



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 03:42 AM EDT

PDB ID : 8TLA  
EMDB ID : EMD-41366  
Title : Human Type 3 IP3 Receptor - Higher-Order Inhibited State - Symmetry Mate  
1  
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.  
Deposited on : 2023-07-26  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

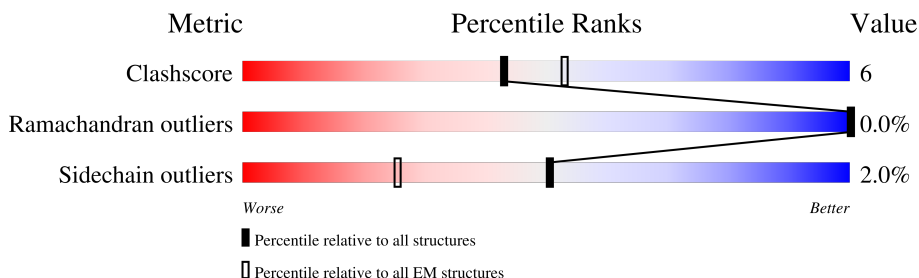
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>30%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	B	2671	<div> <div>34%</div> <div>61%</div> <div>13%</div> <div>26%</div> </div>
1	C	2671	<div> <div>17%</div> <div>65%</div> <div>10%</div> <div>25%</div> </div>
1	D	2671	<div> <div>14%</div> <div>65%</div> <div>11%</div> <div>24%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 130502 atoms, of which 65433 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.

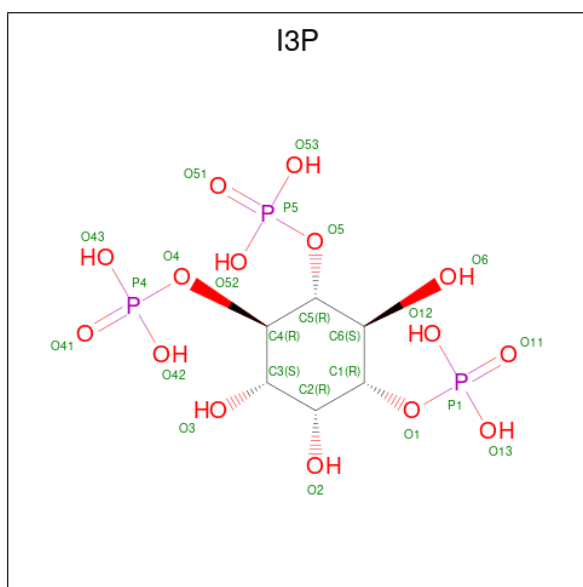
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

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	2004	Total	C	H	N	O	S	0	0
			32571	10370	16344	2767	2986	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	

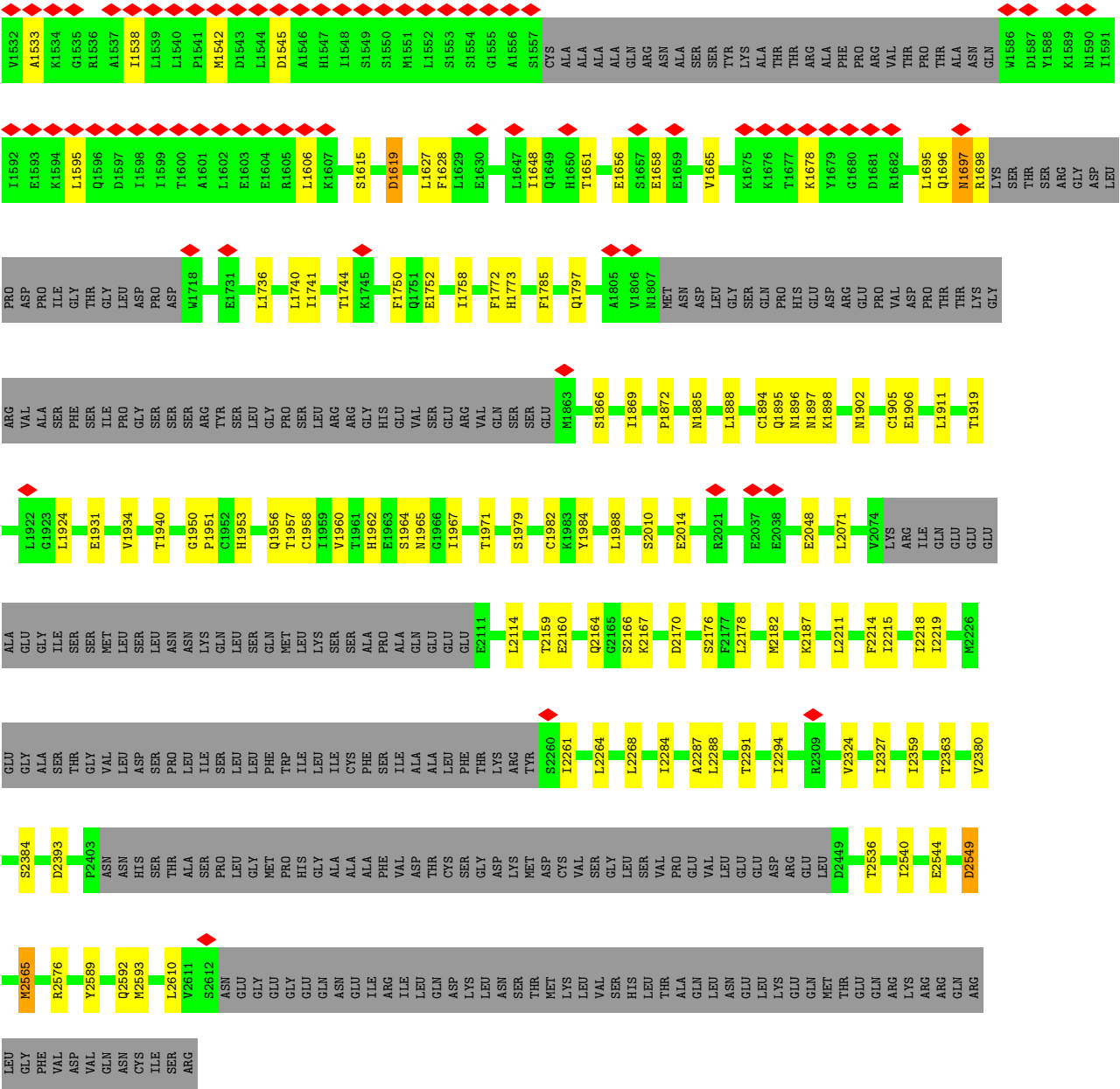
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



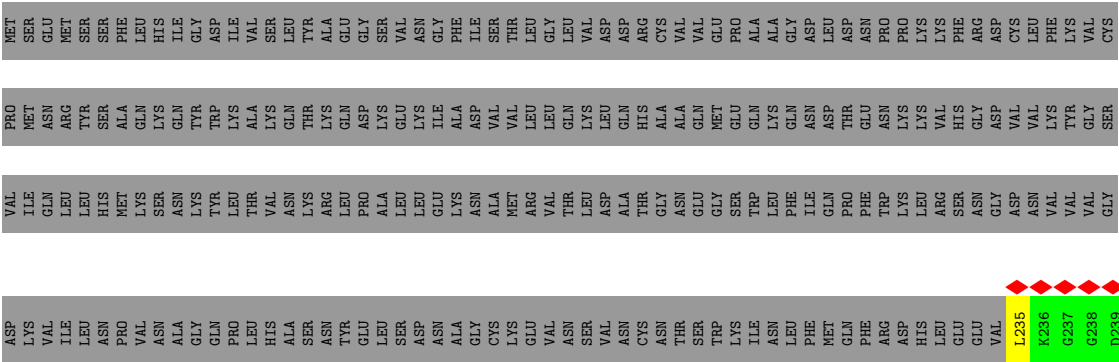
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
5	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	







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





PRO	ALA	M1022	M1023	M1024	M1025	D1026	R1027	E1030	Q1031	A1032	M1035	F1036	G1037	VAL	GLN	ASN	GLY	LYS	THR	SER	ASP	ALA	ASP	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
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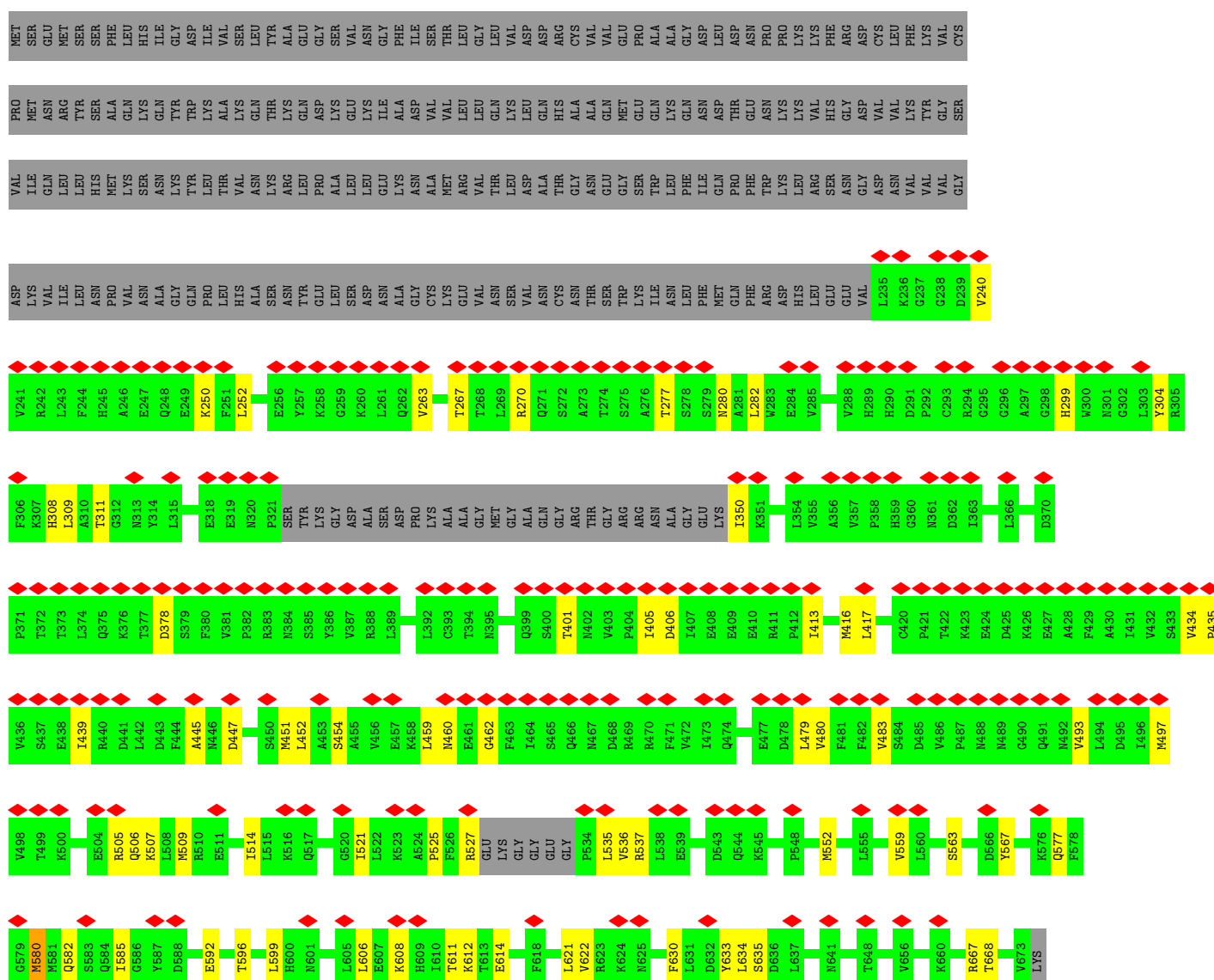








• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





ASN	LYS	GLN	LEU	ARG	TYR	S2260	I2261	G2277	T2281	S2299	D2449	S2450	H2468	V2476	I2479	L2480	R2524	L2569	I2594	A2607	L2610	V2611	S2612	ASN	GLU	GLY	THR	SER	PRO	LEU	GLY	MET	PRO	HIS	GLY	ALA	PRO	SER	ASP	LEU	ILE	SER	THR	PHE	TRP	LEU	CYS	ILE	PHE	SER	VAL	ALA	LEU
ASN	LYS	GLN	LEU	ARG	TYR	S2260	I2261	G2277	T2281	S2299	D2449	S2450	H2468	V2476	I2479	L2480	R2524	L2569	I2594	A2607	L2610	V2611	S2612	ASN	GLU	GLY	THR	SER	PRO	LEU	GLY	MET	PRO	HIS	GLY	ALA	PRO	SER	ASP	LEU	ILE	SER	THR	PHE	TRP	LEU	CYS	ILE	PHE	SER	VAL	ALA	LEU
THR	ALA	GLN	LEU	ASN	GLU	LEU	LEU	LYS	GLU	ASP	ARG	GLU	THR	GLU	GLN	ARG	LYS	ARG	GLN	ARG	LEU	PHE	VAL	ASP	VAL	GLN	ASN	GLU	ILE	ARG	ILE	LEU	GLN	ASP	LYS	LEU	ASN	THR	MET	LYS	LEU	VAL	SER	HIS	LEU								
THR	ALA	GLN	LEU	ASN	GLU	LEU	LEU	LYS	GLU	ASP	ARG	GLU	THR	GLU	GLN	ARG	LYS	ARG	GLN	ARG	LEU	PHE	VAL	ASP	VAL	GLN	ASN	GLU	ILE	ARG	ILE	LEU	GLN	ASP	LYS	LEU	ASN	THR	MET	LYS	LEU	VAL	SER	HIS	LEU								

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85139	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	0.885	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: ATP, ZN, 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	0.46	0/22156
1	B	0.25	0/16384	0.46	0/22131
1	C	0.24	0/16528	0.45	0/22327
1	D	0.25	0/16726	0.46	0/22603
All	All	0.25	0/66041	0.46	0/89217

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	235	0
1	B	16087	16225	16224	236	0
1	C	16227	16344	16353	178	0
1	D	16421	16536	16535	194	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	1	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	1	0
3	D	24	9	9	1	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	65069	65433	65439	837	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 6.

