



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:47 PM UTC

PDB ID : 7T3P / pdb_00007t3p
EMDB ID : EMD-25667
Title : IP3 and ATP bound type 3 IP3 receptor in the pre-active A state
Authors : Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on : 2021-12-08
Resolution : 3.20 Å (reported)
Based on initial model : 6UQK

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

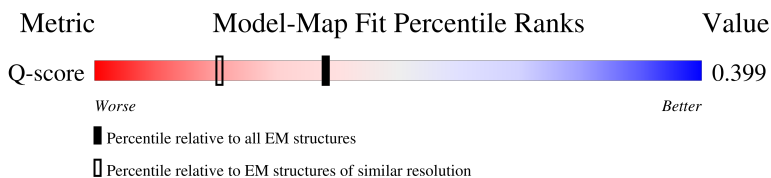
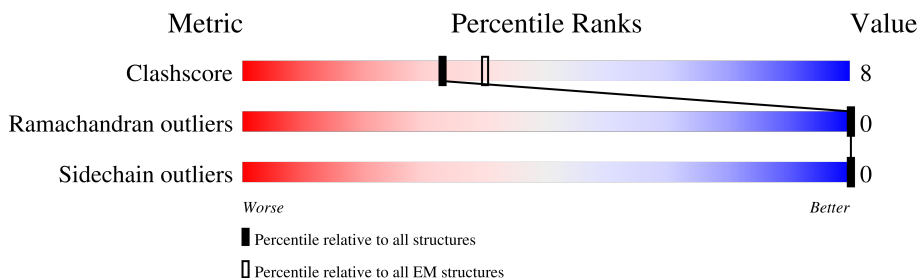
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	2633	 6% 64% 15% 22%
1	B	2633	 7% 63% 15% 22%
1	C	2633	 6% 64% 15% 22%
1	D	2633	 6% 63% 15% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 66992 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.

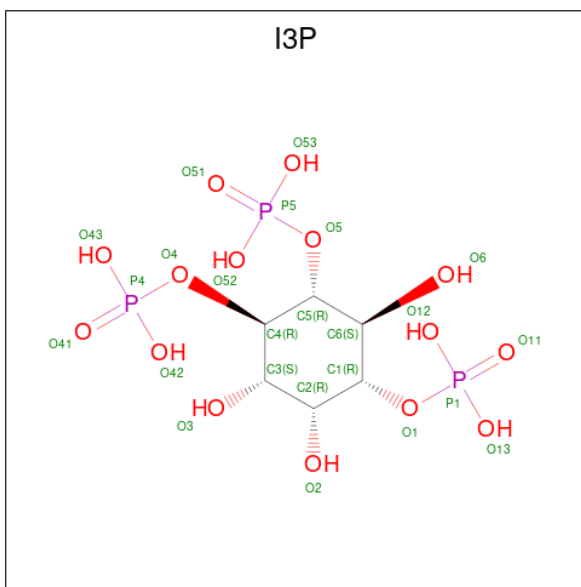
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	B	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	C	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		
1	D	2066	Total	C	N	O	S	0	0
			16692	10684	2850	3057	101		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

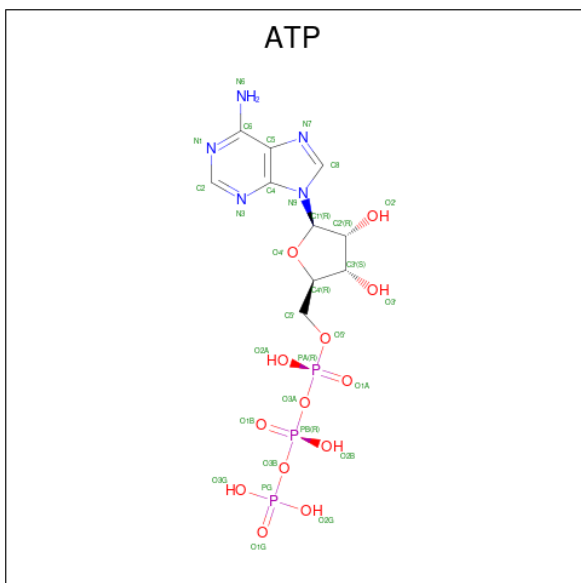
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			24	6	15	3	
3	B	1	Total	C	O	P	0
			24	6	15	3	
3	C	1	Total	C	O	P	0
			24	6	15	3	
3	D	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

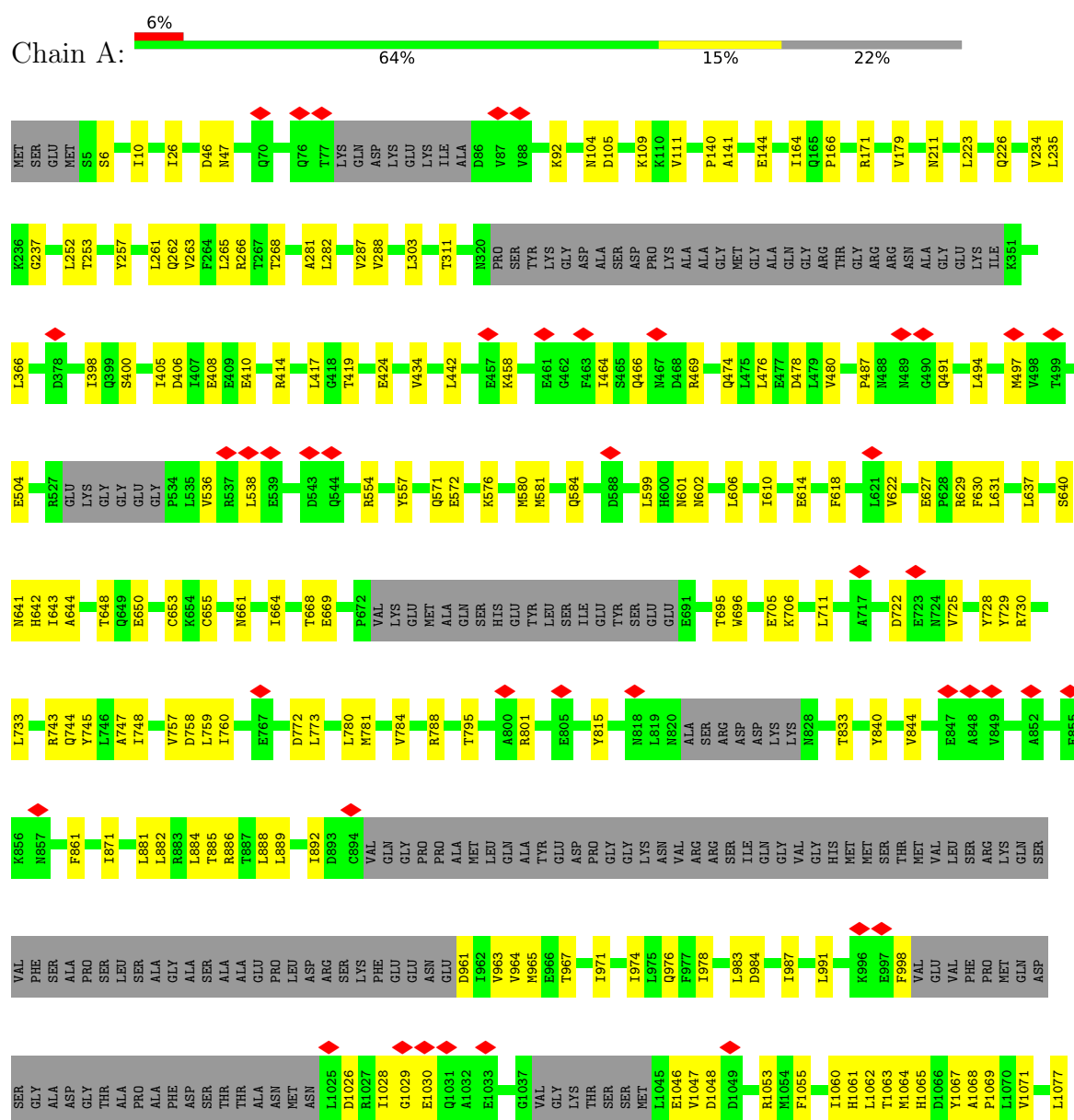


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0

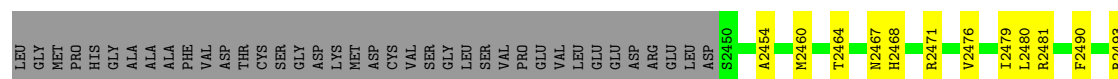
3 Residue-property plots

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.

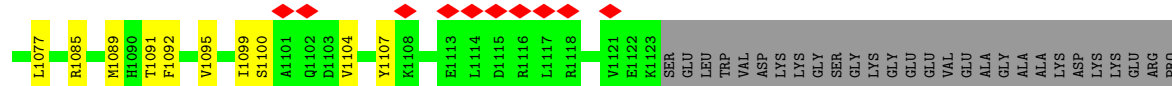
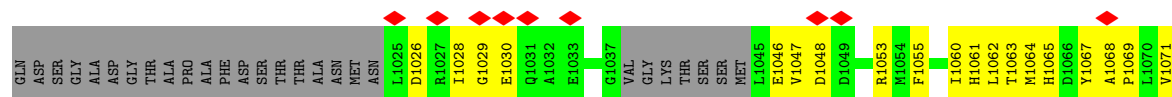
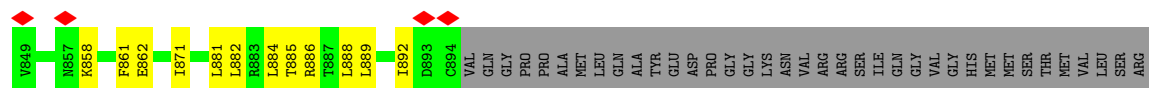
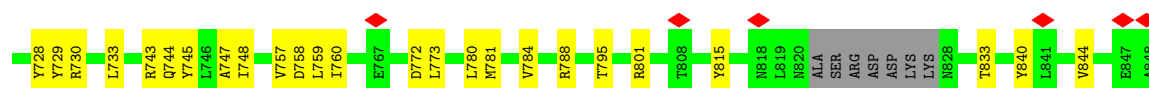
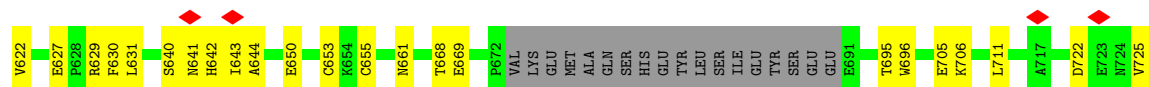
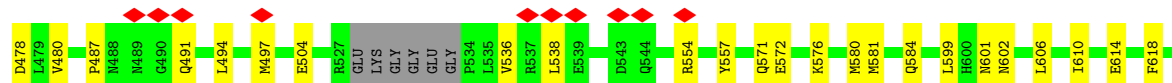
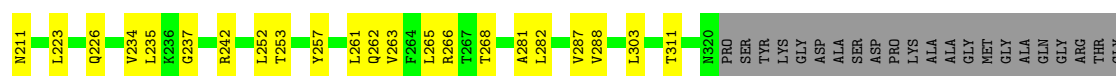
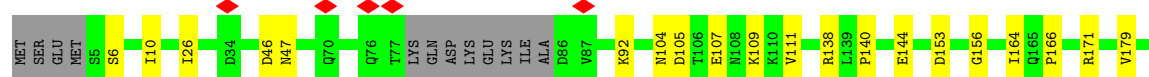
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







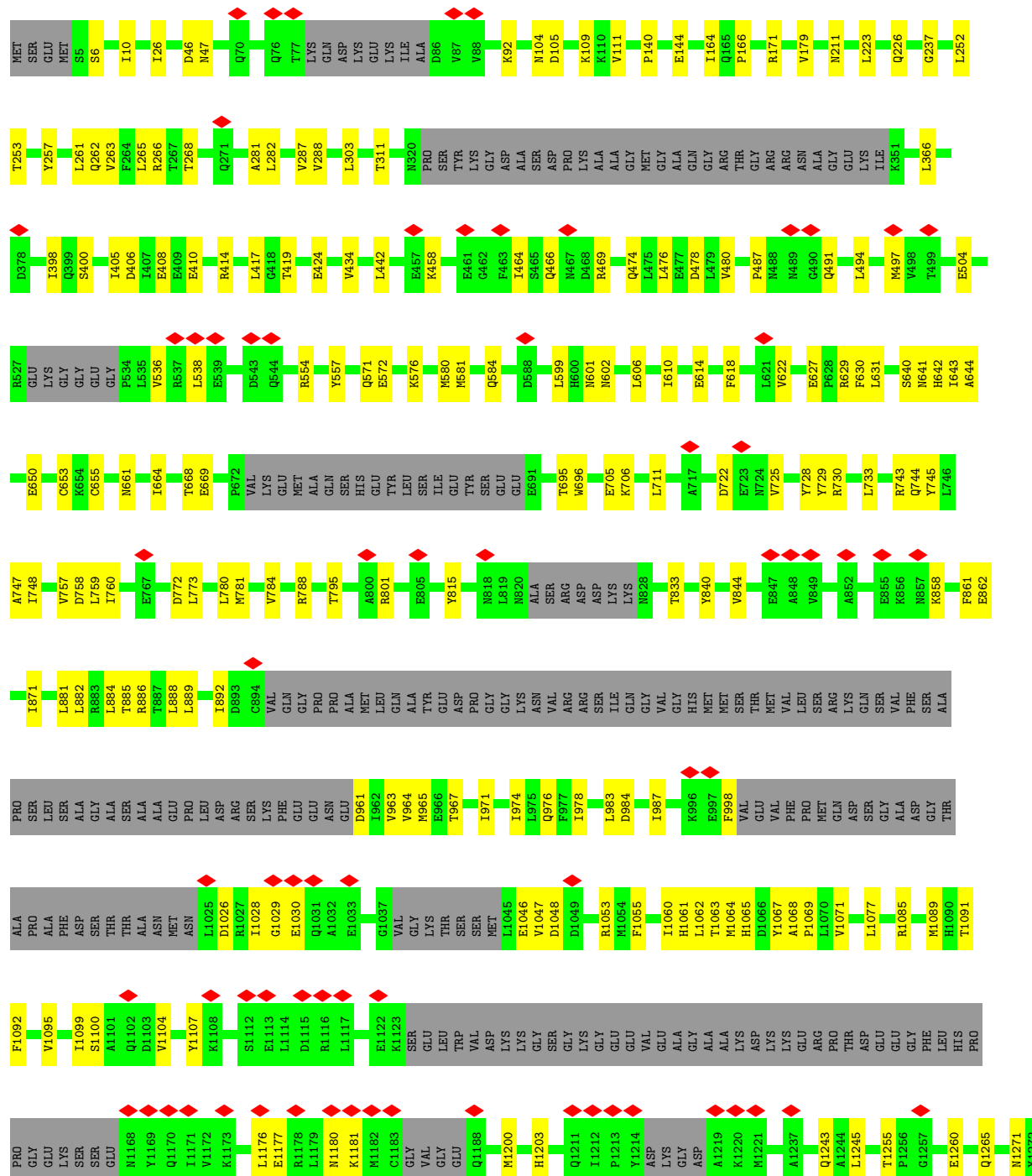
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3







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E2532	Q1273	ARG	GLU	ALA	ALA	R1687	R1784	VAL	ASN	Q2123	LEU	ASP	THR	E2532
R2545	S1279	ASP	ALA	ASN	ASN	L1696	F1785	SER	SER	M2133	PHE	THR	CYS	R2545
V2553	E1280	GLY	VAL	GLN	GLN	Q1696	F1786	GLU	GLU	E2134	THR	LYS	GLY	V2553
S2554	P1281	ASP	ALA	TRP	TRP	ASN	K1787	VAL	VAL	Q2135	TYR	ARG	ASP	S2554
F2555	V1282	LYS	ASP	TYR	TYR	ARG	V1788	SER	SER	C2144	SER	LYS	ASP	F2555
E2556	L1283	MET	HIS	GLN	GLN	LYS	R1792	SER	SER	L2155	SER	MET	ASP	E2556
V2573	Q1284	ASP	HIS	LYS	LYS	THR	R1803	GLU	GLU	D2162	LYS	CYS	ASP	V2573
L2574	V1287	CYS	VAL	ALA	ALA	ARG	VAL	MET	MET	E2163	VAL	VAL	VAL	L2574
V2575	H1288	GLY	LYS	GLY	GLY	ASP	VAL	ASN	ASN	S2169	GLY	SER	GLY	V2575
F2576	A1291	LEU	ARG	GLY	GLY	LEU	ASN	THR	THR	L2178	ARG	VAL	VAL	F2576
V2577	T1292	LEU	ALA	ASP	ASP	PRO	VAL	GLN	GLN	E2183	GLY	GLU	GLU	V2577
Y2583	H1293	SER	ARG	ASP	ASP	THR	ASN	THR	THR	F2184	GLY	GLU	GLU	Y2583
T2584	G1294	PRO	GLY	ASP	ASP	LYS	GLN	TYR	TYR	L2188	GLY	GLU	GLU	T2584
G2585	R1295	VAL	ARG	ASP	ASP	GLY	GLY	ASN	ASN	L2188	GLY	GLU	GLU	G2585
Y2589	Q1298	LEU	ASP	ASP	ASP	THR	ASP	GLU	GLU	R2200	ASP	ARG	ARG	Y2589
M2593	D1301	GLY	ASP	ASP	ASP	GLY	GLY	GLY	GLY	V2204	ASP	GLY	GLY	M2593
M2608	T1305	LEU	ASP	ASP	ASP	GLY	GLY	GLY	GLY	A2212	ASP	ARG	ARG	M2608
X2628	V1306	LEU	ASP	ASP	ASP	GLY	GLY	GLY	GLY	M2216	ASP	GLY	GLY	X2628
X2629	I1307	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	Y2225	ASP	GLY	GLY	X2629
X2630	H1312	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ME1	ASP	GLY	GLY	X2630
X2631	Y1314	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLU	ASP	GLY	GLY	X2631
X2635	K1316	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	ASP	GLY	GLY	X2635
X2639	C1317	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2639
X2642	M1320	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2642
X2643	I1321	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2643
X2644	M1322	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2644
X2645	T1323	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2645
X2646	E1324	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	X2646
UNK	D1330	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	D1331	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	V1332	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	V1333	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	V1334	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	D1338	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	K1339	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	A1340	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	S1341	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	L1342	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	A1343	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	H1344	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	L1345	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	L1346	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	D1347	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	M1348	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	M1349	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	K1350	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	A1351	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK
UNK	A1352	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA	ASP	GLY	GLY	UNK

Chain D: 6% 63% 15% 22%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	116925	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.847	Depositor
Minimum map value	-1.846	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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: ATP, ZN, 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	0.18	0/16897	0.29	0/22813
1	B	0.18	0/16897	0.29	0/22813
1	C	0.18	0/16897	0.29	0/22813
1	D	0.18	0/16897	0.29	0/22813
All	All	0.18	0/67588	0.29	0/91252

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	16692	0	16773	286	0
1	B	16692	0	16773	295	0
1	C	16692	0	16773	290	0
1	D	16692	0	16773	287	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	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	9	2	0
3	C	24	0	9	2	0
3	D	24	0	9	2	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
All	All	66992	0	67176	1124	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 8.

