



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 12:48 PM JST

PDB ID : 5YWB
EMDB ID : EMD-6851
Title : Structure of pancreatic ATP-sensitive potassium channel bound with Mg-ADP
(CTD class2 at 5.2Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-11-29
Resolution : 5.20 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

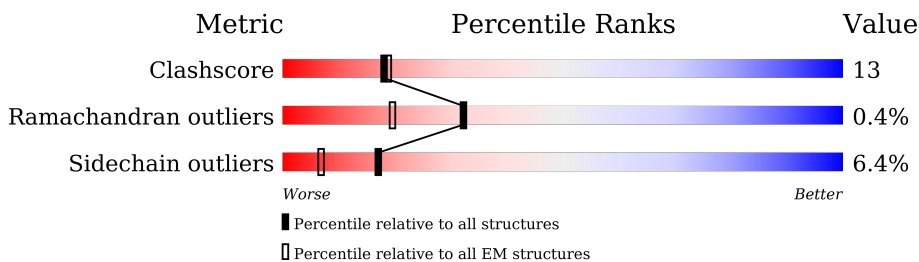
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>7%</div> <div>54%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	C	390	<div> <div>7%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	E	390	<div> <div>7%</div> <div>54%</div> <div>25%</div> <div>•</div> <div>17%</div> </div>
1	G	390	<div> <div>7%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
2	B	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	D	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	F	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	H	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50928 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
			2424	1565	417	427	15		
1	C	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	E	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	G	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	D	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	F	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	H	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		

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



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

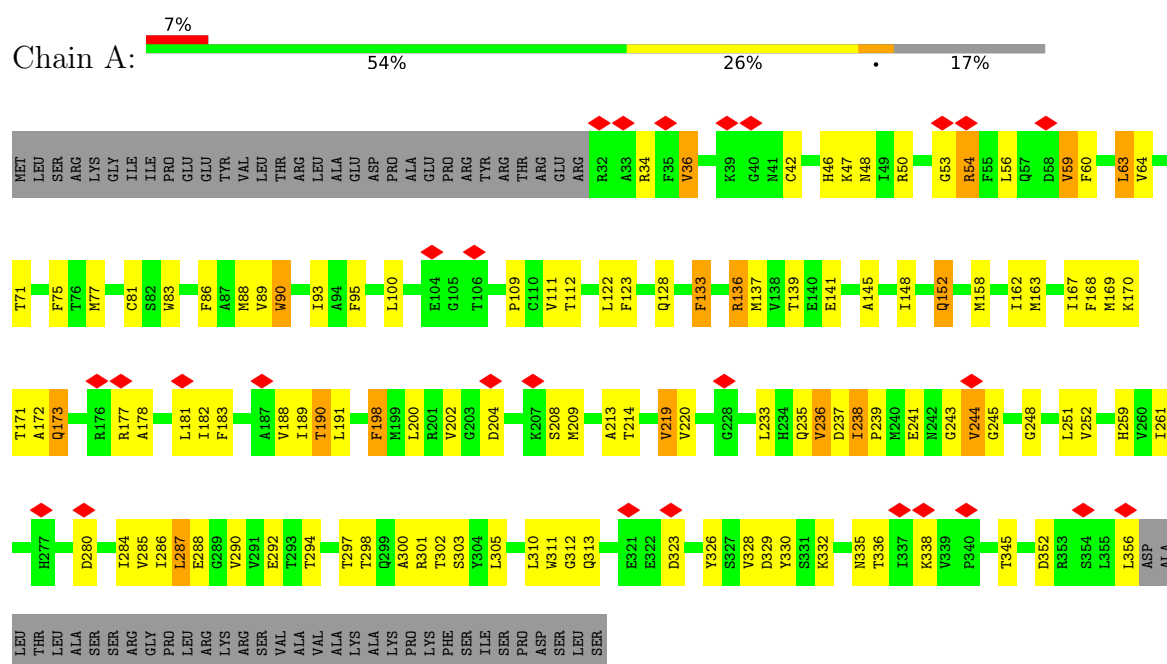
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

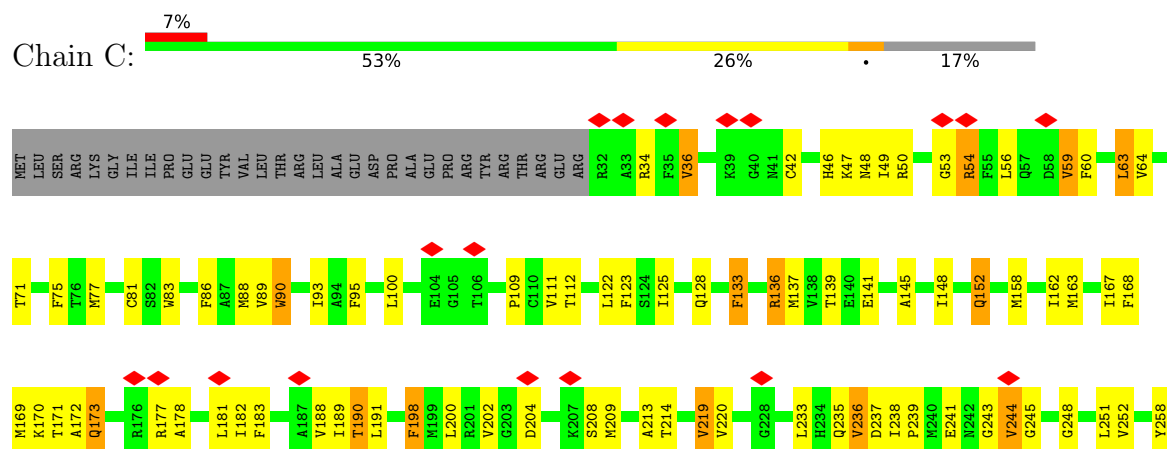
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

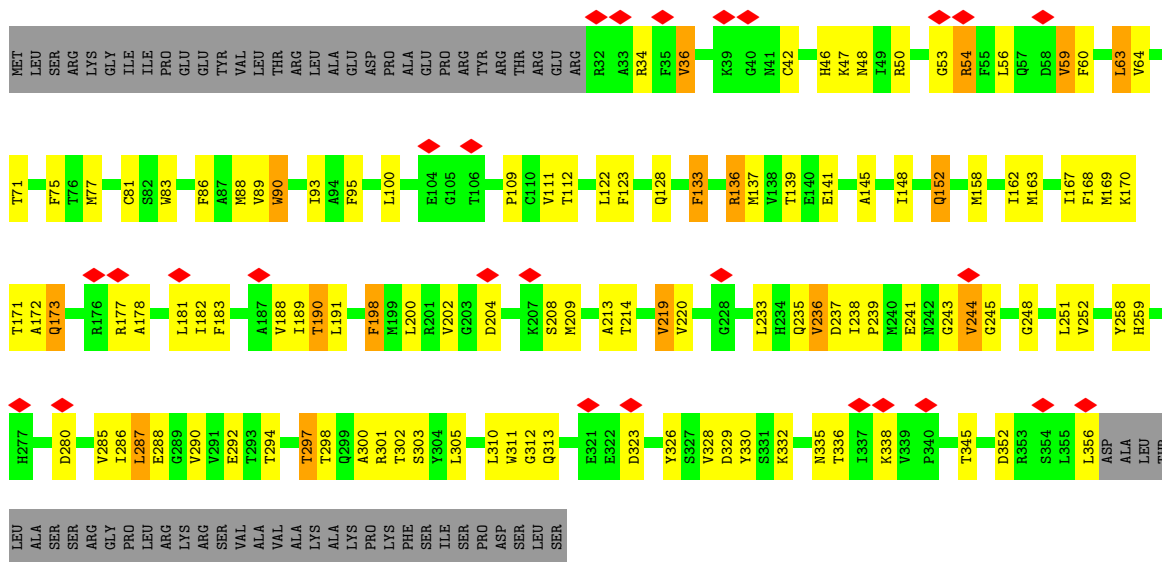
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



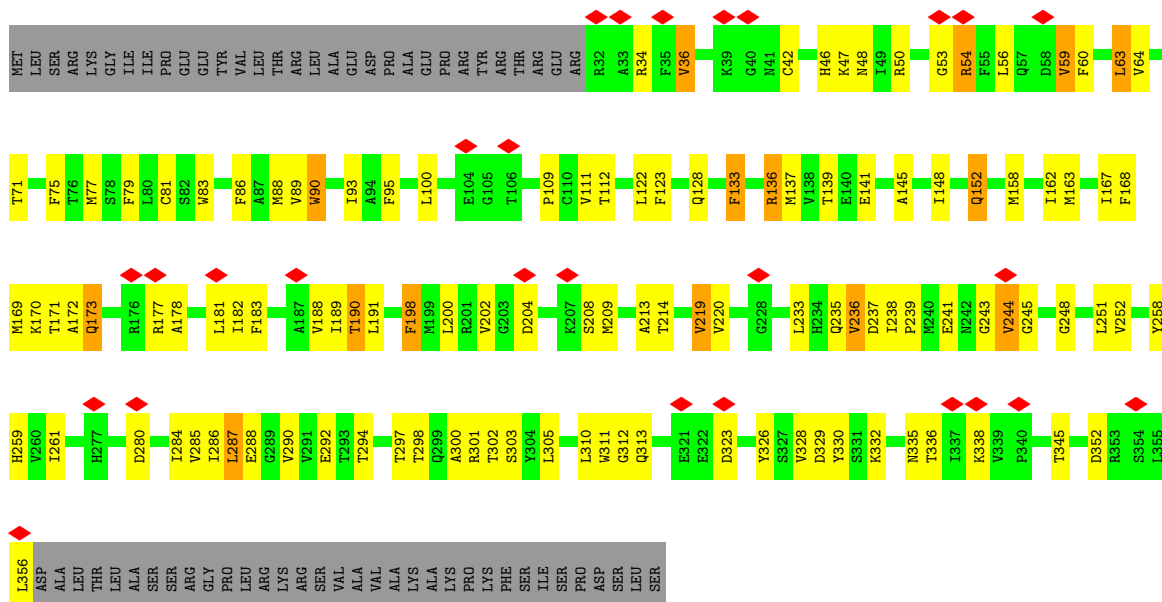
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



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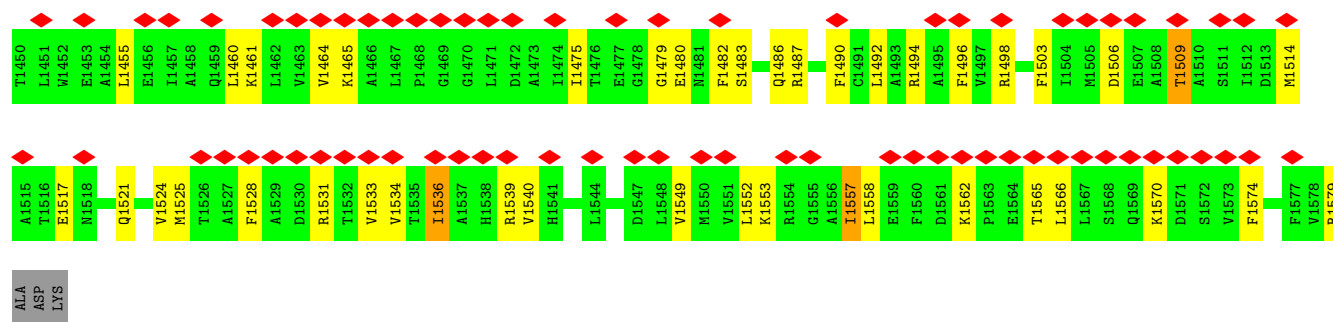
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



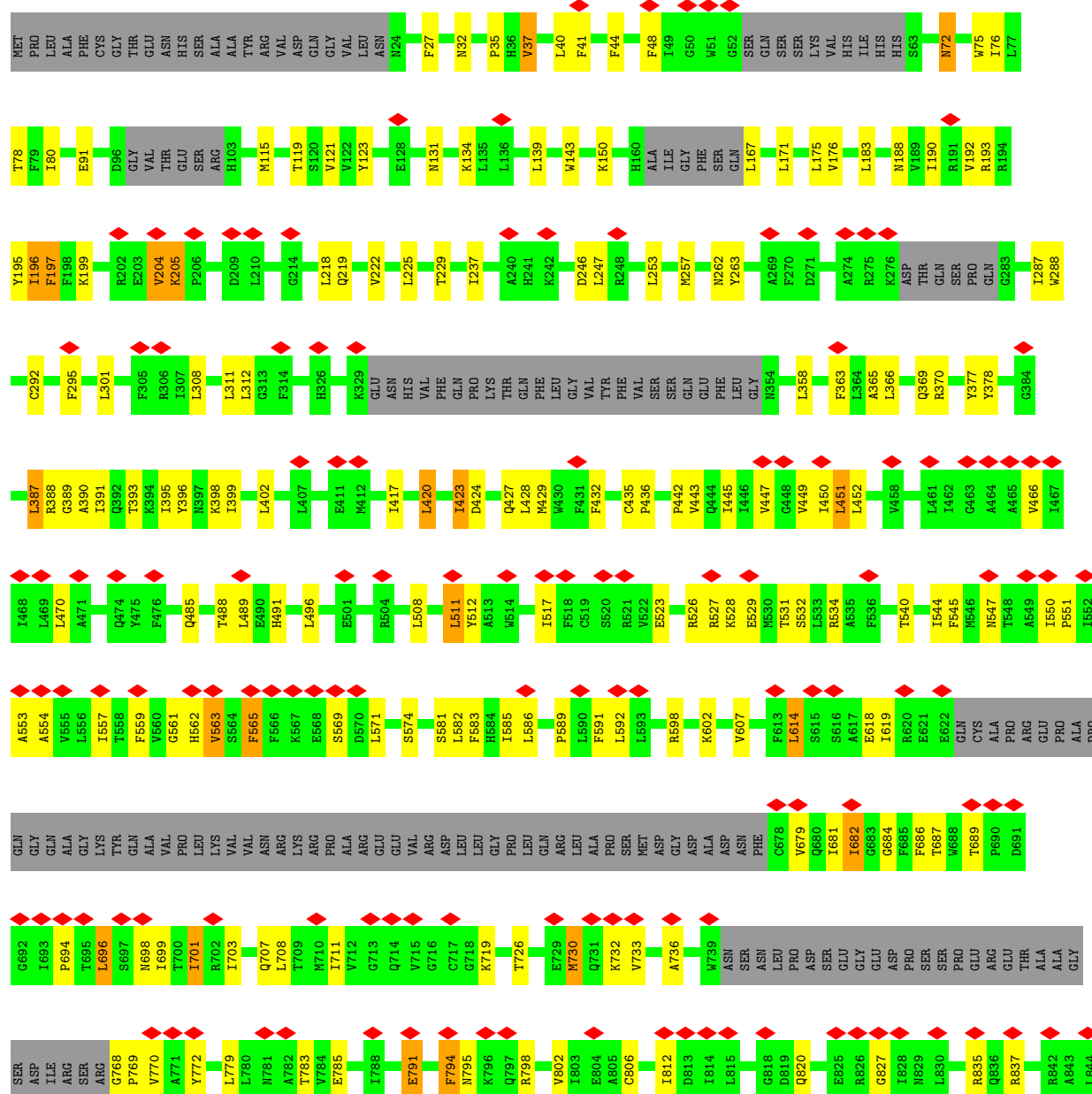
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2







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LEU	A1391	L1462	A1529	◆
ALA	F1392	V1463	D1530	◆
P1332	F1393	V1464	R1531	◆
S1333	R1394	K1465	T1532	◆
L1334	M1395	A1466	V1533	◆
I1335	V1396	L1467	V1534	◆
P1336	D1397	P1468	T1535	◆
K1337	M1398	G1469	I1536	◆
N1338	F1399	G1470	A1537	◆
V1339	E1400	L1471	H1538	◆
P1340	G1401	D1472	R1539	◆
D1341	R1402	A1473	V1540	◆
Q1342	I1403	I1474	H1541	◆
G1343	D1406	I1475	L1544	◆
K1344	G1407	T1476	D1547	◆
I1345	I1408	E1477	L1548	◆
Q1346	I1409	G1478	V1549	◆
I1347	I1410	E1480	M1550	◆
Q1348	A1411	N1481	V1551	◆
N1349	K1412	F1482	K1552	◆
L1350	L1413	S1483	K1553	◆
S1351	P1414	Q1486	R1554	◆
V1352	L1415	R1487	G1555	◆
R1353	R1421	F1490	A1556	◆
Y1354	L1422	C1491	I1557	◆
D1355	L1425	L1492	L1558	◆
S1356	I1426	A1493	E1559	◆
S1357	Q1427	R1494	F1560	◆
L1358	D1428	A1495	D1561	◆
K1359	P1429	F1496	K1562	◆
P1360	V1430	V1497	P1563	◆
V1361	L1431	R1498	E1564	◆
L1362	F1432	F1503	T1565	◆
K1363	F1438	I1504	L1566	◆
H1364	N1439	M1505	L1567	◆
V1365	L1440	D1506	S1568	◆
N1366	E1443	E1507	Q1569	◆
A1367	K1444	A1508	K1570	◆
L1368	K1445	T1509	D1571	◆
I1369	C1446	A1510	S1572	◆
S1370	S1447	S1511	V1573	◆
P1371	D1448	I1512	F1574	◆
K1374	D1449	D1513	F1577	◆
I1375	T1450	M1514	V1578	◆
G1376	L1451	A1515	R1579	◆
I1377	W1452	T1516	ALA	◆
C1378	E1453	E1517	ASP	◆
G1379	A1454	N1518	LYS	◆
R1380	L1455	Q1521		
T1381	E1456	V1524		
G1382	I1457	M1525		
S1383	A1458	T1526		
K1384	Q1459	A1527		
K1385	L1460	F1528		
S1386	K1461			
S1387				
F1388				
S1389				
L1390				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56433	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	0.080	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/2477	0.48	0/3380
1	C	0.27	0/2477	0.48	0/3380
1	E	0.27	0/2477	0.48	0/3380
1	G	0.27	0/2477	0.48	0/3380
2	B	0.29	0/10430	0.46	0/14168
2	D	0.29	0/10430	0.46	0/14168
2	F	0.29	0/10430	0.46	0/14168
2	H	0.29	0/10430	0.46	0/14168
All	All	0.29	0/51628	0.47	0/70192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2424	0	2383	105	0
1	C	2424	0	2383	105	0
1	E	2424	0	2383	104	0
1	G	2424	0	2383	105	0
2	B	10225	0	10456	245	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10225	0	10456	248	0
2	F	10225	0	10456	250	0
2	H	10225	0	10456	242	0
3	A	27	0	12	0	0
3	B	54	0	24	4	0
3	C	27	0	12	0	0
3	D	54	0	24	3	0
3	E	27	0	12	0	0
3	F	54	0	24	3	0
3	G	27	0	12	0	0
3	H	54	0	24	4	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
All	All	50928	0	51500	1335	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 13.

