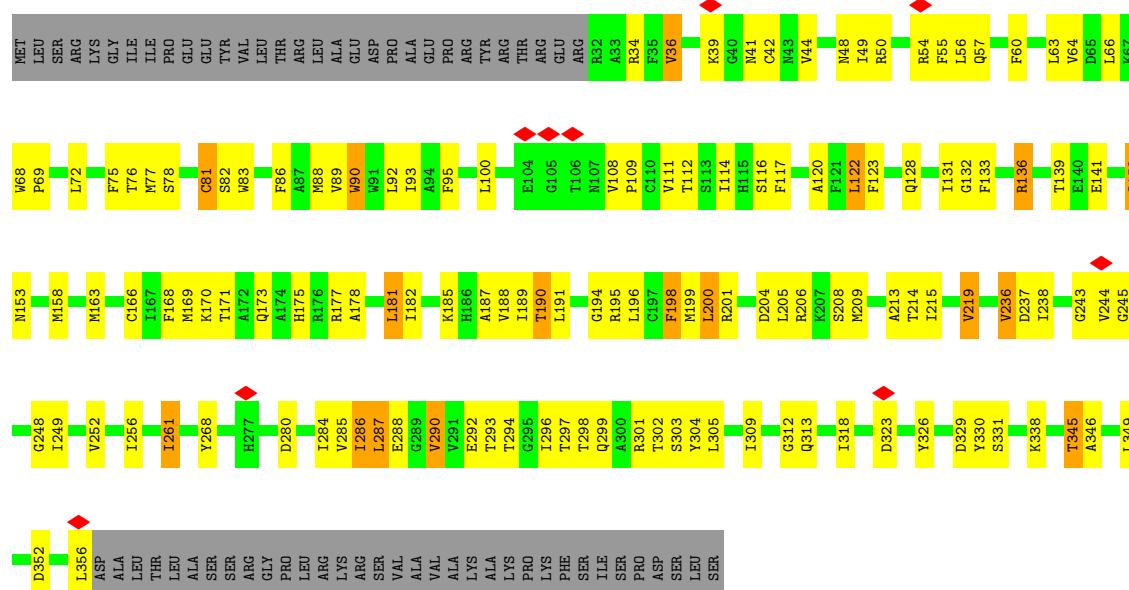
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain E: 48% 31% 5% 17%



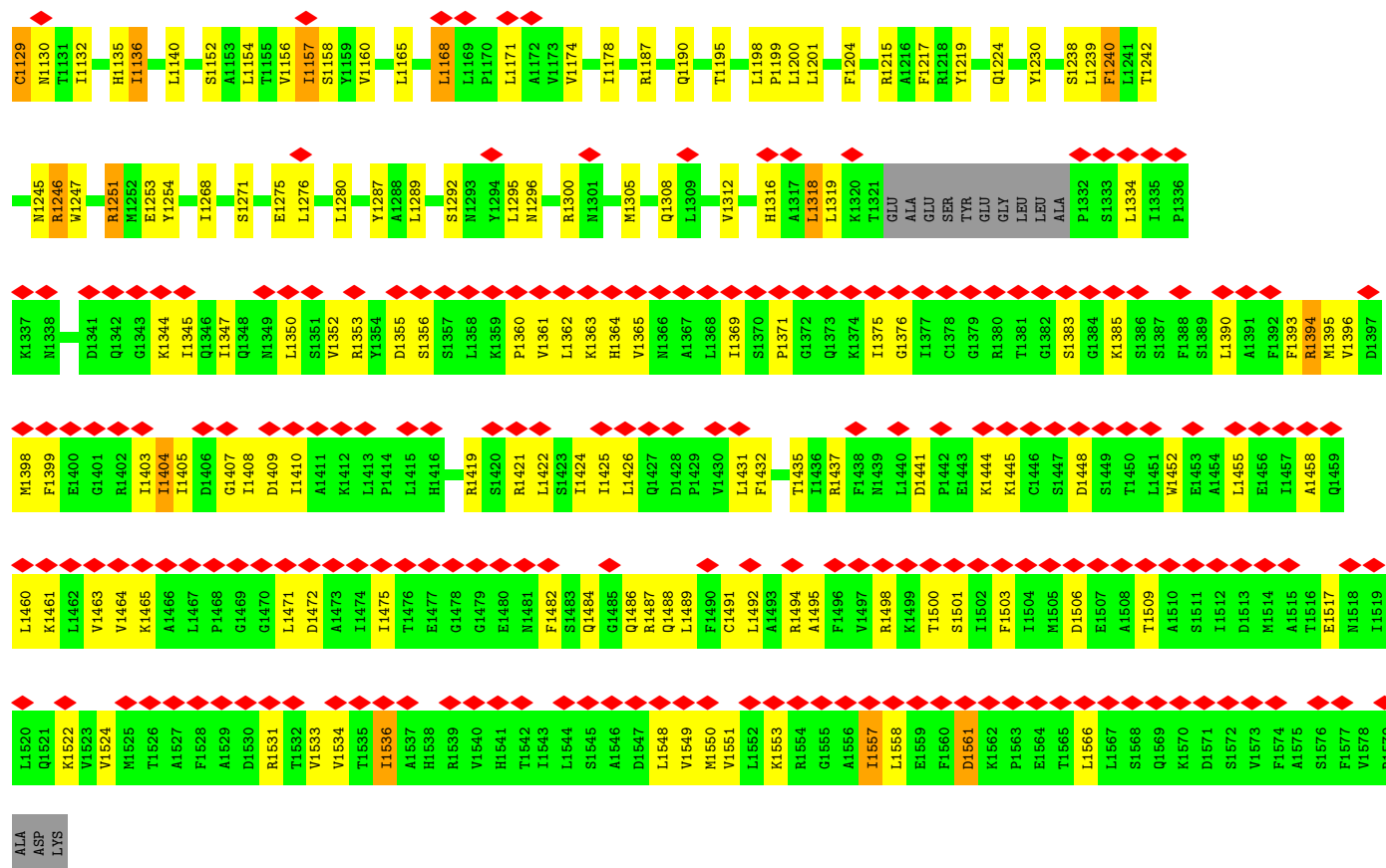
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain G: 49% 30% 17%

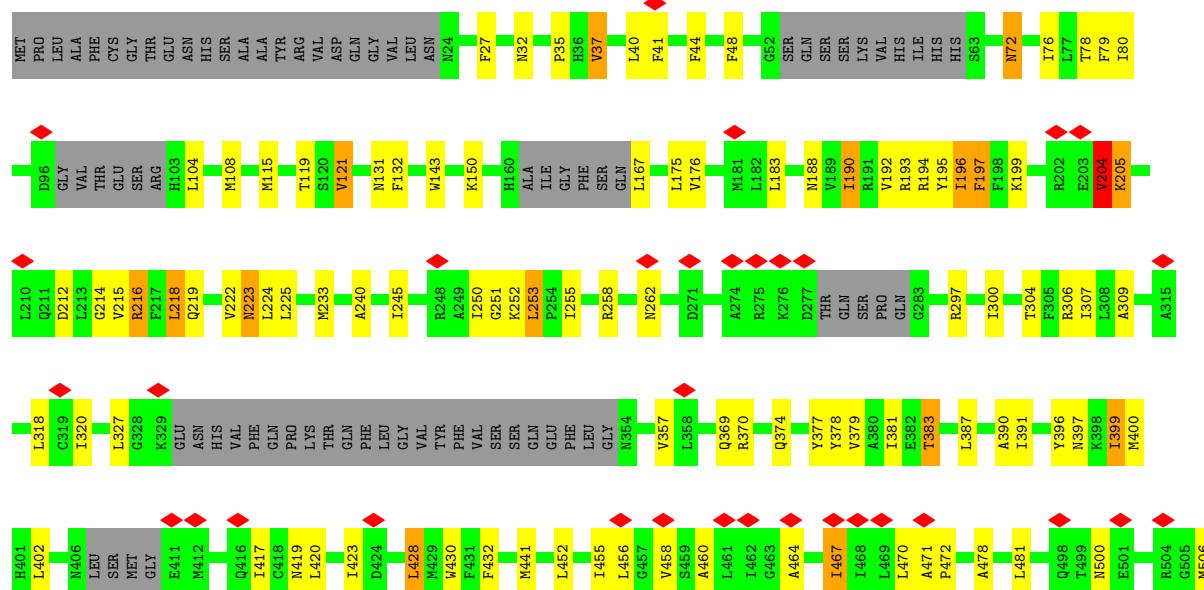


Chain B:

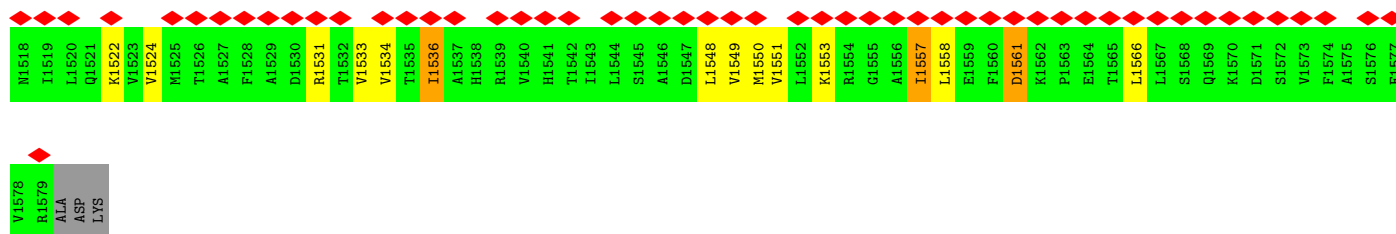




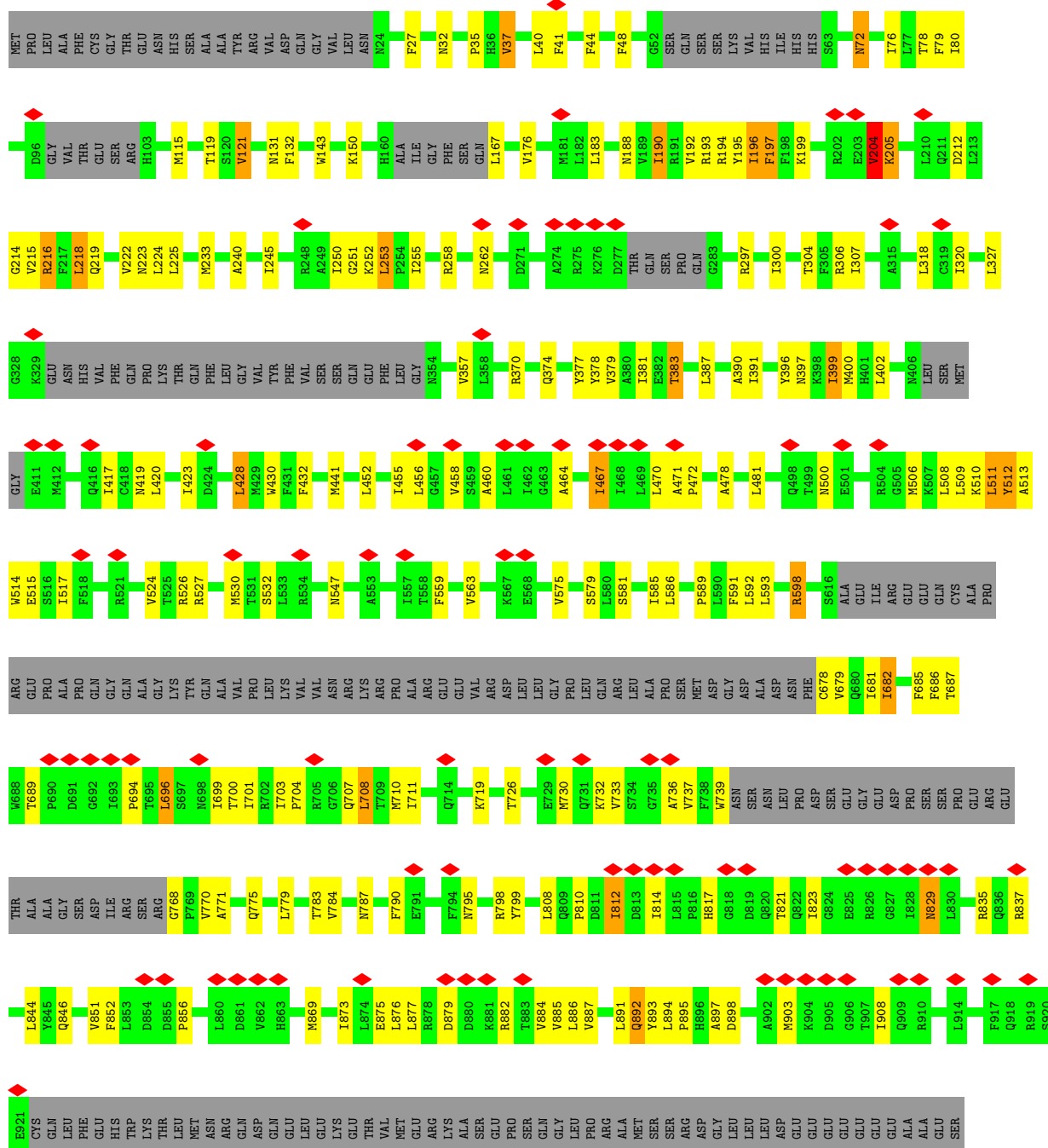
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