All (1124) 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:B:140:PRO:HD2	1:C:1428:MET:HE2	1.33	1.10
1:B:140:PRO:CD	1:C:1428:MET:HE2	1.87	1.03
1:A:1428:MET:HE2	1:D:140:PRO:HD2	1.45	0.99
1:C:140:PRO:HD2	1:D:1428:MET:HE2	1.46	0.97
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.09	0.86
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.09	0.86
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.09	0.85
1:A:627:GLU:OE1	1:A:629:ARG:NH1	2.10	0.84
1:A:801:ARG:NH2	1:A:984:ASP:OD1	2.09	0.84
1:B:627:GLU:OE1	1:B:629:ARG:NH1	2.10	0.84
1:C:1071:VAL:HG21	1:C:1650:HIS:ND1	1.93	0.84
1:A:1071:VAL:HG21	1:A:1650:HIS:ND1	1.93	0.84
1:B:1071:VAL:HG21	1:B:1650:HIS:ND1	1.93	0.84
1:D:1071:VAL:HG21	1:D:1650:HIS:ND1	1.93	0.84
1:D:627:GLU:OE1	1:D:629:ARG:NH1	2.10	0.83
1:C:627:GLU:OE1	1:C:629:ARG:NH1	2.10	0.83
1:A:1243:GLN:NE2	1:A:1271:ASN:OD1	2.12	0.82
1:D:1243:GLN:NE2	1:D:1271:ASN:OD1	2.12	0.82
1:B:1243:GLN:NE2	1:B:1271:ASN:OD1	2.12	0.82
1:C:1243:GLN:NE2	1:C:1271:ASN:OD1	2.12	0.82
1:B:1974:ILE:HD12	1:B:2000:LEU:HD12	1.63	0.81
1:A:1428:MET:HE2	1:D:140:PRO:CD	2.11	0.81
1:C:1974:ILE:HD12	1:C:2000:LEU:HD12	1.63	0.81
1:D:487:PRO:O	1:D:491:GLN:NE2	2.14	0.81
1:C:487:PRO:O	1:C:491:GLN:NE2	2.14	0.80
1:C:743:ARG:NH1	1:C:788:ARG:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:PRO:O	1:A:491:GLN:NE2	2.14	0.80
1:D:1974:ILE:HD12	1:D:2000:LEU:HD12	1.63	0.80
1:C:140:PRO:CD	1:D:1428:MET:HE2	2.12	0.80
1:D:743:ARG:NH1	1:D:788:ARG:O	2.14	0.80
1:A:743:ARG:NH1	1:A:788:ARG:O	2.14	0.80
1:B:487:PRO:O	1:B:491:GLN:NE2	2.14	0.79
1:A:1974:ILE:HD12	1:A:2000:LEU:HD12	1.63	0.79
1:B:571:GLN:OE1	1:B:602:ASN:ND2	2.15	0.79
1:B:743:ARG:NH1	1:B:788:ARG:O	2.14	0.79
1:C:571:GLN:OE1	1:C:602:ASN:ND2	2.15	0.79
1:D:571:GLN:OE1	1:D:602:ASN:ND2	2.15	0.79
1:B:2481:ARG:O	1:B:2493:ARG:NH2	2.16	0.79
1:A:571:GLN:OE1	1:A:602:ASN:ND2	2.15	0.78
1:D:2481:ARG:O	1:D:2493:ARG:NH2	2.16	0.78
1:C:2481:ARG:O	1:C:2493:ARG:NH2	2.16	0.78
1:B:1968:ASP:OD1	1:B:2019:SER:OG	2.02	0.77
1:C:1968:ASP:OD1	1:C:2019:SER:OG	2.02	0.77
1:B:1255:THR:OG1	1:B:1260:GLU:OE1	2.02	0.77
1:A:2481:ARG:O	1:A:2493:ARG:NH2	2.16	0.77
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.02	0.77
1:C:1255:THR:OG1	1:C:1260:GLU:OE1	2.02	0.77
1:D:1968:ASP:OD1	1:D:2019:SER:OG	2.02	0.76
1:D:1255:THR:OG1	1:D:1260:GLU:OE1	2.02	0.76
1:A:781:MET:HE1	1:A:833:THR:HG21	1.68	0.76
1:A:1255:THR:OG1	1:A:1260:GLU:OE1	2.02	0.76
1:D:1424:THR:O	1:D:1429:LYS:NZ	2.16	0.76
1:D:772:ASP:OD1	1:D:773:LEU:N	2.19	0.76
1:D:781:MET:HE1	1:D:833:THR:HG21	1.68	0.75
1:A:772:ASP:OD1	1:A:773:LEU:N	2.19	0.75
1:B:1424:THR:O	1:B:1429:LYS:NZ	2.16	0.75
1:D:885:THR:HG23	1:D:978:ILE:HD13	1.69	0.75
1:B:140:PRO:HD2	1:C:1428:MET:CE	2.15	0.75
1:B:650:GLU:OE2	1:B:744:GLN:NE2	2.20	0.75
1:B:1064:MET:O	1:B:1646:LYS:NZ	2.20	0.74
1:A:650:GLU:OE2	1:A:744:GLN:NE2	2.20	0.74
1:B:781:MET:HE1	1:B:833:THR:HG21	1.68	0.74
1:B:886:ARG:NH1	1:B:1046:GLU:O	2.20	0.74
1:A:885:THR:HG23	1:A:978:ILE:HD13	1.69	0.74
1:A:886:ARG:NH1	1:A:1046:GLU:O	2.21	0.74
1:B:772:ASP:OD1	1:B:773:LEU:N	2.19	0.74
1:C:781:MET:HE1	1:C:833:THR:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1659:GLU:OE1	1:A:1746:ASN:ND2	2.21	0.74
1:C:650:GLU:OE2	1:C:744:GLN:NE2	2.20	0.74
1:D:886:ARG:NH1	1:D:1046:GLU:O	2.21	0.74
1:C:885:THR:HG23	1:C:978:ILE:HD13	1.69	0.74
1:C:1941:LEU:O	1:C:1945:THR:HG23	1.88	0.74
1:D:1941:LEU:O	1:D:1945:THR:HG23	1.87	0.74
1:C:772:ASP:OD1	1:C:773:LEU:N	2.19	0.74
1:D:650:GLU:OE2	1:D:744:GLN:NE2	2.20	0.74
1:A:1064:MET:O	1:A:1646:LYS:NZ	2.20	0.74
1:A:1941:LEU:O	1:A:1945:THR:HG23	1.88	0.74
1:A:140:PRO:HD2	1:B:1428:MET:HE2	1.69	0.73
1:A:1424:THR:O	1:A:1429:LYS:NZ	2.16	0.73
1:C:1424:THR:O	1:C:1429:LYS:NZ	2.16	0.73
1:B:1659:GLU:OE1	1:B:1746:ASN:ND2	2.21	0.73
1:C:1064:MET:O	1:C:1646:LYS:NZ	2.20	0.73
1:C:886:ARG:NH1	1:C:1046:GLU:O	2.21	0.73
1:C:1659:GLU:OE1	1:C:1746:ASN:ND2	2.21	0.73
1:D:1053:ARG:NH2	1:D:1627:LEU:O	2.22	0.73
1:D:1064:MET:O	1:D:1646:LYS:NZ	2.20	0.73
1:B:1941:LEU:O	1:B:1945:THR:HG23	1.87	0.73
1:D:1659:GLU:OE1	1:D:1746:ASN:ND2	2.21	0.73
1:B:885:THR:HG23	1:B:978:ILE:HD13	1.69	0.73
1:C:1053:ARG:NH2	1:C:1627:LEU:O	2.22	0.73
1:D:1107:TYR:CE1	1:D:1200:MET:HE3	2.24	0.73
1:B:1053:ARG:NH2	1:B:1627:LEU:O	2.22	0.73
1:A:1107:TYR:CE1	1:A:1200:MET:HE3	2.24	0.72
1:B:1107:TYR:CE1	1:B:1200:MET:HE3	2.24	0.72
1:C:1107:TYR:CE1	1:C:1200:MET:HE3	2.24	0.72
1:A:1053:ARG:NH2	1:A:1627:LEU:O	2.22	0.72
1:D:706:LYS:NZ	1:D:722:ASP:OD1	2.24	0.71
1:C:998:PHE:O	1:C:1594:LYS:NZ	2.21	0.71
1:B:1974:ILE:CD1	1:B:2000:LEU:HD12	2.21	0.71
1:A:2511:LEU:HD21	1:B:2362:VAL:HG23	1.73	0.70
1:A:1974:ILE:CD1	1:A:2000:LEU:HD12	2.21	0.70
1:C:1654:LEU:HD23	1:C:1654:LEU:O	1.92	0.70
1:D:1974:ILE:CD1	1:D:2000:LEU:HD12	2.21	0.70
1:A:706:LYS:NZ	1:A:722:ASP:OD1	2.24	0.70
1:B:889:LEU:HD13	1:B:1048:ASP:OD1	1.92	0.70
1:C:1974:ILE:CD1	1:C:2000:LEU:HD12	2.21	0.70
1:D:1654:LEU:O	1:D:1654:LEU:HD23	1.92	0.70
1:A:1028:ILE:HD13	1:A:1598:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:LYS:NZ	1:C:722:ASP:OD1	2.24	0.69
1:C:1028:ILE:HD13	1:C:1598:ILE:HD12	1.74	0.69
1:B:882:LEU:O	1:B:885:THR:OG1	2.11	0.69
1:D:2048:GLU:N	1:D:2048:GLU:OE1	2.25	0.69
1:C:889:LEU:HD13	1:C:1048:ASP:OD1	1.92	0.69
1:C:2048:GLU:N	1:C:2048:GLU:OE1	2.25	0.69
1:A:889:LEU:HD13	1:A:1048:ASP:OD1	1.92	0.69
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.26	0.69
1:A:2048:GLU:OE1	1:A:2048:GLU:N	2.25	0.69
1:C:466:GLN:OE1	1:C:469:ARG:NH2	2.26	0.69
1:A:1654:LEU:O	1:A:1654:LEU:HD23	1.92	0.69
1:B:706:LYS:NZ	1:B:722:ASP:OD1	2.24	0.69
1:C:10:ILE:HD11	1:C:111:VAL:HG13	1.75	0.69
1:D:466:GLN:OE1	1:D:469:ARG:NH2	2.26	0.69
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.26	0.68
1:B:2048:GLU:N	1:B:2048:GLU:OE1	2.25	0.68
1:A:882:LEU:O	1:A:885:THR:OG1	2.11	0.68
1:B:2545:ARG:NH1	1:B:2556:GLU:OE2	2.26	0.68
1:D:10:ILE:HD11	1:D:111:VAL:HG13	1.75	0.68
1:D:2545:ARG:NH1	1:D:2556:GLU:OE2	2.26	0.68
1:B:1654:LEU:HD23	1:B:1654:LEU:O	1.92	0.68
1:A:1960:VAL:HG23	1:A:1961:THR:HG23	1.75	0.68
1:D:1960:VAL:HG23	1:D:1961:THR:HG23	1.75	0.68
1:C:2584:THR:HG22	1:C:2585:GLY:H	1.58	0.68
1:D:1028:ILE:HD13	1:D:1598:ILE:HD12	1.74	0.68
1:A:2545:ARG:NH1	1:A:2556:GLU:OE2	2.26	0.68
1:D:889:LEU:HD13	1:D:1048:ASP:OD1	1.92	0.68
1:C:696:TRP:CE2	1:C:725:VAL:HG21	2.29	0.68
1:B:998:PHE:O	1:B:1594:LYS:NZ	2.21	0.68
1:B:1028:ILE:HD13	1:B:1598:ILE:HD12	1.74	0.68
1:D:696:TRP:CE2	1:D:725:VAL:HG21	2.29	0.68
1:D:1774:ASN:OD1	1:D:1775:LEU:N	2.27	0.68
1:B:140:PRO:HG2	1:C:1428:MET:CE	2.24	0.67
1:C:2545:ARG:NH1	1:C:2556:GLU:OE2	2.26	0.67
1:B:10:ILE:CD1	1:B:111:VAL:HG13	2.25	0.67
1:B:10:ILE:HD11	1:B:111:VAL:HG13	1.75	0.67
1:B:1774:ASN:OD1	1:B:1775:LEU:N	2.27	0.67
1:D:881:LEU:HD22	1:D:978:ILE:HG12	1.76	0.67
1:A:10:ILE:CD1	1:A:111:VAL:HG13	2.25	0.67
1:B:881:LEU:HD22	1:B:978:ILE:HG12	1.77	0.67
1:B:1960:VAL:HG23	1:B:1961:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1774:ASN:OD1	1:C:1775:LEU:N	2.27	0.67
1:C:1960:VAL:HG23	1:C:1961:THR:HG23	1.76	0.67
1:D:10:ILE:CD1	1:D:111:VAL:HG13	2.25	0.67
1:A:10:ILE:HD11	1:A:111:VAL:HG13	1.75	0.67
1:A:696:TRP:CE2	1:A:725:VAL:HG21	2.29	0.67
1:D:2584:THR:HG22	1:D:2585:GLY:H	1.59	0.67
1:B:696:TRP:CE2	1:B:725:VAL:HG21	2.29	0.67
1:B:2584:THR:HG22	1:B:2585:GLY:H	1.59	0.67
1:A:1092:PHE:O	1:A:1095:VAL:HG12	1.95	0.67
1:D:998:PHE:O	1:D:1594:LYS:NZ	2.21	0.67
1:D:1092:PHE:O	1:D:1095:VAL:HG12	1.95	0.67
1:D:882:LEU:O	1:D:885:THR:OG1	2.11	0.67
1:B:1092:PHE:O	1:B:1095:VAL:HG12	1.95	0.67
1:A:1774:ASN:OD1	1:A:1775:LEU:N	2.27	0.66
1:C:1301:ASP:O	1:C:1305:THR:HG23	1.95	0.66
1:C:2322:TYR:OH	1:C:2347:ASP:OD1	2.13	0.66
1:C:268:THR:OG1	3:C:2702:I3P:O42	2.13	0.66
1:D:1301:ASP:O	1:D:1305:THR:HG23	1.95	0.66
1:A:881:LEU:HD22	1:A:978:ILE:HG12	1.76	0.66
1:C:10:ILE:CD1	1:C:111:VAL:HG13	2.25	0.66
1:C:1092:PHE:O	1:C:1095:VAL:HG12	1.95	0.66
1:A:2322:TYR:OH	1:A:2347:ASP:OD1	2.13	0.66
1:B:1063:THR:HA	1:B:1071:VAL:HG23	1.78	0.66
1:C:881:LEU:HD22	1:C:978:ILE:HG12	1.77	0.66
1:C:1933:ASN:ND2	1:C:1933:ASN:O	2.29	0.66
1:A:2584:THR:HG22	1:A:2585:GLY:H	1.59	0.66
1:C:695:THR:HG22	1:C:705:GLU:HG2	1.77	0.66
1:D:1933:ASN:O	1:D:1933:ASN:ND2	2.29	0.66
1:B:1301:ASP:O	1:B:1305:THR:HG23	1.95	0.66
1:D:2322:TYR:OH	1:D:2347:ASP:OD1	2.13	0.66
1:D:695:THR:HG22	1:D:705:GLU:HG2	1.77	0.66
1:A:1063:THR:HA	1:A:1071:VAL:HG23	1.78	0.65
1:A:1933:ASN:ND2	1:A:1933:ASN:O	2.29	0.65
1:C:882:LEU:O	1:C:885:THR:OG1	2.11	0.65
1:B:2322:TYR:OH	1:B:2347:ASP:OD1	2.13	0.65
1:A:695:THR:HG22	1:A:705:GLU:HG2	1.77	0.65
1:B:1933:ASN:O	1:B:1933:ASN:ND2	2.29	0.65
1:D:1063:THR:HA	1:D:1071:VAL:HG23	1.78	0.65
1:A:1301:ASP:O	1:A:1305:THR:HG23	1.95	0.65
1:C:410:GLU:OE1	1:C:410:GLU:N	2.30	0.65
1:C:2184:TRP:CZ2	1:C:2188:LEU:HD13	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:THR:HG22	1:B:705:GLU:HG2	1.77	0.65
1:A:2184:TRP:CZ2	1:A:2188:LEU:HD13	2.32	0.65
1:D:410:GLU:N	1:D:410:GLU:OE1	2.30	0.65
1:D:963:VAL:O	1:D:967:THR:HG23	1.97	0.65
1:A:2362:VAL:HG23	1:D:2511:LEU:HD21	1.78	0.64
1:A:963:VAL:O	1:A:967:THR:HG23	1.97	0.64
1:C:963:VAL:O	1:C:967:THR:HG23	1.97	0.64
1:C:1063:THR:HA	1:C:1071:VAL:HG23	1.78	0.64
1:C:2511:LEU:HD21	1:D:2362:VAL:HG23	1.78	0.64
1:B:2184:TRP:CZ2	1:B:2188:LEU:HD13	2.32	0.64
1:B:963:VAL:O	1:B:967:THR:HG23	1.97	0.64
1:D:268:THR:OG1	3:D:2702:I3P:O42	2.13	0.64
1:B:1619:ASP:OD2	1:B:1687:ARG:NH1	2.31	0.64
1:D:696:TRP:CZ2	1:D:725:VAL:HG21	2.33	0.64
1:D:2184:TRP:CZ2	1:D:2188:LEU:HD13	2.32	0.64
1:A:696:TRP:CZ2	1:A:725:VAL:HG21	2.33	0.63
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	1.98	0.63
1:B:410:GLU:N	1:B:410:GLU:OE1	2.30	0.63
1:C:1651:THR:OG1	1:C:1665:VAL:HG11	1.98	0.63
1:D:1651:THR:OG1	1:D:1665:VAL:HG11	1.98	0.63
1:B:696:TRP:CZ2	1:B:725:VAL:HG21	2.33	0.63
1:A:888:LEU:HD22	1:A:971:ILE:HG12	1.79	0.63
1:C:888:LEU:HD22	1:C:971:ILE:HG12	1.79	0.63
1:C:1176:LEU:O	1:C:1180:ASN:ND2	2.32	0.63
1:B:668:THR:OG1	1:B:729:TYR:OH	2.14	0.63
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	1.98	0.63
1:C:696:TRP:CZ2	1:C:725:VAL:HG21	2.33	0.63
1:D:1176:LEU:O	1:D:1180:ASN:ND2	2.32	0.63
1:B:1176:LEU:O	1:B:1180:ASN:ND2	2.32	0.63
1:D:2133:MET:HE3	1:D:2608:MET:HG3	1.81	0.63
1:C:1619:ASP:OD2	1:C:1687:ARG:NH1	2.31	0.63
1:D:1619:ASP:OD2	1:D:1687:ARG:NH1	2.31	0.63
1:A:410:GLU:N	1:A:410:GLU:OE1	2.30	0.63
1:D:1652:LYS:O	1:D:1655:MET:HE3	1.99	0.63
1:A:998:PHE:O	1:A:1594:LYS:NZ	2.21	0.62
1:A:2467:ASN:OD1	1:A:2471:ARG:NH1	2.32	0.62
1:B:1177:GLU:OE1	1:B:1181:LYS:NZ	2.32	0.62
1:B:1652:LYS:O	1:B:1655:MET:HE3	1.99	0.62
1:D:1655:MET:HE2	1:D:1740:LEU:HD12	1.81	0.62
1:B:1655:MET:HE2	1:B:1740:LEU:HD12	1.82	0.62
1:C:1265:GLN:HG3	1:C:1305:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:LEU:O	1:A:1180:ASN:ND2	2.32	0.62
1:A:1655:MET:HE2	1:A:1740:LEU:HD12	1.81	0.62
1:B:888:LEU:HD22	1:B:971:ILE:HG12	1.79	0.62
1:B:2467:ASN:OD1	1:B:2471:ARG:NH1	2.32	0.62
1:A:1619:ASP:OD2	1:A:1687:ARG:NH1	2.31	0.62
1:A:2468:HIS:HB2	1:A:2479:ILE:HD13	1.82	0.62
1:C:2468:HIS:HB2	1:C:2479:ILE:HD13	1.82	0.62
1:D:1177:GLU:OE1	1:D:1181:LYS:NZ	2.33	0.62
1:D:2123:GLN:OE1	1:D:2135:GLN:NE2	2.33	0.62
1:D:2467:ASN:OD1	1:D:2471:ARG:NH1	2.32	0.62
1:A:1652:LYS:O	1:A:1655:MET:HE3	1.99	0.62
1:D:888:LEU:HD22	1:D:971:ILE:HG12	1.79	0.62
1:D:1265:GLN:HG3	1:D:1305:THR:HG21	1.81	0.62
1:C:1655:MET:HE2	1:C:1740:LEU:HD12	1.81	0.62
1:A:252:LEU:HD13	1:A:417:LEU:CD1	2.30	0.62
1:C:1652:LYS:O	1:C:1655:MET:HE3	1.99	0.62
1:A:983:LEU:HD21	1:A:1091:THR:HG21	1.81	0.62
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.33	0.62
1:B:2133:MET:HE3	1:B:2608:MET:HG3	1.81	0.62
1:C:252:LEU:HD13	1:C:417:LEU:CD1	2.30	0.62
1:C:1177:GLU:OE1	1:C:1181:LYS:NZ	2.32	0.62
1:C:1886:ARG:NH1	1:C:1951:PRO:O	2.33	0.62
1:A:268:THR:OG1	3:A:2702:I3P:O42	2.13	0.62
1:D:2468:HIS:HB2	1:D:2479:ILE:HD13	1.82	0.62
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.82	0.61
1:A:2133:MET:HE3	1:A:2608:MET:HG3	1.81	0.61
1:A:223:LEU:HD21	1:A:226:GLN:HG2	1.82	0.61
1:A:1177:GLU:OE1	1:A:1181:LYS:NZ	2.32	0.61
1:A:2123:GLN:OE1	1:A:2135:GLN:NE2	2.33	0.61
1:C:2123:GLN:OE1	1:C:2135:GLN:NE2	2.33	0.61
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.30	0.61
1:D:1886:ARG:NH1	1:D:1951:PRO:O	2.33	0.61
1:B:1886:ARG:NH1	1:B:1951:PRO:O	2.33	0.61
1:C:668:THR:OG1	1:C:729:TYR:OH	2.14	0.61
1:C:2467:ASN:OD1	1:C:2471:ARG:NH1	2.32	0.61
1:B:268:THR:OG1	3:B:2702:I3P:O42	2.13	0.61
1:C:1314:VAL:HG23	1:C:1317:CYS:HB2	1.83	0.61
1:A:1265:GLN:HG3	1:A:1305:THR:HG21	1.81	0.61
1:B:1265:GLN:HG3	1:B:1305:THR:HG21	1.81	0.61
1:C:2133:MET:HE3	1:C:2608:MET:HG3	1.81	0.61
1:B:1314:VAL:HG23	1:B:1317:CYS:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:983:LEU:HD21	1:C:1091:THR:HG21	1.81	0.61
1:B:252:LEU:HD13	1:B:417:LEU:CD1	2.30	0.61
1:B:983:LEU:HD21	1:B:1091:THR:HG21	1.81	0.61
1:D:983:LEU:HD21	1:D:1091:THR:HG21	1.81	0.61
1:B:758:ASP:OD1	1:B:759:LEU:N	2.34	0.61
1:D:758:ASP:OD1	1:D:759:LEU:N	2.34	0.61
1:D:223:LEU:HD21	1:D:226:GLN:HG2	1.82	0.61
1:A:2054:TYR:OH	1:A:2118:GLU:OE1	2.19	0.60
1:C:2054:TYR:OH	1:C:2118:GLU:OE1	2.19	0.60
1:C:2062:ARG:NH2	1:C:2135:GLN:OE1	2.34	0.60
1:C:758:ASP:OD1	1:C:759:LEU:N	2.34	0.60
1:A:1886:ARG:NH1	1:A:1951:PRO:O	2.33	0.60
1:A:2062:ARG:NH2	1:A:2135:GLN:OE1	2.34	0.60
1:B:140:PRO:CD	1:C:1428:MET:CE	2.74	0.60
1:B:2468:HIS:HB3	1:B:2479:ILE:HG21	1.84	0.60
1:C:400:SER:HA	1:C:417:LEU:HD23	1.84	0.60
1:D:2062:ARG:NH2	1:D:2135:GLN:OE1	2.34	0.60
1:B:2054:TYR:OH	1:B:2118:GLU:OE1	2.19	0.60
1:B:2062:ARG:NH2	1:B:2135:GLN:OE1	2.34	0.60
1:B:223:LEU:HD21	1:B:226:GLN:HG2	1.82	0.60
1:D:2054:TYR:OH	1:D:2118:GLU:OE1	2.20	0.60
1:B:400:SER:HA	1:B:417:LEU:HD23	1.84	0.59
1:D:400:SER:HA	1:D:417:LEU:HD23	1.84	0.59
1:A:758:ASP:OD1	1:A:759:LEU:N	2.34	0.59
1:B:138:ARG:HG3	1:C:1427:GLU:HG3	1.84	0.59
1:A:780:LEU:O	1:A:784:VAL:HG12	2.03	0.59
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.85	0.59
1:D:892:ILE:HD11	1:D:971:ILE:HG21	1.85	0.59
1:D:1314:VAL:HG23	1:D:1317:CYS:HB2	1.83	0.59
1:D:2468:HIS:HB3	1:D:2479:ILE:HG21	1.84	0.59
1:A:1314:VAL:HG23	1:A:1317:CYS:HB2	1.83	0.59
1:B:780:LEU:O	1:B:784:VAL:HG12	2.03	0.59
1:C:780:LEU:O	1:C:784:VAL:HG12	2.03	0.59
1:C:892:ILE:HD11	1:C:971:ILE:HG21	1.85	0.59
1:A:2468:HIS:HB3	1:A:2479:ILE:HG21	1.84	0.59
1:C:223:LEU:HD21	1:C:226:GLN:HG2	1.82	0.59
1:C:871:ILE:HD13	1:C:974:ILE:HG23	1.85	0.59
1:A:892:ILE:HD11	1:A:971:ILE:HG21	1.85	0.59
1:A:2144:CYS:HA	1:A:2182:MET:HE2	1.85	0.59
1:D:1203:HIS:CD2	1:D:1245:LEU:HD21	2.38	0.59
1:B:282:LEU:CD2	1:B:434:VAL:HG21	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1203:HIS:CD2	1:B:1245:LEU:HD21	2.38	0.58
1:C:282:LEU:CD2	1:C:434:VAL:HG21	2.33	0.58
1:B:266:ARG:NH2	3:B:2702:I3P:O43	2.36	0.58
1:C:266:ARG:NH2	3:C:2702:I3P:O43	2.36	0.58
1:C:1740:LEU:O	1:C:1744:THR:OG1	2.09	0.58
1:A:871:ILE:HD13	1:A:974:ILE:HG23	1.85	0.58
1:C:1203:HIS:CD2	1:C:1245:LEU:HD21	2.38	0.58
1:D:2144:CYS:HA	1:D:2182:MET:HE2	1.85	0.58
1:D:2155:LEU:HD22	1:D:2178:LEU:HD11	1.85	0.58
1:A:400:SER:HA	1:A:417:LEU:HD23	1.84	0.58
1:C:2144:CYS:HA	1:C:2182:MET:HE2	1.85	0.58
1:D:780:LEU:O	1:D:784:VAL:HG12	2.03	0.58
1:A:557:TYR:OH	1:A:584:GLN:OE1	2.18	0.58
1:B:892:ILE:HD11	1:B:971:ILE:HG21	1.85	0.58
1:B:2468:HIS:CB	1:B:2479:ILE:HD13	2.34	0.58
1:D:2353:GLU:O	1:D:2357:ASN:ND2	2.37	0.58
1:D:282:LEU:CD2	1:D:434:VAL:HG21	2.33	0.58
1:A:2468:HIS:CB	1:A:2479:ILE:HD13	2.34	0.58
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.84	0.58
1:A:889:LEU:HD11	1:A:1047:VAL:HG12	1.85	0.58
1:C:6:SER:O	1:C:179:VAL:HG22	2.04	0.58
1:D:6:SER:O	1:D:179:VAL:HG22	2.04	0.58
1:A:733:LEU:HD22	1:A:780:LEU:HD22	1.86	0.58
1:A:1203:HIS:CD2	1:A:1245:LEU:HD21	2.38	0.58
1:B:6:SER:O	1:B:179:VAL:HG22	2.04	0.58
1:A:282:LEU:CD2	1:A:434:VAL:HG21	2.33	0.58
1:B:2144:CYS:HA	1:B:2182:MET:HE2	1.85	0.58
1:A:6:SER:O	1:A:179:VAL:HG22	2.04	0.57
1:D:266:ARG:NH2	3:D:2702:I3P:O43	2.36	0.57
1:A:266:ARG:NH2	3:A:2702:I3P:O43	2.36	0.57
1:A:2353:GLU:O	1:A:2357:ASN:ND2	2.37	0.57
1:D:733:LEU:HD22	1:D:780:LEU:HD22	1.86	0.57
1:C:2155:LEU:HD22	1:C:2178:LEU:HD11	1.85	0.57
1:C:2353:GLU:O	1:C:2357:ASN:ND2	2.37	0.57
1:C:2468:HIS:CB	1:C:2479:ILE:HD13	2.34	0.57
1:D:976:GLN:HG2	1:D:1077:LEU:HD11	1.86	0.57
1:A:976:GLN:HG2	1:A:1077:LEU:HD11	1.86	0.57
1:B:1934:VAL:HG21	1:B:1988:LEU:HD13	1.87	0.57
1:B:2353:GLU:O	1:B:2357:ASN:ND2	2.37	0.57
1:A:536:VAL:HG12	1:A:538:LEU:H	1.68	0.57
1:A:1428:MET:CE	1:D:140:PRO:HD2	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:ILE:HD11	1:B:884:LEU:CD2	2.35	0.57
1:B:871:ILE:HD13	1:B:974:ILE:HG23	1.85	0.57
1:B:889:LEU:HD11	1:B:1047:VAL:HG12	1.85	0.57
1:C:976:GLN:HG2	1:C:1077:LEU:HD11	1.86	0.57
1:D:536:VAL:HG12	1:D:538:LEU:H	1.68	0.57
1:D:889:LEU:HD11	1:D:1047:VAL:HG12	1.85	0.57
1:B:1396:VAL:HG22	1:B:1413:TYR:HD2	1.69	0.57
1:B:2155:LEU:HD22	1:B:2178:LEU:HD11	1.85	0.57
1:C:536:VAL:HG12	1:C:538:LEU:H	1.68	0.57
1:A:1396:VAL:HG22	1:A:1413:TYR:HD2	1.69	0.57
1:C:1060:ILE:O	1:C:1063:THR:OG1	2.22	0.57
1:C:1026:ASP:O	1:C:1030:GLU:OE1	2.23	0.57
1:D:2468:HIS:CB	1:D:2479:ILE:HD13	2.33	0.57
1:B:733:LEU:HD22	1:B:780:LEU:HD22	1.86	0.57
1:D:557:TYR:OH	1:D:584:GLN:OE1	2.18	0.57
1:D:1333:VAL:HG13	1:D:1333:VAL:O	2.05	0.57
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.35	0.57
1:A:1100:SER:O	1:A:1104:VAL:HG23	2.05	0.56
1:B:1100:SER:O	1:B:1104:VAL:HG23	2.05	0.56
1:A:1934:VAL:HG21	1:A:1988:LEU:HD13	1.86	0.56
1:A:2155:LEU:HD22	1:A:2178:LEU:HD11	1.85	0.56
1:B:1333:VAL:HG13	1:B:1333:VAL:O	2.05	0.56
1:C:140:PRO:HD2	1:D:1428:MET:CE	2.28	0.56
1:C:733:LEU:HD22	1:C:780:LEU:HD22	1.86	0.56
1:D:1934:VAL:HG21	1:D:1988:LEU:HD13	1.86	0.56
1:A:140:PRO:CD	1:B:1428:MET:HE2	2.33	0.56
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.35	0.56
1:A:1026:ASP:O	1:A:1030:GLU:OE1	2.23	0.56
1:B:976:GLN:HG2	1:B:1077:LEU:HD11	1.86	0.56
1:B:2020:LEU:HD13	1:B:2025:LEU:HD11	1.88	0.56
1:C:889:LEU:HD11	1:C:1047:VAL:HG12	1.85	0.56
1:C:1333:VAL:HG13	1:C:1333:VAL:O	2.05	0.56
1:D:1060:ILE:O	1:D:1063:THR:OG1	2.22	0.56
1:D:1288:HIS:O	1:D:1292:THR:HG22	2.06	0.56
1:B:1288:HIS:O	1:B:1292:THR:HG22	2.06	0.56
1:D:1945:THR:HG22	1:D:1999:LEU:HA	1.87	0.56
1:A:1288:HIS:O	1:A:1292:THR:HG22	2.06	0.56
1:B:252:LEU:HD11	1:B:263:VAL:CG2	2.36	0.56
1:B:2589:TYR:OH	1:B:2593:MET:HE2	2.06	0.56
1:D:2506:ILE:O	1:D:2510:ASN:ND2	2.39	0.56
1:A:252:LEU:HD11	1:A:263:VAL:CG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:LEU:HD13	1:A:2025:LEU:HD11	1.87	0.56
1:B:1026:ASP:O	1:B:1030:GLU:OE1	2.23	0.56
1:B:2506:ILE:O	1:B:2510:ASN:ND2	2.39	0.56
1:B:2511:LEU:HD21	1:C:2362:VAL:HG23	1.86	0.56
1:C:2506:ILE:O	1:C:2510:ASN:ND2	2.39	0.56
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.35	0.56
1:D:1100:SER:O	1:D:1104:VAL:HG23	2.05	0.56
1:D:1396:VAL:HG22	1:D:1413:TYR:HD2	1.69	0.56
1:A:1333:VAL:O	1:A:1333:VAL:HG13	2.05	0.56
1:C:1100:SER:O	1:C:1104:VAL:HG23	2.05	0.56
1:D:252:LEU:HD11	1:D:263:VAL:CG2	2.36	0.56
1:D:1026:ASP:O	1:D:1030:GLU:OE1	2.23	0.56
1:B:536:VAL:HG12	1:B:538:LEU:H	1.68	0.56
1:B:557:TYR:OH	1:B:584:GLN:OE1	2.18	0.56
1:B:1945:THR:HG22	1:B:1999:LEU:HA	1.87	0.56
1:C:2589:TYR:OH	1:C:2593:MET:HE2	2.06	0.56
1:A:2506:ILE:O	1:A:2510:ASN:ND2	2.39	0.56
1:C:1934:VAL:HG21	1:C:1988:LEU:HD13	1.86	0.56
1:C:1945:THR:HG22	1:C:1999:LEU:HA	1.87	0.56
1:B:10:ILE:HD11	1:B:111:VAL:O	2.06	0.56
1:C:252:LEU:HD11	1:C:263:VAL:CG2	2.36	0.56
1:C:1396:VAL:HG22	1:C:1413:TYR:HD2	1.69	0.56
1:D:2004:MET:O	1:D:2059:GLN:NE2	2.39	0.56
1:D:2589:TYR:OH	1:D:2593:MET:HE2	2.06	0.56
1:A:631:LEU:HD11	1:A:728:TYR:CE1	2.41	0.55
1:A:2004:MET:O	1:A:2059:GLN:NE2	2.39	0.55
1:B:406:ASP:OD2	1:B:414:ARG:NH1	2.38	0.55
1:C:2020:LEU:HD13	1:C:2025:LEU:HD11	1.87	0.55
1:B:2004:MET:O	1:B:2059:GLN:NE2	2.39	0.55
1:D:631:LEU:HD11	1:D:728:TYR:CE1	2.41	0.55
1:D:1969:ILE:O	1:D:1973:LEU:HD23	2.06	0.55
1:A:2584:THR:HG22	1:A:2585:GLY:N	2.22	0.55
1:A:2589:TYR:OH	1:A:2593:MET:HE2	2.06	0.55
1:D:1747:GLU:OE1	1:D:1792:ARG:NH2	2.40	0.55
1:A:1085:ARG:NH1	1:A:1613:GLU:OE1	2.40	0.55
1:A:1945:THR:HG22	1:A:1999:LEU:HA	1.87	0.55
1:B:1085:ARG:NH1	1:B:1613:GLU:OE1	2.40	0.55
1:B:2584:THR:HG22	1:B:2585:GLY:N	2.22	0.55
1:A:10:ILE:HD11	1:A:111:VAL:O	2.06	0.55
1:A:109:LYS:HE2	1:A:109:LYS:HA	1.88	0.55
1:C:631:LEU:HD11	1:C:728:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:ARG:NH1	1:C:1613:GLU:OE1	2.40	0.55
1:C:1969:ILE:O	1:C:1973:LEU:HD23	2.06	0.55
1:C:655:CYS:O	1:C:661:ASN:ND2	2.40	0.55
1:C:1288:HIS:O	1:C:1292:THR:HG22	2.06	0.55
1:B:1060:ILE:O	1:B:1063:THR:OG1	2.22	0.55
1:C:2004:MET:O	1:C:2059:GLN:NE2	2.39	0.55
1:D:109:LYS:HA	1:D:109:LYS:HE2	1.88	0.55
1:D:1085:ARG:NH1	1:D:1613:GLU:OE1	2.40	0.55
1:A:406:ASP:OD2	1:A:414:ARG:NH1	2.38	0.55
1:A:424:GLU:OE1	1:A:424:GLU:N	2.40	0.55
1:A:1969:ILE:O	1:A:1973:LEU:HD23	2.06	0.55
1:B:631:LEU:HD11	1:B:728:TYR:CE1	2.41	0.55
1:B:1969:ILE:O	1:B:1973:LEU:HD23	2.06	0.55
1:A:237:GLY:HA2	1:A:287:VAL:HG23	1.89	0.54
1:A:601:ASN:O	1:A:641:ASN:ND2	2.39	0.54
1:A:2511:LEU:HD21	1:B:2362:VAL:CG2	2.35	0.54
1:B:1760:LEU:O	1:B:1768:ILE:HD13	2.08	0.54
1:C:10:ILE:HD11	1:C:111:VAL:O	2.06	0.54
1:D:2020:LEU:HD13	1:D:2025:LEU:HD11	1.87	0.54
1:A:655:CYS:O	1:A:661:ASN:ND2	2.40	0.54
1:A:2155:LEU:CD2	1:A:2178:LEU:HD11	2.38	0.54
1:B:601:ASN:O	1:B:641:ASN:ND2	2.39	0.54
1:C:424:GLU:N	1:C:424:GLU:OE1	2.40	0.54
1:C:601:ASN:O	1:C:641:ASN:ND2	2.39	0.54
1:D:10:ILE:HD11	1:D:111:VAL:O	2.06	0.54
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.38	0.54
1:D:2584:THR:HG22	1:D:2585:GLY:N	2.22	0.54
1:A:2005:GLU:O	1:A:2007:ARG:N	2.40	0.54
1:B:237:GLY:HA2	1:B:287:VAL:HG23	1.89	0.54
1:B:1746:ASN:OD1	1:B:1747:GLU:N	2.41	0.54
1:C:109:LYS:HE2	1:C:109:LYS:HA	1.88	0.54
1:A:1747:GLU:OE1	1:A:1792:ARG:NH2	2.40	0.54
1:B:138:ARG:O	1:C:1427:GLU:HG3	2.07	0.54
1:B:614:GLU:OE1	1:B:614:GLU:N	2.41	0.54
1:C:557:TYR:OH	1:C:584:GLN:OE1	2.18	0.54
1:C:2155:LEU:CD2	1:C:2178:LEU:HD11	2.38	0.54
1:A:1060:ILE:O	1:A:1063:THR:OG1	2.22	0.54
1:A:1746:ASN:OD1	1:A:1747:GLU:N	2.41	0.54
1:B:109:LYS:HA	1:B:109:LYS:HE2	1.88	0.54
1:B:140:PRO:CG	1:C:1428:MET:HE2	2.36	0.54
1:B:2155:LEU:CD2	1:B:2178:LEU:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:CYS:O	1:D:661:ASN:ND2	2.40	0.54
1:D:1760:LEU:O	1:D:1768:ILE:HD13	2.08	0.54
1:A:2490:PHE:CZ	1:B:2460:MET:HE1	2.43	0.54
1:C:1068:ALA:HB3	1:C:1069:PRO:HD3	1.89	0.54
1:D:2051:HIS:NE2	1:D:2121:THR:OG1	2.36	0.54
1:A:1948:CYS:SG	1:A:1959:ILE:HD12	2.48	0.54
1:B:1871:GLN:HB3	1:B:1872:PRO:HD3	1.90	0.54
1:C:92:LYS:HE3	1:C:92:LYS:HA	1.90	0.54
1:C:760:ILE:HG21	1:C:781:MET:HB2	1.90	0.54
1:C:1747:GLU:OE1	1:C:1792:ARG:NH2	2.40	0.54
1:C:1760:LEU:O	1:C:1768:ILE:HD13	2.08	0.54
1:D:92:LYS:HE3	1:D:92:LYS:HA	1.90	0.54
1:D:406:ASP:OD2	1:D:414:ARG:NH1	2.38	0.54
1:D:1871:GLN:HB3	1:D:1872:PRO:HD3	1.90	0.54
1:A:614:GLU:OE1	1:A:614:GLU:N	2.41	0.54
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.48	0.54
1:B:424:GLU:N	1:B:424:GLU:OE1	2.40	0.54
1:D:424:GLU:OE1	1:D:424:GLU:N	2.40	0.54
1:A:398:ILE:CD1	1:A:419:THR:HG22	2.39	0.53
1:C:2584:THR:HG22	1:C:2585:GLY:N	2.22	0.53
1:D:1948:CYS:SG	1:D:1959:ILE:HD12	2.48	0.53
1:B:655:CYS:O	1:B:661:ASN:ND2	2.40	0.53
1:C:398:ILE:CD1	1:C:419:THR:HG22	2.39	0.53
1:C:1746:ASN:OD1	1:C:1747:GLU:N	2.41	0.53
1:A:1068:ALA:HB3	1:A:1069:PRO:HD3	1.89	0.53
1:A:1760:LEU:O	1:A:1768:ILE:HD13	2.08	0.53
1:B:2005:GLU:O	1:B:2007:ARG:N	2.40	0.53
1:D:601:ASN:O	1:D:641:ASN:ND2	2.39	0.53
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	1.90	0.53
1:D:1068:ALA:HB3	1:D:1069:PRO:HD3	1.89	0.53
1:A:1871:GLN:HB3	1:A:1872:PRO:HD3	1.90	0.53
1:B:398:ILE:CD1	1:B:419:THR:HG22	2.39	0.53
1:B:1068:ALA:HB3	1:B:1069:PRO:HD3	1.89	0.53
1:B:2454:ALA:HB1	1:B:2464:THR:OG1	2.09	0.53
1:C:2005:GLU:O	1:C:2007:ARG:N	2.40	0.53
1:B:760:ILE:HG21	1:B:781:MET:HB2	1.90	0.53
1:C:2511:LEU:HD21	1:D:2362:VAL:CG2	2.39	0.53
1:D:398:ILE:CD1	1:D:419:THR:HG22	2.39	0.53
1:D:760:ILE:HG21	1:D:781:MET:HB2	1.90	0.53
1:D:1060:ILE:HG22	1:D:1064:MET:HE2	1.91	0.53
1:A:1060:ILE:HG22	1:A:1064:MET:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:GLU:OE1	1:C:504:GLU:N	2.41	0.53
1:D:237:GLY:HA2	1:D:287:VAL:HG23	1.89	0.53
1:D:2005:GLU:O	1:D:2007:ARG:N	2.40	0.53
1:C:237:GLY:HA2	1:C:287:VAL:HG23	1.89	0.52
1:C:2454:ALA:HB1	1:C:2464:THR:OG1	2.09	0.52
1:D:282:LEU:HD12	1:D:442:LEU:HD22	1.92	0.52
1:A:26:ILE:HG23	1:A:26:ILE:O	2.09	0.52
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.90	0.52
1:B:26:ILE:HG23	1:B:26:ILE:O	2.09	0.52
1:B:1060:ILE:HG22	1:B:1064:MET:HE2	1.91	0.52
1:B:1747:GLU:OE1	1:B:1792:ARG:NH2	2.40	0.52
1:C:1948:CYS:SG	1:C:1959:ILE:HD12	2.48	0.52
1:D:614:GLU:OE1	1:D:614:GLU:N	2.41	0.52
1:D:2454:ALA:HB1	1:D:2464:THR:OG1	2.09	0.52
1:B:140:PRO:CG	1:C:1428:MET:CE	2.88	0.52
1:C:643:ILE:HG13	1:C:644:ALA:H	1.75	0.52
1:D:1746:ASN:OD1	1:D:1747:GLU:N	2.41	0.52
1:A:282:LEU:HD12	1:A:442:LEU:HD22	1.92	0.52
1:A:760:ILE:HG21	1:A:781:MET:HB2	1.90	0.52
1:A:2454:ALA:HB1	1:A:2464:THR:OG1	2.09	0.52
1:B:92:LYS:HE3	1:B:92:LYS:HA	1.90	0.52
1:D:643:ILE:HG13	1:D:644:ALA:H	1.75	0.52
1:C:1060:ILE:HG22	1:C:1064:MET:HE2	1.91	0.52
1:D:26:ILE:O	1:D:26:ILE:HG23	2.09	0.52
1:B:643:ILE:HG13	1:B:644:ALA:H	1.75	0.52
1:B:1974:ILE:HD12	1:B:2000:LEU:CD1	2.38	0.52
1:C:1414:VAL:HG21	1:C:1467:TYR:OH	2.10	0.52
1:A:1089:MET:HE3	1:A:1089:MET:HA	1.92	0.52
1:B:282:LEU:HD12	1:B:442:LEU:HD22	1.92	0.52
1:C:26:ILE:HG23	1:C:26:ILE:O	2.09	0.52
1:D:10:ILE:HD11	1:D:111:VAL:C	2.35	0.52
1:D:164:ILE:HG23	1:D:164:ILE:O	2.10	0.52
1:C:282:LEU:HD12	1:C:442:LEU:HD22	1.92	0.52
1:A:643:ILE:HG13	1:A:644:ALA:H	1.75	0.52
1:D:497:MET:SD	1:D:497:MET:N	2.83	0.52
1:D:504:GLU:N	1:D:504:GLU:OE1	2.41	0.52
1:A:1414:VAL:HG21	1:A:1467:TYR:OH	2.10	0.51
1:A:2051:HIS:NE2	1:A:2121:THR:OG1	2.36	0.51
1:C:406:ASP:OD2	1:C:414:ARG:NH1	2.38	0.51
1:D:1089:MET:HA	1:D:1089:MET:HE3	1.92	0.51
1:D:1414:VAL:HG21	1:D:1467:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:THR:HG23	1:A:1293:HIS:N	2.25	0.51
1:B:10:ILE:HD11	1:B:111:VAL:C	2.35	0.51
1:B:1028:ILE:HD13	1:B:1598:ILE:CD1	2.41	0.51
1:B:1292:THR:HG23	1:B:1293:HIS:N	2.25	0.51