All (1335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:ILE:HG13	2:D:195:TYR:CB	1.79	1.13
2:F:190:ILE:HG13	2:F:195:TYR:CB	1.79	1.13
2:H:190:ILE:HG13	2:H:195:TYR:CB	1.79	1.12
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
1:A:172:ALA:HA	1:G:169:MET:HE1	1.34	1.05
1:E:169:MET:HE1	1:G:172:ALA:HA	1.42	1.00
1:C:169:MET:HE1	1:E:172:ALA:HA	1.44	0.99
1:A:169:MET:HE1	1:C:172:ALA:HA	1.39	0.98
2:H:295:PHE:CZ	2:H:387:LEU:HB2	2.01	0.96
2:D:190:ILE:CG1	2:D:195:TYR:CB	2.44	0.95
2:D:295:PHE:CZ	2:D:387:LEU:HB2	2.01	0.94
2:F:190:ILE:CG1	2:F:195:TYR:CB	2.44	0.94
2:H:190:ILE:CG1	2:H:195:TYR:CB	2.44	0.94
2:B:295:PHE:CZ	2:B:387:LEU:HB2	2.01	0.94
2:F:295:PHE:CZ	2:F:387:LEU:HB2	2.01	0.94
2:B:190:ILE:CG1	2:B:195:TYR:CB	2.44	0.94
1:E:169:MET:CE	1:G:172:ALA:HA	2.02	0.90
1:A:169:MET:CE	1:C:172:ALA:HA	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ALA:HA	1:G:169:MET:CE	2.02	0.89
1:C:169:MET:CE	1:E:172:ALA:HA	2.02	0.89
2:D:91:GLU:CD	2:D:171:LEU:HD12	1.96	0.85
1:E:168:PHE:O	1:E:171:THR:CG2	2.25	0.85
1:G:168:PHE:O	1:G:171:THR:CG2	2.25	0.85
1:A:168:PHE:O	1:A:171:THR:CG2	2.25	0.84
1:C:168:PHE:O	1:C:171:THR:CG2	2.25	0.84
1:A:172:ALA:CA	1:G:169:MET:HE1	2.08	0.82
1:A:243:GLY:HA3	1:G:237:ASP:HB3	1.62	0.81
1:A:182:ILE:HD12	1:A:182:ILE:O	1.81	0.81
1:E:237:ASP:HB3	1:G:243:GLY:HA3	1.62	0.81
1:C:237:ASP:HB3	1:E:243:GLY:HA3	1.62	0.81
1:C:182:ILE:HD12	1:C:182:ILE:O	1.81	0.81
1:G:182:ILE:HD12	1:G:182:ILE:O	1.81	0.81
1:A:237:ASP:HB3	1:C:243:GLY:HA3	1.62	0.80
1:E:182:ILE:HD12	1:E:182:ILE:O	1.81	0.80
1:G:168:PHE:HA	1:G:171:THR:CG2	2.12	0.80
1:G:168:PHE:O	1:G:171:THR:HG23	1.81	0.80
1:C:168:PHE:O	1:C:171:THR:HG23	1.81	0.80
1:C:168:PHE:HA	1:C:171:THR:CG2	2.12	0.80
1:A:168:PHE:HA	1:A:171:THR:CG2	2.12	0.80
1:E:168:PHE:HA	1:E:171:THR:CG2	2.12	0.79
1:A:169:MET:HE1	1:C:172:ALA:CA	2.13	0.79
1:E:168:PHE:O	1:E:171:THR:HG23	1.81	0.79
2:D:1124:ARG:HH11	2:D:1314:ARG:HD3	1.49	0.78
2:D:1271:SER:HA	2:D:1275:GLU:HB3	1.66	0.78
2:F:1271:SER:HA	2:F:1275:GLU:HB3	1.66	0.78
1:A:168:PHE:O	1:A:171:THR:HG23	1.81	0.78
2:F:1124:ARG:HH11	2:F:1314:ARG:HD3	1.49	0.78
1:G:214:THR:HA	1:G:248:GLY:HA2	1.65	0.78
1:E:214:THR:HA	1:E:248:GLY:HA2	1.65	0.78
2:B:204:VAL:O	2:B:205:LYS:HB3	1.83	0.77
2:D:204:VAL:O	2:D:205:LYS:HB3	1.83	0.77
2:H:1271:SER:HA	2:H:1275:GLU:HB3	1.66	0.77
1:C:214:THR:HA	1:C:248:GLY:HA2	1.65	0.77
2:B:1271:SER:HA	2:B:1275:GLU:HB3	1.66	0.77
2:B:1421:ARG:HG3	2:B:1422:LEU:HG	1.67	0.77
2:B:196:ILE:O	2:B:197:PHE:O	2.03	0.77
1:A:214:THR:HA	1:A:248:GLY:HA2	1.65	0.76
2:D:1421:ARG:HG3	2:D:1422:LEU:HG	1.67	0.76
2:F:204:VAL:O	2:F:205:LYS:HB3	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:MET:HE1	1:G:172:ALA:CA	2.15	0.76
2:B:150:LYS:HB3	2:B:176:VAL:HG22	1.67	0.76
2:H:204:VAL:O	2:H:205:LYS:HB3	1.83	0.76
2:B:150:LYS:HE3	2:B:175:LEU:HD13	1.67	0.76
2:F:1421:ARG:HG3	2:F:1422:LEU:HG	1.67	0.76
2:H:1124:ARG:HH11	2:H:1314:ARG:HD3	1.49	0.76
2:H:150:LYS:HB3	2:H:176:VAL:HG22	1.67	0.76
2:B:1124:ARG:HH11	2:B:1314:ARG:HD3	1.49	0.76
2:D:150:LYS:HE3	2:D:175:LEU:HD13	1.67	0.76
2:D:196:ILE:O	2:D:197:PHE:O	2.03	0.76
2:H:1421:ARG:HG3	2:H:1422:LEU:HG	1.67	0.75
1:A:177:ARG:HH22	1:A:208:SER:HB2	1.51	0.75
2:D:150:LYS:HB3	2:D:176:VAL:HG22	1.67	0.75
2:F:196:ILE:O	2:F:197:PHE:O	2.03	0.75
1:G:177:ARG:HH22	1:G:208:SER:HB2	1.51	0.75
2:H:150:LYS:HE3	2:H:175:LEU:HD13	1.67	0.75
2:H:196:ILE:O	2:H:197:PHE:O	2.03	0.75
2:F:150:LYS:HE3	2:F:175:LEU:HD13	1.67	0.75
1:C:169:MET:HE1	1:E:172:ALA:CA	2.17	0.74
1:C:177:ARG:HH22	1:C:208:SER:HB2	1.51	0.74
2:D:387:LEU:HD21	2:D:428:LEU:HB3	1.69	0.74
2:F:150:LYS:HB3	2:F:176:VAL:HG22	1.67	0.74
1:E:177:ARG:HH22	1:E:208:SER:HB2	1.51	0.73
2:B:387:LEU:HD21	2:B:428:LEU:HB3	1.69	0.73
2:H:387:LEU:HD21	2:H:428:LEU:HB3	1.69	0.73
2:F:387:LEU:HD21	2:F:428:LEU:HB3	1.69	0.72
2:H:1334:LEU:HD13	2:H:1408:ILE:HG23	1.72	0.72
1:E:177:ARG:NH2	1:E:208:SER:HB2	2.05	0.72
1:G:177:ARG:NH2	1:G:208:SER:HB2	2.05	0.72
1:C:219:VAL:HG13	1:C:236:VAL:HG23	1.72	0.71
2:B:150:LYS:CE	2:B:175:LEU:HD13	2.21	0.71
1:E:219:VAL:HG13	1:E:236:VAL:HG23	1.72	0.71
2:B:1334:LEU:HD13	2:B:1408:ILE:HG23	1.72	0.71
1:E:36:VAL:HG12	1:E:42:CYS:HA	1.72	0.71
1:G:36:VAL:HG12	1:G:42:CYS:HA	1.72	0.71
2:F:1334:LEU:HD13	2:F:1408:ILE:HG23	1.72	0.71
2:D:150:LYS:CE	2:D:175:LEU:HD13	2.21	0.71
1:A:36:VAL:HG12	1:A:42:CYS:HA	1.72	0.71
1:A:219:VAL:HG13	1:A:236:VAL:HG23	1.72	0.71
2:H:150:LYS:CE	2:H:175:LEU:HD13	2.21	0.70
2:F:682:ILE:HG23	2:F:736:ALA:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:NH2	1:C:208:SER:HB2	2.05	0.70
1:G:219:VAL:HG13	1:G:236:VAL:HG23	1.72	0.70
2:D:682:ILE:HG23	2:D:736:ALA:HB3	1.73	0.70
1:A:177:ARG:NH2	1:A:208:SER:HB2	2.05	0.70
2:D:204:VAL:O	2:D:205:LYS:CB	2.39	0.70
2:D:1334:LEU:HD13	2:D:1408:ILE:HG23	1.72	0.70
2:F:204:VAL:O	2:F:205:LYS:CB	2.39	0.70
2:B:682:ILE:HG23	2:B:736:ALA:HB3	1.73	0.70
2:F:150:LYS:CE	2:F:175:LEU:HD13	2.21	0.69
2:H:1394:ARG:HD2	2:H:1410:ILE:HG21	1.73	0.69
2:D:1394:ARG:HD2	2:D:1410:ILE:HG21	1.73	0.69
1:C:168:PHE:O	1:C:171:THR:HG22	1.92	0.69
2:B:562:HIS:NE2	2:B:569:SER:O	2.26	0.69
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.72	0.69
2:D:287:ILE:HD11	2:D:607:VAL:HG13	1.74	0.69
2:B:1394:ARG:HD2	2:B:1410:ILE:HG21	1.73	0.69
2:F:287:ILE:HD11	2:F:607:VAL:HG13	1.74	0.68
2:H:562:HIS:NE2	2:H:569:SER:O	2.26	0.68
2:H:682:ILE:HG23	2:H:736:ALA:HB3	1.73	0.68
2:B:287:ILE:HD11	2:B:607:VAL:HG13	1.74	0.68
1:C:183:PHE:CD2	1:C:202:VAL:HG12	2.29	0.68
1:A:168:PHE:O	1:A:171:THR:HG22	1.92	0.68
1:A:168:PHE:HA	1:A:171:THR:HG22	1.76	0.68
2:D:562:HIS:NE2	2:D:569:SER:O	2.26	0.68
1:A:183:PHE:CD2	1:A:202:VAL:HG12	2.29	0.68
2:F:562:HIS:NE2	2:F:569:SER:O	2.26	0.68
1:E:168:PHE:O	1:E:171:THR:HG22	1.92	0.68
2:B:869:MET:HA	2:B:873:ILE:HD12	1.75	0.68
2:F:1394:ARG:HD2	2:F:1410:ILE:HG21	1.73	0.68
2:H:287:ILE:HD11	2:H:607:VAL:HG13	1.74	0.68
1:G:168:PHE:O	1:G:171:THR:HG22	1.92	0.67
1:E:167:ILE:O	1:E:171:THR:HG22	1.94	0.67
1:C:168:PHE:HA	1:C:171:THR:HG22	1.76	0.67
1:A:53:GLY:O	1:A:54:ARG:CB	2.43	0.67
1:E:168:PHE:HA	1:E:171:THR:HG22	1.76	0.67
1:G:168:PHE:HA	1:G:171:THR:HG22	1.76	0.67
2:B:204:VAL:O	2:B:205:LYS:CB	2.39	0.67
1:C:167:ILE:O	1:C:171:THR:HG22	1.94	0.67
2:B:873:ILE:HA	2:B:877:LEU:HD12	1.77	0.67
2:D:873:ILE:HA	2:D:877:LEU:HD12	1.77	0.67
1:E:183:PHE:CD2	1:E:202:VAL:HG12	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:551:PRO:HB3	2:F:583:PHE:CZ	2.30	0.67
2:F:869:MET:HA	2:F:873:ILE:HD12	1.75	0.67
2:F:873:ILE:HA	2:F:877:LEU:HD12	1.77	0.67
1:G:53:GLY:O	1:G:54:ARG:CB	2.43	0.67
1:G:183:PHE:CD2	1:G:202:VAL:HG12	2.29	0.67
2:H:869:MET:HA	2:H:873:ILE:HD12	1.75	0.67
2:H:873:ILE:HA	2:H:877:LEU:HD12	1.77	0.67
2:H:551:PRO:HB3	2:H:583:PHE:CZ	2.30	0.67
2:D:869:MET:HA	2:D:873:ILE:HD12	1.75	0.66
2:D:466:VAL:HG11	2:D:554:ALA:HB2	1.76	0.66
1:G:167:ILE:O	1:G:171:THR:HG22	1.94	0.66
2:H:466:VAL:HG11	2:H:554:ALA:HB2	1.76	0.66
1:A:167:ILE:O	1:A:171:THR:HG22	1.94	0.66
1:G:168:PHE:CA	1:G:171:THR:HG22	2.26	0.66
2:H:204:VAL:O	2:H:205:LYS:CB	2.39	0.66
2:B:466:VAL:HG11	2:B:554:ALA:HB2	1.76	0.66
2:B:551:PRO:HB3	2:B:583:PHE:CZ	2.30	0.66
1:C:53:GLY:O	1:C:54:ARG:CB	2.43	0.66
2:D:551:PRO:HB3	2:D:583:PHE:CZ	2.30	0.66
2:H:301:LEU:C	2:H:301:LEU:HD23	2.17	0.66
1:A:168:PHE:CA	1:A:171:THR:HG22	2.26	0.66
2:F:466:VAL:HG11	2:F:554:ALA:HB2	1.76	0.66
1:G:123:PHE:HD2	1:G:136:ARG:HG3	1.61	0.66
1:E:53:GLY:O	1:E:54:ARG:CB	2.43	0.65
1:E:123:PHE:HD2	1:E:136:ARG:HG3	1.61	0.65
2:B:301:LEU:C	2:B:301:LEU:HD23	2.17	0.65
1:A:168:PHE:C	1:A:171:THR:HG22	2.17	0.65
1:C:181:LEU:N	1:C:181:LEU:HD22	2.12	0.65
1:G:168:PHE:C	1:G:171:THR:HG22	2.17	0.65
1:A:181:LEU:N	1:A:181:LEU:HD22	2.12	0.65
2:B:1509:THR:HG23	2:B:1517:GLU:HG2	1.79	0.65
2:D:301:LEU:HD23	2:D:301:LEU:C	2.17	0.65
1:E:168:PHE:CA	1:E:171:THR:HG22	2.26	0.65
1:A:123:PHE:HD2	1:A:136:ARG:HG3	1.61	0.65
2:D:511:LEU:HD23	2:D:1426:LEU:HD21	1.79	0.65
2:F:511:LEU:HD23	2:F:1426:LEU:HD21	1.79	0.65
2:D:1509:THR:HG23	2:D:1517:GLU:HG2	1.79	0.65
2:F:301:LEU:C	2:F:301:LEU:HD23	2.17	0.65
2:H:1509:THR:HG23	2:H:1517:GLU:HG2	1.79	0.65
1:C:123:PHE:HD2	1:C:136:ARG:HG3	1.61	0.64
1:C:168:PHE:CA	1:C:171:THR:HG22	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:C	1:C:171:THR:HG22	2.17	0.64
1:G:183:PHE:HZ	1:G:287:LEU:HD23	1.62	0.64
2:D:1480:GLU:OE1	3:D:2501:ADP:N6	2.30	0.64
2:H:1480:GLU:OE1	3:H:2501:ADP:N6	2.30	0.64
2:F:1480:GLU:OE1	3:F:2501:ADP:N6	2.30	0.64
1:E:181:LEU:HD22	1:E:181:LEU:N	2.12	0.64
2:B:1032:TYR:HA	2:B:1283:LEU:HD11	1.80	0.64
2:F:150:LYS:NZ	2:F:175:LEU:HD13	2.13	0.64
2:H:365:ALA:O	2:H:369:GLN:HG3	1.98	0.64
2:H:681:ILE:HB	2:H:701:ILE:HG23	1.79	0.64
2:B:1480:GLU:OE1	3:B:2501:ADP:N6	2.30	0.64
2:D:365:ALA:O	2:D:369:GLN:HG3	1.98	0.64
2:D:1032:TYR:HA	2:D:1283:LEU:HD11	1.80	0.64
1:E:168:PHE:C	1:E:171:THR:HG22	2.17	0.64
2:D:1506:ASP:HA	2:D:1536:ILE:HG13	1.80	0.64
2:B:365:ALA:O	2:B:369:GLN:HG3	1.98	0.63
2:D:681:ILE:HB	2:D:701:ILE:HG23	1.79	0.63
2:B:190:ILE:CB	2:B:195:TYR:CB	2.77	0.63
2:B:783:THR:HB	2:B:820:GLN:HA	1.80	0.63
1:G:181:LEU:N	1:G:181:LEU:HD22	2.12	0.63
2:D:190:ILE:CB	2:D:195:TYR:CB	2.77	0.63
2:D:592:LEU:HD11	2:D:1297:TRP:HH2	1.63	0.63
2:F:1347:ILE:HG23	2:F:1403:ILE:HG12	1.80	0.63
2:H:190:ILE:CB	2:H:195:TYR:CB	2.77	0.63
1:A:183:PHE:HZ	1:A:287:LEU:HD23	1.62	0.63
1:E:109:PRO:HG2	1:E:112:THR:HA	1.81	0.63
1:E:183:PHE:HZ	1:E:287:LEU:HD23	1.62	0.63
2:F:1509:THR:HG23	2:F:1517:GLU:HG2	1.79	0.63
2:B:1506:ASP:HA	2:B:1536:ILE:HG13	1.80	0.63
2:H:1506:ASP:HA	2:H:1536:ILE:HG13	1.80	0.63
2:B:511:LEU:HD23	2:B:1426:LEU:HD21	1.79	0.63
1:C:109:PRO:HG2	1:C:112:THR:HA	1.81	0.63
2:D:1347:ILE:HG23	2:D:1403:ILE:HG12	1.80	0.63
2:H:150:LYS:NZ	2:H:175:LEU:HD13	2.13	0.63
2:F:681:ILE:HB	2:F:701:ILE:HG23	1.79	0.63
2:H:511:LEU:HD23	2:H:1426:LEU:HD21	1.79	0.63
2:H:551:PRO:HB3	2:H:583:PHE:HZ	1.64	0.63
2:B:592:LEU:HD11	2:B:1297:TRP:HH2	1.63	0.63
2:F:295:PHE:HZ	2:F:387:LEU:HB2	1.63	0.63
2:B:150:LYS:NZ	2:B:175:LEU:HD13	2.13	0.62
2:D:295:PHE:HZ	2:D:387:LEU:HB2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:ALA:O	2:F:369:GLN:HG3	1.98	0.62
2:F:1506:ASP:HA	2:F:1536:ILE:HG13	1.80	0.62
2:H:783:THR:HB	2:H:820:GLN:HA	1.80	0.62
2:D:150:LYS:NZ	2:D:175:LEU:HD13	2.13	0.62
2:F:783:THR:HB	2:F:820:GLN:HA	1.80	0.62
1:C:183:PHE:HZ	1:C:287:LEU:HD23	1.62	0.62
2:D:551:PRO:HB3	2:D:583:PHE:HZ	1.64	0.62
2:F:1032:TYR:HA	2:F:1283:LEU:HD11	1.80	0.62
2:H:592:LEU:HD11	2:H:1297:TRP:HH2	1.63	0.62
2:H:369:GLN:HB2	2:H:370:ARG:NH2	2.15	0.62
2:D:783:THR:HB	2:D:820:GLN:HA	1.80	0.62
2:H:1032:TYR:HA	2:H:1283:LEU:HD11	1.80	0.62
2:B:681:ILE:HB	2:B:701:ILE:HG23	1.79	0.61
2:D:561:GLY:HA2	2:D:565:PHE:HB3	1.82	0.61
2:H:1347:ILE:HG23	2:H:1403:ILE:HG12	1.80	0.61
2:B:551:PRO:HB3	2:B:583:PHE:HZ	1.64	0.61
2:F:190:ILE:CB	2:F:195:TYR:CB	2.77	0.61
2:F:592:LEU:HD11	2:F:1297:TRP:HH2	1.63	0.61
2:B:369:GLN:HB2	2:B:370:ARG:NH2	2.15	0.61
2:F:369:GLN:HB2	2:F:370:ARG:NH2	2.15	0.61
1:G:109:PRO:HG2	1:G:112:THR:HA	1.81	0.61
1:A:213:ALA:HA	1:A:288:GLU:O	2.01	0.61
2:B:561:GLY:HA2	2:B:565:PHE:HB3	1.82	0.61
2:B:1347:ILE:HG23	2:B:1403:ILE:HG12	1.80	0.61
1:A:109:PRO:HG2	1:A:112:THR:HA	1.81	0.61
1:C:237:ASP:HB3	1:E:243:GLY:CA	2.31	0.61
2:D:369:GLN:HB2	2:D:370:ARG:NH2	2.15	0.61
2:F:551:PRO:HB3	2:F:583:PHE:HZ	1.64	0.61
2:H:699:ILE:HG23	2:H:908:ILE:HD11	1.82	0.61
2:D:301:LEU:HD23	2:D:301:LEU:O	2.01	0.61
2:D:1350:LEU:HB3	2:D:1365:VAL:HB	1.83	0.61
2:D:699:ILE:HG23	2:D:908:ILE:HD11	1.82	0.61
1:E:183:PHE:CE2	1:E:202:VAL:HG12	2.36	0.61
2:F:301:LEU:HD23	2:F:301:LEU:O	2.01	0.61
2:B:1350:LEU:HB3	2:B:1365:VAL:HB	1.83	0.60
1:C:181:LEU:HD22	1:C:181:LEU:H	1.66	0.60
2:D:1362:LEU:HD13	2:D:1365:VAL:HG21	1.84	0.60
2:F:561:GLY:HA2	2:F:565:PHE:HB3	1.82	0.60
2:B:1171:LEU:HD11	2:B:1255:ILE:HG23	1.84	0.60
1:C:183:PHE:CE2	1:C:202:VAL:HG12	2.36	0.60
1:C:213:ALA:HA	1:C:288:GLU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:699:ILE:HG23	2:F:908:ILE:HD11	1.82	0.60
2:H:1171:LEU:HD11	2:H:1255:ILE:HG23	1.84	0.60
1:E:213:ALA:HA	1:E:288:GLU:O	2.01	0.60
1:G:312:GLY:O	1:G:313:GLN:NE2	2.35	0.60
2:H:389:GLY:O	2:H:393:THR:HG22	2.02	0.60
2:H:561:GLY:HA2	2:H:565:PHE:HB3	1.82	0.60
1:A:183:PHE:CE2	1:A:202:VAL:HG12	2.36	0.60
1:C:170:LYS:O	1:C:173:GLN:NE2	2.35	0.60
2:H:295:PHE:HZ	2:H:387:LEU:HB2	1.63	0.60
1:A:168:PHE:HA	1:A:171:THR:HG21	1.84	0.60
2:D:1171:LEU:HD11	2:D:1255:ILE:HG23	1.84	0.60
2:F:1171:LEU:HD11	2:F:1255:ILE:HG23	1.84	0.60
1:G:183:PHE:CE2	1:G:202:VAL:HG12	2.36	0.60
2:H:301:LEU:HD23	2:H:301:LEU:O	2.01	0.60
2:F:1362:LEU:HD13	2:F:1365:VAL:HG21	1.84	0.60
1:A:312:GLY:O	1:A:313:GLN:NE2	2.35	0.60
2:B:190:ILE:HB	2:B:195:TYR:CB	2.32	0.60
2:B:295:PHE:HZ	2:B:387:LEU:HB2	1.63	0.60
2:B:301:LEU:HD23	2:B:301:LEU:O	2.01	0.60
1:C:168:PHE:HA	1:C:171:THR:HG21	1.84	0.60
2:D:190:ILE:HB	2:D:195:TYR:CB	2.32	0.60
2:D:312:LEU:HB2	2:D:369:GLN:HG2	1.84	0.60
2:D:389:GLY:O	2:D:393:THR:HG22	2.02	0.60
1:E:95:PHE:HD1	1:E:100:LEU:HD23	1.67	0.60
1:E:181:LEU:HD22	1:E:181:LEU:H	1.66	0.60
1:G:213:ALA:HA	1:G:288:GLU:O	2.01	0.60
1:A:95:PHE:HD1	1:A:100:LEU:HD23	1.67	0.59
2:F:389:GLY:O	2:F:393:THR:HG22	2.02	0.59
2:F:1350:LEU:HB3	2:F:1365:VAL:HB	1.83	0.59
1:G:183:PHE:CZ	1:G:287:LEU:HD23	2.37	0.59
2:H:190:ILE:HB	2:H:195:TYR:CB	2.32	0.59
2:H:785:GLU:HB3	2:H:794:PHE:HZ	1.67	0.59
1:E:312:GLY:O	1:E:313:GLN:NE2	2.35	0.59
2:F:190:ILE:HB	2:F:195:TYR:CB	2.32	0.59
2:H:1362:LEU:HD13	2:H:1365:VAL:HG21	1.84	0.59
2:B:785:GLU:HB3	2:B:794:PHE:HZ	1.67	0.59
2:B:1553:LYS:HE3	2:B:1558:LEU:HB2	1.83	0.59
2:F:785:GLU:HB3	2:F:794:PHE:HZ	1.67	0.59
1:G:95:PHE:HD1	1:G:100:LEU:HD23	1.67	0.59
1:G:168:PHE:HA	1:G:171:THR:HG21	1.84	0.59
1:G:181:LEU:HD22	1:G:181:LEU:H	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1350:LEU:HB3	2:H:1365:VAL:HB	1.83	0.59
1:E:168:PHE:HA	1:E:171:THR:HG21	1.84	0.59
2:F:312:LEU:HB2	2:F:369:GLN:HG2	1.84	0.59
2:H:1553:LYS:HE3	2:H:1558:LEU:HB2	1.83	0.59
1:C:95:PHE:HD1	1:C:100:LEU:HD23	1.67	0.59
2:D:785:GLU:HB3	2:D:794:PHE:HZ	1.67	0.59
1:E:170:LYS:O	1:E:173:GLN:NE2	2.35	0.59
1:A:170:LYS:O	1:A:173:GLN:NE2	2.35	0.59
2:B:699:ILE:HG23	2:B:908:ILE:HD11	1.82	0.59
2:D:1377:ILE:HB	2:D:1536:ILE:HG23	1.85	0.59
2:D:1553:LYS:HE3	2:D:1558:LEU:HB2	1.83	0.59
1:G:170:LYS:O	1:G:173:GLN:NE2	2.35	0.59
2:B:389:GLY:O	2:B:393:THR:HG22	2.02	0.59
1:A:243:GLY:CA	1:G:237:ASP:HB3	2.31	0.59
1:A:183:PHE:CZ	1:A:287:LEU:HD23	2.37	0.58
1:C:312:GLY:O	1:C:313:GLN:NE2	2.35	0.58
2:H:312:LEU:HB2	2:H:369:GLN:HG2	1.84	0.58
2:F:1553:LYS:HE3	2:F:1558:LEU:HB2	1.83	0.58
2:B:1362:LEU:HD13	2:B:1365:VAL:HG21	1.84	0.58
1:C:183:PHE:CZ	1:C:287:LEU:HD23	2.37	0.58
1:A:181:LEU:HD22	1:A:181:LEU:H	1.66	0.58
2:B:312:LEU:HB2	2:B:369:GLN:HG2	1.84	0.58
2:D:75:TRP:CZ3	2:D:225:LEU:CB	2.87	0.58
1:E:183:PHE:CZ	1:E:287:LEU:HD23	2.37	0.58
2:H:545:PHE:HB2	2:H:1080:LEU:HD13	1.86	0.58
2:B:686:PHE:H	2:B:696:LEU:HB3	1.69	0.58
2:H:1377:ILE:HB	2:H:1536:ILE:HG23	1.85	0.58
2:D:366:LEU:O	2:D:370:ARG:HG2	2.04	0.58
2:F:1344:LYS:HB2	2:F:1371:PRO:HG3	1.85	0.58
2:F:1377:ILE:HB	2:F:1536:ILE:HG23	1.85	0.58
2:B:75:TRP:CZ3	2:B:225:LEU:CB	2.87	0.58
2:H:75:TRP:CZ3	2:H:225:LEU:CB	2.87	0.58
2:B:1377:ILE:HB	2:B:1536:ILE:HG23	1.85	0.58
2:H:686:PHE:H	2:H:696:LEU:HB3	1.69	0.58
1:A:237:ASP:HB3	1:C:243:GLY:CA	2.31	0.57
2:F:686:PHE:H	2:F:696:LEU:HB3	1.69	0.57
2:H:366:LEU:O	2:H:370:ARG:HG2	2.04	0.57
2:D:686:PHE:H	2:D:696:LEU:HB3	1.69	0.57
1:E:237:ASP:HB3	1:G:243:GLY:CA	2.31	0.57
2:F:1385:LYS:HB2	2:F:1536:ILE:HG21	1.86	0.57
2:B:681:ILE:HD11	2:B:726:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1344:LYS:HB2	2:B:1371:PRO:HG3	1.85	0.57
2:H:681:ILE:HD11	2:H:726:THR:HG22	1.87	0.57
2:B:366:LEU:O	2:B:370:ARG:HG2	2.04	0.57
2:B:377:TYR:HB3	2:B:1246:ARG:HE	1.70	0.57
2:B:545:PHE:HB2	2:B:1080:LEU:HD13	1.86	0.57
2:F:75:TRP:CZ3	2:F:225:LEU:CB	2.87	0.57
2:F:366:LEU:O	2:F:370:ARG:HG2	2.04	0.57
2:H:1344:LYS:HB2	2:H:1371:PRO:HG3	1.85	0.57
2:D:545:PHE:HB2	2:D:1080:LEU:HD13	1.86	0.57
2:D:681:ILE:HD11	2:D:726:THR:HG22	1.87	0.57
2:F:545:PHE:HB2	2:F:1080:LEU:HD13	1.86	0.57
2:D:1344:LYS:HB2	2:D:1371:PRO:HG3	1.85	0.57
2:B:466:VAL:HG13	2:B:550:ILE:HG22	1.87	0.56
2:D:91:GLU:OE2	2:D:171:LEU:HD12	2.04	0.56
2:F:377:TYR:HB3	2:F:1246:ARG:HE	1.70	0.56
1:E:352:ASP:O	1:E:356:LEU:N	2.39	0.56
2:F:681:ILE:HD11	2:F:726:THR:HG22	1.87	0.56
1:A:352:ASP:O	1:A:356:LEU:N	2.39	0.56
2:B:1385:LYS:HB2	2:B:1536:ILE:HG21	1.86	0.56
2:D:466:VAL:HG13	2:D:550:ILE:HG22	1.87	0.56
2:D:1475:ILE:HD12	2:D:1482:PHE:HE2	1.71	0.56
2:B:1475:ILE:HD12	2:B:1482:PHE:HE2	1.71	0.56
2:H:1475:ILE:HD12	2:H:1482:PHE:HE2	1.71	0.56
1:C:168:PHE:CA	1:C:171:THR:CG2	2.83	0.56
1:C:352:ASP:O	1:C:356:LEU:N	2.39	0.56
2:D:377:TYR:HB3	2:D:1246:ARG:HE	1.70	0.56
2:F:466:VAL:HG13	2:F:550:ILE:HG22	1.87	0.56
1:G:181:LEU:H	1:G:181:LEU:CD2	2.19	0.56
2:H:377:TYR:HB3	2:H:1246:ARG:HE	1.70	0.56
2:H:466:VAL:HG13	2:H:550:ILE:HG22	1.87	0.56
1:A:34:ARG:HG2	1:A:305:LEU:HD21	1.88	0.56
2:D:1385:LYS:HB2	2:D:1536:ILE:HG21	1.86	0.56
1:E:34:ARG:HG2	1:E:305:LEU:HD21	1.88	0.56
2:H:1385:LYS:HB2	2:H:1536:ILE:HG21	1.86	0.56
2:H:1528:PHE:HD1	2:H:1531:ARG:HD2	1.71	0.56
1:A:168:PHE:CA	1:A:171:THR:CG2	2.83	0.55
2:B:1528:PHE:HD1	2:B:1531:ARG:HD2	1.71	0.55
2:B:1540:VAL:HG11	2:B:1579:ARG:HA	1.88	0.55
2:D:1540:VAL:HG11	2:D:1579:ARG:HA	1.88	0.55
2:H:1455:LEU:HD13	2:H:1464:VAL:HG21	1.88	0.55
2:B:686:PHE:HD1	2:B:733:VAL:HG23	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:ASP:O	1:G:356:LEU:N	2.39	0.55
2:B:1086:VAL:HG11	2:B:1141:GLU:HB2	1.89	0.55
1:E:181:LEU:H	1:E:181:LEU:CD2	2.19	0.55
1:C:34:ARG:HG2	1:C:305:LEU:HD21	1.88	0.55
2:F:1475:ILE:HD12	2:F:1482:PHE:HE2	1.71	0.55
2:D:1086:VAL:HG11	2:D:1141:GLU:HB2	1.89	0.55
2:D:1455:LEU:HD13	2:D:1464:VAL:HG21	1.88	0.55
1:G:168:PHE:CA	1:G:171:THR:CG2	2.83	0.55
1:A:181:LEU:H	1:A:181:LEU:CD2	2.19	0.55
2:D:686:PHE:HD1	2:D:733:VAL:HG23	1.71	0.55
2:F:1455:LEU:HD13	2:F:1464:VAL:HG21	1.88	0.55
2:B:363:PHE:HB2	2:B:1261:LEU:HD13	1.90	0.55
2:H:686:PHE:HD1	2:H:733:VAL:HG23	1.71	0.55
2:H:1226:LYS:HG2	2:H:1230:TYR:HE1	1.72	0.55
2:B:1226:LYS:HG2	2:B:1230:TYR:HE1	1.72	0.54
1:E:83:TRP:CD1	1:E:128:GLN:HG2	2.43	0.54
2:F:686:PHE:HD1	2:F:733:VAL:HG23	1.71	0.54
2:F:1086:VAL:HG11	2:F:1141:GLU:HB2	1.89	0.54
1:C:83:TRP:CD1	1:C:128:GLN:HG2	2.43	0.54
2:D:526:ARG:HE	2:D:1098:HIS:CG	2.25	0.54
2:H:363:PHE:HB2	2:H:1261:LEU:HD13	1.90	0.54
2:B:1455:LEU:HD13	2:B:1464:VAL:HG21	1.88	0.54
2:F:1562:LYS:HB3	2:F:1565:THR:HB	1.89	0.54
1:G:83:TRP:CD1	1:G:128:GLN:HG2	2.43	0.54
2:H:1086:VAL:HG11	2:H:1141:GLU:HB2	1.89	0.54
1:A:83:TRP:CD1	1:A:128:GLN:HG2	2.43	0.54
1:C:181:LEU:H	1:C:181:LEU:CD2	2.19	0.54
2:D:1562:LYS:HB3	2:D:1565:THR:HB	1.89	0.54
2:F:1528:PHE:HD1	2:F:1531:ARG:HD2	1.71	0.54
1:G:34:ARG:HG2	1:G:305:LEU:HD21	1.88	0.54
2:D:1528:PHE:HD1	2:D:1531:ARG:HD2	1.71	0.54
2:F:526:ARG:HE	2:F:1098:HIS:CG	2.25	0.54
2:B:1311:ALA:O	2:B:1314:ARG:HG2	2.08	0.54
2:F:366:LEU:HD23	2:F:1260:VAL:HG11	1.89	0.54
2:F:719:LYS:HB3	2:F:887:VAL:HG11	1.90	0.54
2:F:791:GLU:HB3	2:F:1219:TYR:HE2	1.73	0.54
2:H:1562:LYS:HB3	2:H:1565:THR:HB	1.89	0.54
2:D:363:PHE:HB2	2:D:1261:LEU:HD13	1.90	0.54
2:D:366:LEU:HD23	2:D:1260:VAL:HG11	1.89	0.54
2:F:1311:ALA:O	2:F:1314:ARG:HG2	2.08	0.54
2:F:1540:VAL:HG11	2:F:1579:ARG:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1540:VAL:HG11	2:H:1579:ARG:HA	1.88	0.54
2:B:719:LYS:HB3	2:B:887:VAL:HG11	1.90	0.54
2:B:366:LEU:HD23	2:B:1260:VAL:HG11	1.89	0.53
2:B:526:ARG:HE	2:B:1098:HIS:CG	2.25	0.53
2:B:442:PRO:O	2:B:445:ILE:HG13	2.08	0.53
2:D:1226:LYS:HG2	2:D:1230:TYR:HE1	1.72	0.53
2:F:1226:LYS:HG2	2:F:1230:TYR:HE1	1.72	0.53
2:D:791:GLU:HB3	2:D:1219:TYR:HE2	1.73	0.53
2:H:366:LEU:HD23	2:H:1260:VAL:HG11	1.89	0.53
2:H:562:HIS:CD2	2:H:571:LEU:HD23	2.44	0.53
2:H:1311:ALA:O	2:H:1314:ARG:HG2	2.08	0.53
2:B:1562:LYS:HB3	2:B:1565:THR:HB	1.89	0.53
2:F:363:PHE:HB2	2:F:1261:LEU:HD13	1.90	0.53
2:H:526:ARG:HE	2:H:1098:HIS:CG	2.25	0.53
2:B:517:ILE:HD11	2:B:1443:GLU:HG2	1.91	0.53