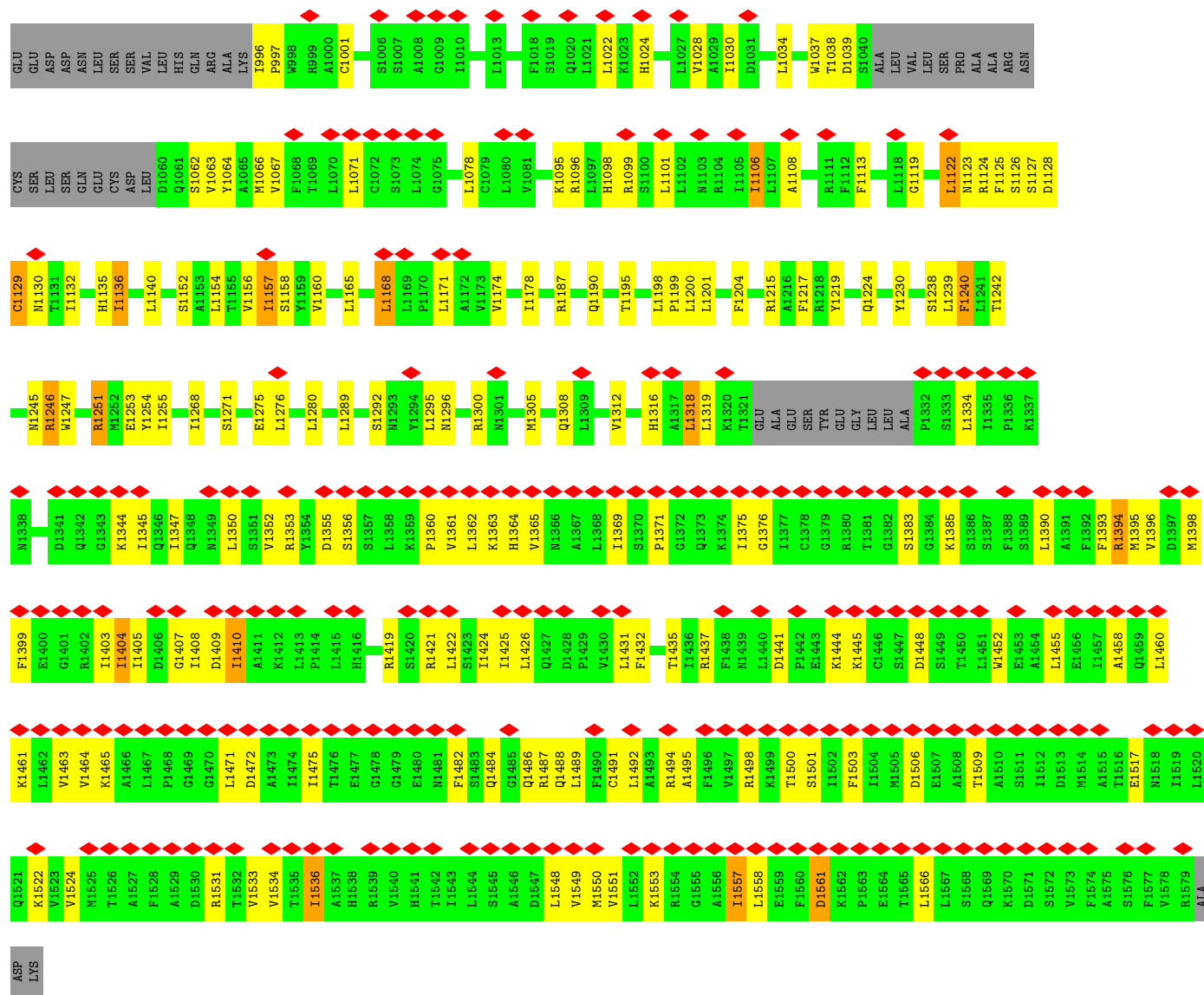


A1458	Q1459	L1460	K1461	L1462	V1463	V1464	K1465	A1466	L1467	P1468	G1469	G1470	L1471	D1472	A1473	I1474	I1475	T1476	E1477	G1478	G1479	E1480	N1481	F1482	S1483	Q1484	G1485	Q1486	R1487	Q1488	L1489	F1490	C1491	L1492	A1493	R1494	A1495	F1496	V1497	R1498	K1499	T1500	S1501	I1502	F1503	I1504	D1506	E1507	A1508	T1509	A1510	S1511	I1512	D1513	M1514	A1515	T1516	E1517
V1396	D1397	M1398	F1399	E1400	G1401	R1402	I1403	I1404	I1405	D1406	G1407	I1408	D1409	I1410	A1411	K1412	L1413	P1414	L1415	H1416	R1419	S1420	R1421	L1422	S1423	I1424	I1425	L1426	Q1427	D1428	P1429	V1430	L1431	F1432	T1435	I1436	R1437	F1438	N1439	L1440	D1441	P1442	E1443	K1444	K1445	C1446	S1447	D1448	T1449	T1450	W1452	E1453	A1454	L1455	E1456	I1457		
I1335	P1336	K1337	N1338	D1341	Q1342	G1343	K1344	I1345	I1346	Q1347	Q1348	N1349	L1350	S1351	V1352	R1353	Y1354	D1355	S1356	S1357	L1358	K1359	P1360	V1361	L1362	K1363	H1364	V1365	N1366	A1367	L1368	I1369	S1370	P1371	G1372	Q1373	K1374	I1375	G1376	I1377	C1378	G1379	K1380	T1381	G1382	S1383	K1384	K1385	S1386	F1387	S1388	S1389	L1390	A1391	F1392	R1393	M1395	
L1241	T1242	N1245	R1246	W1247	R1251	M1252	E1253	Y1254	I1268	S1271	E1275	L1276	L1280	Y1287	A1288	L1289	S1292	N1293	Y1294	L1295	N1296	R1300	N1301	M1305	Q1308	L1309	V1312	H1316	A1317	L1318	L1319	K1320	T1321	GLU	ALA	GLU	SER	TYR	GLU	GLY	LEU	LEU	ALA	P1332	S1333	L1334												
S1126	S1127	D1128	N1130	T1131	I1132	H1135	I1136	L1140	S1152	A1153	L1154	T1155	V1156	I1157	S1158	Y1159	V1160	L1165	L1168	L1169	P1170	L1171	A1172	V1173	V1174	I1178	R1187	Q1190	T1195	L1198	P1199	L1200	F1204	R1215	A1216	F1217	R1218	Y1219	Q1224	Y1230	S1238	L1239	F1240															
LEU	SER	PRO	ALA	ALA	ASN	CYS	ARG	GLN	CYS	GLU	CYS	LEU	D1060	Y1064	F1068	T1069	L1070	L1071	C1072	S1073	L1074	G1075	L1078	C1079	L1080	V1081	K1095	R1096	L1097	H1098	R1099	S1100	L1101	L1102	N1103	R1104	I1105	L1106	L1107	A1108	R1111	F1112	F1113	L1118	G1119	L1122	L1123	R1124	F1125									
GLU	GLU	GLU	ALA	ALA	GLU	SER	GLU	ASP	ASN	GLN	SER	VAL	HIS	TRP	LYS	THR	LEU	MET	ARG	ALA	LYS	I996	W998	R999	A1000	C1001	S1006	S1007	A1008	G1009	I1010	L1013	F1018	S1019	Q1020	L1021	K1023	H1024	L1027	V1028	A1029	I1030	D1031	L1034	W1037	T1038	D1039	S1040	ALA	LEU	VAL							
ASP	PRO	SER	SER	GLU	ARG	GLU	THR	ALA	GLY	SER	ILE	ARG	SER	ARG	G768	P769	V770	A771	Q775	L779	T783	V784	N787	F790	E791	F794	N795	Y799	L808	Q809	P810	D811	I812	D813	I814	L815	P816	H817	G818	D819	Q820	T821	I823	G824	E825	R826	G827											
V679	Q680	I681	I682	F685	F686	T687	W688	T689	P690	D691	G692	I693	P694	T695	L696	S697	M698	I699	T700	I701	R702	I703	P704	R705	G706	Q707	L708	T709	M710	I711	Q714	K719	T726	E729	M730	Q731	K732	V733	S734	G735	A736	V737	F738	W739	ASN	ASN	PRO	ASP	SER	GLY	GLY	ALA	ASN	PHE	C678			
ILE	ARG	GLU	GLU	GLN	CYS	ALA	PRO	GLU	ALA	PRO	GLN	PRO	GLN	ALA	ALA	PRO	GLN	ALA	VAL	PRO	LEU	VAL	ASN	ARG	ARG	PRO	ALA	ARG	GLU	GLU	VAL	ARG	ASP	LEU	LEU	GLY	PRO	LEU	LEU	ARG	ALA	PRO	SER	MET	ASP	GLY	ASP	ALA	ASP	ASN	ASP	ASP	ASP	ASP	ALA	GLU	GLY	



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





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







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	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 ($\text{\AA}$)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.33	0/2518	0.56	0/3430
1	C	0.33	0/2518	0.56	0/3430
1	E	0.33	0/2518	0.56	0/3430
1	G	0.33	0/2518	0.56	0/3430
2	B	0.21	1/10394 (0.0%)	0.44	7/14113 (0.0%)
2	D	0.21	1/10394 (0.0%)	0.44	7/14113 (0.0%)
2	F	0.21	1/10394 (0.0%)	0.44	7/14113 (0.0%)
2	H	0.21	1/10394 (0.0%)	0.44	7/14113 (0.0%)
All	All	0.23	4/51648 (0.0%)	0.46	28/70172 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	ARG	C-N	-5.31	1.26	1.33
2	D	216	ARG	C-N	-5.31	1.26	1.33
2	F	216	ARG	C-N	-5.31	1.26	1.33
2	H	216	ARG	C-N	-5.31	1.26	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	532	SER	CA-C-N	7.34	130.85	120.28
2	B	532	SER	C-N-CA	7.34	130.85	120.28
2	D	532	SER	CA-C-N	7.34	130.85	120.28
2	D	532	SER	C-N-CA	7.34	130.85	120.28
2	F	532	SER	CA-C-N	7.34	130.85	120.28
2	F	532	SER	C-N-CA	7.34	130.85	120.28
2	H	532	SER	CA-C-N	7.34	130.85	120.28
2	H	532	SER	C-N-CA	7.34	130.85	120.28
2	B	1404	ILE	N-CA-C	6.95	120.41	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1404	ILE	N-CA-C	6.95	120.41	108.95
2	F	1404	ILE	N-CA-C	6.95	120.41	108.95
2	H	1404	ILE	N-CA-C	6.95	120.41	108.95
2	B	1448	ASP	N-CA-C	6.83	119.30	111.11
2	D	1448	ASP	N-CA-C	6.83	119.30	111.11
2	F	1448	ASP	N-CA-C	6.83	119.30	111.11
2	H	1448	ASP	N-CA-C	6.83	119.30	111.11
2	B	194	ARG	N-CA-C	6.12	120.80	109.24
2	D	194	ARG	N-CA-C	6.12	120.80	109.24
2	F	194	ARG	N-CA-C	6.12	120.80	109.24
2	H	194	ARG	N-CA-C	6.12	120.80	109.24
2	B	1135	HIS	N-CA-C	5.67	121.62	114.31
2	D	1135	HIS	N-CA-C	5.67	121.62	114.31
2	F	1135	HIS	N-CA-C	5.67	121.62	114.31
2	H	1135	HIS	N-CA-C	5.67	121.62	114.31
2	B	204	VAL	N-CA-C	5.26	115.99	110.62
2	D	204	VAL	N-CA-C	5.26	115.99	110.62
2	F	204	VAL	N-CA-C	5.26	115.99	110.62
2	H	204	VAL	N-CA-C	5.26	115.99	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2451	117	0
1	C	2463	0	2451	113	0
1	E	2463	0	2451	116	0
1	G	2463	0	2451	116	0
2	B	10189	0	10510	300	0
2	D	10189	0	10510	294	0
2	F	10189	0	10510	298	0
2	H	10189	0	10510	294	0
3	A	62	0	24	10	0
3	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1583	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 (1583) 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
1:A:198:PHE:HD1	1:A:198:PHE:C	1.56	1.11
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
1:C:198:PHE:C	1:C:198:PHE:HD1	1.56	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
1:E:198:PHE:HD1	1:E:198:PHE:C	1.56	1.09
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:512:TYR:HB3	2:H:1498:ARG:NH1	1.67	1.09
1:G:198:PHE:HD1	1:G:198:PHE:C	1.56	1.08
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
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
2:B:1350:LEU:HD13	2:B:1403:ILE:CG1	1.85	1.06
2:D:530:MET:HE3	2:D:1095:LYS:HG2	1.38	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
2:F:1350:LEU:HD13	2:F:1403:ILE:CG1	1.85	1.04
2:B:530:MET:HE3	2:B:1095:LYS:HG2	1.38	1.04
2:F:530:MET:HE3	2:F:1095:LYS:HG2	1.38	1.04
2:H:1124:ARG:HD2	2:H:1318:LEU:HD12	1.41	1.03
1:E:198:PHE:C	1:E:198:PHE:CD1	2.30	1.03
2:H:530:MET:HE3	2:H:1095:LYS:HG2	1.38	1.02
1:G:198:PHE:C	1:G:198:PHE:CD1	2.30	1.02
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
1:C:198:PHE:C	1:C:198:PHE:CD1	2.30	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1350:LEU:CD1	2:H:1403:ILE:HD11	1.92	0.98
1:A:198:PHE:C	1:A:198:PHE:CD1	2.30	0.97
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:200:LEU:HD12	1:A:200:LEU:C	1.93	0.93
1:E:200:LEU:HD12	1:E:200:LEU:C	1.93	0.93
1:C:200:LEU:HD12	1:C:200:LEU:C	1.93	0.93
1:G:200:LEU:HD12	1:G:200:LEU:C	1.93	0.92
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:F:530:MET:HE3	2:F:1095:LYS:CG	2.00	0.92
2:H:530:MET:HE3	2:H:1095:LYS:CG	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
2:D:530:MET:HE3	2:D:1095:LYS:CG	2.00	0.91
2:B:530:MET:HE3	2:B:1095:LYS:CG	2.00	0.90
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:200:LEU:CD1	1:G:200:LEU:C	2.50	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:1422:LEU:C	2:B:1500:THR:HG21	2.10	0.76
2:F:1422:LEU:C	2:F:1500:THR:HG21	2.10	0.76
2:H:1422:LEU:C	2:H:1500:THR:HG21	2.10	0.76
2:D:216:ARG:HD2	2:D:250:ILE:C	2.11	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:B:216:ARG:HD2	2:B:250:ILE:C	2.11	0.75
2:D:1422:LEU:C	2:D:1500:THR:HG21	2.10	0.75
2:H:216:ARG:HD2	2:H:250:ILE:C	2.11	0.75
2:F:1132:ILE:HD11	2:F:1312:VAL:HG22	1.67	0.75
2:F:204:VAL:O	2:F:205:LYS:HB3	1.83	0.75
2:H:196:ILE:O	2:H:197:PHE:O	2.03	0.75
2:F:216:ARG:HD2	2:F:250:ILE:C	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:213:ALA:HA	1:G:288:GLU:O	1.90	0.72
2:B:72:ASN:HA	2:B:224:LEU:HD13	1.72	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1165:LEU:HA	2:H:1168:LEU:HD23	1.76	0.67
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
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:1125:PHE:C	2:H:1129:CYS:HG	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:512:TYR:HB2	2:D:1498:ARG:HH22	1.60	0.65
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:B:1125:PHE:C	2:B:1129:CYS:HG	2.06	0.64
2:B:72:ASN:HB3	2:B:224:LEU:HD11	1.79	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:D:1245:ASN:OD1	2:D:1300:ARG:NH2	2.33	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1125:PHE:C	2:F:1129:CYS:HG	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:1125:PHE:C	2:D:1129:CYS:HG	2.10	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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:1422:LEU:O	2:B:1500:THR:HG21	2.05	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:H:1422:LEU:O	2:H:1500:THR:HG21	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1422:LEU:O	2:F:1500:THR:HG21	2.05	0.55
2:B:1495:ALA:HB1	2:B:1503:PHE:HE2	1.72	0.55
1:E:200:LEU:HD12	1:E:201:ARG:C	2.32	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:B:1127:SER:O	2:B:1128:ASP:C	2.50	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
1:G:200:LEU:HD12	1:G:201:ARG:C	2.32	0.55
2:H:215:VAL:HG13	2:H:252:LYS:O	2.06	0.55
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.88	0.55
1:A:200:LEU:HD12	1:A:201:ARG:C	2.32	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:H:1127:SER:O	2:H:1128:ASP:C	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:MET:HE3	1:E:168:PHE:CE1	2.42	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
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
1:E:169:MET:HE3	1:G:168:PHE:CE1	2.42	0.54
2:H:514:TRP:CZ2	2:H:1498:ARG:NH2	2.75	0.54
1:A:169:MET:HE3	1:C:168:PHE:CE1	2.42	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
1:C:200:LEU:HD12	1:C:201:ARG:C	2.32	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
1:A:168:PHE:CE1	1:G:169:MET:HE3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.88	0.54
2:D:1127:SER:O	2:D:1128:ASP:C	2.50	0.54
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.89	0.54
2:F:1127:SER:O	2:F:1128:ASP:C	2.50	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
1:A:75:PHE:HD2	1:G:158:MET:HE1	1.74	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
1:A:158:MET:HE1	1:C:75:PHE:HD2	1.74	0.53
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.89	0.53
1:C:158:MET:HE1	1:E:75:PHE:HD2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:158:MET:HE1	1:G:75:PHE:HD2	1.74	0.53
2:F:1125:PHE:C	2:F:1129:CYS:SG	2.92	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
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
2:D:1125:PHE:C	2:D:1129:CYS:SG	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1125:PHE:C	2:B:1129:CYS:SG	2.92	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
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:H:1125:PHE:C	2:H:1129:CYS:SG	2.92	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:F:1441:ASP:OD2	2:F:1444:LYS:C	2.53	0.51
2:B:1404:ILE:HG12	2:B:1409:ASP:HB3	1.92	0.51
2:B:1441:ASP:OD2	2:B:1444:LYS:C	2.53	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:H:1441:ASP:OD2	2:H:1444:LYS:C	2.53	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
2:D:1441:ASP:OD2	2:D:1444:LYS:C	2.53	0.51
1:G:175:HIS:O	1:G:178:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
1:A:75:PHE:CD2	1:G:158:MET:HE1	2.47	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:196:ILE:C	2:F:197:PHE:O	2.55	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
1:A:158:MET:HE1	1:C:75:PHE:CD2	2.47	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:158:MET:HE1	1:E:75:PHE:CD2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:196:ILE:C	2:D:197:PHE:O	2.55	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: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
3:F:2002:AGS:O2A	3:F:2002:AGS:S1G	2.70	0.49
2:H:196:ILE:C	2:H:197:PHE:O	2.55	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.95	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:511:LEU:HD13	2:F:1395:MET:HE2	1.95	0.49
2:F:512:TYR:HB2	2:F:1498:ARG:NH1	2.11	0.49
2:B:196:ILE:C	2:B:197:PHE:O	2.55	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
1:A:123:PHE:HD2	1:A:136:ARG:HG3	1.78	0.48
1:E:158:MET:HE1	1:G:75:PHE:CD2	2.47	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:OD1	1:C:280:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:511:LEU:HD13	2:H:1395:MET:HE2	1.95	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: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:511:LEU:HD13	2:B:1395:MET:HE2	1.95	0.48
2:B:1024:HIS:O	2:B:1028:VAL:HG12	2.13	0.48
2:D:511:LEU:HD13	2:D:1395:MET:HE2	1.95	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
2:H:563:VAL:HG21	2:H:1037:TRP:CH2	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:F:1561:ASP:OD1	2:F:1561:ASP:N	2.46	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
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: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: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:710:MET:HE3	2:H:893:TYR:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:F:710:MET:HE3	2:F:893:TYR:HB3	1.97	0.46
2:B:710:MET:HE3	2:B:893:TYR:HB3	1.97	0.46
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.97	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
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
2:D:710:MET:HE3	2:D:893:TYR:HB3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:869:MET:HE3	2:D:869:MET:HB3	1.87	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
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: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:H:1140:LEU:HD13	2:H:1305:MET:HE2	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:B:370:ARG:HG3	2:B:1253:GLU:CD	2.42	0.45
2:D:196:ILE:O	2:D:197:PHE:C	2.60	0.45
2:D:379:VAL:O	2:D:383:THR:OG1	2.35	0.45
2:D:1140:LEU:HD13	2:D:1305:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:LEU:CB	1:G:261:ILE:HD11	2.47	0.45
2:H:196:ILE:O	2:H:197:PHE:C	2.60	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: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: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
1:E:116:SER:OG	1:E:117:PHE:N	2.50	0.45
2:F:1140:LEU:HD13	2:F:1305:MET:HE2	1.98	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:F:530:MET:CE	2:F:1095:LYS:HG2	2.28	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
2:B:196:ILE:O	2:B:197:PHE:C	2.60	0.45
2:B:1140:LEU:HD13	2:B:1305:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LYS:O	1:G:173:GLN:N	2.48	0.44
2:H:530:MET:CE	2:H:1095:LYS:HG2	2.28	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
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
2:D:370:ARG:HG3	2:D:1253:GLU:CD	2.42	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:370:ARG:HG3	2:F:1253:GLU:CD	2.42	0.44
2:F:511:LEU:HG	2:F:1424:ILE:HG21	1.98	0.44
2:H:370:ARG:HG3	2:H:1253:GLU:CD	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	2:F:1039:ASP:N	2.50	0.44
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.52	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: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: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
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:H:1122:LEU:HD12	2:H:1122:LEU:C	2.42	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
2:D:1353:ARG:HH11	2:D:1398:MET:HE3	1.84	0.43
1:E:77:MET:HG3	2:F:48:PHE:HE2	1.83	0.43
2:F:400:MET:HA	2:F:400:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.99	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:169:MET:HE3	1:G:168:PHE:HE1	1.83	0.43
1:E:284:ILE:HA	1:E:302:THR:O	2.19	0.43
2:F:196:ILE:O	2:F:197:PHE:C	2.60	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:400:MET:HE2	2:D:400:MET:HA	2.00	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
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
1:E:297:THR:O	1:E:297:THR:OG1	2.37	0.43
2:F:686:PHE:CE2	2:F:730:MET:HB3	2.54	0.43
2:F:1122:LEU:HD12	2:F:1122:LEU:C	2.42	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
1:A:169:MET:HE3	1:C:168:PHE:HE1	1.83	0.43
2:B:400:MET:HE2	2:B:400:MET:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:LEU:HB2	1:E:261:ILE:HD11	2.01	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:B:530:MET:CE	2:B:1095:LYS:HG2	2.28	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
1:E:169:MET:HE1	1:G:171:THR:C	2.44	0.43
2:F:869:MET:HE3	2:F:869:MET:HB3	1.87	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
2:H:400:MET:HA	2:H:400:MET:HE2	2.00	0.43
1:A:56:LEU:HB2	2:B:132:PHE:HZ	1.84	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:530:MET:CE	2:D:1095:LYS:HG2	2.28	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
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:C:169:MET:HE1	1:E:171:THR:C	2.44	0.42
2:D:598:ARG:HD3	2:D:598:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:1353:ARG:HH11	2:H:1398:MET:HE3	1.84	0.42
1:A:187:ALA:O	1:A:309:ILE:HG13	2.19	0.42
2:B:216:ARG:HD2	2:B:251:GLY:N	2.32	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
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
2:B:1353:ARG:HH11	2:B:1398:MET:HE3	1.84	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
2:H:869:MET:HE3	2:H:869:MET:HB3	1.87	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
1:C:169:MET:HE3	1:E:168:PHE:HE1	1.83	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
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:171:THR:C	1:G:169:MET:HE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:168:PHE:HE1	1:G:169:MET:HE3	1.83	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:1353:ARG:HH11	2:F:1398:MET:HE3	1.84	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:598:ARG:HD3	2:F:598:ARG:C	2.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:598:ARG:HD3	2:B:598:ARG:C	2.44	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:598:ARG:HD3	2:H:598:ARG:C	2.44	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
1:A:169:MET:HE1	1:C:171:THR:C	2.44	0.41
2:B:710:MET:HG2	2:B:897:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	2.02	0.41
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: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:530:MET:HE3	2:F:1095:LYS:HG3	1.97	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:869:MET:HE3	2:B:869:MET:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:G:169:MET:HB2	1:G:169:MET:HE3	1.96	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:286:ILE:HG23	1:C:301:ARG:HG2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:708:LEU:HB3	2:D:897:ALA:HA	2.02	0.41
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: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:530:MET:HE3	2:B:1095:LYS:HG3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	2.02	0.40
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: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: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
1:A:198:PHE:CE1	1:A:199:MET:C	3.00	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
1:E:169:MET:HB2	1:E:169:MET:HE3	1.96	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%)	36	71
1	C	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	36	71
1	E	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	36	71
1	G	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	36	71
2	B	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	24	62
2	D	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	24	62
2	F	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	24	62
2	H	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	24	62
All	All	6432/7888 (82%)	6120 (95%)	284 (4%)	28 (0%)	31	66

