



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 08:02 PM EDT

PDB ID : 8TL9
EMDB ID : EMD-41365
Title : Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-26
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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

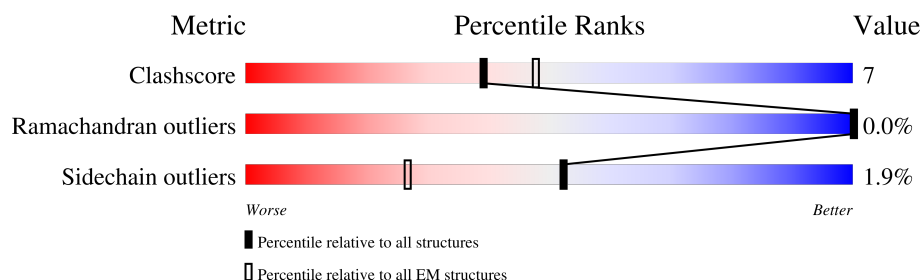
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	2671	
1	B	2671	
1	C	2671	
1	D	2671	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 130518 atoms, of which 65442 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.

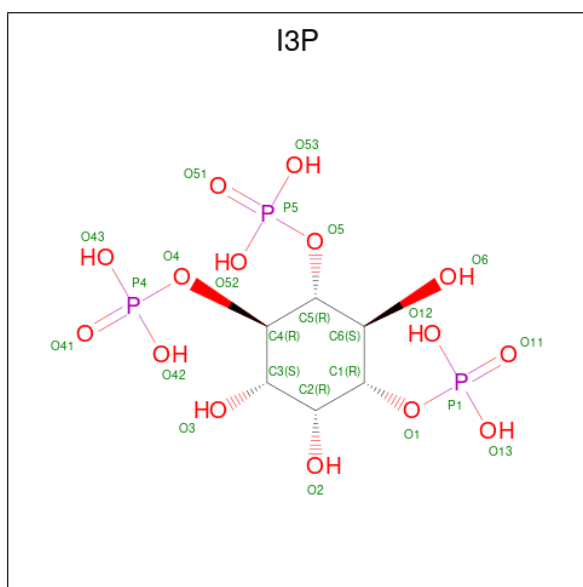
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1989	Total	C	H	N	O	S	0	0
			32350	10293	16244	2749	2960	104		
1	B	1987	Total	C	H	N	O	S	0	0
			32312	10283	16225	2743	2957	104		
1	C	2005	Total	C	H	N	O	S	0	0
			32587	10375	16353	2768	2987	104		
1	D	2034	Total	C	H	N	O	S	0	0
			32957	10480	16536	2807	3029	105		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

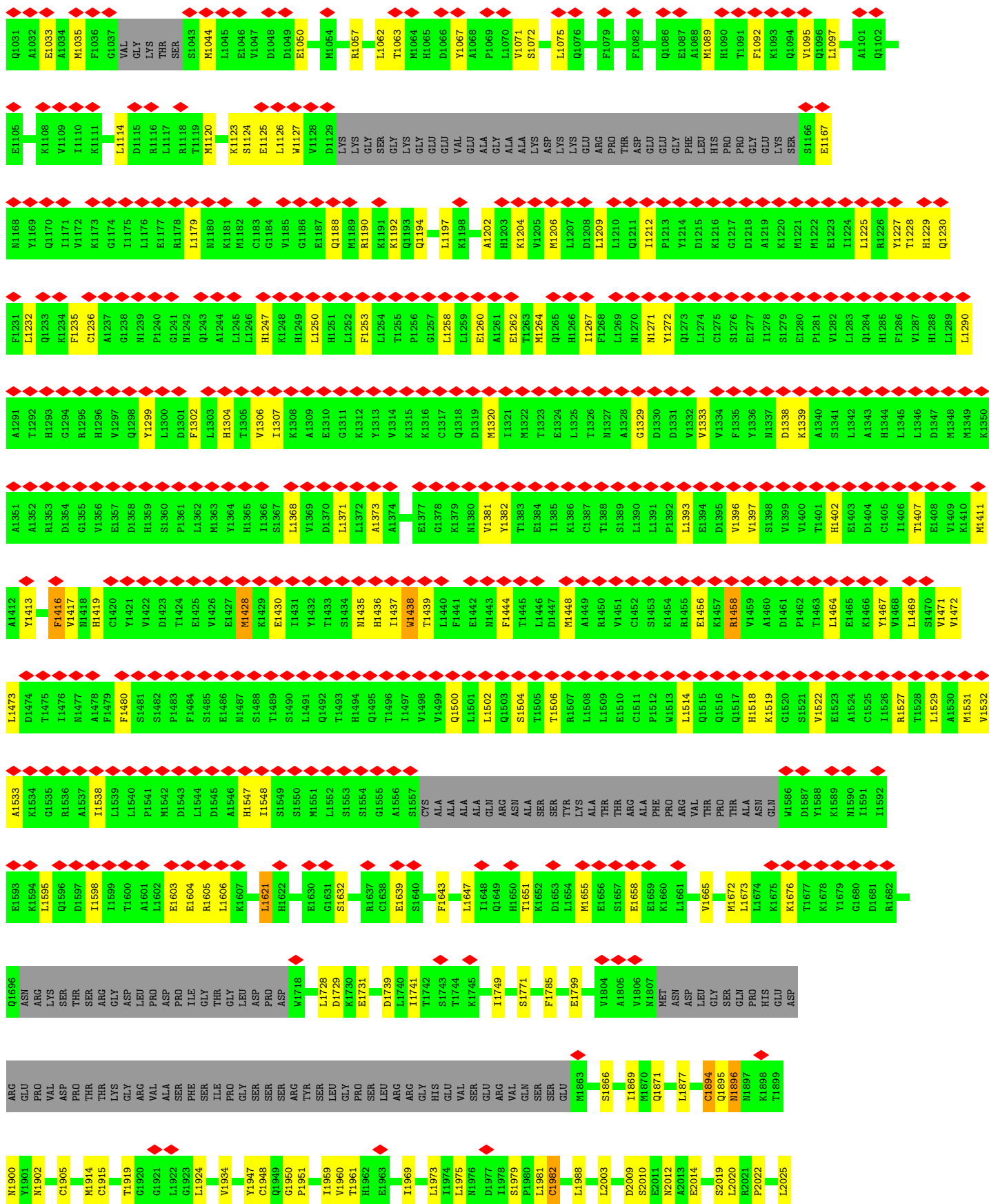


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

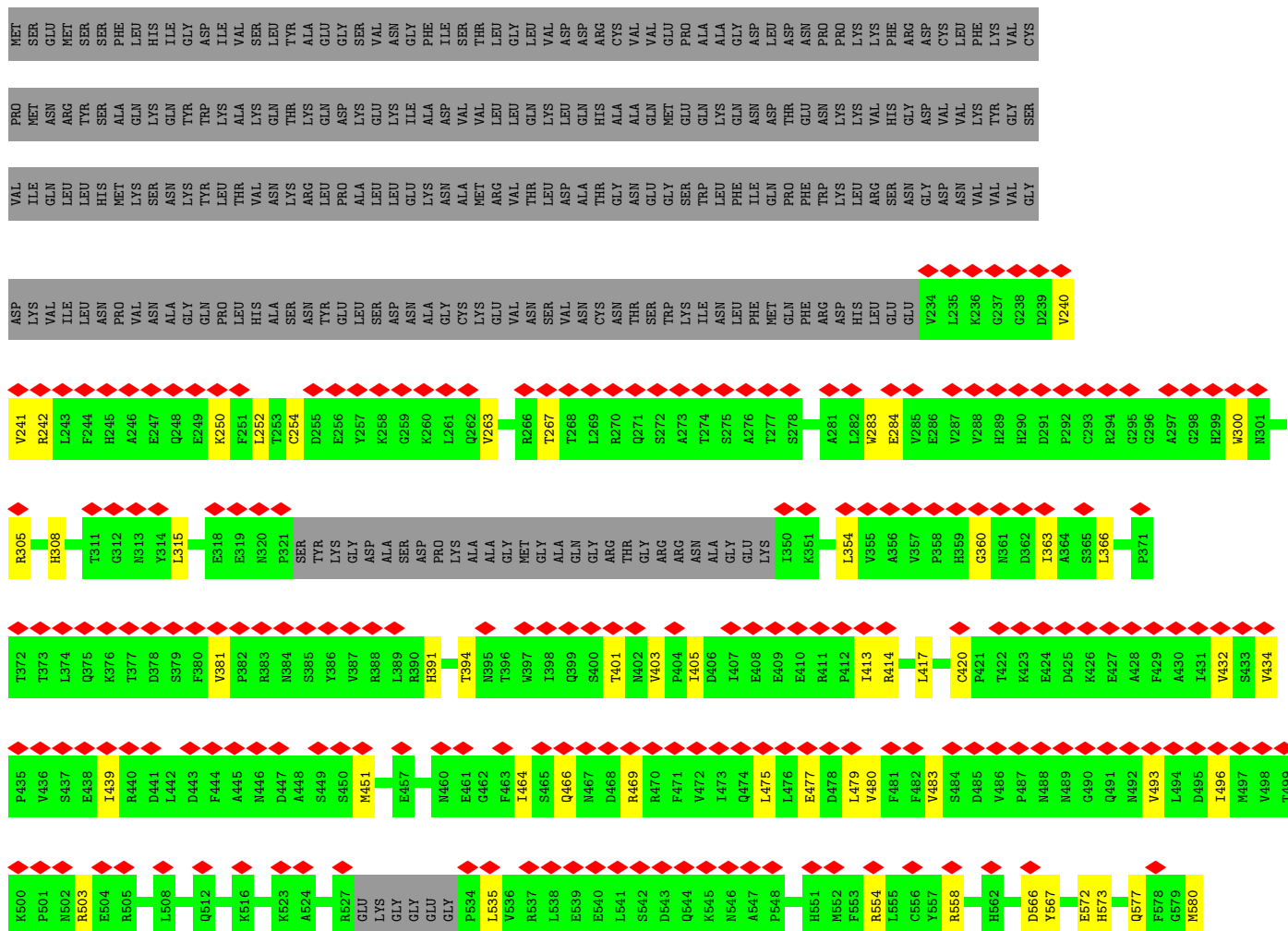


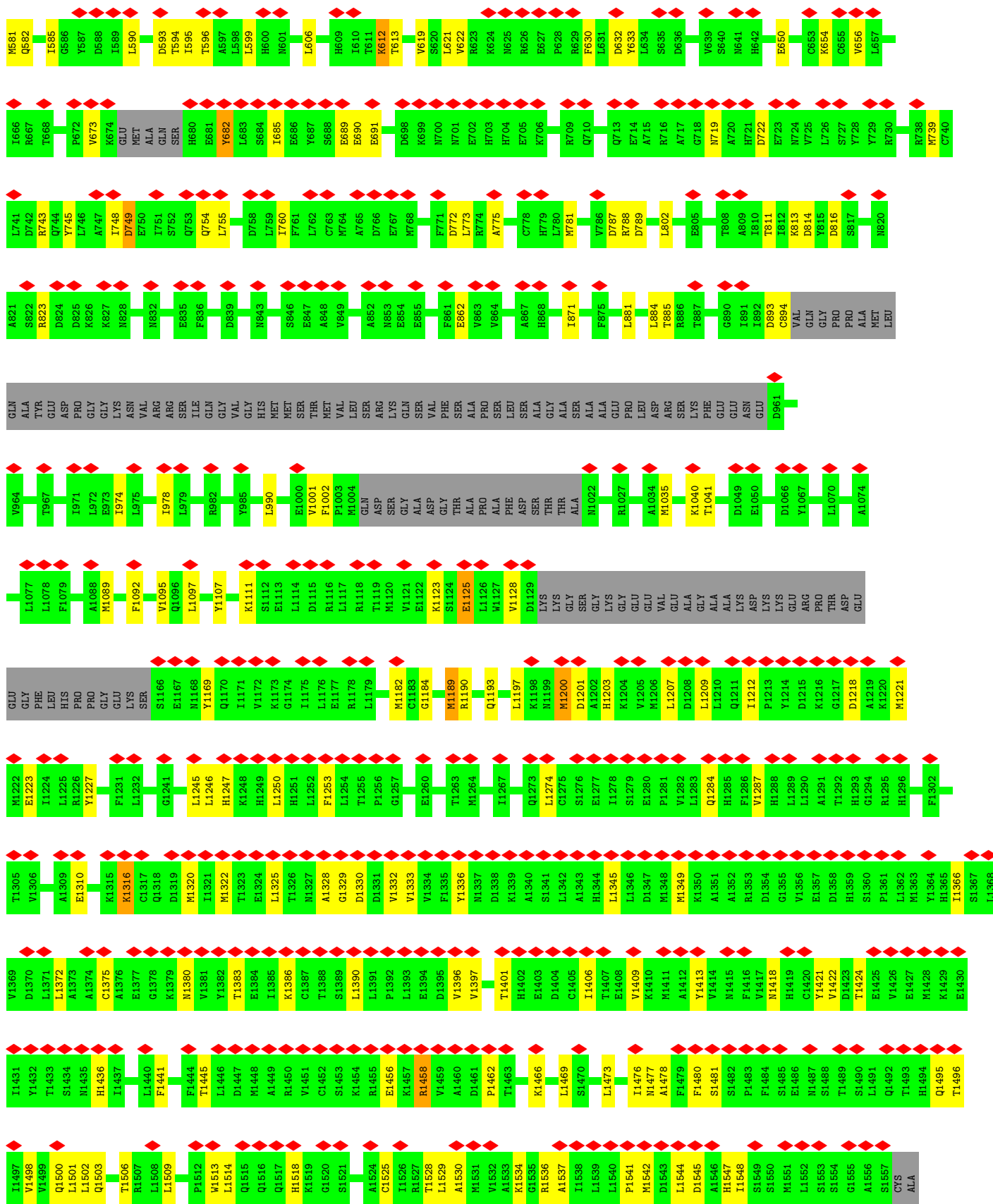


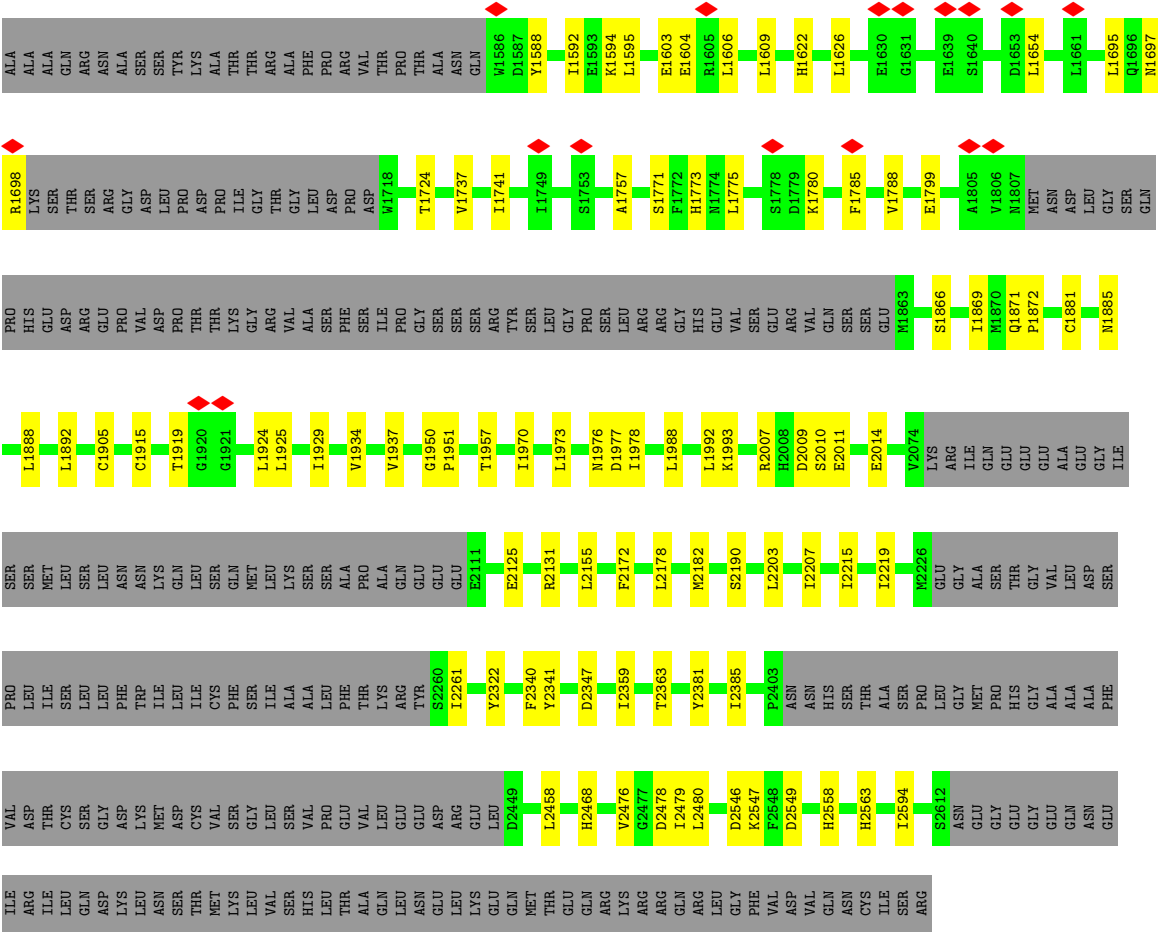




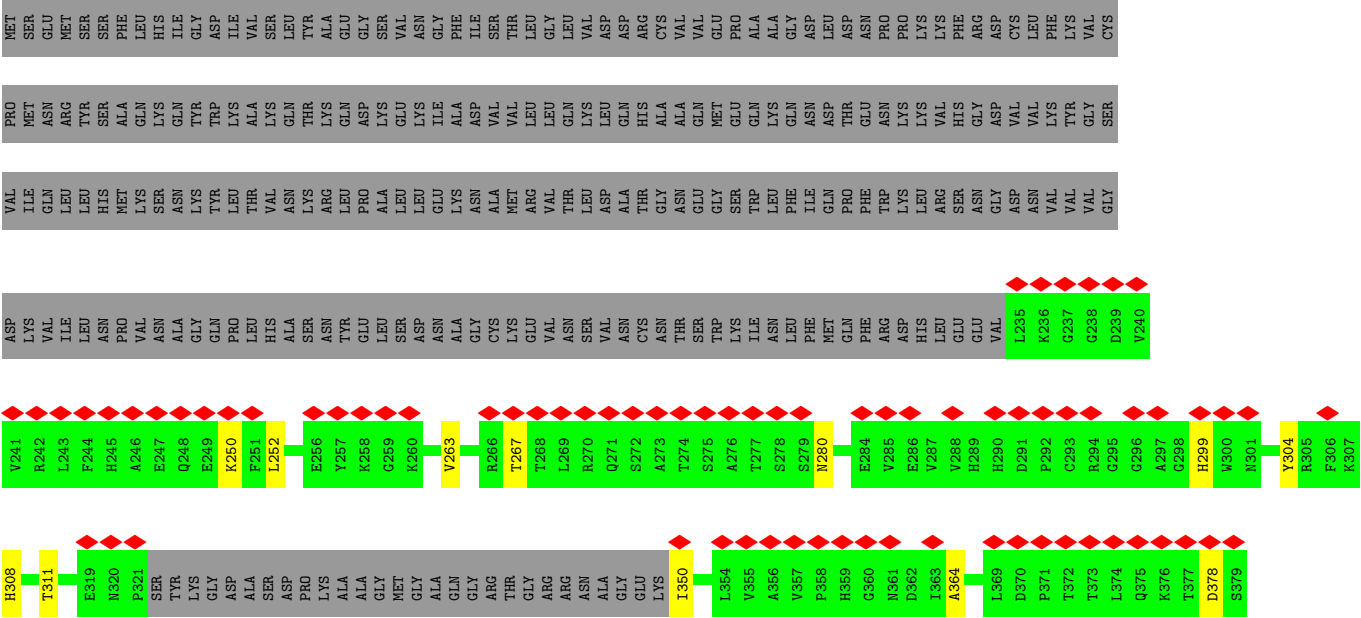
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