2:F:827:GLY:O	2:F:835:ARG:NH2	2.42	0.53
2:H:791:GLU:HB3	2:H:1219:TYR:HE2	1.73	0.53
2:H:827:GLY:O	2:H:835:ARG:NH2	2.42	0.53
2:B:562:HIS:CD2	2:B:571:LEU:HD23	2.44	0.53
2:D:719:LYS:HB3	2:D:887:VAL:HG11	1.90	0.53
2:D:1311:ALA:O	2:D:1314:ARG:HG2	2.08	0.53
2:D:517:ILE:HD11	2:D:1443:GLU:HG2	1.91	0.53
2:D:1124:ARG:NH1	2:D:1314:ARG:HD3	2.22	0.53
1:E:168:PHE:CA	1:E:171:THR:CG2	2.83	0.53
2:F:442:PRO:O	2:F:445:ILE:HG13	2.08	0.53
2:B:1393:PHE:CZ	2:B:1422:LEU:HB2	2.44	0.53
2:D:442:PRO:O	2:D:445:ILE:HG13	2.08	0.53
2:H:442:PRO:O	2:H:445:ILE:HG13	2.08	0.53
2:H:719:LYS:HB3	2:H:887:VAL:HG11	1.90	0.53
2:B:559:PHE:O	2:B:563:VAL:HG22	2.10	0.52
2:B:827:GLY:O	2:B:835:ARG:NH2	2.42	0.52
2:D:562:HIS:CD2	2:D:571:LEU:HD23	2.44	0.52
2:H:1393:PHE:CZ	2:H:1422:LEU:HB2	2.44	0.52
2:B:791:GLU:HB3	2:B:1219:TYR:HE2	1.73	0.52
2:F:517:ILE:HD11	2:F:1443:GLU:HG2	1.91	0.52
2:F:1393:PHE:CZ	2:F:1422:LEU:HB2	2.44	0.52
2:H:559:PHE:O	2:H:563:VAL:HG22	2.10	0.52
2:F:562:HIS:CD2	2:F:571:LEU:HD23	2.44	0.52
2:H:1528:PHE:CD1	2:H:1531:ARG:HD2	2.45	0.52
2:H:517:ILE:HD11	2:H:1443:GLU:HG2	1.91	0.52
2:F:1124:ARG:NH1	2:F:1314:ARG:HD3	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:LYS:NZ	2:B:175:LEU:CD1	2.73	0.52
2:B:1528:PHE:CD1	2:B:1531:ARG:HD2	2.45	0.52
2:D:1393:PHE:CZ	2:D:1422:LEU:HB2	2.44	0.52
2:F:150:LYS:NZ	2:F:175:LEU:CD1	2.73	0.52
2:H:779:LEU:HD11	2:H:835:ARG:HG2	1.92	0.52
2:D:91:GLU:CD	2:D:171:LEU:CD1	2.76	0.52
2:D:779:LEU:HD11	2:D:835:ARG:HG2	1.92	0.52
2:B:143:TRP:HB3	2:B:183:LEU:HG	1.92	0.52
2:F:559:PHE:O	2:F:563:VAL:HG22	2.10	0.52
2:D:827:GLY:O	2:D:835:ARG:NH2	2.42	0.52
2:H:687:THR:HB	2:H:694:PRO:HA	1.92	0.52
2:H:1455:LEU:HD22	2:H:1460:LEU:HD23	1.92	0.52
2:B:679:VAL:HB	2:B:703:ILE:HD12	1.92	0.51
2:D:308:LEU:O	2:D:311:LEU:HG	2.11	0.51
2:F:1528:PHE:CD1	2:F:1531:ARG:HD2	2.45	0.51
2:B:1124:ARG:NH1	2:B:1314:ARG:HD3	2.22	0.51
2:F:679:VAL:HB	2:F:703:ILE:HD12	1.92	0.51
2:F:779:LEU:HD11	2:F:835:ARG:HG2	1.92	0.51
2:F:1455:LEU:HD22	2:F:1460:LEU:HD23	1.92	0.51
2:H:150:LYS:NZ	2:H:175:LEU:CD1	2.73	0.51
2:H:423:ILE:O	2:H:427:GLN:HG2	2.11	0.51
2:H:1124:ARG:NH1	2:H:1314:ARG:HD3	2.22	0.51
2:H:308:LEU:O	2:H:311:LEU:HG	2.11	0.51
2:H:679:VAL:HB	2:H:703:ILE:HD12	1.92	0.51
2:B:779:LEU:HD11	2:B:835:ARG:HG2	1.92	0.51
2:F:687:THR:HB	2:F:694:PRO:HA	1.92	0.51
2:H:686:PHE:HB2	2:H:732:LYS:HA	1.93	0.51
2:D:423:ILE:O	2:D:427:GLN:HG2	2.11	0.51
2:D:679:VAL:HB	2:D:703:ILE:HD12	1.92	0.51
2:F:768:GLY:O	2:F:1218:ARG:NH2	2.44	0.51
2:H:143:TRP:HB3	2:H:183:LEU:HG	1.92	0.51
2:H:295:PHE:CE1	2:H:387:LEU:HB2	2.46	0.51
2:D:150:LYS:NZ	2:D:175:LEU:CD1	2.73	0.51
2:D:559:PHE:O	2:D:563:VAL:HG22	2.10	0.51
1:E:169:MET:CE	1:G:172:ALA:CA	2.79	0.51
2:F:143:TRP:HB3	2:F:183:LEU:HG	1.92	0.51
2:H:686:PHE:CD1	2:H:733:VAL:HG23	2.46	0.51
2:D:687:THR:HB	2:D:694:PRO:HA	1.92	0.51
2:F:308:LEU:O	2:F:311:LEU:HG	2.11	0.51
2:F:847:GLN:HA	2:F:882:ARG:HH12	1.76	0.51
1:A:239:PRO:HG3	1:C:244:VAL:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:VAL:HG22	1:A:302:THR:HG22	1.93	0.51
2:B:768:GLY:O	2:B:1218:ARG:NH2	2.44	0.51
1:C:239:PRO:HG3	1:E:244:VAL:CB	2.41	0.51
2:D:1528:PHE:CD1	2:D:1531:ARG:HD2	2.45	0.51
2:F:686:PHE:HB2	2:F:732:LYS:HA	1.93	0.51
1:C:285:VAL:HG22	1:C:302:THR:HG22	1.93	0.50
2:D:768:GLY:O	2:D:1218:ARG:NH2	2.44	0.50
2:B:686:PHE:CD1	2:B:733:VAL:HG23	2.46	0.50
1:C:202:VAL:HG23	1:C:251:LEU:HD21	1.94	0.50
2:D:1455:LEU:HD22	2:D:1460:LEU:HD23	1.92	0.50
1:E:285:VAL:HG22	1:E:302:THR:HG22	1.93	0.50
2:F:76:ILE:O	2:F:80:ILE:HG13	2.12	0.50
2:H:76:ILE:O	2:H:80:ILE:HG13	2.12	0.50
2:B:686:PHE:HB2	2:B:732:LYS:HA	1.93	0.50
2:D:686:PHE:CD1	2:D:733:VAL:HG23	2.46	0.50
2:H:768:GLY:O	2:H:1218:ARG:NH2	2.44	0.50
2:H:798:ARG:NH2	2:H:847:GLN:OE1	2.45	0.50
2:B:769:PRO:O	2:B:848:THR:OG1	2.26	0.50
2:D:76:ILE:O	2:D:80:ILE:HG13	2.12	0.50
2:D:143:TRP:HB3	2:D:183:LEU:HG	1.92	0.50
2:D:847:GLN:HA	2:D:882:ARG:HH12	1.76	0.50
1:E:239:PRO:HG3	1:G:244:VAL:CB	2.41	0.50
1:A:202:VAL:HG23	1:A:251:LEU:HD21	1.94	0.50
2:B:423:ILE:O	2:B:427:GLN:HG2	2.11	0.50
2:B:798:ARG:NH2	2:B:847:GLN:OE1	2.45	0.50
2:D:402:LEU:O	2:D:1215:ARG:NH1	2.45	0.50
2:D:864:LEU:HD11	2:D:1381:THR:HG21	1.94	0.50
2:F:295:PHE:CE1	2:F:387:LEU:HB2	2.46	0.50
1:G:202:VAL:HG23	1:G:251:LEU:HD21	1.94	0.50
1:A:244:VAL:CB	1:G:239:PRO:HG3	2.41	0.50
2:B:308:LEU:O	2:B:311:LEU:HG	2.11	0.50
2:B:402:LEU:O	2:B:1215:ARG:NH1	2.45	0.50
2:B:847:GLN:HA	2:B:882:ARG:HH12	1.76	0.50
1:G:47:LYS:HG3	1:G:48:ASN:ND2	2.27	0.50
2:H:769:PRO:O	2:H:848:THR:OG1	2.26	0.50
1:A:46:HIS:HA	1:C:328:VAL:CG2	2.42	0.50
2:B:508:LEU:HD13	2:B:1430:VAL:HG12	1.94	0.50
2:B:1455:LEU:HD22	2:B:1460:LEU:HD23	1.92	0.50
1:E:202:VAL:HG23	1:E:251:LEU:HD21	1.94	0.50
2:F:423:ILE:O	2:F:427:GLN:HG2	2.11	0.50
1:G:285:VAL:HG22	1:G:302:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:847:GLN:HA	2:H:882:ARG:HH12	1.76	0.50
1:A:47:LYS:HG3	1:A:48:ASN:ND2	2.27	0.50
2:D:1004:TYR:HE1	2:D:1093:VAL:HG11	1.77	0.50
1:E:46:HIS:HA	1:G:328:VAL:CG2	2.42	0.50
2:F:798:ARG:NH2	2:F:847:GLN:OE1	2.45	0.50
2:F:1004:TYR:HE1	2:F:1093:VAL:HG11	1.77	0.50
2:H:508:LEU:HD13	2:H:1430:VAL:HG12	1.94	0.50
1:A:328:VAL:CG2	1:G:46:HIS:HA	2.42	0.50
2:B:1496:PHE:HA	2:B:1528:PHE:HZ	1.77	0.50
1:E:47:LYS:HG3	1:E:48:ASN:ND2	2.27	0.50
1:E:198:PHE:HE1	1:E:200:LEU:HB2	1.77	0.50
2:B:687:THR:HB	2:B:694:PRO:HA	1.92	0.49
1:C:169:MET:CE	1:E:172:ALA:CA	2.79	0.49
2:D:686:PHE:HB2	2:D:732:LYS:HA	1.93	0.49
2:F:508:LEU:HD13	2:F:1430:VAL:HG12	1.94	0.49
1:A:172:ALA:CA	1:G:169:MET:CE	2.79	0.49
1:C:36:VAL:HG23	1:C:303:SER:OG	2.13	0.49
2:D:1347:ILE:HG21	2:D:1350:LEU:HD22	1.93	0.49
2:F:864:LEU:HD11	2:F:1381:THR:HG21	1.94	0.49
1:A:198:PHE:HE1	1:A:200:LEU:HB2	1.77	0.49
1:A:220:VAL:HG12	1:A:235:GLN:HG2	1.95	0.49
2:B:1004:TYR:HE1	2:B:1093:VAL:HG11	1.77	0.49
2:F:686:PHE:CD1	2:F:733:VAL:HG23	2.46	0.49
2:F:1347:ILE:HG21	2:F:1350:LEU:HD22	1.93	0.49
2:B:76:ILE:O	2:B:80:ILE:HG13	2.12	0.49
2:H:1353:ARG:HE	2:H:1398:MET:HB3	1.77	0.49
1:C:220:VAL:HG12	1:C:235:GLN:HG2	1.95	0.49
2:D:1570:LYS:HD3	2:D:1574:PHE:HB2	1.95	0.49
2:F:1496:PHE:HA	2:F:1528:PHE:HZ	1.77	0.49
1:A:328:VAL:HG23	1:G:46:HIS:HA	1.94	0.49
2:D:798:ARG:NH2	2:D:847:GLN:OE1	2.45	0.49
1:E:36:VAL:HG23	1:E:303:SER:OG	2.13	0.49
1:G:198:PHE:HE1	1:G:200:LEU:HB2	1.77	0.49
2:H:131:ASN:OD1	2:H:131:ASN:N	2.43	0.49
2:B:1353:ARG:HE	2:B:1398:MET:HB3	1.77	0.49
2:B:1553:LYS:HZ1	2:B:1558:LEU:HD13	1.77	0.49
1:C:46:HIS:HA	1:E:328:VAL:CG2	2.42	0.49
1:C:243:GLY:O	1:C:245:GLY:N	2.46	0.49
2:D:508:LEU:HD13	2:D:1430:VAL:HG12	1.94	0.49
2:H:864:LEU:HD11	2:H:1381:THR:HG21	1.94	0.49
1:A:46:HIS:HA	1:C:328:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:PHE:CD2	2:B:1248:LEU:HD22	2.48	0.49
2:B:1347:ILE:HG21	2:B:1350:LEU:HD22	1.93	0.49
2:D:295:PHE:CE1	2:D:387:LEU:HB2	2.46	0.49
1:E:220:VAL:HG12	1:E:235:GLN:HG2	1.95	0.49
2:F:402:LEU:O	2:F:1215:ARG:NH1	2.45	0.49
2:F:785:GLU:OE1	2:F:820:GLN:NE2	2.41	0.49
2:F:1339:TRP:CD2	2:F:1340:PRO:HD2	2.48	0.49
1:A:36:VAL:HG23	1:A:303:SER:OG	2.13	0.49
2:B:864:LEU:HD11	2:B:1381:THR:HG21	1.94	0.49
2:B:1570:LYS:HD3	2:B:1574:PHE:HB2	1.95	0.49
1:C:47:LYS:HG3	1:C:48:ASN:ND2	2.27	0.49
1:G:243:GLY:O	1:G:245:GLY:N	2.46	0.49
2:H:1182:PHE:CD2	2:H:1248:LEU:HD22	2.48	0.49
2:B:363:PHE:CD1	2:B:1261:LEU:HB2	2.48	0.49
2:B:526:ARG:NH1	2:B:529:GLU:OE1	2.46	0.49
1:C:139:THR:HG23	1:C:141:GLU:H	1.77	0.49
2:D:1353:ARG:HE	2:D:1398:MET:HB3	1.77	0.49
2:F:363:PHE:CD1	2:F:1261:LEU:HB2	2.48	0.49
1:G:139:THR:HG23	1:G:141:GLU:H	1.77	0.49
2:H:526:ARG:NH1	2:H:529:GLU:OE1	2.46	0.49
2:H:1004:TYR:HE1	2:H:1093:VAL:HG11	1.77	0.49
2:B:1339:TRP:CD2	2:B:1340:PRO:HD2	2.48	0.48
2:D:253:LEU:HD13	2:D:1236:ILE:HB	1.95	0.48
1:G:220:VAL:HG12	1:G:235:GLN:HG2	1.95	0.48
2:H:402:LEU:O	2:H:1215:ARG:NH1	2.45	0.48
2:H:1347:ILE:HG21	2:H:1350:LEU:HD22	1.93	0.48
2:H:1496:PHE:HA	2:H:1528:PHE:HZ	1.77	0.48
1:A:139:THR:HG23	1:A:141:GLU:H	1.77	0.48
2:B:795:ASN:HB2	2:B:798:ARG:HB3	1.95	0.48
2:D:795:ASN:HB2	2:D:798:ARG:HB3	1.95	0.48
2:D:1182:PHE:CD2	2:D:1248:LEU:HD22	2.48	0.48
2:F:253:LEU:HD13	2:F:1236:ILE:HB	1.95	0.48
1:A:169:MET:CE	1:C:172:ALA:CA	2.79	0.48
2:B:1461:LYS:HE2	2:B:1465:LYS:HE2	1.95	0.48
2:D:526:ARG:NH1	2:D:529:GLU:OE1	2.46	0.48
2:D:1553:LYS:HZ1	2:D:1558:LEU:HD13	1.78	0.48
2:F:449:VAL:HA	2:F:452:LEU:HG	1.96	0.48
2:F:526:ARG:NH1	2:F:529:GLU:OE1	2.46	0.48
2:F:1353:ARG:HE	2:F:1398:MET:HB3	1.77	0.48
2:F:1570:LYS:HD3	2:F:1574:PHE:HB2	1.95	0.48
1:A:181:LEU:N	1:A:181:LEU:CD2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:SER:O	2:D:585:ILE:HG12	2.14	0.48
1:E:46:HIS:HA	1:G:328:VAL:HG23	1.94	0.48
2:F:1182:PHE:CD2	2:F:1248:LEU:HD22	2.48	0.48
2:F:1553:LYS:HZ1	2:F:1558:LEU:HD13	1.78	0.48
2:H:449:VAL:HA	2:H:452:LEU:HG	1.96	0.48
2:H:1226:LYS:HG2	2:H:1230:TYR:CE1	2.48	0.48
2:H:1339:TRP:CD2	2:H:1340:PRO:HD2	2.48	0.48
2:B:449:VAL:HA	2:B:452:LEU:HG	1.96	0.48
1:C:198:PHE:HE1	1:C:200:LEU:HB2	1.77	0.48
2:D:363:PHE:CD1	2:D:1261:LEU:HB2	2.48	0.48
2:D:449:VAL:HA	2:D:452:LEU:HG	1.96	0.48
2:D:1496:PHE:HA	2:D:1528:PHE:HZ	1.77	0.48
1:E:181:LEU:N	1:E:181:LEU:CD2	2.76	0.48
2:H:32:ASN:O	2:H:35:PRO:HD2	2.14	0.48
1:A:243:GLY:O	1:A:245:GLY:N	2.46	0.48
2:B:32:ASN:O	2:B:35:PRO:HD2	2.14	0.48
2:D:711:ILE:HB	2:D:887:VAL:HG13	1.96	0.48
1:E:77:MET:HG2	2:F:48:PHE:CE2	2.48	0.48
2:F:581:SER:O	2:F:585:ILE:HG12	2.14	0.48
2:F:1461:LYS:HE2	2:F:1465:LYS:HE2	1.95	0.48
1:G:36:VAL:HG23	1:G:303:SER:OG	2.13	0.48
2:H:526:ARG:HE	2:H:1098:HIS:CD2	2.32	0.48
2:H:1570:LYS:HD3	2:H:1574:PHE:HB2	1.95	0.48
2:B:1226:LYS:HG2	2:B:1230:TYR:CE1	2.48	0.48
2:D:526:ARG:HE	2:D:1098:HIS:CD2	2.32	0.48
2:D:1339:TRP:CD2	2:D:1340:PRO:HD2	2.48	0.48
1:E:243:GLY:O	1:E:245:GLY:N	2.46	0.48
2:H:363:PHE:CD1	2:H:1261:LEU:HB2	2.48	0.48
2:H:1128:ASP:OD1	2:H:1311:ALA:HB1	2.14	0.48
2:H:1553:LYS:HZ1	2:H:1558:LEU:HD13	1.78	0.48
1:C:46:HIS:HA	1:E:328:VAL:HG23	1.94	0.48
2:H:488:THR:OG1	2:H:532:SER:HB3	2.14	0.48
2:B:253:LEU:HD13	2:B:1236:ILE:HB	1.95	0.48
2:B:550:ILE:HB	2:B:551:PRO:HD3	1.96	0.48
2:D:1079:CYS:O	2:D:1082:THR:OG1	2.27	0.48
1:G:168:PHE:C	1:G:171:THR:CG2	2.81	0.48
2:H:581:SER:O	2:H:585:ILE:HG12	2.14	0.48
1:A:64:VAL:HG13	1:A:170:LYS:CB	2.44	0.47
1:C:77:MET:HG2	2:D:48:PHE:CE2	2.48	0.47
1:C:128:GLN:NE2	1:C:152:GLN:OE1	2.47	0.47
2:D:32:ASN:O	2:D:35:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:GLN:NE2	1:E:152:GLN:OE1	2.47	0.47
1:G:77:MET:HG2	2:H:48:PHE:CE2	2.48	0.47
2:H:553:ALA:O	2:H:557:ILE:HG12	2.15	0.47
2:D:550:ILE:HB	2:D:551:PRO:HD3	1.96	0.47
2:D:1246:ARG:HA	2:D:1246:ARG:HD3	1.65	0.47
1:E:139:THR:HG23	1:E:141:GLU:H	1.77	0.47
2:B:396:TYR:CD1	2:B:1227:LEU:HD13	2.50	0.47
2:B:1128:ASP:OD1	2:B:1311:ALA:HB1	2.14	0.47
2:D:1078:LEU:O	2:D:1082:THR:HG23	2.15	0.47
1:E:46:HIS:HD2	1:G:330:TYR:OH	1.98	0.47
2:F:526:ARG:HE	2:F:1098:HIS:CD2	2.32	0.47
1:G:181:LEU:N	1:G:181:LEU:CD2	2.76	0.47
2:B:1078:LEU:O	2:B:1082:THR:HG23	2.15	0.47
2:D:396:TYR:CD1	2:D:1227:LEU:HD13	2.50	0.47
1:E:95:PHE:HE2	2:F:27:PHE:HB2	1.80	0.47
2:F:711:ILE:HB	2:F:887:VAL:HG13	1.96	0.47
2:F:1375:ILE:HB	2:F:1534:VAL:HG22	1.97	0.47
2:H:550:ILE:HB	2:H:551:PRO:HD3	1.96	0.47
2:H:802:VAL:HG11	2:H:845:TYR:HB2	1.97	0.47
2:H:1078:LEU:O	2:H:1082:THR:HG23	2.15	0.47
2:H:1461:LYS:HE2	2:H:1465:LYS:HE2	1.95	0.47
1:A:128:GLN:NE2	1:A:152:GLN:OE1	2.47	0.47
2:B:131:ASN:OD1	2:B:131:ASN:N	2.43	0.47
2:D:553:ALA:O	2:D:557:ILE:HG12	2.15	0.47
2:D:785:GLU:OE1	2:D:820:GLN:NE2	2.41	0.47
2:F:550:ILE:HB	2:F:551:PRO:HD3	1.96	0.47
2:F:1425:ILE:HD13	2:F:1492:LEU:HD12	1.97	0.47
1:G:64:VAL:HG13	1:G:170:LYS:CB	2.44	0.47
1:G:95:PHE:HE2	2:H:27:PHE:HB2	1.80	0.47
1:A:46:HIS:HD2	1:C:330:TYR:OH	1.98	0.47
1:A:77:MET:HG2	2:B:48:PHE:CE2	2.48	0.47
1:A:330:TYR:OH	1:G:46:HIS:HD2	1.98	0.47
2:B:526:ARG:HE	2:B:1098:HIS:CD2	2.32	0.47
2:D:1425:ILE:HD13	2:D:1492:LEU:HD12	1.97	0.47
2:F:795:ASN:HB2	2:F:798:ARG:HB3	1.95	0.47
2:H:253:LEU:HD13	2:H:1236:ILE:HB	1.95	0.47
2:B:581:SER:O	2:B:585:ILE:HG12	2.14	0.47
1:C:46:HIS:HD2	1:E:330:TYR:OH	1.98	0.47
2:D:488:THR:OG1	2:D:532:SER:HB3	2.14	0.47
2:F:32:ASN:O	2:F:35:PRO:HD2	2.14	0.47
2:F:485:GLN:HE22	2:F:598:ARG:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:592:LEU:HD11	2:F:1297:TRP:CH2	2.48	0.47
2:F:1128:ASP:OD1	2:F:1311:ALA:HB1	2.14	0.47
2:F:1226:LYS:HG2	2:F:1230:TYR:CE1	2.48	0.47
2:F:1345:ILE:HD11	2:F:1369:ILE:HD12	1.97	0.47
2:H:396:TYR:CD1	2:H:1227:LEU:HD13	2.50	0.47
2:H:711:ILE:HB	2:H:887:VAL:HG13	1.96	0.47
2:H:795:ASN:HB2	2:H:798:ARG:HB3	1.95	0.47
2:H:1345:ILE:HD11	2:H:1369:ILE:HD12	1.97	0.47
2:B:553:ALA:O	2:B:557:ILE:HG12	2.15	0.47
1:E:181:LEU:HG	1:E:300:ALA:HB2	1.97	0.47
2:F:488:THR:OG1	2:F:532:SER:HB3	2.14	0.47
1:A:95:PHE:HE2	2:B:27:PHE:HB2	1.80	0.47
2:B:488:THR:OG1	2:B:532:SER:HB3	2.14	0.47
2:B:853:LEU:HB2	2:B:886:LEU:HG	1.97	0.47
2:B:1425:ILE:HD13	2:B:1492:LEU:HD12	1.97	0.47
2:D:853:LEU:HB2	2:D:886:LEU:HG	1.97	0.47
2:D:1128:ASP:OD1	2:D:1311:ALA:HB1	2.14	0.47
2:F:396:TYR:OH	2:F:1223:PHE:HB3	2.15	0.47
2:F:489:LEU:HD11	2:F:602:LYS:HE3	1.97	0.47
2:B:1375:ILE:HB	2:B:1534:VAL:HG22	1.97	0.47
1:G:128:GLN:NE2	1:G:152:GLN:OE1	2.47	0.47
1:A:280:ASP:N	1:A:280:ASP:OD1	2.48	0.46
2:B:1503:PHE:HB2	2:B:1533:VAL:HG22	1.97	0.46
1:C:64:VAL:HG13	1:C:170:LYS:CB	2.44	0.46
2:D:769:PRO:O	2:D:848:THR:OG1	2.26	0.46
2:F:388:ARG:HD3	2:F:429:MET:SD	2.55	0.46
2:D:1345:ILE:HD11	2:D:1369:ILE:HD12	1.97	0.46
2:F:91:GLU:CD	2:F:171:LEU:HD12	2.36	0.46
2:F:853:LEU:HB2	2:F:886:LEU:HG	1.97	0.46
2:H:190:ILE:CD1	2:H:195:TYR:CB	2.94	0.46
2:H:398:LYS:HE3	2:H:398:LYS:HB3	1.81	0.46
2:H:447:VAL:HA	2:H:450:ILE:HG22	1.98	0.46
2:H:1375:ILE:HB	2:H:1534:VAL:HG22	1.97	0.46
2:H:1503:PHE:HB2	2:H:1533:VAL:HG22	1.97	0.46
2:B:396:TYR:OH	2:B:1223:PHE:HB3	2.15	0.46
2:B:785:GLU:OE1	2:B:820:GLN:NE2	2.41	0.46
1:C:95:PHE:HE2	2:D:27:PHE:HB2	1.80	0.46
2:D:1375:ILE:HB	2:D:1534:VAL:HG22	1.97	0.46
2:D:1503:PHE:HB2	2:D:1533:VAL:HG22	1.97	0.46
2:F:553:ALA:O	2:F:557:ILE:HG12	2.15	0.46
2:H:1352:VAL:HG13	2:H:1361:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:LYS:HB3	2:B:176:VAL:CG2	2.41	0.46
2:B:711:ILE:HB	2:B:887:VAL:HG13	1.96	0.46
2:D:150:LYS:HB3	2:D:176:VAL:CG2	2.41	0.46
2:D:388:ARG:HD3	2:D:429:MET:SD	2.55	0.46
2:D:396:TYR:OH	2:D:1223:PHE:HB3	2.15	0.46
2:D:701:ILE:HD11	2:D:703:ILE:HD11	1.98	0.46
2:D:1226:LYS:HG2	2:D:1230:TYR:CE1	2.48	0.46
2:D:1260:VAL:HG23	2:D:1288:ALA:HB1	1.98	0.46
1:E:177:ARG:HH22	1:E:208:SER:CB	2.25	0.46
2:H:701:ILE:HD11	2:H:703:ILE:HD11	1.98	0.46
2:B:1345:ILE:HD11	2:B:1369:ILE:HD12	1.97	0.46
2:D:489:LEU:HD11	2:D:602:LYS:HE3	1.97	0.46
2:D:802:VAL:HG11	2:D:845:TYR:HB2	1.97	0.46
2:F:398:LYS:CD	2:F:614:LEU:HA	2.45	0.46
2:F:1490:PHE:O	2:F:1494:ARG:HG3	2.16	0.46
2:H:396:TYR:OH	2:H:1223:PHE:HB3	2.15	0.46
1:A:181:LEU:HG	1:A:300:ALA:HB2	1.97	0.46
2:B:190:ILE:CD1	2:B:195:TYR:CB	2.94	0.46
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.98	0.46
2:B:1514:MET:HG2	2:B:1539:ARG:NH2	2.31	0.46
2:D:1461:LYS:HE2	2:D:1465:LYS:HE2	1.95	0.46
2:F:396:TYR:CD1	2:F:1227:LEU:HD13	2.50	0.46
2:F:802:VAL:HG11	2:F:845:TYR:HB2	1.97	0.46
2:F:1514:MET:HG2	2:F:1539:ARG:NH2	2.31	0.46
2:H:489:LEU:HD11	2:H:602:LYS:HE3	1.97	0.46
2:H:853:LEU:HB2	2:H:886:LEU:HG	1.97	0.46
2:B:388:ARG:HD3	2:B:429:MET:SD	2.55	0.46
2:B:398:LYS:CD	2:B:614:LEU:HA	2.45	0.46
2:B:485:GLN:HE22	2:B:598:ARG:HG3	1.80	0.46
2:B:802:VAL:HG11	2:B:845:TYR:HB2	1.97	0.46
2:D:263:TYR:HB2	2:D:393:THR:HG21	1.98	0.46
2:D:398:LYS:CD	2:D:614:LEU:HA	2.45	0.46
2:D:1352:VAL:HG13	2:D:1361:VAL:HB	1.97	0.46
2:F:1260:VAL:HG23	2:F:1288:ALA:HB1	1.98	0.46
1:G:190:THR:HG22	1:G:191:LEU:H	1.81	0.46
1:A:190:THR:HG22	1:A:191:LEU:H	1.81	0.46
2:B:1260:VAL:HG23	2:B:1288:ALA:HB1	1.98	0.46
2:B:1490:PHE:O	2:B:1494:ARG:HG3	2.16	0.46
1:C:181:LEU:HG	1:C:300:ALA:HB2	1.97	0.46
1:E:190:THR:HG22	1:E:191:LEU:H	1.81	0.46
1:E:280:ASP:OD1	1:E:280:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1078:LEU:O	2:F:1082:THR:HG23	2.15	0.46
1:G:181:LEU:HG	1:G:300:ALA:HB2	1.97	0.46
1:G:280:ASP:OD1	1:G:280:ASP:N	2.48	0.46
2:H:253:LEU:HG	2:H:257:MET:HB3	1.98	0.46
2:H:388:ARG:HD3	2:H:429:MET:SD	2.55	0.46
2:H:398:LYS:CD	2:H:614:LEU:HA	2.45	0.46
2:B:253:LEU:HG	2:B:257:MET:HB3	1.98	0.46
1:C:90:TRP:HA	1:C:93:ILE:HG22	1.98	0.46
1:C:178:ALA:O	1:C:181:LEU:CD2	2.64	0.46
1:E:168:PHE:C	1:E:171:THR:CG2	2.81	0.46
2:F:701:ILE:HD11	2:F:703:ILE:HD11	1.98	0.46
2:F:1352:VAL:HG13	2:F:1361:VAL:HB	1.97	0.46
2:F:1503:PHE:HB2	2:F:1533:VAL:HG22	1.97	0.46
1:G:313:GLN:HB3	1:G:336:THR:CG2	2.46	0.46
2:H:485:GLN:HE22	2:H:598:ARG:HG3	1.80	0.46
2:H:1425:ILE:HD13	2:H:1492:LEU:HD12	1.97	0.46
1:A:178:ALA:O	1:A:181:LEU:CD2	2.64	0.46
1:A:261:ILE:H	1:A:261:ILE:HG13	1.61	0.46
2:B:447:VAL:HA	2:B:450:ILE:HG22	1.98	0.46
2:B:1352:VAL:HG13	2:B:1361:VAL:HB	1.97	0.46
1:C:177:ARG:HH22	1:C:208:SER:CB	2.25	0.46
2:D:253:LEU:HG	2:D:257:MET:HB3	1.98	0.46
1:E:64:VAL:HG13	1:E:170:LYS:CB	2.44	0.46
1:E:178:ALA:O	1:E:181:LEU:CD2	2.64	0.46
2:D:447:VAL:HA	2:D:450:ILE:HG22	1.98	0.45
2:D:1102:LEU:HD23	2:D:1102:LEU:HA	1.76	0.45
1:E:90:TRP:HA	1:E:93:ILE:HG22	1.98	0.45
2:F:190:ILE:CD1	2:F:195:TYR:CB	2.94	0.45
2:H:1327:GLU:HB3	2:H:1415:LEU:H	1.82	0.45
2:B:196:ILE:C	2:B:197:PHE:O	2.55	0.45
1:C:280:ASP:N	1:C:280:ASP:OD1	2.48	0.45
2:F:263:TYR:HB2	2:F:393:THR:HG21	1.98	0.45
2:F:447:VAL:HA	2:F:450:ILE:HG22	1.98	0.45
1:G:313:GLN:HE22	1:G:338:LYS:HD2	1.82	0.45
1:A:313:GLN:HE22	1:A:338:LYS:HD2	1.82	0.45
1:C:190:THR:HG22	1:C:191:LEU:H	1.81	0.45
2:D:485:GLN:HE22	2:D:598:ARG:HG3	1.80	0.45
2:D:511:LEU:HD12	2:D:511:LEU:HA	1.73	0.45
2:D:1514:MET:HG2	2:D:1539:ARG:NH2	2.31	0.45
1:G:90:TRP:HA	1:G:93:ILE:HG22	1.98	0.45
2:H:196:ILE:C	2:H:197:PHE:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:HB3	1:A:336:THR:CG2	2.46	0.45
2:B:489:LEU:HD11	2:B:602:LYS:HE3	1.97	0.45
1:C:313:GLN:HE22	1:C:338:LYS:HD2	1.82	0.45
2:D:190:ILE:CD1	2:D:195:TYR:CB	2.94	0.45
2:D:398:LYS:HE3	2:D:398:LYS:HB3	1.81	0.45
2:F:150:LYS:CB	2:F:176:VAL:HG22	2.44	0.45
2:F:892:GLN:H	2:F:892:GLN:HG3	1.41	0.45
2:F:1079:CYS:O	2:F:1082:THR:OG1	2.27	0.45
1:G:177:ARG:HH22	1:G:208:SER:CB	2.25	0.45
1:G:178:ALA:O	1:G:181:LEU:CD2	2.64	0.45
2:H:785:GLU:OE1	2:H:820:GLN:NE2	2.41	0.45
2:H:1260:VAL:HG23	2:H:1288:ALA:HB1	1.98	0.45
2:B:246:ASP:OD1	2:B:247:LEU:N	2.49	0.45
2:B:288:TRP:CE3	2:B:607:VAL:HG11	2.52	0.45
2:B:312:LEU:CB	2:B:369:GLN:HG2	2.47	0.45
2:B:1327:GLU:HB3	2:B:1415:LEU:H	1.82	0.45
1:C:313:GLN:HB3	1:C:336:THR:CG2	2.46	0.45
2:D:1327:GLU:HB3	2:D:1415:LEU:H	1.82	0.45
2:D:1490:PHE:O	2:D:1494:ARG:HG3	2.16	0.45
1:E:56:LEU:O	1:E:59:VAL:HG22	2.17	0.45
2:F:37:VAL:HG13	2:F:41:PHE:CE2	2.52	0.45
2:F:769:PRO:O	2:F:848:THR:OG1	2.26	0.45
2:F:1353:ARG:O	2:F:1398:MET:HB2	2.17	0.45
2:H:1030:ILE:HD11	2:H:1068:PHE:CE1	2.52	0.45
2:H:1102:LEU:HD23	2:H:1102:LEU:HA	1.76	0.45
2:H:1490:PHE:O	2:H:1494:ARG:HG3	2.16	0.45
2:H:1514:MET:HG2	2:H:1539:ARG:NH2	2.31	0.45
2:D:196:ILE:C	2:D:197:PHE:O	2.55	0.45
1:E:313:GLN:HB3	1:E:336:THR:CG2	2.46	0.45
2:F:253:LEU:HG	2:F:257:MET:HB3	1.98	0.45
2:H:37:VAL:HG13	2:H:41:PHE:CE2	2.52	0.45
1:A:90:TRP:HA	1:A:93:ILE:HG22	1.98	0.45
2:D:37:VAL:HG13	2:D:41:PHE:CE2	2.52	0.45
2:D:540:THR:O	2:D:544:ILE:HG12	2.17	0.45
1:E:313:GLN:HE22	1:E:338:LYS:HD2	1.82	0.45
2:F:196:ILE:C	2:F:197:PHE:O	2.55	0.45
2:F:511:LEU:HD12	2:F:511:LEU:HA	1.73	0.45
1:G:56:LEU:O	1:G:59:VAL:HG22	2.17	0.45
2:D:288:TRP:CE3	2:D:607:VAL:HG11	2.52	0.45
2:F:540:THR:O	2:F:544:ILE:HG12	2.17	0.45
2:H:1353:ARG:O	2:H:1398:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:O	1:A:59:VAL:HG22	2.17	0.45
1:A:177:ARG:HH22	1:A:208:SER:CB	2.25	0.45
2:B:1246:ARG:HA	2:B:1246:ARG:HD3	1.65	0.45
1:C:56:LEU:O	1:C:59:VAL:HG22	2.17	0.45
2:D:592:LEU:HD21	2:D:1297:TRP:CH2	2.52	0.45
2:D:853:LEU:HD23	2:D:856:PRO:HG3	1.99	0.45
2:F:288:TRP:CE3	2:F:607:VAL:HG11	2.52	0.45
2:F:312:LEU:CB	2:F:369:GLN:HG2	2.47	0.45
2:H:592:LEU:HD11	2:H:1297:TRP:CH2	2.48	0.45
2:H:1460:LEU:HD21	2:H:1490:PHE:CE1	2.52	0.45