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 ⓘ

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%)	219 (85%)	39 (15%)	3	14
1	C	258/339 (76%)	219 (85%)	39 (15%)	3	14
1	E	258/339 (76%)	219 (85%)	39 (15%)	3	14
1	G	258/339 (76%)	219 (85%)	39 (15%)	3	14
2	B	1102/1371 (80%)	1030 (94%)	72 (6%)	15	38
2	D	1102/1371 (80%)	1030 (94%)	72 (6%)	15	38
2	F	1102/1371 (80%)	1030 (94%)	72 (6%)	15	38
2	H	1102/1371 (80%)	1030 (94%)	72 (6%)	15	38
All	All	5440/6840 (80%)	4996 (92%)	444 (8%)	13	31

All (444) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	78	SER
1	A	81	CYS
1	A	82	SER
1	A	88	MET
1	A	90	TRP
1	A	92	LEU
1	A	108	VAL
1	A	111	VAL
1	A	122	LEU
1	A	133	PHE
1	A	136	ARG
1	A	152	GLN
1	A	153	ASN
1	A	166	CYS
1	A	181	LEU
1	A	182	ILE
1	A	188	VAL
1	A	190	THR
1	A	198	PHE
1	A	200	LEU
1	A	204	ASP
1	A	205	LEU
1	A	219	VAL
1	A	236	VAL
1	A	238	ILE
1	A	249	ILE
1	A	252	VAL
1	A	256	ILE
1	A	261	ILE
1	A	286	ILE
1	A	287	LEU
1	A	290	VAL
1	A	293	THR
1	A	294	THR
1	A	297	THR
1	A	298	THR
1	A	323	ASP
1	A	345	THR
2	B	37	VAL
2	B	72	ASN
2	B	119	THR

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Mol	Chain	Res	Type
2	B	121	VAL
2	B	167	LEU
2	B	190	ILE
2	B	193	ARG
2	B	204	VAL
2	B	218	LEU
2	B	222	VAL
2	B	223	ASN
2	B	253	LEU
2	B	318	LEU
2	B	327	LEU
2	B	357	VAL
2	B	374	GLN
2	B	383	THR
2	B	391	ILE
2	B	399	ILE
2	B	420	LEU
2	B	428	LEU
2	B	430	TRP
2	B	432	PHE
2	B	458	VAL
2	B	467	ILE
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	737	VAL
2	B	770	VAL
2	B	812	ILE
2	B	829	ASN
2	B	892	GLN
2	B	1001	CYS
2	B	1106	ILE
2	B	1122	LEU
2	B	1129	CYS
2	B	1136	ILE
2	B	1157	ILE

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Mol	Chain	Res	Type
2	B	1168	LEU
2	B	1178	ILE
2	B	1195	THR
2	B	1204	PHE
2	B	1238	SER
2	B	1240	PHE
2	B	1246	ARG
2	B	1251	ARG
2	B	1254	TYR
2	B	1268	ILE
2	B	1276	LEU
2	B	1296	ASN
2	B	1318	LEU
2	B	1383	SER
2	B	1394	ARG
2	B	1396	VAL
2	B	1410	ILE
2	B	1432	PHE
2	B	1488	GLN
2	B	1522	LYS
2	B	1524	VAL
2	B	1536	ILE
2	B	1550	MET
2	B	1551	VAL
2	B	1557	ILE
2	B	1561	ASP
2	B	1566	LEU
1	C	36	VAL
1	C	78	SER
1	C	81	CYS
1	C	82	SER
1	C	88	MET
1	C	90	TRP
1	C	92	LEU
1	C	108	VAL
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

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Mol	Chain	Res	Type
1	C	181	LEU
1	C	182	ILE
1	C	188	VAL
1	C	190	THR
1	C	198	PHE
1	C	200	LEU
1	C	204	ASP
1	C	205	LEU
1	C	219	VAL
1	C	236	VAL
1	C	238	ILE
1	C	249	ILE
1	C	252	VAL
1	C	256	ILE
1	C	261	ILE
1	C	286	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
2	D	72	ASN
2	D	119	THR
2	D	121	VAL
2	D	167	LEU
2	D	190	ILE
2	D	193	ARG
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	223	ASN
2	D	253	LEU
2	D	318	LEU
2	D	327	LEU
2	D	357	VAL
2	D	374	GLN
2	D	383	THR
2	D	391	ILE

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Mol	Chain	Res	Type
2	D	399	ILE
2	D	420	LEU
2	D	428	LEU
2	D	430	TRP
2	D	432	PHE
2	D	458	VAL
2	D	467	ILE
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	737	VAL
2	D	770	VAL
2	D	812	ILE
2	D	829	ASN
2	D	892	GLN
2	D	1001	CYS
2	D	1106	ILE
2	D	1122	LEU
2	D	1129	CYS
2	D	1136	ILE
2	D	1157	ILE
2	D	1168	LEU
2	D	1178	ILE
2	D	1195	THR
2	D	1204	PHE
2	D	1238	SER
2	D	1240	PHE
2	D	1246	ARG
2	D	1251	ARG
2	D	1254	TYR
2	D	1268	ILE
2	D	1276	LEU
2	D	1296	ASN
2	D	1318	LEU
2	D	1383	SER
2	D	1394	ARG

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Mol	Chain	Res	Type
2	D	1396	VAL
2	D	1410	ILE
2	D	1432	PHE
2	D	1488	GLN
2	D	1522	LYS
2	D	1524	VAL
2	D	1536	ILE
2	D	1550	MET
2	D	1551	VAL
2	D	1557	ILE
2	D	1561	ASP
2	D	1566	LEU
1	E	36	VAL
1	E	78	SER
1	E	81	CYS
1	E	82	SER
1	E	88	MET
1	E	90	TRP
1	E	92	LEU
1	E	108	VAL
1	E	111	VAL
1	E	122	LEU
1	E	133	PHE
1	E	136	ARG
1	E	152	GLN
1	E	153	ASN
1	E	166	CYS
1	E	181	LEU
1	E	182	ILE
1	E	188	VAL
1	E	190	THR
1	E	198	PHE
1	E	200	LEU
1	E	204	ASP
1	E	205	LEU
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	249	ILE
1	E	252	VAL
1	E	256	ILE
1	E	261	ILE

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Mol	Chain	Res	Type
1	E	286	ILE
1	E	287	LEU
1	E	290	VAL
1	E	293	THR
1	E	294	THR
1	E	297	THR
1	E	298	THR
1	E	323	ASP
1	E	345	THR
2	F	37	VAL
2	F	72	ASN
2	F	119	THR
2	F	121	VAL
2	F	167	LEU
2	F	190	ILE
2	F	193	ARG
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	223	ASN
2	F	253	LEU
2	F	318	LEU
2	F	327	LEU
2	F	357	VAL
2	F	374	GLN
2	F	383	THR
2	F	391	ILE
2	F	399	ILE
2	F	420	LEU
2	F	428	LEU
2	F	430	TRP
2	F	432	PHE
2	F	458	VAL
2	F	467	ILE
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

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Mol	Chain	Res	Type
2	F	708	LEU
2	F	737	VAL
2	F	770	VAL
2	F	812	ILE
2	F	829	ASN
2	F	892	GLN
2	F	1001	CYS
2	F	1106	ILE
2	F	1122	LEU
2	F	1129	CYS
2	F	1136	ILE
2	F	1157	ILE
2	F	1168	LEU
2	F	1178	ILE
2	F	1195	THR
2	F	1204	PHE
2	F	1238	SER
2	F	1240	PHE
2	F	1246	ARG
2	F	1251	ARG
2	F	1254	TYR
2	F	1268	ILE
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	1410	ILE
2	F	1432	PHE
2	F	1488	GLN
2	F	1522	LYS
2	F	1524	VAL
2	F	1536	ILE
2	F	1550	MET
2	F	1551	VAL
2	F	1557	ILE
2	F	1561	ASP
2	F	1566	LEU
1	G	36	VAL
1	G	78	SER
1	G	81	CYS

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Mol	Chain	Res	Type
1	G	82	SER
1	G	88	MET
1	G	90	TRP
1	G	92	LEU
1	G	108	VAL
1	G	111	VAL
1	G	122	LEU
1	G	133	PHE
1	G	136	ARG
1	G	152	GLN
1	G	153	ASN
1	G	166	CYS
1	G	181	LEU
1	G	182	ILE
1	G	188	VAL
1	G	190	THR
1	G	198	PHE
1	G	200	LEU
1	G	204	ASP
1	G	205	LEU
1	G	219	VAL
1	G	236	VAL
1	G	238	ILE
1	G	249	ILE
1	G	252	VAL
1	G	256	ILE
1	G	261	ILE
1	G	286	ILE
1	G	287	LEU
1	G	290	VAL
1	G	293	THR
1	G	294	THR
1	G	297	THR
1	G	298	THR
1	G	323	ASP
1	G	345	THR
2	H	37	VAL
2	H	72	ASN
2	H	119	THR
2	H	121	VAL
2	H	167	LEU
2	H	190	ILE

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Mol	Chain	Res	Type
2	H	193	ARG
2	H	204	VAL
2	H	218	LEU
2	H	222	VAL
2	H	223	ASN
2	H	253	LEU
2	H	318	LEU
2	H	327	LEU
2	H	357	VAL
2	H	374	GLN
2	H	383	THR
2	H	391	ILE
2	H	399	ILE
2	H	420	LEU
2	H	428	LEU
2	H	430	TRP
2	H	432	PHE
2	H	458	VAL
2	H	467	ILE
2	H	470	LEU
2	H	511	LEU
2	H	512	TYR
2	H	598	ARG
2	H	682	ILE
2	H	689	THR
2	H	696	LEU
2	H	701	ILE
2	H	708	LEU
2	H	737	VAL
2	H	770	VAL
2	H	812	ILE
2	H	829	ASN
2	H	892	GLN
2	H	1001	CYS
2	H	1106	ILE
2	H	1122	LEU
2	H	1129	CYS
2	H	1136	ILE
2	H	1157	ILE
2	H	1168	LEU
2	H	1178	ILE
2	H	1195	THR

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Mol	Chain	Res	Type
2	H	1204	PHE
2	H	1238	SER
2	H	1240	PHE
2	H	1246	ARG
2	H	1251	ARG
2	H	1254	TYR
2	H	1268	ILE
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	1410	ILE
2	H	1432	PHE
2	H	1488	GLN
2	H	1522	LYS
2	H	1524	VAL
2	H	1536	ILE
2	H	1550	MET
2	H	1551	VAL
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 (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	48	ASN
1	A	128	GLN
1	A	152	GLN
1	A	173	GLN
1	A	259	HIS
1	A	299	GLN
1	A	313	GLN
1	A	348	GLN
2	B	219	GLN
2	B	326	HIS
2	B	491	HIS
2	B	834	GLN
2	B	1020	GLN

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Mol	Chain	Res	Type
2	B	1135	HIS
2	B	1190	GLN
2	B	1518	ASN
2	B	1521	GLN
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
1	C	313	GLN
1	C	348	GLN
2	D	219	GLN
2	D	326	HIS
2	D	491	HIS
2	D	834	GLN
2	D	1020	GLN
2	D	1135	HIS
2	D	1190	GLN
2	D	1518	ASN
2	D	1521	GLN
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	152	GLN
1	E	173	GLN
1	E	299	GLN
1	E	313	GLN
1	E	348	GLN
2	F	219	GLN
2	F	326	HIS
2	F	491	HIS
2	F	834	GLN
2	F	1020	GLN
2	F	1135	HIS
2	F	1190	GLN
2	F	1518	ASN
2	F	1521	GLN
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN

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Mol	Chain	Res	Type
1	G	152	GLN
1	G	173	GLN
1	G	299	GLN
1	G	313	GLN
1	G	348	GLN
2	H	219	GLN
2	H	326	HIS
2	H	491	HIS
2	H	834	GLN
2	H	1020	GLN
2	H	1135	HIS
2	H	1190	GLN
2	H	1518	ASN
2	H	1521	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	E	401	-	32,33,33	2.76	10 (31%)	45,52,52	1.88	13 (28%)
4	GBM	H	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.88	8 (16%)
3	AGS	H	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
3	AGS	A	401	-	32,33,33	2.76	10 (31%)	45,52,52	1.88	13 (28%)
3	AGS	A	402	-	32,33,33	2.76	10 (31%)	45,52,52	1.88	13 (28%)
3	AGS	D	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
4	GBM	D	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.88	8 (16%)
3	AGS	B	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
4	GBM	F	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.88	8 (16%)
4	GBM	B	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.88	8 (16%)
3	AGS	F	2002	-	32,33,33	2.06	8 (25%)	45,52,52	1.85	9 (20%)
3	AGS	C	401	-	32,33,33	2.76	10 (31%)	45,52,52	1.88	13 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	E	401	-	-	6/21/38/38	0/3/3/3
4	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	H	2002	-	-	2/21/38/38	0/3/3/3
3	AGS	A	401	-	-	6/21/38/38	0/3/3/3
3	AGS	A	402	-	-	6/21/38/38	0/3/3/3
3	AGS	D	2002	-	-	2/21/38/38	0/3/3/3
4	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	B	2002	-	-	2/21/38/38	0/3/3/3
4	GBM	F	2001	-	-	8/27/35/35	0/3/3/3
4	GBM	B	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	F	2002	-	-	2/21/38/38	0/3/3/3
3	AGS	C	401	-	-	6/21/38/38	0/3/3/3

