



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 02:09 AM EST

PDB ID : 5UJM
EMDB ID : EMD-8541
Title : Structure of the active form of human Origin Recognition Complex and its ATPase motor module
Authors : Tocilj, A.; On, K.; Yuan, Z.; Sun, J.; Elkayam, E.; Li, H.; Stillman, B.; Joshua-Tor, L.
Deposited on : 2017-01-18
Resolution : 18.00 Å (reported)
Based on initial models : 4XGC, 5UJ7, 5UJ8

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

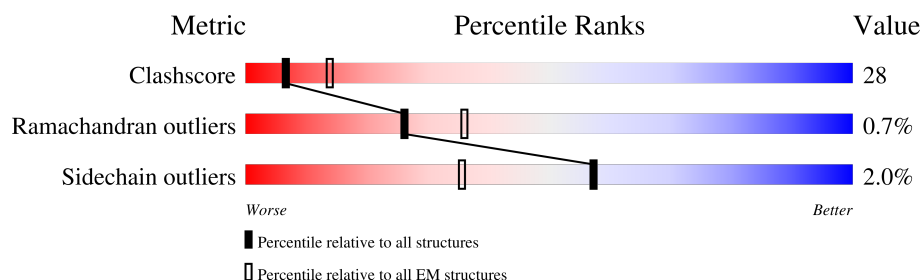
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 18.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	522	
2	B	347	
3	C	712	
4	D	436	
5	E	435	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15673 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	337	Total	C	N	O	S	0	0
			2683	1693	471	498	21		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	MET	-	expression tag	UNP Q13415
A	341	SER	-	expression tag	UNP Q13415
A	342	ALA	-	expression tag	UNP Q13415
A	343	TRP	-	expression tag	UNP Q13415
A	344	SER	-	expression tag	UNP Q13415
A	345	HIS	-	expression tag	UNP Q13415
A	346	PRO	-	expression tag	UNP Q13415
A	347	GLN	-	expression tag	UNP Q13415
A	348	PHE	-	expression tag	UNP Q13415
A	349	GLU	-	expression tag	UNP Q13415
A	350	LYS	-	expression tag	UNP Q13415
A	351	GLY	-	expression tag	UNP Q13415
A	352	GLY	-	expression tag	UNP Q13415
A	353	GLY	-	expression tag	UNP Q13415
A	354	SER	-	expression tag	UNP Q13415
A	355	GLY	-	expression tag	UNP Q13415
A	356	GLY	-	expression tag	UNP Q13415
A	357	GLY	-	expression tag	UNP Q13415
A	358	SER	-	expression tag	UNP Q13415
A	359	GLY	-	expression tag	UNP Q13415
A	360	GLY	-	expression tag	UNP Q13415
A	361	SER	-	expression tag	UNP Q13415
A	362	ALA	-	expression tag	UNP Q13415
A	363	TRP	-	expression tag	UNP Q13415
A	364	SER	-	expression tag	UNP Q13415
A	365	HIS	-	expression tag	UNP Q13415
A	366	PRO	-	expression tag	UNP Q13415
A	367	GLN	-	expression tag	UNP Q13415

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Chain	Residue	Modelled	Actual	Comment	Reference
A	368	PHE	-	expression tag	UNP Q13415
A	369	GLU	-	expression tag	UNP Q13415
A	370	LYS	-	expression tag	UNP Q13415
A	371	THR	-	expression tag	UNP Q13415
A	372	GLY	-	expression tag	UNP Q13415
A	373	SER	-	expression tag	UNP Q13415
A	374	LEU	-	expression tag	UNP Q13415
A	375	GLN	-	expression tag	UNP Q13415
A	376	ASP	-	expression tag	UNP Q13415
A	377	SER	-	expression tag	UNP Q13415
A	378	GLU	-	expression tag	UNP Q13415
A	379	VAL	-	expression tag	UNP Q13415
A	380	ASN	-	expression tag	UNP Q13415
A	381	GLN	-	expression tag	UNP Q13415
A	382	GLU	-	expression tag	UNP Q13415
A	383	ALA	-	expression tag	UNP Q13415
A	384	LYS	-	expression tag	UNP Q13415
A	385	PRO	-	expression tag	UNP Q13415
A	386	GLU	-	expression tag	UNP Q13415
A	387	VAL	-	expression tag	UNP Q13415
A	388	LYS	-	expression tag	UNP Q13415
A	389	PRO	-	expression tag	UNP Q13415
A	390	GLU	-	expression tag	UNP Q13415
A	391	VAL	-	expression tag	UNP Q13415
A	392	LYS	-	expression tag	UNP Q13415
A	393	PRO	-	expression tag	UNP Q13415
A	394	GLU	-	expression tag	UNP Q13415
A	395	THR	-	expression tag	UNP Q13415
A	396	HIS	-	expression tag	UNP Q13415
A	397	ILE	-	expression tag	UNP Q13415
A	398	ASN	-	expression tag	UNP Q13415
A	399	LEU	-	expression tag	UNP Q13415
A	400	LYS	-	expression tag	UNP Q13415
A	401	VAL	-	expression tag	UNP Q13415
A	402	SER	-	expression tag	UNP Q13415
A	403	ASP	-	expression tag	UNP Q13415
A	404	GLY	-	expression tag	UNP Q13415
A	405	SER	-	expression tag	UNP Q13415
A	406	SER	-	expression tag	UNP Q13415
A	407	GLU	-	expression tag	UNP Q13415
A	408	ILE	-	expression tag	UNP Q13415
A	409	PHE	-	expression tag	UNP Q13415

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Chain	Residue	Modelled	Actual	Comment	Reference
A	410	PHE	-	expression tag	UNP Q13415
A	411	LYS	-	expression tag	UNP Q13415
A	412	ILE	-	expression tag	UNP Q13415
A	413	LYS	-	expression tag	UNP Q13415
A	414	LYS	-	expression tag	UNP Q13415
A	415	THR	-	expression tag	UNP Q13415
A	416	THR	-	expression tag	UNP Q13415
A	417	PRO	-	expression tag	UNP Q13415
A	418	LEU	-	expression tag	UNP Q13415
A	419	ARG	-	expression tag	UNP Q13415
A	420	ARG	-	expression tag	UNP Q13415
A	421	LEU	-	expression tag	UNP Q13415
A	422	MET	-	expression tag	UNP Q13415
A	423	GLU	-	expression tag	UNP Q13415
A	424	ALA	-	expression tag	UNP Q13415
A	425	PHE	-	expression tag	UNP Q13415
A	426	ALA	-	expression tag	UNP Q13415
A	427	LYS	-	expression tag	UNP Q13415
A	428	ARG	-	expression tag	UNP Q13415
A	429	GLN	-	expression tag	UNP Q13415
A	430	GLY	-	expression tag	UNP Q13415
A	431	LYS	-	expression tag	UNP Q13415
A	432	GLU	-	expression tag	UNP Q13415
A	433	MET	-	expression tag	UNP Q13415
A	434	ASP	-	expression tag	UNP Q13415
A	435	SER	-	expression tag	UNP Q13415
A	436	LEU	-	expression tag	UNP Q13415
A	437	THR	-	expression tag	UNP Q13415
A	438	PHE	-	expression tag	UNP Q13415
A	439	LEU	-	expression tag	UNP Q13415
A	440	TYR	-	expression tag	UNP Q13415
A	441	ASP	-	expression tag	UNP Q13415
A	442	GLY	-	expression tag	UNP Q13415
A	443	ILE	-	expression tag	UNP Q13415
A	444	GLU	-	expression tag	UNP Q13415
A	445	ILE	-	expression tag	UNP Q13415
A	446	GLN	-	expression tag	UNP Q13415
A	447	ALA	-	expression tag	UNP Q13415
A	448	ASP	-	expression tag	UNP Q13415
A	449	GLN	-	expression tag	UNP Q13415
A	450	THR	-	expression tag	UNP Q13415
A	451	PRO	-	expression tag	UNP Q13415

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Chain	Residue	Modelled	Actual	Comment	Reference
A	452	GLU	-	expression tag	UNP Q13415
A	453	ASP	-	expression tag	UNP Q13415
A	454	LEU	-	expression tag	UNP Q13415
A	455	ASP	-	expression tag	UNP Q13415
A	456	MET	-	expression tag	UNP Q13415
A	457	GLU	-	expression tag	UNP Q13415
A	458	ASP	-	expression tag	UNP Q13415
A	459	ASN	-	expression tag	UNP Q13415
A	460	ASP	-	expression tag	UNP Q13415
A	461	ILE	-	expression tag	UNP Q13415
A	462	ILE	-	expression tag	UNP Q13415
A	463	GLU	-	expression tag	UNP Q13415
A	464	ALA	-	expression tag	UNP Q13415
A	465	HIS	-	expression tag	UNP Q13415
A	466	ARG	-	expression tag	UNP Q13415
A	467	GLU	-	expression tag	UNP Q13415
A	468	GLN	-	expression tag	UNP Q13415
A	469	ILE	-	expression tag	UNP Q13415
A	470	GLY	-	expression tag	UNP Q13415
A	624	ILE	LEU	conflict	UNP Q13415

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	287	Total	C	N	O	S	5	0
			2362	1518	396	442	6		

- Molecule 3 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	553	Total	C	N	O	S	0	0
			4524	2920	767	812	25		