1:D:1292:THR:HG23	1:D:1293:HIS:N	2.25	0.51
1:B:1089:MET:HE3	1:B:1089:MET:HA	1.92	0.51
1:C:10:ILE:HD11	1:C:111:VAL:C	2.35	0.51
1:C:881:LEU:HD22	1:C:978:ILE:CG1	2.41	0.51
1:C:1089:MET:HE3	1:C:1089:MET:HA	1.92	0.51
1:C:1292:THR:HG23	1:C:1293:HIS:N	2.25	0.51
1:D:2162:ASP:OD2	1:D:2169:SER:OG	2.25	0.51
1:A:668:THR:OG1	1:A:729:TYR:OH	2.14	0.51
1:C:1028:ILE:HD13	1:C:1598:ILE:CD1	2.41	0.51
1:C:2490:PHE:CZ	1:D:2460:MET:HE1	2.45	0.51
1:A:10:ILE:HD11	1:A:111:VAL:C	2.35	0.51
1:A:164:ILE:O	1:A:164:ILE:HG23	2.10	0.51
1:C:1974:ILE:HD12	1:C:2000:LEU:CD1	2.38	0.51
1:D:1912:ASP:OD2	1:D:1964:SER:OG	2.27	0.51
1:A:1028:ILE:HD13	1:A:1598:ILE:CD1	2.41	0.51
1:A:2460:MET:HE1	1:D:2490:PHE:CZ	2.46	0.51
1:B:164:ILE:HG23	1:B:164:ILE:O	2.10	0.51
1:B:1414:VAL:HG21	1:B:1467:TYR:OH	2.10	0.51
1:C:164:ILE:HG23	1:C:164:ILE:O	2.10	0.51
1:C:614:GLU:N	1:C:614:GLU:OE1	2.41	0.51
1:A:892:ILE:HD11	1:A:971:ILE:CG2	2.41	0.51
1:A:2362:VAL:CG2	1:D:2511:LEU:HD21	2.40	0.51
1:C:2200:ARG:O	1:C:2204:TRP:NE1	2.44	0.51
1:D:1451:VAL:HG22	1:D:1464:LEU:HD22	1.93	0.51
1:A:2200:ARG:O	1:A:2204:TRP:NE1	2.44	0.51
1:B:1048:ASP:OD2	1:B:1055:PHE:N	2.38	0.51
1:C:2051:HIS:NE2	1:C:2121:THR:OG1	2.36	0.51
1:C:892:ILE:HD11	1:C:971:ILE:CG2	2.41	0.50
1:D:892:ILE:HD11	1:D:971:ILE:CG2	2.41	0.50
1:B:2162:ASP:OD2	1:B:2169:SER:OG	2.25	0.50
1:C:1451:VAL:HG22	1:C:1464:LEU:HD22	1.93	0.50
1:B:458:LYS:HZ1	1:B:464:ILE:HG13	1.77	0.50
1:B:892:ILE:HD11	1:B:971:ILE:CG2	2.41	0.50
1:B:504:GLU:OE1	1:B:504:GLU:N	2.41	0.50
1:B:1451:VAL:HG22	1:B:1464:LEU:HD22	1.93	0.50
1:D:881:LEU:HD22	1:D:978:ILE:CG1	2.41	0.50
1:D:976:GLN:CG	1:D:1077:LEU:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1028:ILE:HD13	1:D:1598:ILE:CD1	2.41	0.50
1:B:2200:ARG:O	1:B:2204:TRP:NE1	2.44	0.50
1:A:458:LYS:HZ1	1:A:464:ILE:HG13	1.77	0.50
1:A:1451:VAL:HG22	1:A:1464:LEU:HD22	1.93	0.50
1:B:1751:GLN:O	1:B:1751:GLN:NE2	2.45	0.50
1:D:1741:ILE:HD11	1:D:1754:ILE:HD13	1.94	0.50
1:B:881:LEU:HD22	1:B:978:ILE:CG1	2.40	0.50
1:C:1751:GLN:O	1:C:1751:GLN:NE2	2.45	0.50
1:D:2200:ARG:O	1:D:2204:TRP:NE1	2.44	0.50
1:A:1751:GLN:O	1:A:1751:GLN:NE2	2.45	0.50
1:A:1912:ASP:OD2	1:A:1964:SER:OG	2.27	0.50
1:A:1974:ILE:HD12	1:A:2000:LEU:CD1	2.38	0.50
1:C:1986:MET:HE2	1:C:1986:MET:HA	1.94	0.50
1:D:1751:GLN:O	1:D:1751:GLN:NE2	2.45	0.50
1:C:1048:ASP:OD2	1:C:1055:PHE:N	2.38	0.50
1:D:1986:MET:HE2	1:D:1986:MET:HA	1.94	0.50
1:A:1617:LEU:O	1:A:1621:LEU:HD23	2.12	0.49
1:B:2054:TYR:CZ	1:B:2058:LEU:HD11	2.47	0.49
1:A:606:LEU:HD22	1:A:640:SER:HB2	1.94	0.49
1:C:1741:ILE:HD11	1:C:1754:ILE:HD13	1.94	0.49
1:D:1974:ILE:HD12	1:D:2000:LEU:CD1	2.38	0.49
1:A:881:LEU:HD22	1:A:978:ILE:CG1	2.40	0.49
1:A:1741:ILE:HD11	1:A:1754:ILE:HD13	1.94	0.49
1:B:1617:LEU:O	1:B:1621:LEU:HD23	2.12	0.49
1:B:2051:HIS:NE2	1:B:2121:THR:OG1	2.36	0.49
1:C:664:ILE:O	1:C:728:TYR:OH	2.23	0.49
1:B:1741:ILE:HD11	1:B:1754:ILE:HD13	1.94	0.49
1:A:504:GLU:OE1	1:A:504:GLU:N	2.41	0.49
1:B:1986:MET:HE2	1:B:1986:MET:HA	1.94	0.49
1:B:1061:HIS:HA	1:B:1064:MET:HE3	1.94	0.49
1:B:1736:LEU:HD12	1:B:1740:LEU:HD13	1.95	0.49
1:C:1298:GLN:N	1:C:1298:GLN:OE1	2.46	0.49
1:B:618:PHE:O	1:B:622:VAL:HG23	2.13	0.49
1:B:1298:GLN:OE1	1:B:1298:GLN:N	2.46	0.49
1:C:976:GLN:CG	1:C:1077:LEU:HD11	2.42	0.49
1:C:2054:TYR:CZ	1:C:2058:LEU:HD11	2.47	0.49
1:D:861:PHE:HA	1:D:967:THR:HG22	1.95	0.49
1:A:599:LEU:HD13	1:A:610:ILE:HG12	1.95	0.49
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.46	0.49
1:B:599:LEU:HD13	1:B:610:ILE:HG12	1.95	0.49
1:C:458:LYS:HZ1	1:C:464:ILE:HG13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2575:VAL:O	1:C:2583:TYR:OH	2.18	0.49
1:C:1061:HIS:HA	1:C:1064:MET:HE3	1.94	0.49
1:D:1617:LEU:O	1:D:1621:LEU:HD23	2.13	0.49
1:A:976:GLN:CG	1:A:1077:LEU:HD11	2.42	0.49
1:A:1085:ARG:HB2	1:A:1610:VAL:HG12	1.95	0.49
1:B:1085:ARG:HB2	1:B:1610:VAL:HG12	1.95	0.49
1:B:1448:MET:HA	1:B:1451:VAL:HG23	1.95	0.49
1:C:599:LEU:HD13	1:C:610:ILE:HG12	1.95	0.49
1:C:618:PHE:O	1:C:622:VAL:HG23	2.13	0.49
1:D:1061:HIS:HA	1:D:1064:MET:HE3	1.94	0.49
1:D:1736:LEU:HD12	1:D:1740:LEU:HD13	1.95	0.49
1:A:2054:TYR:CZ	1:A:2058:LEU:HD11	2.47	0.48
1:B:2490:PHE:CZ	1:C:2460:MET:HE1	2.48	0.48
1:C:965:MET:SD	1:C:1067:TYR:CD2	3.06	0.48
1:A:1448:MET:HA	1:A:1451:VAL:HG23	1.95	0.48
1:C:861:PHE:HA	1:C:967:THR:HG22	1.95	0.48
1:D:1298:GLN:OE1	1:D:1298:GLN:N	2.46	0.48
1:C:1617:LEU:O	1:C:1621:LEU:HD23	2.12	0.48
1:D:815:TYR:OH	1:D:984:ASP:OD2	2.32	0.48
1:D:2054:TYR:CZ	1:D:2058:LEU:HD11	2.47	0.48
1:D:2476:VAL:O	1:D:2480:LEU:HD13	2.14	0.48
1:A:965:MET:SD	1:A:1067:TYR:CD2	3.06	0.48
1:A:1986:MET:HA	1:A:1986:MET:HE2	1.94	0.48
1:A:2476:VAL:O	1:A:2480:LEU:HD13	2.14	0.48
1:C:606:LEU:HD22	1:C:640:SER:HB2	1.94	0.48
1:C:1912:ASP:OD2	1:C:1964:SER:OG	2.27	0.48
1:D:618:PHE:O	1:D:622:VAL:HG23	2.13	0.48
1:B:398:ILE:HD13	1:B:419:THR:HG22	1.95	0.48
1:B:815:TYR:OH	1:B:984:ASP:OD2	2.32	0.48
1:B:976:GLN:CG	1:B:1077:LEU:HD11	2.42	0.48
1:C:1085:ARG:HB2	1:C:1610:VAL:HG12	1.95	0.48
1:D:965:MET:SD	1:D:1067:TYR:CD2	3.06	0.48
1:A:618:PHE:O	1:A:622:VAL:HG23	2.13	0.48
1:B:965:MET:SD	1:B:1067:TYR:CD2	3.06	0.48
1:C:1448:MET:HA	1:C:1451:VAL:HG23	1.95	0.48
1:D:599:LEU:HD13	1:D:610:ILE:HG12	1.95	0.48
1:D:1048:ASP:OD2	1:D:1055:PHE:N	2.38	0.48
1:A:815:TYR:OH	1:A:984:ASP:OD2	2.32	0.48
1:D:606:LEU:HD22	1:D:640:SER:HB2	1.94	0.48
1:D:1085:ARG:HB2	1:D:1610:VAL:HG12	1.95	0.48
1:B:2476:VAL:O	1:B:2480:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1283:LEU:HG	1:C:1320:MET:HE1	1.96	0.48
1:C:1736:LEU:HD12	1:C:1740:LEU:HD13	1.95	0.48
1:A:622:VAL:HG22	1:A:630:PHE:HB3	1.96	0.48
1:A:1061:HIS:HA	1:A:1064:MET:HE3	1.94	0.48
1:D:261:LEU:HD21	1:D:311:THR:HG21	1.96	0.48
1:D:1281:PRO:HD2	1:D:1282:VAL:H	1.79	0.48
1:D:1448:MET:HA	1:D:1451:VAL:HG23	1.95	0.48
1:A:1283:LEU:HG	1:A:1320:MET:HE1	1.96	0.47
1:B:606:LEU:HD22	1:B:640:SER:HB2	1.94	0.47
1:A:861:PHE:HA	1:A:967:THR:HG22	1.95	0.47
1:B:261:LEU:HD21	1:B:311:THR:HG21	1.96	0.47
1:C:622:VAL:HG22	1:C:630:PHE:HB3	1.96	0.47
1:C:885:THR:CG2	1:C:978:ILE:HD13	2.43	0.47
1:C:2476:VAL:O	1:C:2480:LEU:HD13	2.14	0.47
1:D:303:LEU:HD23	1:D:366:LEU:HD22	1.96	0.47
1:D:1422:VAL:O	1:D:1432:TYR:OH	2.28	0.47
1:A:104:ASN:OD1	1:A:105:ASP:N	2.48	0.47
1:A:398:ILE:HD13	1:A:419:THR:HG22	1.96	0.47
1:A:1736:LEU:HD12	1:A:1740:LEU:HD13	1.95	0.47
1:A:2163:GLU:OE1	1:A:2163:GLU:N	2.45	0.47
1:B:622:VAL:HG22	1:B:630:PHE:HB3	1.96	0.47
1:B:861:PHE:HA	1:B:967:THR:HG22	1.95	0.47
1:B:885:THR:CG2	1:B:978:ILE:HD13	2.43	0.47
1:A:262:GLN:OE1	1:A:405:ILE:HG21	2.14	0.47
1:B:104:ASN:OD1	1:B:105:ASP:N	2.48	0.47
1:C:262:GLN:OE1	1:C:405:ILE:HG21	2.14	0.47
1:C:1422:VAL:O	1:C:1432:TYR:OH	2.28	0.47
1:D:622:VAL:HG22	1:D:630:PHE:HB3	1.96	0.47
1:D:2573:VAL:O	1:D:2577:VAL:HG23	2.14	0.47
1:A:2573:VAL:O	1:A:2577:VAL:HG23	2.14	0.47
1:B:1281:PRO:HD2	1:B:1282:VAL:H	1.79	0.47
1:C:815:TYR:OH	1:C:984:ASP:OD2	2.32	0.47
1:D:253:THR:HG22	1:D:281:ALA:HB2	1.97	0.47
1:A:253:THR:HG22	1:A:281:ALA:HB2	1.97	0.47
1:A:261:LEU:HD21	1:A:311:THR:HG21	1.96	0.47
1:A:303:LEU:HD23	1:A:366:LEU:HD22	1.97	0.47
1:A:1924:LEU:HD23	1:A:1924:LEU:H	1.80	0.47
1:B:1283:LEU:HG	1:B:1320:MET:HE1	1.96	0.47
1:C:303:LEU:HD23	1:C:366:LEU:HD22	1.97	0.47
1:D:104:ASN:OD1	1:D:105:ASP:N	2.48	0.47
1:D:1283:LEU:HG	1:D:1320:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:GLU:N	1:A:669:GLU:OE1	2.48	0.47
1:A:1281:PRO:HD2	1:A:1282:VAL:H	1.79	0.47
1:B:303:LEU:HD23	1:B:366:LEU:HD22	1.97	0.47
1:B:669:GLU:N	1:B:669:GLU:OE1	2.48	0.47
1:B:1422:VAL:O	1:B:1432:TYR:OH	2.28	0.47
1:B:2163:GLU:N	1:B:2163:GLU:OE1	2.45	0.47
1:C:253:THR:HG22	1:C:281:ALA:HB2	1.97	0.47
1:C:398:ILE:HD13	1:C:419:THR:HG22	1.95	0.47
1:C:669:GLU:N	1:C:669:GLU:OE1	2.48	0.47
1:D:1924:LEU:H	1:D:1924:LEU:HD23	1.80	0.47
1:D:2163:GLU:OE1	1:D:2163:GLU:N	2.45	0.47
1:B:2573:VAL:O	1:B:2577:VAL:HG23	2.15	0.47
1:C:2163:GLU:OE1	1:C:2163:GLU:N	2.46	0.47
1:C:1965:ASN:CG	1:C:1965:ASN:O	2.58	0.47
1:A:1307:ILE:HD12	1:A:1371:LEU:CD1	2.45	0.47
1:C:261:LEU:HD21	1:C:311:THR:HG21	1.96	0.47
1:C:1281:PRO:HD2	1:C:1282:VAL:H	1.79	0.47
1:D:262:GLN:OE1	1:D:405:ILE:HG21	2.14	0.47
1:A:606:LEU:HD22	1:A:640:SER:CB	2.45	0.46
1:C:2573:VAL:O	1:C:2577:VAL:HG23	2.14	0.46
1:D:669:GLU:OE1	1:D:669:GLU:N	2.48	0.46
1:B:253:THR:HG22	1:B:281:ALA:HB2	1.97	0.46
1:B:606:LEU:HD22	1:B:640:SER:CB	2.45	0.46
1:B:1307:ILE:HD12	1:B:1371:LEU:CD1	2.45	0.46
1:D:1965:ASN:CG	1:D:1965:ASN:O	2.58	0.46
1:B:265:LEU:HD11	1:B:417:LEU:HD21	1.98	0.46
1:C:757:VAL:HG23	1:C:781:MET:HE3	1.97	0.46
1:D:757:VAL:HG23	1:D:781:MET:HE3	1.97	0.46
1:A:885:THR:CG2	1:A:978:ILE:HD13	2.43	0.46
1:C:265:LEU:HD11	1:C:417:LEU:HD21	1.98	0.46
1:C:1464:LEU:O	1:C:1464:LEU:HD23	2.16	0.46
1:D:458:LYS:HZ1	1:D:464:ILE:HG13	1.79	0.46
1:A:664:ILE:O	1:A:728:TYR:OH	2.23	0.46
1:A:1744:THR:HG21	1:A:1749:ILE:HG21	1.98	0.46
1:B:2054:TYR:O	1:B:2058:LEU:HD13	2.16	0.46
1:C:104:ASN:OD1	1:C:105:ASP:N	2.48	0.46
1:C:961:ASP:CB	1:C:964:VAL:HG22	2.46	0.46
1:C:2054:TYR:O	1:C:2058:LEU:HD13	2.16	0.46
1:D:1785:PHE:O	1:D:1788:VAL:HG12	2.16	0.46
1:A:961:ASP:CB	1:A:964:VAL:HG22	2.46	0.46
1:B:1924:LEU:H	1:B:1924:LEU:HD23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:LEU:HD22	1:C:640:SER:CB	2.45	0.46
1:D:1307:ILE:HD12	1:D:1371:LEU:CD1	2.46	0.46
1:A:1965:ASN:CG	1:A:1965:ASN:O	2.58	0.46
1:B:961:ASP:CB	1:B:964:VAL:HG22	2.46	0.46
1:B:1785:PHE:O	1:B:1788:VAL:HG12	2.16	0.46
1:D:961:ASP:CB	1:D:964:VAL:HG22	2.46	0.46
1:D:1744:THR:HG21	1:D:1749:ILE:HG21	1.98	0.46
1:A:757:VAL:HG23	1:A:781:MET:HE3	1.97	0.46
1:A:1245:LEU:HD23	1:A:1245:LEU:C	2.41	0.46
1:B:1965:ASN:CG	1:B:1965:ASN:O	2.58	0.46
1:C:1744:THR:HG21	1:C:1749:ILE:HG21	1.98	0.46
1:C:1924:LEU:HD23	1:C:1924:LEU:H	1.80	0.46
1:D:398:ILE:HD13	1:D:419:THR:HG22	1.96	0.46
1:D:730:ARG:NH1	1:D:772:ASP:OD2	2.49	0.46
1:D:795:THR:HG23	1:D:795:THR:O	2.16	0.46
1:D:2054:TYR:O	1:D:2058:LEU:HD13	2.16	0.46
1:A:1464:LEU:O	1:A:1464:LEU:HD23	2.16	0.46
1:A:1785:PHE:O	1:A:1788:VAL:HG12	2.16	0.46
1:C:1307:ILE:HD12	1:C:1371:LEU:CD1	2.45	0.46
1:A:1048:ASP:OD2	1:A:1055:PHE:N	2.38	0.46
1:B:497:MET:SD	1:B:497:MET:N	2.83	0.46
1:B:1912:ASP:OD2	1:B:1964:SER:OG	2.27	0.46
1:B:2553:VAL:O	1:B:2554:SER:OG	2.22	0.46
1:D:606:LEU:HD22	1:D:640:SER:CB	2.45	0.46
1:B:262:GLN:OE1	1:B:405:ILE:HG21	2.14	0.45
1:B:1245:LEU:C	1:B:1245:LEU:HD23	2.41	0.45
1:B:1464:LEU:HD23	1:B:1464:LEU:O	2.15	0.45
1:D:1464:LEU:HD23	1:D:1464:LEU:O	2.16	0.45
1:A:1650:HIS:O	1:A:1654:LEU:CB	2.65	0.45
1:A:2054:TYR:O	1:A:2058:LEU:HD13	2.16	0.45
1:D:1650:HIS:O	1:D:1654:LEU:CB	2.65	0.45
1:A:730:ARG:NH1	1:A:772:ASP:OD2	2.49	0.45
1:A:795:THR:HG23	1:A:795:THR:O	2.16	0.45
1:B:1681:ASP:N	1:B:1681:ASP:OD1	2.49	0.45
1:B:1744:THR:HG21	1:B:1749:ILE:HG21	1.98	0.45
1:C:2162:ASP:OD2	1:C:2169:SER:OG	2.25	0.45
1:A:265:LEU:HD11	1:A:417:LEU:HD21	1.98	0.45
1:B:2027:ASP:O	1:B:2031:LYS:HE2	2.17	0.45
1:B:795:THR:HG23	1:B:795:THR:O	2.16	0.45
1:C:1287:VAL:HG11	1:C:1324:GLU:HB3	1.99	0.45
1:D:288:VAL:HG21	1:D:366:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:ARG:NH1	1:B:772:ASP:OD2	2.49	0.45
1:B:2511:LEU:HD21	1:C:2362:VAL:CG2	2.47	0.45
1:A:1422:VAL:O	1:A:1432:TYR:OH	2.28	0.45
1:C:1245:LEU:HD23	1:C:1245:LEU:C	2.41	0.45
1:C:2027:ASP:O	1:C:2031:LYS:HE2	2.17	0.45
1:D:2002:ALA:HA	1:D:2005:GLU:HG3	1.99	0.45
1:A:2027:ASP:O	1:A:2031:LYS:HE2	2.17	0.45
1:A:2575:VAL:O	1:A:2583:TYR:OH	2.18	0.45
1:B:1287:VAL:HG11	1:B:1324:GLU:HB3	1.99	0.45
1:A:166:PRO:HB3	1:A:171:ARG:HB2	1.98	0.45
1:A:288:VAL:HG21	1:A:366:LEU:HD21	1.99	0.45
1:B:288:VAL:HG21	1:B:366:LEU:HD21	1.99	0.45
1:B:757:VAL:HG23	1:B:781:MET:HE3	1.97	0.45
1:C:1650:HIS:O	1:C:1654:LEU:CB	2.65	0.45
1:A:1287:VAL:HG11	1:A:1324:GLU:HB3	1.99	0.45
1:A:2002:ALA:HA	1:A:2005:GLU:HG3	1.99	0.45
1:C:288:VAL:HG21	1:C:366:LEU:HD21	1.99	0.45
1:C:1785:PHE:O	1:C:1788:VAL:HG12	2.16	0.45
1:D:265:LEU:HD11	1:D:417:LEU:HD21	1.98	0.45
1:D:2027:ASP:O	1:D:2031:LYS:HE2	2.17	0.45
1:A:1681:ASP:OD1	1:A:1681:ASP:N	2.49	0.44
1:B:140:PRO:HD3	1:C:1426:VAL:CG1	2.47	0.44
1:C:730:ARG:NH1	1:C:772:ASP:OD2	2.49	0.44
1:C:795:THR:HG23	1:C:795:THR:O	2.16	0.44
1:C:2002:ALA:HA	1:C:2005:GLU:HG3	1.99	0.44
1:D:1464:LEU:HD23	1:D:1464:LEU:C	2.42	0.44
1:A:1067:TYR:CD1	1:A:1069:PRO:HD2	2.52	0.44
1:B:1067:TYR:CD1	1:B:1069:PRO:HD2	2.52	0.44
1:B:1451:VAL:HG22	1:B:1464:LEU:CD2	2.48	0.44
1:C:622:VAL:HG22	1:C:630:PHE:CB	2.47	0.44
1:D:1245:LEU:C	1:D:1245:LEU:HD23	2.41	0.44
1:D:1725:GLN:HB3	1:D:1768:ILE:CD1	2.47	0.44
1:B:1464:LEU:HD23	1:B:1464:LEU:C	2.42	0.44
1:B:1650:HIS:O	1:B:1654:LEU:CB	2.65	0.44
1:C:166:PRO:HB3	1:C:171:ARG:HB2	1.98	0.44
1:C:963:VAL:HG13	1:C:964:VAL:N	2.33	0.44
1:D:622:VAL:HG22	1:D:630:PHE:CB	2.47	0.44
1:D:1287:VAL:HG11	1:D:1324:GLU:HB3	1.99	0.44
1:B:144:GLU:OE1	1:B:211:ASN:ND2	2.51	0.44
1:B:166:PRO:HB3	1:B:171:ARG:HB2	1.98	0.44
1:B:961:ASP:HB3	1:B:964:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:TYR:HA	1:C:748:ILE:HB	2.00	0.44
1:D:961:ASP:HB3	1:D:964:VAL:HG22	2.00	0.44
1:A:696:TRP:HZ2	1:A:711:LEU:HD11	1.83	0.44
1:C:961:ASP:HB3	1:C:964:VAL:HG22	2.00	0.44
1:C:1451:VAL:HG22	1:C:1464:LEU:CD2	2.48	0.44
1:C:1464:LEU:HD23	1:C:1464:LEU:C	2.42	0.44
1:C:1725:GLN:HB3	1:C:1768:ILE:CD1	2.47	0.44
1:D:166:PRO:HB3	1:D:171:ARG:HB2	1.98	0.44
1:D:892:ILE:CD1	1:D:971:ILE:HG21	2.47	0.44
1:D:2553:VAL:HG13	1:D:2554:SER:N	2.33	0.44
1:A:961:ASP:HB3	1:A:964:VAL:HG22	2.00	0.44
1:C:144:GLU:OE1	1:C:211:ASN:ND2	2.51	0.44
1:B:1945:THR:HG22	1:B:1999:LEU:CA	2.48	0.44
1:B:2002:ALA:HA	1:B:2005:GLU:HG3	1.99	0.44
1:C:1067:TYR:CD1	1:C:1069:PRO:HD2	2.52	0.44
1:D:1067:TYR:CD1	1:D:1069:PRO:HD2	2.52	0.44
1:D:1784:ARG:HA	1:D:1787:LYS:HB3	2.00	0.44
1:A:1626:LEU:HB2	1:A:1695:LEU:HD22	2.00	0.44
1:A:1725:GLN:HB3	1:A:1768:ILE:CD1	2.47	0.44
1:A:1784:ARG:HA	1:A:1787:LYS:HB3	2.00	0.44
1:D:745:TYR:HA	1:D:748:ILE:HB	2.00	0.44
1:D:1279:SER:OG	1:D:1282:VAL:HG12	2.18	0.44
1:A:622:VAL:HG22	1:A:630:PHE:CB	2.47	0.43
1:A:840:TYR:O	1:A:844:VAL:HG23	2.18	0.43
1:A:892:ILE:CD1	1:A:971:ILE:HG21	2.47	0.43
1:A:1945:THR:HG22	1:A:1999:LEU:CA	2.48	0.43
1:A:2020:LEU:CD1	1:A:2025:LEU:HD11	2.48	0.43
1:B:840:TYR:O	1:B:844:VAL:HG23	2.18	0.43
1:B:1279:SER:OG	1:B:1282:VAL:HG12	2.18	0.43
1:B:2553:VAL:HG13	1:B:2554:SER:N	2.33	0.43
1:D:144:GLU:OE1	1:D:211:ASN:ND2	2.51	0.43
1:D:1681:ASP:N	1:D:1681:ASP:OD1	2.49	0.43
1:A:1464:LEU:HD23	1:A:1464:LEU:C	2.42	0.43
1:B:745:TYR:HA	1:B:748:ILE:HB	2.00	0.43
1:C:1925:LEU:HD21	1:C:1973:LEU:HD13	2.00	0.43
1:D:696:TRP:HZ2	1:D:711:LEU:HD11	1.83	0.43
1:D:1451:VAL:HG22	1:D:1464:LEU:CD2	2.48	0.43
1:A:46:ASP:OD1	1:A:47:ASN:N	2.52	0.43
1:A:1451:VAL:HG22	1:A:1464:LEU:CD2	2.48	0.43
1:B:622:VAL:HG22	1:B:630:PHE:CB	2.47	0.43
1:B:696:TRP:HZ2	1:B:711:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1784:ARG:HA	1:B:1787:LYS:HB3	2.00	0.43
1:C:1681:ASP:OD1	1:C:1681:ASP:N	2.49	0.43
1:C:1945:THR:HG22	1:C:1999:LEU:CA	2.48	0.43
1:A:144:GLU:OE1	1:A:211:ASN:ND2	2.51	0.43
1:A:2225:TYR:OH	1:A:2338:GLU:OE1	2.29	0.43
1:A:2553:VAL:HG13	1:A:2554:SER:N	2.33	0.43
1:B:476:LEU:O	1:B:480:VAL:HG23	2.18	0.43
1:B:1925:LEU:HD21	1:B:1973:LEU:HD13	2.00	0.43
1:C:2553:VAL:HG13	1:C:2554:SER:N	2.33	0.43
1:A:497:MET:SD	1:A:497:MET:N	2.83	0.43
1:B:963:VAL:HG13	1:B:964:VAL:N	2.33	0.43
1:D:668:THR:OG1	1:D:729:TYR:OH	2.14	0.43
1:D:1322:MET:HE1	1:D:1387:CYS:SG	2.59	0.43
1:D:1925:LEU:HD21	1:D:1973:LEU:HD13	2.00	0.43
1:A:1322:MET:HE1	1:A:1387:CYS:SG	2.59	0.43
1:B:46:ASP:OD1	1:B:47:ASN:N	2.52	0.43
1:B:572:GLU:O	1:B:576:LYS:HD2	2.19	0.43
1:C:572:GLU:O	1:C:576:LYS:HD2	2.19	0.43
1:C:1956:GLN:NE2	1:C:2002:ALA:O	2.51	0.43
1:A:745:TYR:HA	1:A:748:ILE:HB	2.00	0.43
1:A:963:VAL:HG13	1:A:964:VAL:N	2.33	0.43
1:B:1725:GLN:HB3	1:B:1768:ILE:CD1	2.47	0.43
1:B:2454:ALA:O	1:B:2460:MET:CG	2.67	0.43
1:C:46:ASP:OD1	1:C:47:ASN:N	2.52	0.43
1:C:840:TYR:O	1:C:844:VAL:HG23	2.18	0.43
1:D:1977:ASP:OD1	1:D:1977:ASP:N	2.51	0.43
1:A:476:LEU:O	1:A:480:VAL:HG23	2.18	0.43
1:B:1626:LEU:HB2	1:B:1695:LEU:HD22	2.00	0.43
1:C:476:LEU:O	1:C:480:VAL:HG23	2.18	0.43
1:C:696:TRP:HZ2	1:C:711:LEU:HD11	1.83	0.43
1:C:1281:PRO:HA	1:C:1284:GLN:HG3	2.01	0.43
1:D:1626:LEU:HB2	1:D:1695:LEU:HD22	2.00	0.43
1:A:1279:SER:OG	1:A:1282:VAL:HG12	2.18	0.43
1:B:257:TYR:OH	1:B:408:GLU:OE1	2.36	0.43
1:B:1646:LYS:O	1:B:1650:HIS:CD2	2.72	0.43
1:D:963:VAL:HG13	1:D:964:VAL:N	2.33	0.43
1:D:1443:ASN:C	1:D:1443:ASN:HD22	2.26	0.43
1:D:1646:LYS:O	1:D:1650:HIS:CD2	2.72	0.43
1:A:1393:LEU:O	1:A:1397:VAL:HG23	2.19	0.43
1:B:1443:ASN:HD22	1:B:1443:ASN:C	2.26	0.43
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:892:ILE:CD1	1:C:971:ILE:HG21	2.47	0.43
1:C:1089:MET:HE3	1:C:1089:MET:CA	2.49	0.43
1:C:1626:LEU:HB2	1:C:1695:LEU:HD22	2.00	0.43
1:D:476:LEU:O	1:D:480:VAL:HG23	2.18	0.43
1:D:840:TYR:O	1:D:844:VAL:HG23	2.18	0.43
1:D:1393:LEU:O	1:D:1397:VAL:HG23	2.19	0.43
1:C:987:ILE:HD11	1:C:1091:THR:OG1	2.19	0.42
1:C:1322:MET:HE1	1:C:1387:CYS:SG	2.59	0.42
1:C:1393:LEU:O	1:C:1397:VAL:HG23	2.19	0.42
1:C:2020:LEU:CD1	1:C:2025:LEU:HD11	2.48	0.42
1:D:1945:THR:HG22	1:D:1999:LEU:CA	2.48	0.42
1:B:987:ILE:HD11	1:B:1091:THR:OG1	2.19	0.42
1:B:1322:MET:HE1	1:B:1387:CYS:SG	2.59	0.42
1:B:2020:LEU:CD1	1:B:2025:LEU:HD11	2.48	0.42
1:C:1607:LYS:O	1:C:1610:VAL:HG22	2.19	0.42
1:C:1933:ASN:O	1:C:1937:VAL:HG23	2.19	0.42
1:C:2454:ALA:O	1:C:2460:MET:CG	2.67	0.42
1:A:474:GLN:NE2	1:A:478:ASP:OD1	2.52	0.42
1:A:1099:ILE:HG13	1:A:1100:SER:N	2.34	0.42
1:B:1099:ILE:HG13	1:B:1100:SER:N	2.34	0.42
1:B:1950:GLY:O	1:B:1951:PRO:C	2.62	0.42
1:C:1279:SER:OG	1:C:1282:VAL:HG12	2.18	0.42
1:C:1646:LYS:O	1:C:1650:HIS:CD2	2.72	0.42
1:C:2212:ALA:O	1:C:2216:ASN:ND2	2.48	0.42
1:D:2020:LEU:CD1	1:D:2025:LEU:HD11	2.48	0.42
1:A:257:TYR:OH	1:A:408:GLU:OE1	2.36	0.42
1:A:572:GLU:O	1:A:576:LYS:HD2	2.19	0.42
1:A:1646:LYS:O	1:A:1650:HIS:CD2	2.72	0.42
1:A:1925:LEU:HD21	1:A:1973:LEU:HD13	2.00	0.42
1:A:1950:GLY:O	1:A:1951:PRO:C	2.62	0.42
1:B:1933:ASN:O	1:B:1937:VAL:HG23	2.19	0.42
1:C:1334:VAL:O	1:C:1334:VAL:HG13	2.20	0.42
1:C:1448:MET:HG3	1:C:1468:VAL:HG11	2.02	0.42
1:C:1784:ARG:HA	1:C:1787:LYS:HB3	2.00	0.42
1:C:1950:GLY:O	1:C:1951:PRO:C	2.62	0.42
1:D:1334:VAL:O	1:D:1334:VAL:HG13	2.20	0.42
1:A:171:ARG:NH2	1:B:372:THR:O	2.46	0.42
1:A:1281:PRO:HA	1:A:1284:GLN:HG3	2.01	0.42
1:A:1442:GLU:O	1:A:1445:THR:OG1	2.34	0.42
1:A:1933:ASN:O	1:A:1937:VAL:HG23	2.19	0.42
1:B:1607:LYS:O	1:B:1610:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:GLN:NE2	1:C:478:ASP:OD1	2.52	0.42
1:A:1607:LYS:O	1:A:1610:VAL:HG22	2.20	0.42
1:B:138:ARG:HD3	1:C:1427:GLU:HG2	2.01	0.42
1:B:1393:LEU:O	1:B:1397:VAL:HG23	2.19	0.42
1:C:1907:THR:HG21	1:C:1947:TYR:HE2	1.85	0.42
1:D:46:ASP:OD1	1:D:47:ASN:N	2.52	0.42
1:B:153:ASP:OD1	1:B:156:GLY:N	2.50	0.42
1:B:892:ILE:CD1	1:B:971:ILE:HG21	2.47	0.42
1:C:642:HIS:O	1:C:642:HIS:ND1	2.53	0.42
1:C:2529:LYS:O	1:C:2532:GLU:HG3	2.19	0.42
1:D:572:GLU:O	1:D:576:LYS:HD2	2.19	0.42
1:D:1099:ILE:HG13	1:D:1100:SER:N	2.34	0.42
1:D:1307:ILE:O	1:D:1314:VAL:HG22	2.20	0.42
1:D:2454:ALA:O	1:D:2460:MET:CG	2.67	0.42
1:D:2529:LYS:O	1:D:2532:GLU:HG3	2.19	0.42
1:A:653:CYS:SG	1:A:747:ALA:HB2	2.60	0.42
1:A:987:ILE:HD11	1:A:1091:THR:OG1	2.19	0.42
1:A:2162:ASP:OD2	1:A:2169:SER:OG	2.25	0.42
1:B:1089:MET:HE3	1:B:1089:MET:CA	2.49	0.42
1:C:653:CYS:SG	1:C:747:ALA:HB2	2.60	0.42
1:C:1099:ILE:HG13	1:C:1100:SER:N	2.34	0.42
1:C:1738:CYS:O	1:C:1742:THR:HG22	2.20	0.42
1:D:987:ILE:HD11	1:D:1091:THR:OG1	2.19	0.42
1:D:1950:GLY:O	1:D:1951:PRO:C	2.62	0.42
1:A:1307:ILE:O	1:A:1314:VAL:HG22	2.20	0.42
1:A:2529:LYS:O	1:A:2532:GLU:HG3	2.19	0.42
1:B:1281:PRO:HA	1:B:1284:GLN:HG3	2.01	0.42
1:D:1281:PRO:HA	1:D:1284:GLN:HG3	2.01	0.42
1:D:1607:LYS:O	1:D:1610:VAL:HG22	2.19	0.42
1:A:642:HIS:O	1:A:642:HIS:ND1	2.53	0.42
1:A:2454:ALA:O	1:A:2460:MET:CG	2.67	0.42
1:B:642:HIS:ND1	1:B:642:HIS:O	2.53	0.42
1:B:1448:MET:HG3	1:B:1468:VAL:HG11	2.02	0.42
1:B:2529:LYS:O	1:B:2532:GLU:HG3	2.19	0.42
1:D:642:HIS:O	1:D:642:HIS:ND1	2.53	0.42
1:D:1907:THR:HG21	1:D:1947:TYR:HE2	1.85	0.42
1:D:1933:ASN:O	1:D:1937:VAL:HG23	2.19	0.42
1:A:494:LEU:HD21	1:A:554:ARG:HB3	2.02	0.41
1:A:1772:PHE:O	1:A:1776:MET:HG3	2.20	0.41
1:B:1738:CYS:O	1:B:1742:THR:HG22	2.20	0.41
1:B:2321:LEU:HA	1:B:2324:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:CYS:SG	1:D:747:ALA:HB2	2.60	0.41
1:D:1448:MET:HG3	1:D:1468:VAL:HG11	2.02	0.41
1:A:1089:MET:HE3	1:A:1089:MET:CA	2.49	0.41
1:B:1334:VAL:O	1:B:1334:VAL:HG13	2.20	0.41
1:B:1937:VAL:CG1	1:B:1992:LEU:HD11	2.50	0.41
1:C:580:MET:HG3	1:C:581:MET:N	2.36	0.41
1:C:1937:VAL:CG1	1:C:1992:LEU:HD11	2.50	0.41
1:D:474:GLN:NE2	1:D:478:ASP:OD1	2.52	0.41
1:D:885:THR:CG2	1:D:978:ILE:HD13	2.43	0.41
1:D:1650:HIS:CD2	1:D:1650:HIS:N	2.88	0.41
1:D:1772:PHE:O	1:D:1776:MET:HG3	2.20	0.41
1:A:2385:ILE:CD1	1:B:2342:SER:OG	2.68	0.41
1:B:474:GLN:NE2	1:B:478:ASP:OD1	2.52	0.41
1:C:858:LYS:O	1:C:862:GLU:OE1	2.39	0.41
1:D:1494:HIS:O	1:D:1498:VAL:HG23	2.21	0.41
1:D:1937:VAL:CG1	1:D:1992:LEU:HD11	2.50	0.41
1:A:1334:VAL:O	1:A:1334:VAL:HG13	2.20	0.41
1:A:2212:ALA:O	1:A:2216:ASN:ND2	2.48	0.41
1:B:1907:THR:HG21	1:B:1947:TYR:HE2	1.85	0.41
1:C:1443:ASN:C	1:C:1443:ASN:HD22	2.26	0.41
1:C:1494:HIS:O	1:C:1498:VAL:HG23	2.21	0.41
1:D:1028:ILE:HG13	1:D:1029:GLY:N	2.36	0.41
1:A:1448:MET:HG3	1:A:1468:VAL:HG11	2.02	0.41
1:B:2376:ALA:HB2	1:B:2508:VAL:HG11	2.02	0.41
1:C:2321:LEU:HA	1:C:2324:VAL:HG22	2.02	0.41
1:D:2014:GLU:O	1:D:2018:ILE:HG13	2.21	0.41
1:D:141:ALA:HB3	1:D:144:GLU:O	2.21	0.41
1:A:2014:GLU:O	1:A:2018:ILE:HG13	2.21	0.41
1:B:580:MET:HG3	1:B:581:MET:N	2.36	0.41
1:B:1494:HIS:O	1:B:1498:VAL:HG23	2.21	0.41
1:B:2014:GLU:O	1:B:2018:ILE:HG13	2.21	0.41
1:B:2027:ASP:HB3	1:B:2031:LYS:HZ1	1.86	0.41
1:B:2212:ALA:O	1:B:2216:ASN:ND2	2.48	0.41
1:C:1062:LEU:O	1:C:1065:HIS:HB2	2.21	0.41
1:C:1307:ILE:O	1:C:1314:VAL:HG22	2.20	0.41
1:D:858:LYS:O	1:D:862:GLU:OE1	2.39	0.41
1:D:1745:LYS:HA	1:D:1745:LYS:HD3	1.95	0.41
1:A:1254:LEU:HD21	1:A:1282:VAL:HG23	2.03	0.41
1:B:2490:PHE:O	1:B:2494:VAL:HG23	2.21	0.41
1:C:257:TYR:OH	1:C:408:GLU:OE1	2.36	0.41
1:C:497:MET:SD	1:C:497:MET:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1089:MET:HE3	1:D:1089:MET:CA	2.49	0.41
1:A:141:ALA:HB3	1:A:144:GLU:O	2.21	0.41
1:A:580:MET:HG3	1:A:581:MET:N	2.36	0.41
1:A:637:LEU:O	1:A:648:THR:HG21	2.21	0.41
1:A:991:LEU:HD11	1:A:1095:VAL:HG21	2.03	0.41
1:A:1937:VAL:CG1	1:A:1992:LEU:HD11	2.50	0.41
1:A:2025:LEU:O	1:A:2028:VAL:HG12	2.21	0.41
1:B:1650:HIS:CD2	1:B:1650:HIS:N	2.88	0.41
1:C:888:LEU:HB3	1:C:971:ILE:HG23	2.03	0.41
1:C:1650:HIS:CD2	1:C:1650:HIS:N	2.88	0.41
1:D:494:LEU:HD21	1:D:554:ARG:HB3	2.02	0.41
1:D:1254:LEU:HD21	1:D:1282:VAL:HG23	2.03	0.41
1:D:2025:LEU:O	1:D:2028:VAL:HG12	2.21	0.41
1:A:1062:LEU:O	1:A:1065:HIS:HB2	2.21	0.41
1:A:2490:PHE:O	1:A:2494:VAL:HG23	2.21	0.41
1:B:653:CYS:SG	1:B:747:ALA:HB2	2.60	0.41
1:B:1307:ILE:O	1:B:1314:VAL:HG22	2.20	0.41
1:B:1772:PHE:O	1:B:1776:MET:HG3	2.20	0.41
1:D:642:HIS:O	1:D:642:HIS:CG	2.74	0.41
1:A:1607:LYS:HA	1:A:1610:VAL:HG22	2.03	0.40
1:A:1957:THR:HA	1:A:1960:VAL:HG22	2.04	0.40
1:B:991:LEU:HD11	1:B:1095:VAL:HG21	2.03	0.40
1:B:1062:LEU:O	1:B:1065:HIS:HB2	2.21	0.40
1:C:1490:SER:O	1:C:1491:LEU:C	2.64	0.40
1:D:242:ARG:HB2	1:D:432:VAL:CG2	2.51	0.40
1:D:888:LEU:HB3	1:D:971:ILE:HG23	2.03	0.40
1:D:1797:GLN:NE2	1:D:1906:GLU:O	2.55	0.40
1:A:1494:HIS:O	1:A:1498:VAL:HG23	2.21	0.40
1:A:1738:CYS:O	1:A:1742:THR:HG22	2.20	0.40
1:B:242:ARG:HB2	1:B:432:VAL:CG2	2.51	0.40
1:B:1443:ASN:O	1:B:1443:ASN:ND2	2.54	0.40
1:B:1490:SER:O	1:B:1491:LEU:C	2.65	0.40
1:C:1028:ILE:HG13	1:C:1029:GLY:N	2.36	0.40
1:D:580:MET:HG3	1:D:581:MET:N	2.36	0.40
1:D:2376:ALA:HB2	1:D:2508:VAL:HG11	2.03	0.40
1:A:6:SER:HA	1:B:374:LEU:HD11	2.03	0.40
1:A:234:VAL:HG12	1:A:235:LEU:N	2.37	0.40
1:A:1028:ILE:HG13	1:A:1029:GLY:N	2.36	0.40
1:A:2020:LEU:O	1:A:2020:LEU:HD12	2.22	0.40
1:B:234:VAL:HG12	1:B:235:LEU:N	2.37	0.40
1:C:643:ILE:HG13	1:C:644:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1607:LYS:HA	1:C:1610:VAL:HG22	2.03	0.40
1:C:1772:PHE:O	1:C:1776:MET:HG3	2.21	0.40
1:D:637:LEU:O	1:D:648:THR:HG21	2.21	0.40
1:D:1738:CYS:O	1:D:1742:THR:HG22	2.20	0.40
1:D:2321:LEU:HA	1:D:2324:VAL:HG22	2.02	0.40
1:A:1797:GLN:NE2	1:A:1906:GLU:O	2.55	0.40
1:A:1904:VAL:O	1:A:1907:THR:HG22	2.22	0.40
1:A:1907:THR:HG21	1:A:1947:TYR:HE2	1.85	0.40
1:B:242:ARG:HB2	1:B:432:VAL:HG22	2.04	0.40
1:B:494:LEU:HD21	1:B:554:ARG:HB3	2.02	0.40
1:B:2025:LEU:O	1:B:2028:VAL:HG12	2.21	0.40
1:C:642:HIS:O	1:C:642:HIS:CG	2.74	0.40
1:C:2014:GLU:O	1:C:2018:ILE:HG13	2.21	0.40
1:D:431:ILE:O	1:D:431:ILE:HG22	2.21	0.40
1:D:640:SER:HB3	1:D:645:ILE:HG13	2.03	0.40
1:D:1062:LEU:O	1:D:1065:HIS:HB2	2.21	0.40
1:D:2212:ALA:O	1:D:2216:ASN:ND2	2.48	0.40
1:A:642:HIS:O	1:A:642:HIS:CG	2.74	0.40
1:A:1956:GLN:NE2	1:A:2003:LEU:O	2.55	0.40
1:B:107:GLU:O	1:B:111:VAL:HG12	2.21	0.40
1:B:858:LYS:O	1:B:862:GLU:OE1	2.39	0.40
1:B:1028:ILE:HG13	1:B:1029:GLY:N	2.36	0.40
1:B:1607:LYS:HA	1:B:1610:VAL:HG22	2.03	0.40
1:C:494:LEU:HD21	1:C:554:ARG:HB3	2.02	0.40
1:C:2025:LEU:O	1:C:2028:VAL:HG12	2.21	0.40
1:C:2376:ALA:HB2	1:C:2508:VAL:HG11	2.03	0.40
1:C:2490:PHE:O	1:C:2494:VAL:HG23	2.21	0.40
1:D:1066:ASP:OD1	1:D:1066:ASP:N	2.54	0.40
1:D:1307:ILE:HD12	1:D:1371:LEU:HD12	2.04	0.40
1:D:1956:GLN:NE2	1:D:2003:LEU:O	2.55	0.40
1:D:1957:THR:HA	1:D:1960:VAL:HG22	2.04	0.40
1:D:2575:VAL:O	1:D:2583:TYR:OH	2.18	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	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	B	1995/2633 (76%)	1912 (96%)	83 (4%)	0	100	100
1	C	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
1	D	1995/2633 (76%)	1913 (96%)	82 (4%)	0	100	100
All	All	7980/10532 (76%)	7651 (96%)	329 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1865/2329 (80%)	1865 (100%)	0	100	100
1	B	1865/2329 (80%)	1865 (100%)	0	100	100
1	C	1865/2329 (80%)	1865 (100%)	0	100	100
1	D	1865/2329 (80%)	1865 (100%)	0	100	100
All	All	7460/9316 (80%)	7460 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	384	ASN
1	A	474	GLN
1	A	701	ASN
1	A	744	GLN
1	A	820	ASN