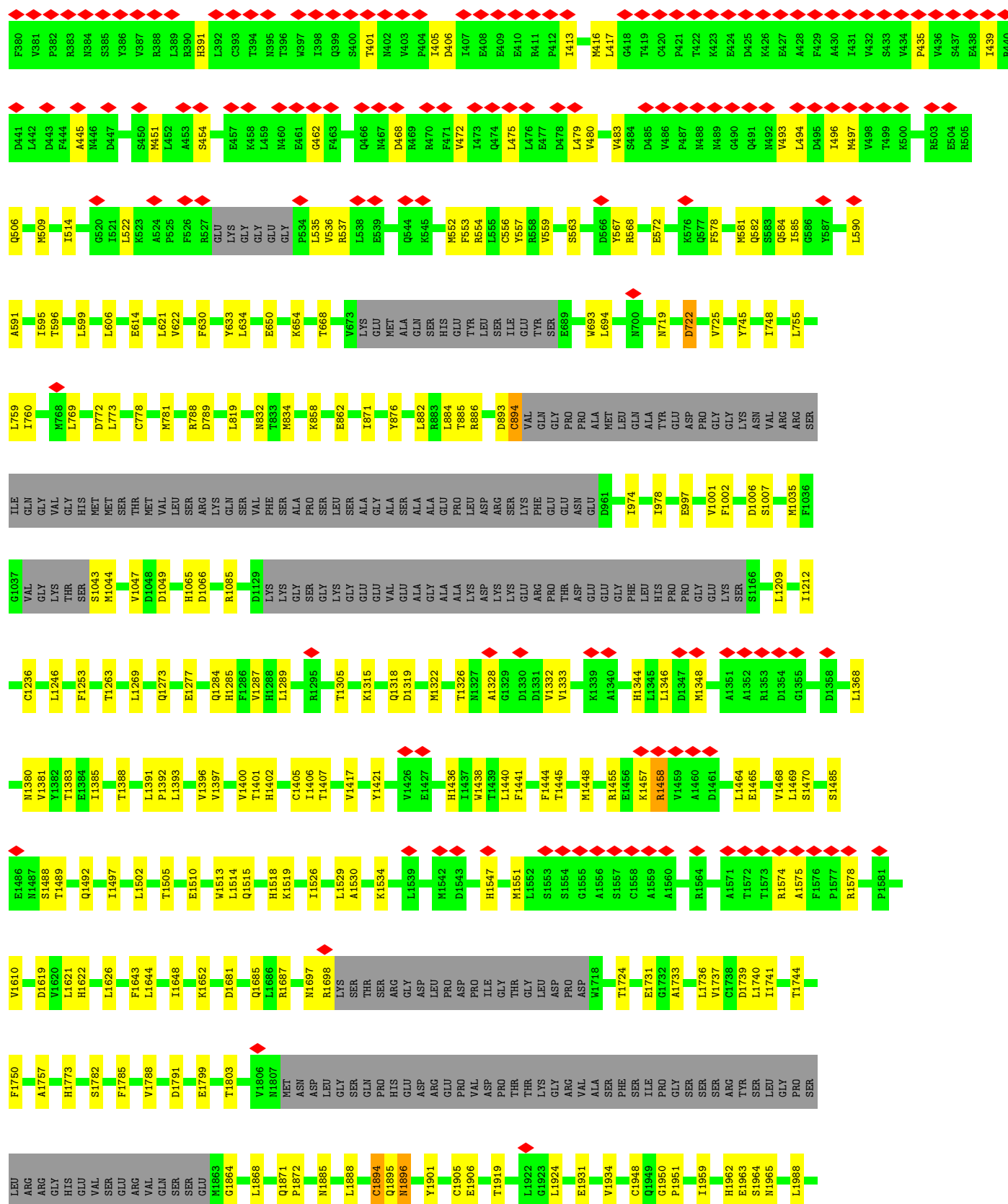


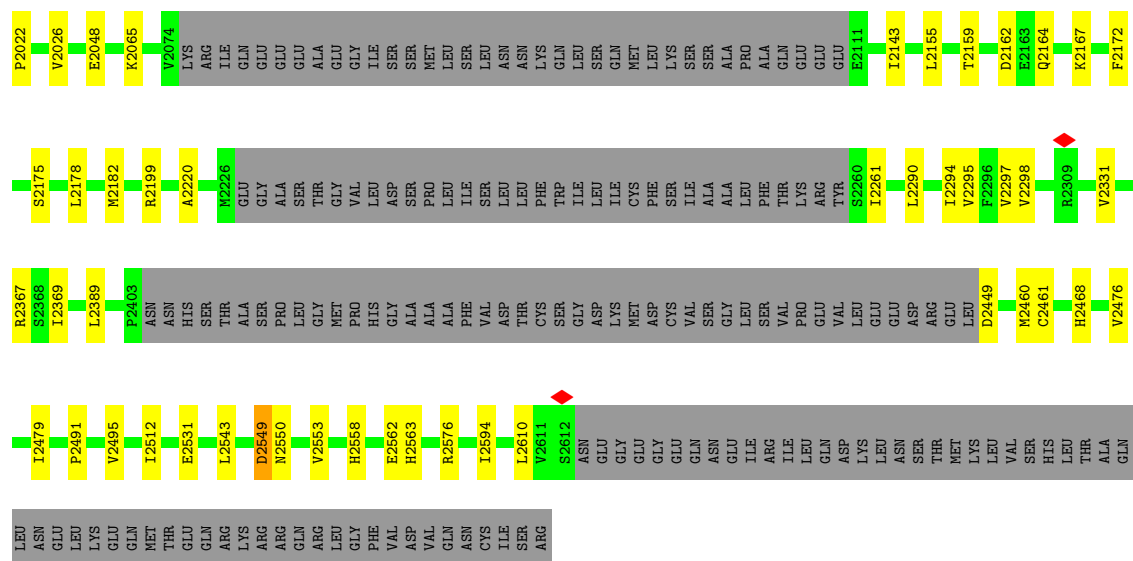




● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88082	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	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: ZN, ATP, CA, I3P

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	0.25	0/16403	0.47	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.25	0/16535	0.46	0/22337
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66048	0.46	0/89227

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	16106	16244	16243	255	0
1	B	16087	16225	16224	248	0
1	C	16234	16353	16362	210	0
1	D	16421	16536	16535	203	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65076	65442	65448	911	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 7.