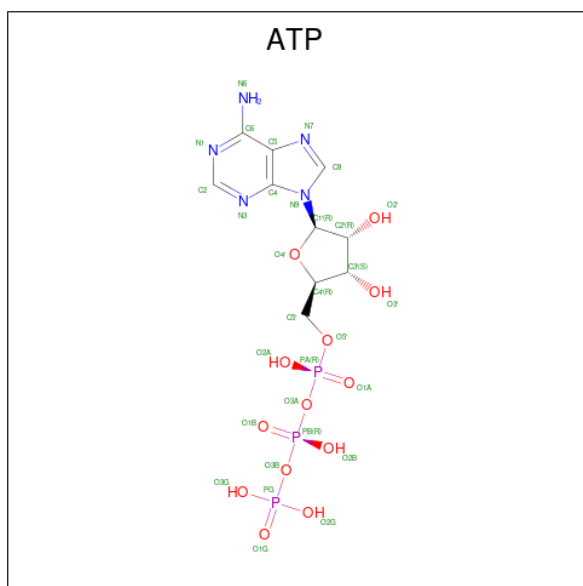
- Molecule 4 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	394	Total	C	N	O	S	0	0
			3205	2053	552	580	20		

- Molecule 5 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	357	Total	C	N	O	S	0	0
			2804	1839	461	494	10		

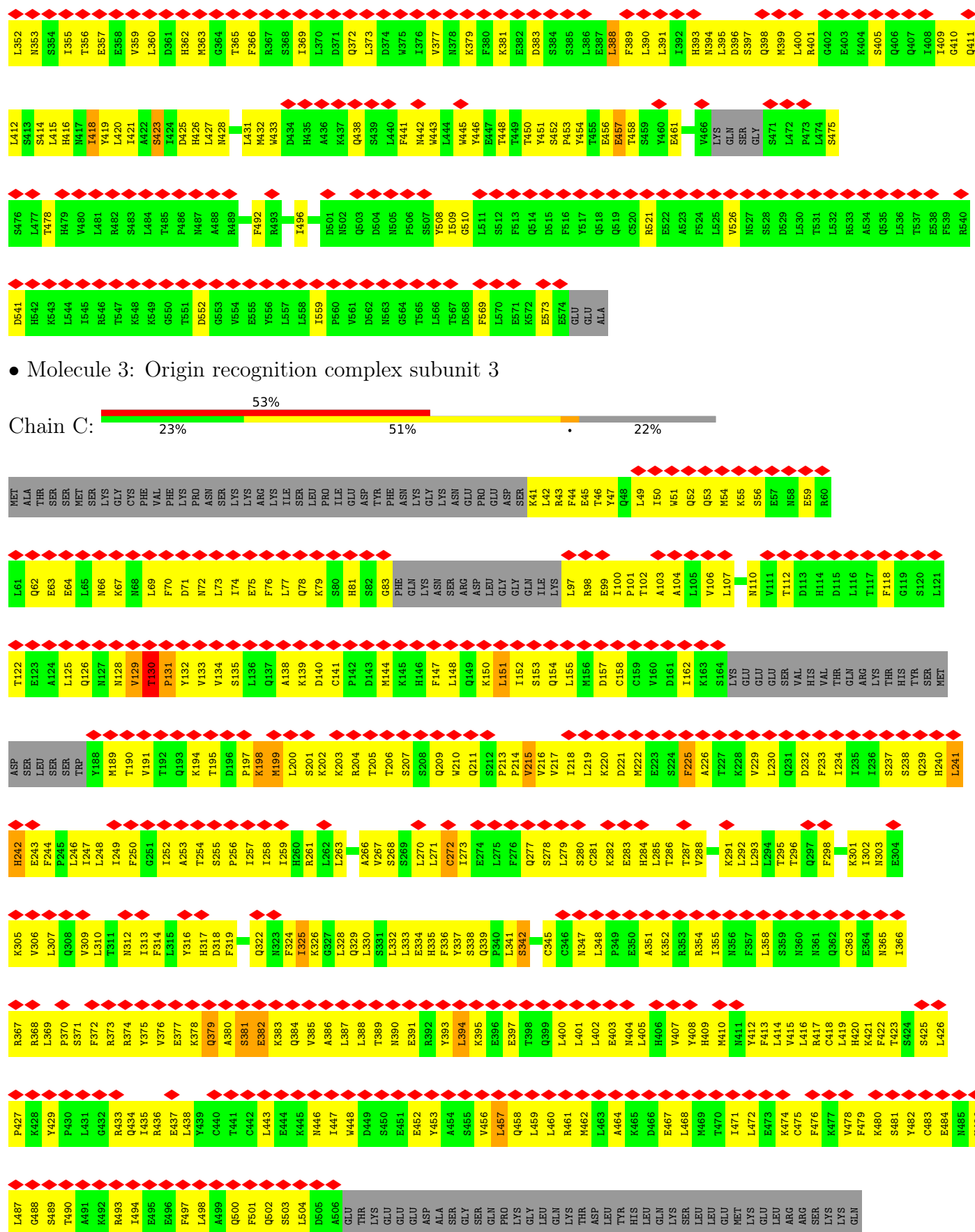
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

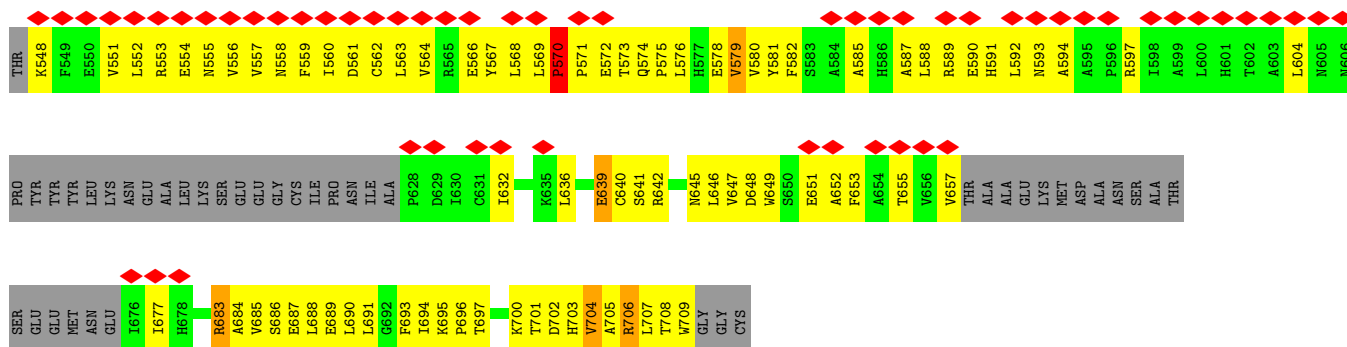


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

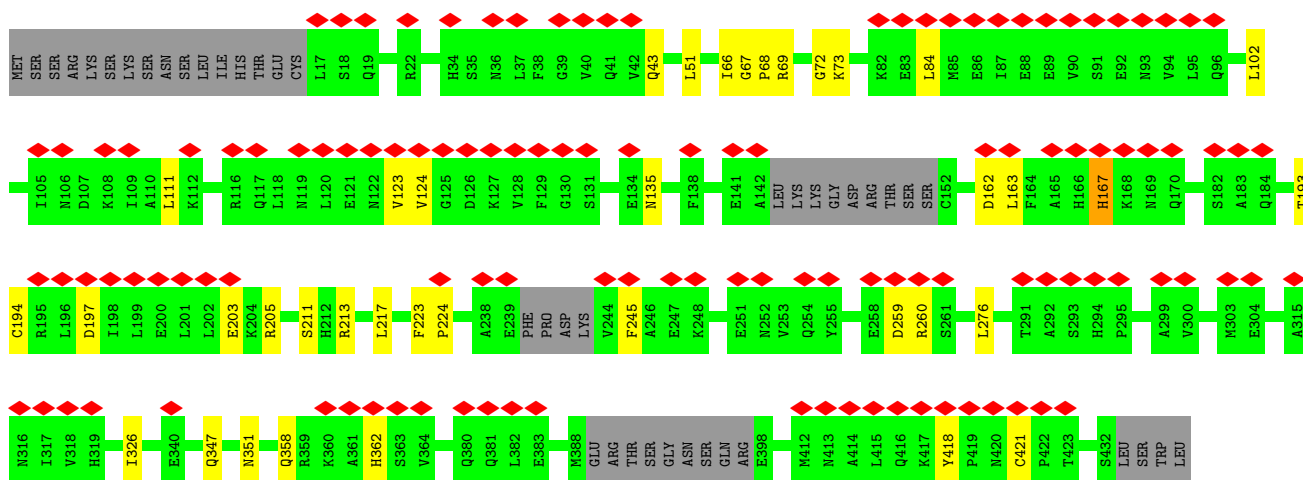
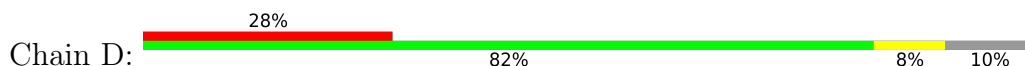
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	