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AGS	PG-S1G	10.14	2.12	1.90
3	A	402	AGS	PG-S1G	10.14	2.12	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	AGS	PG-S1G	10.14	2.12	1.90
3	E	401	AGS	PG-S1G	10.14	2.12	1.90
4	B	2001	GBM	C18-S2	-10.10	1.60	1.76
4	D	2001	GBM	C18-S2	-10.10	1.60	1.76
4	F	2001	GBM	C18-S2	-10.10	1.60	1.76
4	H	2001	GBM	C18-S2	-10.10	1.60	1.76
3	B	2002	AGS	PG-S1G	7.97	2.08	1.90
3	D	2002	AGS	PG-S1G	7.97	2.08	1.90
3	F	2002	AGS	PG-S1G	7.97	2.08	1.90
3	H	2002	AGS	PG-S1G	7.97	2.08	1.90
3	A	401	AGS	PB-O3A	-6.06	1.53	1.59
3	A	402	AGS	PB-O3A	-6.06	1.53	1.59
3	C	401	AGS	PB-O3A	-6.06	1.53	1.59
3	E	401	AGS	PB-O3A	-6.06	1.53	1.59
3	A	401	AGS	PA-O3A	-5.92	1.53	1.59
3	A	402	AGS	PA-O3A	-5.92	1.53	1.59
3	C	401	AGS	PA-O3A	-5.92	1.53	1.59
3	E	401	AGS	PA-O3A	-5.92	1.53	1.59
4	B	2001	GBM	C27-C28	4.77	1.49	1.40
4	D	2001	GBM	C27-C28	4.77	1.49	1.40
4	F	2001	GBM	C27-C28	4.77	1.49	1.40
4	H	2001	GBM	C27-C28	4.77	1.49	1.40
3	B	2002	AGS	C5-C4	4.70	1.47	1.39
3	D	2002	AGS	C5-C4	4.70	1.47	1.39
3	F	2002	AGS	C5-C4	4.70	1.47	1.39
3	H	2002	AGS	C5-C4	4.70	1.47	1.39
3	A	401	AGS	C5-C4	4.52	1.47	1.39
3	A	402	AGS	C5-C4	4.52	1.47	1.39
3	C	401	AGS	C5-C4	4.52	1.47	1.39
3	E	401	AGS	C5-C4	4.52	1.47	1.39
3	A	401	AGS	PG-O2G	3.29	1.65	1.54
3	A	402	AGS	PG-O2G	3.29	1.65	1.54
3	C	401	AGS	PG-O2G	3.29	1.65	1.54
3	E	401	AGS	PG-O2G	3.29	1.65	1.54
3	B	2002	AGS	C5-C6	2.78	1.48	1.41
3	D	2002	AGS	C5-C6	2.78	1.48	1.41
3	F	2002	AGS	C5-C6	2.78	1.48	1.41
3	H	2002	AGS	C5-C6	2.78	1.48	1.41
3	A	401	AGS	C5-N7	-2.65	1.34	1.39
3	A	402	AGS	C5-N7	-2.65	1.34	1.39
3	C	401	AGS	C5-N7	-2.65	1.34	1.39
3	E	401	AGS	C5-N7	-2.65	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	GBM	C31-CL1	2.42	1.80	1.74
4	D	2001	GBM	C31-CL1	2.42	1.80	1.74
4	F	2001	GBM	C31-CL1	2.42	1.80	1.74
4	H	2001	GBM	C31-CL1	2.42	1.80	1.74
3	B	2002	AGS	C8-N7	2.34	1.36	1.31
3	D	2002	AGS	C8-N7	2.34	1.36	1.31
3	F	2002	AGS	C8-N7	2.34	1.36	1.31
3	H	2002	AGS	C8-N7	2.34	1.36	1.31
3	B	2002	AGS	C5-N7	-2.29	1.34	1.39
3	D	2002	AGS	C5-N7	-2.29	1.34	1.39
3	F	2002	AGS	C5-N7	-2.29	1.34	1.39
3	H	2002	AGS	C5-N7	-2.29	1.34	1.39
3	A	401	AGS	C5-C6	2.23	1.47	1.41
3	A	402	AGS	C5-C6	2.23	1.47	1.41
3	C	401	AGS	C5-C6	2.23	1.47	1.41
3	E	401	AGS	C5-C6	2.23	1.47	1.41
4	B	2001	GBM	C17-N9	-2.20	1.34	1.39
4	D	2001	GBM	C17-N9	-2.20	1.34	1.39
4	F	2001	GBM	C17-N9	-2.20	1.34	1.39
4	H	2001	GBM	C17-N9	-2.20	1.34	1.39
3	B	2002	AGS	PB-O3A	2.20	1.61	1.59
3	D	2002	AGS	PB-O3A	2.20	1.61	1.59
3	F	2002	AGS	PB-O3A	2.20	1.61	1.59
3	H	2002	AGS	PB-O3A	2.20	1.61	1.59
3	A	401	AGS	C4-N9	-2.10	1.33	1.37
3	A	402	AGS	C4-N9	-2.10	1.33	1.37
3	C	401	AGS	C4-N9	-2.10	1.33	1.37
3	E	401	AGS	C4-N9	-2.10	1.33	1.37
3	A	401	AGS	PB-O3B	-2.10	1.57	1.59
3	A	402	AGS	PB-O3B	-2.10	1.57	1.59
3	C	401	AGS	PB-O3B	-2.10	1.57	1.59
3	E	401	AGS	PB-O3B	-2.10	1.57	1.59
3	A	401	AGS	C8-N7	2.09	1.35	1.31
3	A	402	AGS	C8-N7	2.09	1.35	1.31
3	C	401	AGS	C8-N7	2.09	1.35	1.31
3	E	401	AGS	C8-N7	2.09	1.35	1.31
3	B	2002	AGS	PA-O3A	2.09	1.61	1.59
3	D	2002	AGS	PA-O3A	2.09	1.61	1.59
3	F	2002	AGS	PA-O3A	2.09	1.61	1.59
3	H	2002	AGS	PA-O3A	2.09	1.61	1.59
3	B	2002	AGS	PG-O2G	2.08	1.61	1.54
3	D	2002	AGS	PG-O2G	2.08	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2002	AGS	PG-O2G	2.08	1.61	1.54
3	H	2002	AGS	PG-O2G	2.08	1.61	1.54

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	GBM	O5-S2-O4	-9.80	107.62	119.52
4	D	2001	GBM	O5-S2-O4	-9.80	107.62	119.52
4	F	2001	GBM	O5-S2-O4	-9.80	107.62	119.52
4	H	2001	GBM	O5-S2-O4	-9.80	107.62	119.52
3	B	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	D	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	F	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	H	2002	AGS	C5-C4-N3	-5.92	118.57	126.72
3	A	401	AGS	C5-C4-N3	-5.51	119.14	126.72
3	A	402	AGS	C5-C4-N3	-5.51	119.14	126.72
3	C	401	AGS	C5-C4-N3	-5.51	119.14	126.72
3	E	401	AGS	C5-C4-N3	-5.51	119.14	126.72
3	B	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	D	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	F	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	H	2002	AGS	N3-C4-N9	4.72	135.20	127.17
3	A	401	AGS	N3-C4-N9	4.51	134.83	127.17
3	A	402	AGS	N3-C4-N9	4.51	134.83	127.17
3	C	401	AGS	N3-C4-N9	4.51	134.83	127.17
3	E	401	AGS	N3-C4-N9	4.51	134.83	127.17
4	B	2001	GBM	O7-C28-C27	3.76	122.01	116.55
4	D	2001	GBM	O7-C28-C27	3.76	122.01	116.55
4	F	2001	GBM	O7-C28-C27	3.76	122.01	116.55
4	H	2001	GBM	O7-C28-C27	3.76	122.01	116.55
3	B	2002	AGS	C2-N3-C4	3.72	120.91	111.83
3	D	2002	AGS	C2-N3-C4	3.72	120.91	111.83
3	F	2002	AGS	C2-N3-C4	3.72	120.91	111.83
3	H	2002	AGS	C2-N3-C4	3.72	120.91	111.83
3	B	2002	AGS	C4-C5-N7	-3.38	106.71	110.58
3	D	2002	AGS	C4-C5-N7	-3.38	106.71	110.58
3	F	2002	AGS	C4-C5-N7	-3.38	106.71	110.58
3	H	2002	AGS	C4-C5-N7	-3.38	106.71	110.58
3	A	401	AGS	C2-N3-C4	3.29	119.87	111.83
3	A	402	AGS	C2-N3-C4	3.29	119.87	111.83
3	C	401	AGS	C2-N3-C4	3.29	119.87	111.83
3	E	401	AGS	C2-N3-C4	3.29	119.87	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	AGS	PB-O3B-PG	-3.28	121.18	133.17
3	D	2002	AGS	PB-O3B-PG	-3.28	121.18	133.17
3	F	2002	AGS	PB-O3B-PG	-3.28	121.18	133.17
3	H	2002	AGS	PB-O3B-PG	-3.28	121.18	133.17
3	B	2002	AGS	N3-C2-N1	-3.23	123.70	128.58
3	D	2002	AGS	N3-C2-N1	-3.23	123.70	128.58
3	F	2002	AGS	N3-C2-N1	-3.23	123.70	128.58
3	H	2002	AGS	N3-C2-N1	-3.23	123.70	128.58
4	B	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	D	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	F	2001	GBM	C18-S2-N9	3.03	110.89	106.06
4	H	2001	GBM	C18-S2-N9	3.03	110.89	106.06
3	A	401	AGS	N3-C2-N1	-2.98	124.08	128.58
3	A	402	AGS	N3-C2-N1	-2.98	124.08	128.58
3	C	401	AGS	N3-C2-N1	-2.98	124.08	128.58
3	E	401	AGS	N3-C2-N1	-2.98	124.08	128.58
3	A	401	AGS	C4-C5-N7	-2.92	107.24	110.58
3	A	402	AGS	C4-C5-N7	-2.92	107.24	110.58
3	C	401	AGS	C4-C5-N7	-2.92	107.24	110.58
3	E	401	AGS	C4-C5-N7	-2.92	107.24	110.58
4	B	2001	GBM	O7-C28-C30	-2.91	119.40	124.30
4	D	2001	GBM	O7-C28-C30	-2.91	119.40	124.30
4	F	2001	GBM	O7-C28-C30	-2.91	119.40	124.30
4	H	2001	GBM	O7-C28-C30	-2.91	119.40	124.30
3	A	401	AGS	PB-O3B-PG	-2.83	122.81	133.17
3	A	402	AGS	PB-O3B-PG	-2.83	122.81	133.17
3	C	401	AGS	PB-O3B-PG	-2.83	122.81	133.17
3	E	401	AGS	PB-O3B-PG	-2.83	122.81	133.17
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-N9-C8	2.61	108.48	105.74
3	D	2002	AGS	C4-N9-C8	2.61	108.48	105.74
3	F	2002	AGS	C4-N9-C8	2.61	108.48	105.74
3	H	2002	AGS	C4-N9-C8	2.61	108.48	105.74
3	A	401	AGS	C3'-C2'-C1'	2.60	106.38	101.46
3	A	402	AGS	C3'-C2'-C1'	2.60	106.38	101.46
3	C	401	AGS	C3'-C2'-C1'	2.60	106.38	101.46
3	E	401	AGS	C3'-C2'-C1'	2.60	106.38	101.46
3	A	401	AGS	O2B-PB-O3A	2.58	114.25	107.27
3	A	402	AGS	O2B-PB-O3A	2.58	114.25	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	AGS	O2B-PB-O3A	2.58	114.25	107.27
3	E	401	AGS	O2B-PB-O3A	2.58	114.25	107.27
3	B	2002	AGS	C5-N7-C8	2.49	107.37	103.45
3	D	2002	AGS	C5-N7-C8	2.49	107.37	103.45
3	F	2002	AGS	C5-N7-C8	2.49	107.37	103.45
3	H	2002	AGS	C5-N7-C8	2.49	107.37	103.45
3	B	2002	AGS	C3'-C2'-C1'	2.46	106.12	101.46
3	D	2002	AGS	C3'-C2'-C1'	2.46	106.12	101.46
3	F	2002	AGS	C3'-C2'-C1'	2.46	106.12	101.46
3	H	2002	AGS	C3'-C2'-C1'	2.46	106.12	101.46
3	A	401	AGS	C4-N9-C8	2.44	108.30	105.74
3	A	402	AGS	C4-N9-C8	2.44	108.30	105.74
3	C	401	AGS	C4-N9-C8	2.44	108.30	105.74
3	E	401	AGS	C4-N9-C8	2.44	108.30	105.74
3	A	401	AGS	O2B-PB-O1B	-2.42	101.20	112.44
3	A	402	AGS	O2B-PB-O1B	-2.42	101.20	112.44
3	C	401	AGS	O2B-PB-O1B	-2.42	101.20	112.44
3	E	401	AGS	O2B-PB-O1B	-2.42	101.20	112.44
4	B	2001	GBM	C25-C20-C19	-2.30	107.66	112.83
4	D	2001	GBM	C25-C20-C19	-2.30	107.66	112.83
4	F	2001	GBM	C25-C20-C19	-2.30	107.66	112.83
4	H	2001	GBM	C25-C20-C19	-2.30	107.66	112.83
4	B	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	D	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	F	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
4	H	2001	GBM	C28-C27-C26	-2.13	122.40	126.24
3	A	401	AGS	C5-N7-C8	2.12	106.79	103.45
3	A	402	AGS	C5-N7-C8	2.12	106.79	103.45
3	C	401	AGS	C5-N7-C8	2.12	106.79	103.45
3	E	401	AGS	C5-N7-C8	2.12	106.79	103.45
4	B	2001	GBM	C33-O7-C28	2.11	120.61	117.51
4	D	2001	GBM	C33-O7-C28	2.11	120.61	117.51
4	F	2001	GBM	C33-O7-C28	2.11	120.61	117.51
4	H	2001	GBM	C33-O7-C28	2.11	120.61	117.51
3	A	401	AGS	C2-N1-C6	2.11	122.19	118.73
3	A	402	AGS	C2-N1-C6	2.11	122.19	118.73
3	C	401	AGS	C2-N1-C6	2.11	122.19	118.73
3	E	401	AGS	C2-N1-C6	2.11	122.19	118.73
4	B	2001	GBM	C30-C32-C31	2.01	121.27	119.24
4	D	2001	GBM	C30-C32-C31	2.01	121.27	119.24
4	F	2001	GBM	C30-C32-C31	2.01	121.27	119.24
4	H	2001	GBM	C30-C32-C31	2.01	121.27	119.24

There are no chirality outliers.

All (64) 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
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
4	D	2001	GBM	C27-C28-O7-C33
4	F	2001	GBM	C27-C28-O7-C33
4	H	2001	GBM	C27-C28-O7-C33
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	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

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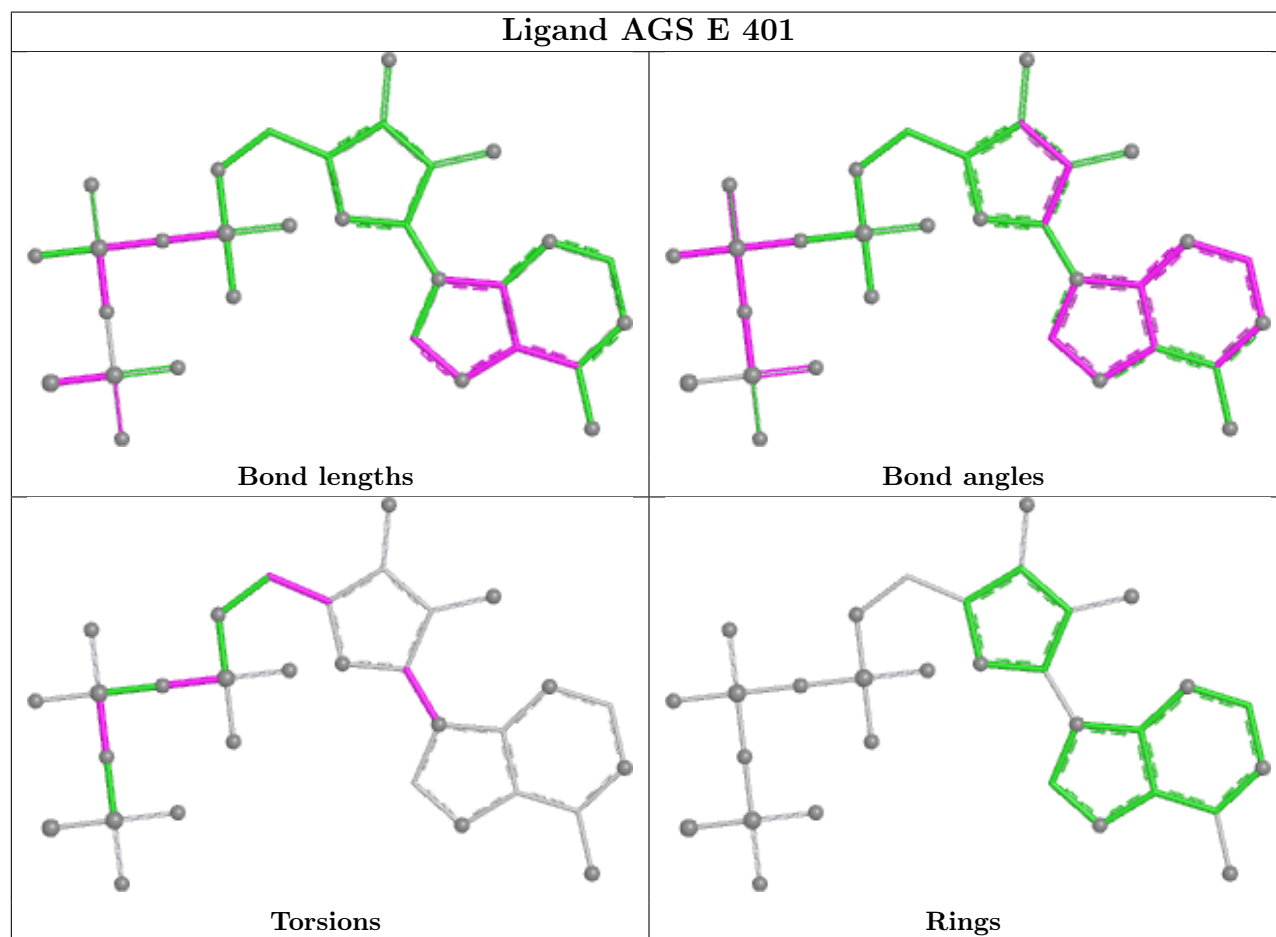
Mol	Chain	Res	Type	Atoms
4	B	2001	GBM	C23-C19-C20-C25
4	D	2001	GBM	C23-C19-C20-C25
4	F	2001	GBM	C23-C19-C20-C25
4	H	2001	GBM	C23-C19-C20-C25
3	A	401	AGS	PG-O3B-PB-O2B
3	A	402	AGS	PG-O3B-PB-O2B
3	C	401	AGS	PG-O3B-PB-O2B
3	E	401	AGS	PG-O3B-PB-O2B
3	A	401	AGS	PB-O3A-PA-O1A
3	A	402	AGS	PB-O3A-PA-O1A
3	C	401	AGS	PB-O3A-PA-O1A
3	E	401	AGS	PB-O3A-PA-O1A
3	A	401	AGS	C2'-C1'-N9-C8
3	A	402	AGS	C2'-C1'-N9-C8
3	C	401	AGS	C2'-C1'-N9-C8
3	E	401	AGS	C2'-C1'-N9-C8
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.