2:B:592:LEU:HD21	2:B:1297:TRP:CH2	2.52	0.45
2:B:1030:ILE:HD11	2:B:1068:PHE:CE1	2.52	0.45
2:D:312:LEU:CB	2:D:369:GLN:HG2	2.47	0.45
2:D:395:ILE:O	2:D:399:ILE:HG13	2.17	0.45
2:F:219:GLN:HG2	2:F:378:TYR:CZ	2.52	0.45
2:H:263:TYR:HB2	2:H:393:THR:HG21	1.98	0.45
2:H:540:THR:O	2:H:544:ILE:HG12	2.17	0.45
2:B:37:VAL:HG13	2:B:41:PHE:CE2	2.52	0.44
2:B:1020:GLN:HB3	2:B:1148:LEU:HD11	1.99	0.44
2:D:246:ASP:OD1	2:D:247:LEU:N	2.49	0.44
2:F:592:LEU:HD21	2:F:1297:TRP:CH2	2.52	0.44
2:H:288:TRP:CE3	2:H:607:VAL:HG11	2.52	0.44
2:H:551:PRO:CB	2:H:583:PHE:HZ	2.30	0.44
2:H:853:LEU:HD23	2:H:856:PRO:HG3	1.99	0.44
1:A:34:ARG:O	1:C:326:TYR:HE1	2.00	0.44
1:A:60:PHE:HA	1:A:63:LEU:HD23	1.99	0.44
1:A:241:GLU:HG3	1:A:259:HIS:HD2	1.82	0.44
2:D:1353:ARG:O	2:D:1398:MET:HB2	2.17	0.44
2:H:312:LEU:CB	2:H:369:GLN:HG2	2.47	0.44
2:H:395:ILE:O	2:H:399:ILE:HG13	2.17	0.44
2:B:853:LEU:HD23	2:B:856:PRO:HG3	1.99	0.44
2:D:1004:TYR:CE1	2:D:1093:VAL:HG11	2.53	0.44
2:H:301:LEU:C	2:H:301:LEU:CD2	2.85	0.44
2:B:219:GLN:HG2	2:B:378:TYR:CZ	2.52	0.44
2:B:1256:GLY:O	2:B:1260:VAL:HG12	2.18	0.44
2:B:1353:ARG:O	2:B:1398:MET:HB2	2.17	0.44
2:D:1020:GLN:HB3	2:D:1148:LEU:HD11	1.99	0.44
2:D:1256:GLY:O	2:D:1260:VAL:HG12	2.18	0.44
2:D:1460:LEU:HD21	2:D:1490:PHE:CE1	2.52	0.44
2:F:395:ILE:O	2:F:399:ILE:HG13	2.17	0.44
2:F:853:LEU:HD23	2:F:856:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1256:GLY:O	2:F:1260:VAL:HG12	2.18	0.44
2:F:1460:LEU:HD21	2:F:1490:PHE:CE1	2.52	0.44
2:B:1483:SER:O	2:B:1487:ARG:HG3	2.18	0.44
2:D:219:GLN:HG2	2:D:378:TYR:CZ	2.52	0.44
2:F:1369:ILE:HD13	2:F:1375:ILE:HG13	2.00	0.44
2:F:1509:THR:HG21	2:F:1539:ARG:HB2	2.00	0.44
1:G:60:PHE:HA	1:G:63:LEU:HD23	1.99	0.44
2:H:219:GLN:HG2	2:H:378:TYR:CZ	2.52	0.44
2:H:491:HIS:CE1	2:H:528:LYS:HB3	2.53	0.44
2:H:1004:TYR:CE1	2:H:1093:VAL:HG11	2.53	0.44
2:B:263:TYR:HB2	2:B:393:THR:HG21	1.98	0.44
2:B:295:PHE:CE1	2:B:387:LEU:HB2	2.46	0.44
2:B:391:ILE:O	2:B:395:ILE:HG23	2.18	0.44
2:D:1030:ILE:HD11	2:D:1068:PHE:CE1	2.52	0.44
2:D:1369:ILE:HD13	2:D:1375:ILE:HG13	2.00	0.44
2:F:40:LEU:O	2:F:44:PHE:HD2	2.01	0.44
2:H:246:ASP:OD1	2:H:247:LEU:N	2.49	0.44
2:H:819:ASP:OD1	2:H:820:GLN:N	2.41	0.44
2:D:391:ILE:O	2:D:395:ILE:HG23	2.18	0.44
2:D:1479:GLY:O	2:D:1487:ARG:NH1	2.51	0.44
2:D:1509:THR:HG21	2:D:1539:ARG:HB2	2.00	0.44
2:F:1030:ILE:HD11	2:F:1068:PHE:CE1	2.52	0.44
2:F:1483:SER:O	2:F:1487:ARG:HG3	2.18	0.44
2:H:40:LEU:O	2:H:44:PHE:HD2	2.01	0.44
2:H:684:GLY:O	2:H:698:ASN:N	2.51	0.44
2:H:1431:LEU:HD12	2:H:1487:ARG:HG2	2.00	0.44
2:B:491:HIS:CE1	2:B:528:LYS:HB3	2.53	0.44
2:B:540:THR:O	2:B:544:ILE:HG12	2.17	0.44
2:B:1460:LEU:HD21	2:B:1490:PHE:CE1	2.52	0.44
2:D:91:GLU:OE1	2:D:171:LEU:HD12	2.18	0.44
2:D:253:LEU:HD12	2:D:253:LEU:HA	1.77	0.44
1:E:241:GLU:HG3	1:E:259:HIS:HD2	1.82	0.44
2:F:684:GLY:O	2:F:698:ASN:N	2.51	0.44
2:F:1192:LEU:HA	2:F:1195:THR:HG22	2.00	0.44
2:F:1327:GLU:HB3	2:F:1415:LEU:H	1.82	0.44
2:B:1004:TYR:CE1	2:B:1093:VAL:HG11	2.53	0.44
2:D:40:LEU:O	2:D:44:PHE:HD2	2.01	0.44
2:D:1386:SER:OG	3:D:2502:ADP:O1A	2.36	0.44
2:F:288:TRP:HE3	2:F:607:VAL:HG11	1.83	0.44
2:F:730:MET:HE3	2:F:730:MET:HB3	1.82	0.44
2:F:1105:ILE:HD11	2:F:1318:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:806:CYS:O	2:H:837:ARG:HD2	2.18	0.44
2:H:1256:GLY:O	2:H:1260:VAL:HG12	2.18	0.44
2:H:1345:ILE:HG12	2:H:1369:ILE:HB	2.00	0.44
2:B:40:LEU:O	2:B:44:PHE:HD2	2.01	0.43
2:B:150:LYS:CB	2:B:176:VAL:HG22	2.44	0.43
2:B:395:ILE:O	2:B:399:ILE:HG13	2.17	0.43
1:C:241:GLU:HG3	1:C:259:HIS:HD2	1.82	0.43
2:D:825:GLU:OE1	2:D:825:GLU:N	2.48	0.43
2:D:1255:ILE:HD13	2:D:1255:ILE:HA	1.93	0.43
2:F:1386:SER:OG	3:F:2502:ADP:O1A	2.36	0.43
2:F:1479:GLY:O	2:F:1487:ARG:NH1	2.51	0.43
2:H:1479:GLY:O	2:H:1487:ARG:NH1	2.51	0.43
2:B:295:PHE:HZ	2:B:387:LEU:CD1	2.30	0.43
2:B:398:LYS:HE3	2:B:398:LYS:HB3	1.81	0.43
2:D:772:TYR:HD1	2:D:852:PHE:HB2	1.83	0.43
2:D:892:GLN:H	2:D:892:GLN:HG3	1.41	0.43
1:E:332:LYS:HD3	1:E:335:ASN:OD1	2.18	0.43
1:A:46:HIS:CD2	1:C:330:TYR:OH	2.72	0.43
2:B:806:CYS:O	2:B:837:ARG:HD2	2.18	0.43
2:B:1105:ILE:HD11	2:B:1318:LEU:HD21	2.00	0.43
2:B:1479:GLY:O	2:B:1487:ARG:NH1	2.51	0.43
2:D:592:LEU:HD11	2:D:1297:TRP:CH2	2.48	0.43
2:D:592:LEU:HD21	2:D:1297:TRP:CZ2	2.54	0.43
2:D:806:CYS:O	2:D:837:ARG:HD2	2.18	0.43
2:D:1105:ILE:HD11	2:D:1318:LEU:HD21	2.00	0.43
2:D:1483:SER:O	2:D:1487:ARG:HG3	2.18	0.43
1:E:60:PHE:HA	1:E:63:LEU:HD23	1.99	0.43
2:F:1020:GLN:HB3	2:F:1148:LEU:HD11	1.99	0.43
2:H:1105:ILE:HD11	2:H:1318:LEU:HD21	2.00	0.43
2:H:1386:SER:OG	3:H:2502:ADP:O1A	2.36	0.43
2:B:1354:TYR:HA	2:B:1396:VAL:HG13	2.00	0.43
1:C:34:ARG:O	1:E:326:TYR:HE1	2.00	0.43
1:C:60:PHE:HA	1:C:63:LEU:HD23	1.99	0.43
2:D:295:PHE:HZ	2:D:387:LEU:CD1	2.30	0.43
1:E:34:ARG:O	1:G:326:TYR:HE1	2.00	0.43
2:F:491:HIS:CE1	2:F:528:LYS:HB3	2.53	0.43
2:F:592:LEU:HD21	2:F:1297:TRP:CZ2	2.54	0.43
2:H:150:LYS:HB3	2:H:176:VAL:CG2	2.41	0.43
2:H:892:GLN:H	2:H:892:GLN:HG3	1.41	0.43
2:H:1114:GLU:OE1	3:H:2502:ADP:N6	2.52	0.43
1:C:332:LYS:HD3	1:C:335:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:684:GLY:O	2:D:698:ASN:N	2.51	0.43
2:F:262:ASN:HB3	2:F:390:ALA:HB2	2.00	0.43
2:H:150:LYS:CB	2:H:176:VAL:HG22	2.44	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CZ2	2.54	0.43
2:H:592:LEU:HD21	2:H:1297:TRP:CH2	2.52	0.43
2:H:1192:LEU:HA	2:H:1195:THR:HG22	2.00	0.43
1:A:326:TYR:HE1	1:G:34:ARG:O	2.00	0.43
2:B:262:ASN:HB3	2:B:390:ALA:HB2	2.00	0.43
2:B:819:ASP:OD1	2:B:820:GLN:N	2.41	0.43
2:B:1431:LEU:HD12	2:B:1487:ARG:HG2	2.00	0.43
2:D:301:LEU:C	2:D:301:LEU:CD2	2.85	0.43
2:D:1353:ARG:NH1	2:D:1400:GLU:OE2	2.45	0.43
2:D:1354:TYR:HA	2:D:1396:VAL:HG13	2.00	0.43
1:E:46:HIS:CD2	1:G:330:TYR:OH	2.72	0.43
2:F:301:LEU:C	2:F:301:LEU:CD2	2.85	0.43
2:F:551:PRO:CB	2:F:583:PHE:HZ	2.30	0.43
2:H:288:TRP:HE3	2:H:607:VAL:HG11	1.83	0.43
2:H:391:ILE:O	2:H:395:ILE:HG23	2.18	0.43
2:H:586:LEU:O	2:H:589:PRO:HD2	2.19	0.43
2:H:825:GLU:OE1	2:H:825:GLU:N	2.48	0.43
2:H:1020:GLN:HB3	2:H:1148:LEU:HD11	1.99	0.43
2:H:1369:ILE:HD13	2:H:1375:ILE:HG13	2.00	0.43
1:C:46:HIS:CD2	1:E:330:TYR:OH	2.72	0.43
2:D:219:GLN:HG2	2:D:378:TYR:OH	2.19	0.43
2:D:491:HIS:CE1	2:D:528:LYS:HB3	2.53	0.43
2:D:1431:LEU:HD12	2:D:1487:ARG:HG2	2.00	0.43
2:F:131:ASN:OD1	2:F:131:ASN:N	2.43	0.43
2:F:295:PHE:HZ	2:F:387:LEU:CD1	2.30	0.43
2:H:219:GLN:HG2	2:H:378:TYR:OH	2.19	0.43
2:H:263:TYR:HB2	2:H:393:THR:CG2	2.49	0.43
2:H:295:PHE:HZ	2:H:387:LEU:CD1	2.30	0.43
2:H:1079:CYS:O	2:H:1082:THR:OG1	2.27	0.43
2:H:1353:ARG:NH1	2:H:1400:GLU:OE2	2.45	0.43
2:B:253:LEU:HA	2:B:253:LEU:HD12	1.77	0.43
2:B:263:TYR:HB2	2:B:393:THR:CG2	2.49	0.43
2:B:592:LEU:HD21	2:B:1297:TRP:CZ2	2.54	0.43
2:B:1369:ILE:HD13	2:B:1375:ILE:HG13	2.00	0.43
1:C:168:PHE:C	1:C:171:THR:CG2	2.81	0.43
2:D:1192:LEU:HA	2:D:1195:THR:HG22	2.00	0.43
2:F:391:ILE:O	2:F:395:ILE:HG23	2.18	0.43
2:F:586:LEU:O	2:F:589:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:772:TYR:HD1	2:F:852:PHE:HB2	1.83	0.43
1:G:241:GLU:HG3	1:G:259:HIS:HD2	1.82	0.43
2:H:1483:SER:O	2:H:1487:ARG:HG3	2.18	0.43
2:B:684:GLY:O	2:B:698:ASN:N	2.51	0.43
2:D:262:ASN:HB3	2:D:390:ALA:HB2	2.00	0.43
2:F:150:LYS:HB3	2:F:176:VAL:CG2	2.41	0.43
2:F:1102:LEU:HD23	2:F:1102:LEU:HA	1.76	0.43
2:F:1106:ILE:HD13	2:F:1106:ILE:HA	1.89	0.43
2:F:1431:LEU:HD12	2:F:1487:ARG:HG2	2.00	0.43
2:H:262:ASN:HB3	2:H:390:ALA:HB2	2.00	0.43
2:H:1494:ARG:O	2:H:1498:ARG:HG3	2.19	0.43
2:B:1114:GLU:OE1	3:B:2502:ADP:N6	2.52	0.43
2:B:1203:HIS:CD2	2:B:1227:LEU:HD12	2.54	0.43
2:F:806:CYS:O	2:F:837:ARG:HD2	2.18	0.43
1:G:332:LYS:HD3	1:G:335:ASN:OD1	2.18	0.43
2:H:772:TYR:HD1	2:H:852:PHE:HB2	1.83	0.43
2:B:288:TRP:HE3	2:B:607:VAL:HG11	1.83	0.42
2:D:1114:GLU:OE1	3:D:2502:ADP:N6	2.52	0.42
2:F:1004:TYR:CE1	2:F:1093:VAL:HG11	2.53	0.42
1:A:178:ALA:O	1:A:181:LEU:HD23	2.20	0.42
1:A:330:TYR:OH	1:G:46:HIS:CD2	2.72	0.42
2:B:586:LEU:O	2:B:589:PRO:HD2	2.19	0.42
2:B:1386:SER:OG	3:B:2502:ADP:O1A	2.36	0.42
2:D:263:TYR:HB2	2:D:393:THR:CG2	2.49	0.42
2:D:1494:ARG:O	2:D:1498:ARG:HG3	2.19	0.42
2:F:44:PHE:HD1	2:F:48:PHE:CE2	2.37	0.42
2:F:1345:ILE:HG12	2:F:1369:ILE:HB	2.00	0.42
2:H:1509:THR:HG21	2:H:1539:ARG:HB2	2.00	0.42
1:A:332:LYS:HD3	1:A:335:ASN:OD1	2.18	0.42
2:B:772:TYR:HD1	2:B:852:PHE:HB2	1.83	0.42
2:B:1509:THR:HG21	2:B:1539:ARG:HB2	2.00	0.42
2:F:263:TYR:HB2	2:F:393:THR:CG2	2.49	0.42
2:F:875:GLU:O	2:F:879:ASP:HB2	2.20	0.42
2:H:78:THR:HG21	2:H:121:VAL:HG23	2.01	0.42
2:H:1521:GLN:HA	2:H:1524:VAL:HG12	2.01	0.42
2:B:370:ARG:HD2	2:B:1253:GLU:CD	2.40	0.42
2:B:1345:ILE:HG12	2:B:1369:ILE:HB	2.00	0.42
2:D:586:LEU:O	2:D:589:PRO:HD2	2.19	0.42
2:F:78:THR:HG21	2:F:121:VAL:HG23	2.01	0.42
2:F:1494:ARG:O	2:F:1498:ARG:HG3	2.19	0.42
2:H:370:ARG:HD2	2:H:1253:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:THR:HG21	2:D:121:VAL:HG23	2.01	0.42
2:D:288:TRP:HE3	2:D:607:VAL:HG11	1.83	0.42
2:D:370:ARG:HD2	2:D:1253:GLU:CD	2.40	0.42
2:D:875:GLU:O	2:D:879:ASP:HB2	2.20	0.42
2:D:1345:ILE:HG12	2:D:1369:ILE:HB	2.00	0.42
2:F:1256:GLY:HA2	2:F:1259:VAL:HG12	2.02	0.42
2:F:1354:TYR:HA	2:F:1396:VAL:HG13	2.00	0.42
1:A:86:PHE:HA	1:A:89:VAL:HG12	2.02	0.42
2:B:592:LEU:HD11	2:B:1297:TRP:CH2	2.48	0.42
2:B:1192:LEU:HA	2:B:1195:THR:HG22	2.00	0.42
2:D:1020:GLN:HB3	2:D:1148:LEU:CD1	2.50	0.42
2:D:1256:GLY:HA2	2:D:1259:VAL:HG12	2.02	0.42
2:D:1521:GLN:O	2:D:1525:MET:HG2	2.20	0.42
2:F:1146:SER:HB3	2:F:1298:MET:HB2	2.02	0.42
1:G:86:PHE:HA	1:G:89:VAL:HG12	2.02	0.42
1:A:286:ILE:HD12	1:A:301:ARG:HG2	2.02	0.42
2:B:219:GLN:HG2	2:B:378:TYR:OH	2.19	0.42
2:B:1020:GLN:HB3	2:B:1148:LEU:CD1	2.50	0.42
2:B:1079:CYS:O	2:B:1082:THR:OG1	2.27	0.42
2:B:1308:GLN:O	2:B:1312:VAL:HG23	2.20	0.42
1:C:188:VAL:HG12	1:C:310:LEU:HD11	2.02	0.42
2:D:1335:ILE:N	2:D:1336:PRO:HD2	2.35	0.42
2:D:1521:GLN:HA	2:D:1524:VAL:HG12	2.01	0.42
2:F:370:ARG:HD2	2:F:1253:GLU:CD	2.40	0.42
2:F:571:LEU:O	2:F:571:LEU:HD12	2.20	0.42
2:F:1521:GLN:HA	2:F:1524:VAL:HG12	2.01	0.42
1:G:286:ILE:HD12	1:G:301:ARG:HG2	2.02	0.42
2:H:44:PHE:HD1	2:H:48:PHE:CE2	2.37	0.42
2:H:1335:ILE:N	2:H:1336:PRO:HD2	2.35	0.42
1:A:209:MET:HB2	1:A:292:GLU:OE2	2.20	0.42
2:D:1164:PHE:HZ	2:D:1259:VAL:HG23	1.85	0.42
1:E:145:ALA:HA	1:E:148:ILE:HG22	2.02	0.42
1:E:178:ALA:O	1:E:181:LEU:HD23	2.20	0.42
2:F:219:GLN:HG2	2:F:378:TYR:OH	2.19	0.42
1:G:79:PHE:HD1	1:G:79:PHE:HA	1.74	0.42
1:G:178:ALA:O	1:G:181:LEU:HD23	2.20	0.42
2:H:531:THR:O	2:H:534:ARG:HG2	2.20	0.42
2:H:571:LEU:HD12	2:H:571:LEU:O	2.20	0.42
2:H:1020:GLN:HB3	2:H:1148:LEU:CD1	2.50	0.42
1:A:137:MET:SD	1:C:133:PHE:HB3	2.60	0.42
2:B:511:LEU:HA	2:B:511:LEU:HD12	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:PHE:HE2	2:B:886:LEU:HD21	1.85	0.42
2:B:875:GLU:O	2:B:879:ASP:HB2	2.20	0.42
2:B:1353:ARG:NH1	2:B:1400:GLU:OE2	2.45	0.42
2:D:44:PHE:HD1	2:D:48:PHE:CE2	2.37	0.42
2:D:1308:GLN:O	2:D:1312:VAL:HG23	2.20	0.42
2:F:1203:HIS:CD2	2:F:1227:LEU:HD12	2.54	0.42
2:H:1226:LYS:O	2:H:1230:TYR:HD1	2.03	0.42
2:B:44:PHE:HD1	2:B:48:PHE:CE2	2.37	0.42
2:B:1335:ILE:N	2:B:1336:PRO:HD2	2.35	0.42
2:B:1494:ARG:O	2:B:1498:ARG:HG3	2.19	0.42
1:C:145:ALA:HA	1:C:148:ILE:HG22	2.02	0.42
2:D:857:PHE:HE2	2:D:886:LEU:HD21	1.85	0.42
2:D:1203:HIS:CD2	2:D:1227:LEU:HD12	2.54	0.42
2:D:1226:LYS:O	2:D:1230:TYR:HD1	2.03	0.42
1:E:220:VAL:HB	1:E:233:LEU:HG	2.02	0.42
1:E:338:LYS:HB3	1:E:338:LYS:HE3	1.87	0.42
2:F:188:ASN:O	2:F:192:VAL:HG23	2.20	0.42
2:F:417:ILE:O	2:F:420:LEU:HB3	2.20	0.42
2:H:451:LEU:HD13	2:H:582:LEU:HD21	2.01	0.42
2:H:1146:SER:HB3	2:H:1298:MET:HB2	2.02	0.42
2:H:1246:ARG:HA	2:H:1246:ARG:HD3	1.65	0.42
2:H:1354:TYR:HA	2:H:1396:VAL:HG13	2.00	0.42
2:B:435:CYS:HB3	2:B:436:PRO:HD3	2.02	0.41
2:B:531:THR:O	2:B:534:ARG:HG2	2.20	0.41
2:B:825:GLU:OE1	2:B:825:GLU:N	2.48	0.41
1:C:49:ILE:H	1:C:49:ILE:HG13	1.58	0.41
1:C:338:LYS:HE3	1:C:338:LYS:HB3	1.87	0.41
2:D:435:CYS:HB3	2:D:436:PRO:HD3	2.02	0.41
1:E:148:ILE:HD12	1:E:148:ILE:HA	1.91	0.41
2:F:531:THR:O	2:F:534:ARG:HG2	2.20	0.41
2:F:857:PHE:HE2	2:F:886:LEU:HD21	1.85	0.41
2:F:1020:GLN:HB3	2:F:1148:LEU:CD1	2.50	0.41
2:F:1255:ILE:HD13	2:F:1255:ILE:HA	1.93	0.41
2:H:888:THR:OG1	2:H:889:HIS:N	2.53	0.41
1:A:329:ASP:OD1	1:G:48:ASN:ND2	2.53	0.41
2:B:892:GLN:H	2:B:892:GLN:HG3	1.41	0.41
2:B:1521:GLN:O	2:B:1525:MET:HG2	2.20	0.41
1:C:137:MET:SD	1:E:133:PHE:HB3	2.60	0.41
1:C:286:ILE:HG23	1:C:301:ARG:HG2	2.02	0.41
2:D:451:LEU:HD13	2:D:582:LEU:HD21	2.01	0.41
1:G:145:ALA:HA	1:G:148:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:435:CYS:HB3	2:H:436:PRO:HD3	2.02	0.41
2:H:1203:HIS:CD2	2:H:1227:LEU:HD12	2.54	0.41
1:A:48:ASN:ND2	1:C:329:ASP:OD1	2.53	0.41
1:A:286:ILE:HG23	1:A:301:ARG:HG2	2.02	0.41
1:C:220:VAL:HB	1:C:233:LEU:HG	2.02	0.41
2:D:571:LEU:HD12	2:D:571:LEU:O	2.20	0.41
2:D:1348:GLN:CG	2:D:1402:ARG:HB2	2.51	0.41
1:E:209:MET:HB2	1:E:292:GLU:OE2	2.20	0.41
2:F:812:ILE:HD13	2:F:812:ILE:HA	1.91	0.41
2:F:1164:PHE:HZ	2:F:1259:VAL:HG23	1.85	0.41
2:H:188:ASN:O	2:H:192:VAL:HG23	2.20	0.41
2:H:417:ILE:O	2:H:420:LEU:HB3	2.20	0.41
2:H:1124:ARG:O	2:H:1128:ASP:HB2	2.21	0.41
1:A:133:PHE:HB3	1:G:137:MET:SD	2.60	0.41
1:A:145:ALA:HA	1:A:148:ILE:HG22	2.02	0.41
1:A:188:VAL:HG12	1:A:310:LEU:HD11	2.02	0.41
2:B:547:ASN:O	2:B:551:PRO:HG2	2.21	0.41
2:B:888:THR:OG1	2:B:889:HIS:N	2.53	0.41
2:B:1553:LYS:CE	2:B:1558:LEU:HB2	2.50	0.41
2:D:40:LEU:HD11	2:D:115:MET:HB2	2.03	0.41
2:D:417:ILE:O	2:D:420:LEU:HB3	2.20	0.41
1:E:137:MET:SD	1:G:133:PHE:HB3	2.60	0.41
2:F:1144:SER:O	2:F:1147:THR:HG22	2.21	0.41
2:F:1521:GLN:O	2:F:1525:MET:HG2	2.20	0.41
1:G:158:MET:O	1:G:162:ILE:HG22	2.20	0.41
2:H:730:MET:HE3	2:H:730:MET:HB3	1.92	0.41
2:H:890:LYS:HB2	2:H:893:TYR:CE2	2.55	0.41
2:B:571:LEU:HD12	2:B:571:LEU:O	2.20	0.41
2:B:1124:ARG:O	2:B:1128:ASP:HB2	2.21	0.41
2:B:1144:SER:O	2:B:1147:THR:HG22	2.21	0.41
2:B:1521:GLN:HA	2:B:1524:VAL:HG12	2.01	0.41
2:D:427:GLN:OE1	2:D:602:LYS:HD3	2.21	0.41
2:D:1146:SER:HB3	2:D:1298:MET:HB2	2.02	0.41
2:F:1246:ARG:HA	2:F:1246:ARG:HD3	1.65	0.41
2:F:1394:ARG:HE	2:F:1415:LEU:HD11	1.86	0.41
1:G:209:MET:HB2	1:G:292:GLU:OE2	2.20	0.41
2:H:1308:GLN:O	2:H:1312:VAL:HG23	2.20	0.41
2:B:78:THR:HG21	2:B:121:VAL:HG23	2.01	0.41
2:B:188:ASN:O	2:B:192:VAL:HG23	2.20	0.41
2:B:427:GLN:OE1	2:B:602:LYS:HD3	2.21	0.41
1:C:158:MET:O	1:C:162:ILE:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:890:LYS:HB2	2:D:893:TYR:CE2	2.55	0.41
2:F:435:CYS:HB3	2:F:436:PRO:HD3	2.02	0.41
2:F:1335:ILE:N	2:F:1336:PRO:HD2	2.35	0.41
2:F:1552:LEU:HD23	2:F:1557:ILE:HG12	2.03	0.41
2:H:875:GLU:O	2:H:879:ASP:HB2	2.20	0.41
2:H:1256:GLY:HA2	2:H:1259:VAL:HG12	2.02	0.41
2:B:40:LEU:HD11	2:B:115:MET:HB2	2.03	0.41
2:B:1552:LEU:HD23	2:B:1557:ILE:HG12	2.03	0.41
1:C:48:ASN:ND2	1:E:329:ASP:OD1	2.53	0.41
1:C:178:ALA:O	1:C:181:LEU:HD23	2.20	0.41
1:C:241:GLU:HB2	1:C:258:TYR:O	2.21	0.41
2:D:188:ASN:O	2:D:192:VAL:HG23	2.20	0.41
2:D:547:ASN:O	2:D:551:PRO:HG2	2.21	0.41
2:D:1394:ARG:HE	2:D:1415:LEU:HD11	1.86	0.41
1:E:86:PHE:HA	1:E:89:VAL:HG12	2.02	0.41
1:E:241:GLU:HB2	1:E:258:TYR:O	2.21	0.41
2:F:1308:GLN:O	2:F:1312:VAL:HG23	2.20	0.41
1:G:286:ILE:HG23	1:G:301:ARG:HG2	2.02	0.41
2:H:1144:SER:O	2:H:1147:THR:HG22	2.21	0.41
1:A:158:MET:O	1:A:162:ILE:HG22	2.20	0.41
2:B:451:LEU:HD13	2:B:582:LEU:HD21	2.01	0.41
2:B:1226:LYS:O	2:B:1230:TYR:HD1	2.03	0.41
2:B:1256:GLY:HA2	2:B:1259:VAL:HG12	2.02	0.41
2:D:531:THR:O	2:D:534:ARG:HG2	2.20	0.41
1:E:158:MET:O	1:E:162:ILE:HG22	2.20	0.41
1:E:297:THR:O	1:E:297:THR:OG1	2.37	0.41
2:F:253:LEU:HD12	2:F:253:LEU:HA	1.77	0.41
2:F:496:LEU:HD23	2:F:496:LEU:HA	1.88	0.41
2:F:1114:GLU:OE1	3:F:2502:ADP:N6	2.52	0.41
1:G:220:VAL:HB	1:G:233:LEU:HG	2.02	0.41
1:G:241:GLU:HB2	1:G:258:TYR:O	2.21	0.41
2:H:253:LEU:HD12	2:H:253:LEU:HA	1.77	0.41
2:H:1164:PHE:HZ	2:H:1259:VAL:HG23	1.85	0.41
1:A:75:PHE:HB3	1:A:163:MET:SD	2.61	0.41
1:A:168:PHE:C	1:A:171:THR:CG2	2.81	0.41
1:A:238:ILE:HA	1:A:239:PRO:HD3	1.96	0.41
2:B:523:GLU:O	2:B:527:ARG:HG3	2.21	0.41
2:B:890:LYS:HB2	2:B:893:TYR:CE2	2.55	0.41
2:B:1102:LEU:HD23	2:B:1102:LEU:HA	1.76	0.41
2:B:1146:SER:HB3	2:B:1298:MET:HB2	2.02	0.41
2:B:1348:GLN:CG	2:B:1402:ARG:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1394:ARG:HE	2:B:1415:LEU:HD11	1.86	0.41
1:C:86:PHE:HA	1:C:89:VAL:HG12	2.02	0.41
2:D:150:LYS:CB	2:D:176:VAL:HG22	2.44	0.41
2:D:414:ALA:HA	2:D:1208:VAL:HG11	2.03	0.41
2:D:1144:SER:O	2:D:1147:THR:HG22	2.21	0.41
2:D:1552:LEU:HD23	2:D:1557:ILE:HG12	2.03	0.41
1:E:75:PHE:HB3	1:E:163:MET:SD	2.61	0.41
1:E:188:VAL:HG12	1:E:310:LEU:HD11	2.02	0.41
1:E:286:ILE:HG23	1:E:301:ARG:HG2	2.02	0.41
2:F:72:ASN:OD1	2:F:72:ASN:N	2.54	0.41
2:F:592:LEU:HD23	2:F:592:LEU:HA	1.89	0.41
2:F:888:THR:OG1	2:F:889:HIS:N	2.53	0.41
2:F:1348:GLN:CG	2:F:1402:ARG:HB2	2.51	0.41
2:F:1553:LYS:CE	2:F:1558:LEU:HB2	2.50	0.41
1:G:75:PHE:HB3	1:G:163:MET:SD	2.61	0.41
1:G:284:ILE:HA	1:G:302:THR:O	2.21	0.41
2:H:547:ASN:O	2:H:551:PRO:HG2	2.21	0.41
1:A:220:VAL:HB	1:A:233:LEU:HG	2.02	0.41
2:B:1164:PHE:HZ	2:B:1259:VAL:HG23	1.85	0.41
1:C:189:ILE:HD11	1:C:311:TRP:CE2	2.56	0.41
1:E:48:ASN:ND2	1:G:329:ASP:OD1	2.53	0.41
2:F:427:GLN:OE1	2:F:602:LYS:HD3	2.21	0.41
2:F:451:LEU:HD13	2:F:582:LEU:HD21	2.01	0.41
2:F:1226:LYS:O	2:F:1230:TYR:HD1	2.03	0.41
2:F:1376:GLY:O	2:F:1549:VAL:HA	2.21	0.41
2:F:1415:LEU:HA	2:F:1418:LEU:HD12	2.03	0.41
2:H:40:LEU:HD11	2:H:115:MET:HB2	2.03	0.41
2:H:423:ILE:HG13	2:H:424:ASP:N	2.36	0.41
2:H:489:LEU:HD21	2:H:602:LYS:HG2	2.03	0.41
2:H:1348:GLN:CG	2:H:1402:ARG:HB2	2.51	0.41
2:H:1521:GLN:O	2:H:1525:MET:HG2	2.20	0.41
1:A:148:ILE:HD12	1:A:148:ILE:HA	1.91	0.40
1:A:189:ILE:HD11	1:A:311:TRP:CE2	2.56	0.40
2:B:597:VAL:O	2:B:601:VAL:HG12	2.21	0.40
2:D:1376:GLY:O	2:D:1549:VAL:HA	2.21	0.40
2:F:246:ASP:OD1	2:F:247:LEU:N	2.49	0.40
2:F:423:ILE:HG13	2:F:424:ASP:N	2.36	0.40
1:G:188:VAL:HG12	1:G:310:LEU:HD11	2.02	0.40
2:H:857:PHE:HE2	2:H:886:LEU:HD21	1.85	0.40
1:A:284:ILE:HA	1:A:302:THR:O	2.21	0.40
2:B:417:ILE:O	2:B:420:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:LEU:HB2	2:B:895:PRO:HD3	2.03	0.40
1:C:284:ILE:HA	1:C:302:THR:O	2.21	0.40
1:C:286:ILE:HD12	1:C:301:ARG:HG2	2.02	0.40
2:D:544:ILE:HD12	2:D:591:PHE:CE2	2.56	0.40
2:D:618:GLU:HG2	2:D:619:ILE:H	1.87	0.40
2:D:1415:LEU:HA	2:D:1418:LEU:HD12	2.03	0.40
1:E:286:ILE:HD12	1:E:301:ARG:HG2	2.02	0.40
2:F:890:LYS:HB2	2:F:893:TYR:CE2	2.55	0.40
2:F:1211:LEU:HD13	2:F:1211:LEU:HA	1.91	0.40
2:H:72:ASN:OD1	2:H:72:ASN:N	2.54	0.40
2:H:1480:GLU:HB2	3:H:2501:ADP:C6	2.57	0.40
2:H:1552:LEU:HD23	2:H:1557:ILE:HG12	2.03	0.40
1:A:169:MET:HE1	1:C:172:ALA:N	2.37	0.40
2:B:489:LEU:HD21	2:B:602:LYS:HG2	2.03	0.40
2:B:871:ALA:O	2:B:875:GLU:HB2	2.22	0.40
2:B:1480:GLU:HB2	3:B:2501:ADP:C6	2.57	0.40
1:C:209:MET:HB2	1:C:292:GLU:OE2	2.20	0.40
2:D:489:LEU:HD21	2:D:602:LYS:HG2	2.03	0.40
2:D:597:VAL:O	2:D:601:VAL:HG12	2.21	0.40
2:D:1486:GLN:O	2:D:1490:PHE:HD1	2.05	0.40
1:E:237:ASP:HB3	1:G:243:GLY:H	1.86	0.40
2:F:139:LEU:HD23	2:F:139:LEU:HA	1.94	0.40
2:F:489:LEU:HD21	2:F:602:LYS:HG2	2.03	0.40
1:A:237:ASP:HB3	1:C:243:GLY:H	1.86	0.40
1:A:243:GLY:H	1:G:237:ASP:HB3	1.86	0.40
2:B:414:ALA:HA	2:B:1208:VAL:HG11	2.03	0.40
1:C:75:PHE:HB3	1:C:163:MET:SD	2.61	0.40
1:C:125:ILE:HD12	1:C:125:ILE:HA	1.95	0.40
1:C:169:MET:HE2	1:E:172:ALA:CB	2.52	0.40
2:D:196:ILE:O	2:D:197:PHE:C	2.60	0.40
2:D:381:ILE:HG21	2:D:1242:THR:HG21	2.04	0.40
1:E:189:ILE:HD11	1:E:311:TRP:CE2	2.56	0.40
2:F:40:LEU:HD11	2:F:115:MET:HB2	2.03	0.40
2:F:618:GLU:HG2	2:F:619:ILE:H	1.87	0.40
1:G:136:ARG:H	1:G:136:ARG:HG2	1.73	0.40
2:H:1486:GLN:O	2:H:1490:PHE:HD1	2.05	0.40
2:B:485:GLN:NE2	2:B:598:ARG:HG3	2.37	0.40
2:B:685:PHE:O	2:B:732:LYS:HB3	2.22	0.40
2:D:131:ASN:OD1	2:D:131:ASN:N	2.43	0.40
2:F:523:GLU:O	2:F:527:ARG:HG3	2.21	0.40
2:F:544:ILE:HD12	2:F:591:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:547:ASN:O	2:F:551:PRO:HG2	2.21	0.40
1:G:189:ILE:HD11	1:G:311:TRP:CE2	2.56	0.40
1:G:261:ILE:H	1:G:261:ILE:HG13	1.61	0.40
2:H:523:GLU:O	2:H:527:ARG:HG3	2.21	0.40
2:H:618:GLU:HG2	2:H:619:ILE:H	1.87	0.40