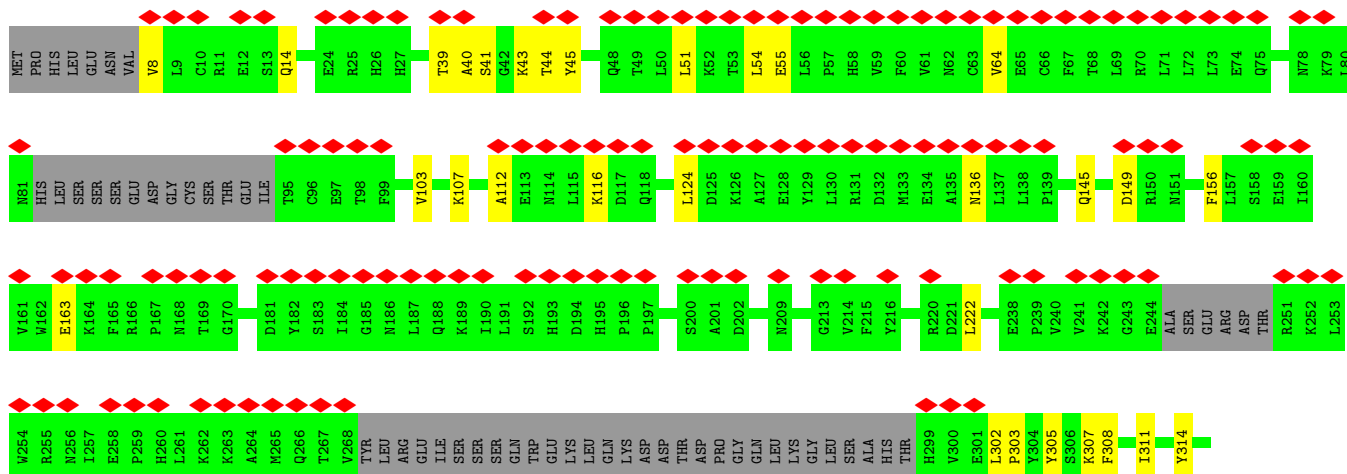


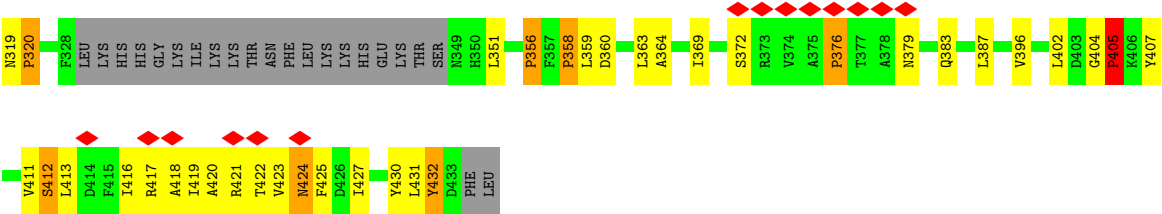


• Molecule 4: Origin recognition complex subunit 4



• Molecule 5: Origin recognition complex subunit 5





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10980	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.020	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.04, 4.04, 4.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/2727	0.46	0/3687
2	B	0.42	1/2430 (0.0%)	0.64	2/3292 (0.1%)
3	C	0.46	0/4616	0.71	5/6244 (0.1%)
4	D	0.26	0/3264	0.43	0/4400
5	E	0.52	2/2862 (0.1%)	0.52	5/3876 (0.1%)
All	All	0.40	3/15899 (0.0%)	0.58	12/21499 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	5
4	D	0	2
5	E	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	432	TYR	CB-CG	19.60	1.81	1.51
5	E	372	SER	CB-OG	7.80	1.52	1.42
2	B	559	ILE	C-N	7.77	1.49	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	151	LEU	CA-CB-CG	10.14	138.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	ARG	NE-CZ-NH2	-9.74	115.43	120.30
5	E	376	PRO	CA-CB-CG	7.32	118.70	104.80
5	E	358	PRO	N-CA-CB	6.84	111.51	103.30
5	E	376	PRO	N-CA-CB	6.58	111.19	103.30
3	C	241	LEU	CB-CG-CD1	-6.50	99.94	111.00
2	B	320	ARG	CG-CD-NE	-5.86	99.49	111.80
3	C	151	LEU	CB-CG-CD1	5.62	120.55	111.00
5	E	356	PRO	N-CA-CB	5.54	109.95	103.30
3	C	198	LYS	CD-CE-NZ	5.47	124.29	111.70
3	C	215	VAL	CA-CB-CG2	-5.26	103.01	110.90
5	E	320	PRO	N-CA-CB	5.12	109.44	103.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	693	ARG	Peptide
1	A	716	SER	Peptide
3	C	130	THR	Peptide
3	C	140	ASP	Peptide
3	C	240	HIS	Peptide
3	C	242	HIS	Peptide
3	C	639	GLU	Peptide
4	D	211	SER	Peptide
4	D	72	GLY	Peptide
5	E	404	GLY	Peptide

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	2683	0	2700	29	0
2	B	2362	0	2330	169	0
3	C	4524	0	4619	615	0
4	D	3205	0	3248	39	0
5	E	2804	0	2733	132	0
6	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	31	0	12	3	0
6	E	31	0	12	4	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
All	All	15673	0	15666	874	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 28.