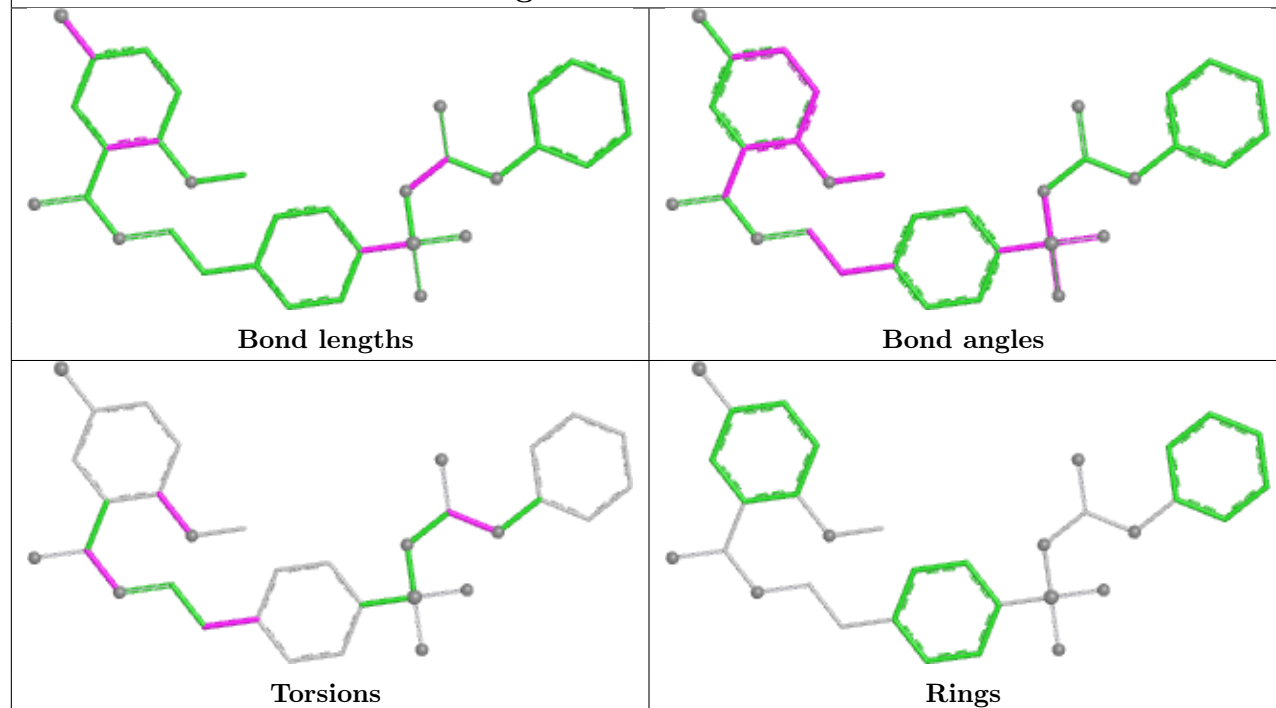
12 monomers are involved in 42 short contacts:

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

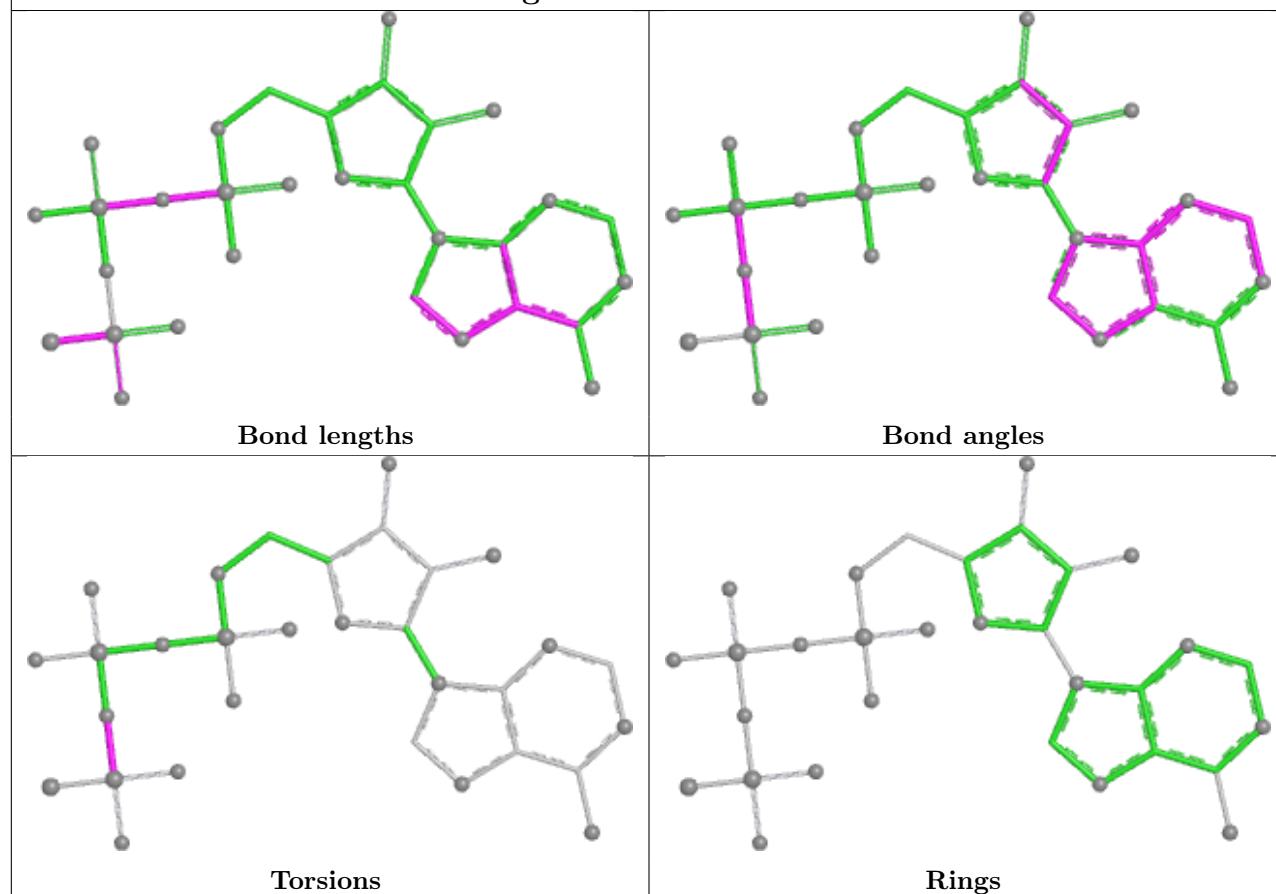
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