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%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	C	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	E	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	G	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
2	B	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	D	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	F	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	H	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
All	All	6492/7888 (82%)	6200 (96%)	264 (4%)	28 (0%)	32	68

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	54	ARG
2	B	197	PHE
2	B	199	LYS
1	C	50	ARG

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Mol	Chain	Res	Type
1	C	54	ARG
2	D	197	PHE
2	D	199	LYS
1	E	50	ARG
1	E	54	ARG
2	F	197	PHE
2	F	199	LYS
1	G	50	ARG
1	G	54	ARG
2	H	197	PHE
2	H	199	LYS
2	B	205	LYS
2	D	205	LYS
2	F	205	LYS
2	H	205	LYS
1	A	244	VAL
1	C	244	VAL
1	E	244	VAL
1	G	244	VAL
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	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	C	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	E	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	G	250/339 (74%)	223 (89%)	27 (11%)	5	19
2	B	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
2	D	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
2	H	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
All	All	5380/6840 (79%)	5036 (94%)	344 (6%)	17	36

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	59	VAL
1	A	63	LEU
1	A	71	THR
1	A	81	CYS
1	A	88	MET
1	A	90	TRP
1	A	111	VAL
1	A	122	LEU
1	A	133	PHE
1	A	136	ARG
1	A	152	GLN
1	A	173	GLN
1	A	190	THR
1	A	198	PHE
1	A	204	ASP
1	A	219	VAL
1	A	236	VAL
1	A	238	ILE
1	A	252	VAL
1	A	287	LEU
1	A	290	VAL
1	A	294	THR
1	A	297	THR
1	A	298	THR
1	A	323	ASP
1	A	345	THR
2	B	37	VAL
2	B	72	ASN
2	B	119	THR
2	B	123	TYR
2	B	134	LYS
2	B	167	LEU
2	B	193	ARG

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Mol	Chain	Res	Type
2	B	204	VAL
2	B	218	LEU
2	B	222	VAL
2	B	229	THR
2	B	237	ILE
2	B	292	CYS
2	B	358	LEU
2	B	387	LEU
2	B	420	LEU
2	B	423	ILE
2	B	432	PHE
2	B	443	VAL
2	B	451	LEU
2	B	470	LEU
2	B	511	LEU
2	B	512	TYR
2	B	563	VAL
2	B	565	PHE
2	B	574	SER
2	B	614	LEU
2	B	682	ILE
2	B	689	THR
2	B	696	LEU
2	B	701	ILE
2	B	707	GLN
2	B	708	LEU
2	B	730	MET
2	B	770	VAL
2	B	791	GLU
2	B	794	PHE
2	B	861	ASP
2	B	869	MET
2	B	891	LEU
2	B	892	GLN
2	B	894	LEU
2	B	1038	THR
2	B	1136	ILE
2	B	1204	PHE
2	B	1211	LEU
2	B	1227	LEU
2	B	1240	PHE
2	B	1258	CYS

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Mol	Chain	Res	Type
2	B	1270	ASN
2	B	1276	LEU
2	B	1315	ILE
2	B	1378	CYS
2	B	1409	ASP
2	B	1432	PHE
2	B	1509	THR
2	B	1536	ILE
2	B	1557	ILE
2	B	1566	LEU
1	C	36	VAL
1	C	59	VAL
1	C	63	LEU
1	C	71	THR
1	C	81	CYS
1	C	88	MET
1	C	90	TRP
1	C	111	VAL
1	C	122	LEU
1	C	133	PHE
1	C	136	ARG
1	C	152	GLN
1	C	173	GLN
1	C	190	THR
1	C	198	PHE
1	C	204	ASP
1	C	219	VAL
1	C	236	VAL
1	C	238	ILE
1	C	252	VAL
1	C	287	LEU
1	C	290	VAL
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	123	TYR
2	D	134	LYS

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Mol	Chain	Res	Type
2	D	167	LEU
2	D	193	ARG
2	D	204	VAL
2	D	218	LEU
2	D	222	VAL
2	D	229	THR
2	D	237	ILE
2	D	292	CYS
2	D	358	LEU
2	D	387	LEU
2	D	420	LEU
2	D	423	ILE
2	D	432	PHE
2	D	443	VAL
2	D	451	LEU
2	D	470	LEU
2	D	511	LEU
2	D	512	TYR
2	D	563	VAL
2	D	565	PHE
2	D	574	SER
2	D	614	LEU
2	D	682	ILE
2	D	689	THR
2	D	696	LEU
2	D	701	ILE
2	D	707	GLN
2	D	708	LEU
2	D	730	MET
2	D	770	VAL
2	D	791	GLU
2	D	794	PHE
2	D	861	ASP
2	D	869	MET
2	D	891	LEU
2	D	892	GLN
2	D	894	LEU
2	D	1038	THR
2	D	1136	ILE
2	D	1204	PHE
2	D	1211	LEU
2	D	1227	LEU