All (837) 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:D:1962:HIS:HD1	1:D:1964:SER:HG	1.08	0.99
1:A:1962:HIS:HD1	1:A:1964:SER:HG	1.06	0.96
1:C:885:THR:HG22	1:C:978:ILE:HD13	1.48	0.93
1:A:729:TYR:CE1	1:A:733:LEU:HD21	2.04	0.92
1:C:2203:LEU:O	1:C:2207:ILE:HD12	1.73	0.89
1:D:445:ALA:HB1	1:D:514:ILE:HD11	1.56	0.86
1:B:885:THR:HG22	1:B:978:ILE:HD13	1.58	0.84
1:A:503:ARG:NH2	1:A:566:ASP:O	2.11	0.83
1:D:1729:ASP:OD1	1:D:1734:THR:OG1	1.96	0.83
1:B:2163:GLU:OE2	1:B:2163:GLU:N	2.13	0.82
1:C:611:THR:OG1	1:C:614:GLU:OE1	1.96	0.82
1:B:1767:GLU:N	1:B:1767:GLU:OE1	2.13	0.80
1:A:1740:LEU:O	1:A:1744:THR:HG22	1.81	0.80
1:C:593:ASP:OD2	1:C:594:THR:N	2.15	0.80
1:A:1658:GLU:N	1:A:1658:GLU:OE1	2.15	0.79
1:B:1895:GLN:NE2	1:B:1901:TYR:O	2.16	0.78
1:A:655:CYS:O	1:A:661:ASN:ND2	2.17	0.78
1:C:698:ASP:OD1	1:C:699:LYS:N	2.16	0.78
1:A:1302:PHE:O	1:A:1306:VAL:HG23	1.84	0.77
1:C:2518:ASP:O	1:D:2524:ARG:NH2	2.18	0.77
1:C:2518:ASP:OD1	1:D:2524:ARG:NH2	2.17	0.77
1:D:1288:HIS:O	1:D:1292:THR:HG23	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ARG:NH2	3:C:3002:I3P:O51	2.19	0.76
1:C:691:GLU:N	1:C:691:GLU:OE1	2.18	0.76
1:D:2048:GLU:N	1:D:2048:GLU:OE1	2.18	0.76
1:B:503:ARG:NH2	1:B:566:ASP:O	2.19	0.75
1:B:2287:ALA:O	1:B:2291:THR:HG23	1.86	0.75
1:A:1056:LEU:HD22	1:A:1627:LEU:HD13	1.69	0.75
1:B:2043:GLU:N	1:B:2043:GLU:OE2	2.19	0.74
1:C:2322:TYR:OH	1:C:2347:ASP:OD1	2.04	0.74
1:D:1418:ASN:OD1	1:D:1475:THR:OG1	2.03	0.74
1:A:2164:GLN:NE2	1:B:2556:GLU:OE2	2.19	0.74
1:A:694:LEU:HD21	1:A:729:TYR:CD2	2.23	0.74
1:B:1954:GLU:OE2	1:B:1954:GLU:N	2.19	0.74
1:B:881:LEU:O	1:B:885:THR:HG23	1.88	0.74
1:B:479:LEU:O	1:B:483:VAL:HG23	1.89	0.73
1:B:2518:ASP:OD1	1:C:2524:ARG:NE	2.19	0.73
1:C:881:LEU:O	1:C:885:THR:HG23	1.88	0.73
1:A:2287:ALA:O	1:A:2291:THR:HG23	1.88	0.73
1:A:451:MET:HG3	1:A:475:LEU:HD22	1.71	0.73
1:B:666:ILE:N	1:B:732:GLN:OE1	2.22	0.73
1:D:2021:ARG:NH1	1:D:2024:GLU:OE2	2.22	0.73
1:C:1397:VAL:HG21	1:C:1436:HIS:CD2	2.23	0.72
1:C:1402:HIS:ND1	1:C:1404:ASP:O	2.22	0.72
1:D:1747:GLU:N	1:D:1747:GLU:OE1	2.22	0.72
1:C:2326:TYR:CE1	1:C:2344:LEU:HD22	2.25	0.72
1:C:2024:GLU:OE2	1:C:2024:GLU:N	2.23	0.71
1:D:1466:LYS:O	1:D:1470:SER:OG	2.06	0.71
1:C:2162:ASP:OD2	1:C:2164:GLN:N	2.23	0.71
1:D:1188:GLN:N	1:D:1188:GLN:OE1	2.24	0.71
1:A:1097:LEU:HD12	1:A:1595:LEU:HD22	1.73	0.70
1:A:2544:GLU:N	1:A:2544:GLU:OE2	2.23	0.70
1:D:1322:MET:O	1:D:1326:THR:HG23	1.90	0.70
1:A:1282:VAL:O	1:A:1285:HIS:ND1	2.24	0.70
1:A:1895:GLN:O	1:A:1896:ASN:ND2	2.25	0.69
1:D:1526:ILE:HG23	1:D:1551:MET:CE	2.21	0.69
1:A:990:LEU:HD23	1:A:1092:PHE:CD1	2.28	0.69
1:A:1297:VAL:HG21	1:A:1363:MET:HE3	1.73	0.69
1:B:1456:GLU:O	1:B:1458:ARG:NH1	2.26	0.68
1:B:1953:HIS:O	1:B:1957:THR:HG23	1.94	0.68
1:A:580:MET:SD	1:A:581:MET:N	2.67	0.67
1:D:299:HIS:ND1	1:D:378:ASP:O	2.27	0.67
1:A:641:ASN:OD1	1:A:641:ASN:O	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:HIS:ND1	1:B:378:ASP:O	2.27	0.67
1:B:2359:ILE:O	1:B:2363:THR:HG23	1.93	0.67
1:A:299:HIS:ND1	1:A:378:ASP:O	2.28	0.66
1:A:621:LEU:HD13	1:A:630:PHE:CE1	2.31	0.66
1:D:277:THR:O	1:D:507:LYS:NZ	2.27	0.66
1:A:299:HIS:O	1:A:304:TYR:OH	2.13	0.66
1:C:299:HIS:ND1	1:C:378:ASP:O	2.28	0.66
1:D:1737:VAL:HG11	1:D:1757:ALA:HB2	1.78	0.66
1:C:608:LYS:HE3	1:C:608:LYS:HA	1.77	0.66
1:B:1648:ILE:HG23	1:B:1736:LEU:HD22	1.77	0.66
1:D:1236:CYS:HB3	1:D:1246:LEU:HD12	1.77	0.65
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.78	0.65
1:A:773:LEU:HD11	1:A:777:PHE:CE2	2.31	0.65
1:C:1445:THR:HG22	1:C:1501:LEU:HA	1.79	0.65
1:A:972:LEU:HD11	1:A:1062:LEU:HD13	1.79	0.65
1:B:299:HIS:O	1:B:304:TYR:OH	2.12	0.65
1:A:716:ARG:NH1	1:A:768:MET:O	2.30	0.65
1:D:479:LEU:O	1:D:483:VAL:HG23	1.97	0.65
1:C:2320:PHE:O	1:C:2324:VAL:HG13	1.98	0.64
1:C:596:THR:HG21	1:C:633:TYR:HD1	1.62	0.64
1:C:2326:TYR:CD1	1:C:2344:LEU:HD22	2.33	0.64
1:A:1186:GLY:O	1:A:1190:ARG:N	2.30	0.64
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.16	0.63
1:C:886:ARG:NE	1:C:1049:ASP:OD2	2.32	0.63
1:A:538:LEU:HD13	1:A:587:TYR:CE2	2.33	0.63
1:B:451:MET:HB2	1:B:475:LEU:HD22	1.81	0.63
1:D:1022:ASN:C	1:D:1022:ASN:HD22	2.01	0.63
1:A:1247:HIS:CD2	1:A:1274:LEU:HD22	2.34	0.63
1:A:1467:TYR:O	1:A:1471:VAL:HG22	1.99	0.63
1:D:299:HIS:O	1:D:304:TYR:OH	2.13	0.62
1:B:1044:MET:SD	1:B:1044:MET:N	2.68	0.62
1:C:1441:PHE:O	1:C:1445:THR:HG23	1.98	0.62
1:B:618:PHE:CE2	1:B:637:LEU:HD11	2.34	0.61
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.30	0.61
1:C:299:HIS:O	1:C:304:TYR:OH	2.13	0.61
1:C:893:ASP:OD1	1:C:894:CYS:N	2.33	0.61
1:A:621:LEU:HD12	1:A:622:VAL:N	2.15	0.61
1:A:972:LEU:HD11	1:A:1062:LEU:CD1	2.30	0.61
1:B:811:THR:N	1:B:814:ASP:OD1	2.33	0.61
1:B:1124:SER:HB2	1:B:1212:ILE:HD11	1.81	0.61
1:C:479:LEU:O	1:C:483:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:LEU:HD21	1:A:729:TYR:CE2	2.36	0.60
1:A:1953:HIS:O	1:A:1957:THR:HG23	2.00	0.60
1:D:460:ASN:OD1	1:D:527:ARG:NH2	2.33	0.60
1:B:1207:LEU:HD13	1:B:1249:HIS:HD2	1.65	0.60
1:D:1300:LEU:HD22	1:D:1371:LEU:HD23	1.83	0.60
1:D:480:VAL:HG11	1:D:493:VAL:HB	1.83	0.60
1:B:515:LEU:HD23	1:B:560:LEU:HD23	1.84	0.60
1:B:695:THR:HG23	1:B:703:HIS:CE1	2.37	0.60
1:A:811:THR:HG22	1:A:812:ILE:H	1.66	0.60
1:B:782:LEU:HD11	1:B:869:ASN:OD1	2.01	0.60
1:B:1207:LEU:HD13	1:B:1249:HIS:CD2	2.36	0.60
1:A:1898:LYS:HA	1:A:1898:LYS:HE3	1.83	0.59
1:A:2536:THR:O	1:A:2536:THR:HG22	2.01	0.59
1:B:2211:LEU:O	1:B:2215:ILE:HD12	2.02	0.59
1:C:1329:GLY:O	1:C:1333:VAL:HG22	2.00	0.59
1:B:2324:VAL:HA	1:B:2327:ILE:HD12	1.83	0.59
1:C:991:LEU:HD11	1:C:1095:VAL:HG21	1.84	0.59
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.36	0.59
1:B:589:ILE:O	1:B:589:ILE:HG22	2.01	0.59
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.02	0.59
1:C:1541:PRO:O	1:C:1545:ASP:N	2.31	0.59
1:D:1978:ILE:HG22	1:D:1978:ILE:O	2.03	0.59
1:B:1260:GLU:N	1:B:1260:GLU:OE1	2.35	0.58
1:D:252:LEU:HD11	1:D:263:VAL:HG12	1.85	0.58
1:A:252:LEU:HD11	1:A:263:VAL:HG12	1.85	0.58
1:A:743:ARG:NE	1:A:787:ASP:OD1	2.36	0.58
1:B:1473:LEU:HD11	1:B:1522:VAL:CG2	2.32	0.58
1:D:596:THR:HG21	1:D:633:TYR:HB3	1.86	0.58
1:B:252:LEU:HD11	1:B:263:VAL:HG12	1.85	0.58
1:C:614:GLU:OE1	1:C:614:GLU:N	2.36	0.58
1:C:1551:MET:SD	1:C:1551:MET:N	2.76	0.58
1:D:1307:ILE:HD11	1:D:1375:CYS:SG	2.43	0.58
1:C:1333:VAL:HG23	1:C:1333:VAL:O	2.03	0.58
1:C:596:THR:HG21	1:C:633:TYR:CD1	2.39	0.58
1:A:812:ILE:HD12	1:A:1044:MET:SD	2.44	0.58
1:B:760:ILE:HG21	1:B:781:MET:HB2	1.85	0.58
1:B:2031:LYS:NZ	1:B:2035:GLN:OE1	2.36	0.58
1:C:1182:MET:HE3	1:C:1182:MET:O	2.04	0.58
1:C:1322:MET:SD	1:C:1322:MET:N	2.76	0.58
1:A:1338:ASP:OD2	1:A:1339:LYS:N	2.37	0.58
1:B:2162:ASP:OD1	1:B:2165:GLY:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2280:PRO:O	1:B:2284:ILE:HG13	2.04	0.58
1:C:252:LEU:HD11	1:C:263:VAL:HG12	1.84	0.58
1:D:1346:LEU:HD21	1:D:1402:HIS:NE2	2.18	0.58
1:A:1089:MET:CE	1:A:1606:LEU:HD12	2.33	0.58
1:A:1325:LEU:HD22	1:A:1333:VAL:CG1	2.33	0.58
1:B:1473:LEU:HD11	1:B:1522:VAL:HG22	1.86	0.57
1:B:1669:LEU:O	1:B:1673:LEU:HD12	2.04	0.57
1:D:435:PRO:O	1:D:439:ILE:HD12	2.04	0.57
1:A:506:GLN:NE2	1:A:563:SER:O	2.37	0.57
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.38	0.57
1:B:1531:MET:SD	1:B:1531:MET:N	2.76	0.57
1:C:621:LEU:HD12	1:C:622:VAL:N	2.19	0.57
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.04	0.57
1:A:1325:LEU:HD22	1:A:1333:VAL:HG12	1.87	0.57
1:B:2536:THR:HG22	1:B:2536:THR:O	2.05	0.57
1:D:2172:PHE:HZ	1:D:2594:ILE:HG23	1.69	0.57
1:B:709:ARG:NH1	1:B:766:ASP:OD2	2.37	0.56
1:A:1243:GLN:OE1	1:A:1271:ASN:ND2	2.38	0.56
1:B:811:THR:OG1	1:B:814:ASP:OD1	2.21	0.56
1:C:760:ILE:HG21	1:C:781:MET:HB2	1.87	0.56
1:A:266:ARG:NH2	3:A:3002:I3P:O43	2.38	0.56
1:B:847:GLU:OE2	1:B:856:LYS:NZ	2.38	0.56
1:C:1542:MET:SD	1:C:1542:MET:N	2.74	0.56
1:A:252:LEU:HD11	1:A:263:VAL:CG1	2.36	0.56
1:B:509:MET:SD	1:B:563:SER:OG	2.63	0.56
1:D:1526:ILE:HG23	1:D:1551:MET:HE2	1.88	0.56
1:A:585:ILE:HD11	1:A:592:GLU:HG3	1.88	0.55
1:C:2207:ILE:HD12	1:C:2207:ILE:H	1.71	0.55
1:B:1960:VAL:HG13	1:B:1961:THR:HG23	1.88	0.55
1:C:1729:ASP:OD2	1:C:1734:THR:OG1	2.19	0.55
1:B:252:LEU:HD11	1:B:263:VAL:CG1	2.36	0.55
1:A:1123:LYS:HD2	1:A:1126:LEU:HD22	1.89	0.55
1:D:1298:GLN:OE1	1:D:1298:GLN:N	2.40	0.55
1:A:1752:GLU:OE1	1:A:1752:GLU:HA	2.06	0.55
1:B:655:CYS:O	1:B:661:ASN:ND2	2.39	0.55
1:B:820:ASN:O	1:B:824:ASP:N	2.35	0.55
1:B:1316:LYS:O	1:B:1320:MET:HE3	2.06	0.55
1:D:1275:CYS:O	1:D:1278:ILE:HG22	2.07	0.55
1:B:1515:GLN:O	1:B:1519:LYS:N	2.36	0.55
1:C:2359:ILE:O	1:C:2363:THR:HG23	2.06	0.55
1:A:1444:PHE:O	1:A:1448:MET:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:GLU:O	1:A:1458:ARG:NH1	2.38	0.54
1:C:2277:GLY:O	1:C:2281:THR:OG1	2.23	0.54
1:A:1290:LEU:HD21	1:A:1299:TYR:HB2	1.89	0.54
1:A:2215:ILE:O	1:A:2219:ILE:HG13	2.06	0.54
1:C:1445:THR:HG22	1:C:1501:LEU:CA	2.36	0.54
1:D:252:LEU:HD11	1:D:263:VAL:CG1	2.37	0.54
1:D:1206:MET:SD	1:D:1228:THR:HG23	2.47	0.54
1:A:705:GLU:N	1:A:705:GLU:OE2	2.40	0.54
1:C:252:LEU:HD11	1:C:263:VAL:CG1	2.36	0.54
1:D:1433:THR:HG22	1:D:1433:THR:O	2.06	0.54
1:B:1123:LYS:HD3	1:B:1126:LEU:HD13	1.89	0.54
1:D:1464:LEU:O	1:D:1468:VAL:HG23	2.07	0.54
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.88	0.54
1:A:1056:LEU:HD23	1:A:1056:LEU:O	2.08	0.54
1:A:1648:ILE:HG23	1:A:1736:LEU:HD22	1.89	0.54
1:D:1097:LEU:HD12	1:D:1595:LEU:HD22	1.90	0.54
1:B:1225:LEU:O	1:B:1229:HIS:ND1	2.41	0.54
1:C:596:THR:HG22	1:C:637:LEU:HD21	1.88	0.54
1:D:1123:LYS:HD2	1:D:1126:LEU:HD13	1.89	0.54
1:D:1407:THR:HG21	1:D:1464:LEU:HA	1.90	0.54
1:A:1089:MET:HE2	1:A:1606:LEU:HD12	1.88	0.54
1:D:1467:TYR:O	1:D:1471:VAL:HG22	2.08	0.54
1:C:1125:GLU:OE2	1:C:1125:GLU:N	2.36	0.53
1:D:1731:GLU:OE1	1:D:1731:GLU:HA	2.08	0.53
1:A:647:VAL:O	1:A:651:LEU:HD23	2.09	0.53
1:C:1737:VAL:HG11	1:C:1757:ALA:HB2	1.89	0.53
1:D:1670:GLN:NE2	1:D:1752:GLU:OE1	2.40	0.53
1:A:599:LEU:HB3	1:A:606:LEU:HD13	1.90	0.53
1:A:990:LEU:HD23	1:A:1092:PHE:HD1	1.72	0.53
1:B:452:LEU:HD22	1:B:521:ILE:CD1	2.38	0.53
1:D:1001:VAL:HG12	1:D:1002:PHE:CD2	2.42	0.53
1:C:1919:THR:HG22	1:C:1924:LEU:HD23	1.89	0.53
1:B:2218:ILE:HD11	1:B:2273:ILE:HD11	1.90	0.53
1:A:1491:LEU:CD2	1:A:1498:VAL:HG11	2.39	0.53
1:B:452:LEU:HD22	1:B:521:ILE:HD11	1.90	0.53
1:B:1247:HIS:O	1:B:1250:LEU:HD22	2.08	0.53
1:D:1397:VAL:O	1:D:1401:THR:HG23	2.09	0.53
1:B:1303:LEU:HD12	1:B:1371:LEU:HD21	1.91	0.53
1:B:1332:VAL:O	1:B:1368:LEU:HD11	2.07	0.53
1:B:1342:LEU:O	1:B:1346:LEU:HD13	2.08	0.53
1:D:1036:PHE:HZ	1:D:1088:ALA:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:LEU:HD23	1:A:1092:PHE:CE1	2.44	0.53
1:D:2023:GLN:NE2	1:D:2027:ASP:OD1	2.42	0.53
1:A:2540:ILE:HD11	1:A:2565:MET:HB3	1.90	0.53
1:B:1067:TYR:O	1:B:1071:VAL:HG23	2.09	0.53
1:B:1125:GLU:HG2	1:B:1126:LEU:HD12	1.90	0.53
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.42	0.53
1:A:760:ILE:HG21	1:A:781:MET:HB2	1.90	0.52
1:B:1407:THR:O	1:B:1411:MET:HG3	2.09	0.52
1:B:1298:GLN:OE1	1:B:1298:GLN:N	2.41	0.52
1:D:833:THR:CG2	1:D:866:LEU:HD21	2.39	0.52
1:A:1332:VAL:HG23	1:A:1333:VAL:HG13	1.91	0.52
1:B:451:MET:N	1:B:451:MET:SD	2.83	0.52
1:B:772:ASP:OD1	1:B:773:LEU:N	2.42	0.52
1:D:2449:ASP:OD1	1:D:2450:SER:N	2.42	0.52
1:B:1393:LEU:O	1:B:1393:LEU:HD12	2.10	0.52
1:C:745:TYR:O	1:C:749:ASP:OD2	2.27	0.52
1:C:816:ASP:O	1:C:823:ARG:NH2	2.42	0.52
1:D:1342:LEU:O	1:D:1346:LEU:HD13	2.09	0.52
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.91	0.52
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.39	0.52
1:A:1491:LEU:HD23	1:A:1498:VAL:HG11	1.91	0.52
1:C:1196:LEU:HD12	1:C:1196:LEU:O	2.09	0.52
1:A:482:PHE:O	1:A:505:ARG:NH1	2.43	0.52
1:A:1533:ALA:HA	1:A:1538:ILE:HD11	1.91	0.52
1:B:599:LEU:HB3	1:B:606:LEU:HD13	1.92	0.52
1:B:1323:THR:O	1:B:1327:ASN:OD1	2.28	0.52
1:C:1316:LYS:O	1:C:1320:MET:HG3	2.08	0.52
1:D:805:GLU:OE1	1:D:805:GLU:HA	2.09	0.52
1:C:1606:LEU:O	1:C:1610:VAL:HG23	2.10	0.52
1:C:655:CYS:O	1:C:661:ASN:ND2	2.40	0.52
1:C:885:THR:HG21	1:C:978:ILE:HG21	1.91	0.52
1:D:1513:TRP:O	1:D:1514:LEU:CB	2.58	0.52
1:B:477:GLU:OE1	1:B:493:VAL:HG11	2.10	0.52
1:D:2476:VAL:HG22	1:D:2480:LEU:HD13	1.92	0.52
1:C:1469:LEU:HD22	1:C:1518:HIS:CG	2.45	0.51
1:A:2178:LEU:O	1:A:2182:MET:HG3	2.10	0.51
1:B:1206:MET:HA	1:B:1206:MET:CE	2.40	0.51
1:B:1287:VAL:HG11	1:B:1324:GLU:HB3	1.92	0.51
1:D:1542:MET:H	1:D:1542:MET:CE	2.23	0.51
1:C:719:ASN:OD1	1:C:721:HIS:N	2.43	0.51
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:LEU:HD12	1:A:780:LEU:O	2.11	0.51
1:C:1421:TYR:HA	1:C:1424:THR:HG23	1.92	0.51
1:A:350:ILE:HD11	1:A:401:THR:HG21	1.93	0.51
1:A:1083:SER:O	1:A:1083:SER:OG	2.29	0.51
1:B:667:ARG:NE	1:B:667:ARG:HA	2.26	0.51
1:B:1379:LYS:NZ	1:B:1425:GLU:OE1	2.43	0.51
1:C:885:THR:CG2	1:C:978:ILE:HD13	2.33	0.51
1:D:506:GLN:NE2	1:D:563:SER:O	2.43	0.51
1:A:772:ASP:OD1	1:A:773:LEU:N	2.44	0.51
1:C:2172:PHE:HZ	1:C:2594:ILE:HG23	1.76	0.51
1:B:606:LEU:HD23	1:B:645:ILE:HD11	1.92	0.51
1:B:568:ARG:NH2	3:B:3002:I3P:O3	2.43	0.51
1:D:832:ASN:HA	1:D:835:GLU:OE1	2.10	0.51
1:B:614:GLU:OE1	1:B:614:GLU:N	2.43	0.51
1:C:708:VAL:HG11	1:C:769:LEU:HD21	1.93	0.51
1:C:1948:CYS:SG	1:C:1959:ILE:HD12	2.51	0.51
1:B:518:VAL:HG11	1:B:560:LEU:HG	1.93	0.51
1:B:279:SER:OG	1:B:511:GLU:OE2	2.19	0.50
1:C:2191:MET:CE	1:C:2194:ILE:HD12	2.40	0.50
1:B:862:GLU:HA	1:B:862:GLU:OE1	2.12	0.50
1:C:1659:GLU:OE1	1:C:1746:ASN:ND2	2.44	0.50
1:A:788:ARG:HG3	1:A:788:ARG:HH11	1.76	0.50
1:B:1533:ALA:HA	1:B:1538:ILE:HD11	1.93	0.50
1:B:2014:GLU:HA	1:B:2014:GLU:OE2	2.10	0.50
1:C:350:ILE:HD11	1:C:401:THR:HG21	1.92	0.50
1:A:656:VAL:HG21	1:A:739:MET:HE1	1.94	0.50
1:A:2264:LEU:O	1:A:2268:LEU:HG	2.11	0.50
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.11	0.50
1:A:1316:LYS:O	1:A:1320:MET:HG3	2.12	0.50
1:B:1441:PHE:CG	1:B:1501:LEU:HD11	2.46	0.50
1:C:1344:HIS:O	1:C:1348:MET:HG2	2.12	0.50
1:C:2388:PHE:HD2	1:C:2458:LEU:HD13	1.77	0.50
1:B:2536:THR:O	1:B:2536:THR:CG2	2.59	0.50
1:D:622:VAL:HG23	1:D:630:PHE:HB2	1.94	0.50
1:B:1106:ASN:ND2	1:B:1193:GLN:OE1	2.45	0.50
1:A:1407:THR:O	1:A:1411:MET:HG3	2.12	0.50
1:B:757:VAL:HG22	1:B:785:HIS:CG	2.46	0.50
1:B:2322:TYR:OH	1:B:2347:ASP:OD1	2.19	0.50
1:A:1514:LEU:HD23	1:A:1519:LYS:HD2	1.93	0.50
1:C:1229:HIS:HA	1:C:1232:LEU:HD12	1.93	0.50
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:ILE:HD13	1:A:2327:ILE:HD11	1.92	0.49
1:B:350:ILE:HD11	1:B:401:THR:HG21	1.92	0.49
1:B:893:ASP:OD1	1:B:894:CYS:N	2.45	0.49
1:B:2218:ILE:HD11	1:B:2273:ILE:CD1	2.41	0.49
1:A:1097:LEU:CD1	1:A:1595:LEU:HD22	2.42	0.49
1:A:1472:VAL:HG12	1:A:1476:ILE:HD12	1.94	0.49
1:A:1956:GLN:O	1:A:1960:VAL:HG23	2.12	0.49
1:D:1799:GLU:C	1:D:1799:GLU:OE1	2.50	0.49
1:A:485:ASP:OD2	1:A:505:ARG:NH1	2.45	0.49
1:A:1050:GLU:OE1	1:A:1053:ARG:NE	2.46	0.49
1:A:2010:SER:O	1:A:2014:GLU:OE1	2.30	0.49
1:C:1323:THR:O	1:C:1326:THR:OG1	2.24	0.49
1:D:599:LEU:HB3	1:D:606:LEU:HD13	1.95	0.49
1:D:976:GLN:HG2	1:D:1077:LEU:HD21	1.93	0.49
1:C:1372:LEU:HA	1:C:1375:CYS:SG	2.52	0.49
1:B:1048:ASP:OD1	1:B:1048:ASP:C	2.50	0.49
1:C:1323:THR:O	1:C:1327:ASN:OD1	2.30	0.49
1:C:1473:LEU:O	1:C:1477:ASN:ND2	2.46	0.49
1:D:1542:MET:SD	1:D:1543:ASP:OD2	2.70	0.49
1:A:811:THR:HG22	1:A:812:ILE:N	2.27	0.49
1:A:1297:VAL:HG12	1:A:1364:TYR:HA	1.94	0.49
1:B:602:ASN:HD22	1:B:605:LEU:HD12	1.78	0.49
1:B:1206:MET:HA	1:B:1206:MET:HE2	1.95	0.49
1:B:1960:VAL:CG1	1:B:1961:THR:HG23	2.41	0.49
1:A:1117:LEU:HD12	1:A:1117:LEU:O	2.13	0.49
1:A:1979:SER:HA	1:A:1982:CYS:SG	2.53	0.49
1:B:1396:VAL:O	1:B:1400:VAL:HG12	2.13	0.49
1:B:1509:LEU:HD21	1:B:1551:MET:CE	2.43	0.49
1:C:405:ILE:HD11	1:C:416:MET:HA	1.95	0.49
1:C:1455:ARG:NH1	1:C:1465:GLU:OE2	2.45	0.49
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.43	0.49
1:A:1627:LEU:HD21	1:A:1695:LEU:HD23	1.94	0.49
1:B:834:MET:O	1:B:837:VAL:HG12	2.13	0.49
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.13	0.49
1:C:1731:GLU:HA	1:C:1731:GLU:OE1	2.12	0.49
1:C:1919:THR:CG2	1:C:1924:LEU:HD23	2.43	0.49
1:C:2476:VAL:HG22	1:C:2480:LEU:HD13	1.95	0.49
1:D:577:GLN:O	1:D:580:MET:SD	2.71	0.49
1:D:1128:VAL:HG23	1:D:1221:MET:HE1	1.95	0.49
1:C:267:THR:HG23	1:C:413:ILE:O	2.13	0.49
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:LEU:HD12	1:D:622:VAL:N	2.26	0.49
1:A:308:HIS:ND1	1:A:311:THR:OG1	2.30	0.48
1:A:1117:LEU:HD12	1:A:1121:VAL:HG23	1.95	0.48
1:B:1256:PRO:HA	1:B:1289:LEU:HD11	1.95	0.48
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.95	0.48
1:A:267:THR:HG23	1:A:413:ILE:O	2.13	0.48
1:A:871:ILE:HD11	1:A:884:LEU:HD23	1.93	0.48
1:A:1656:GLU:OE2	1:A:1656:GLU:N	2.42	0.48
1:B:1288:HIS:O	1:B:1292:THR:HG23	2.13	0.48
1:D:280:ASN:O	1:D:308:HIS:NE2	2.46	0.48
1:D:405:ILE:HD11	1:D:416:MET:HA	1.95	0.48
1:D:969:LEU:HD11	1:D:1069:PRO:HB2	1.95	0.48
1:D:1001:VAL:HG12	1:D:1002:PHE:CE2	2.48	0.48
1:A:694:LEU:HD13	1:A:708:VAL:CG2	2.43	0.48
1:A:1056:LEU:CD2	1:A:1627:LEU:HD13	2.42	0.48
1:D:1509:LEU:HD23	1:D:1509:LEU:O	2.13	0.48
1:A:1358:ASP:O	1:A:1363:MET:CE	2.61	0.48
1:D:1033:GLU:HG2	1:D:1606:LEU:HD21	1.93	0.48
1:A:893:ASP:OD2	1:A:894:CYS:N	2.46	0.48
1:B:1898:LYS:HD2	1:B:1898:LYS:N	2.28	0.48
1:C:972:LEU:HD11	1:C:1062:LEU:HD13	1.95	0.48
1:D:2162:ASP:OD1	1:D:2165:GLY:N	2.47	0.48
1:A:2048:GLU:OE1	1:A:2048:GLU:N	2.47	0.48
1:A:2536:THR:O	1:A:2536:THR:CG2	2.61	0.48
1:B:405:ILE:HD11	1:B:416:MET:HA	1.95	0.48
1:B:782:LEU:HD13	1:B:866:LEU:HD12	1.96	0.48
1:C:482:PHE:O	1:C:505:ARG:NH1	2.45	0.48
1:C:280:ASN:O	1:C:308:HIS:NE2	2.47	0.48
1:D:452:LEU:HB3	1:D:521:ILE:HD11	1.95	0.48
1:D:1626:LEU:HD13	1:D:1698:ARG:HB2	1.95	0.48
1:A:1473:LEU:HD13	1:A:1522:VAL:HG22	1.96	0.48
1:B:1396:VAL:HG13	1:B:1413:TYR:HB3	1.96	0.48
1:A:250:LYS:HE2	1:A:267:THR:HG22	1.96	0.48
1:B:720:ALA:O	1:B:724:ASN:OD1	2.32	0.48
1:B:1434:SER:HB3	1:B:1436:HIS:ND1	2.29	0.48
1:C:682:TYR:HB2	1:C:685:ILE:HD12	1.96	0.48
1:C:1495:GLN:HA	1:C:1498:VAL:HG22	1.95	0.48
1:D:267:THR:HG23	1:D:413:ILE:O	2.14	0.48
1:A:1866:SER:O	1:A:1869:ILE:HG22	2.14	0.48
1:D:1602:LEU:CD2	1:D:1606:LEU:HD12	2.44	0.48
1:D:1924:LEU:N	1:D:1924:LEU:HD22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:LEU:HG	1:A:742:ASP:OD1	2.14	0.47
1:A:1123:LYS:HD3	1:A:1126:LEU:HD13	1.95	0.47
1:A:1773:HIS:HB2	1:A:1888:LEU:HD21	1.96	0.47
1:B:280:ASN:O	1:B:308:HIS:NE2	2.46	0.47
1:B:1467:TYR:O	1:B:1471:VAL:HG22	2.14	0.47
1:C:1315:LYS:N	1:C:1315:LYS:HD3	2.29	0.47
1:A:1345:LEU:O	1:A:1348:MET:HG3	2.14	0.47
1:A:1514:LEU:HD23	1:A:1519:LYS:CD	2.43	0.47
1:A:1902:ASN:ND2	1:A:1905:CYS:SG	2.87	0.47
1:B:1741:ILE:HG21	1:B:1785:PHE:CE1	2.49	0.47
1:A:837:VAL:HG23	1:A:863:VAL:HG13	1.95	0.47
1:A:1248:LYS:HE2	1:A:1248:LYS:HA	1.96	0.47
1:B:1979:SER:HA	1:B:1982:CYS:SG	2.54	0.47
1:D:1290:LEU:HD21	1:D:1299:TYR:HB2	1.96	0.47
1:B:505:ARG:O	1:B:509:MET:HG3	2.14	0.47
1:C:1038:VAL:HG22	1:C:1038:VAL:O	2.13	0.47
1:C:1322:MET:HA	1:C:1322:MET:HE3	1.96	0.47
1:C:1514:LEU:HD23	1:C:1519:LYS:CG	2.44	0.47
1:C:2293:LYS:O	1:C:2297:VAL:HG23	2.14	0.47
1:D:250:LYS:HE2	1:D:267:THR:HG22	1.95	0.47
1:D:2277:GLY:O	1:D:2281:THR:OG1	2.29	0.47
1:A:1967:ILE:O	1:A:1971:THR:HG23	2.14	0.47
1:B:1509:LEU:HD21	1:B:1551:MET:HE2	1.96	0.47
1:D:1381:VAL:O	1:D:1385:ILE:HG13	2.14	0.47
1:B:250:LYS:HE2	1:B:267:THR:HG22	1.95	0.47
1:B:267:THR:HG23	1:B:413:ILE:O	2.14	0.47
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.94	0.47
1:C:1456:GLU:O	1:C:1458:ARG:NH1	2.47	0.47
1:D:2468:HIS:HB2	1:D:2479:ILE:HD13	1.96	0.47
1:A:1187:GLU:OE1	1:A:1190:ARG:NH1	2.48	0.47
1:A:1741:ILE:HG21	1:A:1785:PHE:CE1	2.50	0.47
1:B:585:ILE:HD11	1:B:592:GLU:HG3	1.96	0.47
1:B:1973:LEU:CD2	1:B:1992:LEU:HD21	2.44	0.47
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.30	0.47