All (911) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1962:HIS:HD1	1:A:1964:SER:HG	0.98	0.96
1:B:1799:GLU:OE1	1:B:1866:SER:OG	1.91	0.89
1:C:354:LEU:HD12	1:C:417:LEU:HD12	1.55	0.87
1:D:1510:GLU:OE2	1:D:1547:HIS:NE2	2.08	0.84
1:A:1262:GLU:O	1:A:1266:HIS:ND1	2.11	0.83
1:D:1962:HIS:HD1	1:D:1964:SER:HG	1.26	0.82
1:C:2322:TYR:OH	1:C:2347:ASP:OD2	1.97	0.81
1:D:719:ASN:ND2	1:D:722:ASP:OD1	2.13	0.81
1:B:1448:MET:SD	1:B:1504:SER:OG	2.39	0.81
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.14	0.80
1:B:1895:GLN:O	1:B:1896:ASN:ND2	2.15	0.80
1:B:1302:PHE:O	1:B:1306:VAL:HG23	1.82	0.80
1:D:1322:MET:O	1:D:1326:THR:HG23	1.82	0.79
1:D:445:ALA:HB1	1:D:514:ILE:HD11	1.64	0.79
1:C:503:ARG:NH2	1:C:566:ASP:O	2.16	0.79
1:A:1115:ASP:OD1	1:A:1116:ARG:N	2.17	0.78
1:B:568:ARG:NH2	3:B:3002:I3P:O3	2.16	0.77
1:C:593:ASP:OD2	1:C:594:THR:N	2.18	0.77
1:A:733:LEU:HD22	1:A:780:LEU:HD22	1.66	0.77
1:B:881:LEU:O	1:B:885:THR:HG23	1.86	0.76
1:B:585:ILE:HD13	1:B:595:ILE:HD12	1.67	0.76
1:B:1902:ASN:ND2	1:B:1905:CYS:SG	2.58	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:GLU:N	1:A:1747:GLU:OE2	2.21	0.74
1:C:2011:GLU:N	1:C:2011:GLU:OE1	2.20	0.74
1:C:816:ASP:O	1:C:823:ARG:NH2	2.21	0.74
1:A:2571:PHE:O	1:A:2575:VAL:HG23	1.88	0.74
1:B:1188:GLN:N	1:B:1188:GLN:OE1	2.20	0.74
1:A:1302:PHE:O	1:A:1306:VAL:HG23	1.88	0.73
1:A:252:LEU:HD12	1:A:264:PHE:O	1.88	0.73
1:C:1097:LEU:HD12	1:C:1595:LEU:HD22	1.71	0.73
1:D:1236:CYS:HB3	1:D:1246:LEU:HD12	1.71	0.72
1:C:479:LEU:O	1:C:483:VAL:HG23	1.89	0.72
1:A:800:ALA:N	1:A:1199:ASN:OD1	2.22	0.72
1:D:1737:VAL:HG11	1:D:1757:ALA:HB2	1.72	0.72
1:B:1247:HIS:CD2	1:B:1250:LEU:HD12	2.25	0.72
1:D:886:ARG:NH1	1:D:1047:VAL:O	2.23	0.71
1:C:1169:TYR:OH	1:C:1218:ASP:OD2	2.05	0.70
1:C:673:VAL:HB	1:C:685:ILE:HG22	1.73	0.70
1:A:1127:TRP:CZ3	1:A:1172:VAL:HG21	2.26	0.70
1:D:1648:ILE:HG23	1:D:1736:LEU:HD22	1.72	0.70
1:A:1273:GLN:OE1	1:A:1273:GLN:N	2.24	0.70
1:B:300:TRP:CD2	1:B:381:VAL:HG22	2.27	0.69
1:D:451:MET:O	1:D:454:SER:OG	2.08	0.69
1:A:733:LEU:CD2	1:A:780:LEU:HD22	2.21	0.69
1:A:1028:ILE:HG21	1:A:1598:ILE:HD11	1.74	0.69
1:A:707:SER:O	1:A:711:LEU:HD13	1.91	0.69
1:D:1485:SER:O	1:D:1488:SER:OG	2.10	0.69
1:A:743:ARG:NH1	1:A:787:ASP:OD1	2.24	0.68
1:B:1397:VAL:HG21	1:B:1436:HIS:HB3	1.75	0.68
1:C:1189:MET:SD	1:C:1190:ARG:N	2.66	0.68
1:B:1919:THR:HG22	1:B:1924:LEU:HB2	1.74	0.68
1:C:673:VAL:HB	1:C:685:ILE:CG2	2.24	0.68
1:A:709:ARG:NH2	1:A:766:ASP:OD2	2.26	0.68
1:A:2191:MET:HE2	1:A:2194:ILE:HD12	1.75	0.68
1:B:614:GLU:OE1	1:B:614:GLU:N	2.27	0.68
1:B:314:TYR:O	1:B:357:VAL:HG22	1.94	0.68
1:C:673:VAL:HG12	1:C:691:GLU:OE1	1.93	0.68
1:A:1687:ARG:NH1	1:A:1691:LEU:HD11	2.09	0.68
1:D:299:HIS:ND1	1:D:378:ASP:O	2.26	0.68
1:B:854:GLU:N	1:B:854:GLU:OE1	2.25	0.67
1:C:1456:GLU:O	1:C:1458:ARG:NH1	2.27	0.67
1:C:1919:THR:HG22	1:C:1924:LEU:HD23	1.76	0.67
1:B:631:LEU:HD11	1:B:728:TYR:CE1	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:MET:HE2	1:B:497:MET:HA	1.76	0.67
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.23	0.67
1:C:673:VAL:HG13	1:C:690:GLU:N	2.10	0.67
1:A:1067:TYR:O	1:A:1071:VAL:HG23	1.95	0.66
1:B:1473:LEU:HD11	1:B:1522:VAL:HG22	1.77	0.66
1:C:1397:VAL:HG21	1:C:1436:HIS:HB3	1.76	0.66
1:B:1621:LEU:HD23	1:B:1643:PHE:CE2	2.29	0.66
1:D:1328:ALA:HB3	1:D:1332:VAL:HG21	1.78	0.66
1:A:250:LYS:CE	1:A:267:THR:HG22	2.26	0.66
1:C:1329:GLY:O	1:C:1333:VAL:HG22	1.96	0.66
1:C:974:ILE:O	1:C:978:ILE:HD12	1.95	0.66
1:A:252:LEU:HD13	1:A:417:LEU:HD11	1.76	0.65
1:C:1322:MET:SD	1:C:1322:MET:N	2.70	0.65
1:B:1338:ASP:OD1	1:B:1339:LYS:N	2.29	0.65
1:A:252:LEU:HD11	1:A:263:VAL:HG12	1.76	0.64
1:B:496:ILE:HG23	1:B:562:HIS:NE2	2.12	0.64
1:B:1197:LEU:HD22	1:B:1202:ALA:HB3	1.79	0.64
1:B:1067:TYR:O	1:B:1071:VAL:HG23	1.98	0.64
1:B:1506:THR:HG23	1:B:1547:HIS:ND1	2.12	0.64
1:C:621:LEU:HD12	1:C:622:VAL:N	2.12	0.64
1:C:673:VAL:HA	1:C:691:GLU:OE2	1.98	0.64
1:C:1469:LEU:HD11	1:C:1513:TRP:CZ3	2.32	0.64
1:D:1464:LEU:O	1:D:1468:VAL:HG23	1.98	0.64
1:D:581:MET:HE2	1:D:595:ILE:HD11	1.80	0.63
1:B:480:VAL:CG2	1:B:496:ILE:HG21	2.28	0.63
1:B:503:ARG:NH2	1:B:566:ASP:O	2.31	0.63
1:C:885:THR:HG21	1:C:978:ILE:HG21	1.80	0.63
1:A:1097:LEU:HD11	1:A:1595:LEU:HD22	1.80	0.63
1:C:263:VAL:HG11	1:C:315:LEU:HD13	1.80	0.63
1:C:1441:PHE:O	1:C:1445:THR:HG23	1.98	0.63
1:A:1402:HIS:ND1	1:A:1404:ASP:O	2.31	0.63
1:B:1473:LEU:HD11	1:B:1522:VAL:CG2	2.29	0.63
1:D:1396:VAL:O	1:D:1400:VAL:HG22	1.97	0.63
1:B:445:ALA:HB1	1:B:514:ILE:HD11	1.80	0.63
1:D:299:HIS:O	1:D:304:TYR:OH	2.12	0.63
1:B:840:TYR:O	1:B:844:VAL:HG23	1.99	0.63
1:A:267:THR:HG23	1:A:413:ILE:O	1.98	0.62
1:C:1325:LEU:HD21	1:C:1372:LEU:HD21	1.80	0.62
1:B:1506:THR:HG23	1:B:1547:HIS:CE1	2.34	0.62
1:B:746:LEU:HD21	1:B:1125:GLU:OE2	1.98	0.62
1:C:1541:PRO:O	1:C:1545:ASP:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:ASP:OD2	1:A:894:CYS:N	2.32	0.62
1:D:1441:PHE:O	1:D:1445:THR:HG23	2.00	0.62
1:A:811:THR:OG1	1:A:814:ASP:OD2	2.09	0.62
1:A:2476:VAL:HG22	1:A:2480:LEU:HD13	1.82	0.62
1:B:757:VAL:HG22	1:B:785:HIS:CD2	2.34	0.62
1:D:1948:CYS:SG	1:D:1959:ILE:HD12	2.38	0.62
1:D:893:ASP:OD1	1:D:894:CYS:N	2.33	0.61
1:C:1594:LYS:HE3	1:C:1594:LYS:HA	1.80	0.61
1:A:410:GLU:N	1:A:410:GLU:OE2	2.32	0.61
1:D:2468:HIS:HB2	1:D:2479:ILE:HD13	1.83	0.61
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.34	0.61
1:C:2476:VAL:HG22	1:C:2480:LEU:HD13	1.83	0.61
1:C:315:LEU:HD11	1:C:354:LEU:HB3	1.83	0.61
1:C:789:ASP:OD2	1:C:1123:LYS:NZ	2.28	0.61
1:A:506:GLN:NE2	1:A:563:SER:O	2.33	0.61
1:B:1396:VAL:HG21	1:B:1416:PHE:CE1	2.35	0.61
1:A:769:LEU:HB3	1:A:773:LEU:HD23	1.83	0.60
1:B:833:THR:CG2	1:B:866:LEU:HD21	2.31	0.60
1:B:972:LEU:HD11	1:B:1062:LEU:HD13	1.82	0.60
1:C:300:TRP:CD2	1:C:381:VAL:HG22	2.36	0.60
1:B:812:ILE:HD12	1:B:812:ILE:H	1.66	0.60
1:C:893:ASP:OD1	1:C:894:CYS:N	2.34	0.60
1:C:2546:ASP:OD1	1:C:2547:LYS:N	2.35	0.60
1:C:1445:THR:HG22	1:C:1501:LEU:CA	2.32	0.60
1:A:1127:TRP:CH2	1:A:1172:VAL:HG21	2.37	0.60
1:C:719:ASN:ND2	1:C:722:ASP:OD1	2.33	0.60
1:D:252:LEU:HD11	1:D:263:VAL:HG12	1.84	0.60
1:C:1203:HIS:NE2	1:C:1245:LEU:HD21	2.16	0.60
1:A:1247:HIS:CD2	1:A:1274:LEU:HD22	2.37	0.60
1:B:885:THR:HG22	1:B:978:ILE:HD13	1.84	0.60
1:B:2164:GLN:N	1:B:2164:GLN:OE1	2.35	0.59
1:D:2022:PRO:O	1:D:2026:VAL:HG23	2.01	0.59
1:A:1456:GLU:O	1:A:1458:ARG:NH1	2.34	0.59
1:B:1435:ASN:O	1:B:1439:THR:HG23	2.03	0.59
1:C:1445:THR:HG22	1:C:1501:LEU:HA	1.83	0.59
1:C:267:THR:HG23	1:C:413:ILE:O	2.02	0.59
1:D:568:ARG:NH1	1:D:572:GLU:OE1	2.35	0.59
1:C:439:ILE:H	1:C:439:ILE:HD12	1.68	0.59
1:B:1167:GLU:N	1:B:1167:GLU:OE1	2.34	0.59
1:C:363:ILE:HA	1:C:366:LEU:HD12	1.84	0.59
1:D:2143:ILE:H	1:D:2143:ILE:HD12	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ARG:NH1	1:A:1047:VAL:O	2.36	0.59
1:B:782:LEU:HD13	1:B:866:LEU:HA	1.84	0.59
1:C:254:CYS:SG	1:C:308:HIS:ND1	2.74	0.59
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.85	0.58
1:C:466:GLN:OE1	1:C:469:ARG:NH2	2.36	0.58
1:D:1344:HIS:O	1:D:1348:MET:HG3	2.03	0.58
1:B:1050:GLU:OE1	1:B:1050:GLU:N	2.34	0.58
1:A:773:LEU:HD11	1:A:777:PHE:CE2	2.38	0.58
1:B:782:LEU:HD11	1:B:869:ASN:OD1	2.03	0.58
1:B:1033:GLU:OE2	1:B:1605:ARG:NH1	2.34	0.58
1:B:1621:LEU:HD21	1:B:1647:LEU:HD22	1.84	0.58
1:D:1799:GLU:OE2	1:D:1803:THR:HG23	2.03	0.58
1:B:1961:THR:O	1:B:1961:THR:HG22	2.04	0.58
1:B:2359:ILE:O	1:B:2363:THR:HG23	2.03	0.58
1:C:1469:LEU:HD11	1:C:1513:TRP:HZ3	1.66	0.58
1:D:1736:LEU:O	1:D:1740:LEU:HD23	2.02	0.58
1:A:793:LEU:HD11	1:A:872:TYR:HD1	1.69	0.58
1:A:1028:ILE:HD13	1:A:1598:ILE:HD11	1.84	0.58
1:D:1652:LYS:NZ	1:D:1739:ASP:OD1	2.35	0.58
1:B:2225:TYR:OH	1:B:2338:GLU:OE2	2.13	0.58
1:D:1388:THR:HG22	1:D:1421:TYR:CE1	2.39	0.57
1:A:503:ARG:NH2	1:A:566:ASP:O	2.37	0.57
1:A:844:VAL:HG12	1:A:891:ILE:HD12	1.86	0.57
1:B:442:LEU:HD12	1:B:512:GLN:HE21	1.67	0.57
1:B:1267:ILE:O	1:B:1271:ASN:ND2	2.36	0.57
1:B:1480:PHE:CD1	1:B:1532:VAL:HG21	2.39	0.57
1:B:1866:SER:O	1:B:1869:ILE:HG22	2.04	0.57
1:B:2130:ASP:OD1	1:B:2130:ASP:N	2.38	0.57
1:C:1626:LEU:HD12	1:C:1695:LEU:HD13	1.86	0.57
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.86	0.57
1:B:705:GLU:N	1:B:705:GLU:OE1	2.37	0.57
1:B:2546:ASP:OD1	1:B:2547:LYS:N	2.38	0.57
1:C:1469:LEU:HD22	1:C:1518:HIS:CG	2.39	0.57
1:C:1333:VAL:HG23	1:C:1333:VAL:O	2.05	0.57
1:C:2203:LEU:O	1:C:2207:ILE:HG13	2.04	0.57
1:B:1123:LYS:HD3	1:B:1126:LEU:HD13	1.85	0.57
1:D:479:LEU:O	1:D:483:VAL:HG23	2.04	0.57
1:B:2022:PRO:O	1:B:2026:VAL:HG23	2.05	0.56
1:C:621:LEU:HD13	1:C:630:PHE:CD1	2.39	0.56
1:A:439:ILE:HD12	1:A:439:ILE:H	1.70	0.56
1:A:1773:HIS:HB2	1:A:1888:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2025:LEU:O	1:A:2029:ILE:HG13	2.05	0.56
1:C:1654:LEU:O	1:C:1654:LEU:HD12	2.05	0.56
1:C:2359:ILE:O	1:C:2363:THR:HG23	2.05	0.56
1:A:1941:LEU:HD11	1:A:1973:LEU:CD1	2.35	0.56
1:D:1773:HIS:HB2	1:D:1888:LEU:HD21	1.87	0.56
1:C:2155:LEU:HD22	1:C:2178:LEU:HD21	1.88	0.56
1:D:451:MET:HG3	1:D:475:LEU:HD22	1.86	0.56
1:D:1622:HIS:HE1	1:D:1724:THR:HG23	1.70	0.56
1:A:614:GLU:N	1:A:614:GLU:OE1	2.34	0.56
1:D:480:VAL:HG11	1:D:493:VAL:HB	1.88	0.56
1:C:748:ILE:HG21	1:C:788:ARG:HD3	1.88	0.56
1:C:1092:PHE:O	1:C:1095:VAL:HG12	2.06	0.56
1:B:745:TYR:O	1:B:749:ASP:OD1	2.22	0.56
1:B:2143:ILE:HD13	1:B:2186:ARG:NH2	2.21	0.56
1:C:2468:HIS:HB2	1:C:2479:ILE:HD13	1.87	0.56
1:C:451:MET:HB3	1:C:475:LEU:HD22	1.88	0.56
1:C:2178:LEU:O	1:C:2182:MET:HG3	2.06	0.56
1:D:2172:PHE:HZ	1:D:2594:ILE:HG23	1.71	0.55
1:A:622:VAL:HG21	1:A:631:LEU:HD23	1.87	0.55
1:A:1092:PHE:O	1:A:1095:VAL:HG12	2.07	0.55
1:A:1941:LEU:HD11	1:A:1973:LEU:HD13	1.88	0.55
1:B:451:MET:HE2	1:B:475:LEU:HD22	1.88	0.55
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.88	0.55
1:C:871:ILE:HG23	1:C:881:LEU:HD21	1.88	0.55
1:D:2162:ASP:OD1	1:D:2164:GLN:N	2.39	0.55
1:B:1190:ARG:O	1:B:1194:GLN:HG3	2.06	0.55
1:A:480:VAL:HG13	1:A:496:ILE:HG21	1.87	0.55
1:B:585:ILE:HD13	1:B:595:ILE:CD1	2.35	0.55
1:C:673:VAL:HG13	1:C:689:GLU:C	2.27	0.55
1:D:819:LEU:HD23	1:D:819:LEU:H	1.71	0.55
1:A:2468:HIS:HB2	1:A:2479:ILE:HD13	1.87	0.55
1:C:1603:GLU:OE1	1:C:1604:GLU:N	2.40	0.55
1:D:252:LEU:HD11	1:D:263:VAL:CG1	2.36	0.55
1:B:1320:MET:SD	1:B:1320:MET:N	2.80	0.55
1:D:451:MET:HE2	1:D:472:VAL:HG22	1.89	0.55
1:A:1397:VAL:HG21	1:A:1436:HIS:HB3	1.89	0.55
1:A:1407:THR:O	1:A:1411:MET:HG3	2.07	0.55
1:B:997:GLU:O	1:B:1001:VAL:HG23	2.07	0.55
1:C:1622:HIS:HE1	1:C:1724:THR:HG23	1.72	0.54
1:A:303:LEU:HD22	1:A:392:LEU:HD22	1.89	0.54
1:B:252:LEU:HD12	1:B:264:PHE:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:743:ARG:NE	1:C:787:ASP:OD2	2.40	0.54
1:C:300:TRP:CE2	1:C:381:VAL:HG22	2.42	0.54
1:C:405:ILE:HG22	1:C:414:ARG:HB2	1.90	0.54
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.89	0.54
1:D:1514:LEU:HG	1:D:1519:LYS:HG3	1.89	0.54
1:A:772:ASP:OD1	1:A:773:LEU:N	2.41	0.54
1:A:2468:HIS:CB	1:A:2479:ILE:HD13	2.37	0.54
1:C:1937:VAL:HG12	1:C:1992:LEU:HD11	1.89	0.54
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.37	0.54
1:A:2164:GLN:N	1:A:2164:GLN:OE1	2.40	0.54
1:B:589:ILE:O	1:B:589:ILE:HG22	2.07	0.54
1:A:760:ILE:HG21	1:A:781:MET:HB2	1.89	0.54
1:C:391:HIS:ND1	1:C:394:THR:OG1	2.28	0.54
1:D:886:ARG:NE	1:D:1049:ASP:OD2	2.41	0.54
1:B:1514:LEU:HD23	1:B:1519:LYS:HG2	1.90	0.54
1:D:2553:VAL:HG11	1:D:2562:GLU:OE1	2.08	0.54
1:B:593:ASP:OD1	1:B:594:THR:N	2.41	0.53
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.07	0.53
1:B:1621:LEU:HD21	1:B:1647:LEU:CD2	2.38	0.53
1:C:1203:HIS:CD2	1:C:1245:LEU:HD21	2.43	0.53
1:A:611:THR:HB	1:A:614:GLU:OE1	2.09	0.53
1:A:1625:GLU:OE1	1:A:1625:GLU:N	2.41	0.53
1:A:2352:GLU:OE2	1:D:2367:ARG:NH2	2.42	0.53
1:A:2054:TYR:CD1	1:A:2117:TYR:HB3	2.44	0.53
1:C:811:THR:OG1	1:C:814:ASP:OD2	2.22	0.53
1:D:1896:ASN:OD1	1:D:1896:ASN:O	2.26	0.53
1:B:1329:GLY:O	1:B:1333:VAL:HG22	2.08	0.53
1:C:2215:ILE:O	1:C:2219:ILE:HG13	2.09	0.53
1:D:1397:VAL:HG21	1:D:1436:HIS:HB3	1.91	0.53
1:D:1963:GLU:OE2	1:D:1963:GLU:N	2.38	0.53
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.09	0.53
1:D:506:GLN:NE2	1:D:563:SER:O	2.42	0.53
1:A:538:LEU:HD13	1:A:587:TYR:CE2	2.44	0.53
1:A:1338:ASP:OD2	1:A:1339:LYS:N	2.41	0.53
1:D:468:ASP:O	1:D:472:VAL:HG23	2.08	0.53
1:D:1644:LEU:O	1:D:1648:ILE:HG13	2.09	0.53
1:A:849:VAL:HB	1:A:852:ALA:HB2	1.91	0.53
1:B:695:THR:HG23	1:B:705:GLU:HG3	1.91	0.53
1:B:1120:MET:O	1:B:1127:TRP:NE1	2.35	0.53
1:B:1605:ARG:HG3	1:B:1606:LEU:HD23	1.90	0.53
1:D:1455:ARG:NH1	1:D:1465:GLU:OE2	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:O	1:A:285:VAL:HG12	2.09	0.53
1:B:1120:MET:SD	1:B:1127:TRP:NE1	2.81	0.53
1:B:1502:LEU:HD13	1:B:1529:LEU:HD22	1.91	0.53
1:A:622:VAL:HG23	1:A:630:PHE:HB2	1.90	0.53
1:C:405:ILE:HG22	1:C:414:ARG:CB	2.39	0.53
1:A:2191:MET:CE	1:A:2194:ILE:HD12	2.38	0.52
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.09	0.52
1:C:2476:VAL:HG23	1:C:2479:ILE:HD11	1.91	0.52
1:A:1328:ALA:HB3	1:A:1332:VAL:HG21	1.91	0.52
1:B:1915:CYS:HB3	1:B:1969:ILE:HD12	1.92	0.52
1:D:439:ILE:HD12	1:D:439:ILE:H	1.74	0.52
1:D:480:VAL:HG22	1:D:559:VAL:HG23	1.91	0.52
1:A:882:LEU:O	1:A:885:THR:OG1	2.28	0.52
1:A:2536:THR:O	1:A:2536:THR:HG22	2.09	0.52
1:B:888:LEU:CD1	1:B:974:ILE:HG21	2.40	0.52
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.10	0.52
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.50	0.52
1:C:1089:MET:SD	1:C:1606:LEU:HD12	2.50	0.52
1:C:1502:LEU:HD13	1:C:1529:LEU:HD13	1.91	0.52
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.40	0.51
1:C:1773:HIS:HB2	1:C:1888:LEU:HD21	1.91	0.51
1:D:1346:LEU:HD21	1:D:1402:HIS:NE2	2.26	0.51
1:A:1752:GLU:OE1	1:A:1752:GLU:HA	2.09	0.51
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.91	0.51
1:D:1381:VAL:O	1:D:1385:ILE:HG13	2.11	0.51
1:D:1697:ASN:OD1	1:D:1697:ASN:N	2.44	0.51
1:A:1654:LEU:HD12	1:A:1654:LEU:O	2.09	0.51
1:B:1125:GLU:OE1	1:B:1126:LEU:N	2.44	0.51
1:C:745:TYR:O	1:C:749:ASP:OD2	2.29	0.51
1:D:1502:LEU:HG	1:D:1529:LEU:HD23	1.92	0.51
1:A:1428:MET:HB2	1:A:1431:ILE:HD12	1.91	0.51
1:B:1373:ALA:C	1:B:1419:HIS:HD1	2.13	0.51
1:A:763:CYS:HB3	1:A:777:PHE:CE2	2.46	0.51
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	2.11	0.51
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.41	0.51
1:B:315:LEU:HD11	1:B:354:LEU:HD13	1.92	0.51
1:B:871:ILE:HD11	1:B:884:LEU:HD21	1.93	0.51
1:B:1097:LEU:CD1	1:B:1595:LEU:HD22	2.41	0.51
1:B:1114:LEU:HD11	1:B:1202:ALA:HB2	1.91	0.51
1:B:1469:LEU:HD22	1:B:1518:HIS:CG	2.46	0.51
1:C:1976:ASN:O	1:C:1993:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1533:ALA:HA	1:B:1538:ILE:HD11	1.93	0.51
1:C:656:VAL:HG11	1:C:739:MET:HE1	1.93	0.51
1:D:2543:LEU:CD1	1:D:2610:LEU:HD12	2.41	0.51
1:B:354:LEU:HD12	1:B:417:LEU:HD12	1.93	0.51
1:C:650:GLU:OE2	1:C:654:LYS:NZ	2.44	0.51
1:D:1006:ASP:OD2	1:D:1007:SER:N	2.44	0.51
1:A:599:LEU:HB3	1:A:606:LEU:HD13	1.92	0.50
1:B:398:ILE:HD13	1:B:419:THR:HG22	1.93	0.50
1:C:760:ILE:HG21	1:C:781:MET:HB2	1.92	0.50
1:C:1885:ASN:ND2	1:C:1888:LEU:HD23	2.26	0.50
1:A:1659:GLU:OE2	1:A:1659:GLU:N	2.37	0.50
1:B:300:TRP:CE2	1:B:381:VAL:HG22	2.46	0.50
1:C:1184:GLY:O	1:C:1190:ARG:NH2	2.41	0.50
1:D:1285:HIS:O	1:D:1289:LEU:HD23	2.10	0.50
1:A:1386:LYS:HD3	1:A:1386:LYS:N	2.26	0.50
1:C:240:VAL:HA	1:C:284:GLU:HA	1.94	0.50
1:A:602:ASN:HD22	1:A:605:LEU:HD12	1.75	0.50
1:B:1179:LEU:HD13	1:B:1206:MET:HE1	1.94	0.50
1:C:745:TYR:OH	1:C:789:ASP:OD1	2.28	0.50
1:D:760:ILE:HG21	1:D:781:MET:HB2	1.93	0.50
1:D:1962:HIS:CE1	1:D:1964:SER:HG	2.26	0.50
1:B:476:LEU:O	1:B:480:VAL:HG12	2.12	0.50
1:C:1866:SER:O	1:C:1869:ILE:HG22	2.12	0.50
1:A:282:LEU:HD22	1:A:434:VAL:HG21	1.94	0.50
1:A:647:VAL:O	1:A:651:LEU:HD23	2.11	0.50
1:B:459:LEU:HD13	1:B:525:PRO:HD3	1.93	0.50
1:B:606:LEU:HD12	1:B:610:ILE:HG12	1.94	0.50
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.93	0.50
1:A:1124:SER:HA	1:A:1127:TRP:CD1	2.47	0.50
1:D:755:LEU:HD13	1:D:759:LEU:HD23	1.94	0.50
1:A:1048:ASP:C	1:A:1048:ASP:OD1	2.50	0.50
1:A:2009:ASP:C	1:A:2009:ASP:OD1	2.51	0.50
1:B:2266:VAL:O	1:B:2270:LEU:HG	2.11	0.50
1:C:1506:THR:HG23	1:C:1547:HIS:ND1	2.27	0.50
1:A:1612:ALA:O	1:A:1616:VAL:HG23	2.11	0.50
1:B:1603:GLU:OE2	1:B:1604:GLU:N	2.44	0.50
1:D:2065:LYS:HE2	1:D:2065:LYS:HA	1.92	0.49
1:D:2048:GLU:N	1:D:2048:GLU:OE1	2.44	0.49
1:A:1266:HIS:HD1	1:A:1266:HIS:H	1.59	0.49
1:B:451:MET:CE	1:B:475:LEU:HD22	2.41	0.49
1:D:509:MET:HA	1:D:514:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ASP:OD2	1:A:663:ASP:N	2.44	0.49
1:B:1500:GLN:OE1	1:B:1500:GLN:HA	2.12	0.49
1:A:885:THR:HG23	1:A:978:ILE:HD13	1.93	0.49
1:A:1492:GLN:CD	1:A:1493:THR:HG23	2.32	0.49
1:A:1746:ASN:OD1	1:A:1748:LYS:N	2.45	0.49
1:A:1974:ILE:HD11	1:A:1997:SER:HA	1.95	0.49
1:B:1731:GLU:OE1	1:B:1731:GLU:HA	2.13	0.49
1:C:1780:LYS:HE2	1:C:1780:LYS:HA	1.95	0.49
1:A:585:ILE:HD13	1:A:595:ILE:HD12	1.95	0.49
1:B:1444:PHE:CG	1:B:1472:VAL:HG13	2.48	0.49
1:D:1444:PHE:O	1:D:1448:MET:HG3	2.13	0.49
1:A:1333:VAL:HA	1:A:1368:LEU:HD21	1.95	0.49
1:B:602:ASN:HD22	1:B:605:LEU:HD12	1.78	0.49
1:C:1001:VAL:HG12	1:C:1002:PHE:CD1	2.48	0.49
1:A:871:ILE:HG23	1:A:881:LEU:HD21	1.95	0.49
1:B:833:THR:HG22	1:B:866:LEU:HD21	1.94	0.49
1:C:1970:ILE:HA	1:C:1973:LEU:HD12	1.94	0.49
1:D:522:LEU:HD22	1:D:557:TYR:HE1	1.77	0.49
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.95	0.49
1:A:1025:LEU:HD23	1:A:1601:ALA:CB	2.43	0.49
1:A:1053:ARG:O	1:A:1057:ARG:HG3	2.12	0.49
1:B:581:MET:HG3	1:B:595:ILE:HD11	1.94	0.49
1:C:305:ARG:NE	1:C:360:GLY:O	2.46	0.49
1:A:558:ARG:HD3	1:A:590:LEU:HD23	1.95	0.48
1:B:871:ILE:HD11	1:B:884:LEU:CD2	2.43	0.48
1:B:1260:GLU:O	1:B:1264:MET:HG3	2.13	0.48
1:D:267:THR:HG23	1:D:413:ILE:O	2.13	0.48
1:A:1033:GLU:OE2	1:A:1682:ARG:NH2	2.45	0.48
1:A:2048:GLU:OE1	1:A:2048:GLU:N	2.46	0.48
1:B:745:TYR:HA	1:B:748:ILE:HB	1.93	0.48
1:B:1407:THR:HG21	1:B:1464:LEU:HA	1.95	0.48
1:A:576:LYS:HD2	1:A:576:LYS:N	2.28	0.48
1:B:1960:VAL:HG23	1:B:2003:LEU:HD22	1.94	0.48
1:C:682:TYR:HB2	1:C:685:ILE:HD12	1.95	0.48
1:C:1881:CYS:SG	1:C:1892:LEU:HD12	2.53	0.48
1:D:1333:VAL:HG23	1:D:1333:VAL:O	2.13	0.48
1:D:1513:TRP:O	1:D:1514:LEU:CB	2.62	0.48
1:D:1905:CYS:SG	1:D:1962:HIS:NE2	2.83	0.48
1:A:1595:LEU:O	1:A:1598:ILE:HG22	2.13	0.48
1:A:2014:GLU:O	1:A:2018:ILE:HG13	2.13	0.48
1:D:252:LEU:HD13	1:D:417:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:MET:HG3	1:D:475:LEU:CD2	2.44	0.48
1:D:1397:VAL:O	1:D:1401:THR:HG23	2.12	0.48
1:A:835:GLU:O	1:A:839:ASP:OD1	2.30	0.48
1:B:1894:CYS:O	1:B:1894:CYS:SG	2.72	0.48
1:B:2048:GLU:N	1:B:2048:GLU:OE1	2.47	0.48
1:C:252:LEU:HD11	1:C:417:LEU:HD11	1.95	0.48
1:D:1621:LEU:HD23	1:D:1643:PHE:HE2	1.79	0.48
1:A:1124:SER:HA	1:A:1127:TRP:NE1	2.28	0.48
1:C:1496:THR:O	1:C:1500:GLN:HG2	2.13	0.48
1:D:557:TYR:OH	1:D:584:GLN:OE1	2.31	0.48
1:A:1428:MET:SD	1:A:1428:MET:N	2.87	0.48
1:B:541:LEU:HD13	1:B:550:GLN:HG3	1.94	0.48
1:A:1469:LEU:HD22	1:A:1518:HIS:CG	2.49	0.48
1:B:1437:ILE:N	1:B:1437:ILE:HD12	2.29	0.48
1:A:840:TYR:CD2	1:A:863:VAL:HG11	2.48	0.48
1:B:309:LEU:HD23	1:B:442:LEU:HD22	1.96	0.48
1:B:455:ALA:O	1:B:459:LEU:HG	2.13	0.48
1:C:1366:ILE:HD11	1:C:1409:VAL:HG23	1.94	0.48
1:D:1626:LEU:HD11	1:D:1698:ARG:HB2	1.95	0.48
1:A:250:LYS:HE2	1:A:267:THR:HG22	1.94	0.48
1:B:1097:LEU:HD11	1:B:1595:LEU:HD22	1.96	0.48
1:B:1197:LEU:CD2	1:B:1202:ALA:HB3	2.43	0.48
1:C:581:MET:HB3	1:C:595:ILE:HD11	1.95	0.48
1:D:451:MET:CG	1:D:475:LEU:HD22	2.44	0.48
1:D:2549:ASP:O	1:D:2550:ASN:OD1	2.32	0.48
1:B:1467:TYR:O	1:B:1471:VAL:HG22	2.14	0.47
1:B:1658:GLU:N	1:B:1658:GLU:OE1	2.46	0.47
1:C:1193:GLN:O	1:C:1197:LEU:HD23	2.14	0.47
1:D:882:LEU:O	1:D:885:THR:OG1	2.31	0.47
1:A:354:LEU:HD12	1:A:417:LEU:HD12	1.96	0.47
1:B:782:LEU:HD11	1:B:869:ASN:HB2	1.97	0.47
1:D:614:GLU:OE1	1:D:614:GLU:N	2.47	0.47
1:D:1574:ARG:O	1:D:1575:ALA:HB3	2.14	0.47
1:A:561:ARG:HE	1:A:597:ALA:HB2	1.79	0.47
1:B:667:ARG:NH1	1:B:754:GLN:OE1	2.48	0.47
1:B:1228:THR:O	1:B:1232:LEU:HG	2.14	0.47
1:C:802:LEU:HD11	1:C:1107:TYR:CE1	2.50	0.47
1:C:1203:HIS:O	1:C:1207:LEU:HG	2.13	0.47
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.29	0.47
1:C:1924:LEU:HD22	1:C:1924:LEU:N	2.30	0.47
1:D:250:LYS:HE2	1:D:267:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1864:GLY:O	1:D:1868:LEU:HD23	2.14	0.47
1:A:1736:LEU:HD12	1:A:1740:LEU:HG	1.96	0.47
1:B:1124:SER:HB2	1:B:1212:ILE:HD11	1.96	0.47
1:C:1525:CYS:O	1:C:1528:THR:OG1	2.29	0.47
1:C:1737:VAL:HG11	1:C:1757:ALA:HB2	1.95	0.47
1:D:668:THR:HG21	1:D:755:LEU:HD11	1.96	0.47
1:A:299:HIS:ND1	1:A:378:ASP:O	2.47	0.47
1:A:792:GLU:OE1	1:A:1118:ARG:NE	2.48	0.47
1:A:1626:LEU:HD22	1:A:1698:ARG:HB2	1.96	0.47
1:A:2065:LYS:N	1:A:2065:LYS:HD2	2.29	0.47
1:B:1063:THR:HG23	1:B:1075:LEU:HD21	1.95	0.47
1:B:1381:VAL:HG13	1:B:1382:TYR:N	2.30	0.47
1:B:1621:LEU:HD23	1:B:1643:PHE:HE2	1.74	0.47
1:C:599:LEU:HB3	1:C:606:LEU:HD13	1.96	0.47
1:D:1318:GLN:OE1	1:D:1380:ASN:ND2	2.47	0.47
1:A:1975:LEU:HD22	1:A:2024:GLU:HB3	1.97	0.47
1:A:2172:PHE:HZ	1:A:2594:ILE:HG23	1.78	0.47
1:B:315:LEU:HD12	1:B:316:ALA:N	2.29	0.47
1:B:654:LYS:HE3	1:B:746:LEU:HD13	1.96	0.47
1:B:845:VAL:CG2	1:B:887:THR:HG23	2.45	0.47
1:D:405:ILE:HD11	1:D:416:MET:HA	1.95	0.47
1:D:2159:THR:HG21	1:D:2167:LYS:HB3	1.97	0.47
1:A:1028:ILE:HD13	1:A:1598:ILE:CD1	2.45	0.47
1:B:1290:LEU:HD21	1:B:1299:TYR:HB2	1.97	0.47
1:B:2320:PHE:O	1:B:2324:VAL:HG23	2.15	0.47