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Mol	Chain	Res	Type
2	D	1240	PHE
2	D	1258	CYS
2	D	1270	ASN
2	D	1276	LEU
2	D	1315	ILE
2	D	1378	CYS
2	D	1409	ASP
2	D	1432	PHE
2	D	1509	THR
2	D	1536	ILE
2	D	1557	ILE
2	D	1566	LEU
1	E	36	VAL
1	E	59	VAL
1	E	63	LEU
1	E	71	THR
1	E	81	CYS
1	E	88	MET
1	E	90	TRP
1	E	111	VAL
1	E	122	LEU
1	E	133	PHE
1	E	136	ARG
1	E	152	GLN
1	E	173	GLN
1	E	190	THR
1	E	198	PHE
1	E	204	ASP
1	E	219	VAL
1	E	236	VAL
1	E	238	ILE
1	E	252	VAL
1	E	287	LEU
1	E	290	VAL
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

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Mol	Chain	Res	Type
2	F	123	TYR
2	F	134	LYS
2	F	167	LEU
2	F	193	ARG
2	F	204	VAL
2	F	218	LEU
2	F	222	VAL
2	F	229	THR
2	F	237	ILE
2	F	292	CYS
2	F	358	LEU
2	F	387	LEU
2	F	420	LEU
2	F	423	ILE
2	F	432	PHE
2	F	443	VAL
2	F	451	LEU
2	F	470	LEU
2	F	511	LEU
2	F	512	TYR
2	F	563	VAL
2	F	565	PHE
2	F	574	SER
2	F	614	LEU
2	F	682	ILE
2	F	689	THR
2	F	696	LEU
2	F	701	ILE
2	F	707	GLN
2	F	708	LEU
2	F	730	MET
2	F	770	VAL
2	F	791	GLU
2	F	794	PHE
2	F	861	ASP
2	F	869	MET
2	F	891	LEU
2	F	892	GLN
2	F	894	LEU
2	F	1038	THR
2	F	1136	ILE
2	F	1204	PHE

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Mol	Chain	Res	Type
2	F	1211	LEU
2	F	1227	LEU
2	F	1240	PHE
2	F	1258	CYS
2	F	1270	ASN
2	F	1276	LEU
2	F	1315	ILE
2	F	1378	CYS
2	F	1409	ASP
2	F	1432	PHE
2	F	1509	THR
2	F	1536	ILE
2	F	1557	ILE
2	F	1566	LEU
1	G	36	VAL
1	G	59	VAL
1	G	63	LEU
1	G	71	THR
1	G	81	CYS
1	G	88	MET
1	G	90	TRP
1	G	111	VAL
1	G	122	LEU
1	G	133	PHE
1	G	136	ARG
1	G	152	GLN
1	G	173	GLN
1	G	190	THR
1	G	198	PHE
1	G	204	ASP
1	G	219	VAL
1	G	236	VAL
1	G	238	ILE
1	G	252	VAL
1	G	287	LEU
1	G	290	VAL
1	G	294	THR
1	G	297	THR
1	G	298	THR
1	G	323	ASP
1	G	345	THR
2	H	37	VAL

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Mol	Chain	Res	Type
2	H	72	ASN
2	H	119	THR
2	H	123	TYR
2	H	134	LYS
2	H	167	LEU
2	H	193	ARG
2	H	204	VAL
2	H	218	LEU
2	H	222	VAL
2	H	229	THR
2	H	237	ILE
2	H	292	CYS
2	H	358	LEU
2	H	387	LEU
2	H	420	LEU
2	H	423	ILE
2	H	432	PHE
2	H	443	VAL
2	H	451	LEU
2	H	470	LEU
2	H	511	LEU
2	H	512	TYR
2	H	563	VAL
2	H	565	PHE
2	H	574	SER
2	H	614	LEU
2	H	682	ILE
2	H	689	THR
2	H	696	LEU
2	H	701	ILE
2	H	707	GLN
2	H	708	LEU
2	H	730	MET
2	H	770	VAL
2	H	791	GLU
2	H	794	PHE
2	H	861	ASP
2	H	869	MET
2	H	891	LEU
2	H	892	GLN
2	H	894	LEU
2	H	1038	THR

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Mol	Chain	Res	Type
2	H	1136	ILE
2	H	1204	PHE
2	H	1211	LEU
2	H	1227	LEU
2	H	1240	PHE
2	H	1258	CYS
2	H	1270	ASN
2	H	1276	LEU
2	H	1315	ILE
2	H	1378	CYS
2	H	1409	ASP
2	H	1432	PHE
2	H	1509	THR
2	H	1536	ILE
2	H	1557	ILE
2	H	1566	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	48	ASN
1	A	128	GLN
1	A	173	GLN
1	A	193	HIS
1	A	259	HIS
2	B	474	GLN
2	B	1203	HIS
1	C	46	HIS
1	C	48	ASN
1	C	128	GLN
1	C	173	GLN
1	C	193	HIS
1	C	259	HIS
2	D	474	GLN
1	E	46	HIS
1	E	48	ASN
1	E	128	GLN
1	E	173	GLN
1	E	193	HIS
1	E	259	HIS
2	F	474	GLN

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Mol	Chain	Res	Type
1	G	46	HIS
1	G	48	ASN
1	G	128	GLN
1	G	173	GLN
1	G	193	HIS
1	G	259	HIS
2	H	474	GLN
2	H	1203	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	C	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	D	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	B	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	E	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	H	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	G	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	F	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	H	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	D	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	F	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	A	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	B	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	C	401	-	-	4/12/32/32	0/3/3/3
3	ADP	D	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	B	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	E	401	-	-	4/12/32/32	0/3/3/3
3	ADP	H	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	G	401	-	-	4/12/32/32	0/3/3/3
3	ADP	F	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	H	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	D	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	F	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	A	401	-	-	4/12/32/32	0/3/3/3
3	ADP	B	2501	4	-	2/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ADP	C5-C4	2.46	1.47	1.40
3	C	401	ADP	C5-C4	2.46	1.47	1.40
3	E	401	ADP	C5-C4	2.46	1.47	1.40
3	G	401	ADP	C5-C4	2.46	1.47	1.40
3	B	2502	ADP	C5-C4	2.44	1.47	1.40
3	D	2502	ADP	C5-C4	2.44	1.47	1.40
3	F	2502	ADP	C5-C4	2.44	1.47	1.40
3	H	2502	ADP	C5-C4	2.44	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2501	ADP	C5-C4	2.37	1.47	1.40
3	D	2501	ADP	C5-C4	2.37	1.47	1.40
3	F	2501	ADP	C5-C4	2.37	1.47	1.40
3	H	2501	ADP	C5-C4	2.37	1.47	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	C	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	E	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	G	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	A	401	ADP	C3'-C2'-C1'	3.40	106.09	100.98
3	C	401	ADP	C3'-C2'-C1'	3.40	106.09	100.98
3	E	401	ADP	C3'-C2'-C1'	3.40	106.09	100.98
3	G	401	ADP	C3'-C2'-C1'	3.40	106.09	100.98
3	B	2502	ADP	PA-O3A-PB	-3.38	121.24	132.83
3	D	2502	ADP	PA-O3A-PB	-3.38	121.24	132.83
3	F	2502	ADP	PA-O3A-PB	-3.38	121.24	132.83
3	H	2502	ADP	PA-O3A-PB	-3.38	121.24	132.83
3	B	2501	ADP	C3'-C2'-C1'	3.33	105.99	100.98
3	D	2501	ADP	C3'-C2'-C1'	3.33	105.99	100.98
3	F	2501	ADP	C3'-C2'-C1'	3.33	105.99	100.98
3	H	2501	ADP	C3'-C2'-C1'	3.33	105.99	100.98
3	B	2501	ADP	N3-C2-N1	-3.26	123.58	128.68
3	D	2501	ADP	N3-C2-N1	-3.26	123.58	128.68
3	F	2501	ADP	N3-C2-N1	-3.26	123.58	128.68
3	H	2501	ADP	N3-C2-N1	-3.26	123.58	128.68
3	B	2502	ADP	N3-C2-N1	-3.19	123.69	128.68
3	D	2502	ADP	N3-C2-N1	-3.19	123.69	128.68
3	F	2502	ADP	N3-C2-N1	-3.19	123.69	128.68
3	H	2502	ADP	N3-C2-N1	-3.19	123.69	128.68
3	A	401	ADP	N3-C2-N1	-3.15	123.75	128.68
3	C	401	ADP	N3-C2-N1	-3.15	123.75	128.68
3	E	401	ADP	N3-C2-N1	-3.15	123.75	128.68
3	G	401	ADP	N3-C2-N1	-3.15	123.75	128.68
3	B	2501	ADP	PA-O3A-PB	-2.79	123.27	132.83
3	D	2501	ADP	PA-O3A-PB	-2.79	123.27	132.83
3	F	2501	ADP	PA-O3A-PB	-2.79	123.27	132.83
3	H	2501	ADP	PA-O3A-PB	-2.79	123.27	132.83
3	B	2502	ADP	C3'-C2'-C1'	2.65	104.96	100.98
3	D	2502	ADP	C3'-C2'-C1'	2.65	104.96	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2502	ADP	C3'-C2'-C1'	2.65	104.96	100.98
3	H	2502	ADP	C3'-C2'-C1'	2.65	104.96	100.98
3	A	401	ADP	C4-C5-N7	-2.61	106.67	109.40
3	C	401	ADP	C4-C5-N7	-2.61	106.67	109.40
3	E	401	ADP	C4-C5-N7	-2.61	106.67	109.40
3	G	401	ADP	C4-C5-N7	-2.61	106.67	109.40
3	B	2501	ADP	C4-C5-N7	-2.56	106.73	109.40
3	D	2501	ADP	C4-C5-N7	-2.56	106.73	109.40
3	F	2501	ADP	C4-C5-N7	-2.56	106.73	109.40
3	H	2501	ADP	C4-C5-N7	-2.56	106.73	109.40
3	B	2502	ADP	C4-C5-N7	-2.52	106.78	109.40
3	D	2502	ADP	C4-C5-N7	-2.52	106.78	109.40
3	F	2502	ADP	C4-C5-N7	-2.52	106.78	109.40
3	H	2502	ADP	C4-C5-N7	-2.52	106.78	109.40

There are no chirality outliers.

All (40) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	H	2502	ADP	C5'-O5'-PA-O2A
3	A	401	ADP	PB-O3A-PA-O2A
3	C	401	ADP	PB-O3A-PA-O2A
3	E	401	ADP	PB-O3A-PA-O2A
3	G	401	ADP	PB-O3A-PA-O2A
3	B	2501	ADP	C5'-O5'-PA-O1A
3	D	2501	ADP	C5'-O5'-PA-O1A
3	F	2501	ADP	C5'-O5'-PA-O1A
3	H	2501	ADP	C5'-O5'-PA-O1A
3	B	2501	ADP	O4'-C4'-C5'-O5'
3	D	2501	ADP	O4'-C4'-C5'-O5'
3	F	2501	ADP	O4'-C4'-C5'-O5'
3	H	2501	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	C3'-C4'-C5'-O5'
3	E	401	ADP	C3'-C4'-C5'-O5'
3	G	401	ADP	C3'-C4'-C5'-O5'

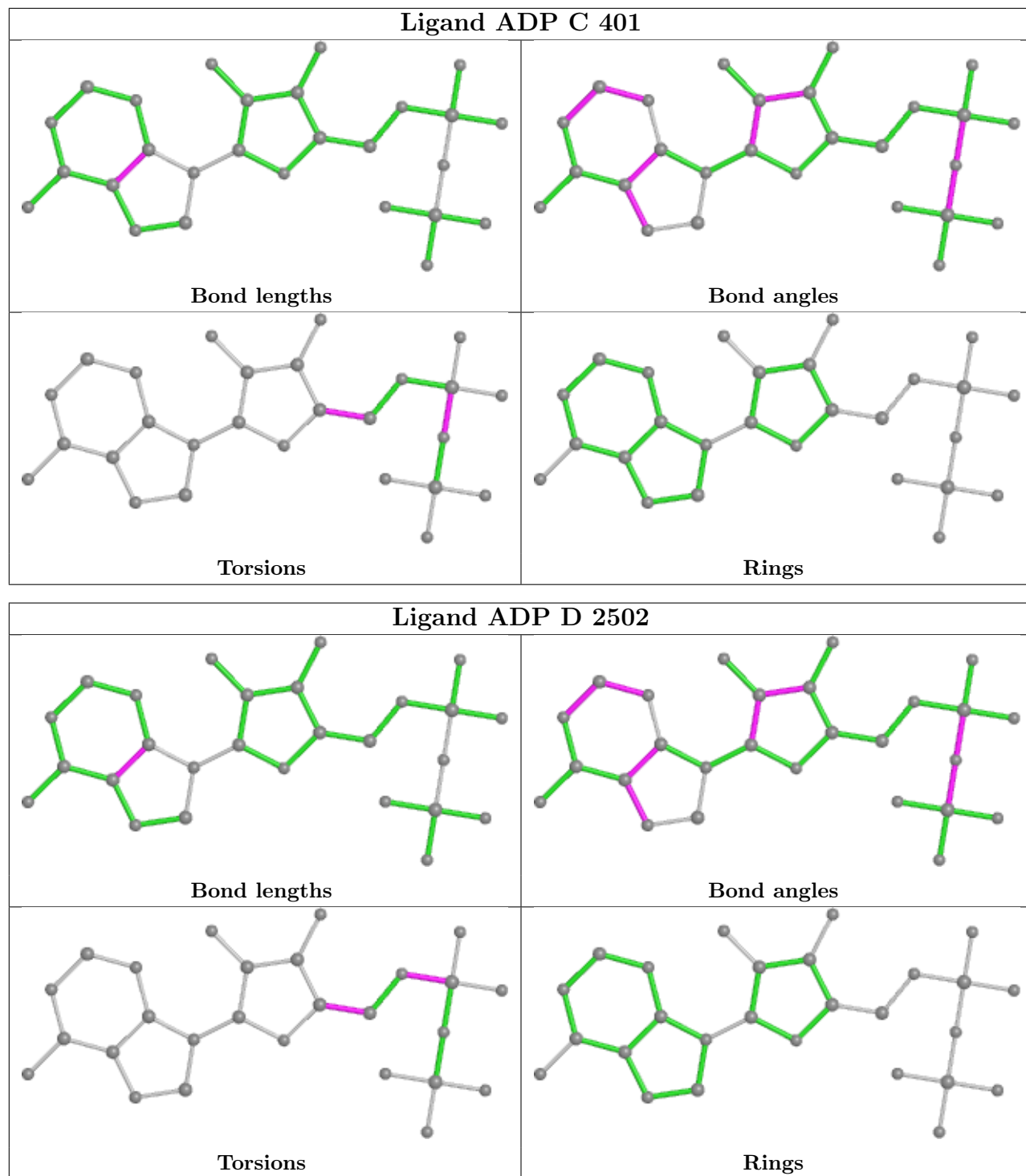
There are no ring outliers.

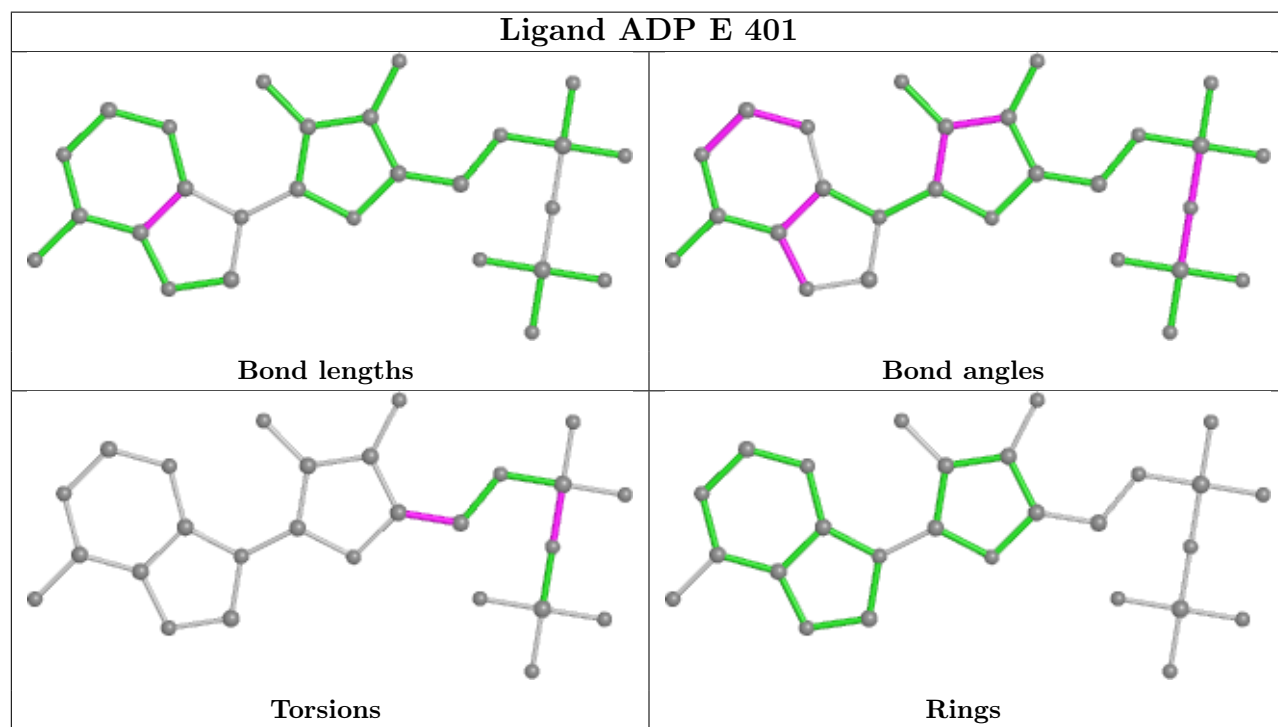
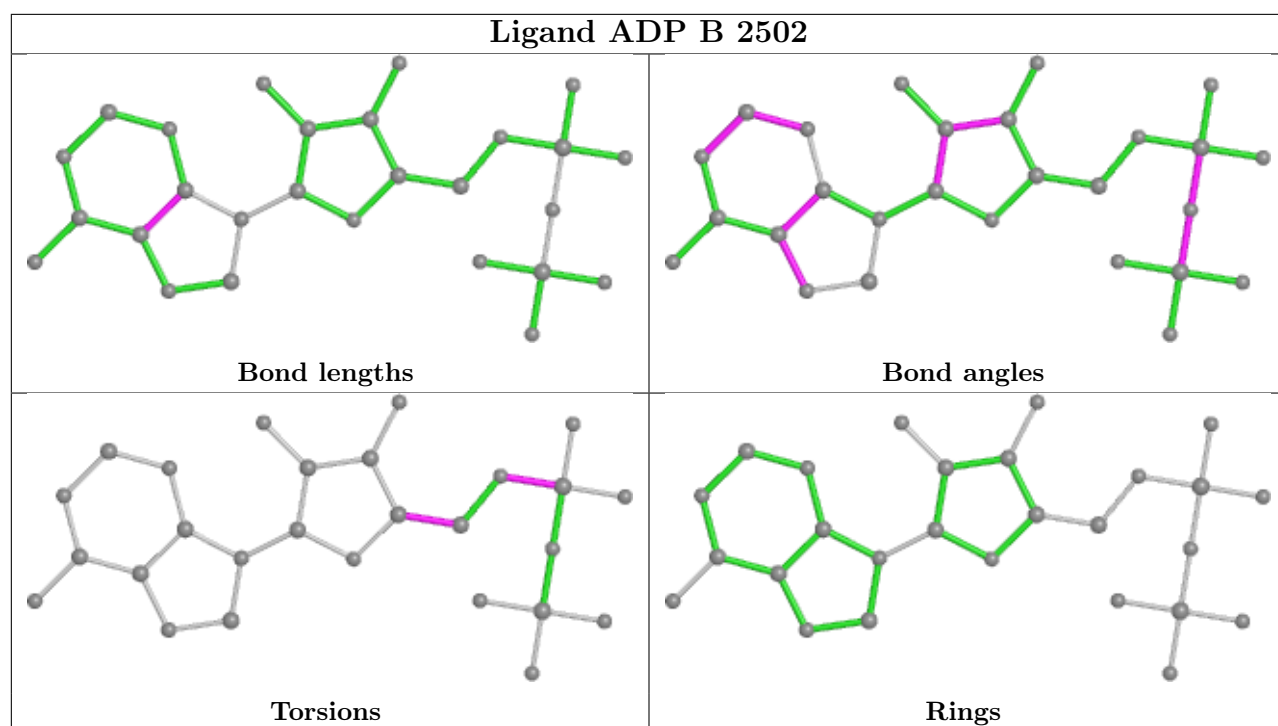
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2502	ADP	2	0
3	B	2502	ADP	2	0
3	H	2502	ADP	2	0
3	F	2502	ADP	2	0
3	H	2501	ADP	2	0
3	D	2501	ADP	1	0
3	F	2501	ADP	1	0
3	B	2501	ADP	2	0

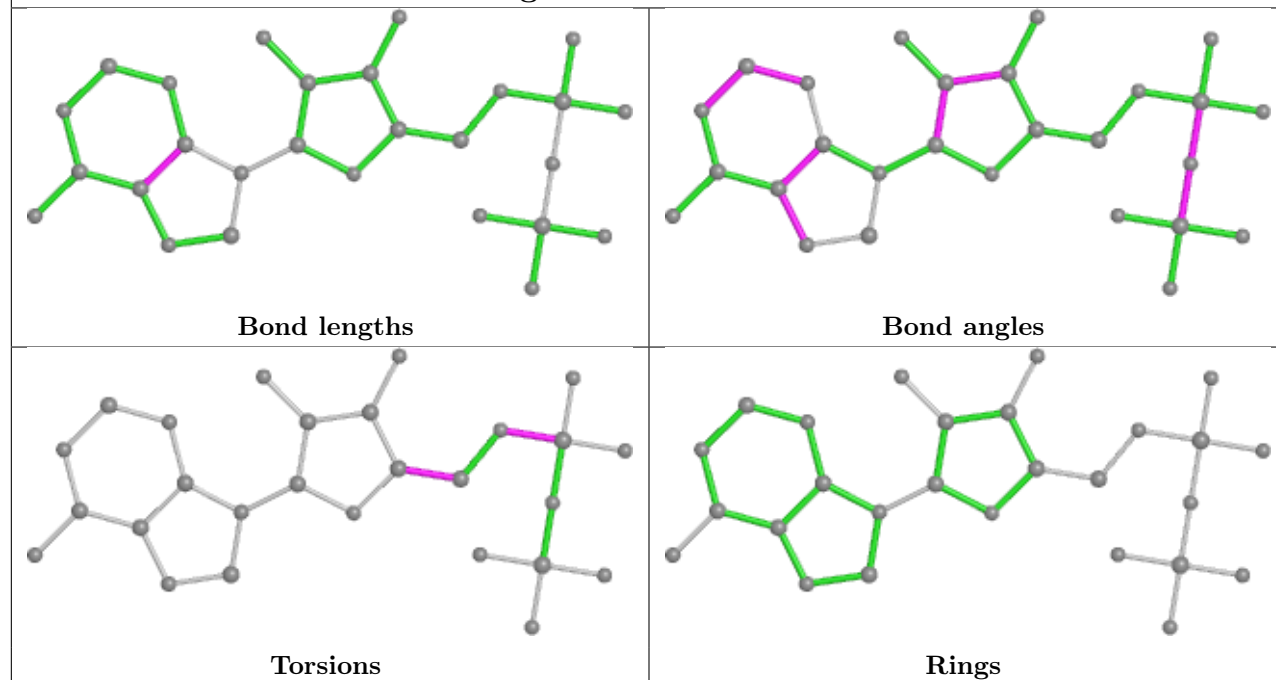
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