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Mol	Chain	Res	Type
1	A	1061	HIS
1	A	1084	GLN
1	A	1243	GLN
1	A	1249	HIS
1	A	1487	ASN
1	A	1930	ASN
1	A	1976	ASN
1	A	2120	HIS
1	A	2179	HIS
1	A	2289	ASN
1	B	112	HIS
1	B	384	ASN
1	B	474	GLN
1	B	744	GLN
1	B	820	ASN
1	B	868	HIS
1	B	1061	HIS
1	B	1084	GLN
1	B	1243	GLN
1	B	1249	HIS
1	B	1487	ASN
1	B	1902	ASN
1	B	1930	ASN
1	B	1976	ASN
1	B	2120	HIS
1	B	2179	HIS
1	B	2289	ASN
1	C	112	HIS
1	C	384	ASN
1	C	744	GLN
1	C	820	ASN
1	C	1061	HIS
1	C	1084	GLN
1	C	1243	GLN
1	C	1487	ASN
1	C	1773	HIS
1	C	1976	ASN
1	C	2120	HIS
1	C	2179	HIS
1	C	2289	ASN
1	D	112	HIS
1	D	384	ASN

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Mol	Chain	Res	Type
1	D	474	GLN
1	D	744	GLN
1	D	820	ASN
1	D	1061	HIS
1	D	1084	GLN
1	D	1243	GLN
1	D	1487	ASN
1	D	1773	HIS
1	D	1976	ASN
1	D	2179	HIS
1	D	2289	ASN