1:C:1502:LEU:HD21	1:C:1548:ILE:HD11	1.96	0.47
1:C:1509:LEU:HD12	1:C:1514:LEU:CD2	2.45	0.47
1:D:451:MET:O	1:D:451:MET:HE3	2.14	0.47
1:D:1621:LEU:HD23	1:D:1643:PHE:CE2	2.50	0.47
1:A:297:ALA:HB3	1:A:380:PHE:CE1	2.50	0.47
1:C:2010:SER:O	1:C:2014:GLU:HG2	2.15	0.47
1:D:435:PRO:O	1:D:439:ILE:HD12	2.14	0.47
1:A:622:VAL:HG23	1:A:630:PHE:CB	2.45	0.46
1:A:893:ASP:OD1	1:A:1057:ARG:NH2	2.48	0.46
1:C:1495:GLN:HA	1:C:1498:VAL:HG22	1.97	0.46
1:C:2155:LEU:CD2	1:C:2178:LEU:HD21	2.45	0.46
1:D:497:MET:SD	1:D:497:MET:C	2.93	0.46
1:D:1388:THR:HG22	1:D:1421:TYR:CD1	2.50	0.46
1:D:1489:THR:O	1:D:1492:GLN:NE2	2.47	0.46
1:A:1866:SER:O	1:A:1869:ILE:HG22	2.15	0.46
1:B:1969:ILE:O	1:B:1973:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:LYS:O	1:C:816:ASP:OD1	2.33	0.46
1:D:997:GLU:N	1:D:997:GLU:OE1	2.48	0.46
1:D:1740:LEU:O	1:D:1744:THR:HG22	2.15	0.46
1:D:2476:VAL:O	1:D:2479:ILE:HG13	2.15	0.46
1:A:2382:LEU:HD11	1:B:2346:PHE:HE1	1.79	0.46
1:B:585:ILE:HD12	1:B:591:ALA:HB3	1.96	0.46
1:B:1444:PHE:CE1	1:B:1472:VAL:HG22	2.50	0.46
1:C:480:VAL:HG13	1:C:496:ILE:HG21	1.97	0.46
1:C:1799:GLU:C	1:C:1799:GLU:OE1	2.54	0.46
1:A:641:ASN:CG	1:A:641:ASN:O	2.53	0.46
1:A:1469:LEU:HD21	1:A:1513:TRP:HZ3	1.80	0.46
1:B:1621:LEU:HD13	1:B:1672:MET:SD	2.56	0.46
1:D:1333:VAL:HA	1:D:1368:LEU:HD21	1.97	0.46
1:A:1066:ASP:OD1	1:A:1067:TYR:N	2.48	0.46
1:B:997:GLU:HG2	1:B:1028:ILE:HD11	1.97	0.46
1:B:1373:ALA:O	1:B:1419:HIS:ND1	2.38	0.46
1:C:477:GLU:HA	1:C:493:VAL:HG11	1.98	0.46
1:C:745:TYR:CZ	1:C:789:ASP:OD1	2.68	0.46
1:B:301:ASN:OD1	1:B:302:GLY:N	2.49	0.46
1:C:1125:GLU:HA	1:C:1128:VAL:HG12	1.97	0.46
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.46	0.46
1:A:252:LEU:HD11	1:A:263:VAL:CG1	2.45	0.46
1:A:1914:MET:CE	1:A:1936:LEU:HD23	2.46	0.46
1:A:2369:ILE:HG23	1:A:2512:ILE:HG23	1.98	0.46
1:A:2536:THR:O	1:A:2536:THR:CG2	2.64	0.46
1:B:391:HIS:HB2	1:B:398:ILE:HD11	1.97	0.46
1:B:442:LEU:HD12	1:B:512:GLN:NE2	2.31	0.46
1:B:702:GLU:OE1	1:B:702:GLU:N	2.49	0.46
1:C:1697:ASN:O	1:C:1698:ARG:C	2.54	0.46
1:D:769:LEU:HB3	1:D:773:LEU:HD23	1.97	0.46
1:A:800:ALA:HB2	1:A:1199:ASN:OD1	2.15	0.46
1:A:1878:GLN:OE1	1:A:1939:GLN:NE2	2.44	0.46
1:B:780:LEU:O	1:B:784:VAL:HG23	2.15	0.46
1:C:242:ARG:HB2	1:C:432:VAL:HB	1.97	0.46
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.50	0.46
1:A:641:ASN:O	1:A:641:ASN:OD1	2.34	0.46
1:A:1979:SER:HA	1:A:1982:CYS:SG	2.55	0.46
1:A:2049:VAL:O	1:A:2053:ILE:HD12	2.15	0.46
1:C:612:LYS:HD2	1:C:613:THR:N	2.30	0.46
1:C:754:GLN:HB3	1:C:755:LEU:HD12	1.98	0.46
1:D:772:ASP:OD1	1:D:773:LEU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1400:VAL:HG21	1:D:1440:LEU:CD1	2.46	0.46
1:D:1505:THR:HG22	1:D:1526:ILE:HD13	1.97	0.46
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.15	0.46
1:B:239:ASP:O	1:B:285:VAL:HG12	2.16	0.46
1:B:282:LEU:CB	1:B:309:LEU:HD22	2.45	0.46
1:C:1189:MET:SD	1:C:1189:MET:C	2.95	0.46
1:D:885:THR:CG2	1:D:978:ILE:HD13	2.46	0.46
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.16	0.46
1:D:1919:THR:HG22	1:D:1924:LEU:HD23	1.98	0.46
1:A:1783:GLU:OE2	1:A:1899:THR:N	2.46	0.45
1:B:1469:LEU:HD21	1:B:1514:LEU:CD1	2.46	0.45
1:B:1961:THR:O	1:B:1961:THR:CG2	2.65	0.45
1:B:599:LEU:HB3	1:B:606:LEU:HD13	1.98	0.45
1:D:280:ASN:O	1:D:308:HIS:NE2	2.48	0.45
1:D:1741:ILE:HG21	1:D:1785:PHE:CE1	2.51	0.45
1:A:803:TRP:HA	1:A:806:ILE:HD12	1.98	0.45
1:A:1527:ARG:O	1:A:1531:MET:HG3	2.16	0.45
1:A:1948:CYS:SG	1:A:1959:ILE:HD12	2.56	0.45
1:C:1697:ASN:N	1:C:1697:ASN:OD1	2.48	0.45
1:D:536:VAL:HG12	1:D:537:ARG:N	2.32	0.45
1:D:599:LEU:HB3	1:D:606:LEU:HD13	1.99	0.45
1:D:1514:LEU:HD11	1:D:1518:HIS:HB2	1.97	0.45
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.30	0.45
1:B:585:ILE:HD11	1:B:592:GLU:HG3	1.98	0.45
1:B:1396:VAL:HG22	1:B:1413:TYR:CE1	2.52	0.45
1:C:582:GLN:O	1:C:585:ILE:HG22	2.16	0.45
1:C:1606:LEU:HD22	1:C:1609:LEU:HD12	1.98	0.45
1:A:580:MET:SD	1:A:581:MET:N	2.89	0.45
1:A:803:TRP:HB2	1:A:1099:ILE:HG12	1.97	0.45
1:A:1285:HIS:HD2	1:A:1289:LEU:HD23	1.81	0.45
1:A:1374:ALA:HA	1:A:1377:GLU:OE1	2.16	0.45
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.45
1:A:2546:ASP:OD1	1:A:2547:LYS:N	2.49	0.45
1:B:1381:VAL:HG13	1:B:1382:TYR:H	1.81	0.45
1:A:745:TYR:HA	1:A:748:ILE:HB	1.99	0.45
1:B:582:GLN:O	1:B:585:ILE:HG22	2.16	0.45
1:B:1225:LEU:O	1:B:1229:HIS:ND1	2.49	0.45
1:B:2476:VAL:O	1:B:2479:ILE:HG13	2.16	0.45
1:C:263:VAL:HG13	1:C:283:TRP:CZ2	2.52	0.45
1:A:473:ILE:HG23	1:A:555:LEU:HD11	1.99	0.45
1:A:789:ASP:C	1:A:789:ASP:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:ASP:C	1:A:984:ASP:OD1	2.55	0.45
1:A:2553:VAL:HG21	1:A:2609:SER:CB	2.47	0.45
1:B:1673:LEU:HD21	1:B:1728:LEU:HD22	1.97	0.45
1:C:1111:LYS:HG3	1:C:1200:MET:HE3	1.99	0.45
1:C:1503:GLN:HG2	1:C:1544:LEU:HD13	1.99	0.45
1:D:630:PHE:O	1:D:634:LEU:HG	2.16	0.45
1:D:1885:ASN:OD1	1:D:1888:LEU:HD23	2.16	0.45
1:A:842:ASN:O	1:A:845:VAL:HG12	2.17	0.45
1:A:1544:LEU:HA	1:A:1547:HIS:ND1	2.32	0.45
1:A:1902:ASN:ND2	1:A:1905:CYS:SG	2.90	0.45
1:B:1124:SER:HA	1:B:1127:TRP:CE2	2.50	0.45
1:B:1877:LEU:HD13	1:B:1947:TYR:OH	2.17	0.45
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.31	0.45
1:C:252:LEU:CD1	1:C:417:LEU:HD11	2.47	0.45
1:C:263:VAL:HG13	1:C:283:TRP:HZ2	1.82	0.45
1:C:2546:ASP:OD1	1:C:2546:ASP:C	2.55	0.45
1:D:1513:TRP:O	1:D:1513:TRP:CD2	2.70	0.45
1:D:1799:GLU:OE2	1:D:1799:GLU:O	2.34	0.45
1:D:2155:LEU:HD21	1:D:2178:LEU:HD11	1.99	0.45
1:A:240:VAL:HA	1:A:284:GLU:HA	1.98	0.45
1:A:1097:LEU:CD1	1:A:1595:LEU:HD22	2.45	0.45
1:A:1488:SER:O	1:A:1536:ARG:NH1	2.50	0.45
1:A:1518:HIS:O	1:A:1522:VAL:HG23	2.17	0.45
1:A:1648:ILE:HG23	1:A:1736:LEU:HD22	1.99	0.45
1:B:749:ASP:O	1:B:753:GLN:HG2	2.17	0.45
1:B:1206:MET:HB3	1:B:1232:LEU:HD21	1.99	0.45
1:C:250:LYS:HD3	1:C:267:THR:HG22	1.98	0.45
1:D:1894:CYS:O	1:D:1894:CYS:SG	2.74	0.45
1:A:300:TRP:CZ2	1:A:381:VAL:HG13	2.53	0.44
1:A:1974:ILE:HD11	1:A:1997:SER:CA	2.47	0.44
1:B:647:VAL:O	1:B:651:LEU:HD23	2.16	0.44
1:B:2468:HIS:CB	1:B:2479:ILE:HD13	2.47	0.44
1:D:1405:CYS:SG	1:D:1406:ILE:N	2.90	0.44
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.18	0.44
1:D:693:TRP:O	1:D:694:LEU:HD12	2.17	0.44
1:A:396:THR:HG21	1:A:419:THR:HB	1.99	0.44
1:A:871:ILE:HD11	1:A:884:LEU:HD21	1.98	0.44
1:C:1785:PHE:O	1:C:1788:VAL:HG22	2.17	0.44
1:D:406:ASP:OD1	1:D:406:ASP:N	2.50	0.44
1:D:1269:LEU:HD12	1:D:1305:THR:HG23	1.99	0.44
1:D:1895:GLN:NE2	1:D:1901:TYR:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:CYS:SG	1:B:747:ALA:HB2	2.57	0.44
1:C:1396:VAL:HG22	1:C:1413:TYR:CE1	2.53	0.44
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.18	0.44
1:D:1085:ARG:HB2	1:D:1610:VAL:HG22	1.98	0.44
1:A:719:ASN:ND2	1:A:722:ASP:OD1	2.50	0.44
1:A:1246:LEU:HD13	1:A:1267:ILE:HG12	1.98	0.44
1:A:1514:LEU:HD11	1:A:1518:HIS:HB3	1.99	0.44
1:A:1885:ASN:OD1	1:A:1888:LEU:HD23	2.18	0.44
1:B:1192:LYS:N	1:B:1192:LYS:HD3	2.33	0.44
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.47	0.44
1:D:308:HIS:ND1	1:D:311:THR:OG1	2.31	0.44
1:D:596:THR:HG21	1:D:633:TYR:HB3	1.99	0.44
1:D:1380:ASN:HB2	1:D:1383:THR:HG22	1.99	0.44
1:D:1457:LYS:O	1:D:1458:ARG:HB2	2.18	0.44
1:D:2162:ASP:OD1	1:D:2162:ASP:C	2.56	0.44
1:A:1525:CYS:O	1:A:1529:LEU:HG	2.17	0.44
1:A:1644:LEU:HD22	1:A:1731:GLU:HG3	2.00	0.44
1:B:536:VAL:HG12	1:B:537:ARG:N	2.33	0.44
1:C:1223:GLU:OE2	1:C:1227:TYR:CE2	2.71	0.44
1:C:1386:LYS:O	1:C:1390:LEU:HD13	2.16	0.44
1:C:2172:PHE:HZ	1:C:2594:ILE:HG23	1.83	0.44
1:D:621:LEU:HD12	1:D:622:VAL:N	2.32	0.44
1:A:477:GLU:HG3	1:A:493:VAL:HG11	1.99	0.44
1:A:1319:ASP:O	1:A:1323:THR:HG23	2.17	0.44
1:B:631:LEU:HD11	1:B:728:TYR:CD1	2.52	0.44
1:B:969:LEU:HD23	1:B:969:LEU:C	2.38	0.44
1:C:464:ILE:HG22	1:C:535:LEU:HD21	2.00	0.44
1:C:1345:LEU:O	1:C:1349:MET:HG3	2.17	0.44
1:C:1422:VAL:CG1	1:C:1478:ALA:HB1	2.48	0.44
1:A:352:TYR:HD2	1:A:419:THR:HG1	1.65	0.44
1:B:464:ILE:HG22	1:B:535:LEU:HD21	2.00	0.44
1:C:577:GLN:O	1:C:580:MET:N	2.47	0.44
1:C:1397:VAL:O	1:C:1401:THR:HG23	2.18	0.44
1:C:1418:ASN:O	1:C:1422:VAL:HB	2.18	0.44
1:D:1514:LEU:HD12	1:D:1515:GLN:N	2.33	0.44
1:A:840:TYR:HD2	1:A:863:VAL:HG11	1.83	0.44
1:A:1115:ASP:OD1	1:A:1115:ASP:C	2.56	0.44
1:A:1740:LEU:O	1:A:1744:THR:HG22	2.18	0.44
1:B:240:VAL:HA	1:B:284:GLU:HA	1.99	0.44
1:B:990:LEU:HD23	1:B:1092:PHE:CD1	2.53	0.44
1:B:1229:HIS:HA	1:B:1232:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2324:VAL:HA	1:B:2327:ILE:HD12	2.00	0.44
1:C:772:ASP:OD1	1:C:773:LEU:N	2.51	0.44
1:C:1372:LEU:HA	1:C:1375:CYS:SG	2.57	0.44
1:D:1284:GLN:HA	1:D:1287:VAL:HG22	2.00	0.44
1:D:1315:LYS:O	1:D:1319:ASP:OD2	2.36	0.44
1:D:2369:ILE:HG23	1:D:2512:ILE:HG23	2.00	0.44
1:A:1182:MET:O	1:A:1182:MET:SD	2.76	0.43
1:B:497:MET:HA	1:B:497:MET:CE	2.48	0.43
1:C:315:LEU:HD11	1:C:354:LEU:HD13	2.00	0.43
1:A:580:MET:SD	1:A:580:MET:C	2.97	0.43
1:A:621:LEU:HD12	1:A:622:VAL:N	2.33	0.43
1:A:836:PHE:CD1	1:A:836:PHE:C	2.89	0.43
1:A:1696:GLN:O	1:A:1697:ASN:CB	2.66	0.43
1:A:2476:VAL:HG22	1:A:2480:LEU:CD1	2.47	0.43
1:B:308:HIS:CE1	1:B:311:THR:HG23	2.53	0.43
1:B:1411:MET:HA	1:B:1471:VAL:HG21	2.00	0.43
1:C:1322:MET:HA	1:C:1322:MET:HE3	2.00	0.43
1:D:2294:ILE:O	1:D:2297:VAL:HG12	2.17	0.43
1:A:1117:LEU:HD11	1:A:1172:VAL:HG13	1.99	0.43
1:A:1284:GLN:HA	1:A:1287:VAL:HG22	2.00	0.43
1:A:1331:ASP:OD2	1:A:1331:ASP:N	2.50	0.43
1:A:1501:LEU:O	1:A:1501:LEU:HD23	2.17	0.43
1:C:596:THR:HG21	1:C:633:TYR:HD1	1.82	0.43
1:A:749:ASP:N	1:A:749:ASP:OD2	2.51	0.43
1:A:2339:LEU:CD1	1:D:2389:LEU:HD11	2.47	0.43
1:B:482:PHE:O	1:B:505:ARG:NH1	2.51	0.43
1:B:1123:LYS:CD	1:B:1126:LEU:HD13	2.48	0.43
1:B:1456:GLU:O	1:B:1458:ARG:NH1	2.51	0.43
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.19	0.43
1:C:1328:ALA:HB3	1:C:1332:VAL:HG21	1.98	0.43
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	2.01	0.43
1:C:2125:GLU:OE1	1:C:2563:HIS:NE2	2.51	0.43
1:D:578:PHE:O	1:D:581:MET:HB2	2.18	0.43
1:A:308:HIS:CE1	1:A:311:THR:HG23	2.53	0.43
1:A:828:ASN:OD1	1:A:829:LYS:N	2.52	0.43
1:A:1253:PHE:CE2	1:A:1267:ILE:HD11	2.53	0.43
1:A:1393:LEU:O	1:A:1397:VAL:HG23	2.18	0.43
1:A:1524:ALA:O	1:A:1528:THR:HG23	2.19	0.43
1:B:608:LYS:N	1:B:608:LYS:HD2	2.32	0.43
1:B:826:LYS:HD3	1:B:875:PHE:CD2	2.53	0.43
1:B:1123:LYS:HD2	1:B:1126:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1246:LEU:HD22	1:C:1253:PHE:CE2	2.53	0.43
1:C:1316:LYS:HD3	1:C:1316:LYS:N	2.34	0.43
1:D:1328:ALA:HB3	1:D:1332:VAL:CG2	2.47	0.43
1:D:1393:LEU:O	1:D:1397:VAL:HG23	2.18	0.43
1:D:2558:HIS:CE1	1:D:2563:HIS:ND1	2.87	0.43
1:A:722:ASP:HA	1:A:725:VAL:HG12	2.01	0.43
1:A:1120:MET:O	1:A:1127:TRP:NE1	2.52	0.43
1:A:1696:GLN:O	1:A:1697:ASN:HB3	2.18	0.43
1:C:1040:LYS:O	1:C:1041:THR:HG23	2.18	0.43
1:C:1530:ALA:O	1:C:1534:LYS:HG2	2.18	0.43
1:C:2215:ILE:HG21	1:C:2341:TYR:CD1	2.54	0.43
1:D:1648:ILE:CG2	1:D:1736:LEU:HD22	2.45	0.43
1:D:1871:GLN:HB3	1:D:1872:PRO:HD3	2.01	0.43
1:A:729:TYR:HE2	1:A:773:LEU:HD13	1.83	0.43
1:A:1616:VAL:HG21	1:A:1690:LEU:HD13	2.00	0.43
1:A:2187:LYS:O	1:A:2191:MET:HG3	2.18	0.43
1:A:2476:VAL:O	1:A:2479:ILE:HG13	2.18	0.43
1:B:240:VAL:CG2	1:B:439:ILE:HD11	2.49	0.43
1:B:405:ILE:HG22	1:B:414:ARG:HB2	2.00	0.43
1:B:867:ALA:O	1:B:871:ILE:HD12	2.19	0.43
1:B:2010:SER:O	1:B:2014:GLU:HG2	2.18	0.43
1:C:466:GLN:O	1:C:466:GLN:NE2	2.52	0.43
1:A:300:TRP:CD2	1:A:381:VAL:HG22	2.54	0.43
1:A:314:TYR:O	1:A:357:VAL:HG22	2.19	0.43
1:A:819:LEU:HD23	1:A:819:LEU:H	1.84	0.43
1:C:1421:TYR:HA	1:C:1424:THR:HG23	2.01	0.43
1:D:557:TYR:CE2	1:D:591:ALA:HA	2.53	0.43
1:A:482:PHE:HE2	1:A:509:MET:SD	2.42	0.43
1:A:1219:ALA:O	1:A:1222:MET:HG2	2.18	0.43
1:B:309:LEU:HD23	1:B:442:LEU:CD2	2.49	0.43
1:B:1975:LEU:HD11	1:B:2020:LEU:HD12	2.01	0.43
1:C:1536:ARG:O	1:C:1537:ALA:HB3	2.19	0.43
1:C:1741:ILE:HG21	1:C:1785:PHE:CE1	2.54	0.43
1:D:858:LYS:O	1:D:862:GLU:HG2	2.18	0.43
1:D:1626:LEU:HD11	1:D:1698:ARG:CB	2.49	0.43
1:A:1914:MET:HE1	1:A:1936:LEU:HD23	2.01	0.43
1:B:1895:GLN:N	1:B:1900:ASN:OD1	2.50	0.43
1:C:2476:VAL:O	1:C:2479:ILE:HG13	2.19	0.43
1:D:493:VAL:O	1:D:496:ILE:HG22	2.19	0.43
1:D:582:GLN:O	1:D:585:ILE:HG22	2.19	0.43
1:D:769:LEU:HD13	1:D:773:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1465:GLU:O	1:D:1469:LEU:HG	2.19	0.43
1:A:398:ILE:HD13	1:A:419:THR:HG22	2.01	0.42
1:A:1062:LEU:HD22	1:A:1070:LEU:HD21	2.01	0.42
1:C:1284:GLN:HA	1:C:1287:VAL:HG22	2.00	0.42
1:D:1530:ALA:O	1:D:1534:LYS:HG2	2.18	0.42
1:D:2491:PRO:O	1:D:2495:VAL:HG23	2.18	0.42
1:A:1971:THR:HG22	1:A:2000:LEU:HD11	2.01	0.42
1:B:760:ILE:HG21	1:B:781:MET:HB2	2.01	0.42
1:B:1979:SER:HA	1:B:1982:CYS:SG	2.58	0.42
1:C:622:VAL:HG23	1:C:630:PHE:HB2	2.01	0.42
1:A:1381:VAL:HA	1:A:1384:GLU:HB3	2.01	0.42
1:A:1523:GLU:HA	1:A:1551:MET:HE3	2.00	0.42
1:B:263:VAL:HG21	1:B:315:LEU:HD13	2.01	0.42
1:C:990:LEU:HG	1:C:1035:MET:HE1	2.01	0.42
1:C:2155:LEU:CD2	1:C:2178:LEU:HD11	2.50	0.42
1:C:2458:LEU:HD23	1:D:2220:ALA:HA	2.01	0.42
1:A:241:VAL:HA	1:A:434:VAL:HG23	2.01	0.42
1:A:482:PHE:O	1:A:505:ARG:NH1	2.52	0.42
1:B:2155:LEU:CD2	1:B:2178:LEU:HD21	2.49	0.42
1:C:572:GLU:OE2	1:C:573:HIS:N	2.53	0.42
1:C:1469:LEU:HD21	1:C:1513:TRP:CZ3	2.54	0.42
1:D:1407:THR:HG21	1:D:1464:LEU:HA	2.02	0.42
1:D:1785:PHE:O	1:D:1788:VAL:HG22	2.19	0.42
1:A:606:LEU:HD23	1:A:645:ILE:CD1	2.49	0.42
1:A:2320:PHE:O	1:A:2324:VAL:HG23	2.19	0.42
1:A:2390:PHE:HB2	1:A:2391:LEU:HD12	2.01	0.42
1:B:469:ARG:HD2	1:B:548:PRO:HB2	2.01	0.42
1:B:1502:LEU:HD13	1:B:1529:LEU:CD2	2.49	0.42
1:B:2020:LEU:HD21	1:B:2025:LEU:HD22	2.02	0.42
1:D:745:TYR:HA	1:D:748:ILE:HB	2.02	0.42
1:D:1001:VAL:HG12	1:D:1002:PHE:CD1	2.54	0.42
1:D:1273:GLN:NE2	1:D:1277:GLU:OE2	2.53	0.42
1:D:1396:VAL:HG11	1:D:1417:VAL:CG2	2.49	0.42
1:A:1469:LEU:HD21	1:A:1513:TRP:CZ3	2.53	0.42
1:B:518:VAL:HG13	1:B:556:CYS:HB3	2.01	0.42
1:B:753:GLN:HA	1:B:753:GLN:OE1	2.20	0.42
1:B:1044:MET:SD	1:B:1044:MET:N	2.76	0.42
1:C:1182:MET:HE2	1:C:1182:MET:O	2.20	0.42
1:C:1380:ASN:HB2	1:C:1383:THR:HG22	2.02	0.42
1:C:1919:THR:CG2	1:C:1924:LEU:HD23	2.46	0.42
1:D:1438:TRP:CE3	1:D:1497:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ILE:HD13	1:A:974:ILE:HG23	2.02	0.42
1:A:1737:VAL:HG11	1:A:1757:ALA:HB2	2.01	0.42
1:B:1529:LEU:HD23	1:B:1529:LEU:C	2.40	0.42
1:B:1924:LEU:N	1:B:1924:LEU:HD22	2.35	0.42
1:D:1253:PHE:CE1	1:D:1263:THR:HG21	2.55	0.42
1:D:451:MET:O	1:D:451:MET:CE	2.67	0.42
1:D:1513:TRP:O	1:D:1513:TRP:CG	2.73	0.42
1:D:1733:ALA:O	1:D:1737:VAL:HG23	2.20	0.42
1:D:2175:SER:HA	1:D:2178:LEU:HD12	2.02	0.42
1:A:1126:LEU:HD12	1:A:1126:LEU:N	2.35	0.42
1:B:519:PHE:HA	1:B:522:LEU:HD12	2.02	0.42
1:C:1929:ILE:HD12	1:C:1978:ILE:HD12	2.01	0.42
1:D:622:VAL:HG23	1:D:630:PHE:HB2	2.02	0.42
1:D:885:THR:HG23	1:D:978:ILE:HD13	2.01	0.42
1:D:1741:ILE:HG23	1:D:1750:PHE:HE1	1.85	0.42
1:A:840:TYR:O	1:A:844:VAL:HG23	2.20	0.42
1:A:1169:TYR:N	1:A:1169:TYR:CD2	2.87	0.42
1:A:2485:LYS:HB2	1:B:2460:MET:CE	2.50	0.42
1:B:505:ARG:O	1:B:509:MET:HG2	2.20	0.42
1:B:518:VAL:HG13	1:B:556:CYS:SG	2.59	0.42
1:B:1981:LEU:HD12	1:B:1981:LEU:O	2.20	0.42
1:C:1201:ASP:HA	1:C:1203:HIS:CE1	2.54	0.42
1:D:483:VAL:HG22	1:D:509:MET:CE	2.50	0.42
1:D:522:LEU:HD21	1:D:556:CYS:HB2	2.01	0.42
1:D:769:LEU:HD13	1:D:773:LEU:HD21	2.02	0.42
1:D:2290:LEU:HD11	1:D:2331:VAL:HG23	2.01	0.42
1:A:702:GLU:OE2	1:A:702:GLU:N	2.53	0.41
1:B:522:LEU:HD22	1:B:557:TYR:CE1	2.54	0.41
1:C:1336:TYR:HB2	1:C:1345:LEU:HD22	2.02	0.41
1:C:2558:HIS:CE1	1:C:2563:HIS:ND1	2.88	0.41
1:D:494:LEU:HD21	1:D:554:ARG:HD2	2.01	0.41
1:D:2199:ARG:HG3	1:D:2199:ARG:HH11	1.85	0.41
1:A:611:THR:HG22	1:A:613:THR:H	1.84	0.41
1:A:1323:THR:O	1:A:1327:ASN:OD1	2.38	0.41
1:B:1435:ASN:HA	1:B:1438:TRP:CD1	2.55	0.41
1:B:2155:LEU:HD22	1:B:2178:LEU:HD21	2.02	0.41
1:C:619:VAL:O	1:C:622:VAL:HG12	2.19	0.41
1:C:1111:LYS:HG3	1:C:1200:MET:CE	2.50	0.41
1:C:1476:ILE:HG22	1:C:1480:PHE:CE2	2.55	0.41
1:D:1455:ARG:HG3	1:D:1513:TRP:NE1	2.34	0.41
1:A:1492:GLN:OE1	1:A:1493:THR:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HG22	1:B:414:ARG:CB	2.51	0.41
1:B:518:VAL:HG11	1:B:560:LEU:HG	2.02	0.41
1:C:1316:LYS:O	1:C:1320:MET:HG2	2.21	0.41
1:C:1322:MET:CE	1:C:1375:CYS:SG	3.08	0.41
1:A:266:ARG:NH1	1:A:267:THR:O	2.53	0.41
1:A:315:LEU:HD12	1:A:316:ALA:N	2.35	0.41
1:A:1258:LEU:HD12	1:A:1259:LEU:HD23	2.03	0.41
1:B:1253:PHE:O	1:B:1264:MET:HE2	2.20	0.41
1:A:1741:ILE:HG23	1:A:1750:PHE:HE1	1.86	0.41
1:A:2184:TRP:CZ3	1:A:2307:PHE:HZ	2.37	0.41
1:B:1333:VAL:HA	1:B:1368:LEU:HD21	2.02	0.41
1:C:401:THR:HG22	1:C:403:VAL:H	1.85	0.41
1:C:871:ILE:HD13	1:C:974:ILE:HG23	2.03	0.41
1:C:1937:VAL:CG1	1:C:1992:LEU:HD11	2.50	0.41
1:D:1731:GLU:OE1	1:D:1731:GLU:HA	2.20	0.41
1:D:2178:LEU:O	1:D:2182:MET:HG3	2.20	0.41
1:A:798:LYS:HA	1:A:798:LYS:HE2	2.03	0.41
1:A:1751:GLN:HG2	1:A:1869:ILE:HD13	2.02	0.41
1:B:240:VAL:HG11	1:B:309:LEU:HD11	2.03	0.41
1:B:267:THR:N	1:B:413:ILE:O	2.52	0.41
1:B:975:LEU:O	1:B:979:LEU:HD23	2.20	0.41
1:B:1307:ILE:HD12	1:B:1371:LEU:HD12	2.03	0.41
1:C:743:ARG:NH1	1:C:788:ARG:O	2.54	0.41
1:C:1223:GLU:OE2	1:C:1227:TYR:CZ	2.74	0.41
1:C:1349:MET:HE2	1:C:1406:ILE:H	1.85	0.41
1:D:462:GLY:O	1:D:535:LEU:HD13	2.21	0.41
1:D:522:LEU:HD23	1:D:553:PHE:HD1	1.85	0.41
1:D:557:TYR:HE2	1:D:591:ALA:HA	1.85	0.41
1:D:1931:GLU:O	1:D:1934:VAL:HG12	2.21	0.41
1:A:451:MET:SD	1:A:451:MET:N	2.94	0.41
1:A:839:ASP:OD1	1:A:839:ASP:N	2.53	0.41
1:A:1124:SER:HA	1:A:1127:TRP:HE1	1.84	0.41
1:A:1533:ALA:HA	1:A:1538:ILE:HD11	2.01	0.41
1:B:558:ARG:HD3	1:B:590:LEU:HD23	2.02	0.41
1:B:841:LEU:HB3	1:B:887:THR:HG21	2.01	0.41
1:B:1227:TYR:HA	1:B:1230:GLN:OE1	2.20	0.41
1:B:1741:ILE:HG21	1:B:1785:PHE:CE1	2.56	0.41
1:B:2267:ALA:HA	1:B:2270:LEU:HD12	2.02	0.41
1:B:2553:VAL:HG21	1:B:2609:SER:HB3	2.02	0.41
1:C:554:ARG:O	1:C:558:ARG:HG2	2.20	0.41
1:C:775:ALA:HB1	1:C:862:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ALA:O	1:D:391:HIS:NE2	2.50	0.41
1:D:451:MET:CE	1:D:472:VAL:HG22	2.51	0.41
1:D:834:MET:CE	1:D:876:TYR:CZ	3.04	0.41
1:D:2295:VAL:O	1:D:2298:VAL:HG22	2.19	0.41
1:A:606:LEU:HD23	1:A:645:ILE:HD13	2.02	0.41
1:A:1746:ASN:HB3	1:A:1749:ILE:HD12	2.01	0.41
1:B:709:ARG:HB2	1:B:709:ARG:NH1	2.36	0.41
1:C:1221:MET:O	1:C:1221:MET:SD	2.79	0.41
1:C:1250:LEU:O	1:C:1250:LEU:HD23	2.20	0.41
1:C:1502:LEU:CD2	1:C:1548:ILE:HD11	2.51	0.41
1:D:590:LEU:N	1:D:590:LEU:HD12	2.35	0.41
1:D:1332:VAL:HG23	1:D:1333:VAL:HG13	2.03	0.41
1:A:1491:LEU:HD22	1:A:1536:ARG:HG3	2.02	0.41
1:A:1587:ASP:HB2	1:A:1590:ASN:HB3	2.03	0.41
1:B:798:LYS:HD3	1:B:798:LYS:N	2.36	0.41
1:B:972:LEU:HD11	1:B:1062:LEU:CD1	2.50	0.41
1:B:1655:MET:HG3	1:B:1749:ILE:HD13	2.01	0.41
1:C:241:VAL:HA	1:C:434:VAL:HG23	2.02	0.41
1:C:1422:VAL:HG11	1:C:1478:ALA:HB1	2.02	0.41
1:C:1462:PRO:O	1:C:1466:LYS:HG2	2.21	0.41
1:C:1469:LEU:O	1:C:1473:LEU:HB3	2.21	0.41
1:C:1915:CYS:HB3	1:C:1925:LEU:HD11	2.02	0.41
1:C:1957:THR:OG1	1:C:2007:ARG:NH2	2.54	0.41
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.54	0.41
1:A:585:ILE:HD11	1:A:592:GLU:HG3	2.01	0.41
1:B:1120:MET:SD	1:B:1127:TRP:CE2	3.14	0.41
1:B:1393:LEU:CD2	1:B:1417:VAL:HG22	2.50	0.41
1:C:554:ARG:HD3	1:C:590:LEU:HD13	2.03	0.41
1:C:1247:HIS:CD2	1:C:1274:LEU:HD22	2.56	0.41
1:C:1771:SER:O	1:C:1775:LEU:HG	2.21	0.41
1:A:698:ASP:OD1	1:A:699:LYS:N	2.52	0.40
1:B:1258:LEU:O	1:B:1262:GLU:HG3	2.21	0.40
1:B:1960:VAL:HG11	1:B:2012:ASN:HD22	1.86	0.40
1:B:2571:PHE:O	1:B:2575:VAL:HG23	2.21	0.40
1:C:1477:ASN:O	1:C:1481:SER:OG	2.30	0.40
1:D:581:MET:HE2	1:D:581:MET:HB3	2.02	0.40
1:D:1044:MET:SD	1:D:1044:MET:N	2.88	0.40
1:D:1391:LEU:HD12	1:D:1392:PRO:HD2	2.04	0.40
1:B:242:ARG:HB2	1:B:432:VAL:HB	2.03	0.40
1:B:1092:PHE:HA	1:B:1095:VAL:HG23	2.02	0.40
1:B:1502:LEU:HD21	1:B:1548:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1527:ARG:O	1:B:1531:MET:HG3	2.21	0.40
1:B:2279:GLY:O	1:B:2283:ASN:OD1	2.39	0.40
1:C:1588:TYR:O	1:C:1592:ILE:HD12	2.22	0.40
1:C:2131:ARG:HH11	1:C:2131:ARG:HG2	1.86	0.40
1:D:788:ARG:HG2	1:D:789:ASP:H	1.87	0.40
1:A:1644:LEU:HD22	1:A:1731:GLU:CG	2.50	0.40
1:A:2068:GLN:O	1:A:2072:LYS:HG3	2.22	0.40
1:B:505:ARG:O	1:B:509:MET:CE	2.70	0.40
1:B:1914:MET:HE3	1:B:1914:MET:HB2	2.00	0.40
1:C:1542:MET:C	1:C:1542:MET:SD	3.00	0.40
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	2.01	0.40
1:D:650:GLU:O	1:D:654:LYS:HG2	2.22	0.40
1:D:1906:GLU:HA	1:D:1906:GLU:OE1	2.21	0.40
1:A:735:LEU:O	1:A:739:MET:HG3	2.21	0.40
1:A:2294:ILE:O	1:A:2297:VAL:HG12	2.21	0.40
1:B:297:ALA:HB3	1:B:380:PHE:CE1	2.57	0.40
1:B:1428:MET:SD	1:B:1430:GLU:HB2	2.62	0.40
1:B:2475:GLY:N	1:B:2478:ASP:OD2	2.54	0.40
1:C:2478:ASP:OD1	1:C:2478:ASP:N	2.54	0.40
1:D:722:ASP:HA	1:D:725:VAL:HG12	2.03	0.40
1:D:1333:VAL:HA	1:D:1368:LEU:CD2	2.52	0.40
1:A:250:LYS:HE3	1:A:267:THR:HG22	2.00	0.40
1:A:1203:HIS:HD2	1:A:1204:LYS:N	2.20	0.40
1:A:1457:LYS:O	1:A:1458:ARG:HB2	2.22	0.40
1:A:1492:GLN:OE1	1:A:1493:THR:N	2.51	0.40
1:B:813:LYS:O	1:B:816:ASP:OD1	2.39	0.40
1:B:1595:LEU:O	1:B:1598:ILE:HG22	2.22	0.40
1:C:1310:GLU:O	1:C:1310:GLU:CG	2.69	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	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	48	76
1	B	1959/2671 (73%)	1937 (99%)	22 (1%)	0	100	100
1	C	1979/2671 (74%)	1948 (98%)	31 (2%)	0	100	100
1	D	2010/2671 (75%)	1975 (98%)	35 (2%)	0	100	100
All	All	7909/10684 (74%)	7790 (98%)	118 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1697	ASN