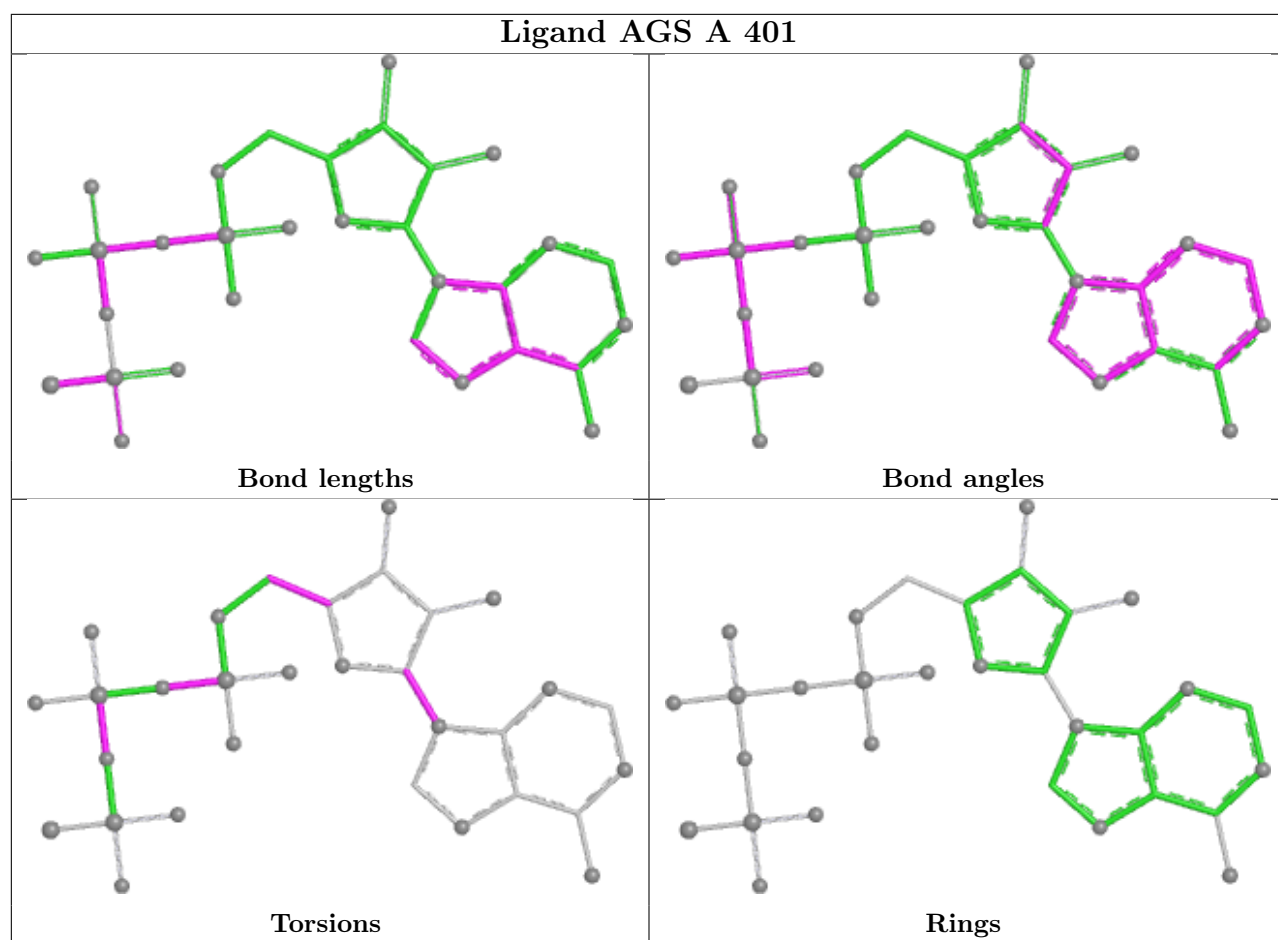


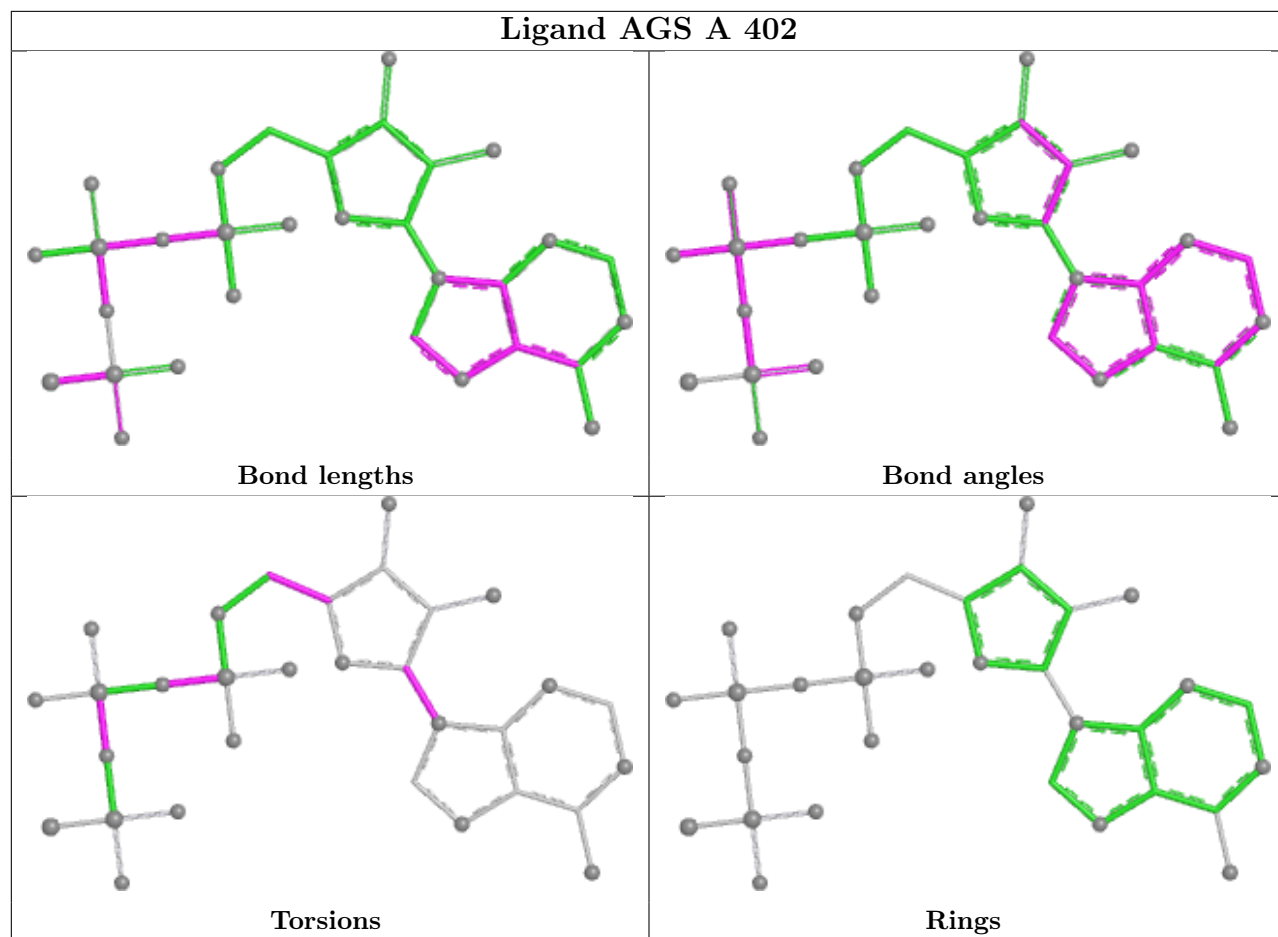
Ligand GBM H 2001

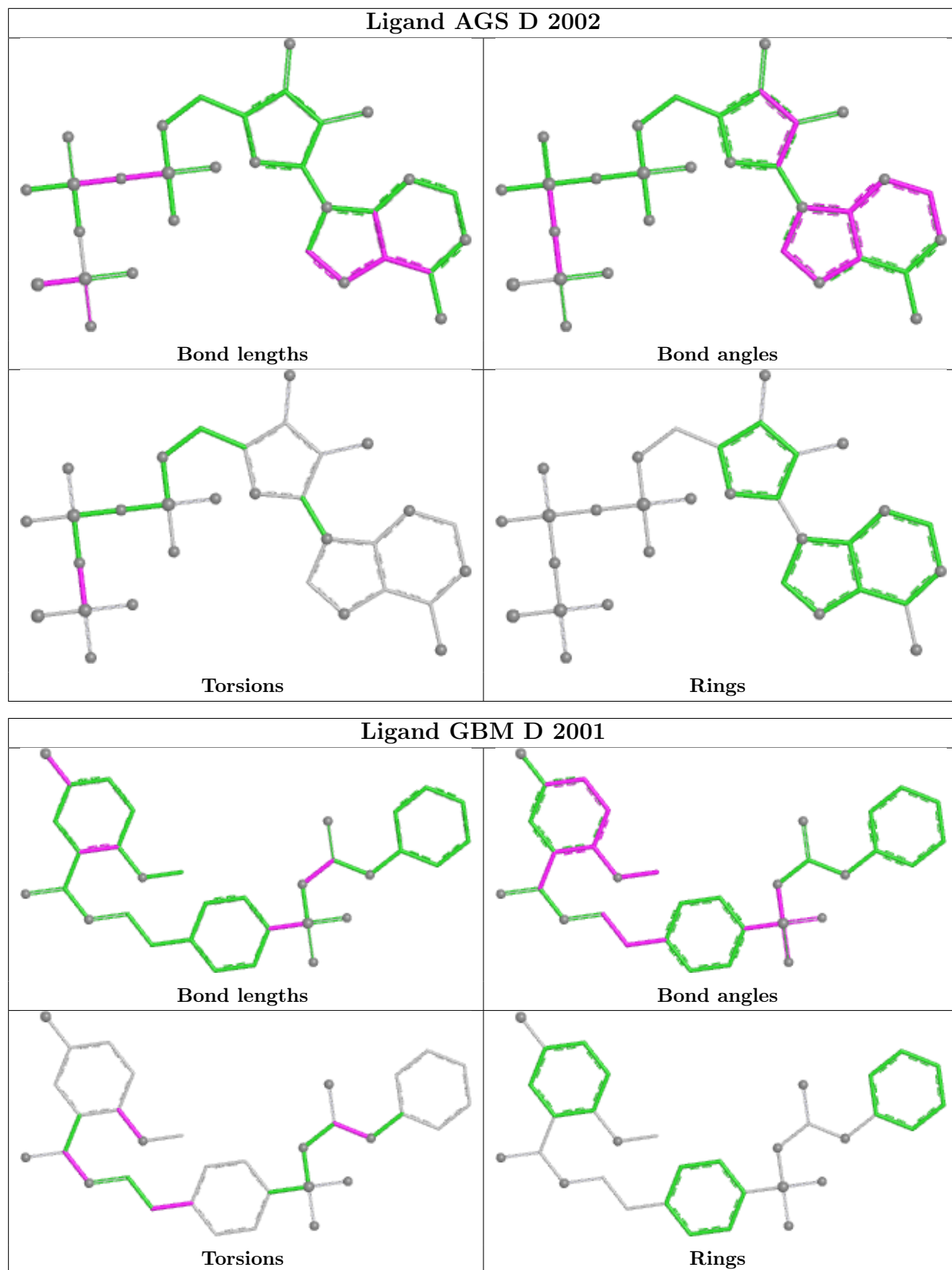


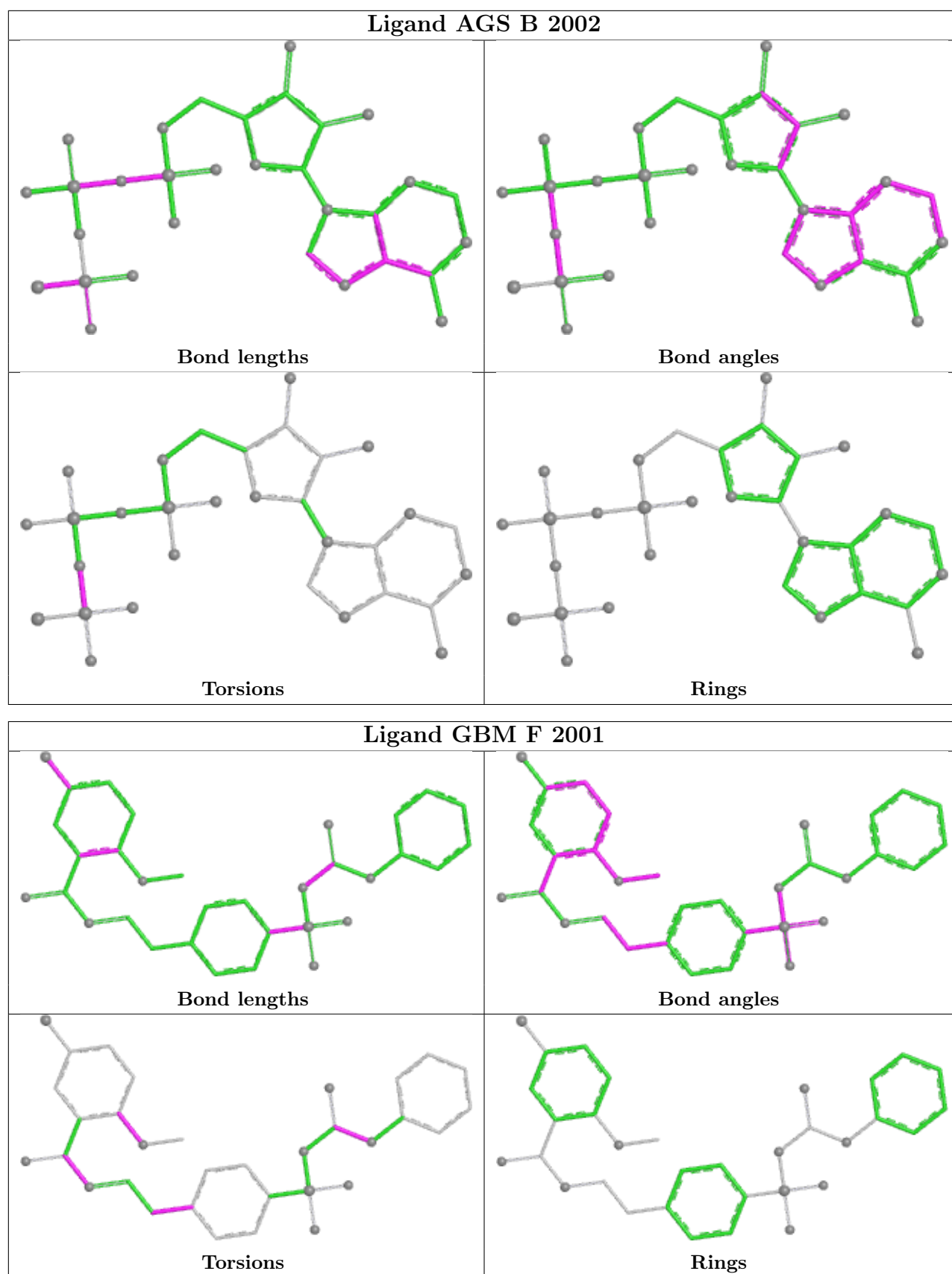
Ligand AGS H 2002



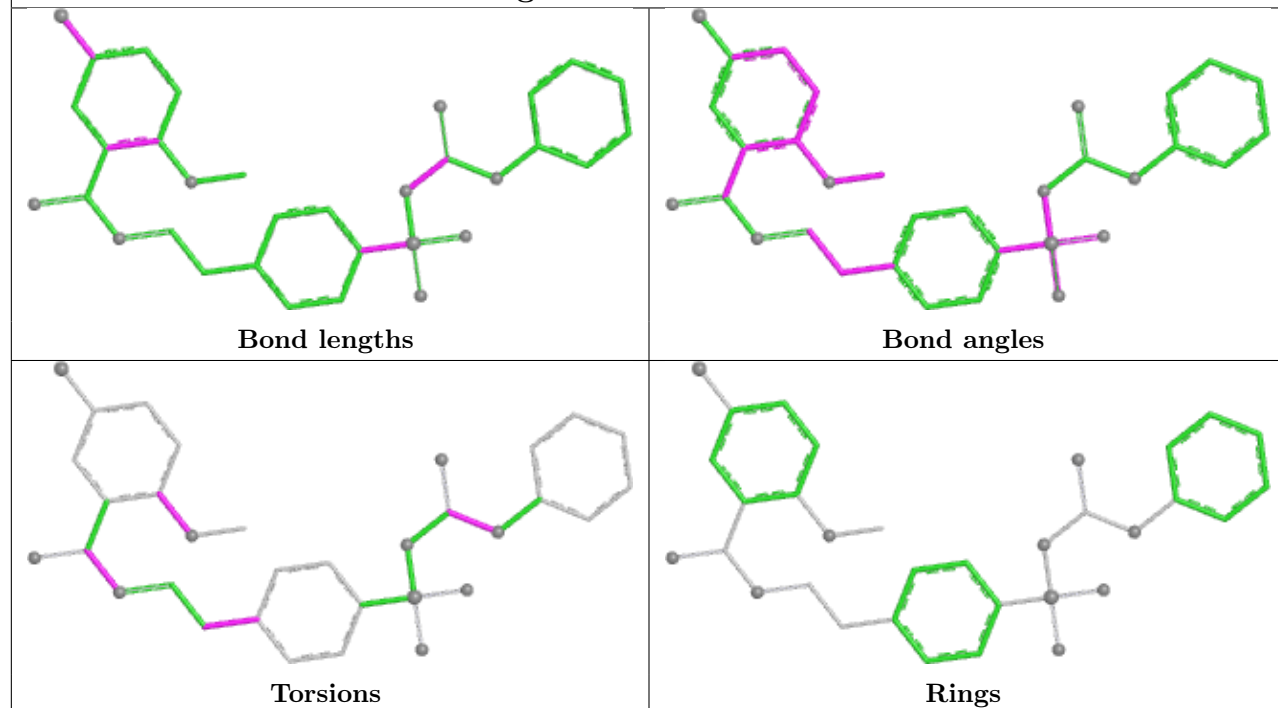




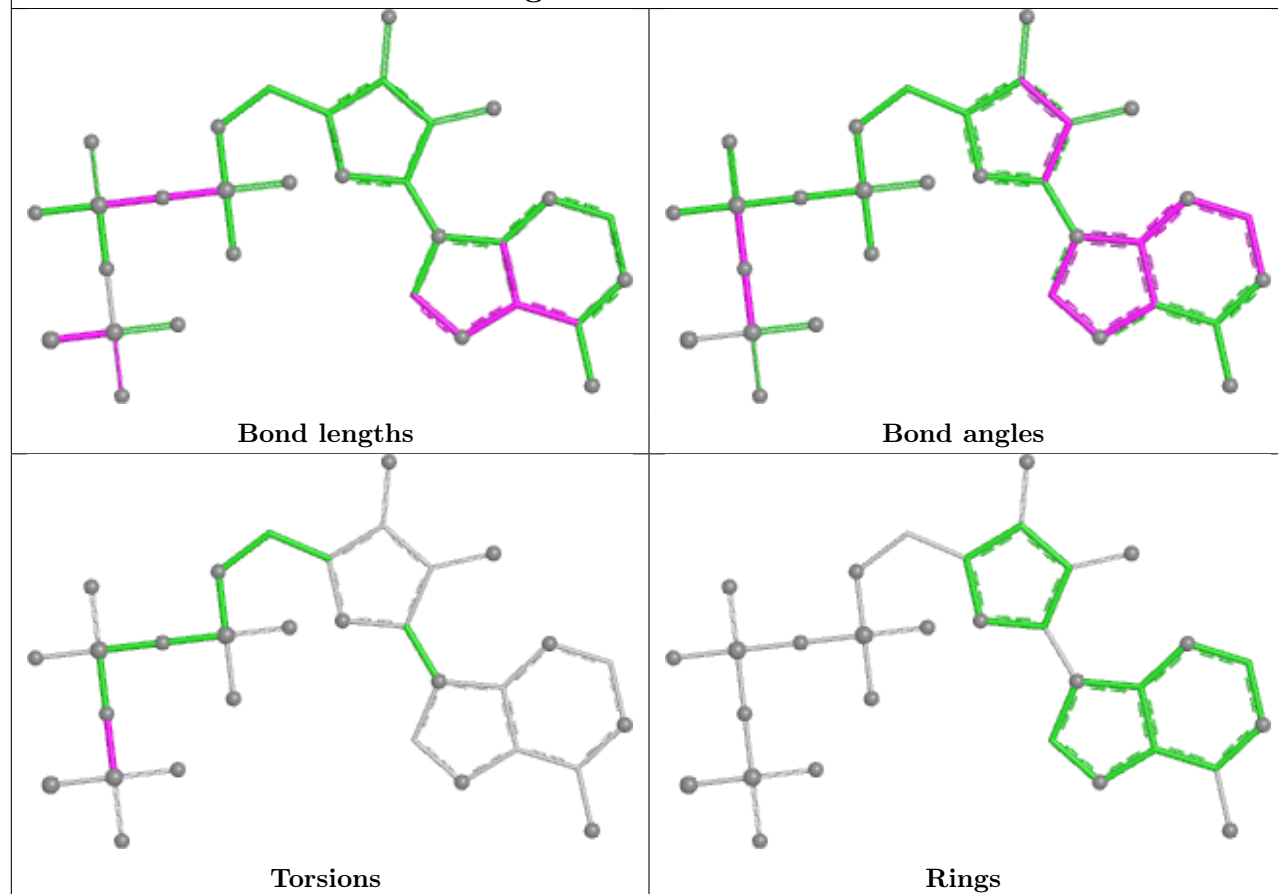


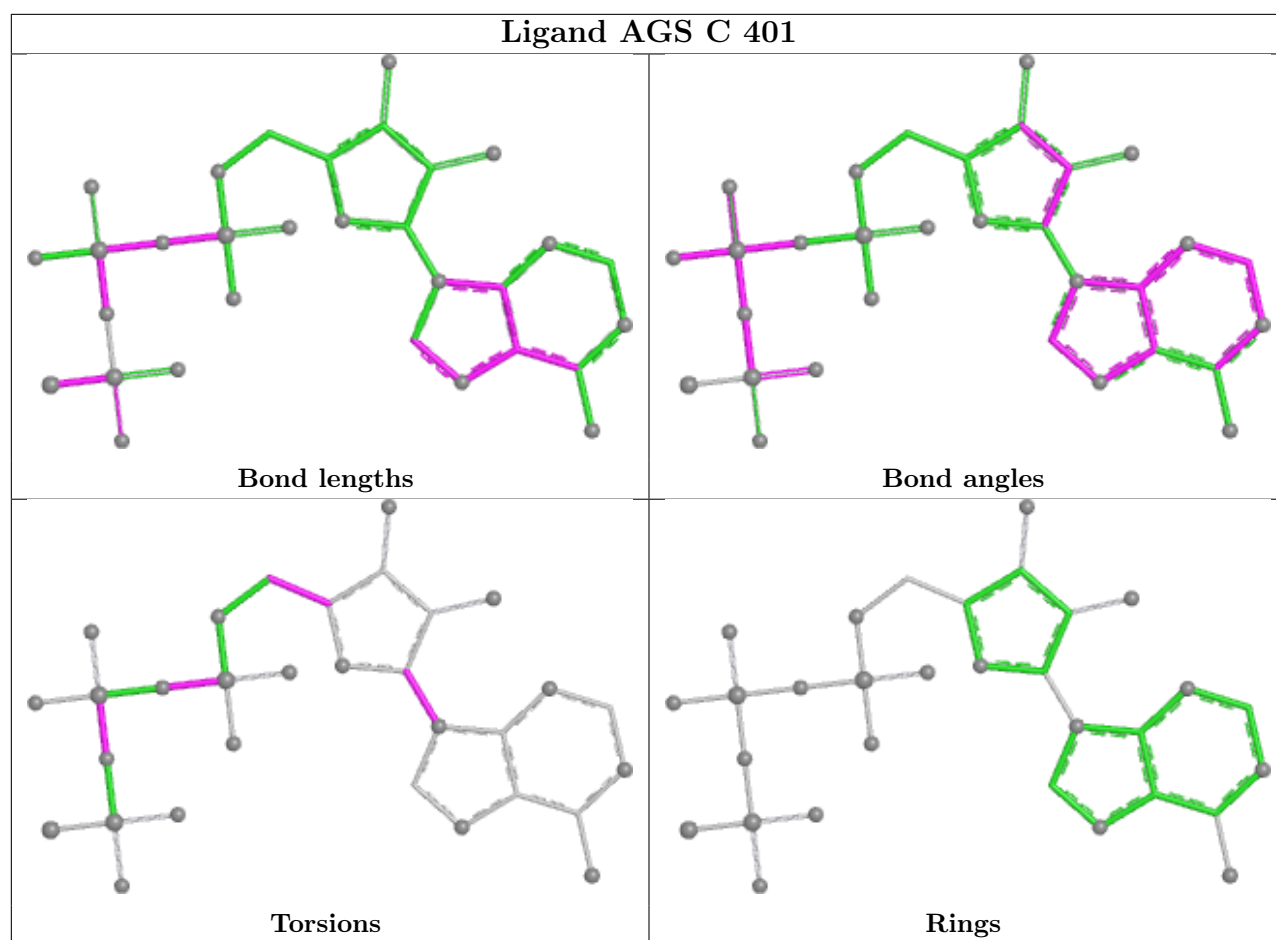


Ligand GBM B 2001



Ligand AGS F 2002





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.

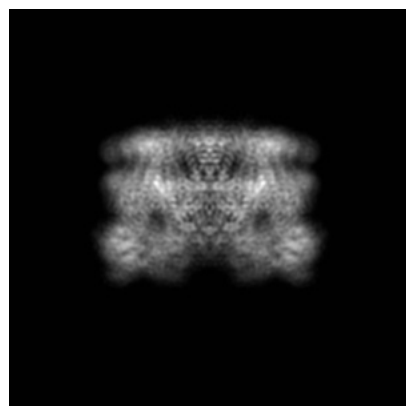
6 Map visualisation [i](#)

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.