All (874) 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)
3:C:709:TRP:CH2	5:E:363:LEU:HB2	1.21	1.66
5:E:432:TYR:CB	5:E:432:TYR:CG	1.81	1.59
2:B:431:LEU:HD12	5:E:402:LEU:CG	1.16	1.56
3:C:319:PHE:CZ	5:E:303:PRO:HG3	1.44	1.52
2:B:431:LEU:CD1	5:E:402:LEU:CG	1.82	1.51
4:D:347:GLN:HG2	5:E:351:LEU:CA	1.41	1.47
4:D:347:GLN:HG3	5:E:351:LEU:CB	1.46	1.45
3:C:709:TRP:CH2	5:E:363:LEU:CB	1.99	1.41
3:C:319:PHE:CE2	5:E:303:PRO:HG3	1.53	1.41
4:D:347:GLN:HG2	5:E:351:LEU:C	1.41	1.39
4:D:347:GLN:CG	5:E:351:LEU:CA	2.02	1.35
3:C:709:TRP:HE1	5:E:360:ASP:CB	1.38	1.34
3:C:319:PHE:CZ	5:E:303:PRO:CG	2.11	1.30
3:C:375:TYR:O	3:C:379:GLN:NE2	1.64	1.30
5:E:413:LEU:O	5:E:416:ILE:HG22	1.24	1.28
4:D:347:GLN:CG	5:E:351:LEU:HB2	1.70	1.22
3:C:709:TRP:NE1	5:E:360:ASP:CB	2.04	1.20
3:C:709:TRP:CZ3	5:E:363:LEU:CB	2.25	1.19
4:D:347:GLN:CG	5:E:351:LEU:CB	2.16	1.19
5:E:359:LEU:CG	5:E:405:PRO:CG	2.19	1.19
3:C:709:TRP:NE1	5:E:360:ASP:HB3	1.60	1.17
3:C:709:TRP:CZ3	5:E:363:LEU:HB2	1.78	1.17
4:D:347:GLN:HG2	5:E:351:LEU:O	1.39	1.17
4:D:347:GLN:CG	5:E:351:LEU:HA	1.69	1.17
3:C:319:PHE:CZ	5:E:303:PRO:CB	2.29	1.14
3:C:709:TRP:CZ3	5:E:364:ALA:N	2.16	1.13
3:C:709:TRP:HE1	5:E:360:ASP:CG	1.50	1.13
3:C:319:PHE:CE2	5:E:303:PRO:CG	2.32	1.10
3:C:709:TRP:CH2	5:E:363:LEU:CA	2.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:709:TRP:CH2	5:E:364:ALA:N	2.20	1.09
3:C:381:SER:O	3:C:384:GLN:N	1.86	1.08
5:E:413:LEU:O	5:E:416:ILE:CG2	2.01	1.06
3:C:709:TRP:CZ3	5:E:363:LEU:C	2.28	1.06
3:C:381:SER:O	3:C:383:LYS:N	1.90	1.04
3:C:709:TRP:CZ2	5:E:363:LEU:HB2	1.92	1.04
2:B:432:MET:SD	5:E:402:LEU:CG	2.48	1.02
3:C:394:LEU:O	3:C:397:GLU:N	1.93	1.01
4:D:347:GLN:HG2	5:E:351:LEU:HA	1.32	1.01
4:D:347:GLN:CD	5:E:351:LEU:HA	1.81	1.01
4:D:347:GLN:CG	5:E:351:LEU:O	2.08	1.01
3:C:709:TRP:HH2	5:E:363:LEU:CA	1.71	0.99
4:D:69:ARG:HG3	6:D:901:ATP:O2G	1.61	0.97
3:C:378:LYS:O	3:C:379:GLN:HG3	1.63	0.97
5:E:420:ALA:HB2	5:E:427:ILE:HG12	1.45	0.96
3:C:709:TRP:HZ3	5:E:363:LEU:C	1.65	0.95
3:C:319:PHE:HZ	5:E:303:PRO:CA	1.79	0.94
3:C:709:TRP:HH2	5:E:363:LEU:N	1.65	0.94
3:C:709:TRP:CE2	5:E:360:ASP:CA	2.38	0.94
3:C:645:ASN:O	3:C:649:TRP:N	2.01	0.93
2:B:347:SER:O	2:B:351:VAL:N	2.02	0.92
2:B:317:GLY:N	2:B:450:THR:O	2.04	0.91
3:C:687:GLU:O	3:C:691:LEU:N	2.05	0.90
2:B:431:LEU:HD11	5:E:402:LEU:CG	1.97	0.90
3:C:239:GLN:HE22	5:E:64:VAL:HG11	1.33	0.90
5:E:413:LEU:C	5:E:416:ILE:HG22	1.92	0.90
3:C:375:TYR:OH	3:C:397:GLU:OE1	1.90	0.89
3:C:319:PHE:CZ	5:E:303:PRO:HB3	2.06	0.88
3:C:200:LEU:O	3:C:204:ARG:N	2.06	0.88
3:C:77:LEU:O	3:C:81:HIS:ND1	2.09	0.86
3:C:107:LEU:N	3:C:252:ILE:O	2.09	0.86
3:C:709:TRP:CH2	5:E:363:LEU:C	2.49	0.86
4:D:347:GLN:CB	5:E:351:LEU:O	2.24	0.85
3:C:201:SER:O	3:C:205:THR:OG1	1.95	0.84
2:B:319:LYS:O	2:B:323:LEU:N	2.12	0.83
2:B:427:LEU:N	3:C:691:LEU:O	2.12	0.83
3:C:112:THR:OG1	3:C:322:GLN:OE1	1.96	0.82
3:C:709:TRP:NE1	5:E:360:ASP:CA	2.42	0.82
5:E:420:ALA:CB	5:E:427:ILE:HG12	2.10	0.82
2:B:320:ARG:NH1	2:B:457:GLU:OE1	2.13	0.82
3:C:709:TRP:CZ3	5:E:363:LEU:HB3	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:375:TYR:O	3:C:379:GLN:CD	2.17	0.81
2:B:475:SER:CB	3:C:702:ASP:OD2	2.28	0.81
4:D:162:ASP:OD1	4:D:193:THR:OG1	1.99	0.81
4:D:347:GLN:HG3	5:E:351:LEU:HB2	0.82	0.80
3:C:43:ARG:NH2	3:C:339:GLN:O	2.15	0.80
3:C:141:CYS:HB3	3:C:147:PHE:CZ	2.17	0.80
3:C:66:ASN:O	3:C:69:LEU:N	2.15	0.80
3:C:375:TYR:CD1	3:C:379:GLN:NE2	2.50	0.80
3:C:319:PHE:HZ	5:E:303:PRO:CB	1.80	0.79
2:B:366:PHE:O	2:B:372:GLN:NE2	2.16	0.78
3:C:203:LYS:O	3:C:207:SER:N	2.16	0.78
3:C:202:LYS:HD2	3:C:244:PHE:CE1	2.19	0.78
2:B:391:LEU:HD22	2:B:421:ILE:HB	1.64	0.77
3:C:319:PHE:CE2	5:E:303:PRO:CD	2.66	0.77
3:C:202:LYS:HD2	3:C:244:PHE:HE1	1.49	0.77
5:E:420:ALA:HB1	5:E:425:PHE:O	1.84	0.77
4:D:347:GLN:CG	5:E:351:LEU:C	2.34	0.77
3:C:709:TRP:NE1	5:E:360:ASP:CG	2.34	0.77
3:C:709:TRP:NE1	5:E:360:ASP:HA	2.00	0.77
2:B:445:TRP:O	3:C:591:HIS:HA	1.84	0.76
3:C:319:PHE:CZ	5:E:303:PRO:CA	2.63	0.76
3:C:319:PHE:CE1	5:E:303:PRO:HG3	2.18	0.76
2:B:475:SER:HB2	3:C:702:ASP:OD2	1.85	0.76
3:C:385:VAL:O	3:C:389:THR:N	2.18	0.75
3:C:239:GLN:NE2	5:E:64:VAL:HG11	2.02	0.75
5:E:411:VAL:O	5:E:412:SER:CB	2.35	0.74
3:C:433:ARG:N	3:C:437:GLU:OE1	2.20	0.74
3:C:302:ILE:CG2	3:C:306:VAL:HG22	2.17	0.74
4:D:351:ASN:HD21	5:E:351:LEU:HB3	1.53	0.74
3:C:452:GLU:OE1	3:C:452:GLU:N	2.22	0.73
3:C:319:PHE:HZ	5:E:303:PRO:HA	1.50	0.73
3:C:199:MET:HA	3:C:244:PHE:CZ	2.23	0.72
3:C:237:SER:O	3:C:241:LEU:HG	1.89	0.72
3:C:709:TRP:CE2	5:E:360:ASP:HA	1.74	0.72
3:C:202:LYS:HE2	3:C:213:PRO:HG2	1.72	0.71
3:C:100:ILE:HG13	3:C:241:LEU:HD11	1.69	0.71
2:B:318:SER:O	2:B:452:SER:OG	2.08	0.71
3:C:375:TYR:CE1	3:C:379:GLN:NE2	2.59	0.71
2:B:356:THR:HA	2:B:360:LEU:HB2	1.73	0.71
3:C:372:PHE:O	3:C:376:VAL:N	2.23	0.71
3:C:556:VAL:HA	3:C:559:PHE:HD2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:314:TYR:CG	5:E:416:ILE:HD12	2.25	0.70
3:C:556:VAL:HA	3:C:559:PHE:HB2	1.73	0.70
3:C:380:ALA:O	3:C:384:GLN:OE1	2.09	0.70
3:C:405:LEU:N	3:C:574:GLN:OE1	2.24	0.69
3:C:130:THR:OG1	3:C:131:PRO:HD3	1.92	0.69
5:E:420:ALA:HB2	5:E:427:ILE:CG1	2.22	0.69
2:B:453:PRO:HA	2:B:454:TYR:HB2	1.75	0.69
3:C:63:GLU:O	3:C:67:LYS:HG3	1.91	0.69
3:C:125:LEU:O	3:C:131:PRO:HD2	1.93	0.69
3:C:291:LYS:O	3:C:295:THR:HG23	1.93	0.69
3:C:335:HIS:NE2	3:C:579:VAL:O	2.25	0.69
2:B:353:ASN:O	2:B:357:GLU:N	2.22	0.69
2:B:352:LEU:HD23	2:B:372:GLN:OE1	1.92	0.68
5:E:359:LEU:CG	5:E:405:PRO:CB	2.71	0.68
3:C:151:LEU:HD12	3:C:198:LYS:NZ	2.09	0.68
3:C:151:LEU:HD12	3:C:198:LYS:HZ2	1.59	0.68
2:B:398:GLN:HB3	2:B:399:MET:HA	1.76	0.68
2:B:431:LEU:HD13	5:E:402:LEU:CG	2.16	0.68