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	1807/2385 (76%)	1760 (97%)	47 (3%)	41	66
1	B	1805/2385 (76%)	1758 (97%)	47 (3%)	41	66
1	C	1821/2385 (76%)	1803 (99%)	18 (1%)	73	84
1	D	1838/2385 (77%)	1811 (98%)	27 (2%)	60	77
All	All	7271/9540 (76%)	7132 (98%)	139 (2%)	52	72

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	PHE
1	A	319	GLU
1	A	405	ILE
1	A	463	PHE
1	A	497	MET
1	A	552	MET
1	A	567	TYR
1	A	580	MET
1	A	624	LYS
1	A	696	TRP

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Mol	Chain	Res	Type
1	A	732	GLN
1	A	801	ARG
1	A	836	PHE
1	A	839	ASP
1	A	1048	ASP
1	A	1120	MET
1	A	1127	TRP
1	A	1203	HIS
1	A	1214	TYR
1	A	1236	CYS
1	A	1249	HIS
1	A	1266	HIS
1	A	1299	TYR
1	A	1304	HIS
1	A	1335	PHE
1	A	1338	ASP
1	A	1458	ARG
1	A	1492	GLN
1	A	1542	MET
1	A	1547	HIS
1	A	1605	ARG
1	A	1644	LEU
1	A	1655	MET
1	A	1687	ARG
1	A	1698	ARG
1	A	1770	LYS
1	A	1799	GLU
1	A	1977	ASP
1	A	2009	ASP
1	A	2017	LEU
1	A	2027	ASP
1	A	2063	HIS
1	A	2129	GLN
1	A	2166	SER
1	A	2170	ASP
1	A	2208	SER
1	A	2318	MET
1	B	251	PHE
1	B	444	PHE
1	B	497	MET
1	B	527	ARG
1	B	567	TYR

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Mol	Chain	Res	Type
1	B	618	PHE
1	B	658	ASP
1	B	671	ARG
1	B	711	LEU
1	B	713	GLN
1	B	742	ASP
1	B	749	ASP
1	B	761	PHE
1	B	778	CYS
1	B	788	ARG
1	B	1035	MET
1	B	1057	ARG
1	B	1072	SER
1	B	1089	MET
1	B	1204	LYS
1	B	1235	PHE
1	B	1236	CYS
1	B	1272	TYR
1	B	1304	HIS
1	B	1402	HIS
1	B	1416	PHE
1	B	1428	MET
1	B	1438	TRP
1	B	1458	ARG
1	B	1621	LEU
1	B	1632	SER
1	B	1639	GLU
1	B	1676	LYS
1	B	1729	ASP
1	B	1739	ASP
1	B	1771	SER
1	B	1871	GLN
1	B	1894	CYS
1	B	1896	ASN
1	B	1982	CYS
1	B	2009	ASP
1	B	2019	SER
1	B	2166	SER
1	B	2170	ASP
1	B	2190	SER
1	B	2198	SER
1	B	2326	TYR

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Mol	Chain	Res	Type
1	C	420	CYS
1	C	567	TYR
1	C	612	LYS
1	C	632	ASP
1	C	682	TYR
1	C	749	ASP
1	C	1125	GLU
1	C	1189	MET
1	C	1200	MET
1	C	1316	LYS
1	C	1330	ASP
1	C	1458	ARG
1	C	1905	CYS
1	C	1977	ASP
1	C	2009	ASP
1	C	2190	SER
1	C	2340	PHE
1	C	2549	ASP
1	D	552	MET
1	D	567	TYR
1	D	722	ASP
1	D	778	CYS
1	D	832	ASN
1	D	894	CYS
1	D	1035	MET
1	D	1043	SER
1	D	1065	HIS
1	D	1066	ASP
1	D	1458	ARG
1	D	1470	SER
1	D	1551	MET
1	D	1578	ARG
1	D	1681	ASP
1	D	1685	GLN
1	D	1782	SER
1	D	1791	ASP
1	D	1894	CYS
1	D	1896	ASN
1	D	1965	ASN
1	D	2449	ASP
1	D	2460	MET
1	D	2461	CYS

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Mol	Chain	Res	Type
1	D	2531	GLU
1	D	2549	ASP
1	D	2576	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	779	HIS
1	A	1090	HIS
1	A	1094	GLN
1	A	1102	GLN
1	A	1285	HIS
1	A	1419	HIS
1	A	2292	ASN
1	B	512	GLN
1	B	649	GLN
1	B	783	HIS
1	B	785	HIS
1	B	1094	GLN
1	B	1622	HIS
1	B	1902	ASN
1	B	2292	ASN
1	C	791	GLN
1	C	1065	HIS
1	C	1622	HIS
1	C	2598	ASN
1	D	573	HIS
1	D	783	HIS
1	D	1061	HIS
1	D	1229	HIS
1	D	1285	HIS
1	D	1622	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.92	0
5	ATP	C	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
3	I3P	C	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
5	ATP	B	3004	-	28,33,33	0.62	0	34,52,52	0.86	1 (2%)
5	ATP	D	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0
5	ATP	A	3004	-	28,33,33	0.61	0	34,52,52	0.86	1 (2%)

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	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	2/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	0/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	4/18/38/38	0/3/3/3
5	ATP	D	3004	-	-	2/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	A	3004	-	-	5/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	C	3002	I3P	P5-O5	5.96	1.70	1.59
3	B	3002	I3P	P5-O5	5.94	1.69	1.59
3	D	3002	I3P	P5-O5	5.94	1.69	1.59
3	A	3002	I3P	P5-O5	5.94	1.69	1.59
3	D	3002	I3P	P1-O1	5.78	1.69	1.59
3	C	3002	I3P	P1-O1	5.72	1.69	1.59
3	B	3002	I3P	P1-O1	5.72	1.69	1.59
3	A	3002	I3P	P1-O1	5.71	1.69	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3004	ATP	C5-C6-N6	2.33	123.86	120.31
5	B	3004	ATP	C5-C6-N6	2.33	123.86	120.31
5	C	3004	ATP	C5-C6-N6	2.32	123.85	120.31
5	D	3004	ATP	C5-C6-N6	2.32	123.85	120.31

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	C3'-C4'-C5'-O5'
5	C	3004	ATP	C3'-C4'-C5'-O5'
3	D	3002	I3P	C6-C1-O1-P1
5	B	3004	ATP	PB-O3B-PG-O2G
5	A	3004	ATP	C5'-O5'-PA-O1A
5	A	3004	ATP	C5'-O5'-PA-O3A
3	B	3002	I3P	C6-C1-O1-P1
3	C	3002	I3P	C6-C1-O1-P1
5	C	3004	ATP	O4'-C4'-C5'-O5'
3	D	3002	I3P	C2-C1-O1-P1
5	B	3004	ATP	C3'-C4'-C5'-O5'
5	B	3004	ATP	PB-O3A-PA-O1A

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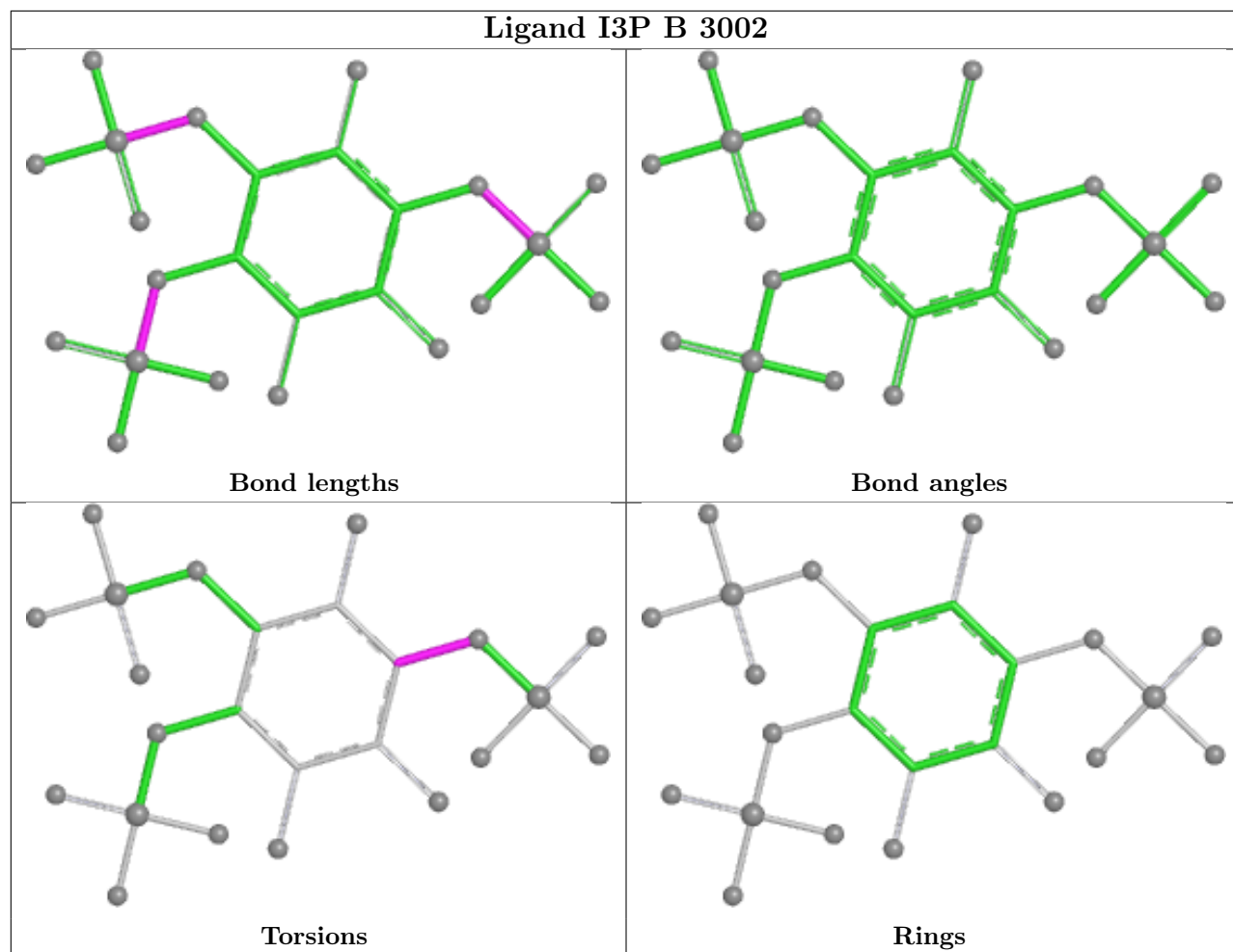
Mol	Chain	Res	Type	Atoms
5	B	3004	ATP	PB-O3A-PA-O2A