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.30	0.47
1:A:892:ILE:CG2	1:A:971:ILE:HD13	2.45	0.47
1:B:1373:ALA:O	1:B:1419:HIS:ND1	2.46	0.47
1:B:1430:GLU:O	1:B:1434:SER:OG	2.21	0.47
1:B:2328:LEU:O	1:B:2331:VAL:HG12	2.15	0.47
1:C:1411:MET:HE3	1:C:1466:LYS:HG3	1.97	0.47
1:C:2162:ASP:OD2	1:C:2162:ASP:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:THR:HG22	1:D:612:LYS:N	2.30	0.47
1:A:715:ALA:N	1:A:722:ASP:OD2	2.48	0.47
1:A:1615:SER:O	1:A:1619:ASP:OD2	2.32	0.47
1:C:606:LEU:HD23	1:C:645:ILE:HD13	1.97	0.47
1:C:1397:VAL:HG21	1:C:1436:HIS:HD2	1.74	0.47
1:D:1956:GLN:NE2	1:D:2002:ALA:O	2.48	0.47
1:A:1399:VAL:HG21	1:A:1413:TYR:HE2	1.79	0.47
1:A:2380:VAL:O	1:A:2384:SER:OG	2.28	0.47
1:B:464:ILE:HG22	1:B:535:LEU:HD21	1.97	0.47
1:B:1344:HIS:O	1:B:1348:MET:HG2	2.15	0.47
1:C:1773:HIS:HB2	1:C:1888:LEU:HD21	1.97	0.47
1:D:614:GLU:OE1	1:D:614:GLU:N	2.48	0.47
1:C:1386:LYS:O	1:C:1390:LEU:HD13	2.15	0.46
1:D:509:MET:HA	1:D:514:ILE:HD12	1.98	0.46
1:A:1229:HIS:CG	1:A:1259:LEU:HD22	2.51	0.46
1:B:455:ALA:O	1:B:459:LEU:HG	2.14	0.46
1:B:2004:MET:O	1:B:2004:MET:HG2	2.14	0.46
1:D:1125:GLU:HA	1:D:1128:VAL:HG12	1.97	0.46
1:A:1124:SER:HA	1:A:1127:TRP:CD1	2.50	0.46
1:C:716:ARG:NH2	1:C:768:MET:O	2.48	0.46
1:C:2546:ASP:OD2	1:C:2547:LYS:N	2.48	0.46
1:D:582:GLN:O	1:D:585:ILE:HG22	2.16	0.46
1:D:976:GLN:CG	1:D:1077:LEU:HD21	2.45	0.46
1:D:1346:LEU:HD21	1:D:1402:HIS:CD2	2.50	0.46
1:A:405:ILE:HD11	1:A:416:MET:HA	1.95	0.46
1:A:755:LEU:HD12	1:A:780:LEU:HD21	1.97	0.46
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	2.16	0.46
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.96	0.46
1:D:1473:LEU:CD1	1:D:1522:VAL:HG22	2.46	0.46
1:A:670:LEU:HD12	1:A:670:LEU:O	2.15	0.46
1:B:469:ARG:HD2	1:B:548:PRO:HB2	1.97	0.46
1:D:803:TRP:HA	1:D:806:ILE:HD12	1.97	0.46
1:A:1545:ASP:OD1	1:A:1545:ASP:C	2.54	0.46
1:B:1976:ASN:O	1:B:1993:LYS:NZ	2.47	0.46
1:C:2131:ARG:HG2	1:C:2131:ARG:HH11	1.79	0.46
1:A:711:LEU:HG	1:A:722:ASP:OD1	2.16	0.46
1:A:715:ALA:CA	1:A:722:ASP:OD2	2.63	0.46
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.32	0.46
1:B:854:GLU:OE2	1:B:854:GLU:N	2.33	0.46
1:B:1226:ARG:HA	1:B:1259:LEU:HD11	1.98	0.46
1:C:1885:ASN:ND2	1:C:1888:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1797:GLN:O	1:B:1800:THR:HG22	2.16	0.46
1:B:2004:MET:O	1:B:2004:MET:CG	2.64	0.46
1:C:250:LYS:HE2	1:C:267:THR:HG22	1.97	0.46
1:D:1919:THR:HG22	1:D:1924:LEU:HD23	1.97	0.46
1:A:2324:VAL:O	1:A:2327:ILE:HG22	2.16	0.46
1:C:1503:GLN:CG	1:C:1544:LEU:HD22	2.45	0.46
1:A:840:TYR:O	1:A:844:VAL:HG23	2.16	0.46
1:B:1396:VAL:HG21	1:B:1416:PHE:CE2	2.50	0.46
1:D:1432:TYR:HE2	1:D:1484:PHE:HB2	1.80	0.46
1:A:2284:ILE:O	1:A:2288:LEU:HD13	2.15	0.45
1:B:745:TYR:HA	1:B:748:ILE:HB	1.98	0.45
1:B:1469:LEU:HA	1:B:1473:LEU:HD12	1.98	0.45
1:B:1654:LEU:HD12	1:B:1654:LEU:O	2.16	0.45
1:C:1321:ILE:HG22	1:C:1325:LEU:HD11	1.98	0.45
1:C:1530:ALA:O	1:C:1534:LYS:HG2	2.17	0.45
1:C:1785:PHE:O	1:C:1788:VAL:HG22	2.15	0.45
1:A:515:LEU:HD11	1:A:570:ASN:ND2	2.31	0.45
1:A:1678:LYS:HA	1:A:1678:LYS:HE3	1.98	0.45
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.16	0.45
1:B:786:VAL:O	1:B:791:GLN:NE2	2.50	0.45
1:B:2185:GLN:O	1:B:2189:ARG:HG3	2.15	0.45
1:C:406:ASP:OD1	1:C:406:ASP:N	2.50	0.45
1:C:1228:THR:O	1:C:1232:LEU:HG	2.16	0.45
1:D:763:CYS:HB2	1:D:777:PHE:CD2	2.52	0.45
1:D:1326:THR:HG21	1:D:1386:LYS:HE3	1.98	0.45
1:A:406:ASP:OD1	1:A:406:ASP:N	2.50	0.45
1:A:1096:GLN:NE2	1:A:1097:LEU:O	2.49	0.45
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.45
1:B:972:LEU:HG	1:B:1077:LEU:HD12	1.99	0.45
1:B:1329:GLY:O	1:B:1333:VAL:HG22	2.17	0.45
1:B:1397:VAL:HA	1:B:1400:VAL:HG12	1.99	0.45
1:B:1494:HIS:O	1:B:1497:ILE:N	2.45	0.45
1:B:1881:CYS:SG	1:B:1892:LEU:HD12	2.57	0.45
1:C:1469:LEU:HD21	1:C:1514:LEU:HD12	1.98	0.45
1:B:966:GLU:O	1:B:970:LYS:HG2	2.17	0.45
1:A:604:LYS:HD3	1:A:604:LYS:N	2.32	0.45
1:A:621:LEU:HD13	1:A:630:PHE:CD1	2.50	0.45
1:B:801:ARG:HD2	1:B:991:LEU:HD12	1.98	0.45
1:C:1405:CYS:SG	1:C:1406:ILE:N	2.89	0.45
1:C:2280:PRO:O	1:C:2284:ILE:HG13	2.17	0.45
1:D:252:LEU:HD13	1:D:417:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1741:ILE:HG21	1:A:1785:PHE:HE1	1.82	0.45
1:A:1931:GLU:O	1:A:1934:VAL:HG12	2.17	0.45
1:C:806:ILE:HG22	1:C:995:LYS:HD2	1.99	0.45
1:C:1385:ILE:O	1:C:1388:THR:OG1	2.32	0.45
1:C:1503:GLN:HG3	1:C:1544:LEU:HD22	1.98	0.45
1:A:1056:LEU:HD23	1:A:1056:LEU:C	2.37	0.45
1:A:2214:PHE:O	1:A:2218:ILE:HG12	2.16	0.45
1:B:1994:ASP:OD1	1:B:1994:ASP:C	2.55	0.45
1:D:2359:ILE:O	1:D:2363:THR:HG23	2.17	0.45
1:A:761:PHE:C	1:A:761:PHE:CD2	2.89	0.45
1:B:1303:LEU:HD12	1:B:1371:LEU:CD2	2.46	0.45
1:C:703:HIS:ND1	1:C:703:HIS:N	2.64	0.45
1:D:1396:VAL:HG13	1:D:1413:TYR:HB3	1.97	0.45
1:D:2352:GLU:HA	1:D:2352:GLU:OE1	2.17	0.45
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.32	0.45
1:C:252:LEU:HD13	1:C:417:LEU:HD12	1.99	0.45
1:C:483:VAL:HG22	1:C:509:MET:SD	2.57	0.45
1:C:997:GLU:HA	1:C:997:GLU:OE1	2.17	0.45
1:C:1924:LEU:HD12	1:C:1927:LEU:HD12	1.99	0.45
1:C:2297:VAL:HG21	1:C:2327:ILE:CD1	2.47	0.45
1:D:2064:ASN:OD1	1:D:2066:GLN:N	2.50	0.45
1:A:1048:ASP:C	1:A:1048:ASP:OD1	2.55	0.45
1:A:1444:PHE:CD2	1:A:1472:VAL:HG13	2.52	0.45
1:D:1432:TYR:N	1:D:1432:TYR:CD1	2.84	0.45
1:D:1436:HIS:O	1:D:1439:THR:OG1	2.30	0.45
1:D:2009:ASP:OD1	1:D:2009:ASP:C	2.55	0.45
1:A:974:ILE:O	1:A:978:ILE:HG12	2.17	0.44
1:A:1434:SER:HB2	1:A:1436:HIS:CE1	2.52	0.44
1:B:871:ILE:HD13	1:B:974:ILE:HG23	1.98	0.44
1:B:1957:THR:HG22	1:B:2007:ARG:HH22	1.82	0.44
1:C:1514:LEU:HD23	1:C:1519:LYS:HG3	1.98	0.44
1:D:240:VAL:HG11	1:D:309:LEU:HD13	1.98	0.44
1:D:758:ASP:O	1:D:762:LEU:HD23	2.17	0.44
1:D:1393:LEU:HD11	1:D:1431:ILE:HG12	1.99	0.44
1:A:280:ASN:O	1:A:308:HIS:NE2	2.47	0.44
1:B:1220:LYS:HD3	1:B:1220:LYS:N	2.32	0.44
1:D:1931:GLU:O	1:D:1934:VAL:HG12	2.17	0.44
1:D:2178:LEU:HD13	1:D:2569:LEU:HD22	1.99	0.44
1:A:518:VAL:HG13	1:A:556:CYS:HB3	1.99	0.44
1:A:2159:THR:HG21	1:A:2167:LYS:HB3	1.99	0.44
1:B:1619:ASP:OD1	1:B:1687:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1333:VAL:HA	1:C:1368:LEU:HD21	1.99	0.44
1:A:252:LEU:HD13	1:A:417:LEU:HD12	1.99	0.44
1:A:729:TYR:O	1:A:733:LEU:HG	2.17	0.44
1:A:1696:GLN:O	1:A:1697:ASN:CB	2.65	0.44
1:B:406:ASP:OD1	1:B:406:ASP:N	2.50	0.44
1:B:2014:GLU:O	1:B:2018:ILE:HG13	2.18	0.44
1:C:621:LEU:HD13	1:C:630:PHE:CD1	2.52	0.44
1:D:1589:LYS:O	1:D:1593:GLU:OE1	2.36	0.44
1:A:607:GLU:OE2	1:A:608:LYS:NZ	2.45	0.44
1:A:1346:LEU:HD21	1:A:1402:HIS:CD2	2.52	0.44
1:C:451:MET:CE	1:C:451:MET:O	2.65	0.44
1:C:477:GLU:OE2	1:C:493:VAL:HG11	2.17	0.44
1:C:1924:LEU:HD22	1:C:1924:LEU:N	2.32	0.44
1:A:1250:LEU:HD23	1:A:1253:PHE:HB2	2.00	0.44
1:B:581:MET:N	1:B:581:MET:HE2	2.33	0.44
1:B:1286:PHE:O	1:B:1290:LEU:HG	2.18	0.44
1:B:1509:LEU:HD11	1:B:1551:MET:HE3	2.00	0.44
1:B:2284:ILE:HG22	1:B:2288:LEU:CD1	2.47	0.44
1:C:1741:ILE:HG21	1:C:1785:PHE:CE1	2.53	0.44
1:D:505:ARG:O	1:D:509:MET:HG3	2.16	0.44
1:D:1885:ASN:ND2	1:D:1888:LEU:HD23	2.33	0.44
1:A:745:TYR:N	1:A:1125:GLU:OE2	2.51	0.44
1:A:761:PHE:CE1	1:A:832:ASN:HB3	2.53	0.44
1:B:2323:HIS:O	1:B:2327:ILE:HG13	2.18	0.44
1:D:406:ASP:OD1	1:D:406:ASP:N	2.50	0.44
1:D:1345:LEU:O	1:D:1349:MET:HG3	2.18	0.44
1:A:1696:GLN:O	1:A:1697:ASN:HB3	2.17	0.44
1:C:1740:LEU:O	1:C:1744:THR:HG22	2.17	0.44
1:D:1334:VAL:HG23	1:D:1334:VAL:O	2.17	0.44
1:A:494:LEU:HD11	1:A:555:LEU:HG	1.99	0.43
1:A:2589:TYR:O	1:A:2593:MET:HG2	2.18	0.43
1:B:252:LEU:HD13	1:B:417:LEU:HD12	1.98	0.43
1:B:826:LYS:HD3	1:B:875:PHE:CD1	2.53	0.43
1:B:1967:ILE:O	1:B:1971:THR:HG23	2.18	0.43
1:D:772:ASP:OD1	1:D:773:LEU:N	2.49	0.43
1:D:1433:THR:O	1:D:1433:THR:CG2	2.66	0.43
1:D:1654:LEU:HD12	1:D:1654:LEU:O	2.17	0.43
1:D:1754:ILE:HG21	1:D:1872:PRO:HB2	2.00	0.43
1:A:834:MET:O	1:A:837:VAL:HG12	2.18	0.43
1:D:1006:ASP:OD2	1:D:1007:SER:N	2.51	0.43
1:D:1773:HIS:HB2	1:D:1888:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:LYS:CD	1:A:1126:LEU:HD13	2.48	0.43
1:A:1435:ASN:HA	1:A:1438:TRP:CD1	2.53	0.43
1:B:1444:PHE:CD2	1:B:1472:VAL:HG13	2.53	0.43
1:A:652:ILE:O	1:A:656:VAL:HG23	2.18	0.43
1:A:1247:HIS:HD2	1:A:1274:LEU:HD22	1.81	0.43
1:A:1379:LYS:NZ	1:A:1425:GLU:OE1	2.49	0.43
1:A:1911:LEU:HB2	1:A:1940:THR:HG21	2.00	0.43
1:B:580:MET:N	1:B:580:MET:CE	2.81	0.43
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.48	0.43
1:D:1377:GLU:O	1:D:1380:ASN:ND2	2.52	0.43
1:D:1530:ALA:O	1:D:1534:LYS:HG2	2.19	0.43
1:D:2015:ARG:HA	1:D:2018:ILE:HD12	2.00	0.43
1:A:1438:TRP:CD1	1:A:1494:HIS:CE1	3.07	0.43
1:A:1542:MET:SD	1:A:1542:MET:C	2.97	0.43
1:B:459:LEU:HD13	1:B:525:PRO:HD3	2.00	0.43
1:B:466:GLN:OE1	1:B:469:ARG:NH2	2.51	0.43
1:B:493:VAL:O	1:B:496:ILE:HG22	2.19	0.43
1:C:252:LEU:HD13	1:C:417:LEU:CD1	2.48	0.43
1:D:833:THR:HG21	1:D:866:LEU:HD21	2.01	0.43
1:D:1310:GLU:HG2	1:D:1310:GLU:O	2.18	0.43
1:B:698:ASP:OD1	1:B:699:LYS:N	2.51	0.43
1:B:1409:VAL:HG13	1:B:1413:TYR:CZ	2.54	0.43
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.52	0.43
1:C:816:ASP:OD1	1:C:817:SER:N	2.52	0.43
1:D:1454:LYS:HB3	1:D:1460:ALA:HA	2.00	0.43
1:D:1518:HIS:O	1:D:1522:VAL:HG23	2.19	0.43
1:A:639:VAL:HG12	1:A:738:ARG:HH21	1.84	0.43
1:A:857:ASN:HA	1:A:860:THR:HG22	2.00	0.43
1:B:743:ARG:NH1	1:B:745:TYR:OH	2.52	0.43
1:B:1514:LEU:HD23	1:B:1519:LYS:HG2	2.00	0.43
1:C:1509:LEU:HA	1:C:1514:LEU:HD22	2.00	0.43
1:A:252:LEU:HD13	1:A:417:LEU:CD1	2.49	0.43
1:A:580:MET:C	1:A:580:MET:HE2	2.38	0.43
1:A:585:ILE:HD13	1:A:595:ILE:HD12	1.99	0.43
1:A:1188:GLN:HA	1:A:1191:LYS:HG2	2.01	0.43
1:A:1885:ASN:ND2	1:A:1888:LEU:HD23	2.33	0.43
1:A:2294:ILE:CD1	1:A:2327:ILE:HD11	2.49	0.43
1:C:1366:ILE:HD11	1:C:1409:VAL:HG23	2.00	0.43
1:D:497:MET:SD	1:D:497:MET:C	2.97	0.43
1:D:1522:VAL:O	1:D:1526:ILE:HG22	2.19	0.43
1:A:882:LEU:O	1:A:886:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LEU:HD13	1:B:417:LEU:CD1	2.48	0.43
1:B:750:GLU:C	1:B:750:GLU:OE2	2.58	0.43
1:B:782:LEU:HD13	1:B:866:LEU:HA	2.00	0.43
1:B:1356:VAL:HG23	1:B:1363:MET:HE2	2.01	0.43
1:C:308:HIS:ND1	1:C:311:THR:OG1	2.30	0.43
1:D:1994:ASP:OD1	1:D:2052:ASN:ND2	2.52	0.43
1:A:1758:ILE:HD11	1:A:1872:PRO:O	2.18	0.43
1:B:974:ILE:HG22	1:B:978:ILE:HD11	2.00	0.43
1:B:1941:LEU:HD12	1:B:1992:LEU:HD12	2.01	0.43
1:C:580:MET:N	1:C:580:MET:CE	2.82	0.43
1:C:1501:LEU:HD23	1:C:1501:LEU:O	2.19	0.43
1:C:2131:ARG:HG2	1:C:2131:ARG:NH1	2.34	0.43
1:D:462:GLY:O	1:D:535:LEU:HD13	2.18	0.43
1:D:1388:THR:HG22	1:D:1421:TYR:CE1	2.54	0.43
1:D:1574:ARG:O	1:D:1575:ALA:HB3	2.19	0.43
1:D:1651:THR:OG1	1:D:1665:VAL:HG11	2.18	0.43
1:B:2159:THR:HG21	1:B:2167:LYS:HB3	2.01	0.42
1:C:2148:THR:OG1	1:C:2151:THR:OG1	2.34	0.42
1:D:1602:LEU:HD23	1:D:1602:LEU:O	2.19	0.42
1:A:842:ASN:O	1:A:845:VAL:HG12	2.19	0.42
1:A:1334:VAL:HG23	1:A:1334:VAL:O	2.19	0.42
1:B:496:ILE:HG23	1:B:562:HIS:NE2	2.35	0.42
1:B:834:MET:HE2	1:B:876:TYR:CE1	2.53	0.42
1:D:1505:THR:HG21	1:D:1526:ILE:HB	2.00	0.42
1:D:2017:LEU:HG	1:D:2060:LEU:HD22	2.01	0.42
1:A:1797:GLN:NE2	1:A:1906:GLU:O	2.52	0.42
1:B:1473:LEU:HD11	1:B:1522:VAL:HG23	2.01	0.42
1:C:1797:GLN:NE2	1:C:1906:GLU:OE2	2.49	0.42
1:D:592:GLU:O	1:D:596:THR:HG23	2.19	0.42
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.20	0.42
1:A:279:SER:OG	1:A:511:GLU:OE2	2.36	0.42
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.60	0.42
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.19	0.42
1:D:729:TYR:O	1:D:733:LEU:HG	2.20	0.42
1:D:2607:ALA:HB3	1:D:2610:LEU:HD12	2.00	0.42
1:A:488:ASN:OD1	1:A:491:GLN:NE2	2.53	0.42
1:B:797:VAL:HG22	1:B:984:ASP:HB2	2.02	0.42
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.53	0.42
1:C:1382:TYR:O	1:C:1386:LYS:HG3	2.19	0.42
1:D:270:ARG:NH2	3:D:3002:I3P:O51	2.46	0.42
1:D:990:LEU:HD13	1:D:1035:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1339:LYS:O	1:D:1339:LYS:HD3	2.20	0.42
1:B:581:MET:HB3	1:B:595:ILE:HD11	2.01	0.42
1:B:760:ILE:HA	1:B:763:CYS:SG	2.59	0.42
1:D:1128:VAL:HG23	1:D:1221:MET:CE	2.50	0.42
1:D:1428:MET:HB3	1:D:1431:ILE:HD12	2.02	0.42
1:D:1513:TRP:O	1:D:1514:LEU:HB3	2.20	0.42
1:D:1666:LEU:HD11	1:D:1740:LEU:HD13	2.01	0.42
1:A:881:LEU:HD22	1:A:978:ILE:CD1	2.50	0.42
1:A:1328:ALA:HB3	1:A:1332:VAL:HG21	2.01	0.42
1:B:1124:SER:HA	1:B:1127:TRP:CE2	2.54	0.42
1:B:1411:MET:HG2	1:B:1467:TYR:HB2	2.01	0.42
1:C:1650:HIS:O	1:C:1654:LEU:HD23	2.19	0.42
1:D:755:LEU:HD13	1:D:780:LEU:HD21	2.01	0.42
1:D:1345:LEU:O	1:D:1348:MET:HG2	2.20	0.42
1:A:882:LEU:O	1:A:885:THR:OG1	2.37	0.42
1:A:1619:ASP:OD2	1:A:1619:ASP:N	2.53	0.42
1:A:2211:LEU:O	1:A:2215:ILE:HD12	2.20	0.42
1:A:2359:ILE:O	1:A:2363:THR:HG23	2.20	0.42
1:B:308:HIS:ND1	1:B:311:THR:OG1	2.30	0.42
1:B:518:VAL:HG13	1:B:556:CYS:SG	2.59	0.42
1:C:581:MET:HB3	1:C:595:ILE:HD11	2.01	0.42
1:C:630:PHE:O	1:C:634:LEU:HD13	2.20	0.42
1:C:1300:LEU:HB3	1:C:1371:LEU:HD22	2.02	0.42
1:D:630:PHE:O	1:D:634:LEU:HG	2.19	0.42
1:B:634:LEU:HA	1:B:637:LEU:HD12	2.02	0.42
1:B:1123:LYS:CD	1:B:1126:LEU:HD13	2.50	0.42
1:B:2369:ILE:HG23	1:B:2512:ILE:HG23	2.02	0.42
1:C:745:TYR:HA	1:C:748:ILE:HB	2.02	0.42
1:A:1023:MET:N	1:A:1023:MET:HE2	2.35	0.41
1:B:1054:MET:O	1:B:1058:VAL:HG22	2.19	0.41
1:B:1941:LEU:HD11	1:B:1973:LEU:HD13	2.02	0.41
1:B:2476:VAL:O	1:B:2479:ILE:HG13	2.20	0.41
1:A:1290:LEU:HD21	1:A:1299:TYR:CB	2.50	0.41
1:A:1457:LYS:O	1:A:1458:ARG:HB2	2.20	0.41
1:B:2294:ILE:O	1:B:2297:VAL:HG12	2.21	0.41
1:C:997:GLU:O	1:C:1001:VAL:HG23	2.20	0.41
1:C:1328:ALA:HB3	1:C:1332:VAL:HG21	2.02	0.41
1:D:1548:ILE:HA	1:D:1551:MET:HG2	2.02	0.41
1:A:653:CYS:SG	1:A:739:MET:HG2	2.60	0.41
1:B:515:LEU:HD21	1:B:563:SER:HB2	2.01	0.41
1:B:1218:ASP:O	1:B:1222:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2608:MET:HA	1:B:2611:VAL:HG12	2.02	0.41
1:C:1525:CYS:O	1:C:1528:THR:OG1	2.32	0.41
1:C:2390:PHE:N	1:C:2390:PHE:CD1	2.89	0.41
1:D:1881:CYS:SG	1:D:1892:LEU:HD12	2.61	0.41
1:A:1492:GLN:OE1	1:A:1492:GLN:N	2.54	0.41
1:A:1515:GLN:O	1:A:1519:LYS:N	2.46	0.41
1:B:991:LEU:HD11	1:B:1097:LEU:HD21	2.02	0.41
1:B:1048:ASP:OD1	1:B:1051:GLY:N	2.47	0.41
1:B:2020:LEU:HD21	1:B:2025:LEU:HD22	2.02	0.41
1:B:2164:GLN:N	1:B:2164:GLN:OE1	2.53	0.41
1:C:694:LEU:HD13	1:C:708:VAL:HG22	2.03	0.41
1:D:1182:MET:HE2	1:D:1182:MET:HA	2.02	0.41
1:B:888:LEU:CD1	1:B:974:ILE:HG21	2.51	0.41
1:C:694:LEU:CD1	1:C:708:VAL:HG22	2.50	0.41
1:D:480:VAL:CG2	1:D:559:VAL:HG23	2.50	0.41
1:D:1117:LEU:HB2	1:D:1175:ILE:HG21	2.02	0.41
1:B:1221:MET:O	1:B:1221:MET:SD	2.78	0.41
1:B:1409:VAL:CG1	1:B:1413:TYR:CZ	3.04	0.41
1:B:1689:MET:HA	1:B:1689:MET:CE	2.50	0.41
1:D:722:ASP:HA	1:D:725:VAL:HG12	2.02	0.41
1:D:1085:ARG:HB2	1:D:1610:VAL:HG22	2.03	0.41
1:D:1626:LEU:HD13	1:D:1698:ARG:CB	2.51	0.41
1:A:466:GLN:OE1	1:A:469:ARG:NH2	2.52	0.41
1:A:1628:PHE:CD1	1:A:1628:PHE:N	2.88	0.41
1:A:2187:LYS:HB2	1:A:2187:LYS:HE3	1.95	0.41
1:A:2549:ASP:OD1	1:A:2549:ASP:N	2.53	0.41
1:C:2389:LEU:HD21	1:D:2339:LEU:CD1	2.51	0.41
1:D:692:VAL:HG21	1:D:763:CYS:SG	2.61	0.41
1:D:1606:LEU:CD2	1:D:1609:LEU:HD12	2.51	0.41
1:D:1869:ILE:O	1:D:1869:ILE:HD12	2.21	0.41
1:A:439:ILE:H	1:A:439:ILE:HD12	1.86	0.41
1:A:1439:THR:HA	1:A:1442:GLU:HG2	2.02	0.41
1:A:1492:GLN:CD	1:A:1493:THR:HG23	2.41	0.41
1:B:722:ASP:HA	1:B:725:VAL:HG12	2.02	0.41
1:B:877:SER:OG	1:B:878:PHE:N	2.53	0.41
1:B:1316:LYS:HD2	1:B:1316:LYS:N	2.36	0.41
1:C:606:LEU:HD23	1:C:645:ILE:CD1	2.50	0.41
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.51	0.41
1:C:1125:GLU:HA	1:C:1128:VAL:HG12	2.03	0.41
1:C:1316:LYS:HD3	1:C:1316:LYS:H	1.86	0.41
1:D:282:LEU:HD22	1:D:434:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:VAL:HG12	1:D:537:ARG:N	2.35	0.41
1:A:253:THR:HG22	1:A:254:CYS:N	2.36	0.41
1:A:596:THR:HG21	1:A:633:TYR:HD1	1.86	0.41
1:A:1501:LEU:HD23	1:A:1501:LEU:O	2.21	0.41
1:A:1919:THR:HG22	1:A:1924:LEU:HD23	2.03	0.41
1:B:581:MET:HE2	1:B:581:MET:H	1.85	0.41
1:B:822:SER:O	1:B:826:LYS:HG2	2.21	0.41
1:B:1551:MET:O	1:B:1551:MET:SD	2.78	0.41
1:B:1771:SER:O	1:B:1775:LEU:HG	2.21	0.41
1:C:1397:VAL:O	1:C:1401:THR:HG23	2.20	0.41
1:C:1439:THR:HA	1:C:1442:GLU:HG2	2.03	0.41
1:C:1469:LEU:HD22	1:C:1518:HIS:CD2	2.55	0.41
1:C:1626:LEU:HD13	1:C:1698:ARG:HB2	2.03	0.41
1:D:459:LEU:HD22	1:D:525:PRO:HG3	2.03	0.41
1:D:1067:TYR:O	1:D:1071:VAL:HG23	2.20	0.41
1:D:1284:GLN:HA	1:D:1287:VAL:HG22	2.03	0.41
1:D:1362:LEU:HD11	1:D:1409:VAL:CG2	2.51	0.41
1:D:1473:LEU:HD11	1:D:1522:VAL:HG22	2.03	0.41
1:D:1740:LEU:O	1:D:1744:THR:HG22	2.21	0.41
1:D:2155:LEU:HD22	1:D:2178:LEU:HD11	2.03	0.41
1:A:235:LEU:N	1:A:381:VAL:O	2.54	0.41
1:A:606:LEU:HD23	1:A:645:ILE:HD13	2.02	0.41
1:A:754:GLN:HA	1:A:754:GLN:OE1	2.21	0.41
1:A:810:ILE:HG21	1:A:989:TYR:HA	2.02	0.41
1:A:1214:TYR:CD2	1:A:1221:MET:HG3	2.56	0.41
1:B:606:LEU:HD12	1:B:610:ILE:HG12	2.02	0.41
1:B:843:ASN:O	1:B:847:GLU:HG3	2.21	0.41
1:B:1674:LEU:HD23	1:B:1674:LEU:HA	1.98	0.41
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	2.02	0.41
1:C:2297:VAL:O	1:C:2301:VAL:HG22	2.21	0.41
1:C:2558:HIS:CE1	1:C:2563:HIS:ND1	2.89	0.41
1:D:1263:THR:HG22	1:D:1267:ILE:CD1	2.51	0.41
1:D:1626:LEU:HD12	1:D:1695:LEU:HD13	2.03	0.41
1:D:1741:ILE:HG21	1:D:1785:PHE:CE1	2.56	0.41
1:A:722:ASP:HA	1:A:725:VAL:HG12	2.03	0.40
1:A:1221:MET:O	1:A:1221:MET:SD	2.80	0.40
1:A:1221:MET:SD	1:A:1225:LEU:HG	2.61	0.40
1:B:235:LEU:N	1:B:381:VAL:O	2.54	0.40
1:B:1056:LEU:HD12	1:B:1694:TYR:CD2	2.55	0.40
1:B:1120:MET:O	1:B:1127:TRP:NE1	2.47	0.40
1:B:1174:GLY:O	1:B:1178:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1266:HIS:CD2	1:B:1266:HIS:N	2.86	0.40
1:B:1646:LYS:HD2	1:B:1646:LYS:O	2.21	0.40
1:C:451:MET:HG3	1:C:475:LEU:HD22	2.03	0.40
1:D:308:HIS:ND1	1:D:311:THR:OG1	2.31	0.40
1:D:608:LYS:C	1:D:608:LYS:HD3	2.42	0.40
1:D:667:ARG:HD3	1:D:668:THR:N	2.36	0.40
1:D:2007:ARG:HG3	1:D:2007:ARG:HH11	1.86	0.40
1:A:2071:LEU:CD2	1:A:2114:LEU:HD22	2.51	0.40
1:B:1297:VAL:HG12	1:B:1364:TYR:HA	2.03	0.40
1:C:591:ALA:O	1:C:595:ILE:HD12	2.21	0.40
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.21	0.40
1:D:1288:HIS:CE1	1:D:1292:THR:HG21	2.56	0.40
1:A:694:LEU:O	1:A:705:GLU:HA	2.21	0.40
1:A:1322:MET:HE1	1:A:1323:THR:HA	2.03	0.40
1:B:253:THR:HG22	1:B:254:CYS:N	2.36	0.40
1:B:1124:SER:CB	1:B:1212:ILE:HD11	2.48	0.40
1:B:1333:VAL:HG23	1:B:1333:VAL:O	2.22	0.40
1:C:582:GLN:O	1:C:585:ILE:HG22	2.21	0.40
1:C:2297:VAL:HG21	1:C:2327:ILE:HD11	2.03	0.40
1:D:447:ASP:O	1:D:451:MET:HG2	2.22	0.40
1:D:1626:LEU:HD22	1:D:1698:ARG:CB	2.51	0.40
1:A:462:GLY:O	1:A:535:LEU:HD13	2.21	0.40
1:A:1421:TYR:O	1:A:1424:THR:HG23	2.22	0.40
1:A:1741:ILE:HG23	1:A:1750:PHE:HE2	1.86	0.40
1:B:439:ILE:H	1:B:439:ILE:HD12	1.87	0.40
1:C:235:LEU:N	1:C:381:VAL:O	2.55	0.40
1:C:554:ARG:O	1:C:558:ARG:HG2	2.21	0.40
1:C:743:ARG:NH1	1:C:788:ARG:O	2.55	0.40
1:C:2518:ASP:CG	1:D:2524:ARG:NH2	2.74	0.40
1:D:480:VAL:HG22	1:D:559:VAL:HG23	2.02	0.40
1:A:694:LEU:HD13	1:A:708:VAL:HG22	2.03	0.40
1:A:1304:HIS:CD2	1:A:1304:HIS:C	2.94	0.40
1:A:2610:LEU:HD23	1:A:2610:LEU:HA	1.99	0.40
1:B:823:ARG:HA	1:B:826:LYS:HG2	2.04	0.40
1:B:1381:VAL:HG13	1:B:1382:TYR:N	2.37	0.40
1:C:1462:PRO:O	1:C:1466:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	80
1	B	1959/2671 (73%)	1933 (99%)	26 (1%)	0	100	100
1	C	1978/2671 (74%)	1951 (99%)	27 (1%)	0	100	100
1	D	2010/2671 (75%)	1979 (98%)	30 (2%)	1 (0%)	100	100
All	All	7908/10684 (74%)	7793 (98%)	113 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1514	LEU
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%)	1764 (98%)	43 (2%)	44	71
1	B	1805/2385 (76%)	1764 (98%)	41 (2%)	45	72
1	C	1820/2385 (76%)	1790 (98%)	30 (2%)	58	79
1	D	1838/2385 (77%)	1805 (98%)	33 (2%)	54	77
All	All	7270/9540 (76%)	7123 (98%)	147 (2%)	50	75