3:C:555:ASN:O	3:C:559:PHE:N	2.26	0.68
3:C:689:GLU:HG3	3:C:694:ILE:HD11	1.75	0.68
3:C:415:VAL:HG12	3:C:567:TYR:CZ	2.29	0.68
4:D:347:GLN:HB3	5:E:351:LEU:O	1.93	0.67
3:C:45:GLU:O	3:C:49:LEU:HG	1.94	0.67
5:E:14:GLN:N	5:E:14:GLN:OE1	2.27	0.67
3:C:132:TYR:O	3:C:215:VAL:HG22	1.93	0.67
3:C:52:GLN:O	3:C:56:SER:OG	2.06	0.66
3:C:151:LEU:HG	3:C:198:LYS:HD2	1.77	0.66
3:C:648:ASP:O	3:C:652:ALA:HB2	1.94	0.66
3:C:102:THR:OG1	3:C:273:ILE:HG12	1.96	0.66
3:C:199:MET:HA	3:C:244:PHE:CE2	2.30	0.66
2:B:328:THR:O	2:B:332:GLN:NE2	2.25	0.65
3:C:381:SER:C	3:C:383:LYS:N	2.49	0.65
3:C:709:TRP:CE2	5:E:360:ASP:CB	2.74	0.65
3:C:397:GLU:HG2	3:C:400:LEU:HD12	1.78	0.65
2:B:311:ILE:HG13	2:B:421:ILE:HG12	1.78	0.65
2:B:478:THR:HG22	3:C:701:THR:HG21	1.78	0.65
3:C:709:TRP:CZ3	5:E:363:LEU:CA	2.71	0.65
3:C:475:CYS:O	3:C:479:PHE:HB2	1.96	0.65
3:C:500:GLN:O	3:C:503:SER:OG	2.13	0.65
3:C:457:LEU:HG	3:C:559:PHE:CZ	2.32	0.64
3:C:476:PHE:O	3:C:480:LYS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:709:TRP:CH2	5:E:363:LEU:N	2.56	0.64
3:C:548:LYS:O	3:C:552:LEU:N	2.29	0.64
4:D:351:ASN:ND2	5:E:351:LEU:HB3	2.12	0.64
2:B:426:HIS:HA	3:C:690:LEU:O	1.98	0.64
3:C:234:ILE:O	3:C:238:SER:CB	2.46	0.64
3:C:319:PHE:CE1	5:E:303:PRO:HB3	2.32	0.64
3:C:397:GLU:O	3:C:401:LEU:HG	1.98	0.64
3:C:562:CYS:O	3:C:566:GLU:N	2.30	0.64
3:C:489:SER:HA	3:C:490:THR:HB	1.80	0.64
2:B:298:PHE:HB3	2:B:330:MET:HG3	1.80	0.64
3:C:381:SER:O	3:C:383:LYS:CA	2.46	0.63
3:C:684:ALA:O	3:C:688:LEU:HD13	1.97	0.63
3:C:556:VAL:HA	3:C:559:PHE:CD2	2.34	0.63
5:E:423:VAL:O	5:E:424:ASN:CB	2.46	0.63
3:C:448:TRP:CZ2	3:C:559:PHE:HB3	2.33	0.63
5:E:418:ALA:O	5:E:422:THR:HG23	1.99	0.63
3:C:694:ILE:HD13	3:C:704:VAL:HG13	1.81	0.63
3:C:476:PHE:CE2	3:C:501:PHE:CD1	2.87	0.62
3:C:597:ARG:NH2	3:C:708:THR:OG1	2.31	0.62
3:C:381:SER:O	3:C:382:GLU:C	2.34	0.62
3:C:147:PHE:HB2	3:C:233:PHE:CZ	2.34	0.62
3:C:569:LEU:HB3	3:C:571:PRO:HD2	1.81	0.62
3:C:418:CYS:HA	3:C:479:PHE:CZ	2.34	0.62
5:E:417:ARG:O	5:E:421:ARG:HG3	2.00	0.62
5:E:314:TYR:HB3	5:E:416:ILE:HD12	1.82	0.62
2:B:298:PHE:HB3	2:B:330:MET:SD	2.39	0.62
2:B:373:LEU:HD22	2:B:412:LEU:HD21	1.81	0.62
3:C:102:THR:HG1	3:C:250:PHE:HE2	1.45	0.61
3:C:475:CYS:O	3:C:479:PHE:CD2	2.53	0.61
3:C:47:TYR:OH	3:C:329:GLN:OE1	2.13	0.61
3:C:688:LEU:HG	3:C:693:PHE:HB2	1.82	0.61
3:C:272:CYS:SG	3:C:272:CYS:O	2.58	0.61
3:C:420:HIS:NE2	3:C:438:LEU:HB2	2.16	0.60
3:C:97:LEU:HA	3:C:242:HIS:CD2	2.36	0.60
3:C:155:LEU:CD1	3:C:198:LYS:HE2	2.31	0.60
3:C:64:GLU:O	3:C:67:LYS:N	2.33	0.60
3:C:155:LEU:CD1	3:C:215:VAL:HG21	2.31	0.60
3:C:420:HIS:CD2	3:C:435:ILE:HA	2.35	0.60
2:B:377:VAL:O	2:B:381:LYS:N	2.30	0.60
2:B:411:GLN:O	2:B:415:LEU:N	2.32	0.60
3:C:104:ALA:HA	3:C:250:PHE:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:429:TYR:HB3	3:C:433:ARG:HG2	1.83	0.60
2:B:287:LEU:HD22	2:B:451:TYR:HB2	1.82	0.60
2:B:348:VAL:HA	2:B:351:VAL:HB	1.84	0.60
3:C:122:THR:HA	3:C:133:VAL:CG2	2.32	0.60
2:B:337:VAL:HG22	2:B:359:VAL:HG21	1.83	0.59
3:C:147:PHE:CD2	3:C:233:PHE:CE2	2.89	0.59
5:E:413:LEU:CA	5:E:416:ILE:HG22	2.33	0.59
2:B:445:TRP:HB2	3:C:590:GLU:O	2.02	0.59
3:C:317:HIS:HB3	5:E:379:ASN:HB3	1.84	0.59
1:A:638:ASP:OD2	1:A:642:HIS:NE2	2.35	0.59
3:C:488:GLY:O	3:C:490:THR:OG1	2.16	0.59
3:C:709:TRP:HH2	5:E:364:ALA:N	1.95	0.59
3:C:209:GLN:N	3:C:210:TRP:HA	2.17	0.59
2:B:305:LEU:O	2:B:419:TYR:CE1	2.56	0.59
2:B:366:PHE:N	2:B:372:GLN:HG2	2.18	0.59
3:C:151:LEU:O	3:C:198:LYS:HE3	2.02	0.59
3:C:189:MET:O	3:C:191:VAL:N	2.35	0.59
3:C:709:TRP:CE2	5:E:360:ASP:HB3	2.34	0.59
3:C:155:LEU:HD11	3:C:215:VAL:HG21	1.83	0.58
3:C:296:THR:HB	3:C:410:MET:SD	2.42	0.58
3:C:489:SER:HA	3:C:490:THR:CB	2.33	0.58
3:C:50:ILE:O	3:C:54:MET:HG2	2.02	0.58
3:C:152:ILE:HG21	3:C:197:PRO:CB	2.34	0.58
3:C:302:ILE:HG23	3:C:306:VAL:HG22	1.84	0.58
3:C:199:MET:CE	3:C:203:LYS:HE3	2.33	0.58
3:C:99:GLU:N	3:C:241:LEU:HD12	2.18	0.58
5:E:314:TYR:CB	5:E:416:ILE:HD12	2.34	0.58
3:C:131:PRO:HB3	3:C:214:PRO:O	2.02	0.58
3:C:216:VAL:HA	3:C:247:ILE:O	2.04	0.57
3:C:416:LEU:O	3:C:420:HIS:ND1	2.37	0.57
3:C:648:ASP:O	3:C:652:ALA:CB	2.51	0.57
2:B:318:SER:N	2:B:452:SER:O	2.30	0.57
3:C:155:LEU:HG	3:C:198:LYS:HE2	1.86	0.57
3:C:418:CYS:HA	3:C:479:PHE:CE2	2.39	0.57
4:D:69:ARG:CG	6:D:901:ATP:O2G	2.44	0.57
3:C:421:LYS:HB2	3:C:479:PHE:CE2	2.40	0.57
2:B:475:SER:HB3	3:C:702:ASP:OD2	2.04	0.57
3:C:152:ILE:HG21	3:C:197:PRO:CG	2.34	0.57
3:C:335:HIS:O	3:C:338:SER:N	2.27	0.57
4:D:68:PRO:O	4:D:73:LYS:NZ	2.38	0.57
5:E:112:ALA:O	5:E:116:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:PHE:HB3	2:B:330:MET:CG	2.34	0.57
3:C:479:PHE:HA	3:C:482:TYR:HD2	1.70	0.57
2:B:352:LEU:HA	2:B:355:ILE:HG22	1.87	0.57
3:C:468:LEU:O	3:C:472:LEU:HG	2.05	0.57
3:C:709:TRP:HE1	5:E:360:ASP:CA	2.04	0.57
2:B:478:THR:CG2	3:C:701:THR:HG21	2.35	0.57
3:C:409:HIS:HA	3:C:412:TYR:HD2	1.69	0.57
2:B:331:LEU:HD11	2:B:391:LEU:HD11	1.87	0.56
3:C:234:ILE:O	3:C:238:SER:HB2	2.05	0.56
3:C:271:LEU:HD13	3:C:273:ILE:HD11	1.87	0.56
2:B:323:LEU:HD22	2:B:391:LEU:HD13	1.87	0.56
2:B:335:ILE:HG22	2:B:388:LEU:HA	1.87	0.56
2:B:400:LEU:O	2:B:405:SER:OG	2.23	0.56
3:C:229:VAL:HG13	3:C:233:PHE:HE2	1.71	0.56
3:C:310:LEU:O	3:C:313:ILE:HG22	2.05	0.56
3:C:378:LYS:O	3:C:379:GLN:CG	2.47	0.56
3:C:648:ASP:HA	3:C:651:GLU:HB2	1.86	0.56
5:E:369:ILE:HD11	5:E:425:PHE:CE1	2.40	0.56
3:C:46:THR:HA	3:C:49:LEU:HD12	1.88	0.56
3:C:560:ILE:HA	3:C:564:VAL:HB	1.87	0.56
3:C:694:ILE:HD12	3:C:695:LYS:N	2.19	0.56
3:C:147:PHE:HE1	3:C:225:PHE:CZ	2.24	0.56
3:C:651:GLU:O	3:C:655:THR:HG23	2.05	0.56
3:C:43:ARG:NH2	3:C:342:SER:OG	2.38	0.56
3:C:458:GLN:O	3:C:462:MET:HG2	2.05	0.56
2:B:428:ASN:O	2:B:431:LEU:HB3	2.05	0.56