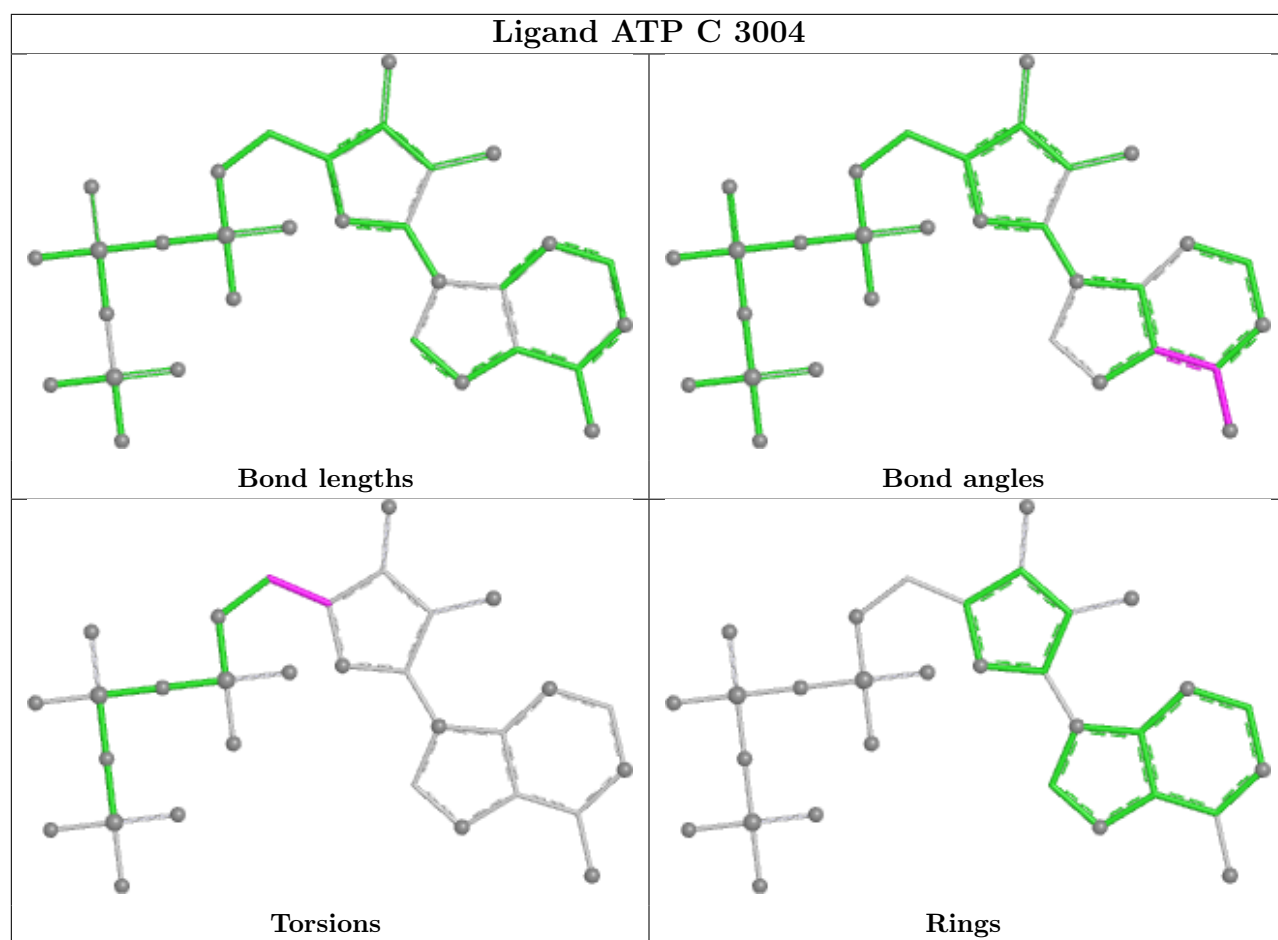
There are no ring outliers.

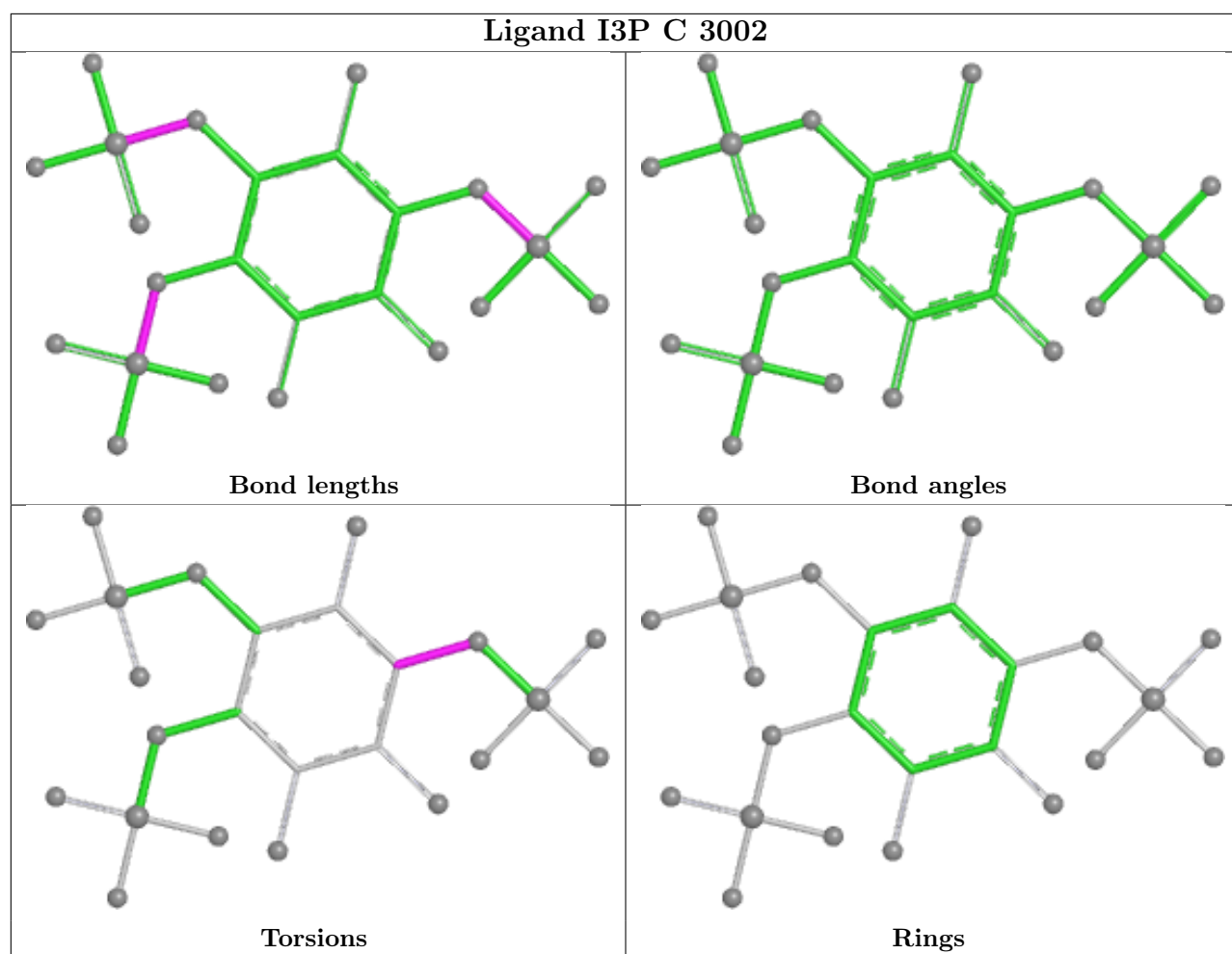
1 monomer is involved in 1 short contact:

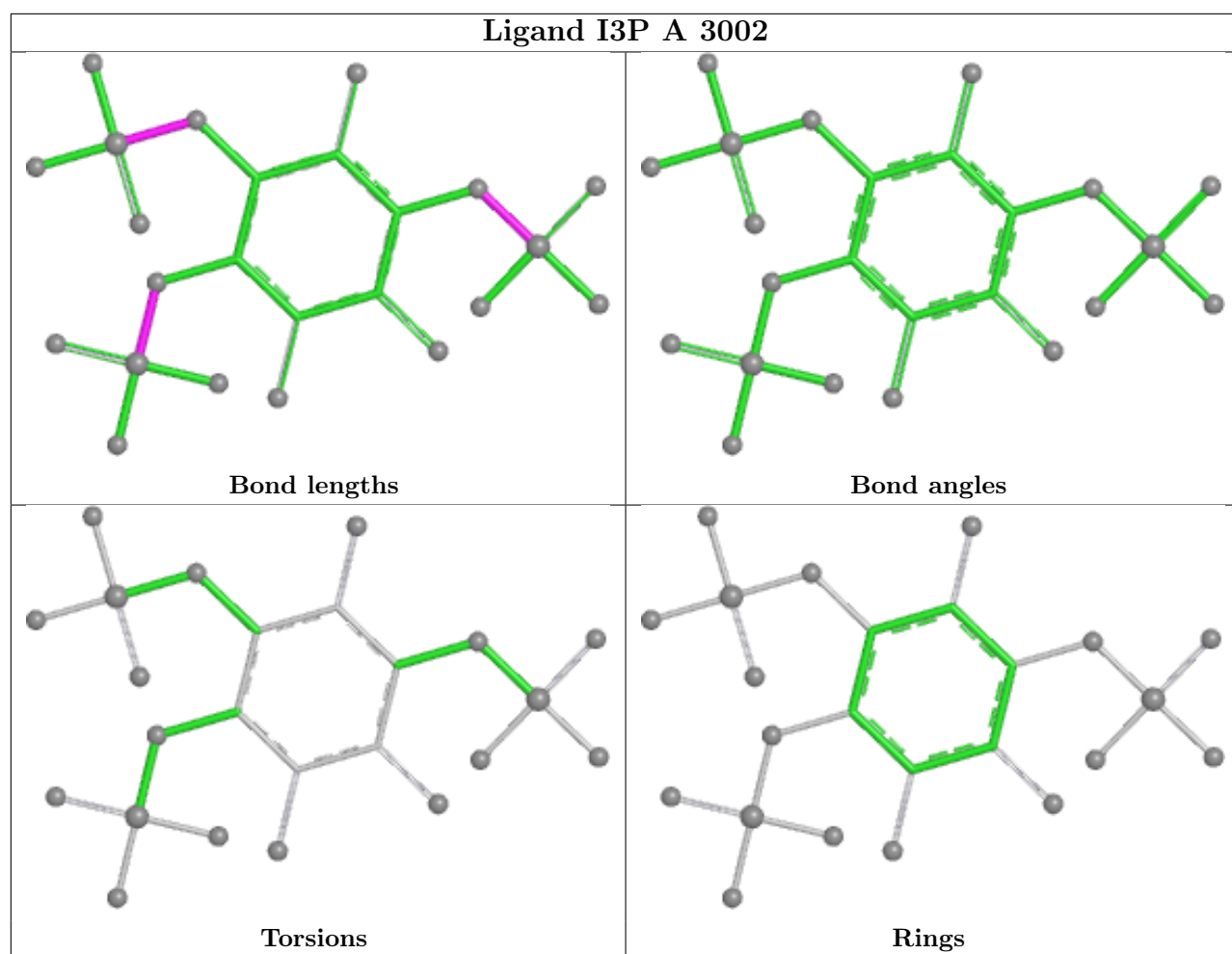
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	1	0

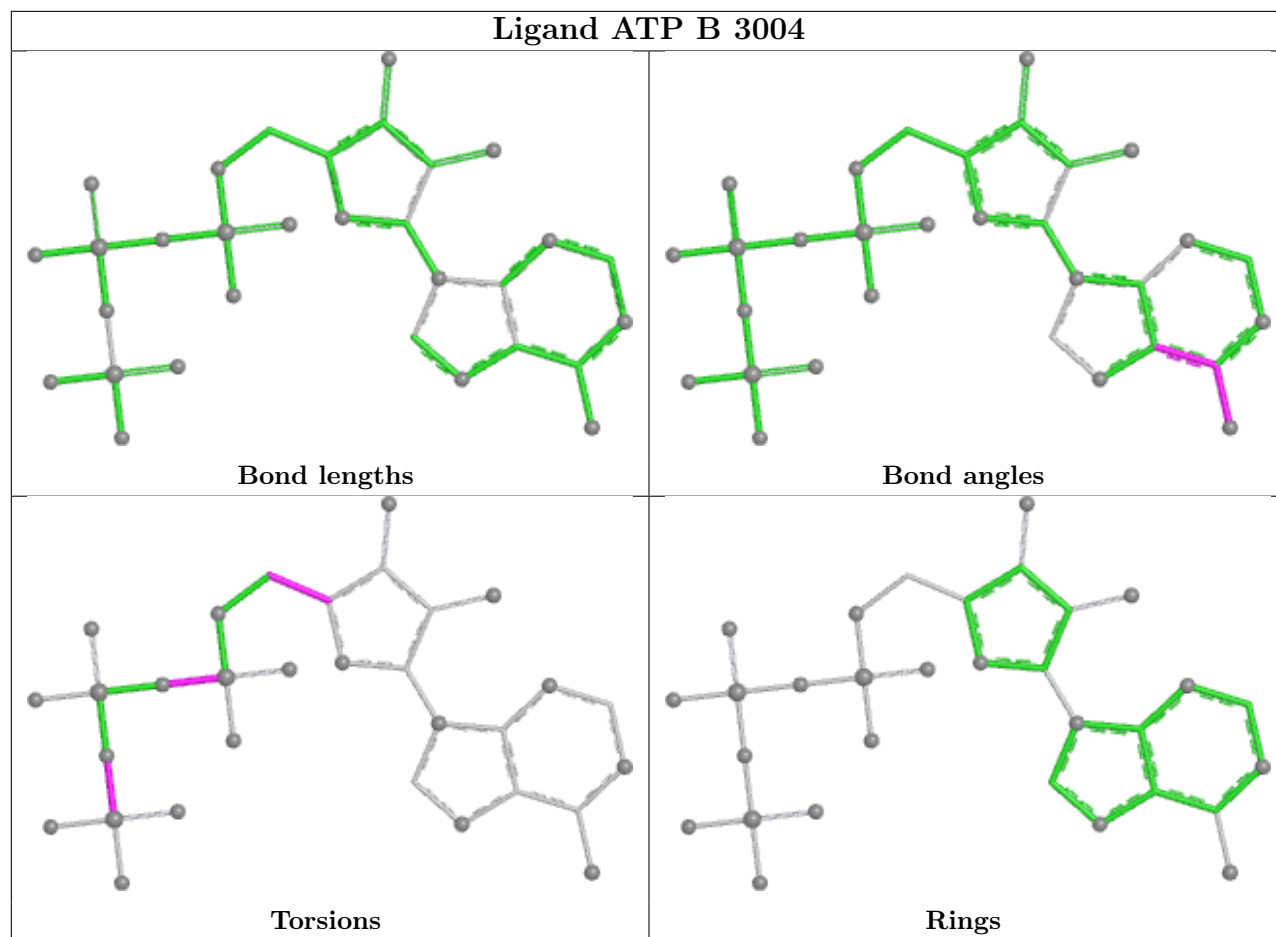
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