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 12 ligands modelled in this entry, 4 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	D	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	D	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	I3P	A	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
3	I3P	C	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
3	I3P	B	2702	-	24,24,24	1.28	3 (12%)	39,39,39	0.73	0
4	ATP	C	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)
4	ATP	A	2703	-	32,33,33	0.35	0	48,52,52	0.69	1 (2%)
4	ATP	B	2703	-	32,33,33	0.35	0	48,52,52	0.69	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	D	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	D	2703	-	-	4/22/38/38	0/3/3/3
3	I3P	A	2702	-	-	3/15/39/39	0/1/1/1
3	I3P	C	2702	-	-	4/15/39/39	0/1/1/1
3	I3P	B	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	C	2703	-	-	4/22/38/38	0/3/3/3
4	ATP	A	2703	-	-	4/22/38/38	0/3/3/3
4	ATP	B	2703	-	-	4/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2702	I3P	P4-O4	3.10	1.65	1.59
3	A	2702	I3P	P4-O4	3.07	1.64	1.59
3	C	2702	I3P	P4-O4	3.07	1.64	1.59
3	D	2702	I3P	P4-O4	3.07	1.64	1.59
3	A	2702	I3P	P5-O5	2.99	1.64	1.59
3	D	2702	I3P	P5-O5	2.99	1.64	1.59
3	A	2702	I3P	P1-O1	2.97	1.64	1.59
3	C	2702	I3P	P1-O1	2.97	1.64	1.59
3	D	2702	I3P	P1-O1	2.97	1.64	1.59
3	B	2702	I3P	P5-O5	2.97	1.64	1.59
3	C	2702	I3P	P5-O5	2.96	1.64	1.59
3	B	2702	I3P	P1-O1	2.92	1.64	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2703	ATP	O3'-C3'-C2'	-2.03	105.32	111.82
4	D	2703	ATP	O3'-C3'-C2'	-2.03	105.32	111.82
4	A	2703	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
4	B	2703	ATP	O3'-C3'-C2'	-2.02	105.33	111.82

There are no chirality outliers.