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	PHE
1	A	552	MET
1	A	567	TYR
1	A	580	MET
1	A	600	HIS
1	A	758	ASP
1	A	761	PHE
1	A	830	PHE
1	A	988	SER
1	A	1092	PHE
1	A	1100	SER
1	A	1107	TYR
1	A	1115	ASP
1	A	1203	HIS
1	A	1214	TYR
1	A	1233	GLN
1	A	1236	CYS
1	A	1253	PHE
1	A	1308	LYS
1	A	1322	MET
1	A	1325	LEU
1	A	1339	LYS
1	A	1348	MET
1	A	1411	MET
1	A	1458	ARG
1	A	1507	ARG
1	A	1619	ASP
1	A	1698	ARG
1	A	1772	PHE
1	A	1894	CYS
1	A	1897	ASN
1	A	1958	CYS
1	A	1965	ASN
1	A	1984	TYR
1	A	2160	GLU
1	A	2166	SER
1	A	2170	ASP
1	A	2176	SER
1	A	2393	ASP
1	A	2549	ASP
1	A	2565	MET
1	A	2576	ARG
1	A	2592	GLN

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Mol	Chain	Res	Type
1	B	552	MET
1	B	567	TYR
1	B	581	MET
1	B	612	LYS
1	B	618	PHE
1	B	632	ASP
1	B	703	HIS
1	B	714	GLU
1	B	724	ASN
1	B	728	TYR
1	B	743	ARG
1	B	818	ASN
1	B	1035	MET
1	B	1044	MET
1	B	1048	ASP
1	B	1072	SER
1	B	1211	GLN
1	B	1249	HIS
1	B	1268	PHE
1	B	1288	HIS
1	B	1327	ASN
1	B	1364	TYR
1	B	1370	ASP
1	B	1382	TYR
1	B	1458	ARG
1	B	1467	TYR
1	B	1619	ASP
1	B	1635	TYR
1	B	1655	MET
1	B	1787	LYS
1	B	1871	GLN
1	B	1895	GLN
1	B	1905	CYS
1	B	1964	SER
1	B	2033	TYR
1	B	2166	SER
1	B	2191	MET
1	B	2292	ASN
1	B	2318	MET
1	B	2466	MET
1	B	2549	ASP
1	C	552	MET