3:C:202:LYS:CE	3:C:215:VAL:HG23	2.36	0.56
3:C:230:LEU:HD21	3:C:263:LEU:HD23	1.86	0.56
2:B:412:LEU:HB3	2:B:418:ILE:HD11	1.87	0.56
3:C:385:VAL:O	3:C:388:LEU:N	2.39	0.56
5:E:432:TYR:CG	5:E:432:TYR:CA	2.81	0.56
3:C:324:PHE:O	3:C:328:LEU:HG	2.05	0.56
5:E:145:GLN:O	5:E:149:ASP:N	2.39	0.56
3:C:695:LYS:HD2	3:C:707:LEU:HD11	1.87	0.55
3:C:222:MET:HG3	3:C:250:PHE:CD1	2.41	0.55
3:C:325:ILE:O	3:C:328:LEU:N	2.40	0.55
3:C:381:SER:O	3:C:383:LYS:C	2.45	0.55
3:C:134:VAL:HG22	3:C:154:GLN:HB3	1.87	0.55
3:C:128:ASN:HB2	3:C:130:THR:OG1	2.06	0.55
3:C:131:PRO:CB	3:C:214:PRO:O	2.55	0.55
3:C:482:TYR:O	3:C:487:LEU:N	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:PHE:O	3:C:151:LEU:HB2	2.06	0.55
2:B:397:SER:HB2	2:B:398:GLN:C	2.27	0.55
3:C:152:ILE:HG12	3:C:198:LYS:CB	2.37	0.55
3:C:453:TYR:OH	3:C:563:LEU:CD1	2.55	0.55
5:E:311:ILE:CG2	5:E:419:ILE:HG21	2.37	0.55
2:B:295:GLU:O	2:B:298:PHE:HB2	2.07	0.55
2:B:352:LEU:HD21	2:B:373:LEU:HD21	1.89	0.55
3:C:482:TYR:O	3:C:486:HIS:N	2.39	0.55
3:C:280:SER:O	3:C:284:HIS:ND1	2.38	0.55
3:C:494:ILE:HA	3:C:497:PHE:HD2	1.72	0.55
2:B:478:THR:CG2	3:C:701:THR:CG2	2.85	0.54
3:C:375:TYR:CZ	3:C:401:LEU:HD21	2.42	0.54
3:C:687:GLU:O	3:C:690:LEU:N	2.40	0.54
5:E:308:PHE:HE1	5:E:423:VAL:HG11	1.73	0.54
2:B:339:ILE:HD13	2:B:351:VAL:HG22	1.90	0.54
3:C:476:PHE:HB3	3:C:480:LYS:HE3	1.89	0.54
3:C:138:ALA:HB2	3:C:221:ASP:O	2.08	0.54
3:C:319:PHE:CE2	5:E:303:PRO:HD3	2.41	0.54
3:C:478:VAL:O	3:C:481:SER:HB3	2.07	0.54
3:C:556:VAL:CA	3:C:559:PHE:HD2	2.21	0.54
3:C:267:VAL:HG12	3:C:271:LEU:HD11	1.89	0.54
3:C:230:LEU:HD11	3:C:263:LEU:HD22	1.89	0.54
3:C:319:PHE:CD2	5:E:303:PRO:HG3	2.30	0.54
3:C:330:LEU:O	3:C:334:GLU:HB2	2.07	0.54
1:A:580:TYR:CE2	1:A:632:ILE:HG22	2.42	0.54
3:C:209:GLN:HE22	3:C:213:PRO:HG3	1.72	0.54
2:B:320:ARG:HH22	2:B:457:GLU:N	2.06	0.54
2:B:333:ASP:HB2	2:B:336:HIS:HE2	1.72	0.54
2:B:366:PHE:O	2:B:372:GLN:CG	2.55	0.54
3:C:554:GLU:O	3:C:558:ASN:N	2.38	0.54
3:C:147:PHE:CE2	3:C:229:VAL:HG11	2.43	0.53
3:C:226:ALA:O	3:C:230:LEU:N	2.40	0.53
3:C:420:HIS:NE2	3:C:435:ILE:HA	2.23	0.53
1:A:500:VAL:HB	1:A:501:PRO:HD3	1.91	0.53
2:B:340:ASN:HB3	2:B:342:PHE:CE2	2.44	0.53
3:C:99:GLU:C	3:C:241:LEU:CD1	2.77	0.53
3:C:152:ILE:HG21	3:C:197:PRO:CD	2.38	0.53
3:C:369:LEU:HD11	3:C:576:LEU:HD23	1.90	0.53
3:C:371:SER:HA	3:C:374:ARG:HB2	1.91	0.53
3:C:403:GLU:O	3:C:407:VAL:HG23	2.08	0.53
3:C:480:LYS:HE2	3:C:498:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:685:VAL:HG11	3:C:704:VAL:HG21	1.90	0.53
2:B:320:ARG:CZ	2:B:456:GLU:HB2	2.38	0.53
2:B:446:TYR:CD1	3:C:591:HIS:CE1	2.96	0.53
3:C:453:TYR:OH	3:C:559:PHE:CE1	2.60	0.53
3:C:412:TYR:O	3:C:415:VAL:N	2.41	0.53
3:C:493:ARG:O	3:C:497:PHE:CD2	2.62	0.53
3:C:330:LEU:O	3:C:334:GLU:CB	2.56	0.53
3:C:375:TYR:CG	3:C:379:GLN:NE2	2.77	0.53
2:B:390:LEU:HD11	2:B:420:LEU:HD13	1.89	0.53
3:C:417:ARG:O	3:C:479:PHE:CZ	2.62	0.53
2:B:365:THR:HB	2:B:372:GLN:CD	2.29	0.53
3:C:420:HIS:CD2	3:C:438:LEU:HD22	2.43	0.53
4:D:347:GLN:NE2	5:E:351:LEU:HA	2.23	0.53
3:C:387:LEU:HD22	3:C:394:LEU:HD13	1.90	0.53
3:C:239:GLN:HE22	5:E:64:VAL:CG1	2.14	0.52
3:C:448:TRP:HZ2	3:C:559:PHE:HB3	1.71	0.52
3:C:483:CYS:HA	3:C:487:LEU:O	2.09	0.52
2:B:458:THR:HA	3:C:683:ARG:NH1	2.25	0.52
3:C:46:THR:O	3:C:50:ILE:HG13	2.08	0.52
3:C:330:LEU:HD13	3:C:592:LEU:HD21	1.91	0.52
3:C:563:LEU:HA	3:C:567:TYR:HB2	1.92	0.52
3:C:404:ASN:C	3:C:574:GLN:OE1	2.48	0.52
3:C:548:LYS:O	3:C:551:VAL:N	2.43	0.52
2:B:337:VAL:HG21	2:B:355:ILE:HG13	1.91	0.52
2:B:420:LEU:HD12	2:B:421:ILE:N	2.25	0.52
3:C:101:PRO:O	3:C:247:ILE:HA	2.10	0.52
2:B:325:ARG:O	2:B:329:THR:N	2.39	0.52
3:C:152:ILE:HG23	3:C:198:LYS:N	2.25	0.52
3:C:244:PHE:O	3:C:246:LEU:N	2.41	0.52
3:C:296:THR:HG22	3:C:413:PHE:CD2	2.45	0.52
3:C:559:PHE:O	3:C:564:VAL:N	2.33	0.52
2:B:416:HIS:O	2:B:419:TYR:CZ	2.62	0.52
2:B:508:TYR:CZ	2:B:510:GLY:HA2	2.45	0.52
3:C:133:VAL:N	3:C:158:CYS:SG	2.83	0.52
3:C:234:ILE:O	3:C:238:SER:HB3	2.10	0.52
3:C:429:TYR:CB	3:C:433:ARG:HG2	2.40	0.52
2:B:314:TYR:N	2:B:448:THR:OG1	2.43	0.52
3:C:100:ILE:O	3:C:270:LEU:O	2.28	0.52
3:C:132:TYR:O	3:C:155:LEU:HD21	2.09	0.52
3:C:335:HIS:CE1	3:C:579:VAL:HA	2.45	0.52
4:D:276:LEU:HB2	6:D:901:ATP:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ARG:HA	3:C:238:SER:O	2.10	0.51
3:C:199:MET:HE2	3:C:244:PHE:HE2	1.75	0.51
5:E:314:TYR:CG	5:E:416:ILE:CD1	2.93	0.51
3:C:301:LYS:N	3:C:580:VAL:O	2.39	0.51
3:C:342:SER:O	3:C:345:CYS:N	2.32	0.51
3:C:347:ASN:O	3:C:351:ALA:N	2.34	0.51
3:C:368:ARG:O	3:C:373:ARG:HG3	2.09	0.51
3:C:553:ARG:O	3:C:557:VAL:HG23	2.10	0.51
3:C:645:ASN:OD1	3:C:648:ASP:N	2.37	0.51
5:E:416:ILE:HG12	5:E:427:ILE:CD1	2.41	0.51
2:B:307:LEU:HD13	3:C:333:LEU:HD13	1.93	0.51
5:E:416:ILE:HG12	5:E:427:ILE:HG13	1.92	0.51
3:C:66:ASN:HB3	3:C:70:PHE:CD2	2.46	0.51
3:C:645:ASN:OD1	3:C:648:ASP:HB2	2.11	0.51
3:C:367:ARG:HA	3:C:372:PHE:CE2	2.46	0.51
3:C:707:LEU:N	3:C:707:LEU:HD12	2.25	0.51
3:C:152:ILE:HG12	3:C:198:LYS:H	1.75	0.51
3:C:155:LEU:HD12	3:C:198:LYS:CD	2.41	0.51
3:C:569:LEU:O	3:C:573:THR:CG2	2.59	0.51
3:C:689:GLU:CG	3:C:694:ILE:HD11	2.41	0.51
3:C:199:MET:CE	3:C:244:PHE:HE2	2.24	0.51
3:C:288:VAL:O	3:C:292:LEU:N	2.33	0.51
3:C:317:HIS:O	5:E:383:GLN:NE2	2.44	0.51
3:C:404:ASN:CB	3:C:574:GLN:OE1	2.59	0.51
3:C:464:ALA:HA	3:C:468:LEU:HD12	1.91	0.51
3:C:709:TRP:HH2	5:E:363:LEU:H	1.56	0.51
3:C:685:VAL:CG1	3:C:704:VAL:HG21	2.40	0.50
1:A:690:LEU:HD11	1:A:722:CYS:HB3	1.94	0.50
3:C:110:ASN:HB3	3:C:281:CYS:SG	2.51	0.50
5:E:427:ILE:O	5:E:431:LEU:HG	2.10	0.50
3:C:342:SER:OG	3:C:579:VAL:HG13	2.12	0.50
5:E:416:ILE:HG12	5:E:427:ILE:HD12	1.93	0.50
3:C:43:ARG:NH2	3:C:342:SER:H	2.10	0.50
3:C:401:LEU:HD22	3:C:575:PRO:CG	2.41	0.50