All (29) torsion outliers are listed below:

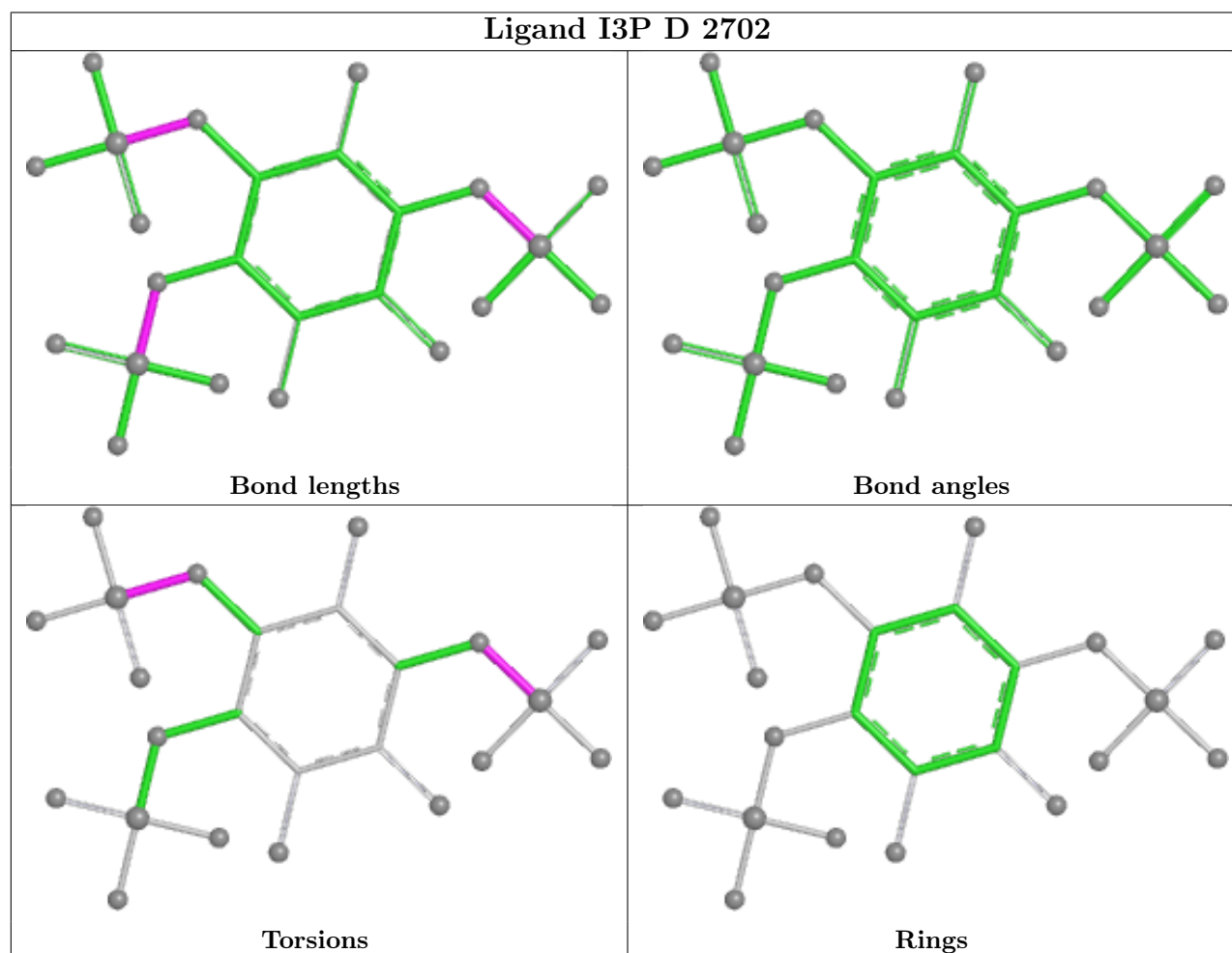
Mol	Chain	Res	Type	Atoms
4	A	2703	ATP	O4'-C4'-C5'-O5'
4	B	2703	ATP	O4'-C4'-C5'-O5'
4	C	2703	ATP	O4'-C4'-C5'-O5'
4	D	2703	ATP	O4'-C4'-C5'-O5'
4	A	2703	ATP	PB-O3A-PA-O5'
4	B	2703	ATP	PB-O3A-PA-O5'
4	C	2703	ATP	PB-O3A-PA-O5'
4	D	2703	ATP	PB-O3A-PA-O5'
4	A	2703	ATP	C5'-O5'-PA-O1A
4	B	2703	ATP	C5'-O5'-PA-O1A
4	C	2703	ATP	C5'-O5'-PA-O1A
4	D	2703	ATP	C5'-O5'-PA-O1A
3	A	2702	I3P	C1-O1-P1-O12
3	A	2702	I3P	C5-O5-P5-O53
3	B	2702	I3P	C1-O1-P1-O12
3	B	2702	I3P	C5-O5-P5-O53
3	C	2702	I3P	C1-O1-P1-O12
3	C	2702	I3P	C5-O5-P5-O53
3	D	2702	I3P	C1-O1-P1-O12
3	D	2702	I3P	C5-O5-P5-O53
3	C	2702	I3P	C1-O1-P1-O13
3	A	2702	I3P	C1-O1-P1-O11
3	B	2702	I3P	C1-O1-P1-O11
3	C	2702	I3P	C1-O1-P1-O11
3	D	2702	I3P	C1-O1-P1-O11
4	B	2703	ATP	C3'-C4'-C5'-O5'
4	D	2703	ATP	C3'-C4'-C5'-O5'
4	A	2703	ATP	C3'-C4'-C5'-O5'
4	C	2703	ATP	C3'-C4'-C5'-O5'

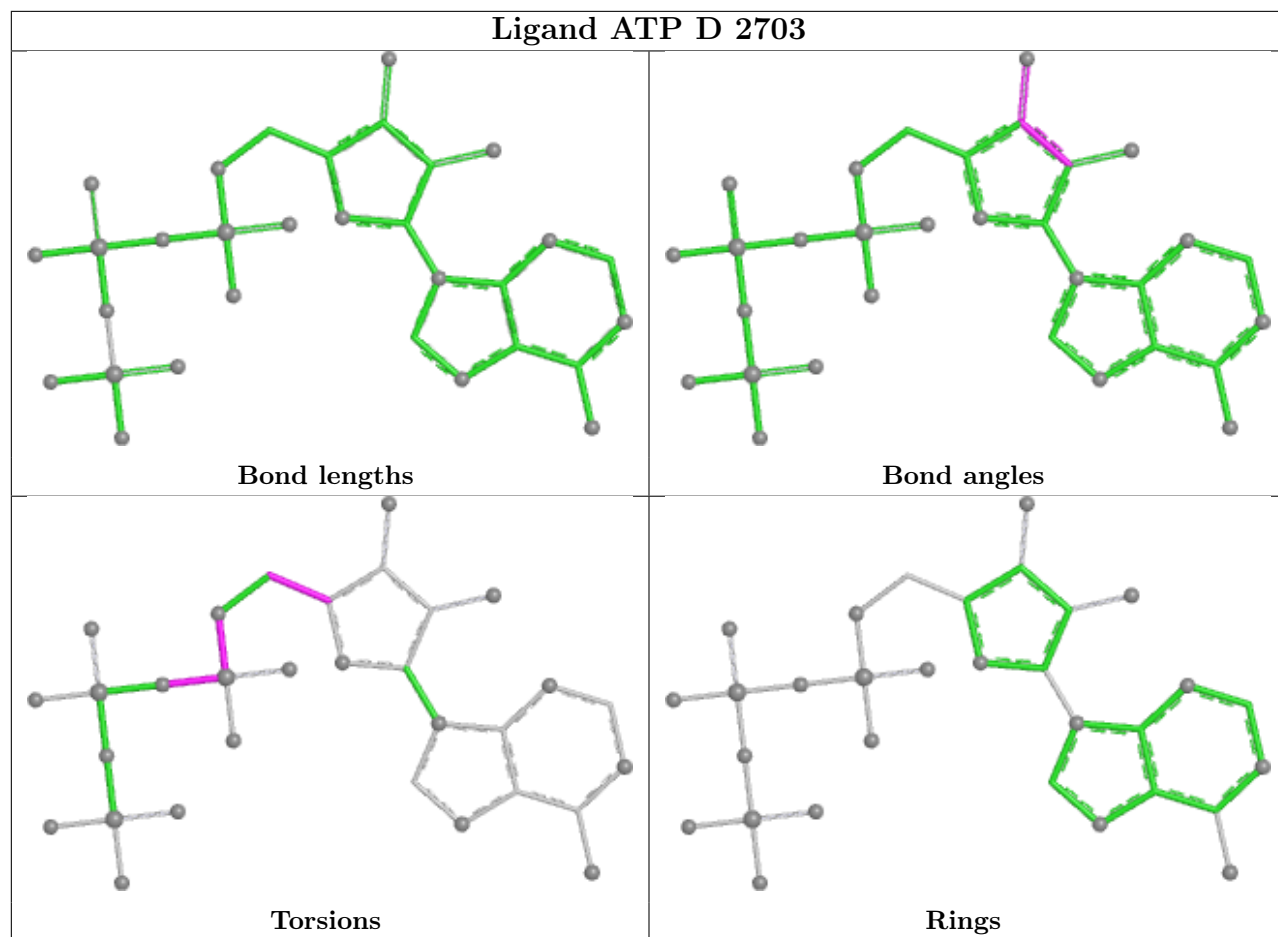
There are no ring outliers.

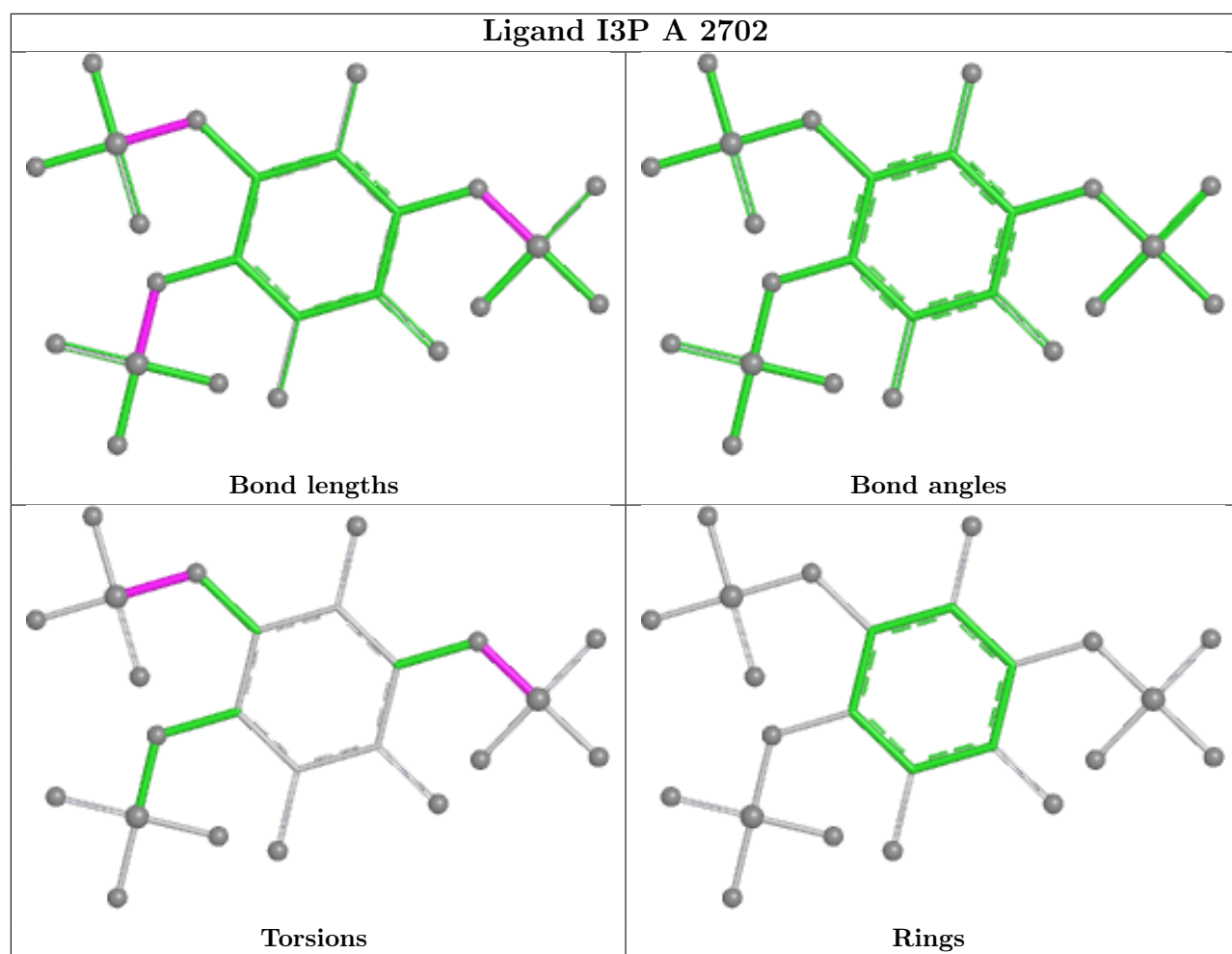
4 monomers are involved in 8 short contacts:

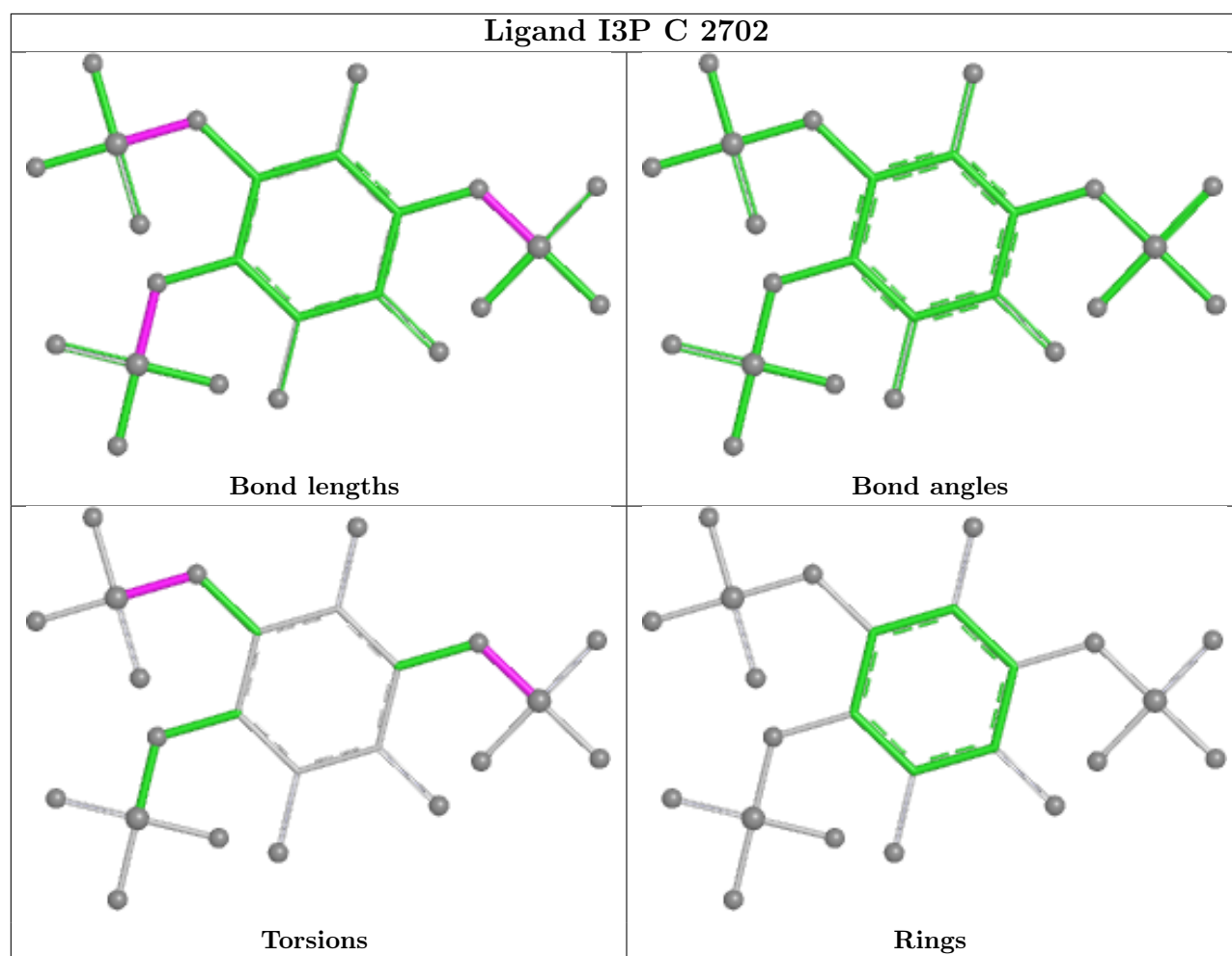
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2702	I3P	2	0
3	A	2702	I3P	2	0
3	C	2702	I3P	2	0
3	B	2702	I3P	2	0

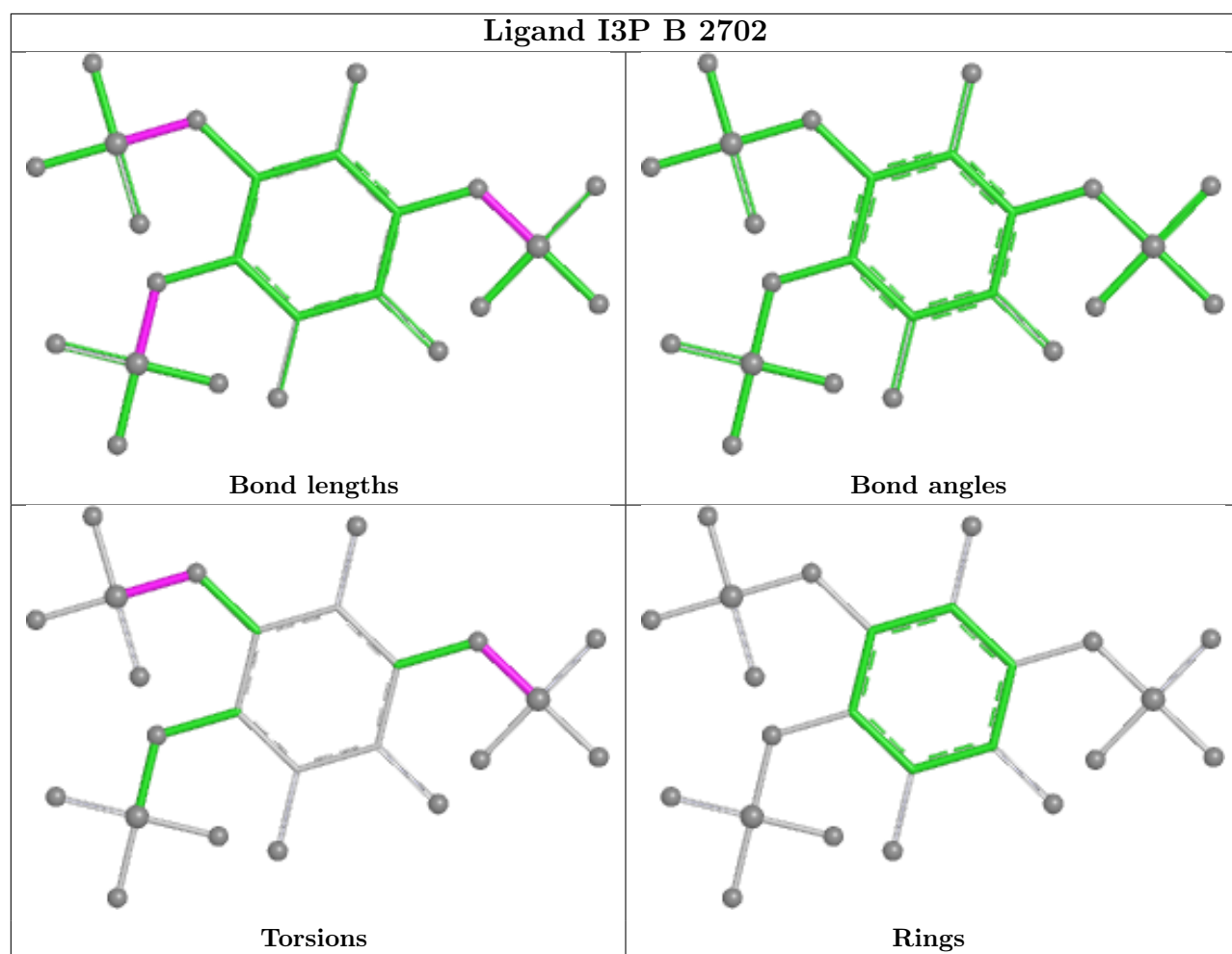
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