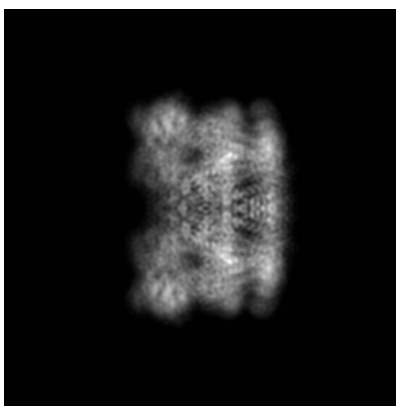
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

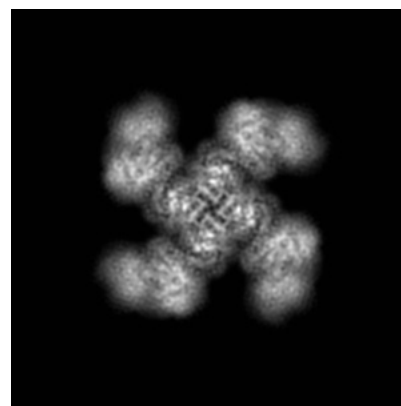
6.1.1 Primary map



X

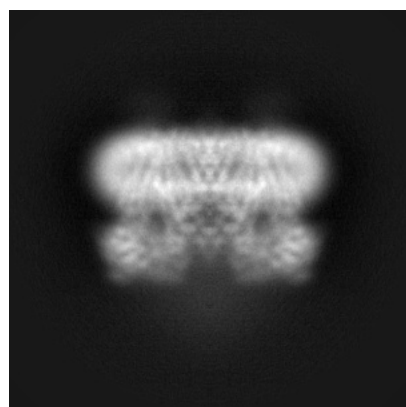


Y

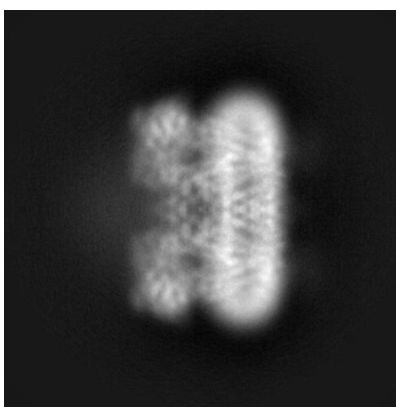


Z

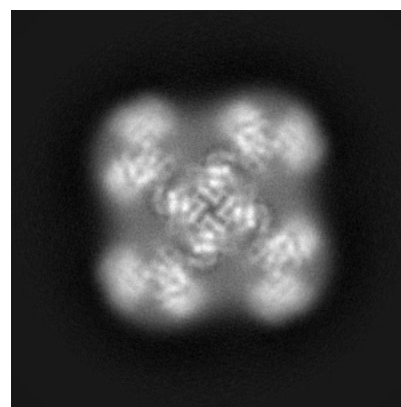
6.1.2 Raw map



X



Y

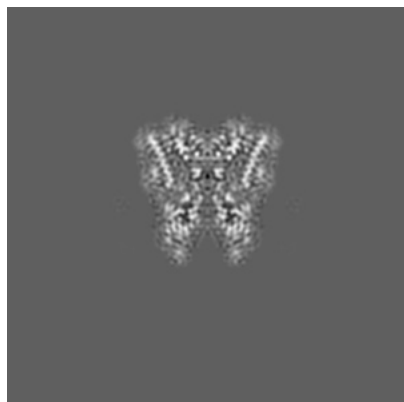


Z

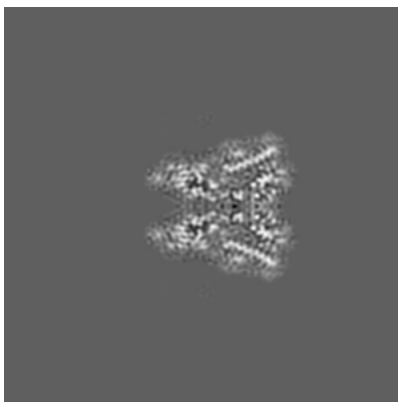
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

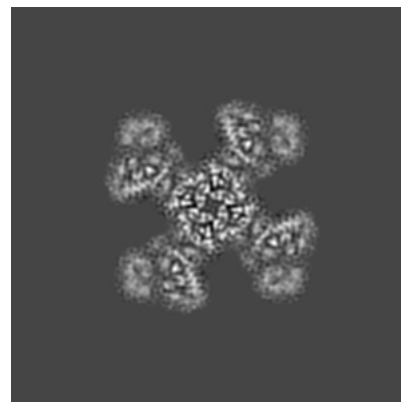
6.2.1 Primary map



X Index: 156

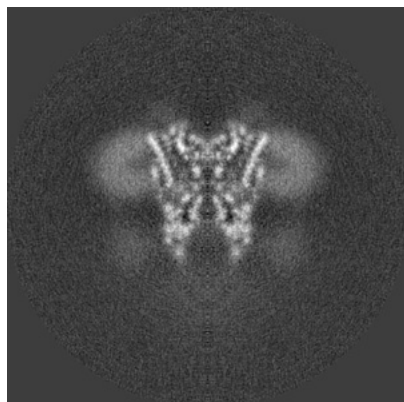


Y Index: 156

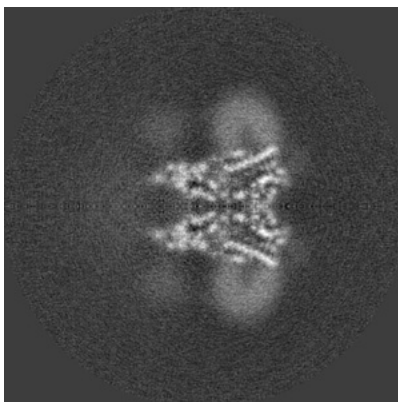


Z Index: 156

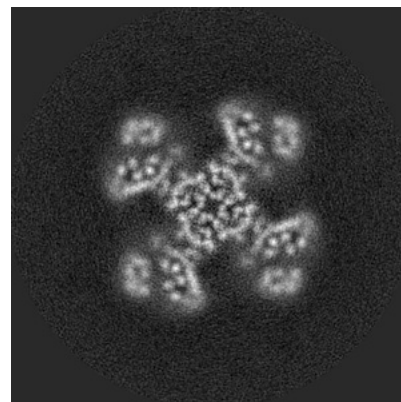
6.2.2 Raw map



X Index: 156



Y Index: 156

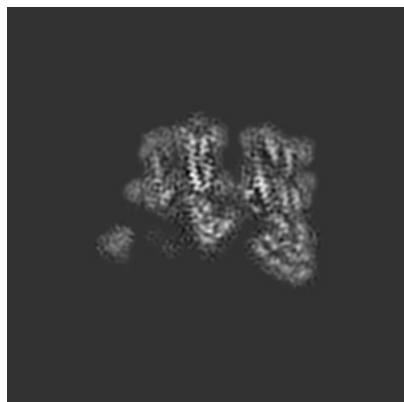


Z Index: 156

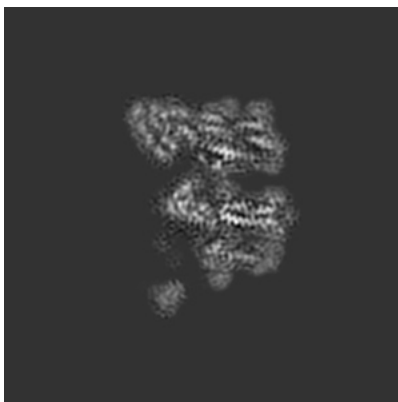
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

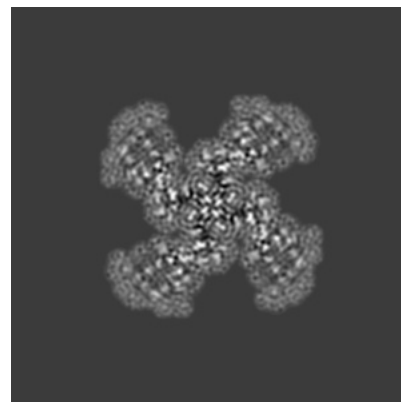
6.3.1 Primary map



X Index: 187

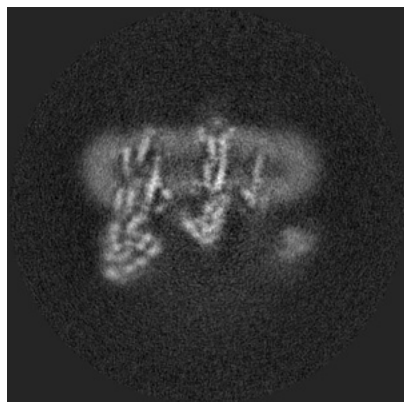


Y Index: 125

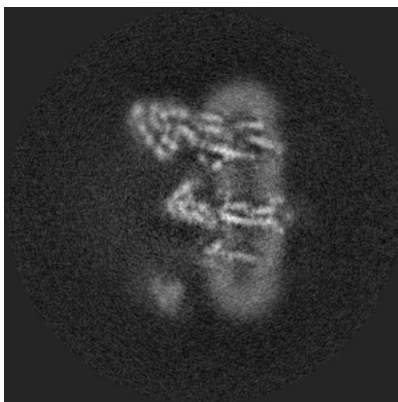


Z Index: 175

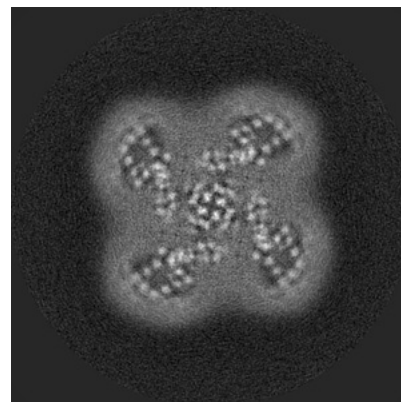
6.3.2 Raw map



X Index: 125



Y Index: 125

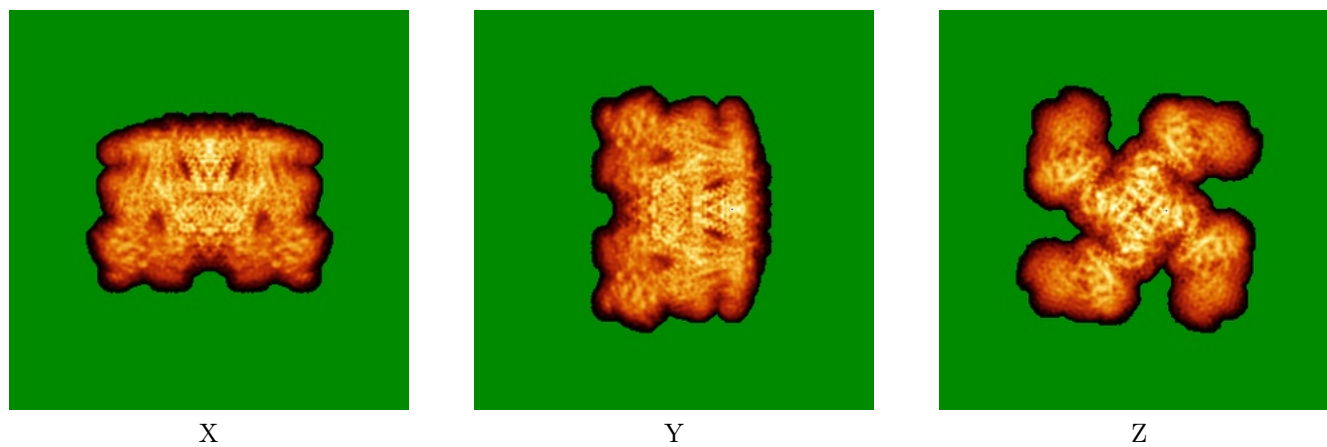


Z Index: 173

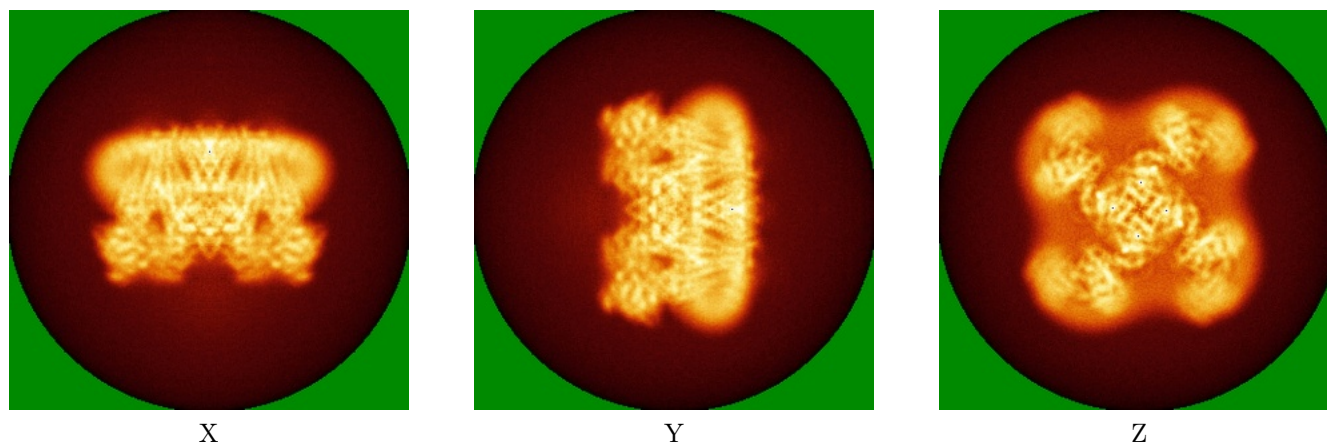
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

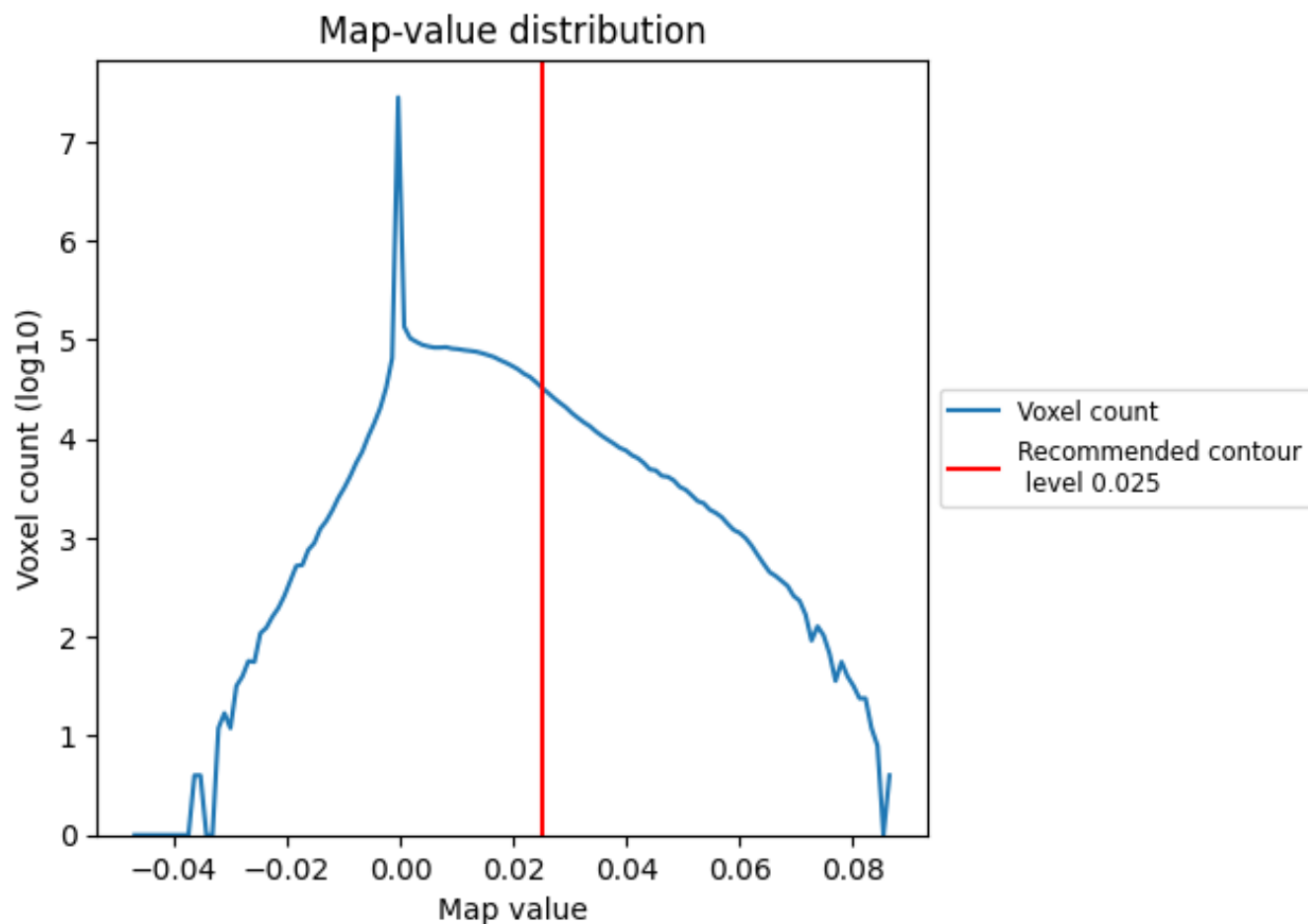
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

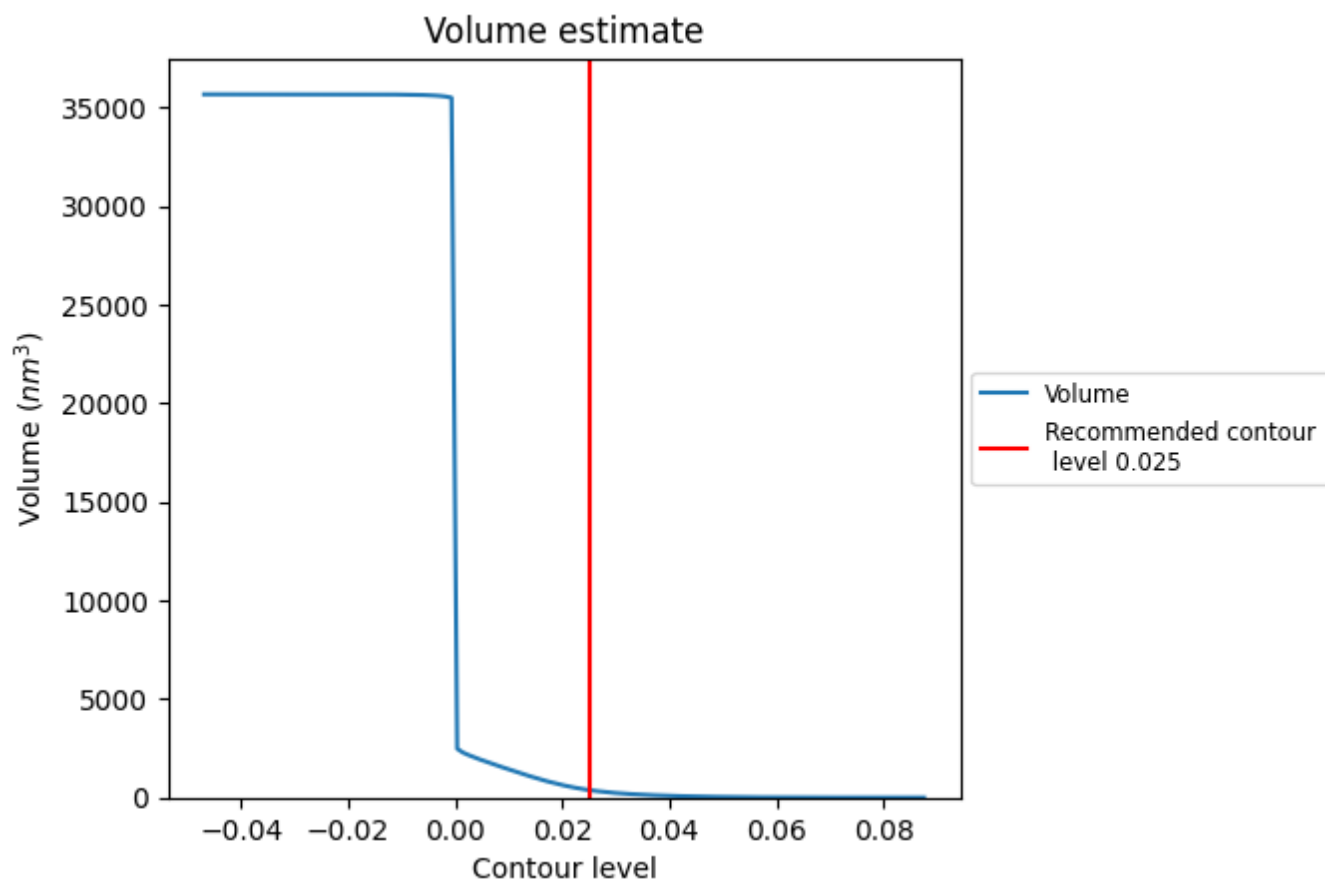
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