3:C:457:LEU:HG	3:C:559:PHE:HZ	1.76	0.50
3:C:480:LYS:HE2	3:C:498:LEU:CB	2.41	0.50
2:B:339:ILE:HD13	2:B:351:VAL:HG13	1.94	0.50
2:B:369:ILE:HG12	2:B:372:GLN:OE1	2.12	0.50
2:B:458:THR:HG23	3:C:683:ARG:CZ	2.42	0.50
2:B:458:THR:OG1	3:C:683:ARG:HD2	2.12	0.50
3:C:152:ILE:HA	3:C:198:LYS:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:MET:HE2	3:C:244:PHE:CE2	2.47	0.50
3:C:316:TYR:HD2	5:E:305:TYR:CE2	2.30	0.50
3:C:417:ARG:HD3	3:C:482:TYR:CE1	2.46	0.50
3:C:429:TYR:CG	3:C:433:ARG:HG2	2.46	0.50
1:A:625:LEU:O	1:A:632:ILE:HD11	2.12	0.50
1:A:785:PHE:O	1:A:789:GLY:N	2.37	0.50
2:B:355:ILE:O	2:B:360:LEU:HB2	2.12	0.50
3:C:202:LYS:HB2	3:C:244:PHE:CE1	2.47	0.50
3:C:461:ARG:HG2	3:C:552:LEU:CD2	2.42	0.50
2:B:320:ARG:NH2	2:B:457:GLU:N	2.60	0.50
3:C:63:GLU:O	3:C:66:ASN:HB2	2.11	0.50
3:C:148:LEU:O	3:C:151:LEU:HB3	2.12	0.50
3:C:148:LEU:HD23	3:C:151:LEU:HD22	1.93	0.50
3:C:286:THR:HG22	3:C:436:ARG:HE	1.77	0.50
3:C:330:LEU:CD1	3:C:592:LEU:HD21	2.42	0.50
3:C:387:LEU:HD21	3:C:397:GLU:CD	2.32	0.50
5:E:302:LEU:O	5:E:307:LYS:NZ	2.44	0.50
3:C:152:ILE:HG12	3:C:198:LYS:HB2	1.93	0.50
3:C:494:ILE:O	3:C:498:LEU:HG	2.12	0.50
3:C:355:ILE:HA	3:C:358:LEU:HG	1.94	0.49
3:C:372:PHE:HA	3:C:375:TYR:HB3	1.94	0.49
3:C:415:VAL:O	3:C:418:CYS:HB3	2.12	0.49
3:C:552:LEU:O	3:C:556:VAL:HG23	2.13	0.49
2:B:311:ILE:HD11	2:B:421:ILE:HG23	1.94	0.49
2:B:332:GLN:O	2:B:336:HIS:CD2	2.66	0.49
3:C:504:LEU:HD11	3:C:554:GLU:CD	2.32	0.49
2:B:410:GLY:HA2	2:B:441:PHE:CE1	2.48	0.49
3:C:155:LEU:CG	3:C:198:LYS:HE2	2.42	0.49
3:C:202:LYS:CD	3:C:244:PHE:CE1	2.92	0.49
3:C:219:LEU:HB2	3:C:222:MET:HG2	1.93	0.49
3:C:369:LEU:HD13	3:C:370:PRO:O	2.12	0.49
1:A:687:GLN:OE1	1:A:691:ARG:NH1	2.45	0.49
3:C:252:ILE:HD13	3:C:259:ILE:HD11	1.95	0.49
3:C:405:LEU:HD23	3:C:574:GLN:HB2	1.94	0.49
3:C:418:CYS:O	3:C:422:PHE:CD2	2.65	0.49
3:C:646:LEU:HA	3:C:649:TRP:HB3	1.94	0.49
4:D:102:LEU:O	5:E:136:ASN:ND2	2.45	0.49
3:C:132:TYR:O	3:C:155:LEU:CD2	2.61	0.49
3:C:480:LYS:NZ	3:C:502:GLN:HG3	2.28	0.49
5:E:39:THR:HG23	5:E:40:ALA:N	2.28	0.49
2:B:302:MET:HA	2:B:305:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:VAL:CG2	2:B:443:TRP:CE3	2.95	0.49
2:B:398:GLN:HG3	2:B:401:ARG:HG3	1.95	0.49
3:C:222:MET:SD	3:C:225:PHE:CE2	3.06	0.49
3:C:381:SER:HA	3:C:384:GLN:HG2	1.95	0.49
3:C:393:TYR:O	3:C:397:GLU:HG3	2.13	0.49
3:C:420:HIS:O	3:C:421:LYS:C	2.50	0.49
2:B:410:GLY:O	2:B:414:SER:CB	2.61	0.49
3:C:446:ASN:HA	3:C:569:LEU:HD21	1.94	0.49
3:C:71:ASP:O	3:C:75:GLU:CG	2.61	0.49
3:C:293:LEU:HD21	3:C:328:LEU:HD13	1.95	0.49
3:C:694:ILE:HA	3:C:706:ARG:HA	1.93	0.49
2:B:352:LEU:CD2	2:B:369:ILE:HG23	2.43	0.48
3:C:285:LEU:O	3:C:288:VAL:HG12	2.13	0.48
3:C:501:PHE:CE1	3:C:554:GLU:CD	2.86	0.48
3:C:341:LEU:HD21	3:C:365:ASN:CB	2.43	0.48
3:C:478:VAL:O	3:C:482:TYR:CD2	2.66	0.48
3:C:480:LYS:O	3:C:484:GLU:CG	2.61	0.48
3:C:387:LEU:HA	3:C:394:LEU:HB2	1.95	0.48
3:C:402:LEU:HA	3:C:405:LEU:HD12	1.96	0.48
3:C:202:LYS:CD	3:C:244:PHE:HE1	2.23	0.48
3:C:263:LEU:HD13	3:C:271:LEU:HD11	1.96	0.48
2:B:412:LEU:O	2:B:415:LEU:N	2.47	0.48
2:B:461:GLU:HB2	3:C:683:ARG:HH12	1.78	0.48
3:C:306:VAL:HG12	3:C:585:ALA:HB2	1.94	0.48
3:C:386:ALA:O	3:C:390:ASN:O	2.31	0.48
3:C:446:ASN:OD1	3:C:569:LEU:HD11	2.13	0.48
2:B:373:LEU:O	2:B:377:VAL:HB	2.14	0.48
3:C:79:LYS:O	3:C:83:GLY:N	2.37	0.48
3:C:100:ILE:O	3:C:271:LEU:HA	2.14	0.48
3:C:418:CYS:SG	3:C:422:PHE:HE2	2.37	0.48
3:C:457:LEU:CG	3:C:559:PHE:CZ	2.96	0.48
3:C:555:ASN:C	3:C:559:PHE:CD2	2.86	0.48
3:C:152:ILE:HG12	3:C:198:LYS:HG3	1.95	0.48
2:B:320:ARG:HH22	2:B:457:GLU:CA	2.27	0.48
2:B:446:TYR:CB	2:B:448:THR:HG23	2.43	0.48
3:C:288:VAL:CG2	3:C:292:LEU:HD12	2.43	0.48
1:A:536:PRO:HA	6:A:901:ATP:O1G	2.14	0.48
2:B:445:TRP:O	3:C:590:GLU:O	2.32	0.48
3:C:126:GLN:HB3	3:C:162:ILE:HD11	1.95	0.48
2:B:298:PHE:CD2	2:B:330:MET:HG2	2.49	0.48
3:C:151:LEU:CD1	3:C:198:LYS:HD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:556:VAL:O	3:C:560:ILE:N	2.42	0.48
4:D:67:GLY:O	4:D:194:CYS:HA	2.14	0.48
2:B:425:ASP:OD1	2:B:454:TYR:OH	2.32	0.47
3:C:302:ILE:CG2	3:C:307:LEU:HG	2.44	0.47
3:C:303:ASN:ND2	3:C:581:TYR:HB3	2.28	0.47
3:C:325:ILE:HG22	3:C:326:LYS:N	2.29	0.47
3:C:478:VAL:O	3:C:482:TYR:HD2	1.96	0.47
2:B:394:ASN:ND2	2:B:425:ASP:OD2	2.36	0.47
2:B:426:HIS:CA	3:C:690:LEU:O	2.61	0.47
2:B:427:LEU:HG	3:C:691:LEU:O	2.14	0.47
3:C:102:THR:HA	3:C:247:ILE:HG23	1.97	0.47
3:C:255:SER:HB2	3:C:256:PRO:HD3	1.95	0.47
3:C:497:PHE:O	3:C:501:PHE:HD2	1.97	0.47
2:B:340:ASN:O	2:B:343:PHE:HB2	2.15	0.47
3:C:100:ILE:HG12	3:C:241:LEU:HD21	1.95	0.47
3:C:475:CYS:O	3:C:479:PHE:CB	2.61	0.47
5:E:54:LEU:N	5:E:55:GLU:HA	2.28	0.47
2:B:327:ARG:HA	2:B:331:LEU:HB2	1.97	0.47
2:B:362:HIS:O	2:B:363:MET:HG2	2.14	0.47
3:C:404:ASN:O	3:C:407:VAL:HB	2.14	0.47
3:C:555:ASN:HA	3:C:558:ASN:HB2	1.97	0.47
3:C:695:LYS:HG3	3:C:696:PRO:HD2	1.95	0.47
3:C:234:ILE:HG21	3:C:267:VAL:HG13	1.96	0.47
3:C:417:ARG:C	3:C:479:PHE:CE1	2.87	0.47
3:C:555:ASN:O	3:C:559:PHE:CD2	2.68	0.47
3:C:645:ASN:HA	3:C:703:HIS:CE1	2.49	0.47
3:C:326:LYS:HA	3:C:329:GLN:HE21	1.79	0.47
1:A:708:VAL:HG13	1:A:751:SER:HB3	1.97	0.47
3:C:44:PHE:HA	3:C:47:TYR:HB3	1.96	0.47
3:C:199:MET:HG2	3:C:244:PHE:CE2	2.50	0.47
3:C:405:LEU:HD21	3:C:575:PRO:O	2.15	0.47
3:C:422:PHE:CE1	3:C:472:LEU:HD22	2.50	0.47
5:E:319:ASN:ND2	5:E:430:TYR:O	2.46	0.47
1:A:694:LEU:O	1:A:696:HIS:N	2.47	0.47
3:C:366:ILE:O	3:C:372:PHE:CD2	2.68	0.47
3:C:447:ILE:HG22	3:C:453:TYR:CG	2.50	0.47
3:C:588:LEU:O	3:C:592:LEU:N	2.48	0.47
4:D:259:ASP:OD1	4:D:260:ARG:N	2.47	0.47
2:B:318:SER:HA	2:B:319:LYS:HZ1	1.80	0.47
3:C:148:LEU:HA	3:C:151:LEU:CD2	2.45	0.47