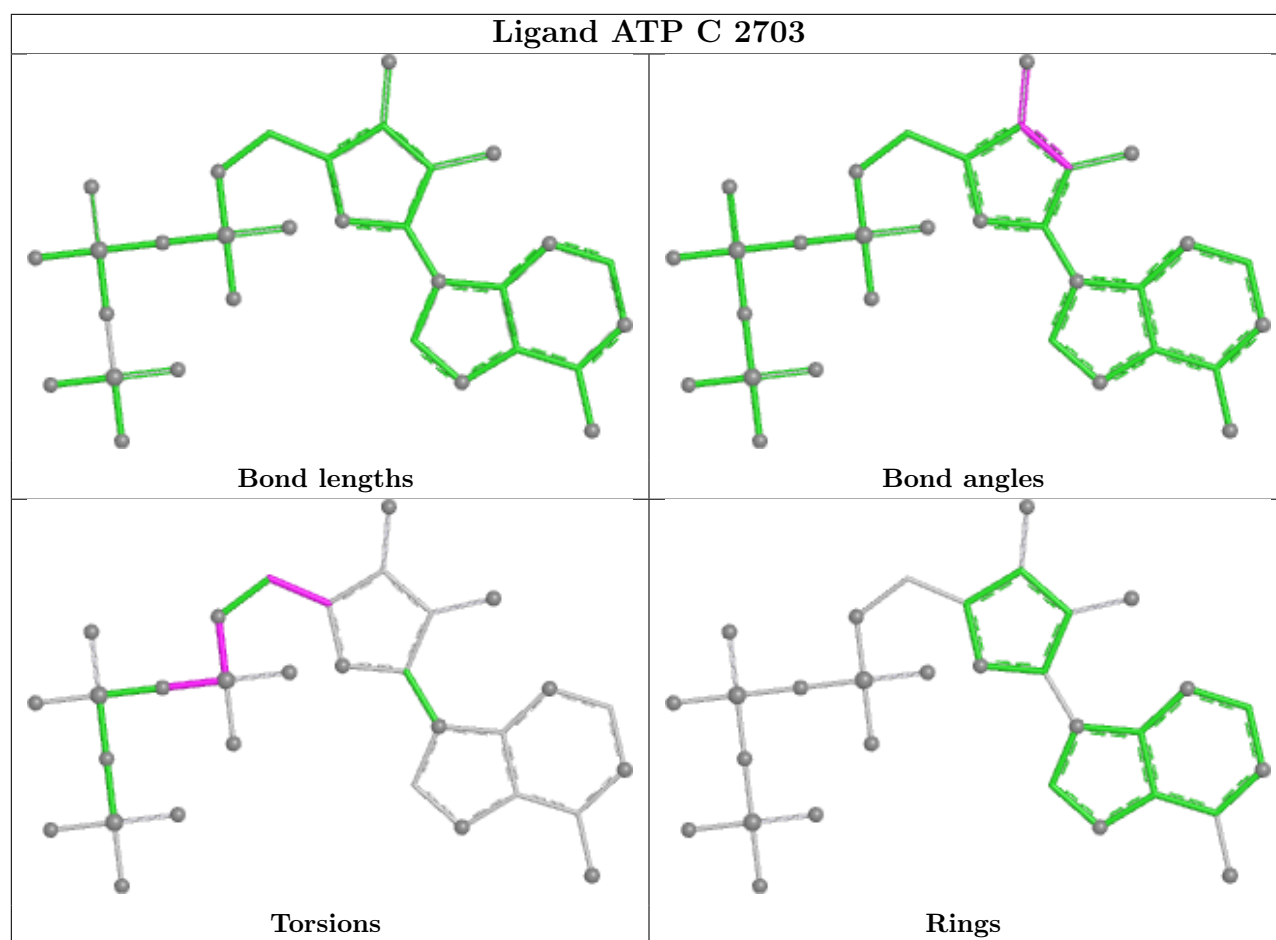


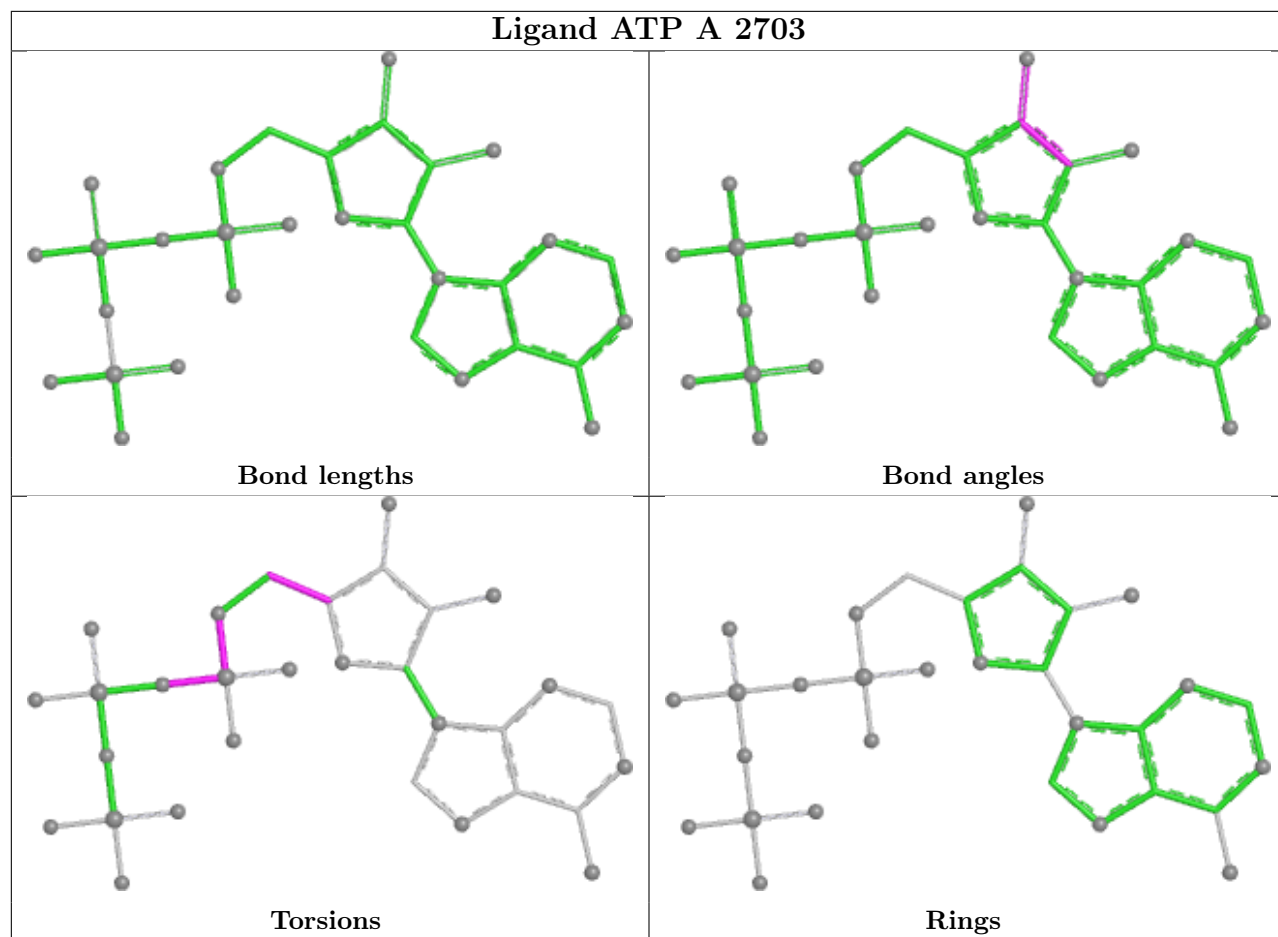


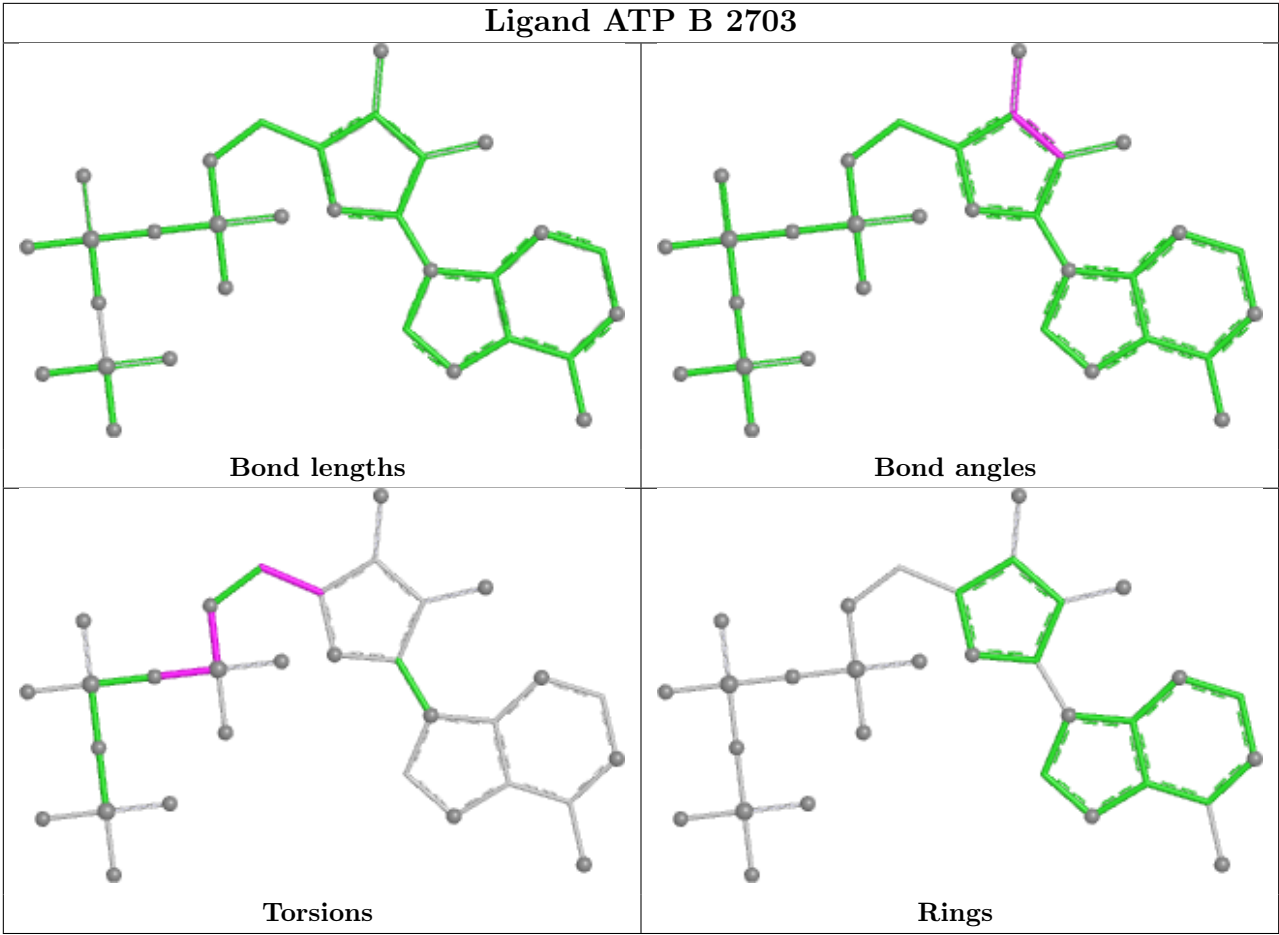












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2611:VAL	C	2628:UNK	N	25.33
1	B	2611:VAL	C	2628:UNK	N	25.33

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2611:VAL	C	2628:UNK	N	25.33
1	D	2611:VAL	C	2628:UNK	N	25.33

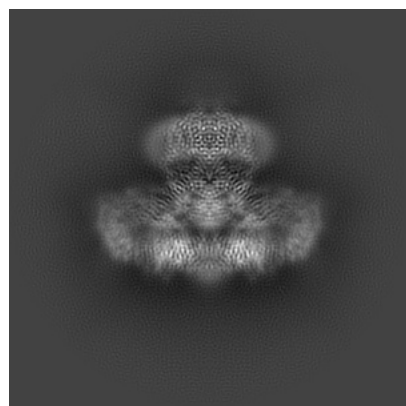
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25667. These allow visual inspection of the internal detail of the map and identification of artifacts.

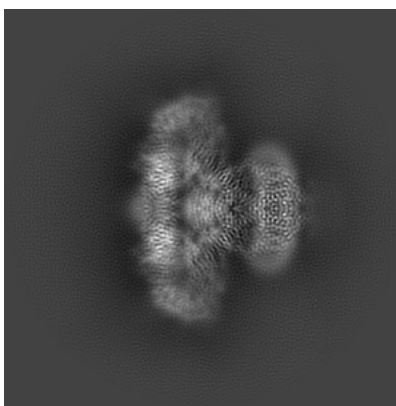
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

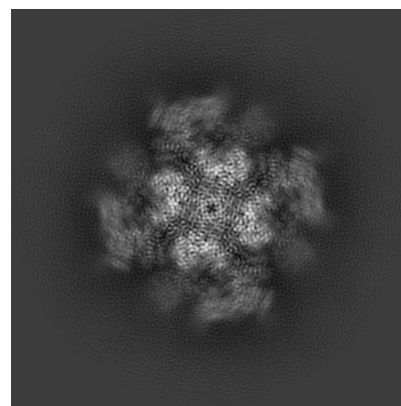
6.1.1 Primary map



X

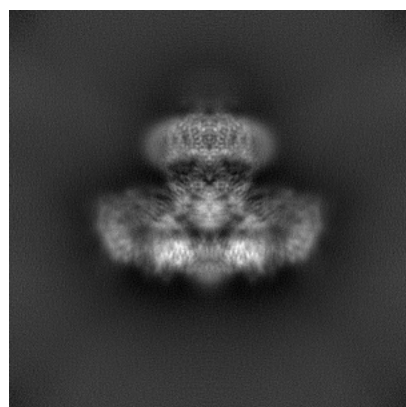


Y

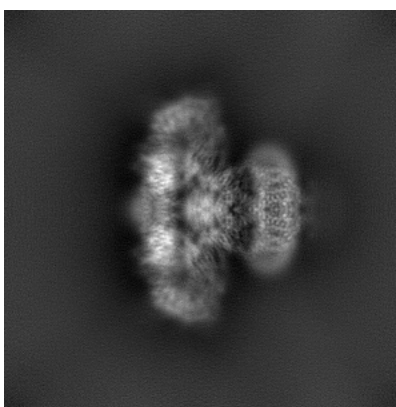


Z

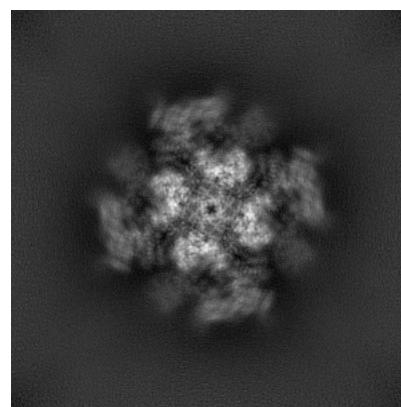
6.1.2 Raw map



X



Y

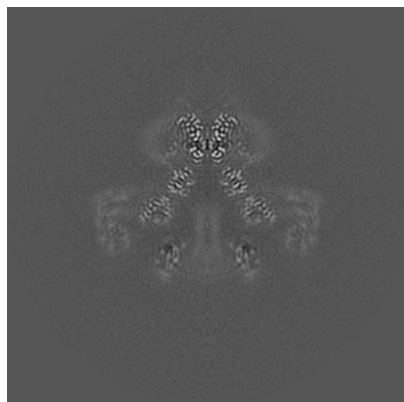


Z

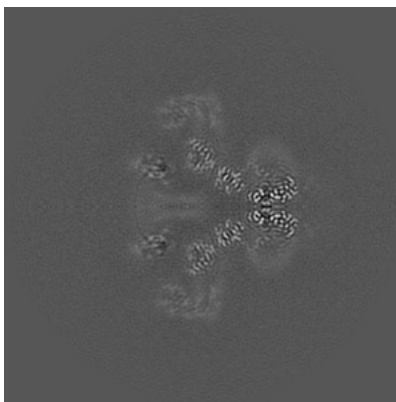
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

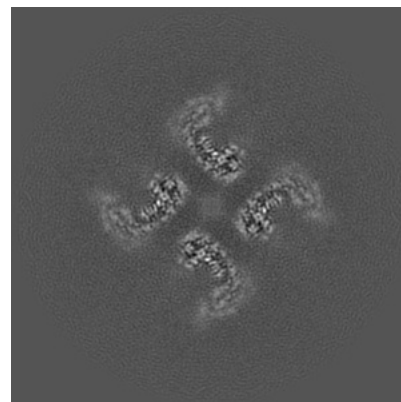
6.2.1 Primary map



X Index: 240

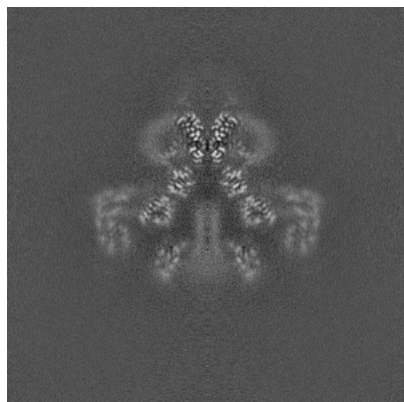


Y Index: 240

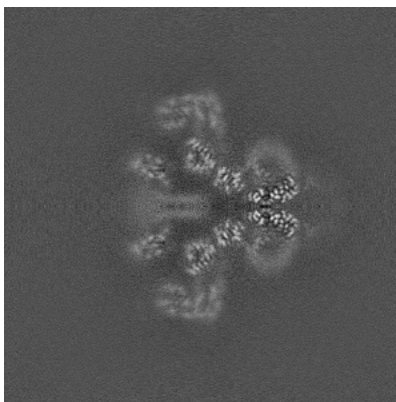


Z Index: 240

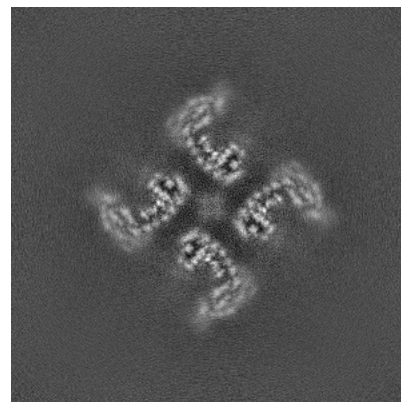
6.2.2 Raw map



X Index: 240



Y Index: 240

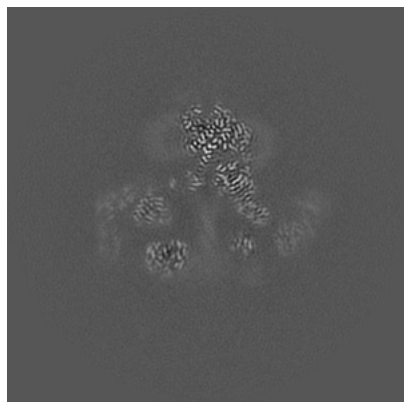


Z Index: 240

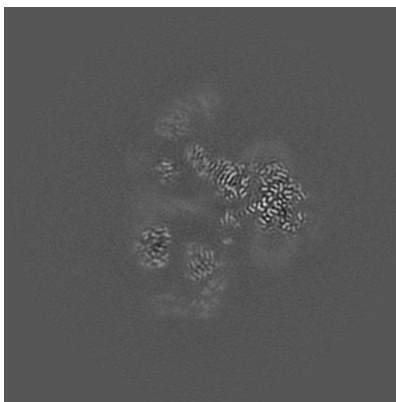
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

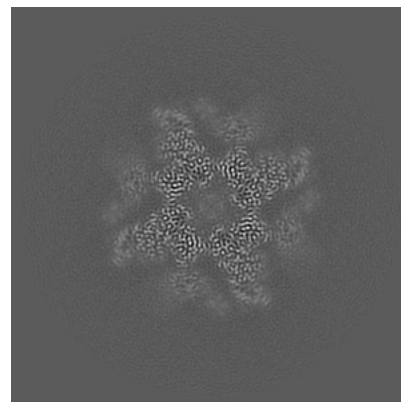
6.3.1 Primary map



X Index: 250

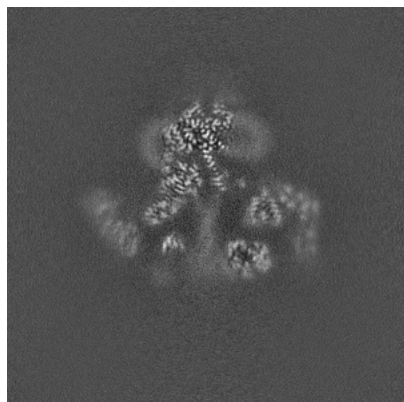


Y Index: 230

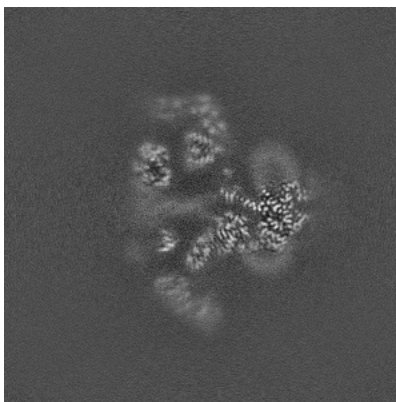


Z Index: 188

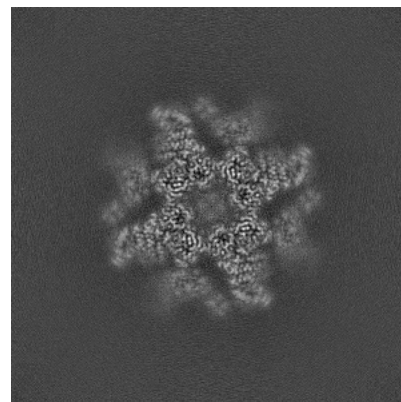
6.3.2 Raw map



X Index: 229



Y Index: 251

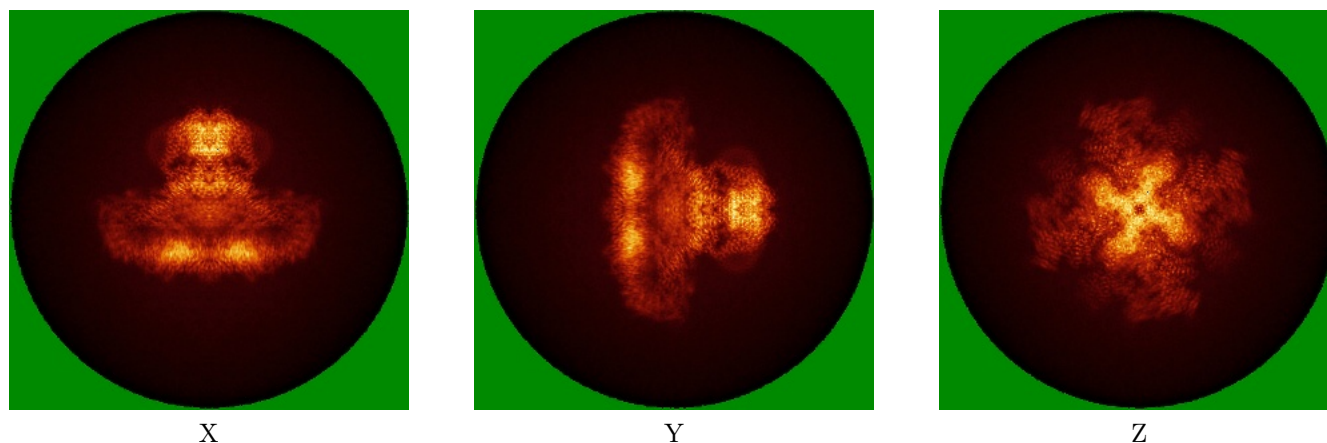


Z Index: 189

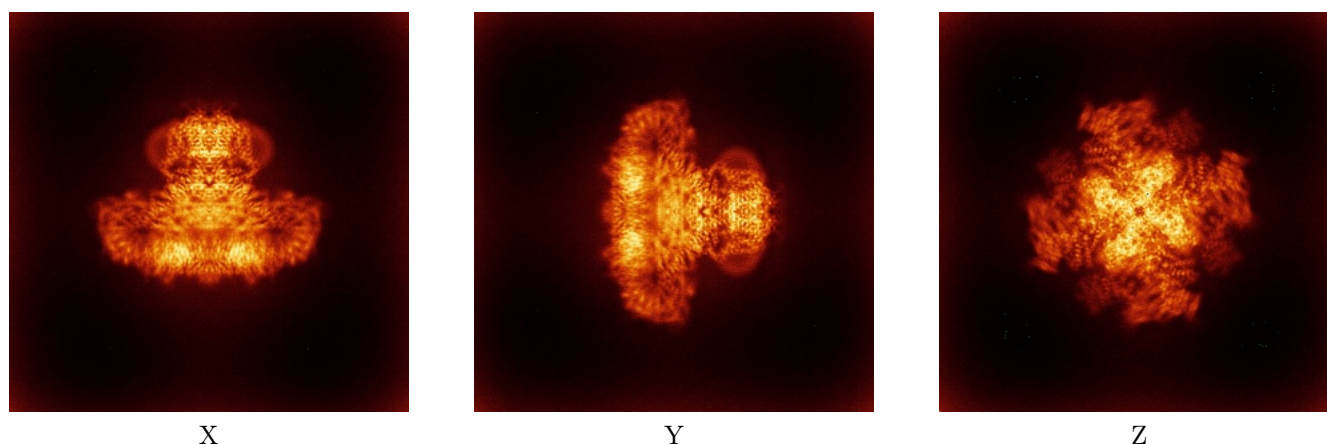
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