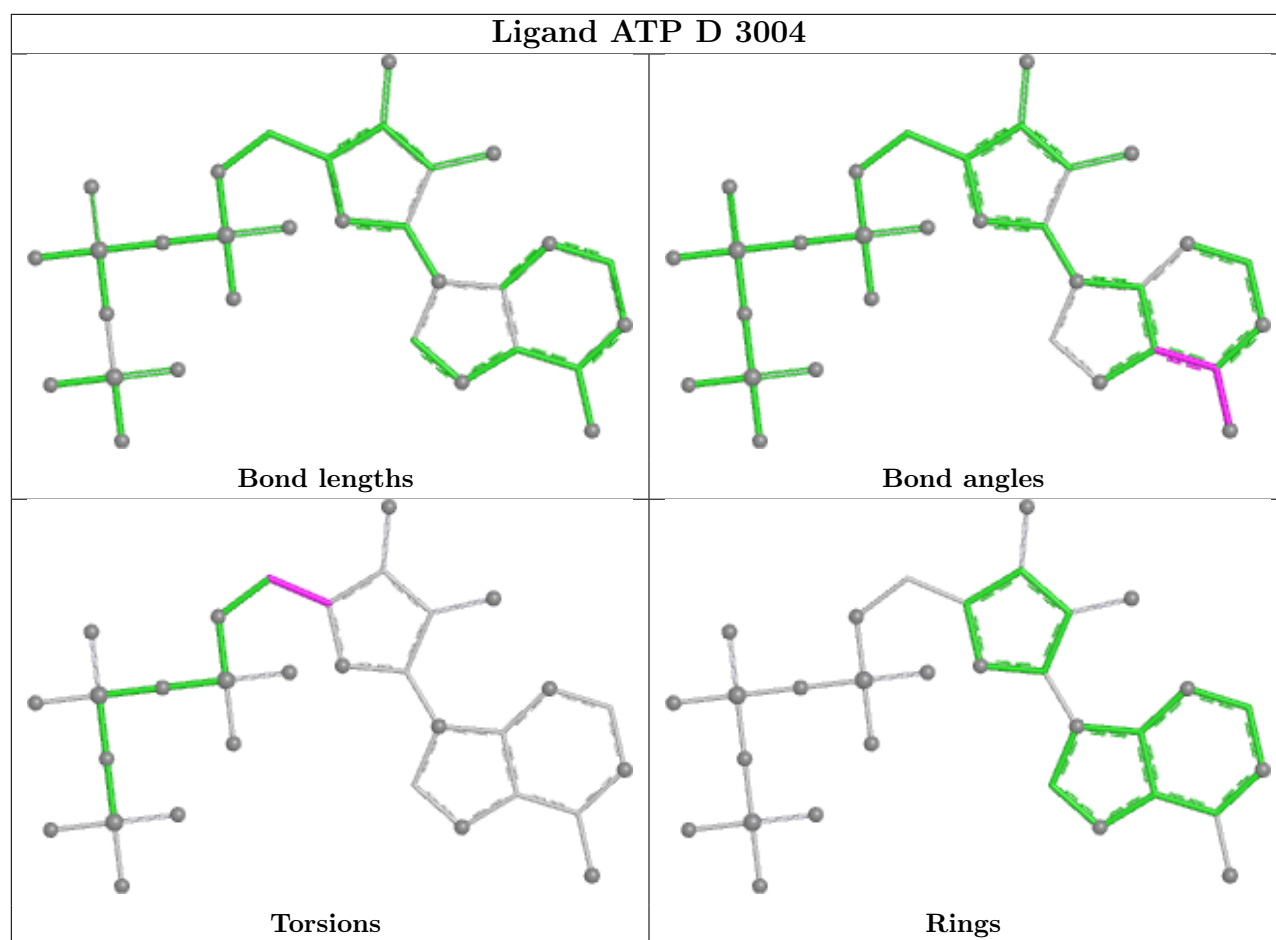


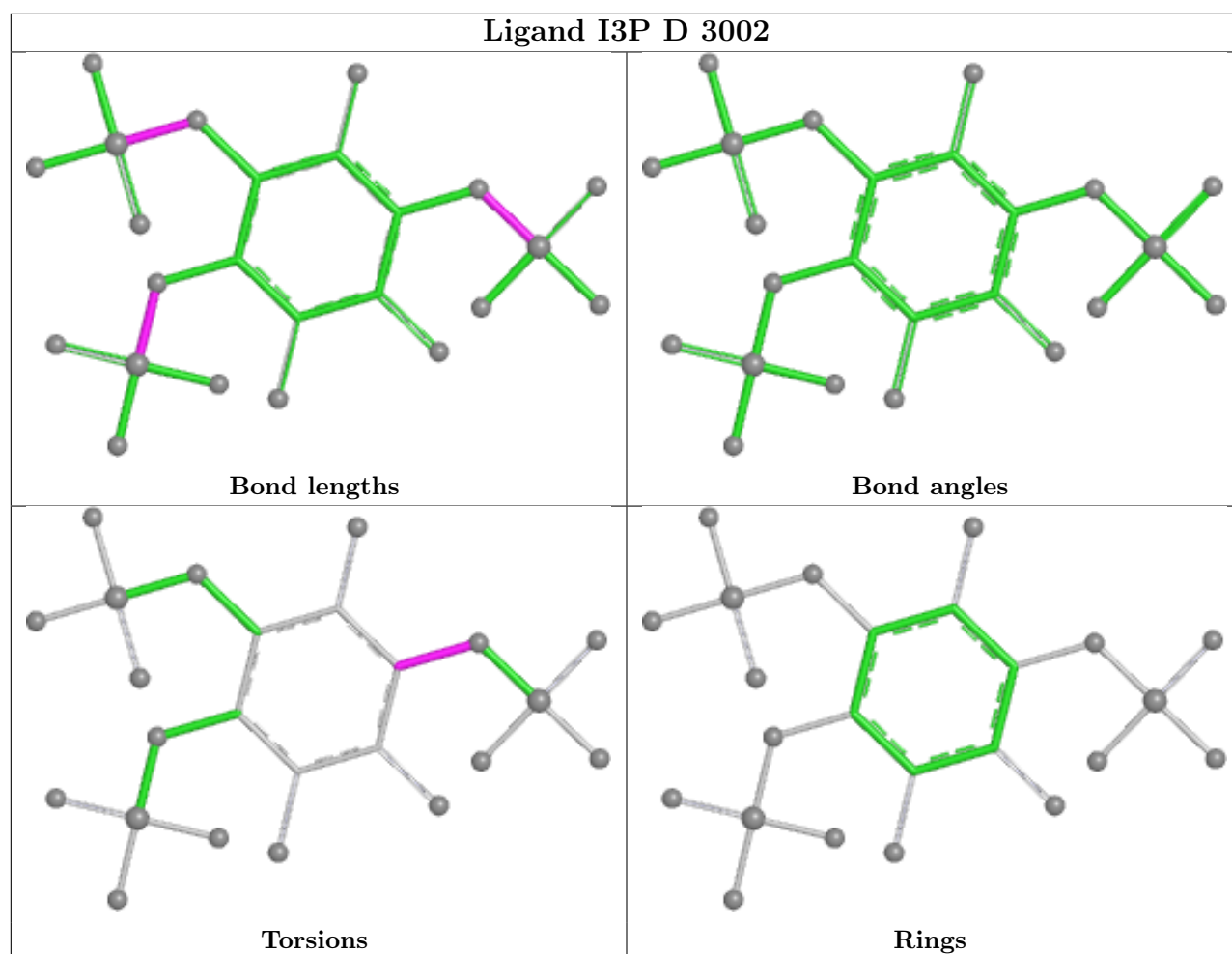


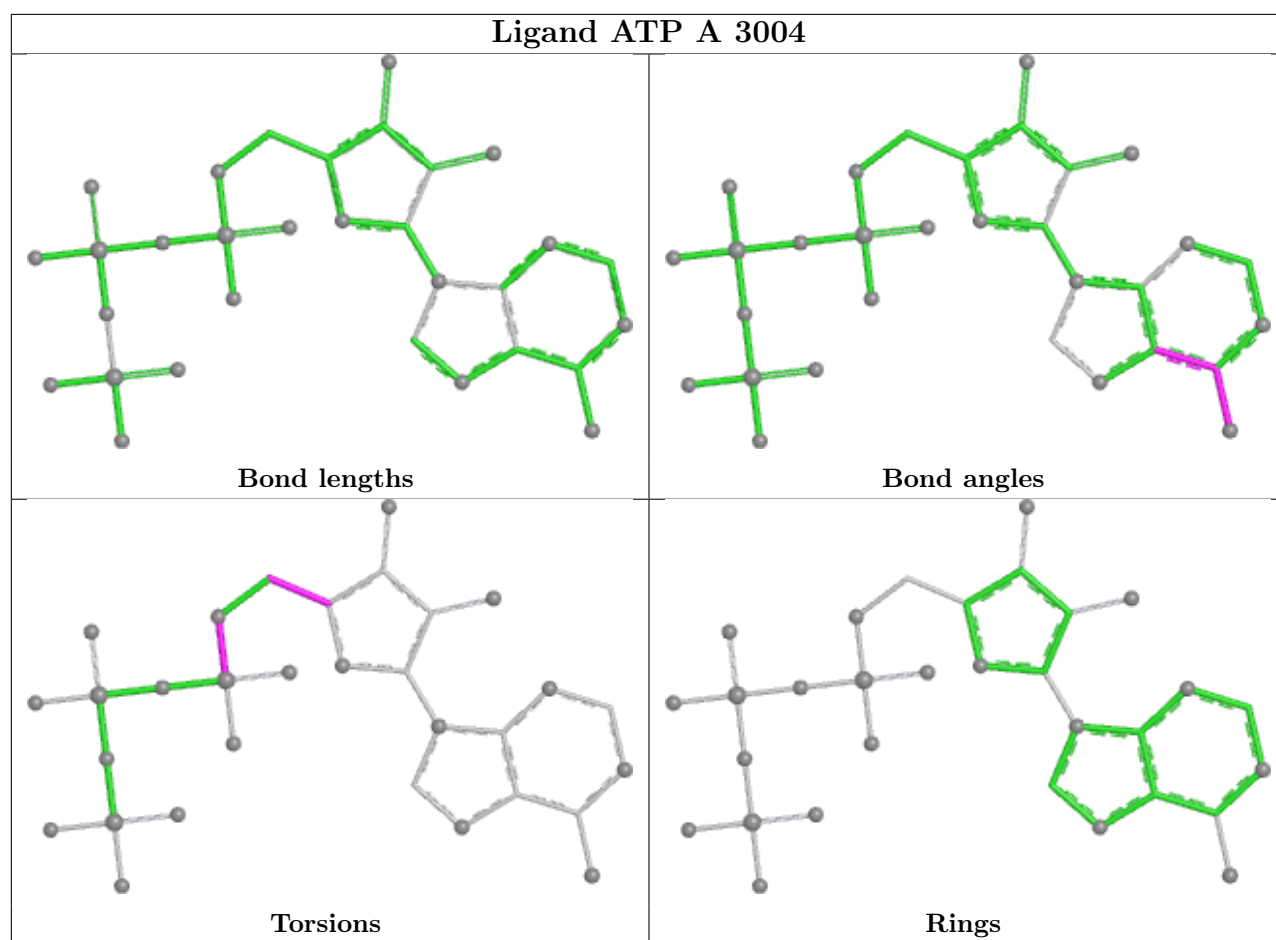












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

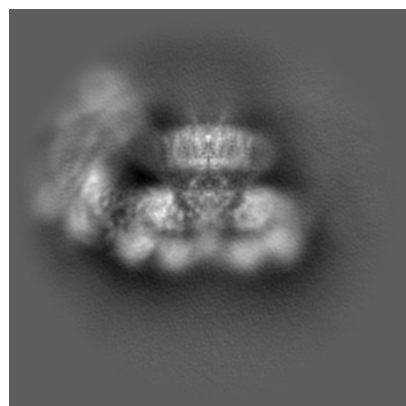
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41365. These allow visual inspection of the internal detail of the map and identification of artifacts.

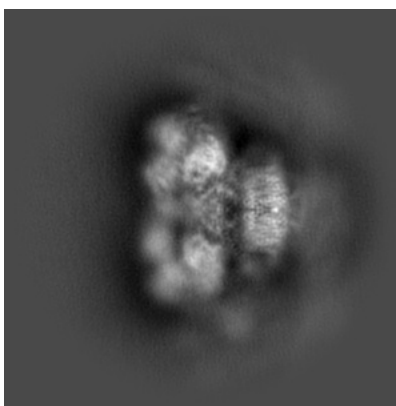
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

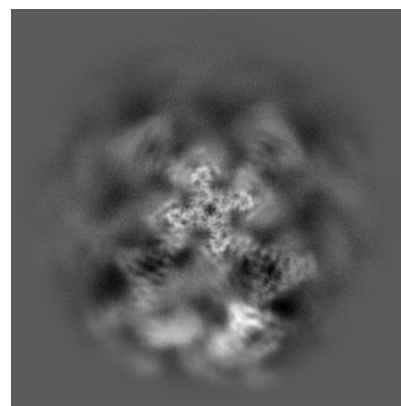
6.1.1 Primary map



X

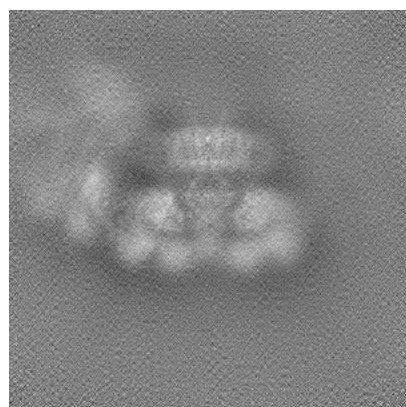


Y

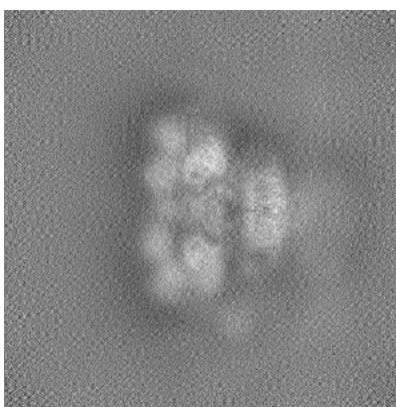


Z

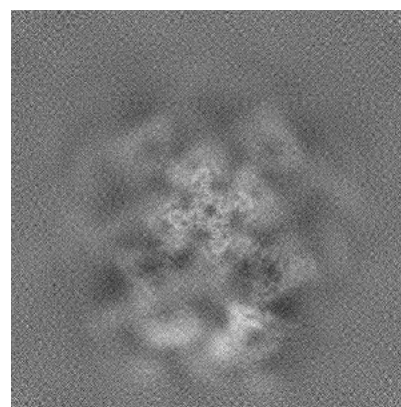
6.1.2 Raw map



X



Y

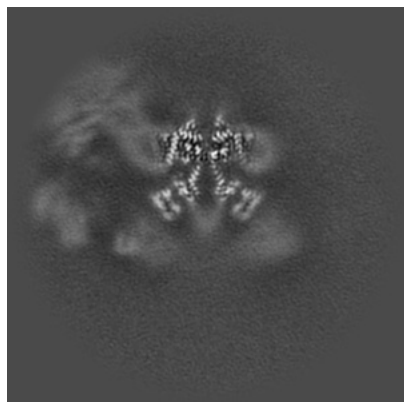


Z

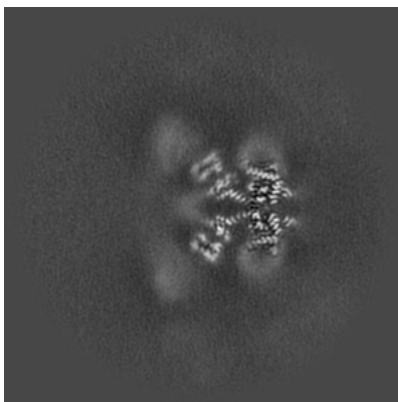
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

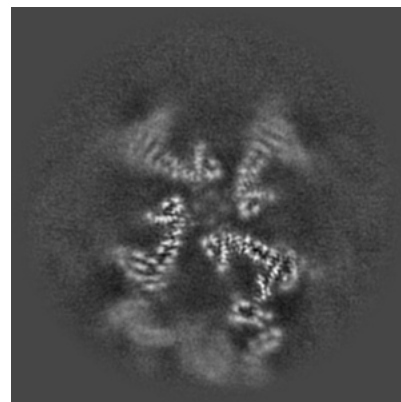
6.2.1 Primary map



X Index: 256

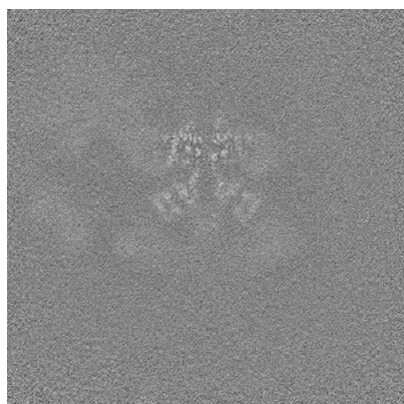


Y Index: 256



Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

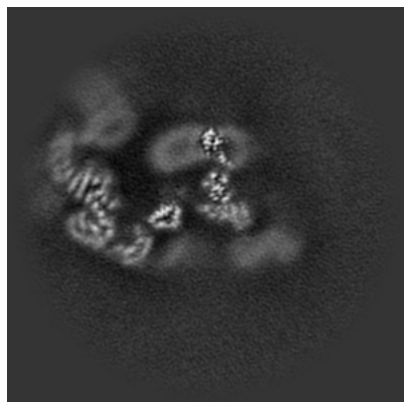


Z Index: 256

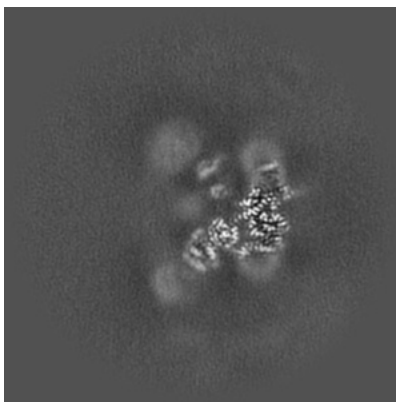
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

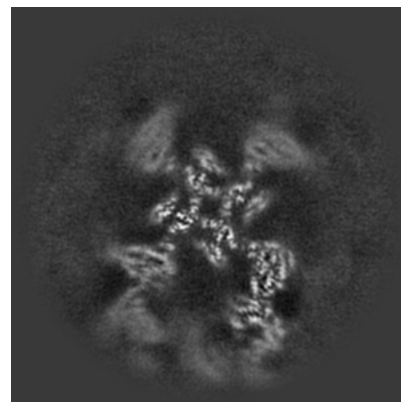
6.3.1 Primary map



X Index: 293

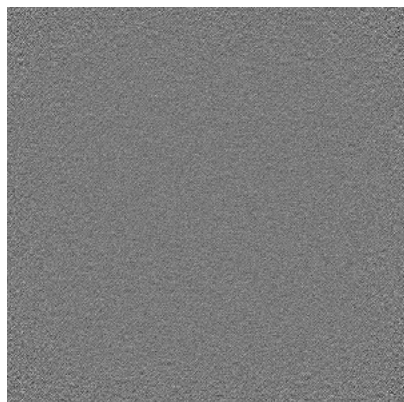


Y Index: 247

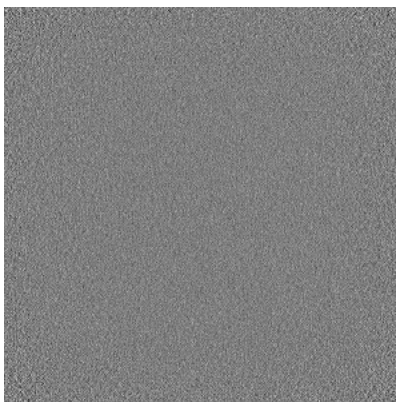


Z Index: 266

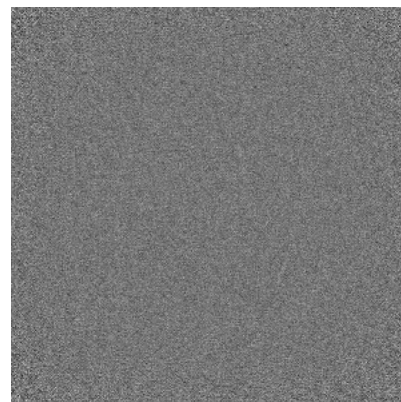
6.3.2 Raw map



X Index: 0



Y Index: 0

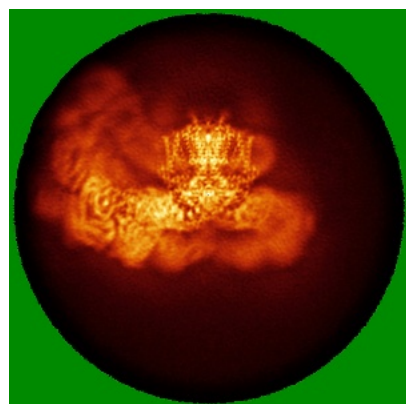


Z Index: 0

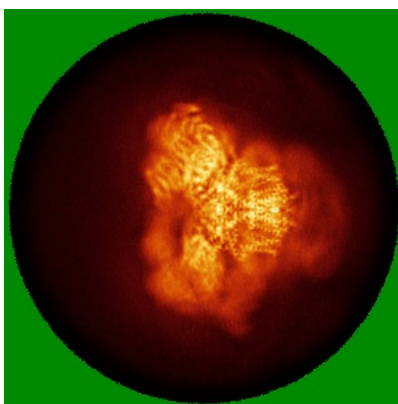
The images above show the largest variance slices of the map in three orthogonal directions.

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

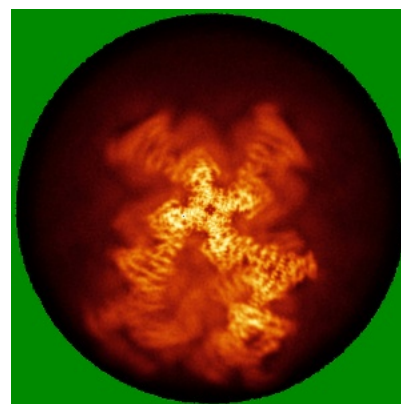
6.4.1 Primary map



X

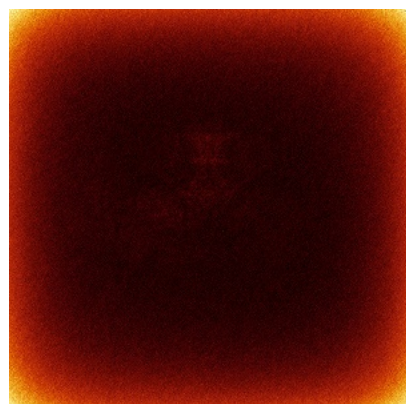


Y

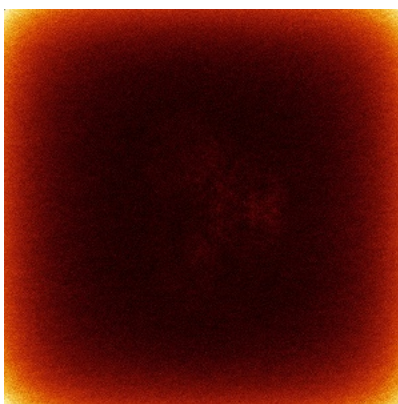


Z

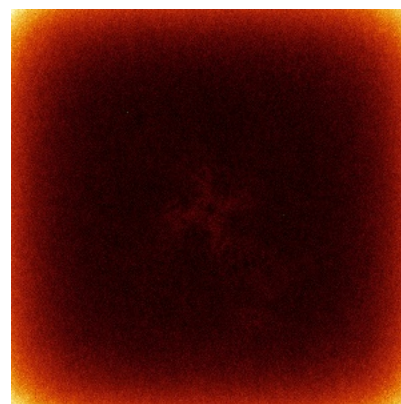
6.4.2 Raw map



X



Y

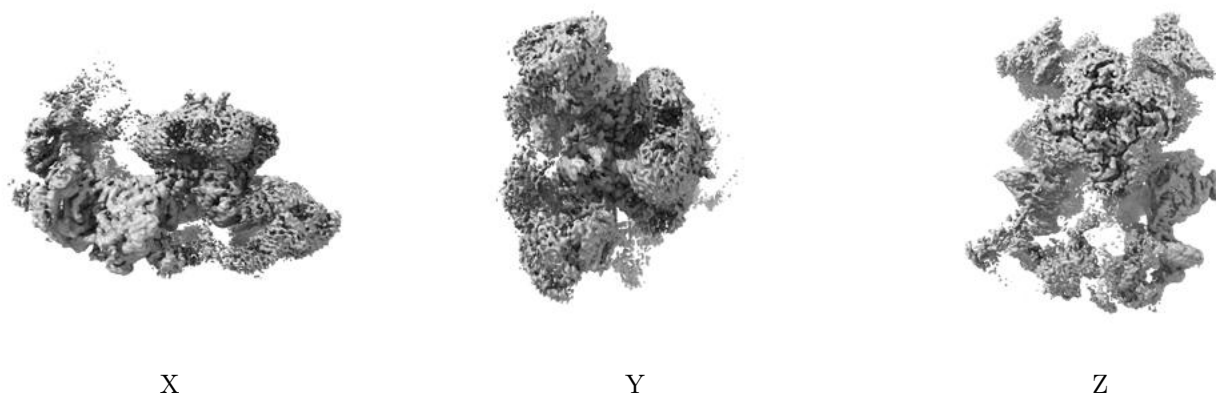


Z

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.

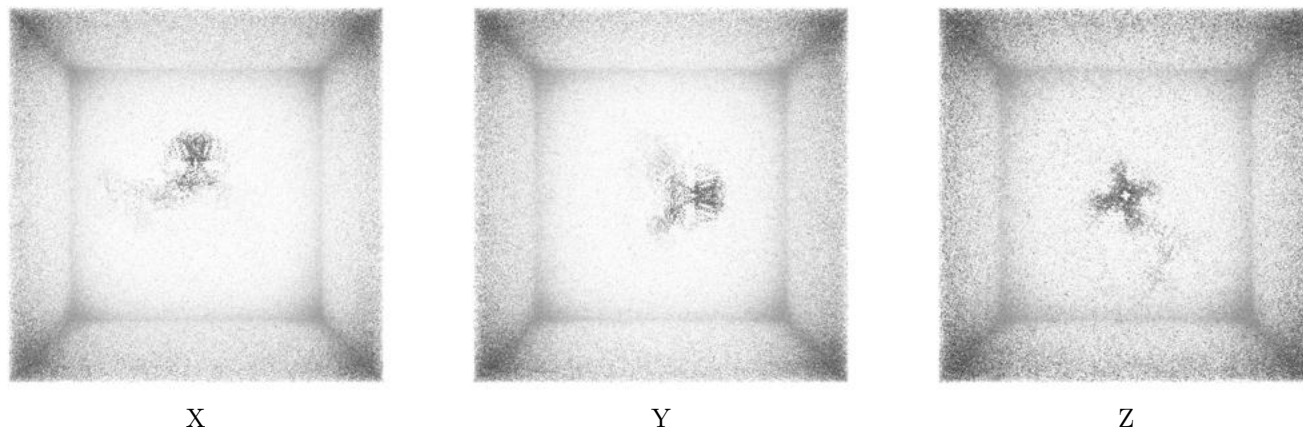
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

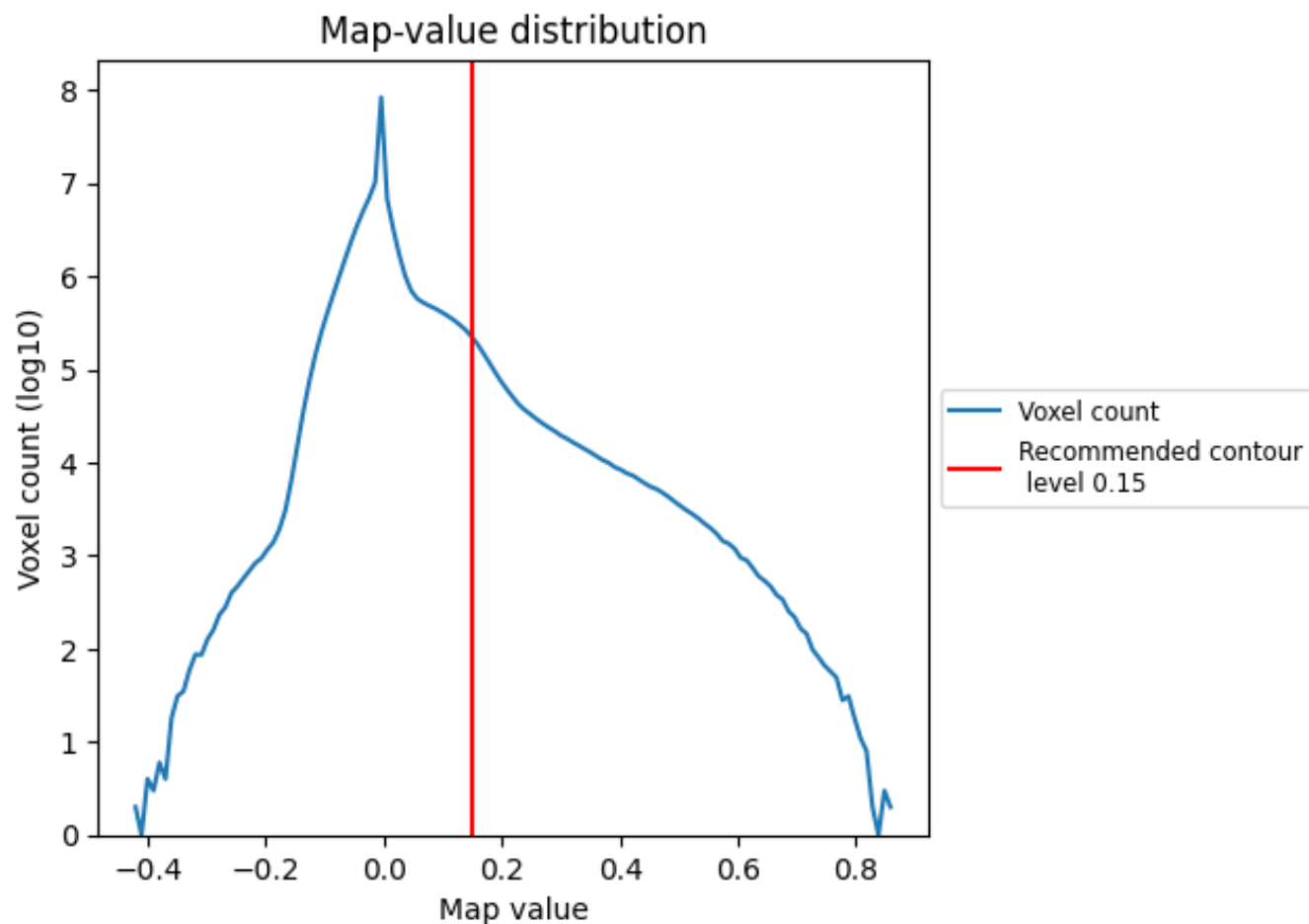
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