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Mol	Chain	Res	Type
1	C	567	TYR
1	C	682	TYR
1	C	703	HIS
1	C	722	ASP
1	C	742	ASP
1	C	749	ASP
1	C	778	CYS
1	C	1040	LYS
1	C	1049	ASP
1	C	1115	ASP
1	C	1203	HIS
1	C	1251	HIS
1	C	1331	ASP
1	C	1348	MET
1	C	1353	ARG
1	C	1458	ARG
1	C	1542	MET
1	C	1698	ARG
1	C	1905	CYS
1	C	1982	CYS
1	C	2010	SER
1	C	2162	ASP
1	C	2198	SER
1	C	2326	TYR
1	C	2361	SER
1	C	2449	ASP
1	C	2461	CYS
1	C	2520	PHE
1	C	2528	GLN
1	D	454	SER
1	D	552	MET
1	D	567	TYR
1	D	580	MET
1	D	635	SER
1	D	722	ASP
1	D	758	ASP
1	D	766	ASP
1	D	846	SER
1	D	1018	SER
1	D	1022	ASN
1	D	1043	SER
1	D	1061	HIS

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Mol	Chain	Res	Type
1	D	1222	MET
1	D	1322	MET
1	D	1360	SER
1	D	1364	TYR
1	D	1458	ARG
1	D	1531	MET
1	D	1542	MET
1	D	1551	MET
1	D	1578	ARG
1	D	1689	MET
1	D	1698	ARG
1	D	1795	ARG
1	D	1802	SER
1	D	1905	CYS
1	D	1987	ASP
1	D	2033	TYR
1	D	2047	ARG
1	D	2173	ASP
1	D	2299	SER
1	D	2330	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	783	HIS
1	A	791	GLN
1	A	1304	HIS
1	B	1065	HIS
1	B	1304	HIS
1	B	1318	GLN
1	B	1418	ASN
1	B	2135	GLN
1	C	573	HIS
1	C	1247	HIS
1	C	1304	HIS
1	D	1229	HIS
1	D	1318	GLN
1	D	1380	ASN
1	D	1622	HIS
1	D	2550	ASN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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$
5	ATP	A	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	0.86	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	C	3004	-	28,33,33	0.63	0	34,52,52	0.90	1 (2%)
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0
3	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.86	0
5	ATP	B	3004	-	28,33,33	0.62	0	34,52,52	0.87	1 (2%)
5	ATP	D	3004	-	28,33,33	0.61	0	34,52,52	0.87	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
5	ATP	A	3004	-	-	7/18/38/38	0/3/3/3
3	I3P	C	3002	-	-	2/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	10/18/38/38	0/3/3/3
3	I3P	D	3002	-	-	3/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	2/15/39/39	0/1/1/1
5	ATP	B	3004	-	-	6/18/38/38	0/3/3/3
5	ATP	D	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	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	A	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	D	3002	I3P	P5-O5	5.96	1.70	1.59
3	B	3002	I3P	P5-O5	5.95	1.70	1.59
3	C	3002	I3P	P5-O5	5.95	1.70	1.59
3	A	3002	I3P	P5-O5	5.95	1.69	1.59
3	D	3002	I3P	P1-O1	5.76	1.69	1.59
3	A	3002	I3P	P1-O1	5.75	1.69	1.59
3	B	3002	I3P	P1-O1	5.72	1.69	1.59
3	C	3002	I3P	P1-O1	5.72	1.69	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3004	ATP	C5-C6-N6	2.34	123.88	120.31
5	B	3004	ATP	C5-C6-N6	2.32	123.85	120.31
5	A	3004	ATP	C5-C6-N6	2.32	123.85	120.31
5	C	3004	ATP	C5-C6-N6	2.32	123.85	120.31

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C5'-O5'-PA-O3A
5	B	3004	ATP	C5'-O5'-PA-O2A
5	C	3004	ATP	PB-O3B-PG-O2G

*Continued on next page...*

*Continued from previous page...*

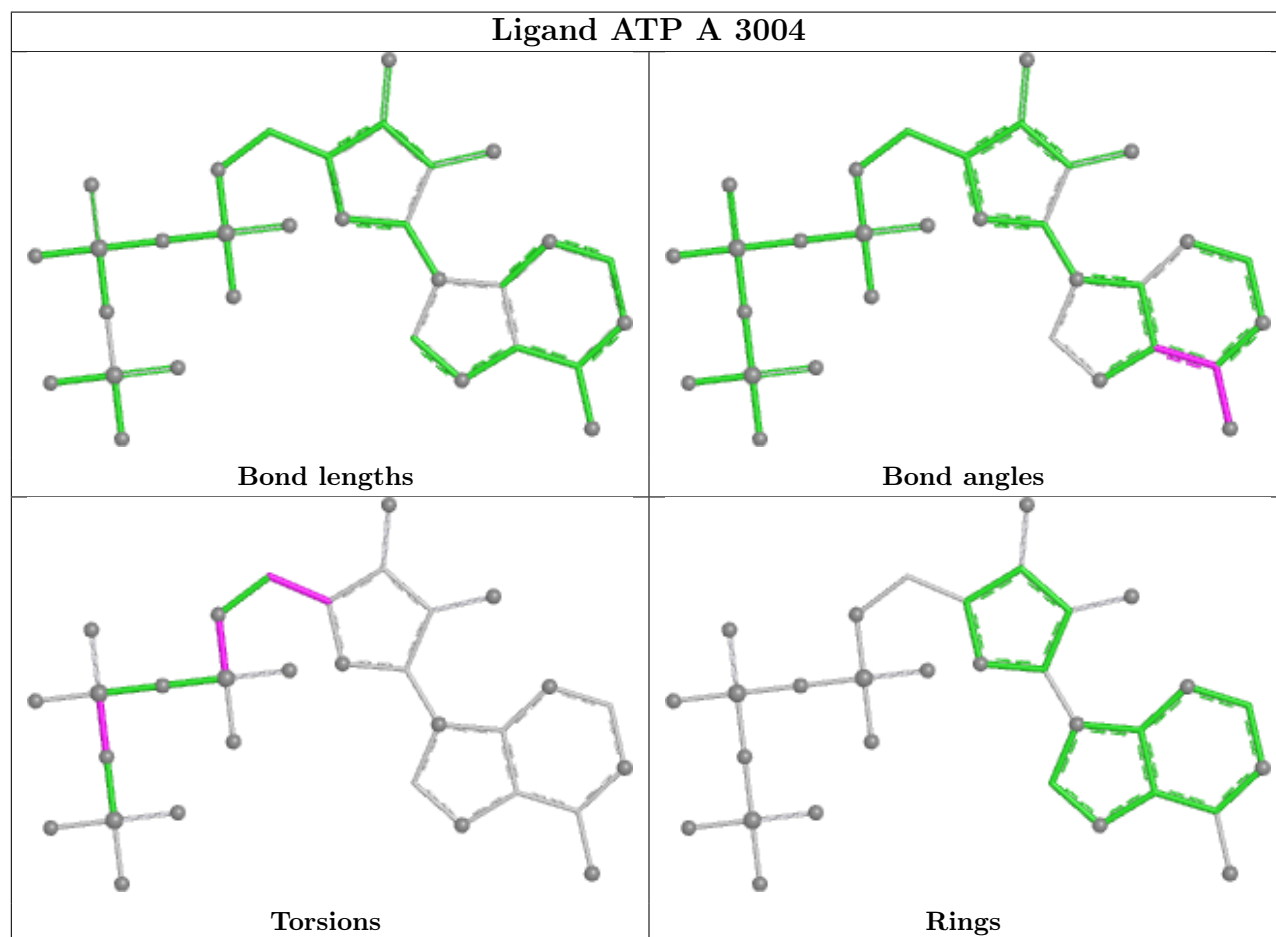
Mol	Chain	Res	Type	Atoms
5	C	3004	ATP	C5'-O5'-PA-O1A
5	C	3004	ATP	C5'-O5'-PA-O2A
5	C	3004	ATP	C5'-O5'-PA-O3A
5	D	3004	ATP	PB-O3B-PG-O2G
5	D	3004	ATP	PB-O3B-PG-O3G
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	C	3004	ATP	O4'-C4'-C5'-O5'
5	C	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	B	3004	ATP	C3'-C4'-C5'-O5'
5	B	3004	ATP	O4'-C4'-C5'-O5'
3	D	3002	I3P	C6-C1-O1-P1
5	A	3004	ATP	C5'-O5'-PA-O1A
5	B	3004	ATP	C5'-O5'-PA-O1A
5	C	3004	ATP	PB-O3A-PA-O2A
3	A	3002	I3P	C6-C1-O1-P1
3	C	3002	I3P	C6-C1-O1-P1
3	D	3002	I3P	C5-O5-P5-O53
3	B	3002	I3P	C6-C1-O1-P1
5	B	3004	ATP	PG-O3B-PB-O2B
5	C	3004	ATP	PG-O3B-PB-O2B
3	D	3002	I3P	C2-C1-O1-P1
5	B	3004	ATP	PG-O3B-PB-O1B
5	D	3004	ATP	PG-O3B-PB-O1B
3	B	3002	I3P	C4-O4-P4-O42
3	C	3002	I3P	C4-O4-P4-O42
5	D	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	PG-O3B-PB-O1B
5	A	3004	ATP	PG-O3B-PB-O2B
5	C	3004	ATP	PG-O3B-PB-O1B
5	C	3004	ATP	PB-O3A-PA-O1A
5	D	3004	ATP	PG-O3B-PB-O2B

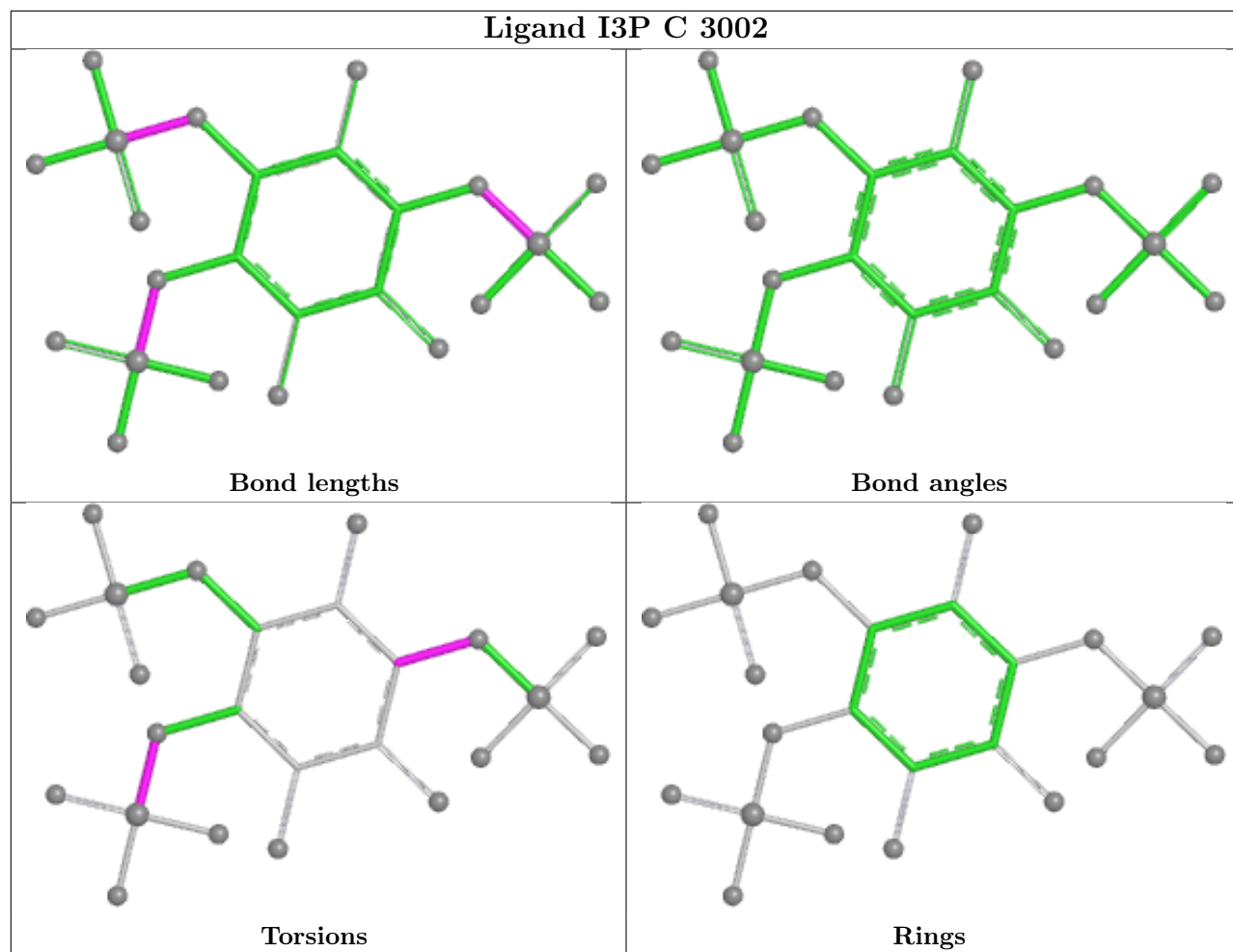
There are no ring outliers.

4 monomers are involved in 4 short contacts:

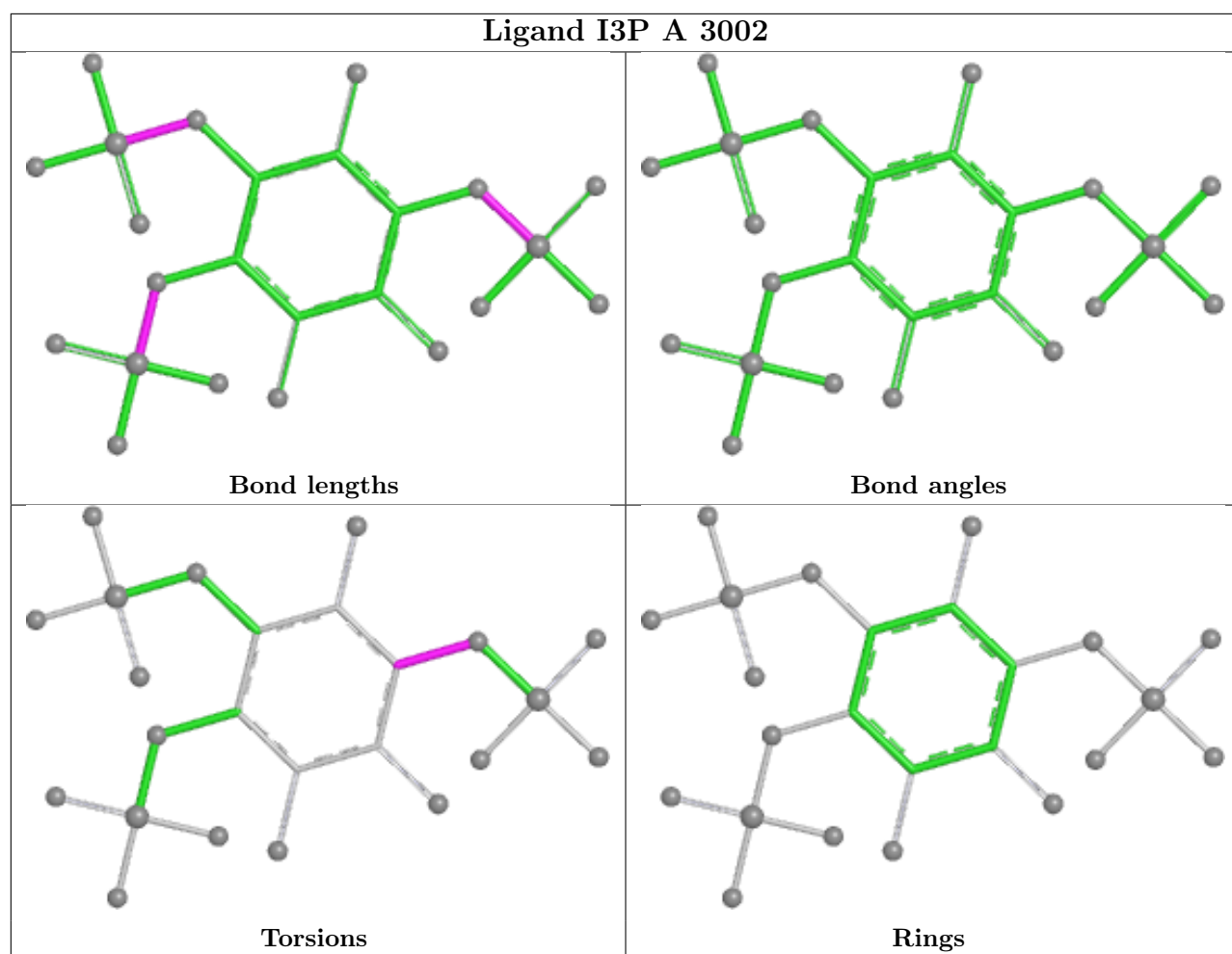
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	1	0
3	A	3002	I3P	1	0
3	D	3002	I3P	1	0
3	B	3002	I3P	1	0