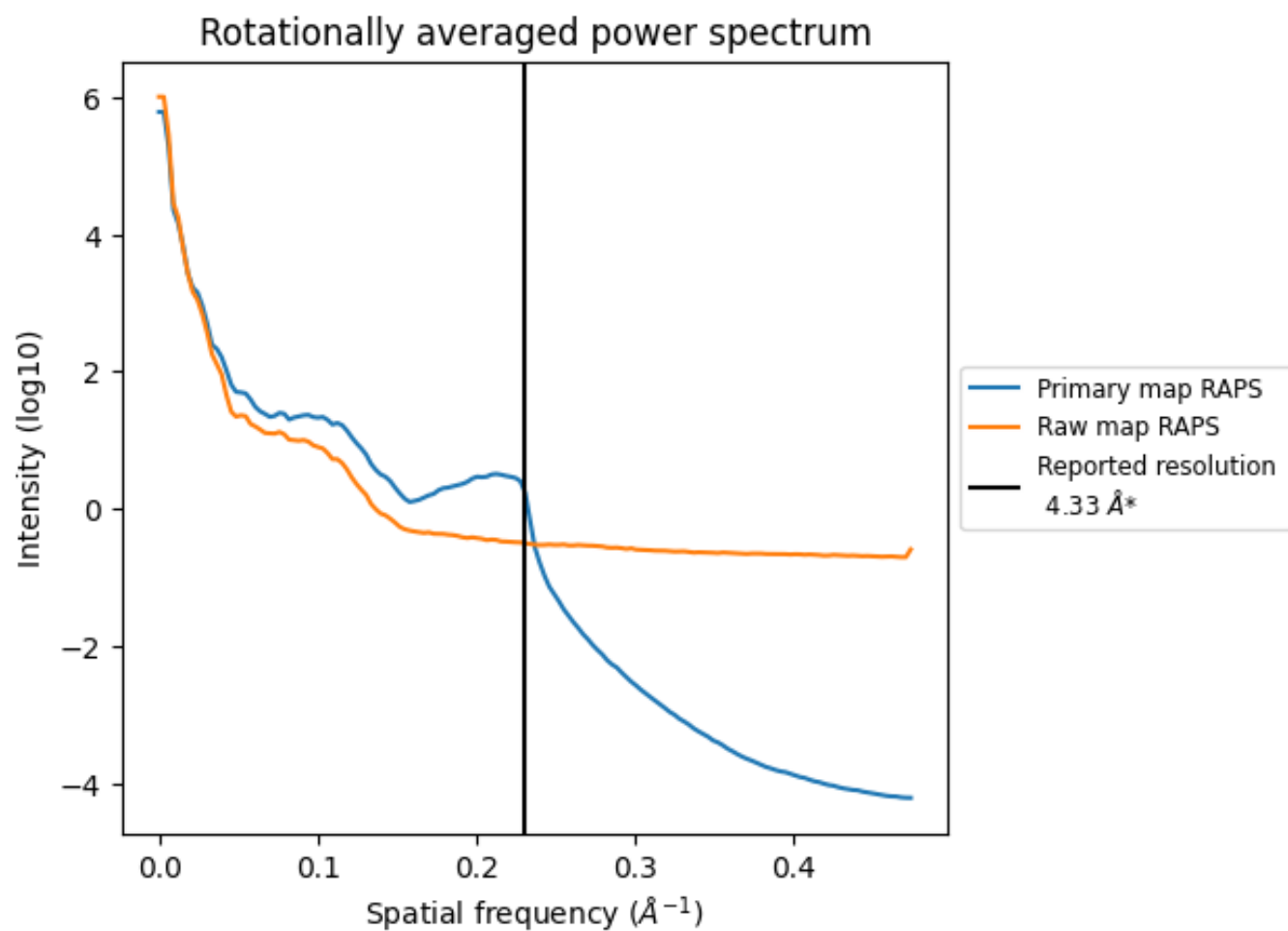
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm³; 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 ⓘ

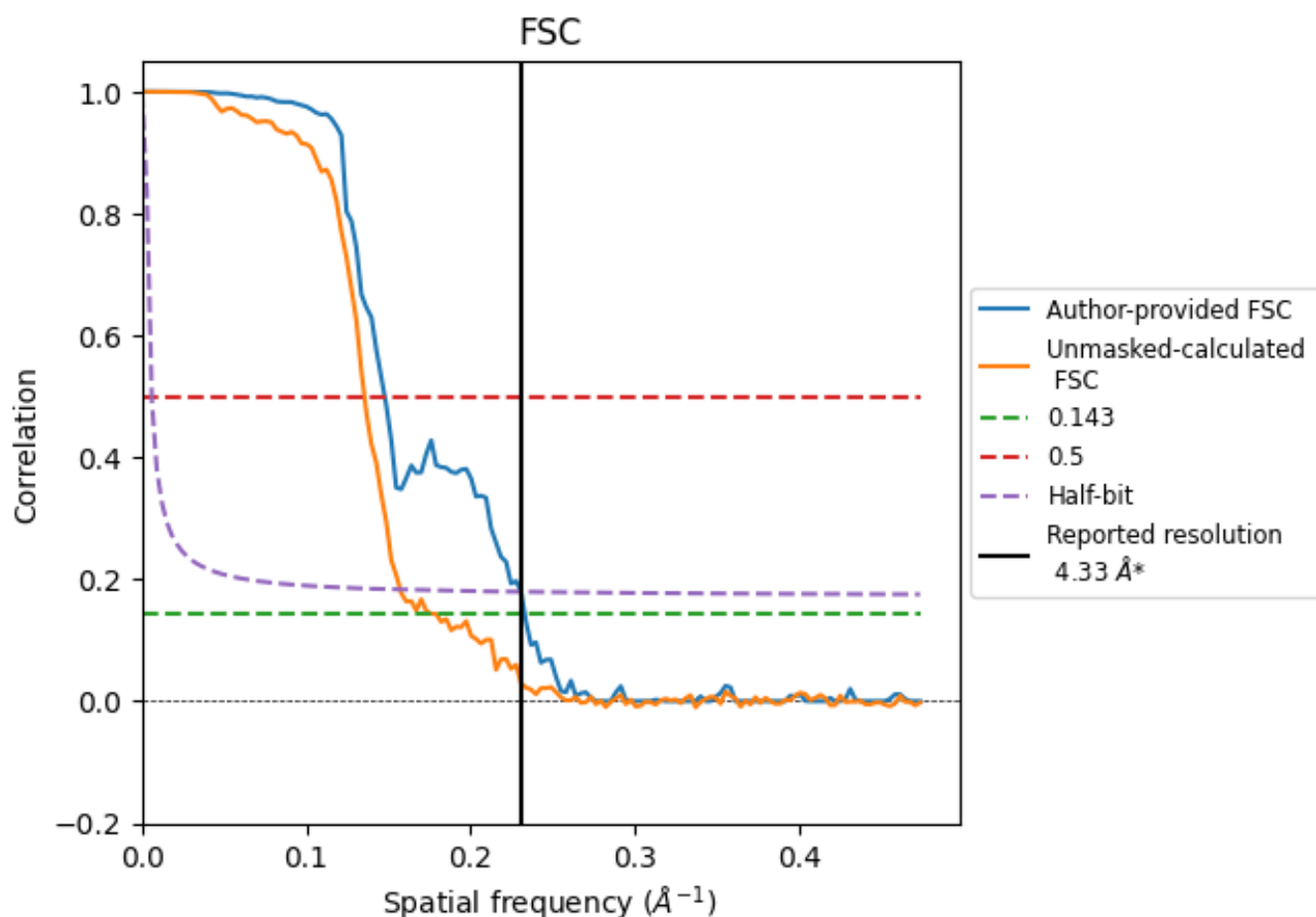


*Reported resolution corresponds to spatial frequency of $0.231 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.231 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

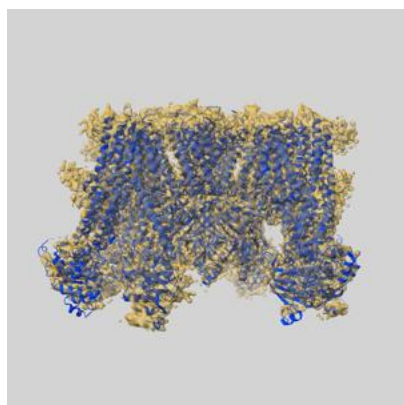
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.29	6.77	4.33
Unmasked-calculated*	5.58	7.38	6.35

*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 %

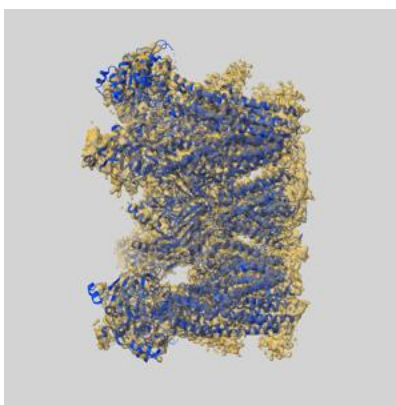
9 Map-model fit [i](#)

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 7.

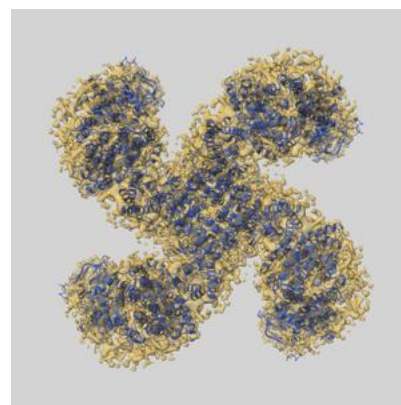
9.1 Map-model overlay [i](#)



X



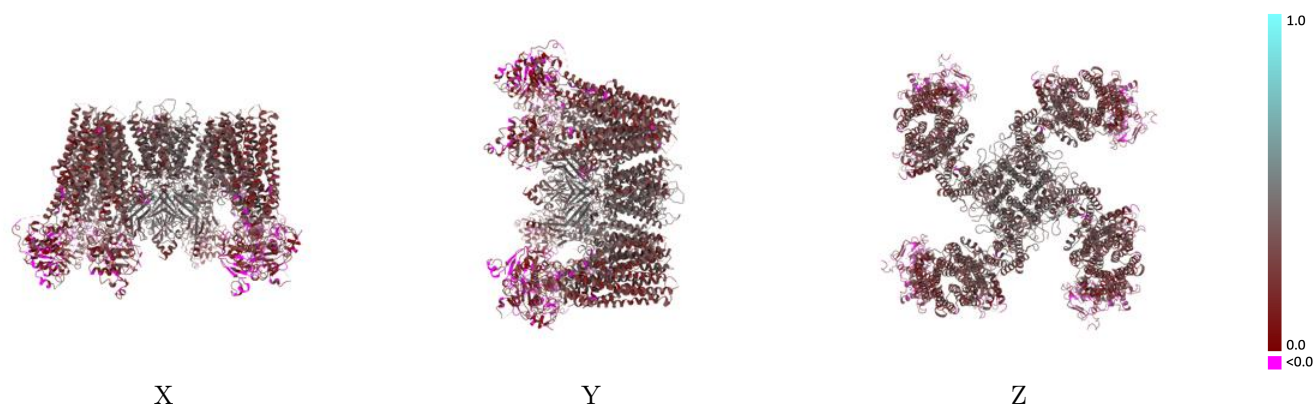
Y



Z

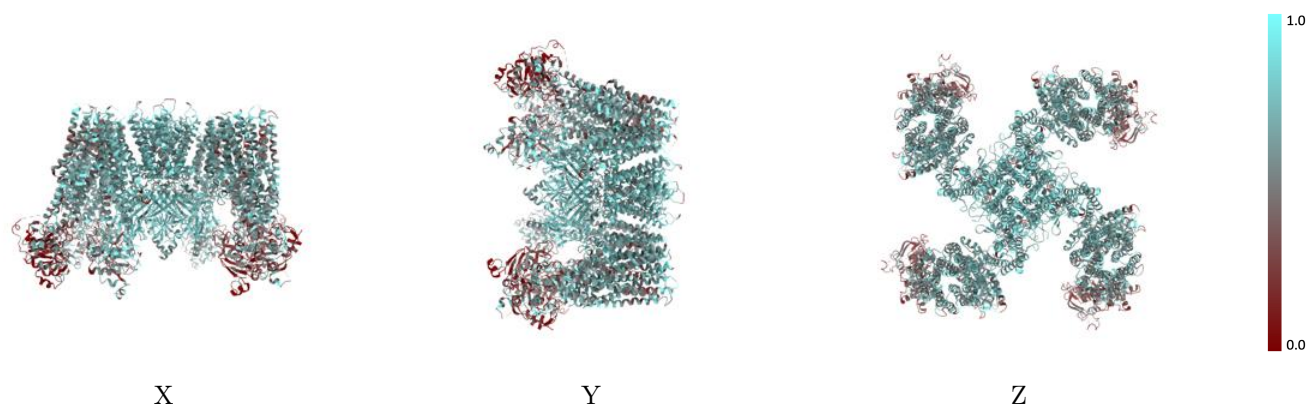
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



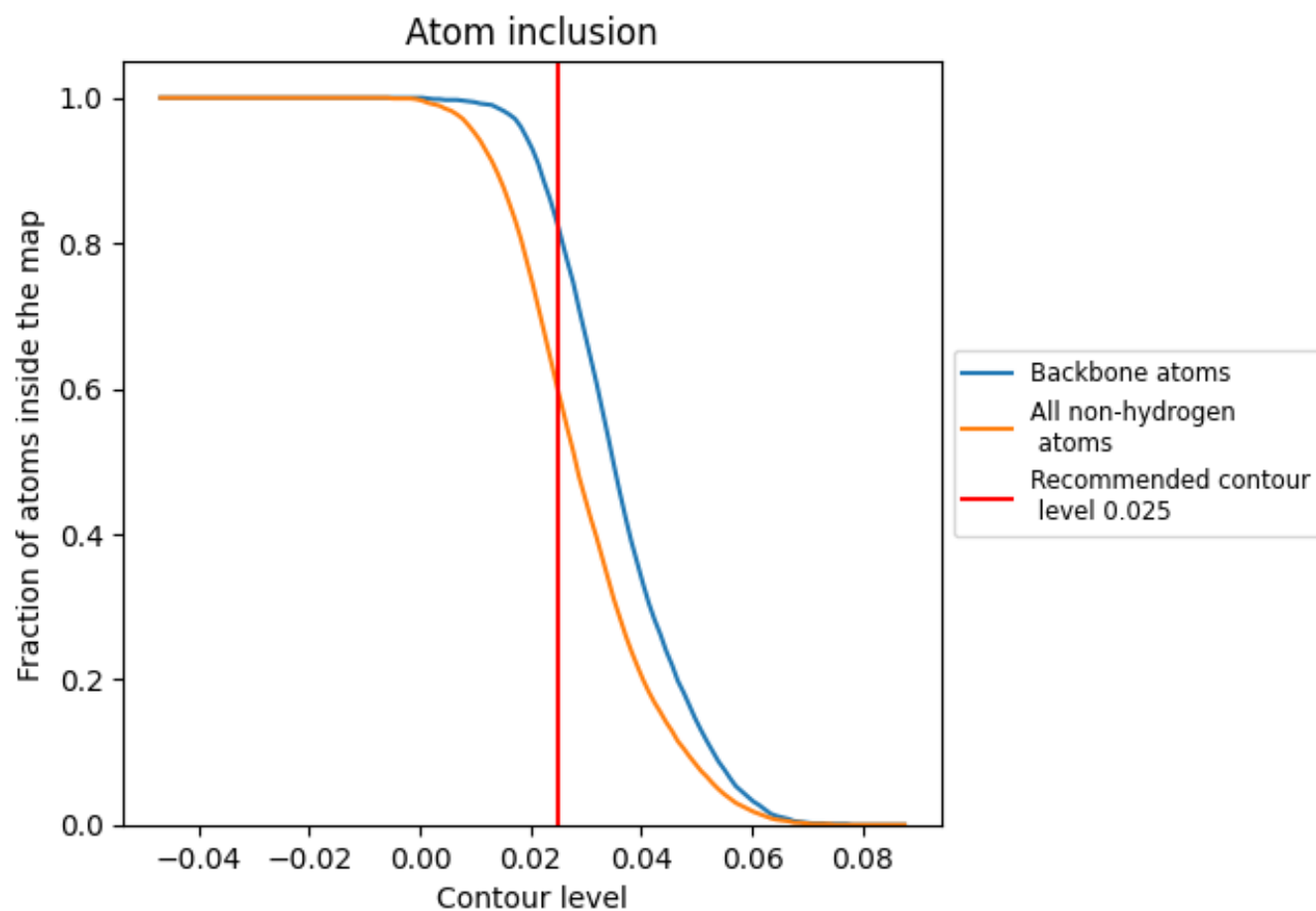
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 60% 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	0.5950	0.2740
A	0.7660	0.3990
B	0.5540	0.2420
C	0.7640	0.3970
D	0.5540	0.2430
E	0.7640	0.3990
F	0.5540	0.2440
G	0.7610	0.4000
H	0.5540	0.2430