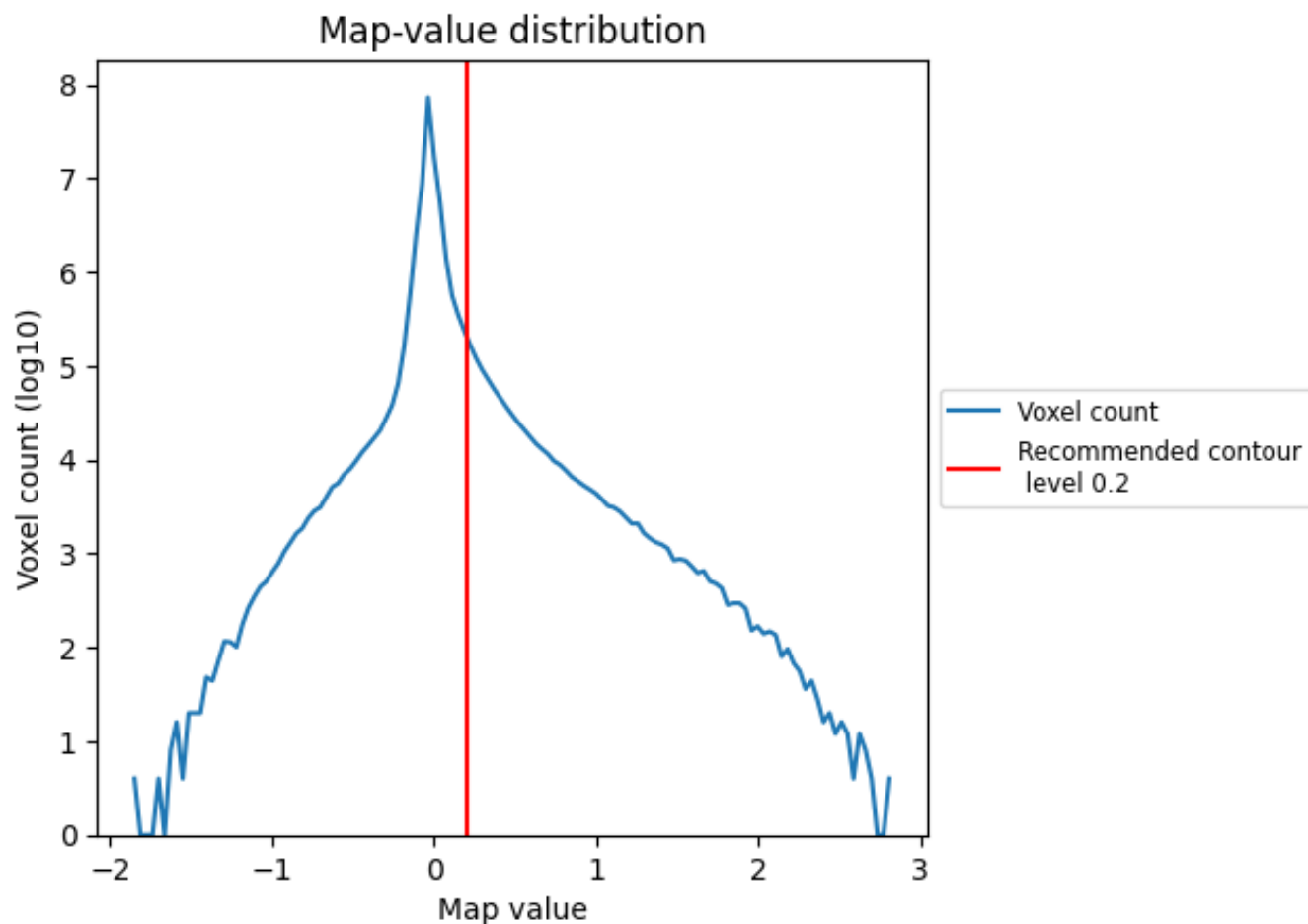
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

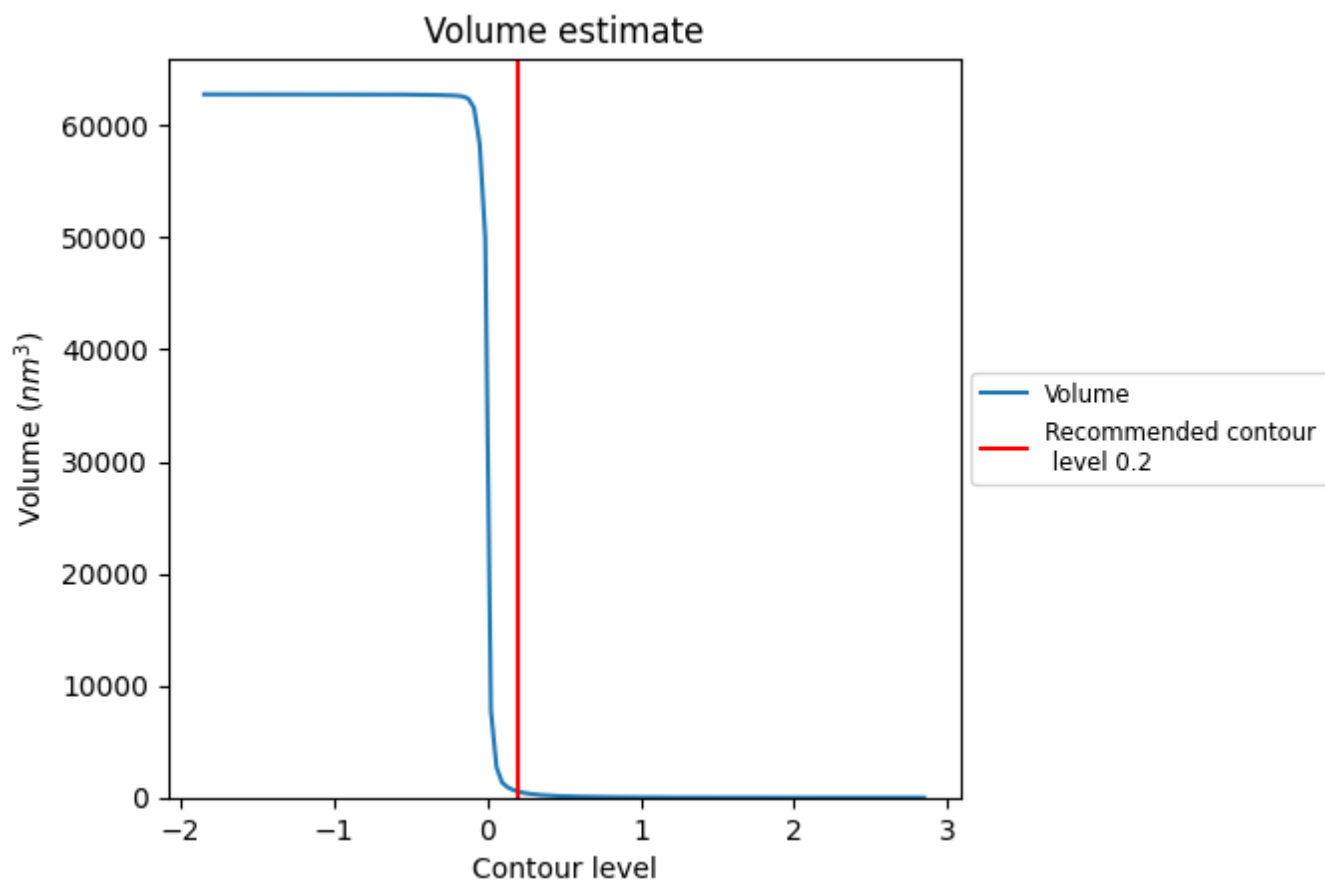
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

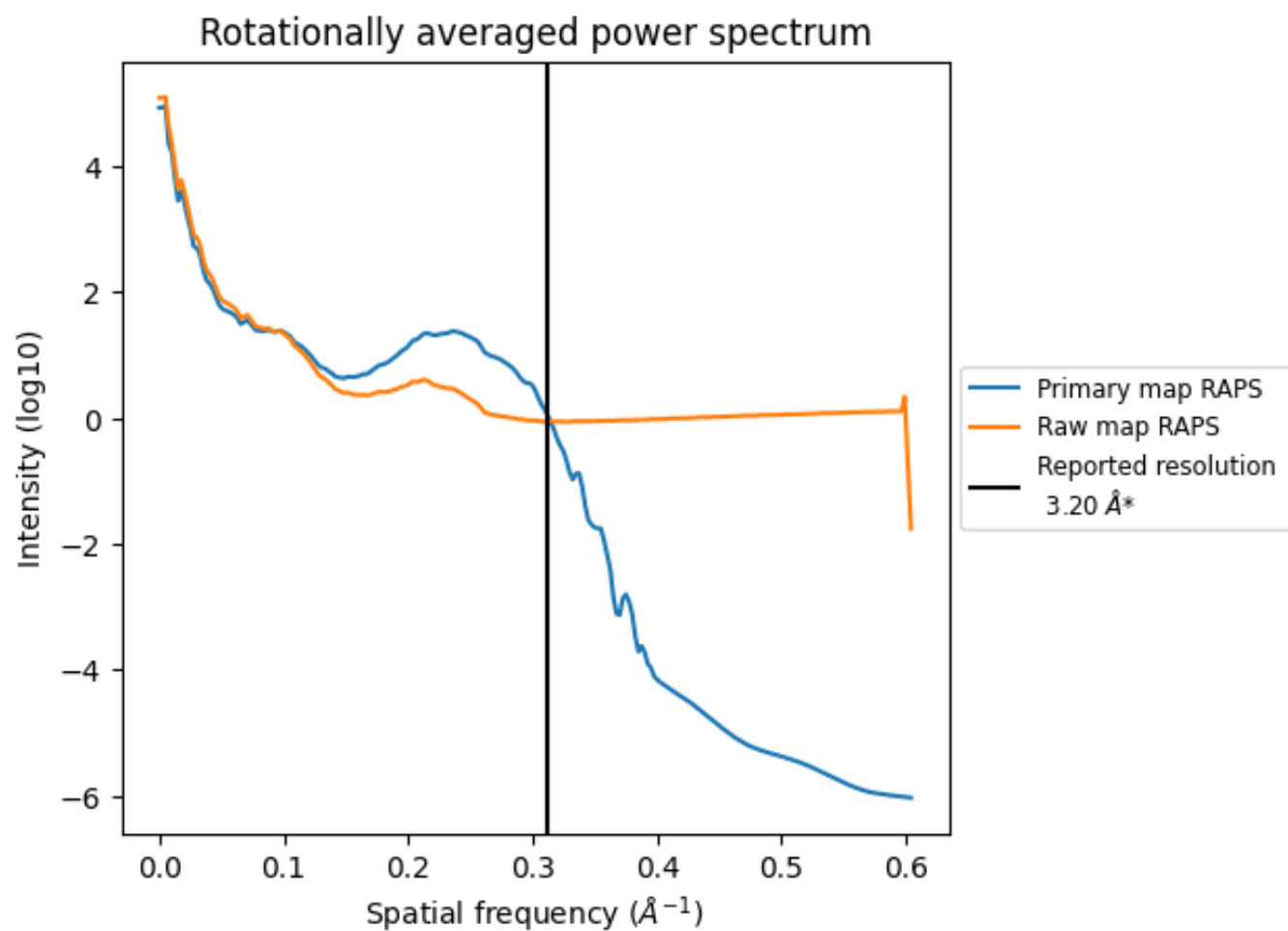
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 544 nm³; this corresponds to an approximate mass of 491 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

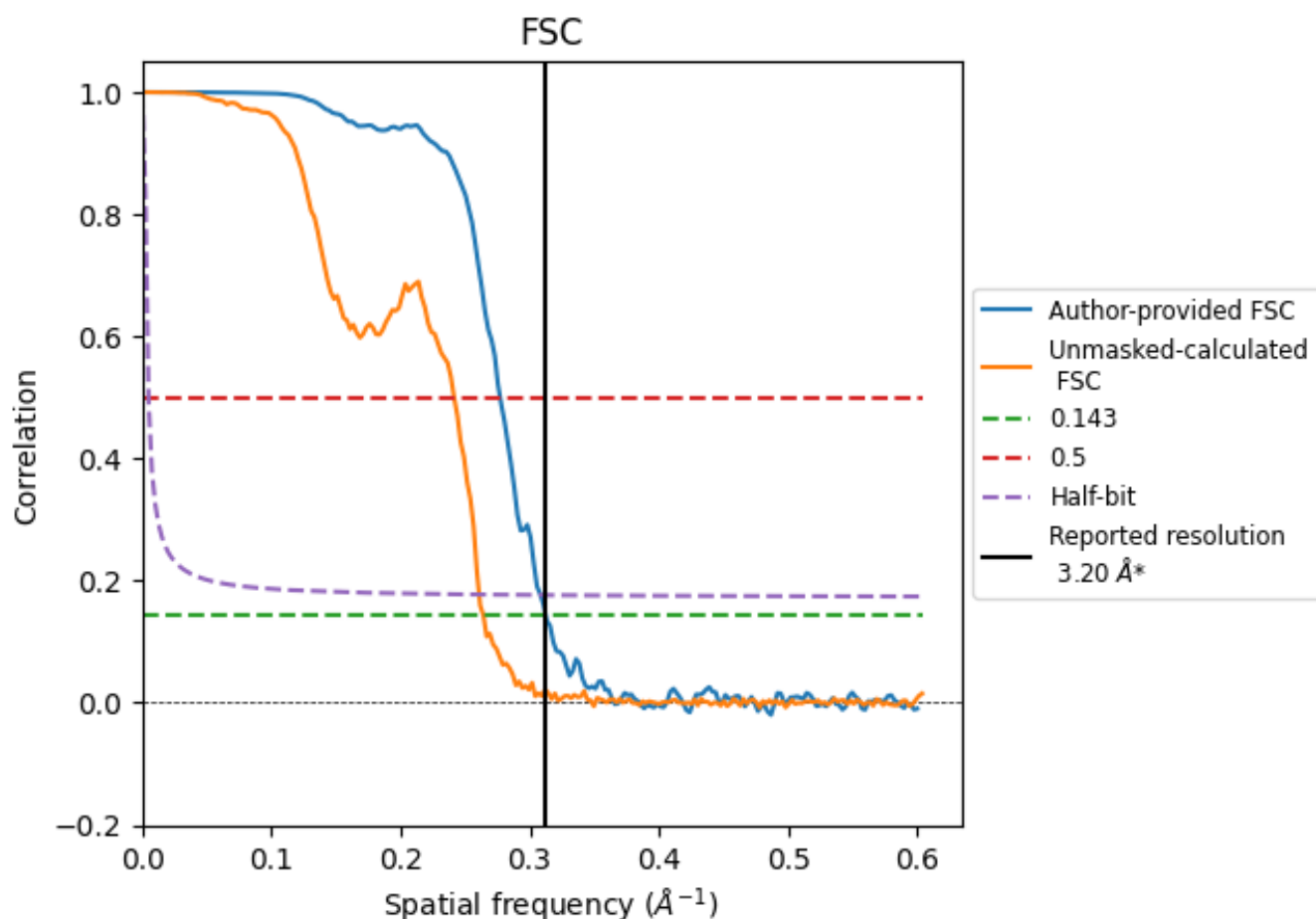


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

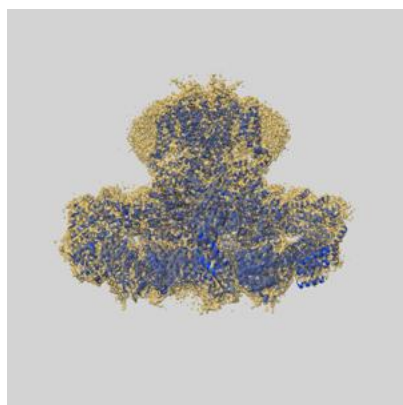
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.61	3.24
Unmasked-calculated*	3.79	4.14	3.83

*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 3.79 differs from the reported value 3.2 by more than 10 %

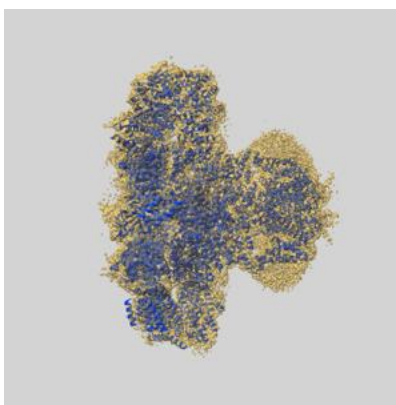
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25667 and PDB model 7T3P. Per-residue inclusion information can be found in section [3](#) on page [6](#).

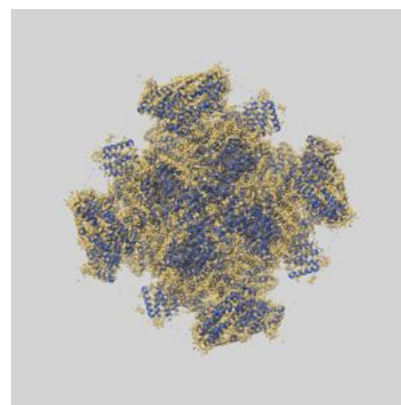
9.1 Map-model overlay [i](#)



X



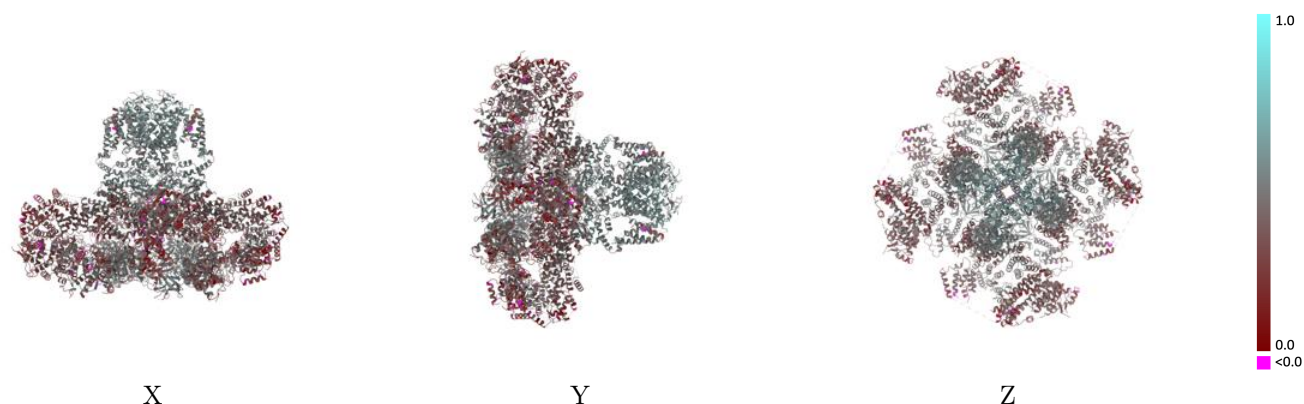
Y



Z

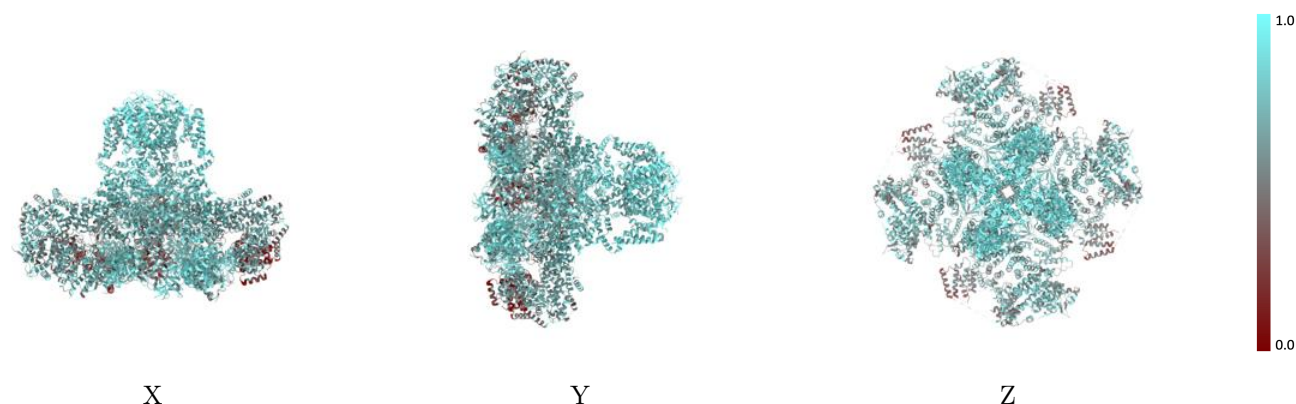
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



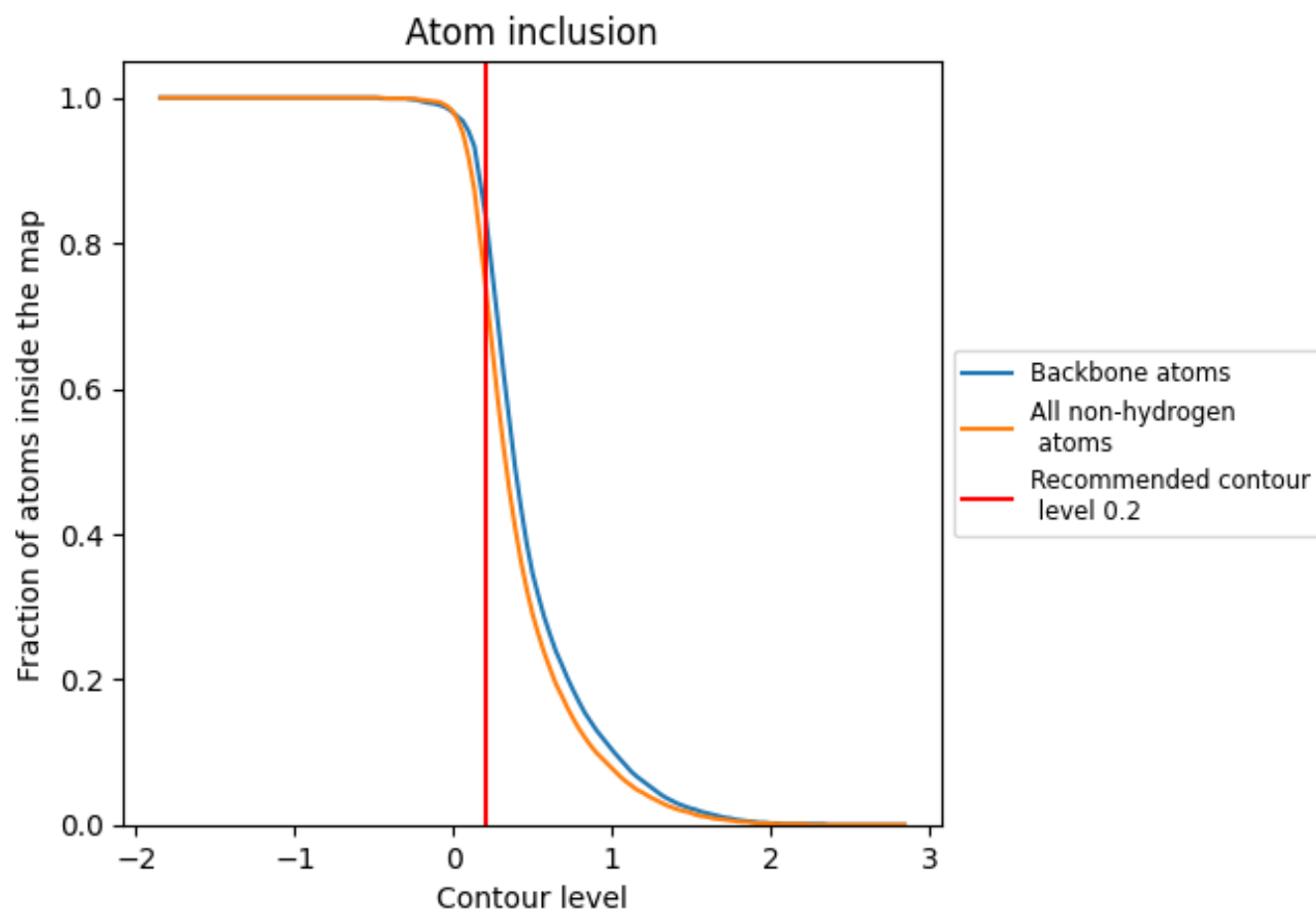
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.3990
A	0.7510	0.4020
B	0.7450	0.3910
C	0.7510	0.4020
D	0.7510	0.4020