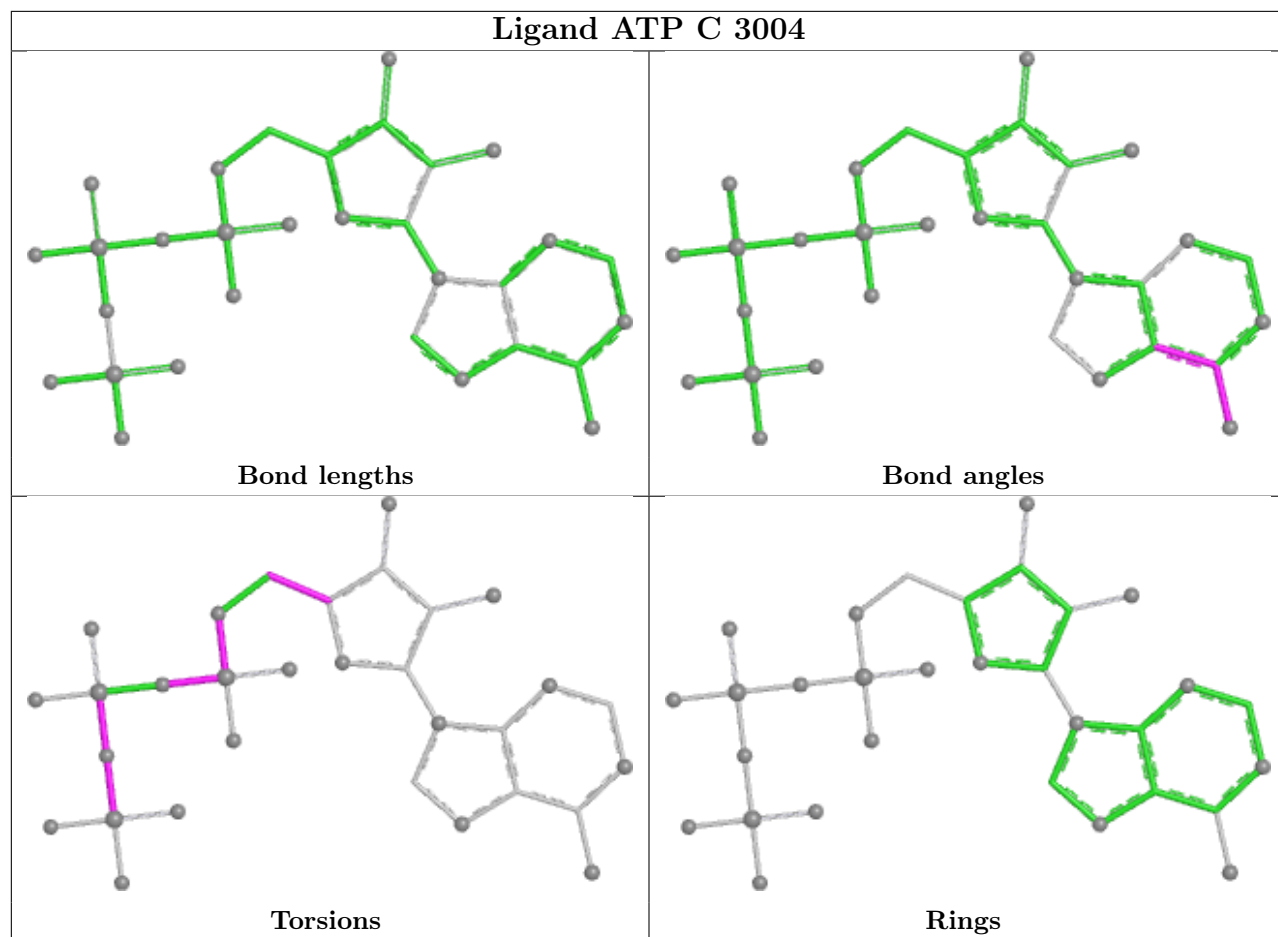
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

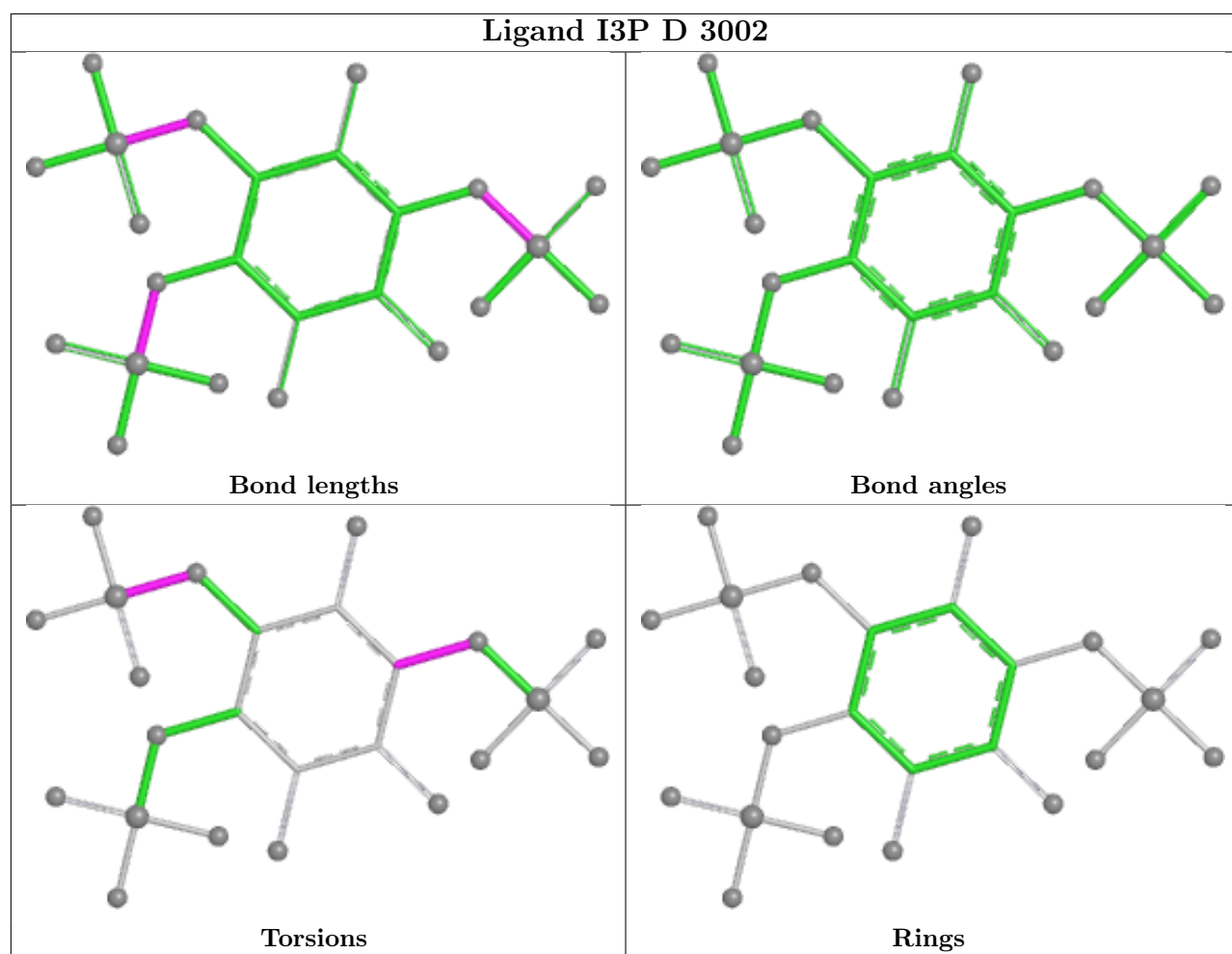


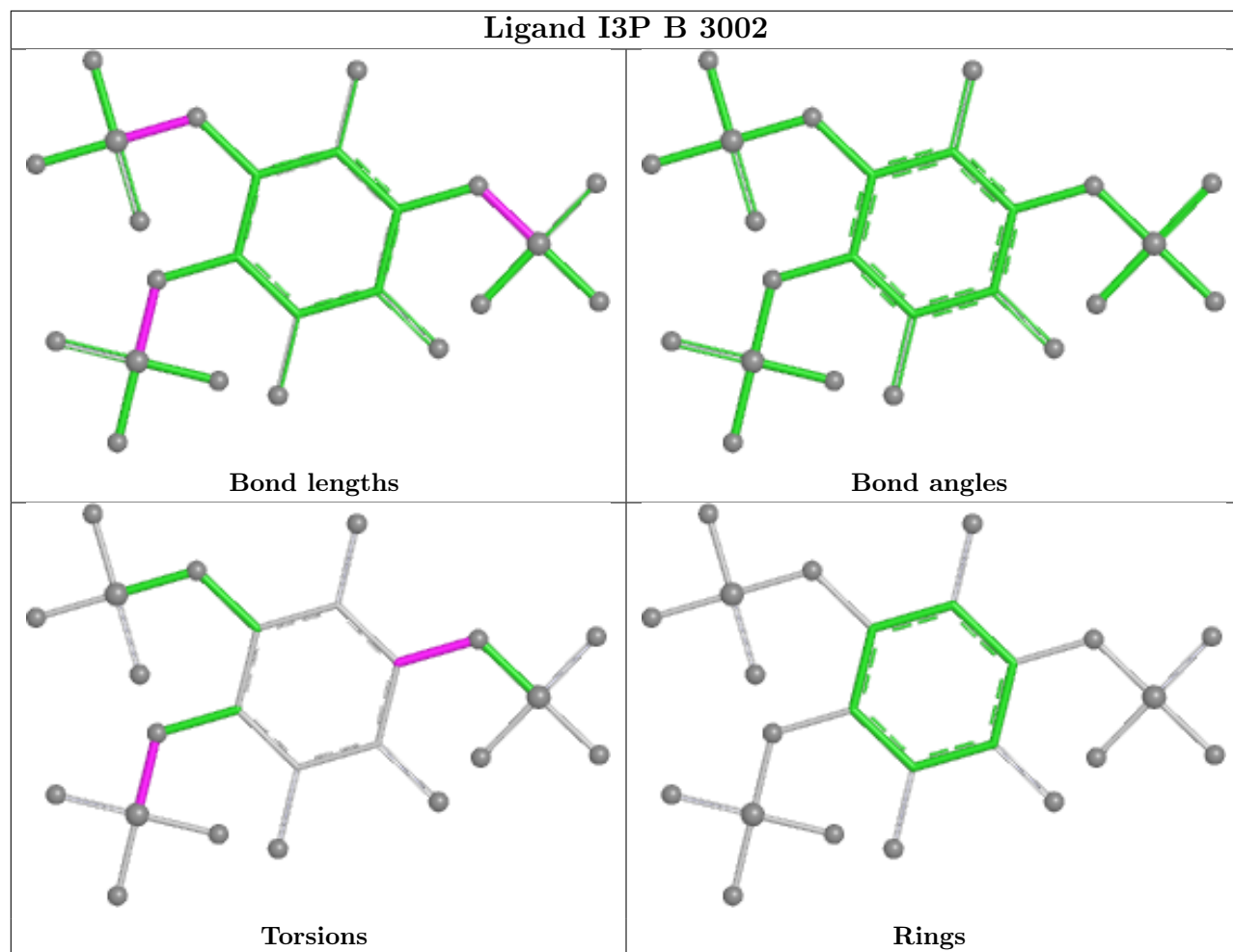


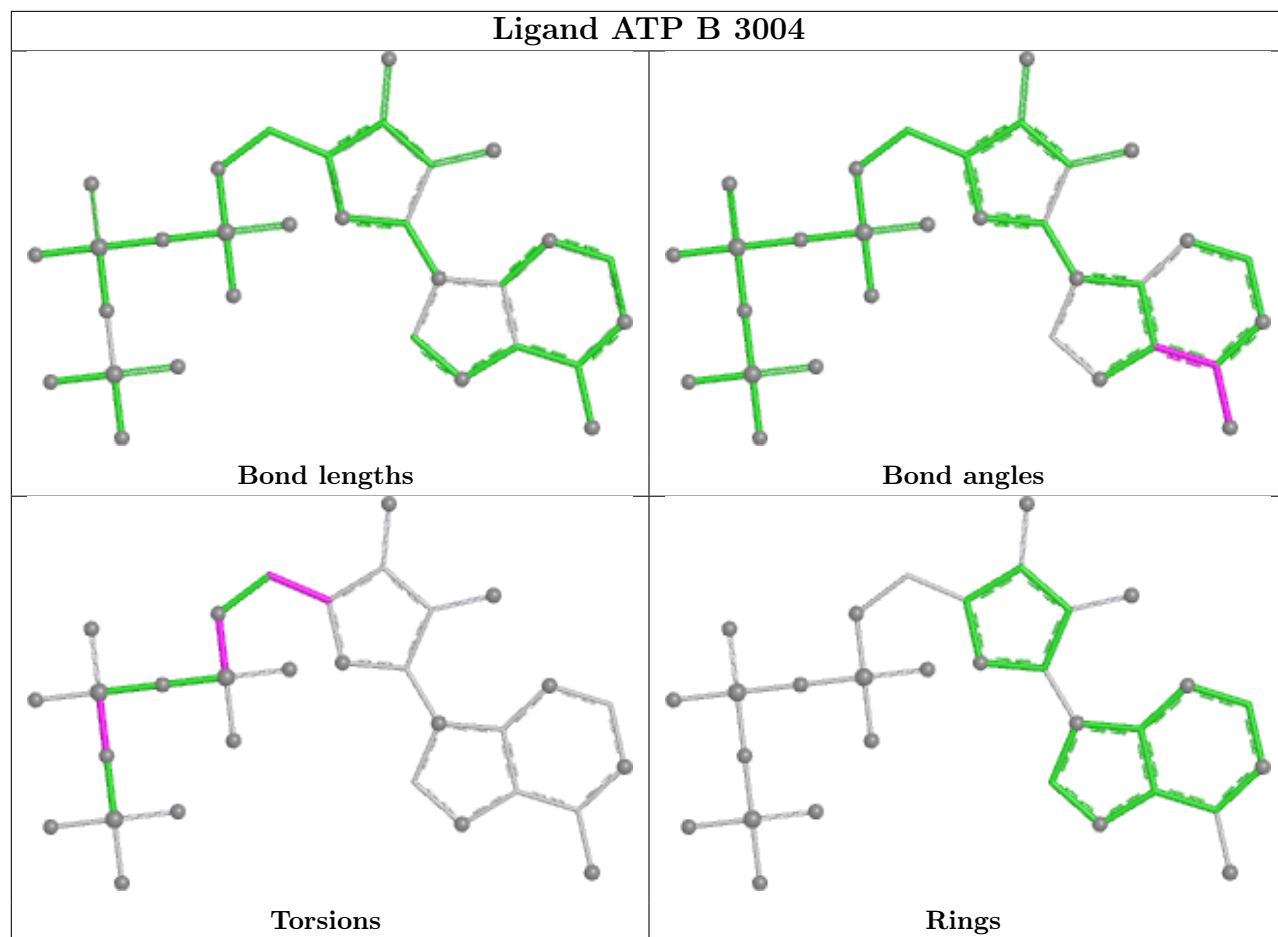


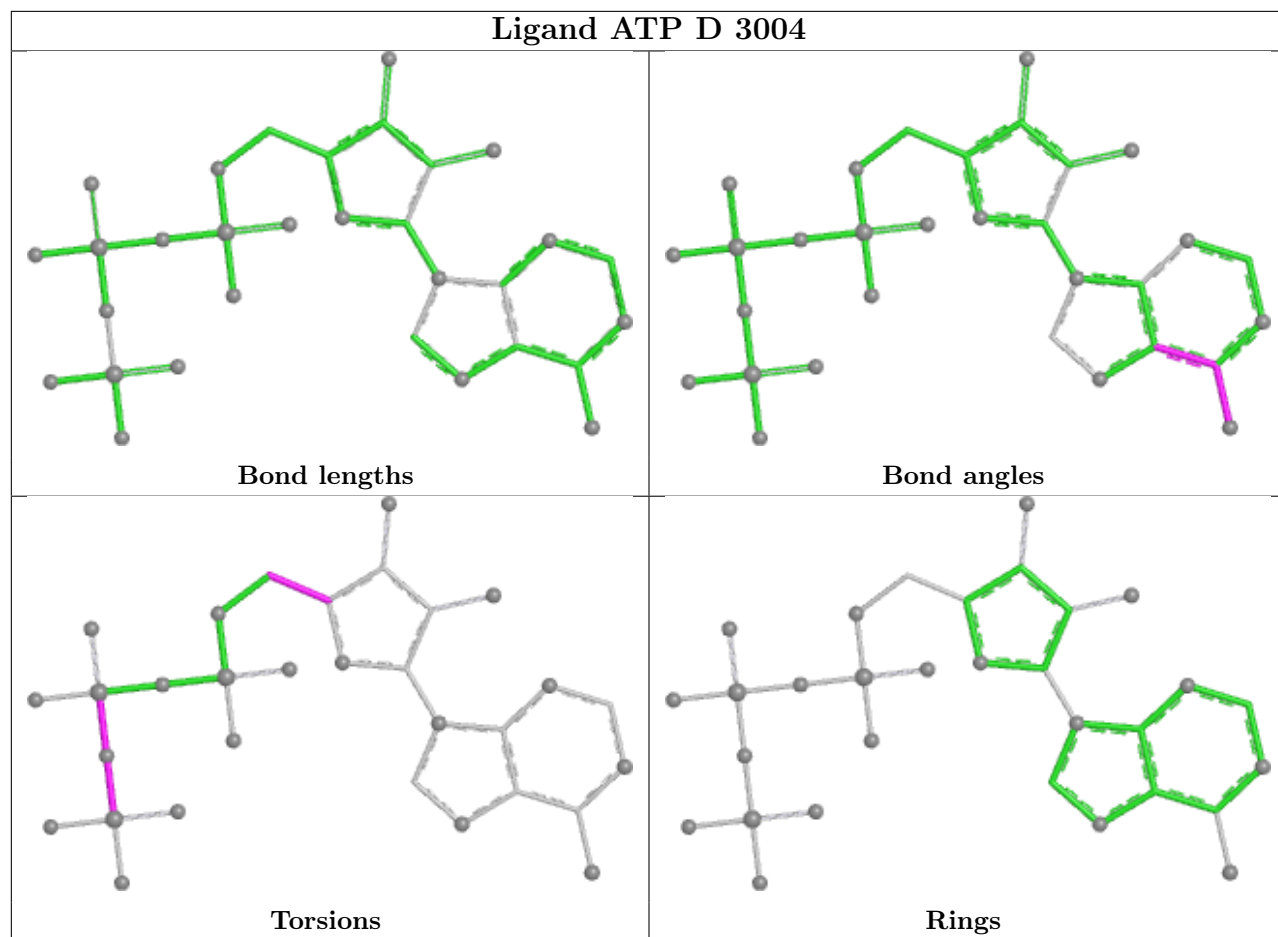












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

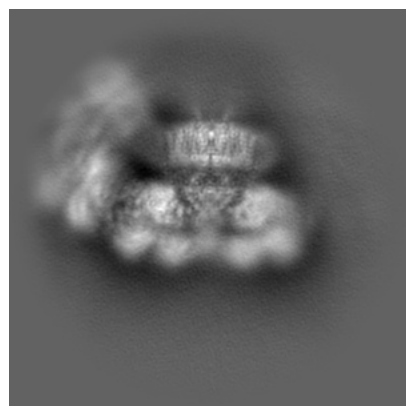
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41366. These allow visual inspection of the internal detail of the map and identification of artifacts.