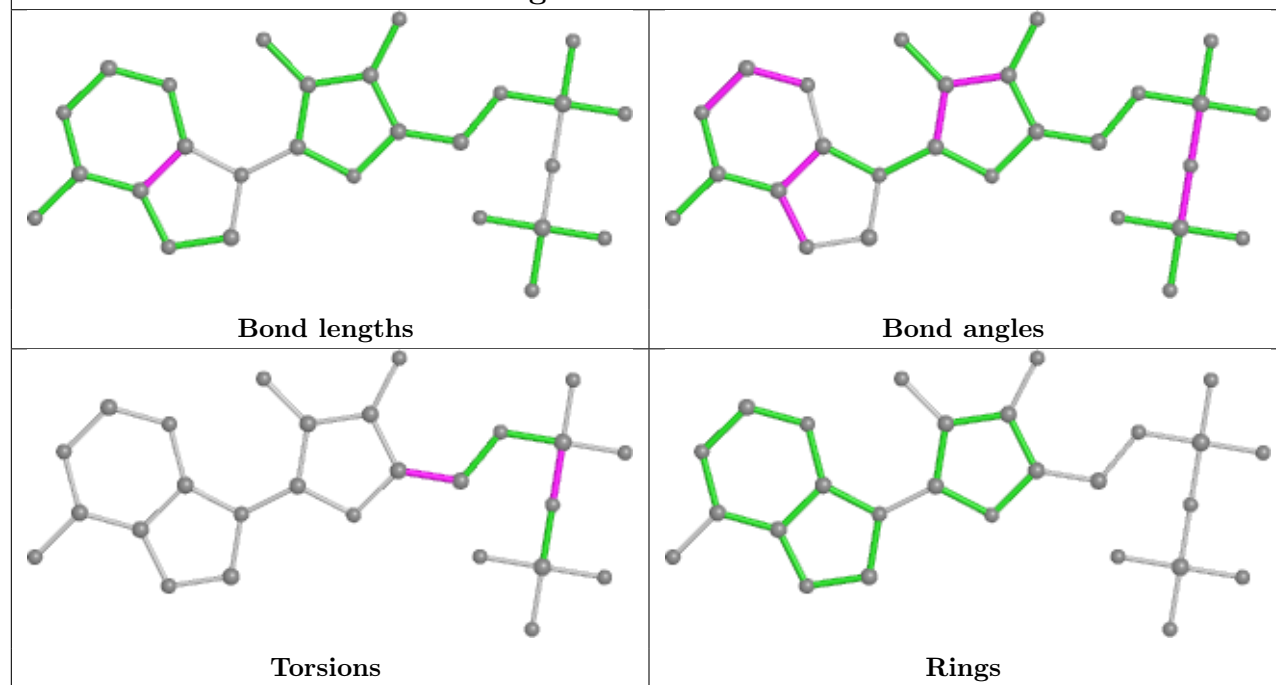




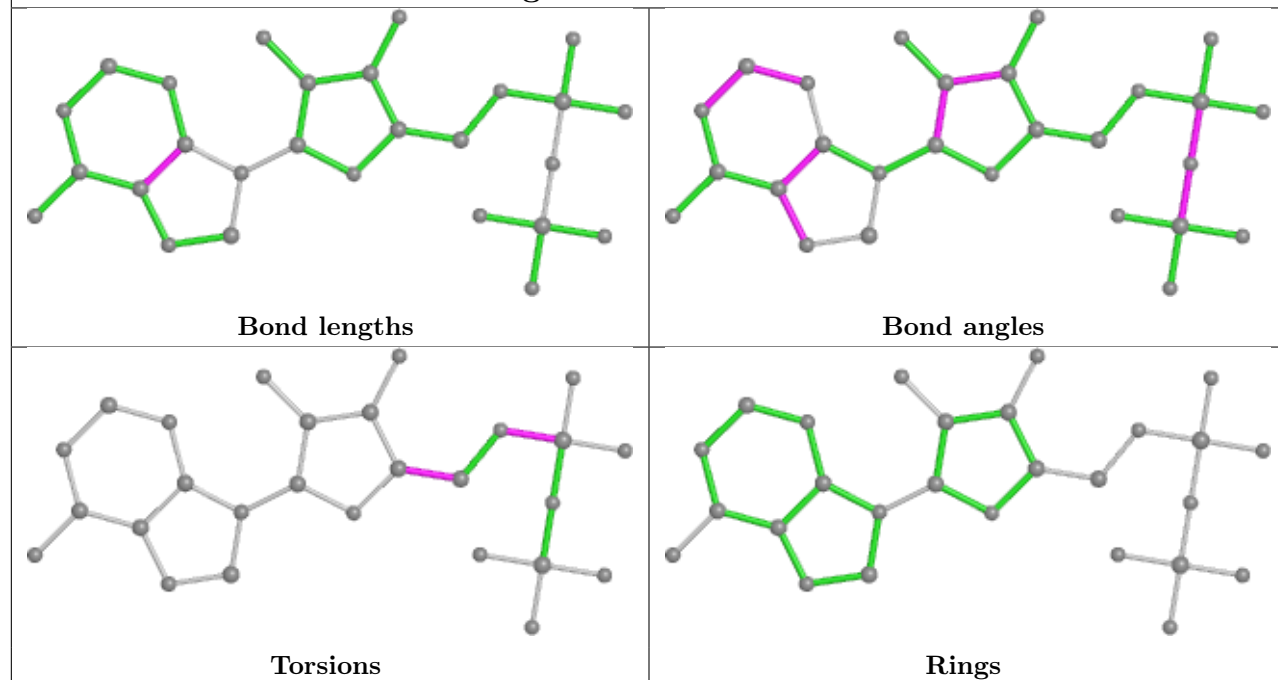
Ligand ADP H 2502



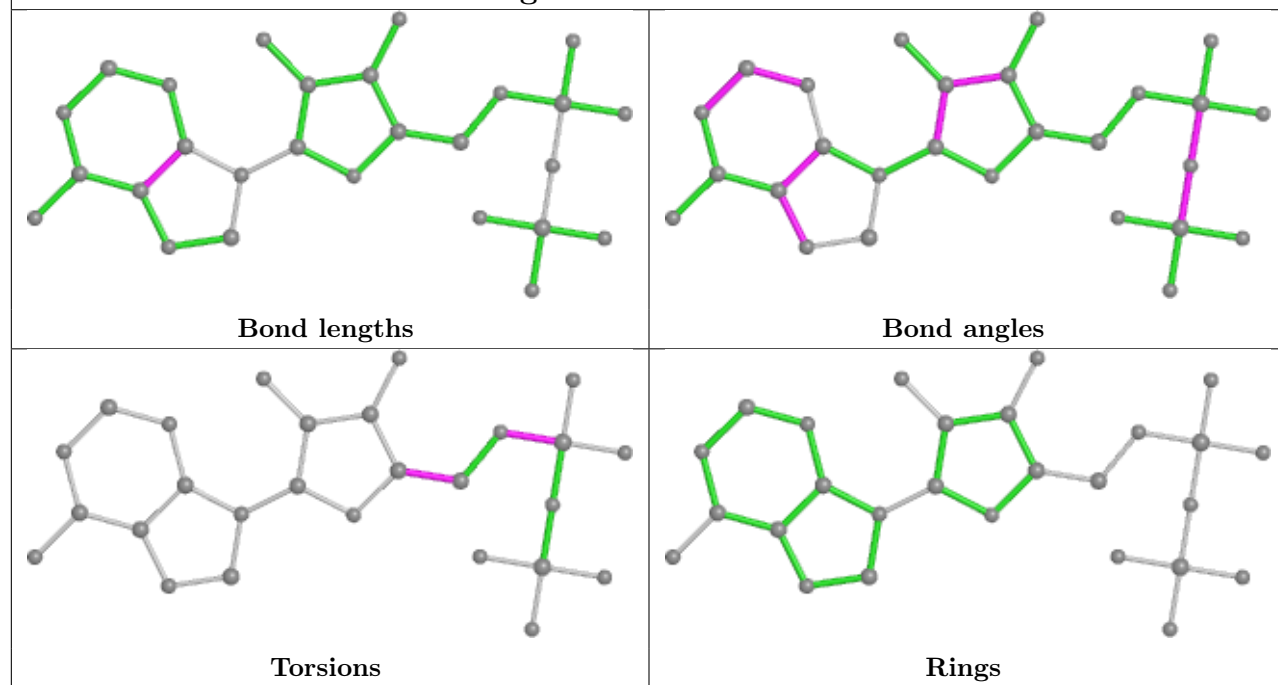
Ligand ADP G 401



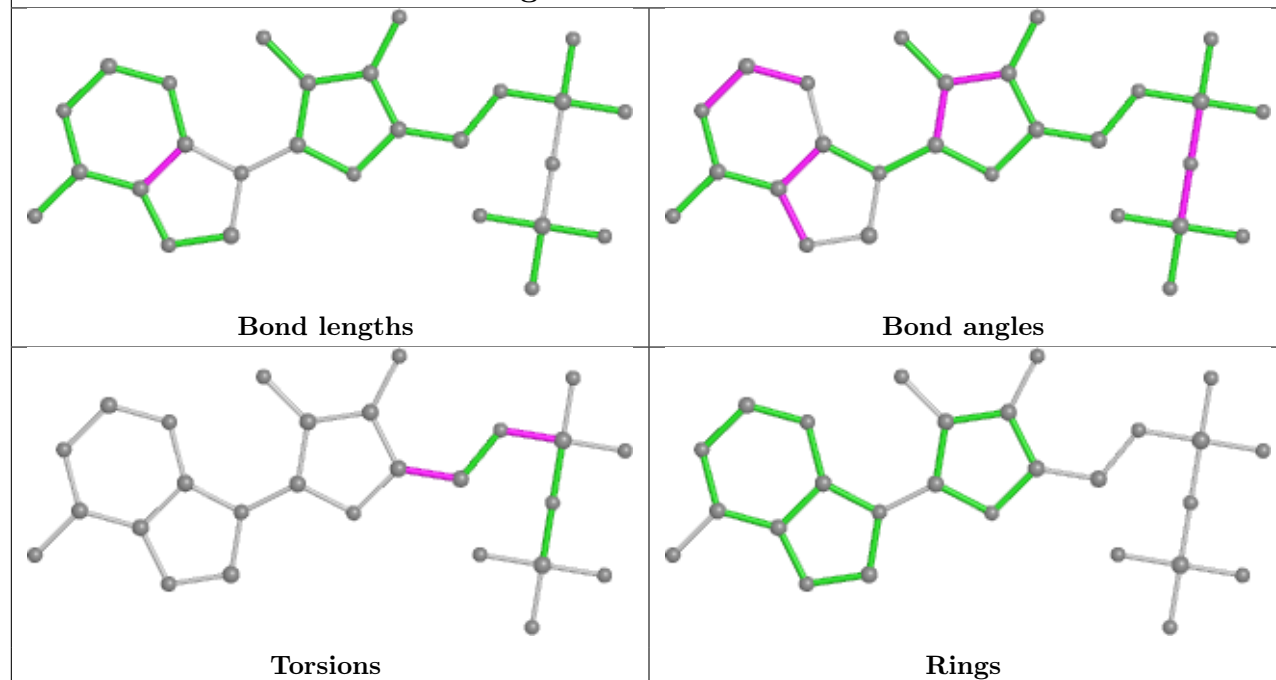
Ligand ADP F 2502



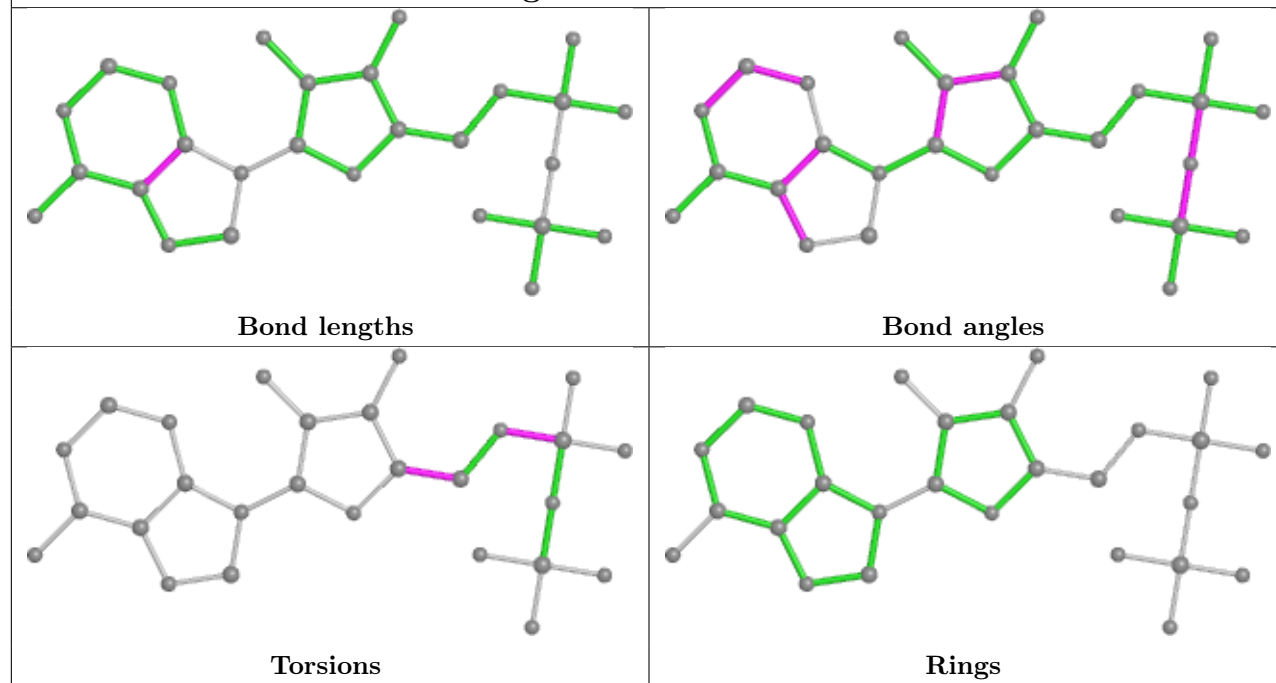
Ligand ADP H 2501

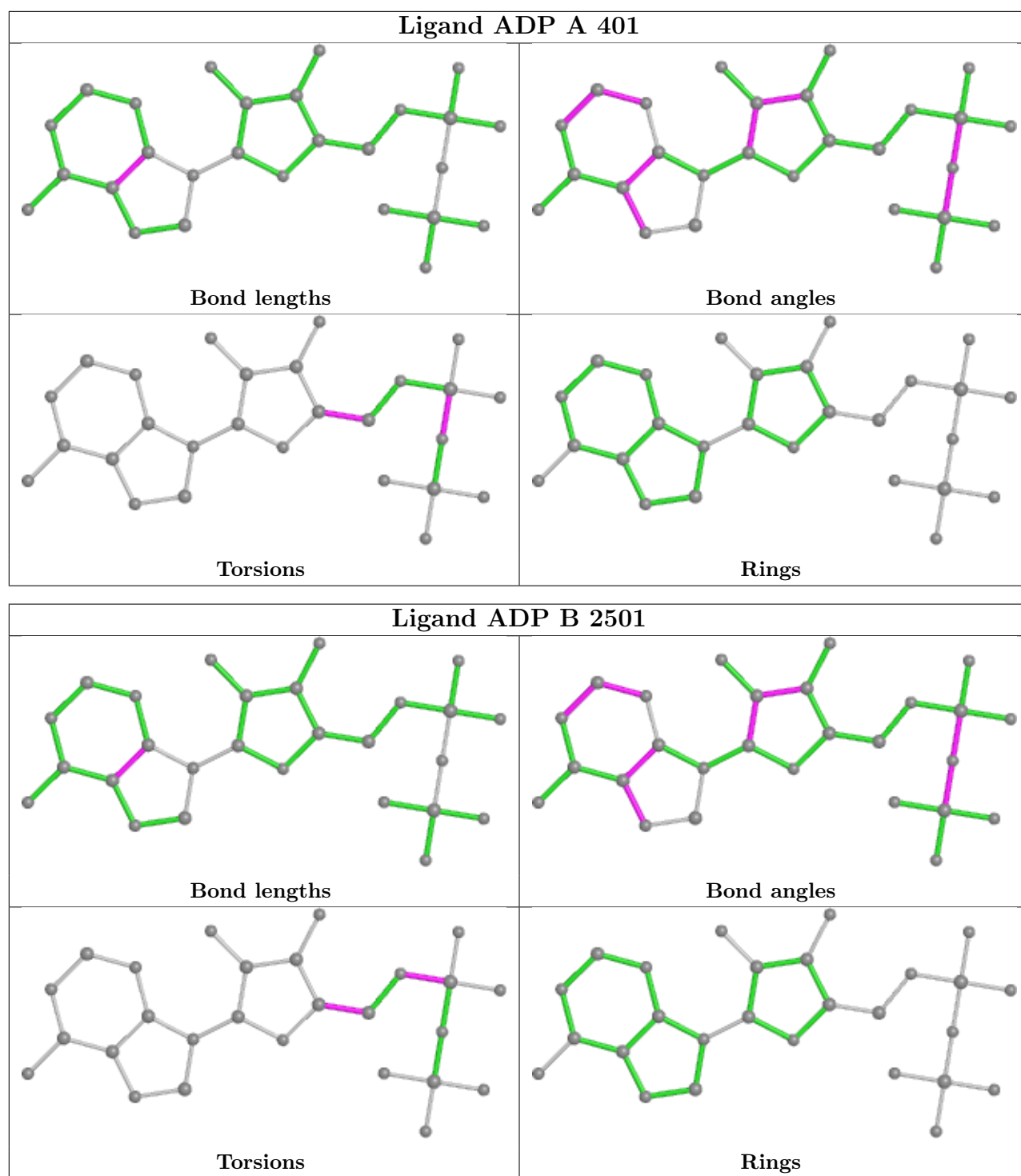


Ligand ADP D 2501



Ligand ADP F 2501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

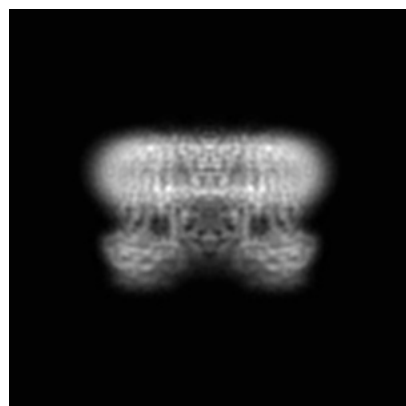
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6851. These allow visual inspection of the internal detail of the map and identification of artifacts.

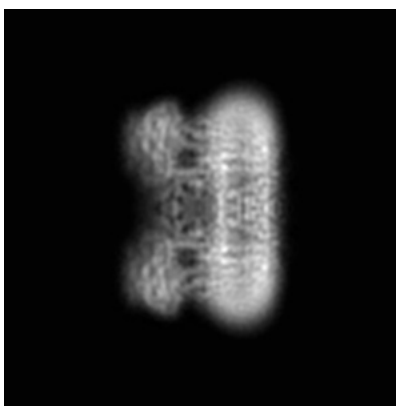
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

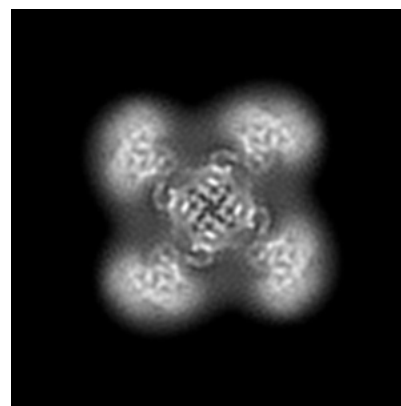
6.1.1 Primary map



X

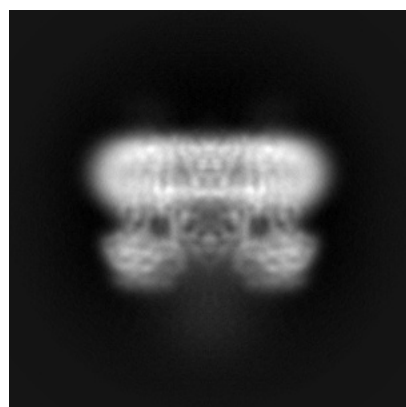


Y

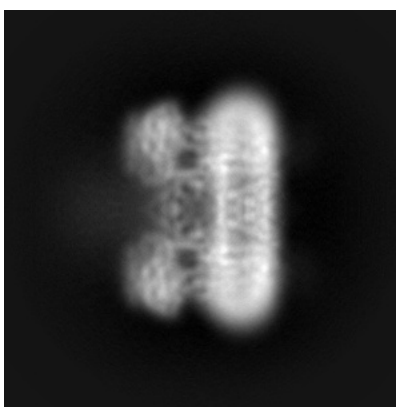


Z

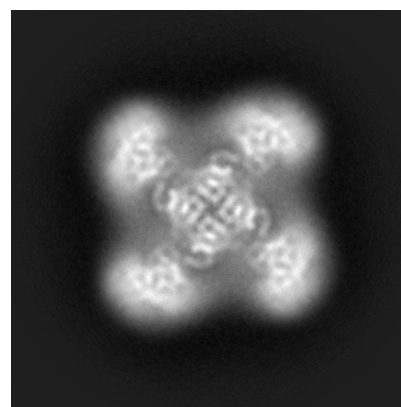
6.1.2 Raw map



X



Y



Z

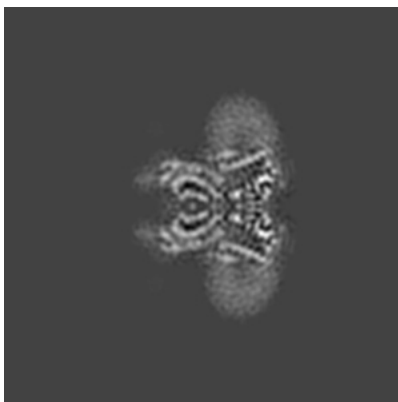
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 156

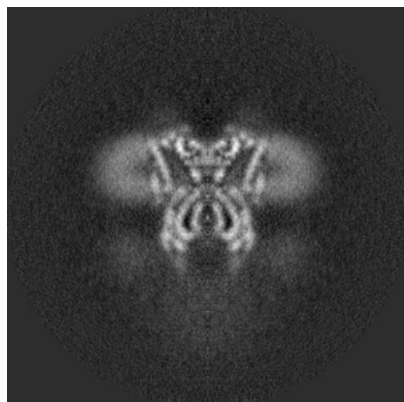


Y Index: 156

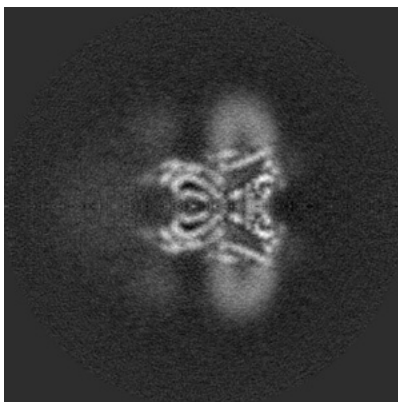


Z Index: 156

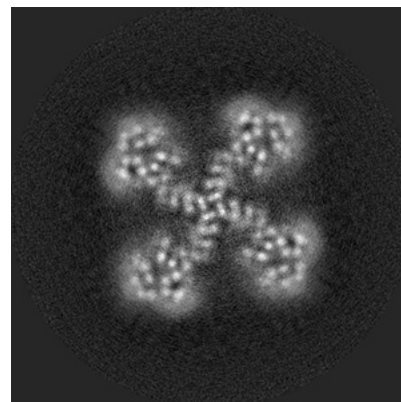
6.2.2 Raw map



X Index: 156



Y Index: 156



Z Index: 156

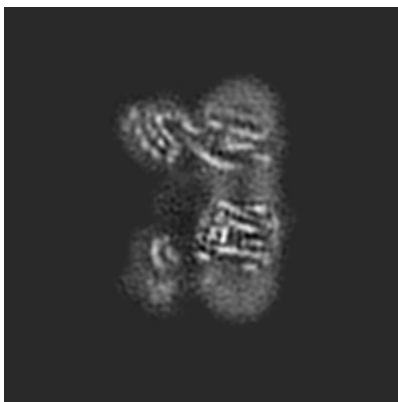
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

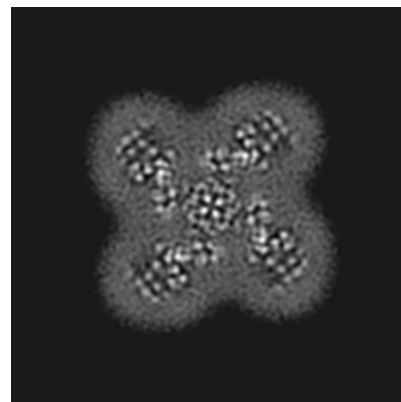
6.3.1 Primary map



X Index: 196

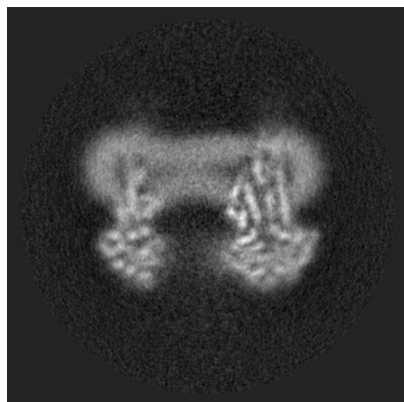


Y Index: 116

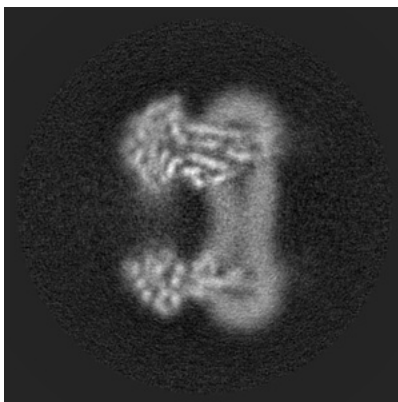


Z Index: 170

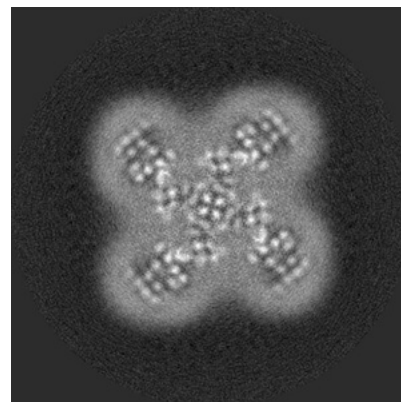
6.3.2 Raw map



X Index: 98



Y Index: 214

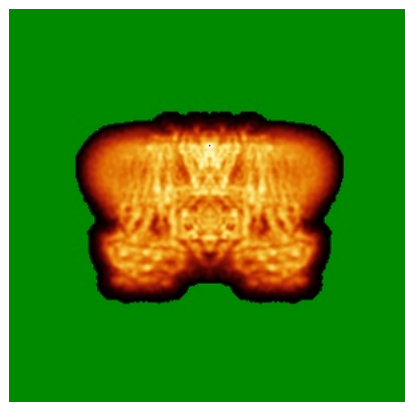


Z Index: 170

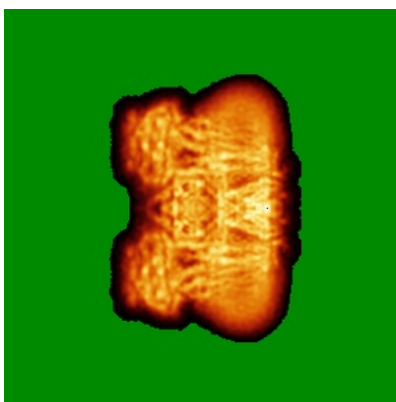
The images above show the largest variance slices of the map in three orthogonal directions.