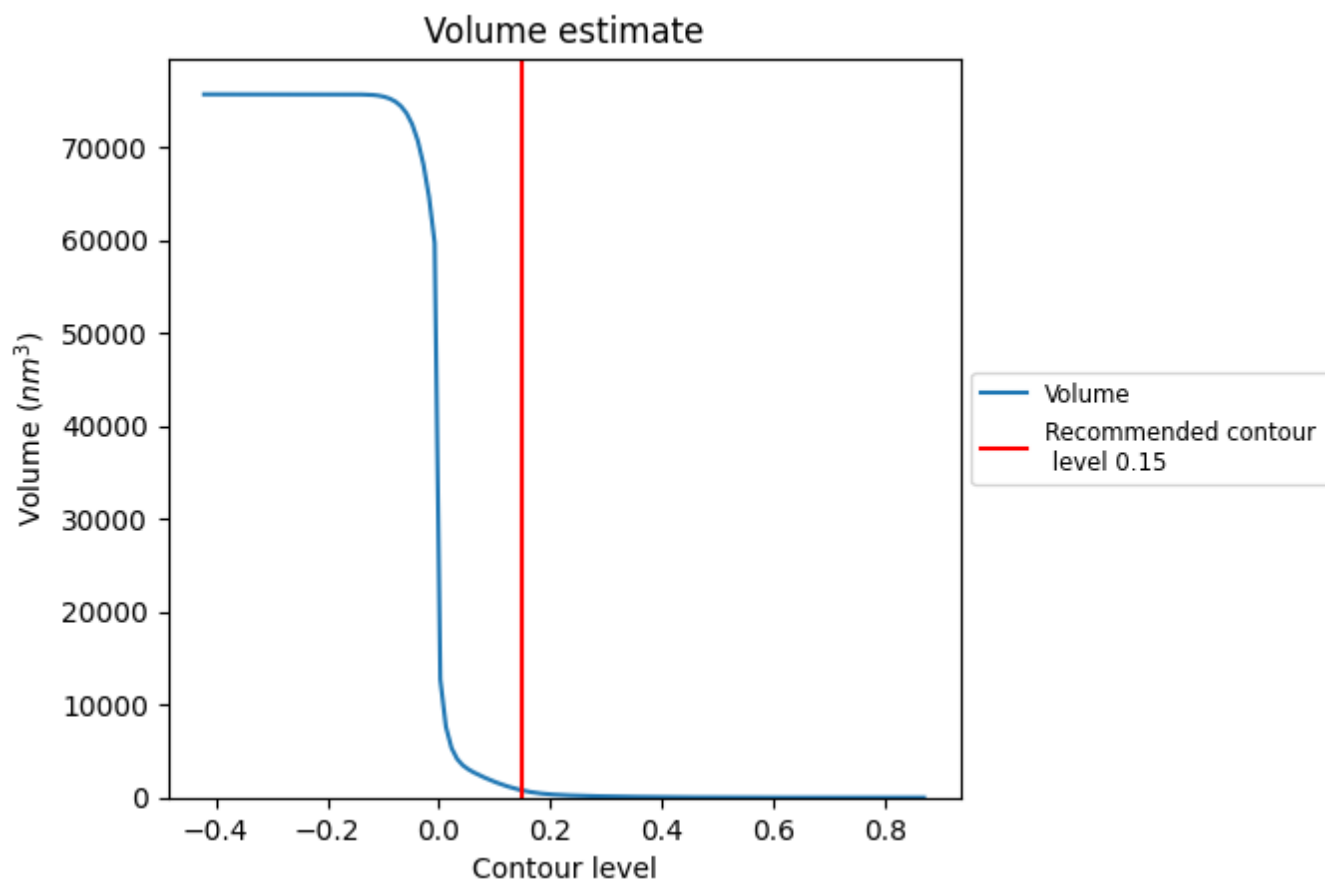
This section contains the results of statistical analysis of the map.

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.

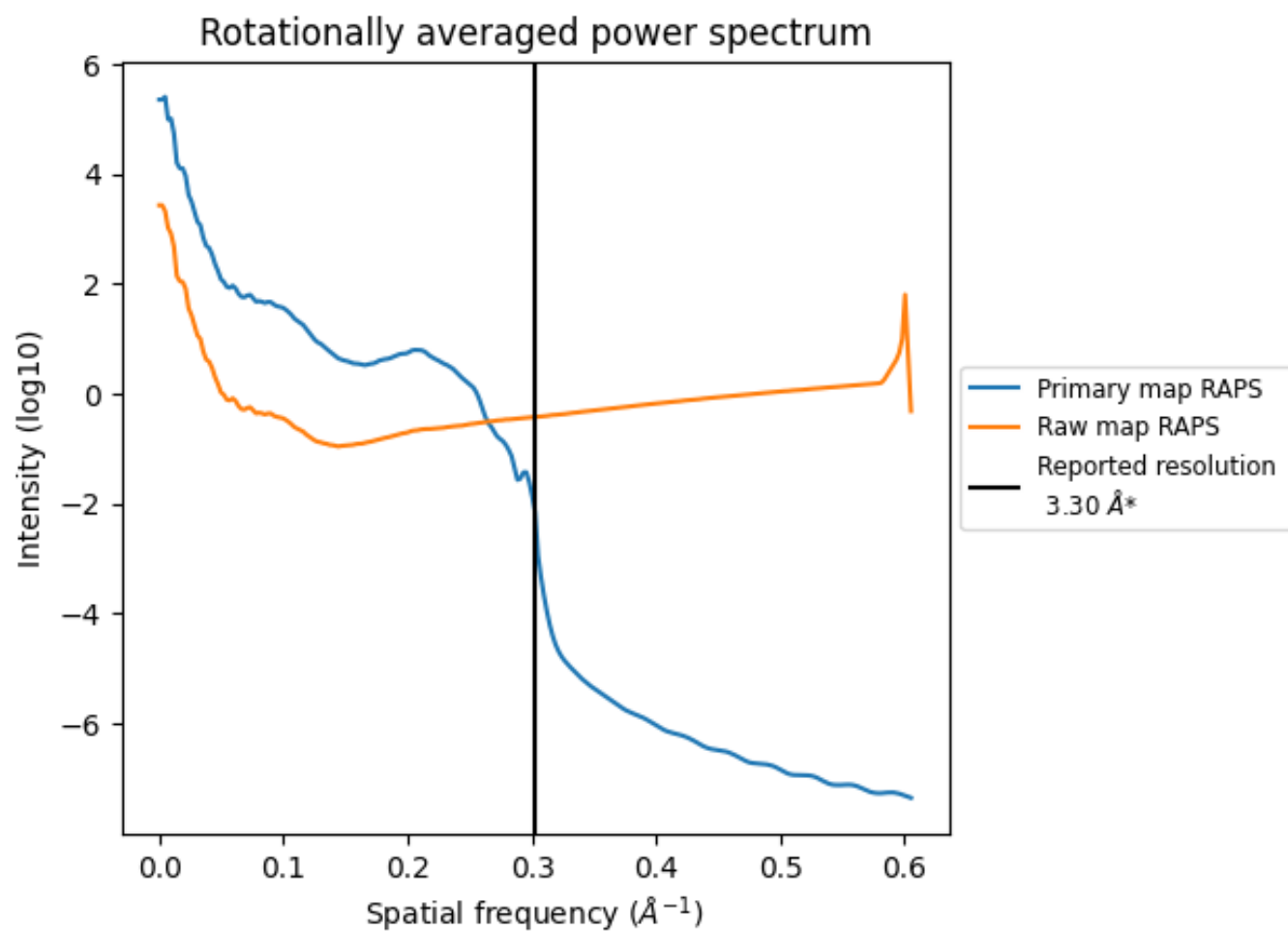
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm³; this corresponds to an approximate mass of 690 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 ⓘ

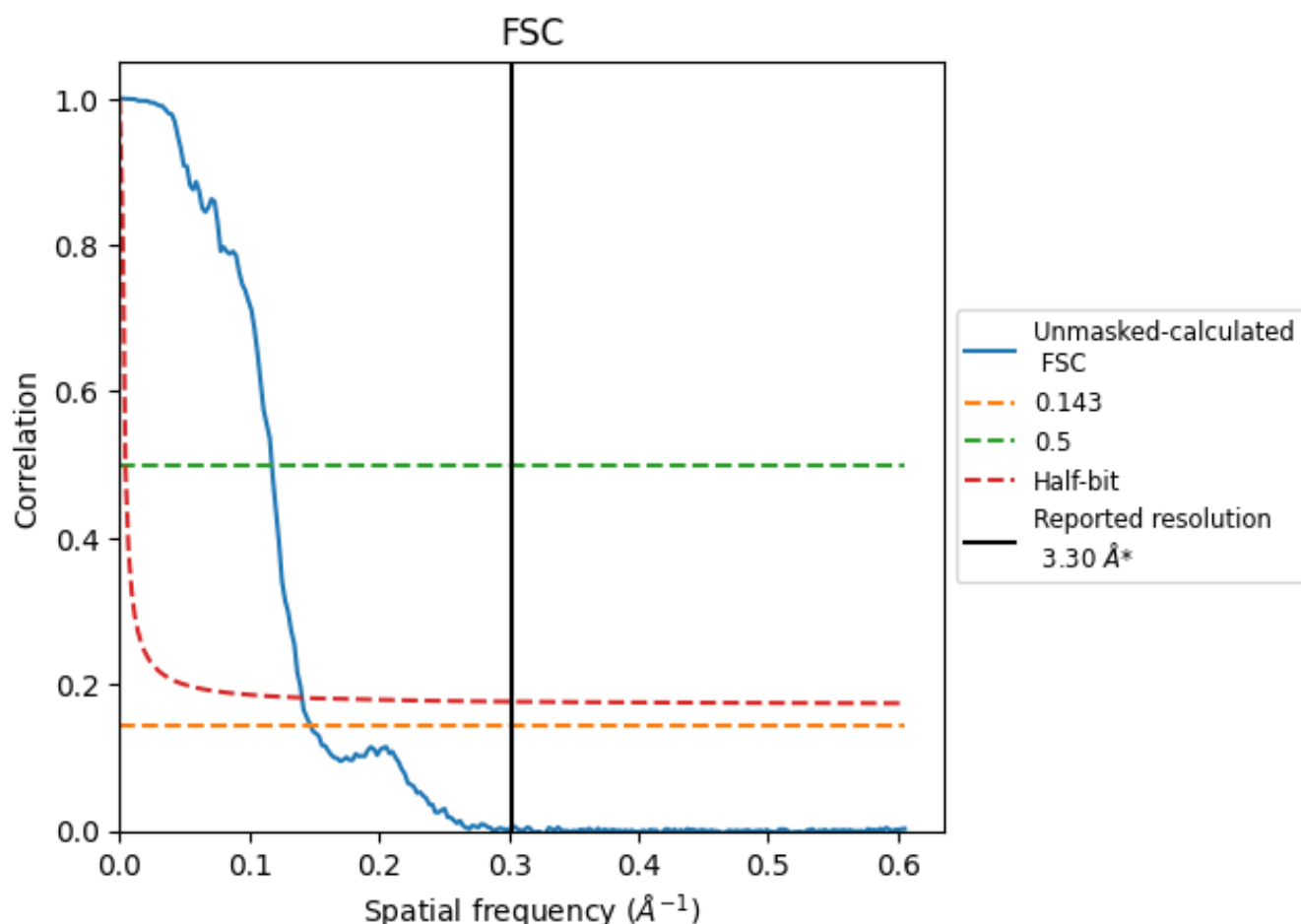


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

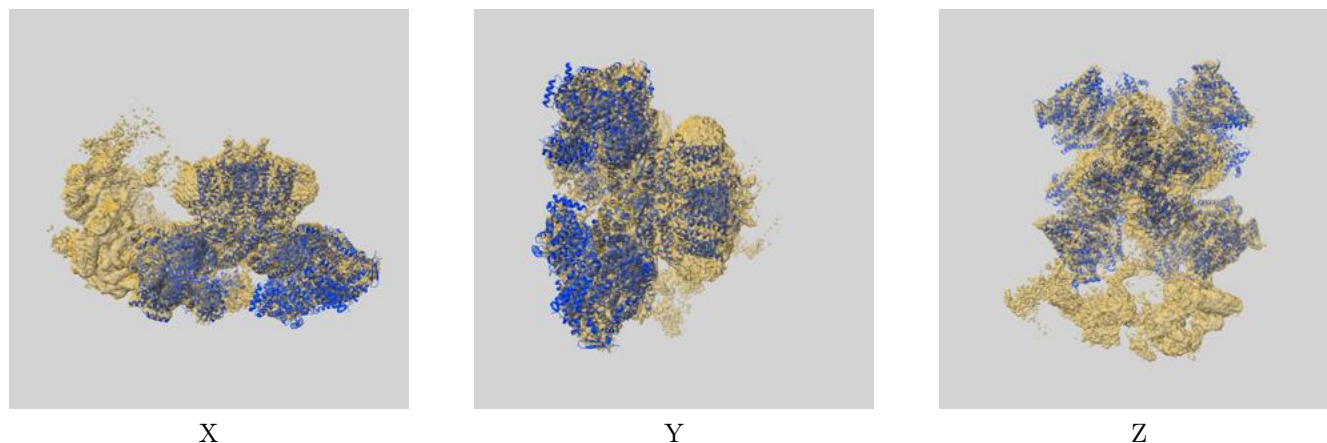
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.78	8.52	7.11

*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 6.78 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

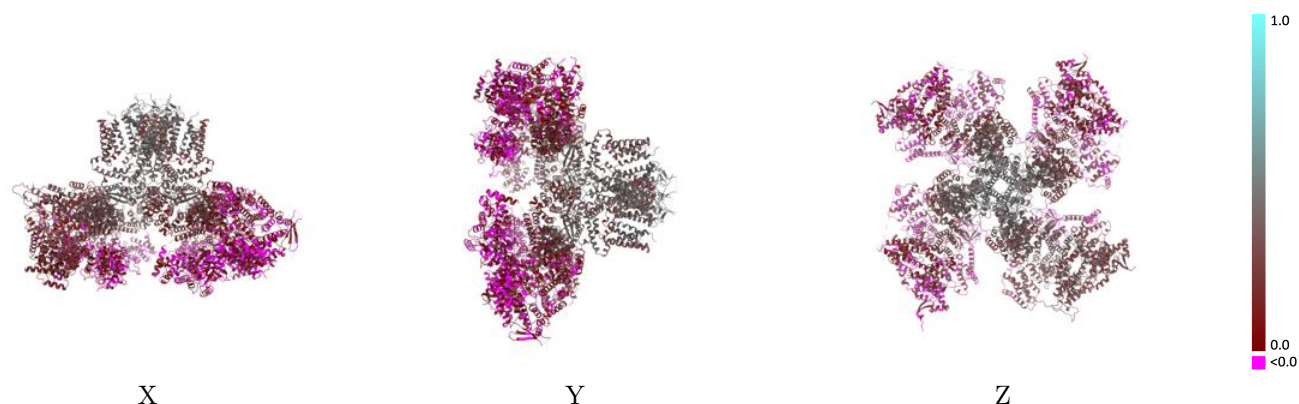
This section contains information regarding the fit between EMDB map EMD-41365 and PDB model 8TL9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



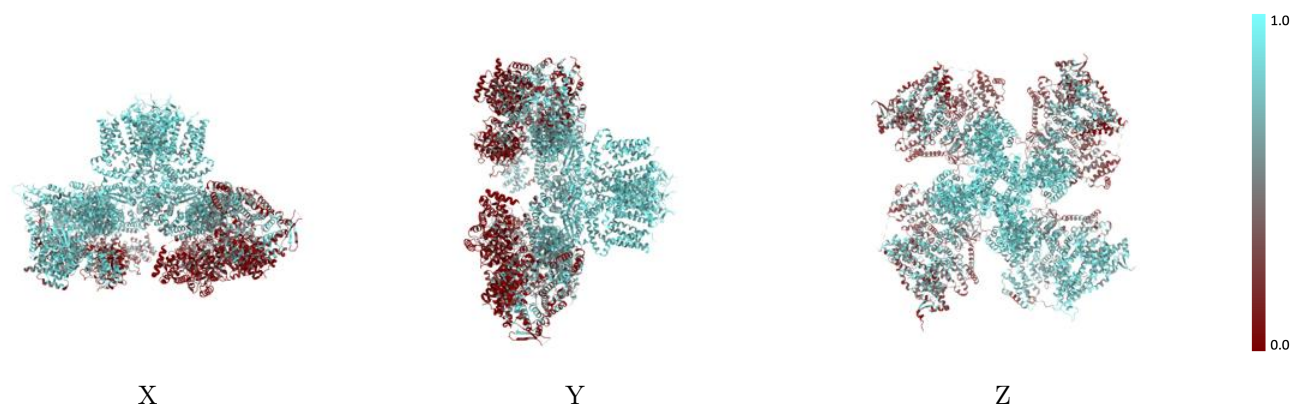
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



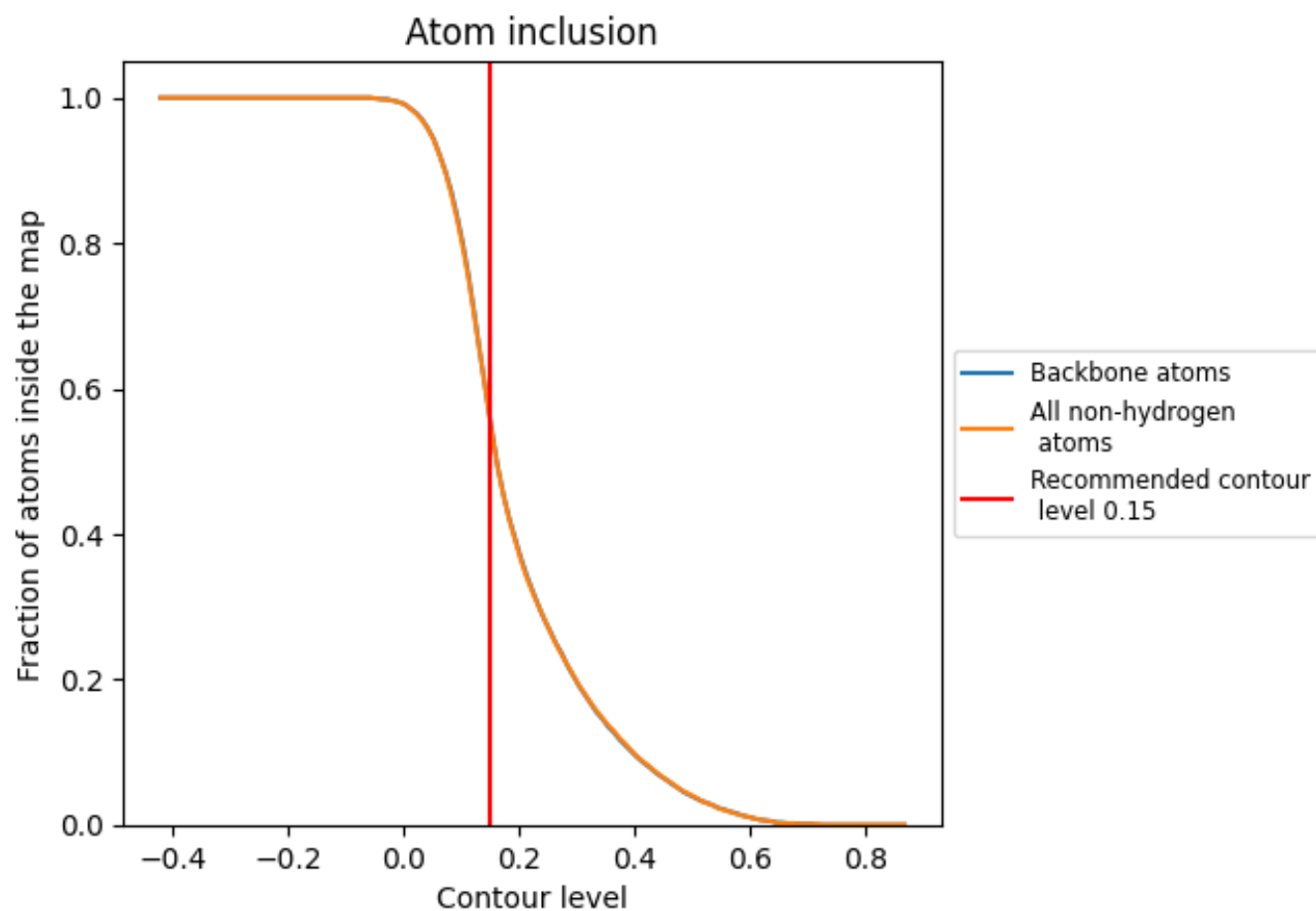
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5580	<div></div> 0.1960
A	<div></div> 0.4890	<div></div> 0.1590
B	<div></div> 0.4520	<div></div> 0.1630
C	<div></div> 0.5790	<div></div> 0.1900
D	<div></div> 0.7300	<div></div> 0.2700