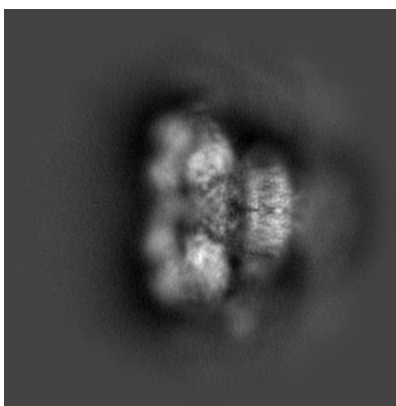
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

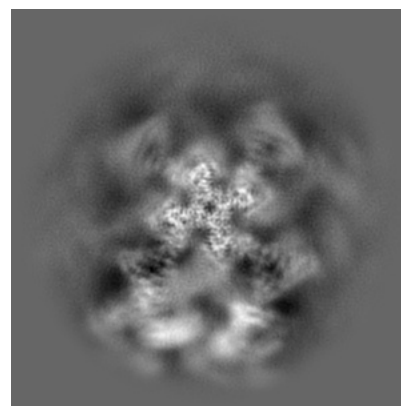
#### 6.1.1 Primary map



X

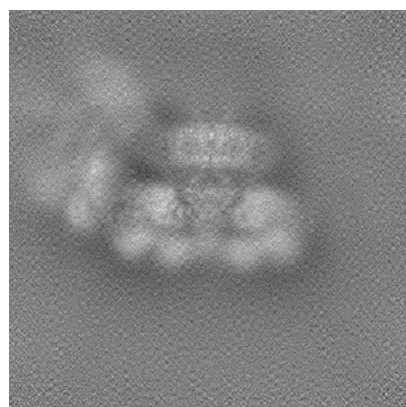


Y

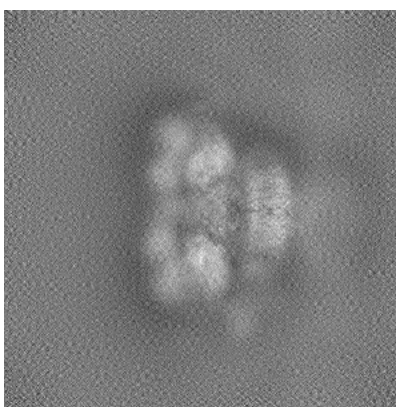


Z

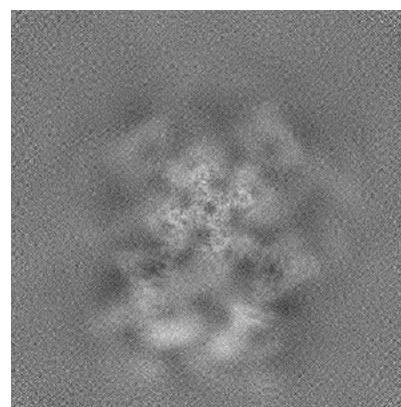
#### 6.1.2 Raw map



X



Y

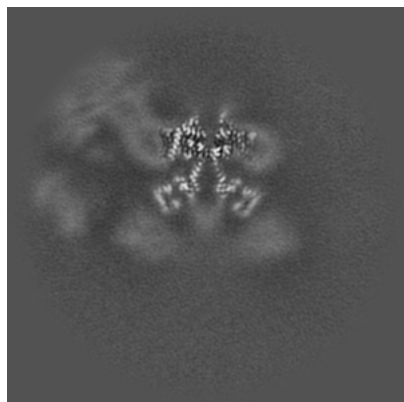


Z

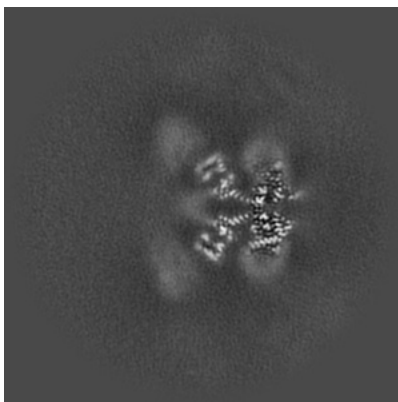
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

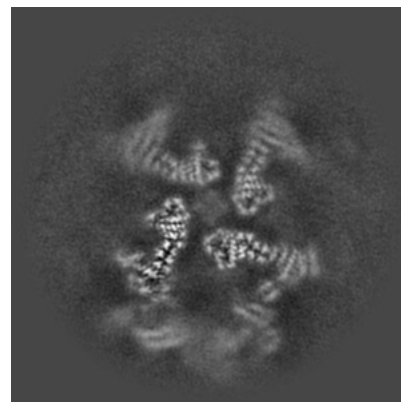
### 6.2.1 Primary map



X Index: 256

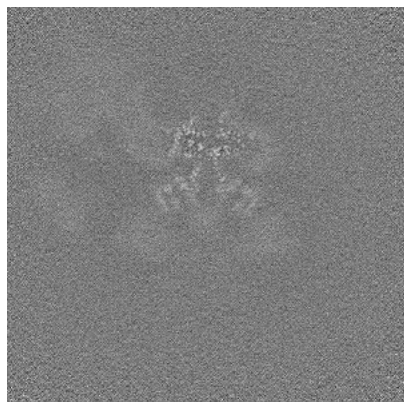


Y Index: 256



Z Index: 256

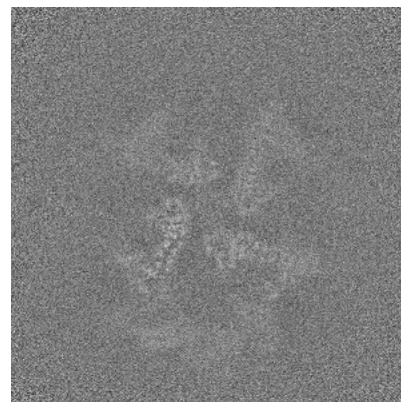
### 6.2.2 Raw map



X Index: 256



Y Index: 256



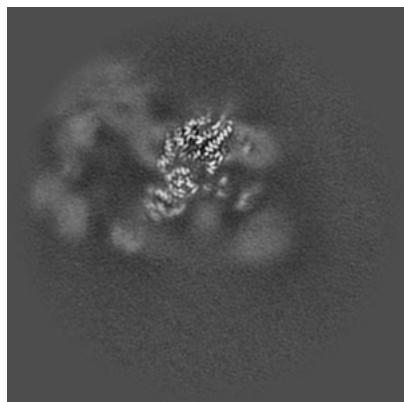
Z Index: 256

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

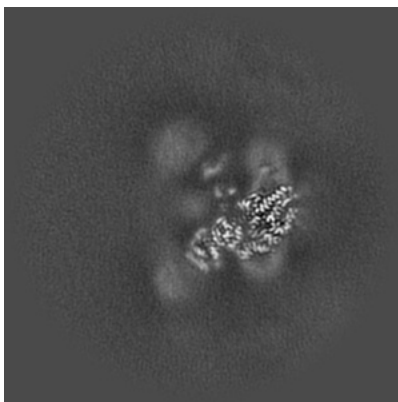


## 6.3 Largest variance slices [i](#)

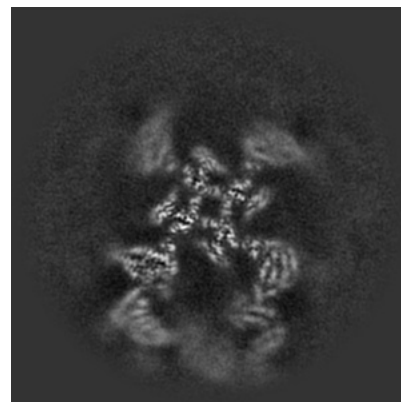
### 6.3.1 Primary map



X Index: 266

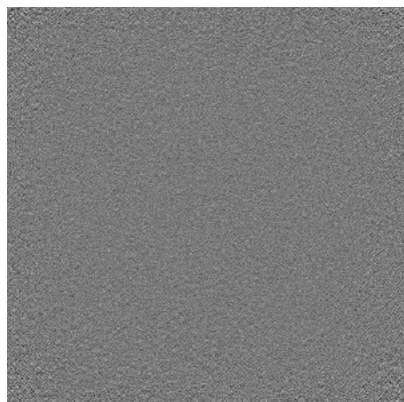


Y Index: 246

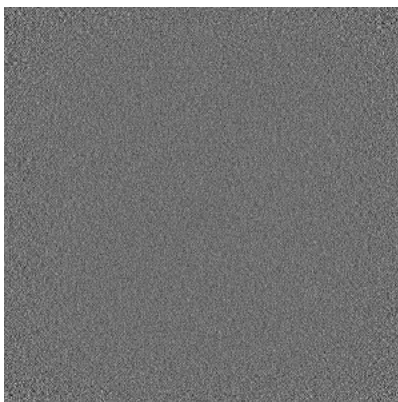


Z Index: 271

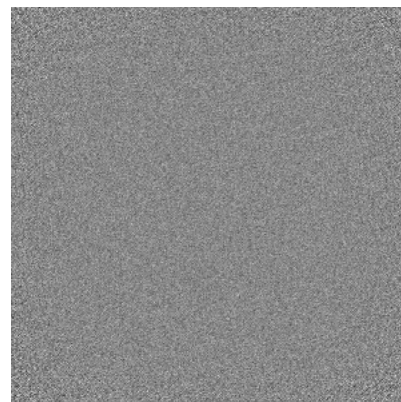
### 6.3.2 Raw map



X Index: 0



Y Index: 0

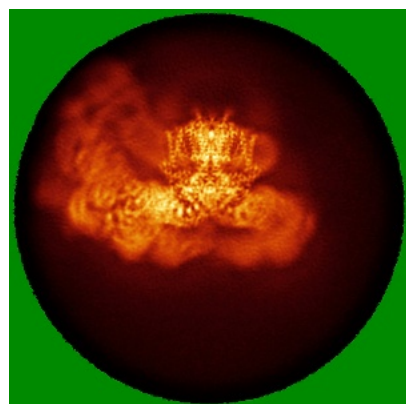


Z Index: 0

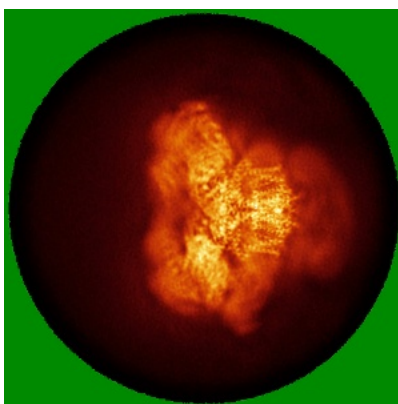
The images above show the largest variance slices of the map in three orthogonal directions.

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

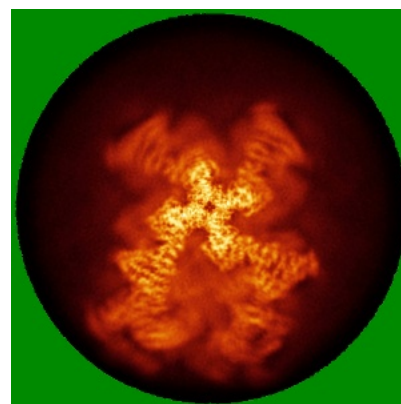
### 6.4.1 Primary map



X

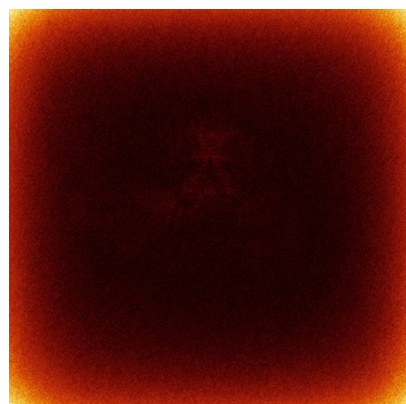


Y

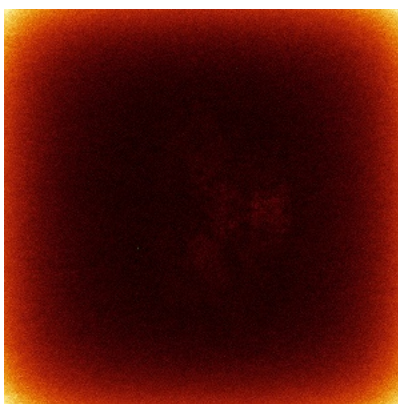


Z

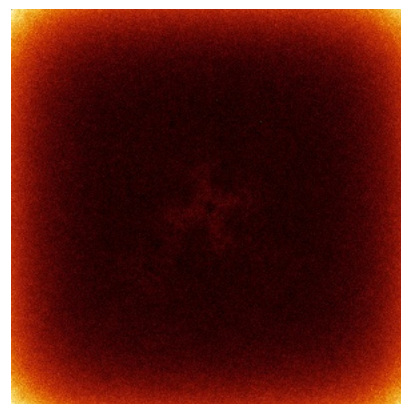
### 6.4.2 Raw map



X



Y

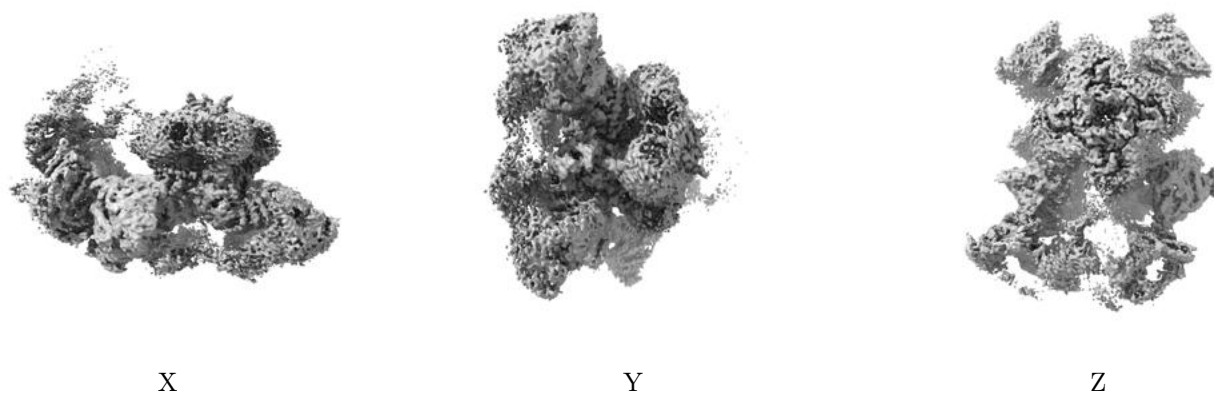


Z

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.

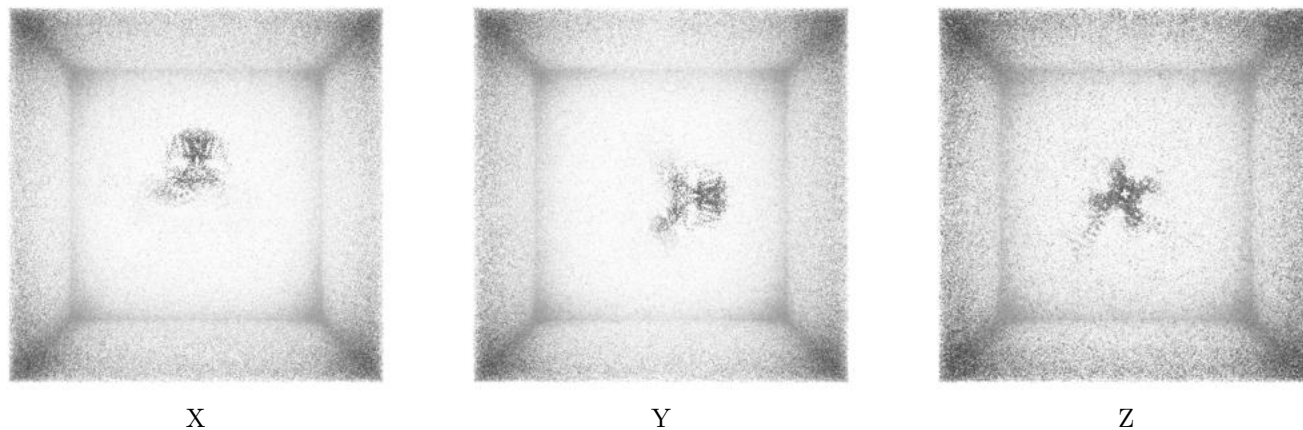
## 6.5 Orthogonal surface views [i](#)

### 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.

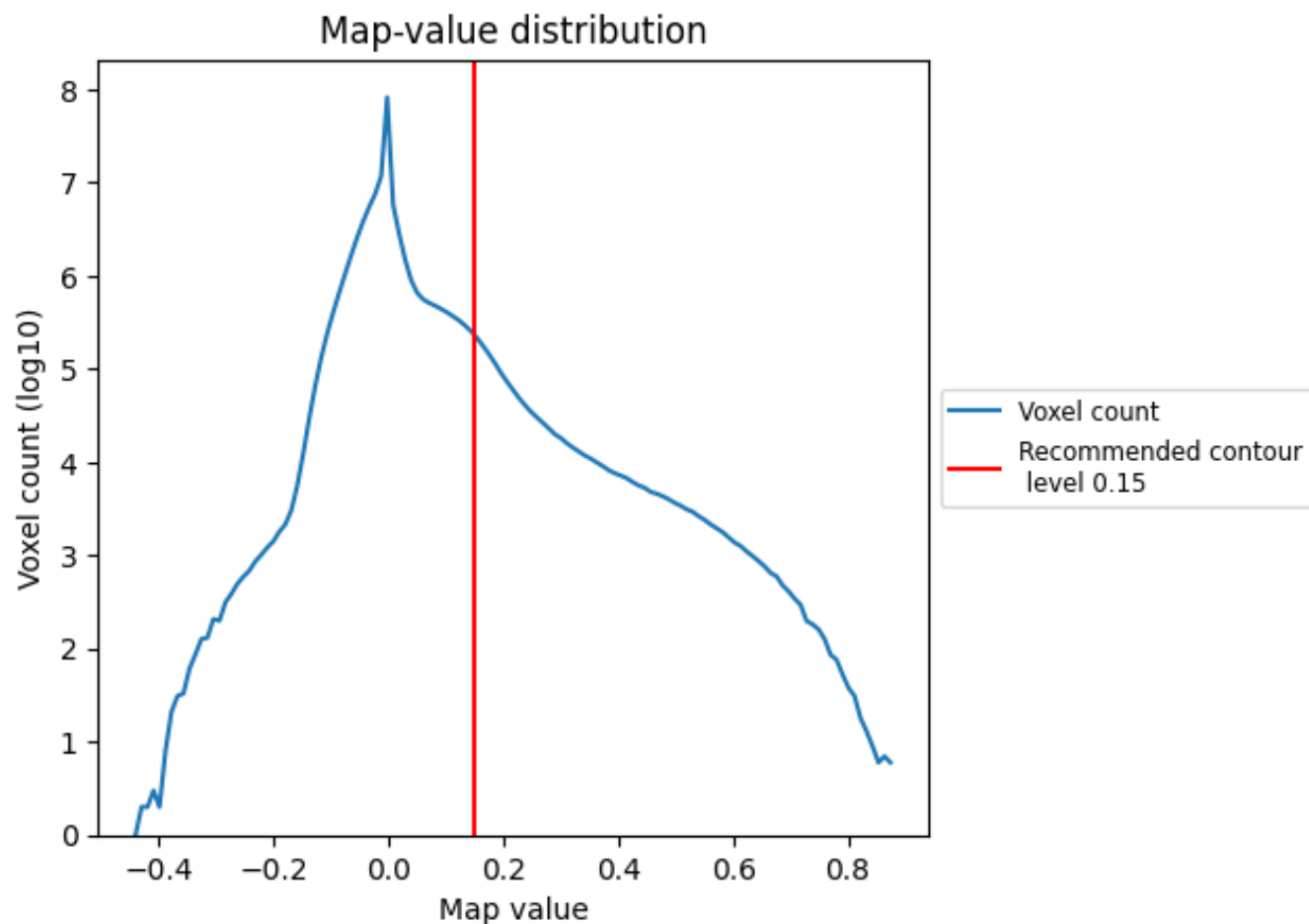
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