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

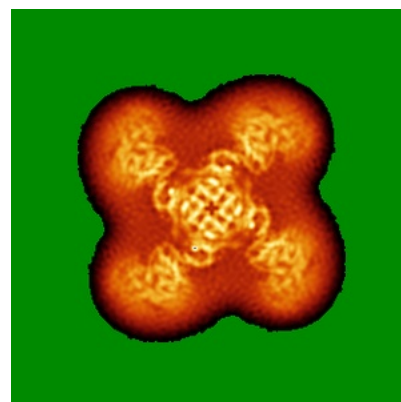
6.4.1 Primary map



X

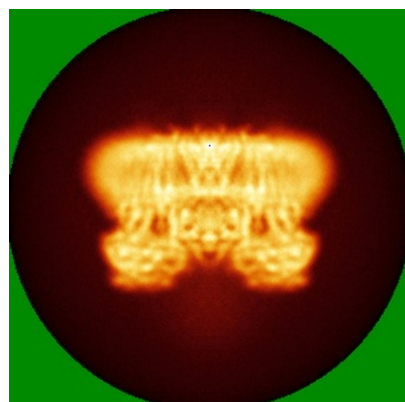


Y

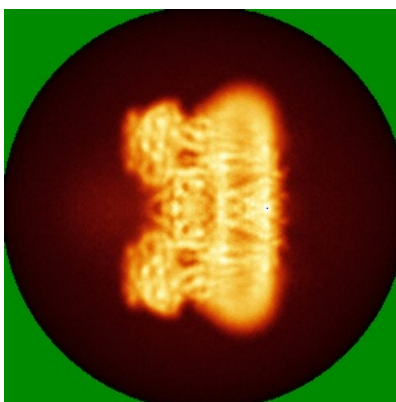


Z

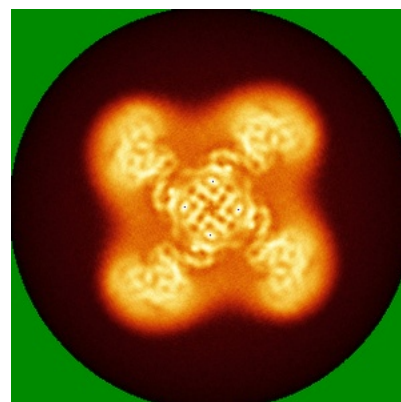
6.4.2 Raw map



X



Y

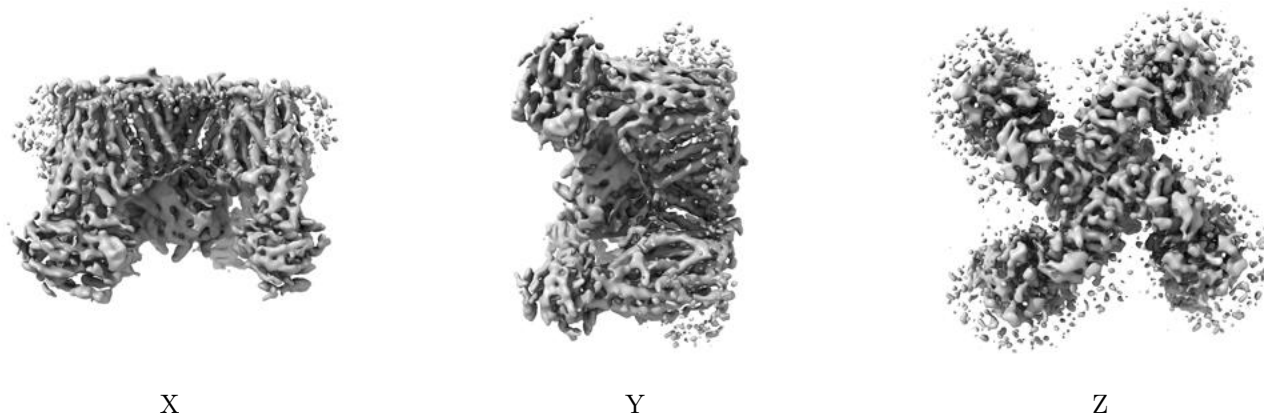


Z

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

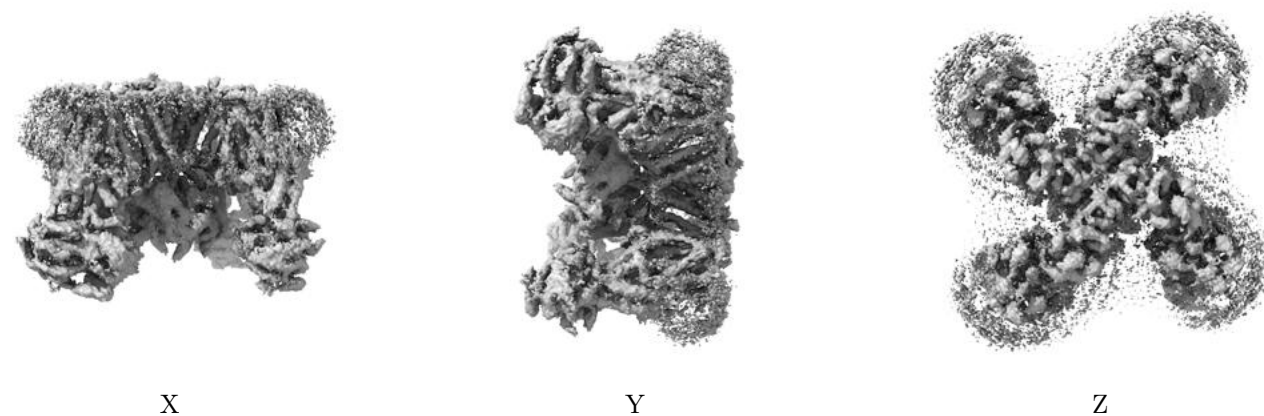
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

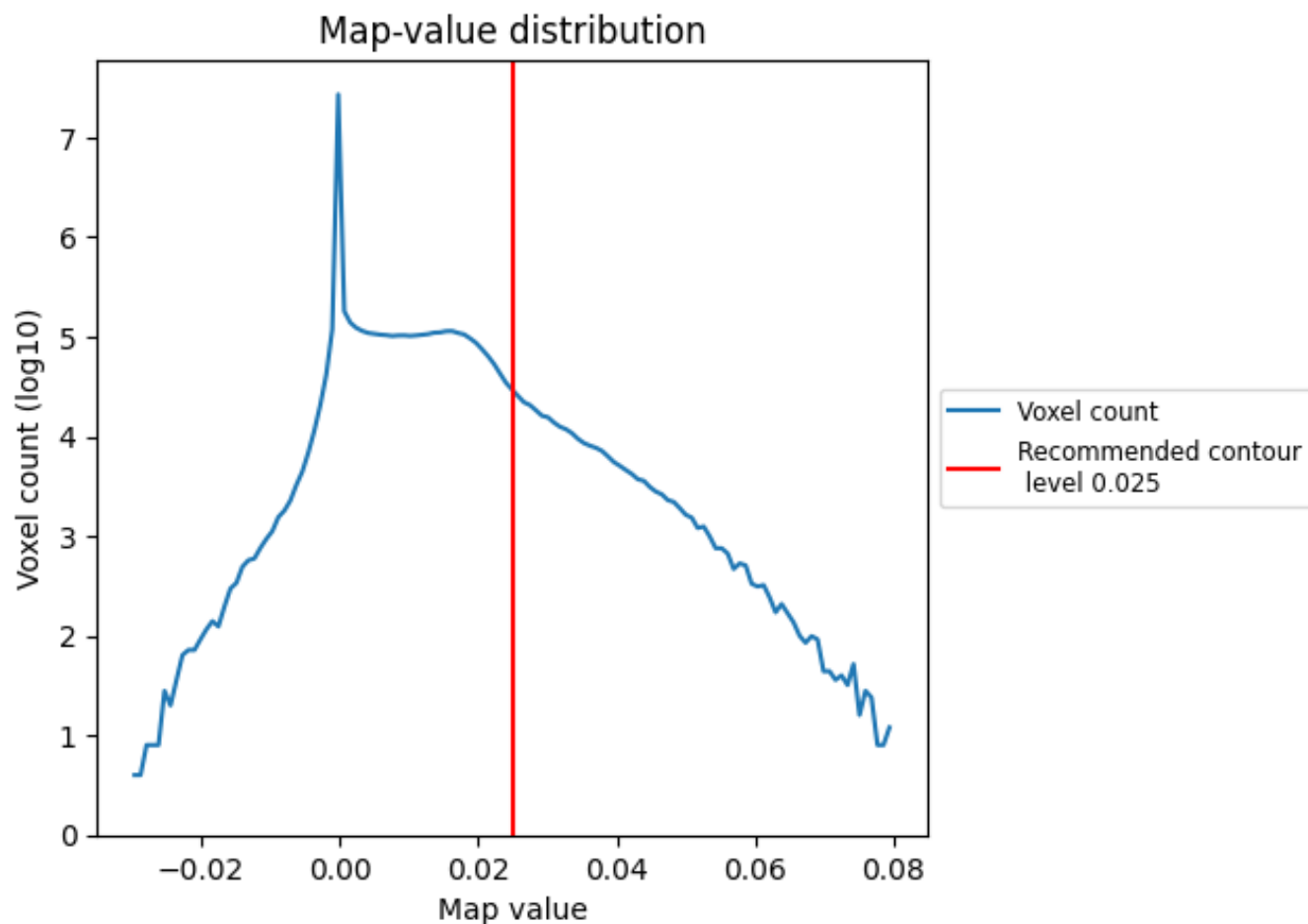
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

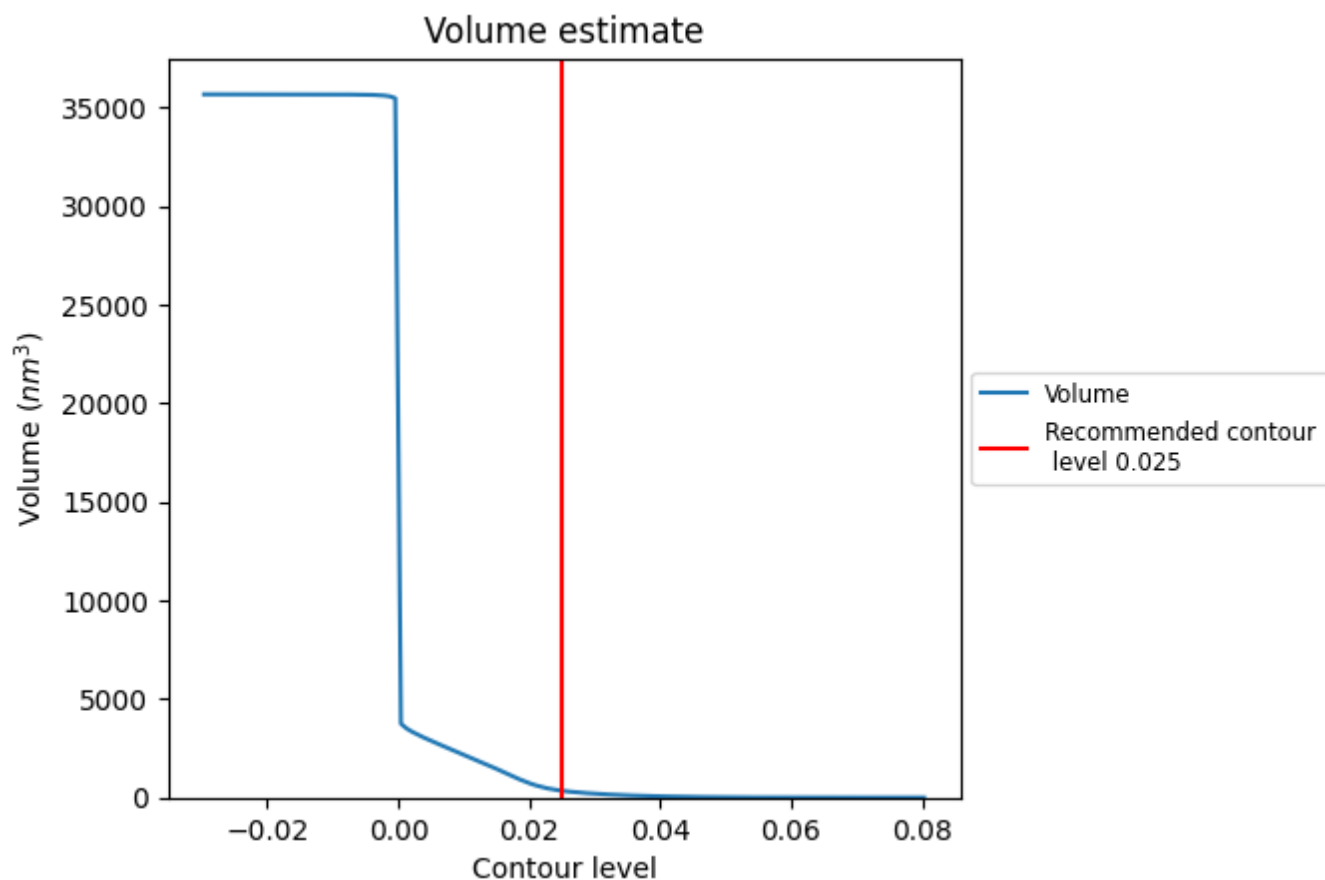
This section contains the results of statistical analysis of the map.

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.

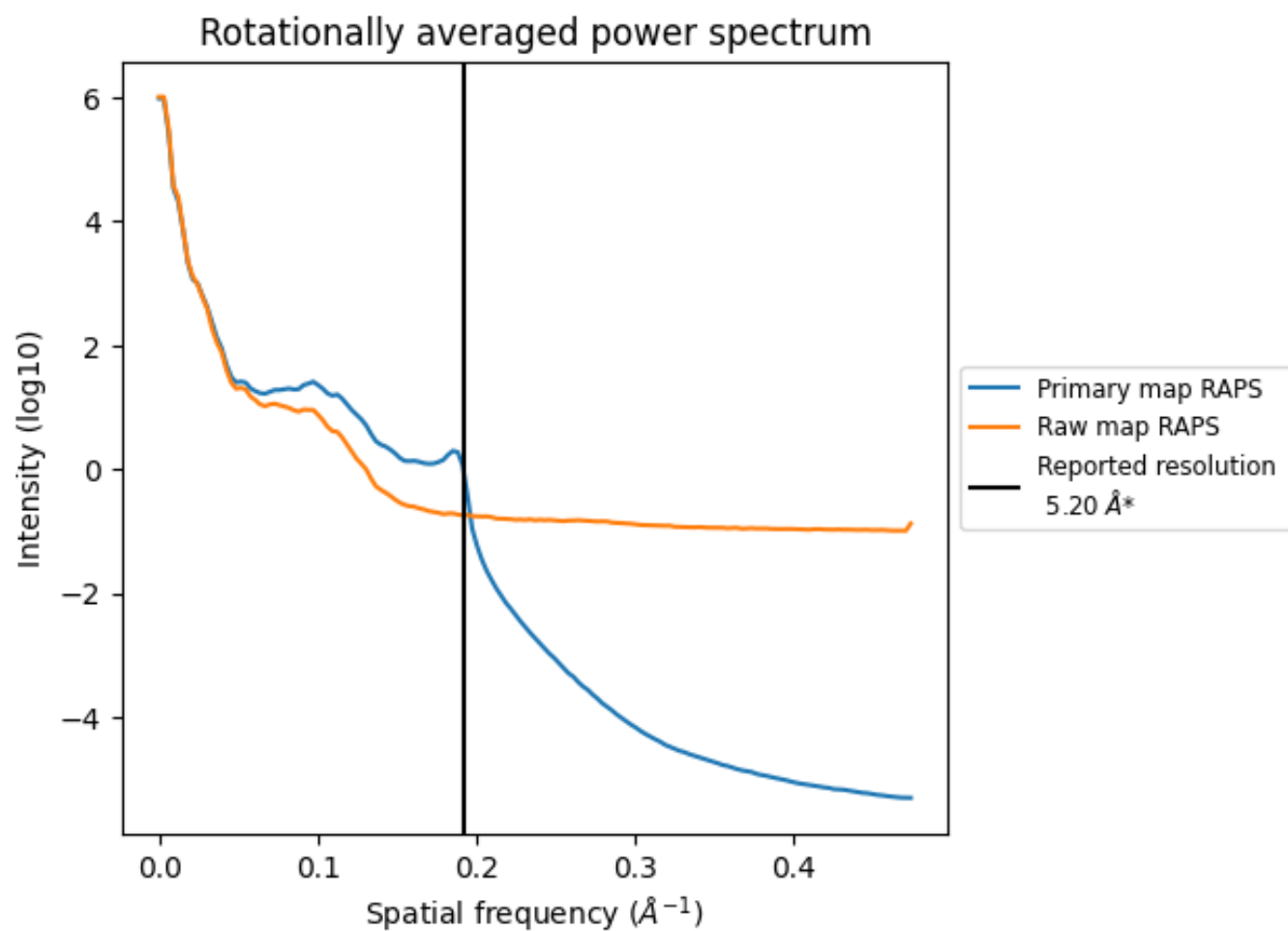
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 314 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 ⓘ

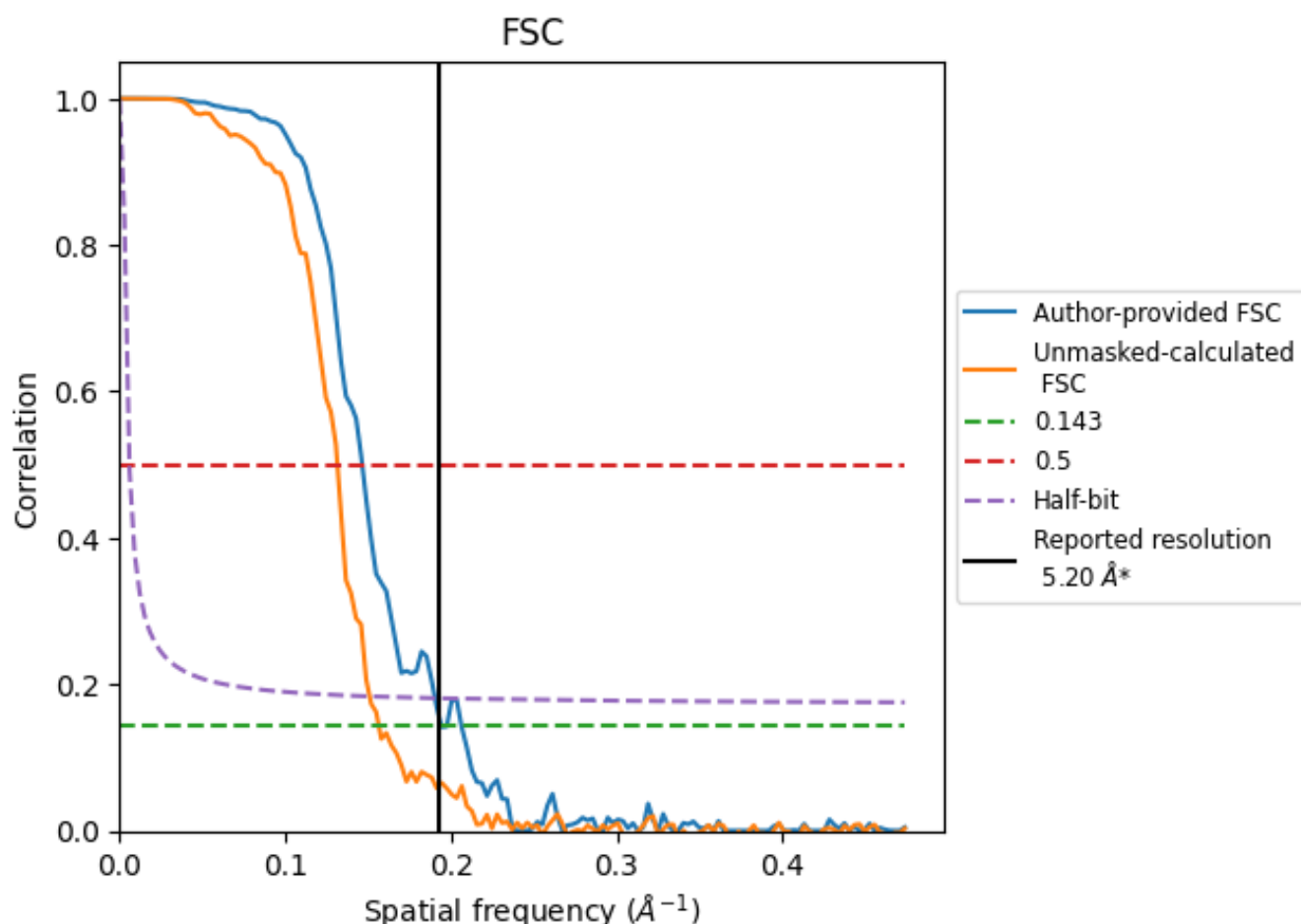


*Reported resolution corresponds to spatial frequency of 0.192 \AA^{-1}

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 0.192 Å⁻¹

8.2 Resolution estimates [i](#)

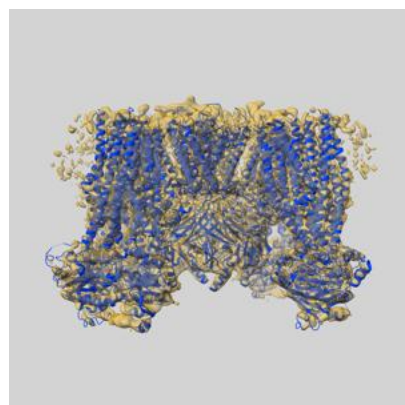
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.15	6.83	5.25
Unmasked-calculated*	6.39	7.60	6.62

*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 6.39 differs from the reported value 5.2 by more than 10 %

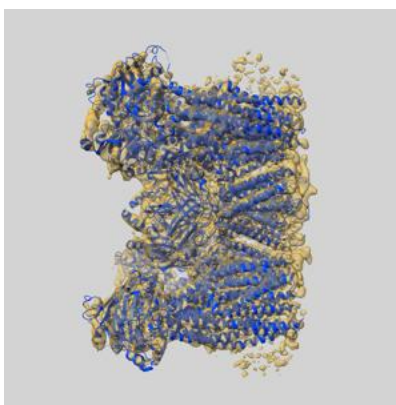
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6851 and PDB model 5YWB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

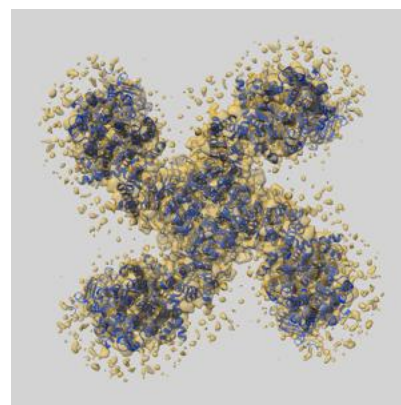
9.1 Map-model overlay [i](#)



X



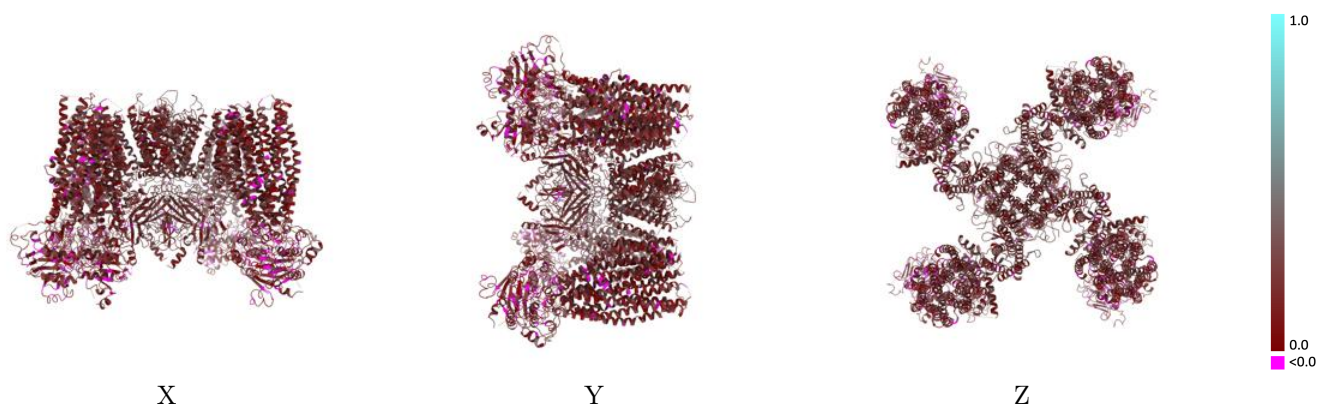
Y



Z

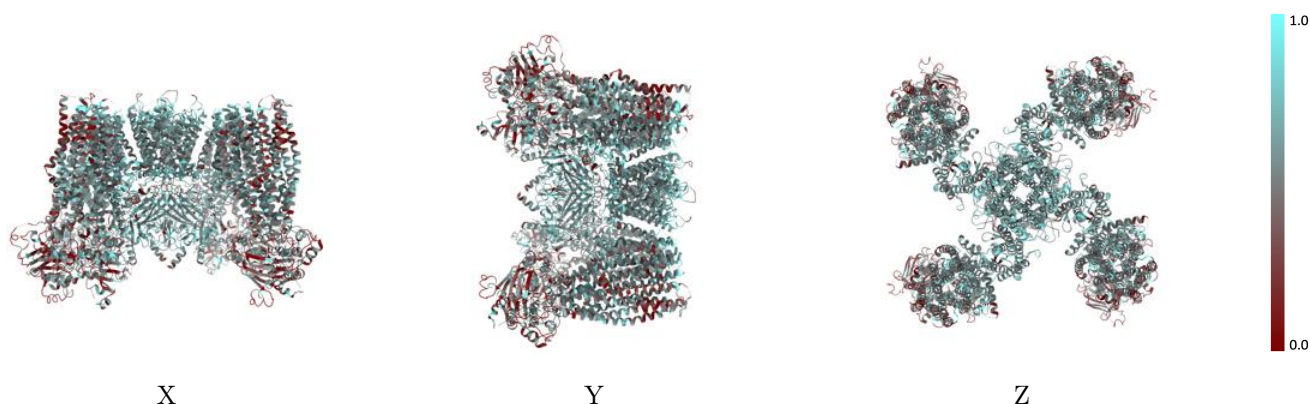
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



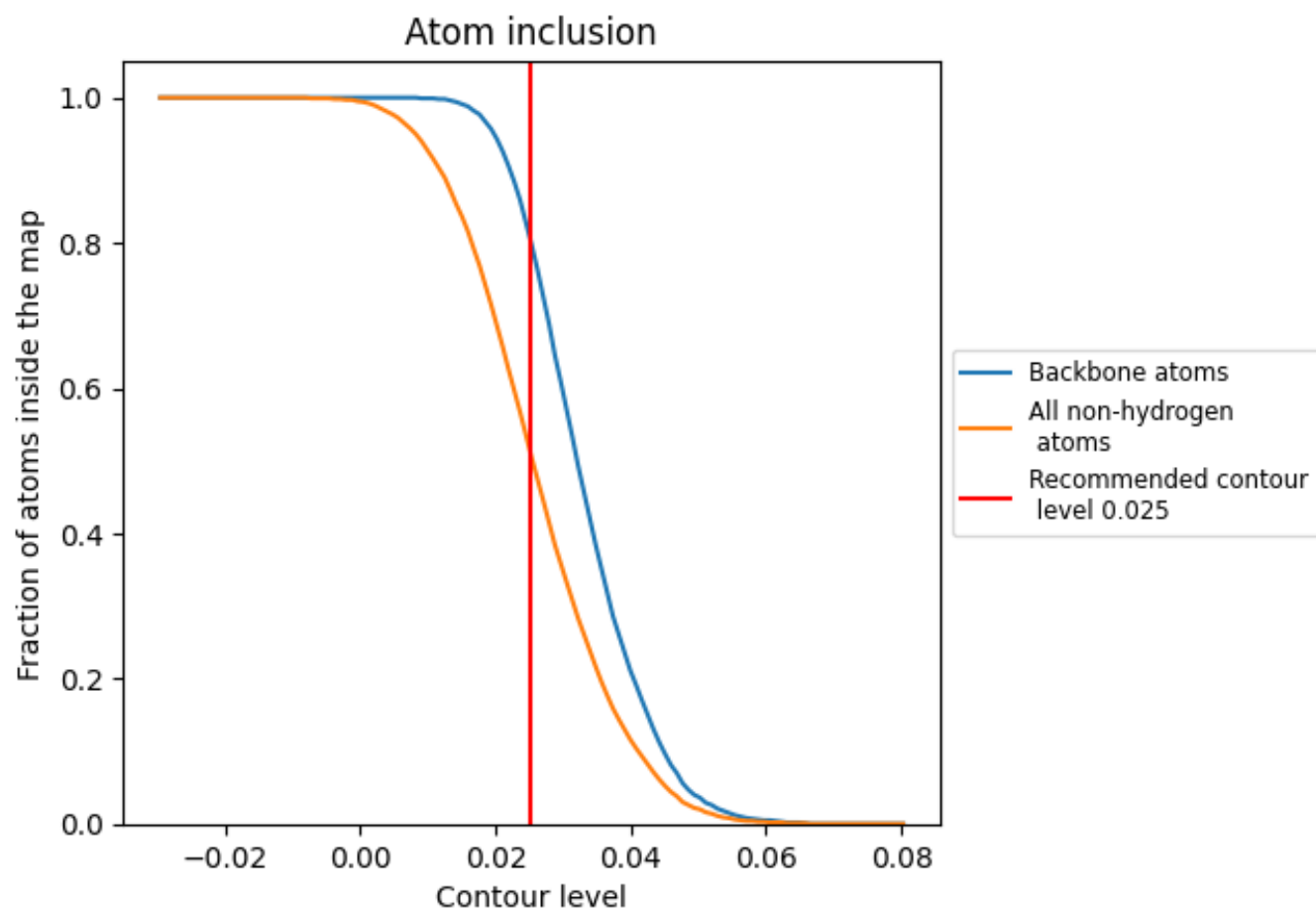
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 52% 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	<div></div> 0.5160	<div></div> 0.1930
A	<div></div> 0.6260	<div></div> 0.2330
B	<div></div> 0.4890	<div></div> 0.1840
C	<div></div> 0.6260	<div></div> 0.2350
D	<div></div> 0.4890	<div></div> 0.1830
E	<div></div> 0.6260	<div></div> 0.2340
F	<div></div> 0.4890	<div></div> 0.1830
G	<div></div> 0.6260	<div></div> 0.2320
H	<div></div> 0.4890	<div></div> 0.1830

1.0

0.0

<0.0