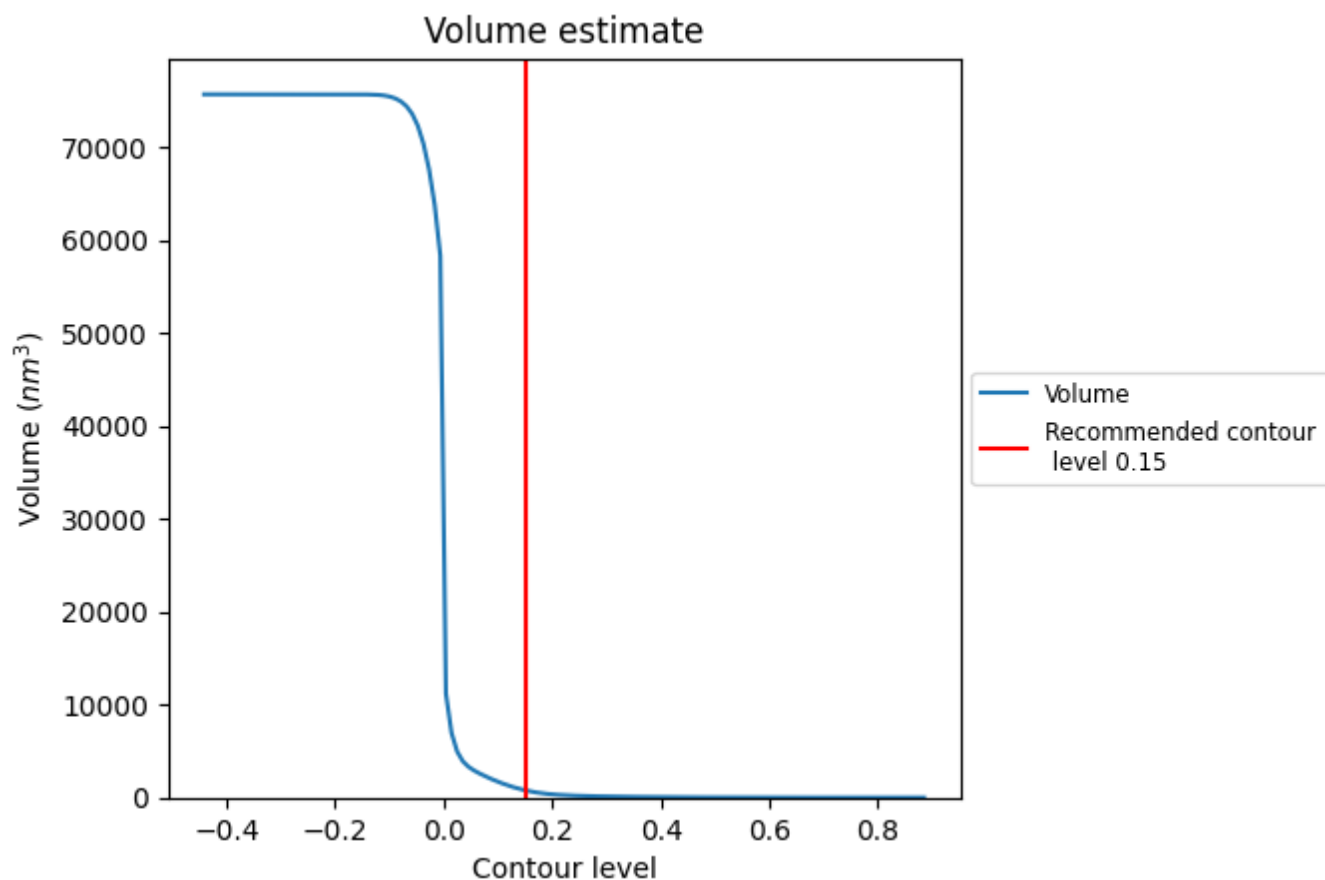
This section contains the results of statistical analysis of the map.

### 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.

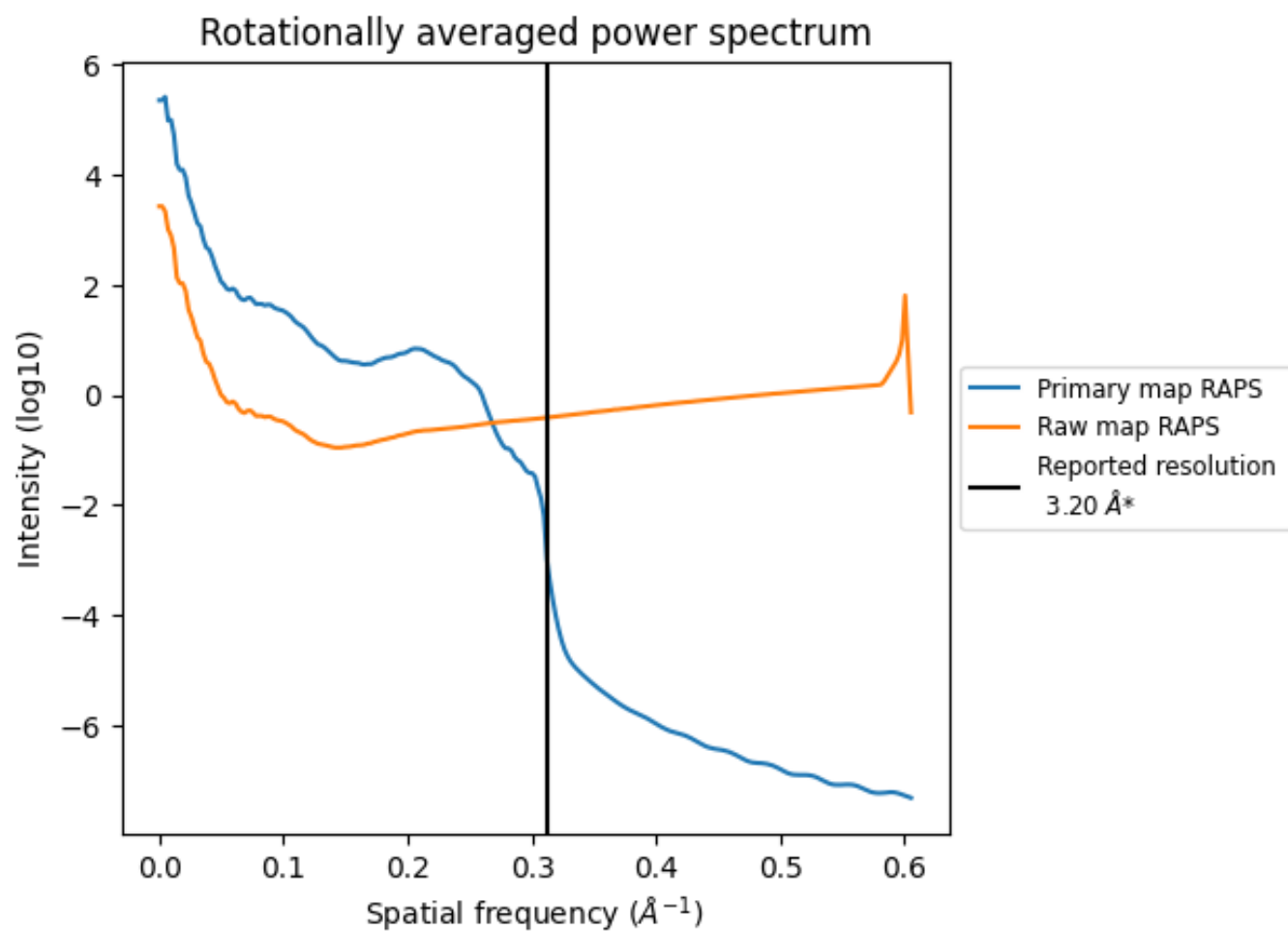
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 788 nm<sup>3</sup>; this corresponds to an approximate mass of 712 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 ⓘ



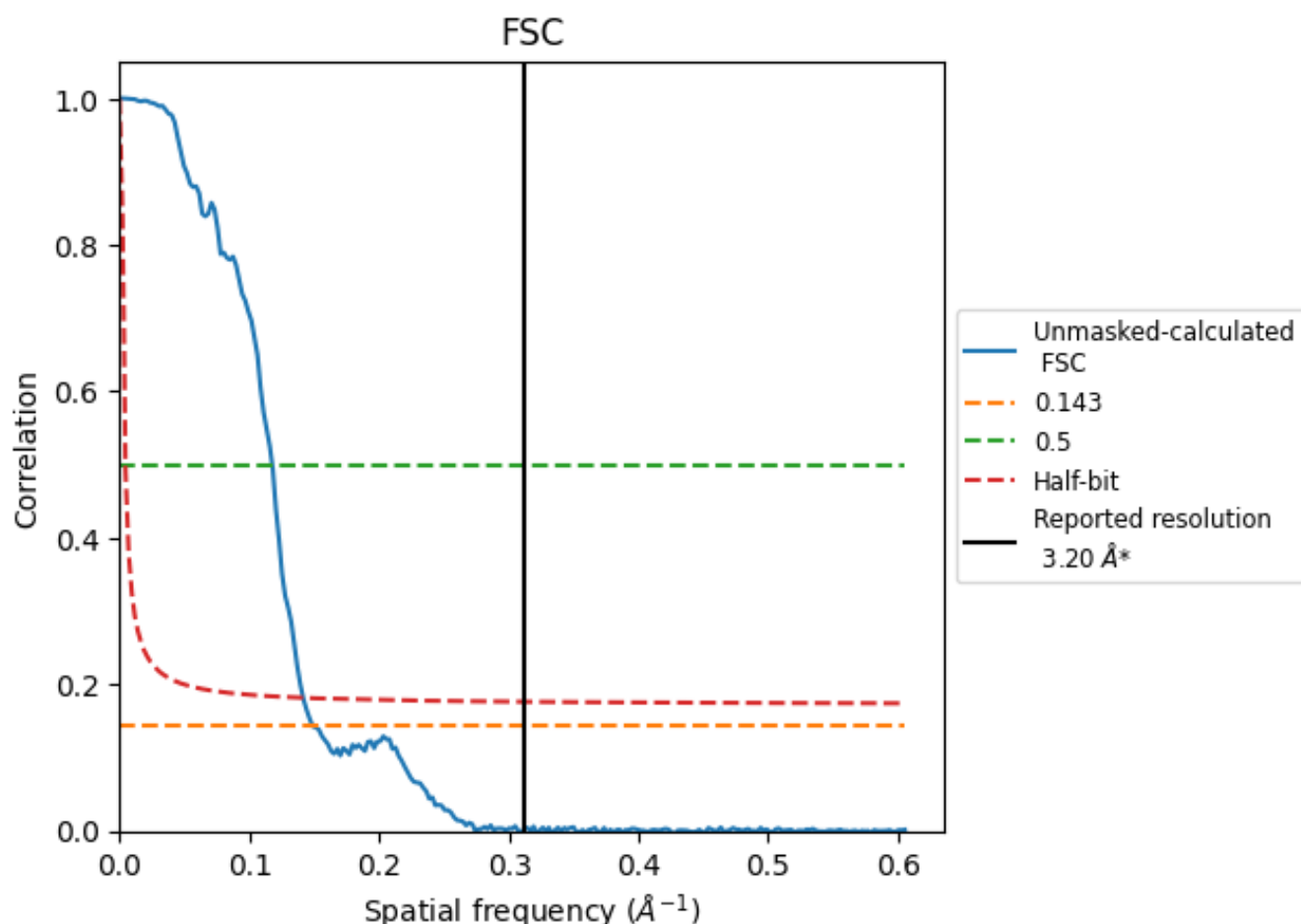
\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>



## 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	-	-	-
Unmasked-calculated*	6.72	8.50	7.06

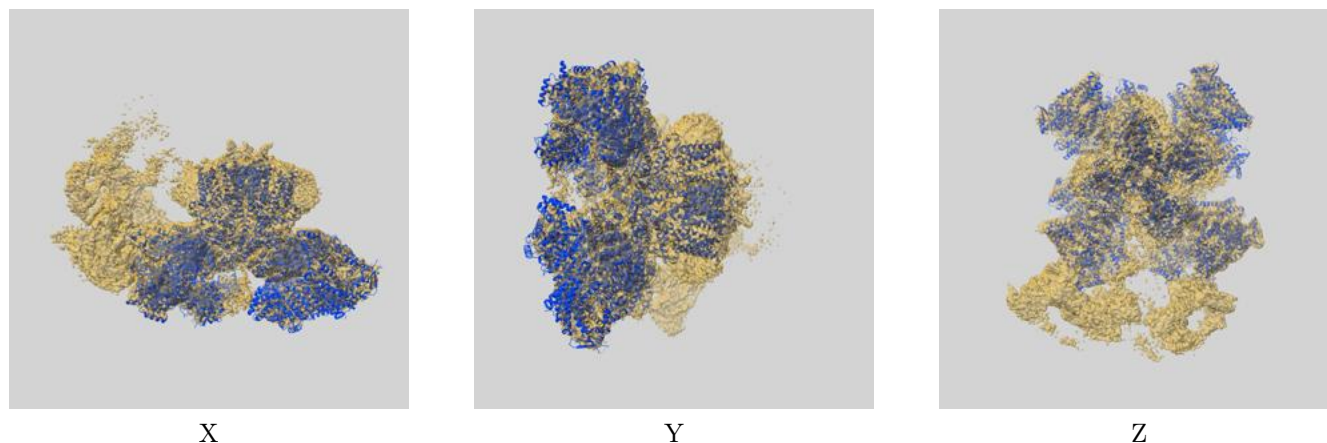
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 3.2 by more than 10 %



## 9 Map-model fit [i](#)

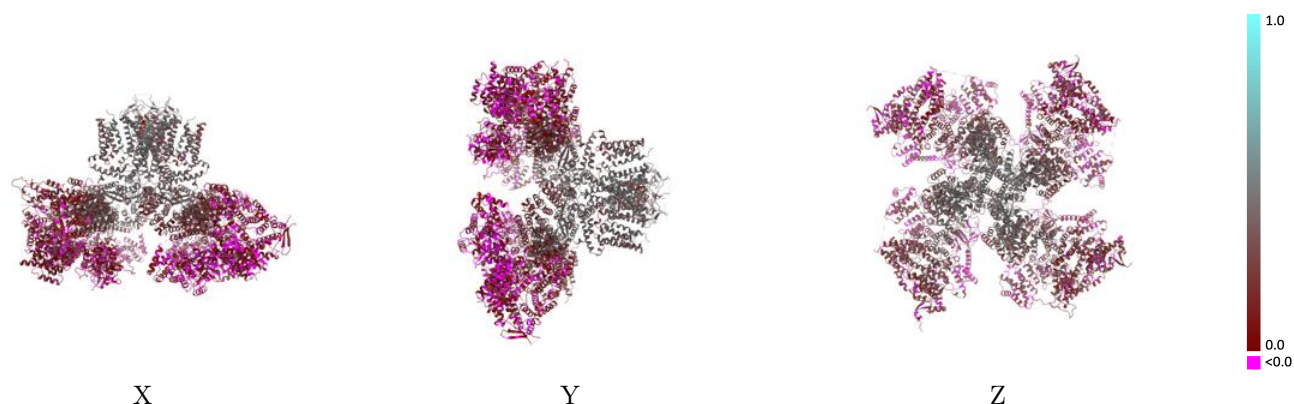
This section contains information regarding the fit between EMDB map EMD-41366 and PDB model 8TLA. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



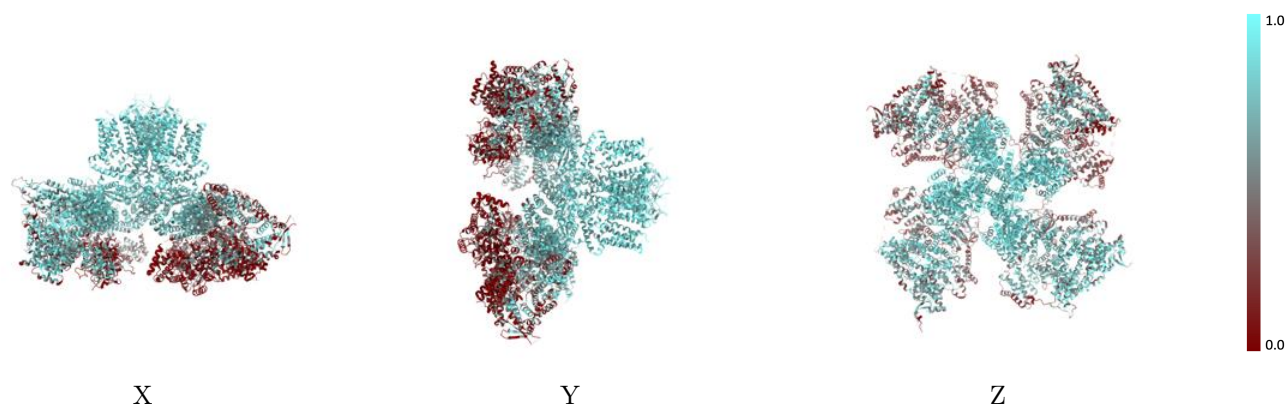
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



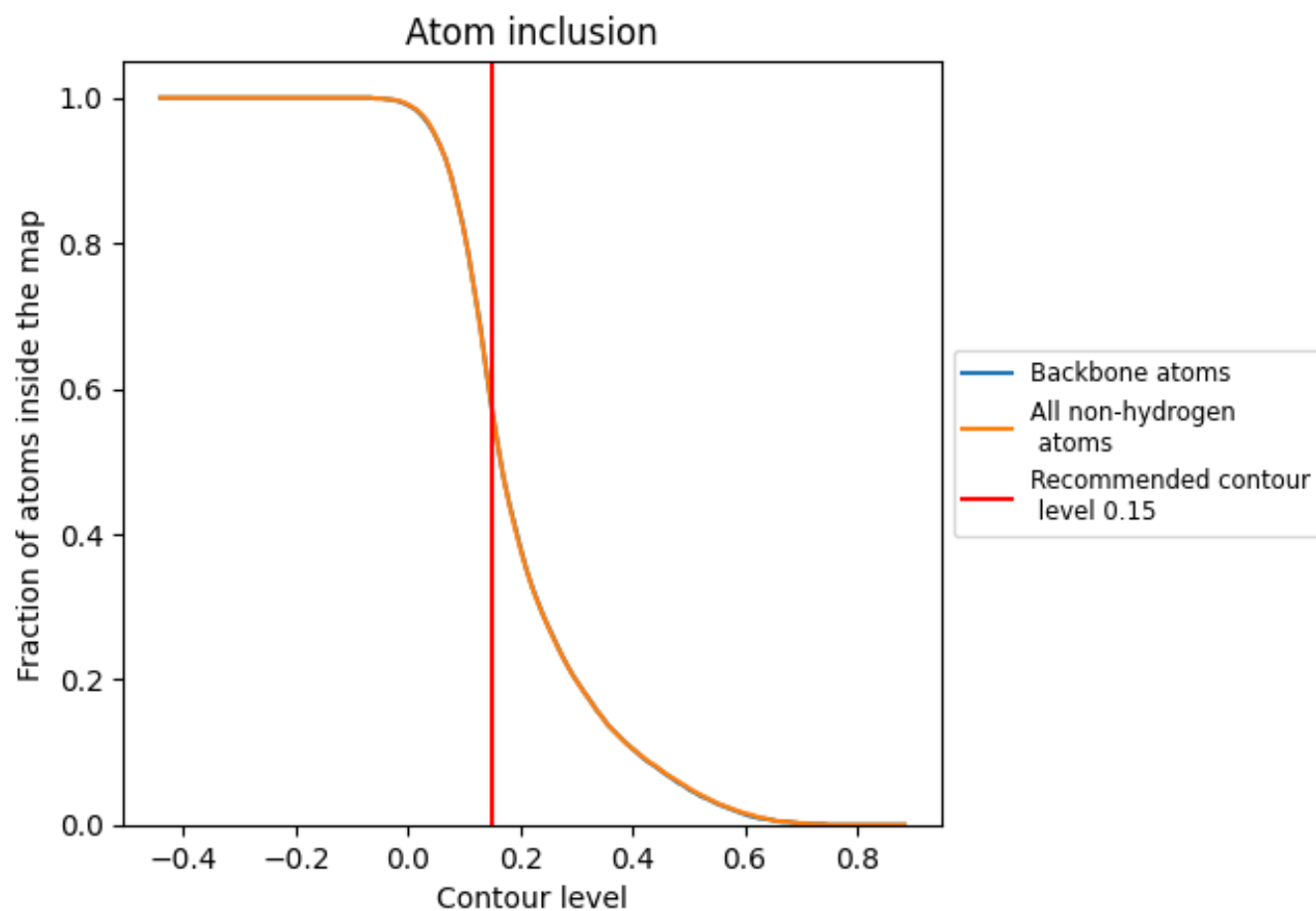
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 57% of all backbone atoms, 57% 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> 0.5720	<div></div> 0.1980
A	<div></div> 0.5100	<div></div> 0.1710
B	<div></div> 0.4700	<div></div> 0.1640
C	<div></div> 0.6520	<div></div> 0.2320
D	<div></div> 0.6740	<div></div> 0.2250