3:C:422:PHE:HE1	3:C:472:LEU:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:HD11	2:B:391:LEU:CD1	2.45	0.47
3:C:130:THR:O	3:C:131:PRO:O	2.33	0.47
3:C:226:ALA:HB3	3:C:229:VAL:HB	1.96	0.47
3:C:252:ILE:CD1	3:C:259:ILE:HD11	2.44	0.47
2:B:409:ILE:HG22	2:B:441:PHE:CE1	2.49	0.46
2:B:441:PHE:HB3	2:B:443:TRP:CE2	2.50	0.46
3:C:421:LYS:NZ	3:C:479:PHE:CE1	2.79	0.46
2:B:397:SER:HB2	2:B:400:LEU:H	1.80	0.46
3:C:202:LYS:HE3	3:C:215:VAL:CG2	2.46	0.46
3:C:267:VAL:O	3:C:271:LEU:HG	2.15	0.46
3:C:497:PHE:HE1	3:C:557:VAL:HG13	1.80	0.46
3:C:569:LEU:O	3:C:573:THR:HG23	2.16	0.46
3:C:222:MET:HG3	3:C:250:PHE:CE1	2.50	0.46
3:C:419:LEU:HB2	3:C:567:TYR:CE1	2.50	0.46
4:D:123:VAL:HB	4:D:124:VAL:HA	1.96	0.46
1:A:694:LEU:O	1:A:697:LEU:N	2.41	0.46
2:B:331:LEU:HB3	2:B:336:HIS:CG	2.50	0.46
2:B:336:HIS:ND1	2:B:389:PHE:HB2	2.30	0.46
3:C:401:LEU:HD22	3:C:575:PRO:HG3	1.97	0.46
5:E:416:ILE:HG12	5:E:427:ILE:CG1	2.46	0.46
2:B:295:GLU:HG2	2:B:298:PHE:CE2	2.51	0.46
2:B:492:PHE:CE2	2:B:496:ILE:HD11	2.51	0.46
3:C:319:PHE:CE1	5:E:303:PRO:CG	2.89	0.46
3:C:695:LYS:CG	3:C:696:PRO:HD2	2.45	0.46
3:C:101:PRO:HB3	3:C:272:CYS:SG	2.56	0.46
3:C:695:LYS:CD	3:C:707:LEU:HD11	2.46	0.46
2:B:317:GLY:O	2:B:319:LYS:NZ	2.49	0.46
3:C:144:MET:SD	3:C:232:ASP:HB2	2.56	0.46
3:C:416:LEU:HD12	3:C:567:TYR:HD1	1.80	0.46
1:A:631:ASP:OD1	1:A:632:ILE:HG23	2.15	0.46
2:B:412:LEU:HB3	2:B:418:ILE:CD1	2.46	0.46
3:C:50:ILE:HG12	3:C:298:PHE:CE1	2.50	0.46
3:C:104:ALA:CA	3:C:250:PHE:HD2	2.29	0.46
3:C:420:HIS:CG	3:C:435:ILE:HG12	2.51	0.46
3:C:475:CYS:O	3:C:479:PHE:HD2	1.97	0.46
5:E:44:THR:HG22	6:E:501:ATP:O3A	2.16	0.46
2:B:309:PHE:CE2	3:C:330:LEU:HD11	2.51	0.46
3:C:306:VAL:O	3:C:310:LEU:HD13	2.15	0.46
3:C:381:SER:C	3:C:384:GLN:HG2	2.36	0.46
3:C:497:PHE:CE1	3:C:557:VAL:CG1	2.98	0.46
3:C:695:LYS:HD2	3:C:707:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:371:SER:O	3:C:575:PRO:HB3	2.15	0.46
3:C:419:LEU:HD23	3:C:438:LEU:HD23	1.97	0.46
2:B:324:GLU:O	2:B:328:THR:HG23	2.16	0.45
2:B:355:ILE:HD11	2:B:388:LEU:HD21	1.98	0.45
3:C:319:PHE:HE2	5:E:303:PRO:CD	2.27	0.45
1:A:631:ASP:OD1	1:A:632:ILE:N	2.49	0.45
3:C:148:LEU:HG	3:C:233:PHE:HE1	1.82	0.45
3:C:348:LEU:CD2	3:C:403:GLU:HA	2.46	0.45
4:D:66:ILE:O	4:D:217:LEU:HA	2.16	0.45
2:B:348:VAL:HG22	2:B:400:LEU:HD23	1.98	0.45
3:C:302:ILE:HG22	3:C:307:LEU:HG	1.98	0.45
3:C:572:GLU:O	3:C:573:THR:HG23	2.16	0.45
2:B:320:ARG:HH22	2:B:457:GLU:HG3	1.82	0.45
2:B:355:ILE:HG23	2:B:356:THR:N	2.31	0.45
3:C:125:LEU:HB3	3:C:133:VAL:HG11	1.97	0.45
2:B:325:ARG:HA	2:B:328:THR:OG1	2.15	0.45
3:C:229:VAL:HG13	3:C:233:PHE:CE2	2.49	0.45
3:C:341:LEU:HD21	3:C:365:ASN:HB3	1.99	0.45
3:C:636:LEU:O	3:C:639:GLU:N	2.49	0.45
3:C:42:LEU:HD13	3:C:354:ARG:NH1	2.32	0.45
3:C:148:LEU:HA	3:C:151:LEU:HD22	1.99	0.45
3:C:414:LEU:HD13	3:C:494:ILE:HD11	1.99	0.45
5:E:41:SER:OG	5:E:43:LYS:HE2	2.17	0.45
1:A:541:THR:HG22	6:A:901:ATP:O3A	2.17	0.45
3:C:151:LEU:HG	3:C:198:LYS:CD	2.46	0.45
3:C:497:PHE:HB3	3:C:501:PHE:HE2	1.82	0.45
3:C:709:TRP:NE1	5:E:360:ASP:OD1	2.43	0.45
2:B:340:ASN:HB2	2:B:343:PHE:CG	2.52	0.44
2:B:433:TRP:HB3	2:B:438:GLN:HG3	1.99	0.44
2:B:569:PHE:CE2	2:B:573[A]:GLU:HG3	2.52	0.44
3:C:216:VAL:HG11	3:C:249:ILE:CD1	2.47	0.44
3:C:254:THR:HB	3:C:258:ILE:HD12	1.99	0.44
2:B:335:ILE:CG2	2:B:388:LEU:HB2	2.47	0.44
3:C:44:PHE:HZ	3:C:337:TYR:CE1	2.35	0.44
3:C:50:ILE:O	3:C:53:GLN:HB2	2.17	0.44
3:C:384:GLN:O	3:C:387:LEU:HB2	2.16	0.44
3:C:587:ALA:O	3:C:591:HIS:CD2	2.71	0.44
3:C:597:ARG:CZ	3:C:708:THR:OG1	2.65	0.44
3:C:50:ILE:HG12	3:C:298:PHE:CD1	2.52	0.44
3:C:67:LYS:O	3:C:71:ASP:HB2	2.18	0.44
3:C:709:TRP:CZ3	5:E:364:ALA:CA	2.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:LYS:HD2	3:C:244:PHE:CD1	2.52	0.44
3:C:268:SER:HA	3:C:271:LEU:HD12	1.99	0.44
3:C:373:ARG:O	3:C:377:GLU:HG3	2.18	0.44
2:B:400:LEU:HD22	2:B:409:ILE:HD11	1.98	0.44
3:C:128:ASN:O	3:C:129:VAL:HB	2.17	0.44
3:C:134:VAL:HG13	3:C:154:GLN:CB	2.48	0.44
3:C:234:ILE:HD13	3:C:267:VAL:HG13	2.00	0.44
3:C:405:LEU:HD11	3:C:576:LEU:HB2	2.00	0.44
2:B:369:ILE:HA	2:B:372:GLN:CG	2.47	0.44
3:C:122:THR:HA	3:C:133:VAL:HG23	1.98	0.44
3:C:199:MET:CE	3:C:244:PHE:CE2	3.01	0.44
3:C:443:LEU:HA	3:C:570:PRO:HD3	1.99	0.44
2:B:323:LEU:HD12	2:B:393:HIS:CE1	2.53	0.44
3:C:138:ALA:O	3:C:141:CYS:HB2	2.17	0.44
3:C:144:MET:SD	3:C:233:PHE:CE2	3.11	0.44
3:C:152:ILE:CG2	3:C:198:LYS:N	2.81	0.44
3:C:415:VAL:HG12	3:C:567:TYR:CE1	2.52	0.44
3:C:694:ILE:HD13	3:C:704:VAL:HG22	2.00	0.44
3:C:144:MET:HE3	3:C:233:PHE:CE1	2.53	0.44
3:C:250:PHE:HB3	3:C:252:ILE:CD1	2.48	0.44
3:C:423:THR:HG21	3:C:438:LEU:HD21	2.00	0.44
3:C:563:LEU:HA	3:C:567:TYR:HD2	1.83	0.44
3:C:134:VAL:O	3:C:218:ILE:HD12	2.18	0.44
3:C:335:HIS:HB2	3:C:582:PHE:CG	2.53	0.44
3:C:415:VAL:HG12	3:C:567:TYR:CE2	2.53	0.44
2:B:339:ILE:HG21	2:B:351:VAL:HG22	1.99	0.43
2:B:369:ILE:HA	2:B:372:GLN:CD	2.38	0.43
2:B:396:ASP:O	2:B:401:ARG:NE	2.51	0.43
3:C:72:ASN:HA	3:C:75:GLU:HB2	1.99	0.43
3:C:104:ALA:HA	3:C:250:PHE:CD2	2.50	0.43
3:C:147:PHE:CE1	3:C:225:PHE:CE1	3.06	0.43
3:C:279:LEU:HD22	3:C:283:GLU:OE1	2.18	0.43
3:C:557:VAL:HG22	3:C:561:ASP:OD2	2.17	0.43
3:C:125:LEU:HB3	3:C:131:PRO:HG2	2.00	0.43
3:C:217:VAL:HG12	3:C:219:LEU:HD21	2.00	0.43
3:C:239:GLN:NE2	5:E:64:VAL:CG1	2.76	0.43
3:C:476:PHE:HB3	3:C:480:LYS:CE	2.49	0.43
3:C:649:TRP:O	3:C:653:PHE:HB3	2.18	0.43
3:C:697:THR:HG21	3:C:705:ALA:HB3	2.00	0.43
2:B:295:GLU:HA	2:B:298:PHE:CD2	2.54	0.43
3:C:70:PHE:HA	3:C:73:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:HIS:CE1	3:C:214:PRO:HG3	2.53	0.43
3:C:139:LYS:C	3:C:141:CYS:H	2.21	0.43
3:C:286:THR:HG21	3:C:434:GLN:NE2	2.33	0.43
3:C:694:ILE:CG1	3:C:704:VAL:HG13	2.49	0.43
1:A:690:LEU:CD2	1:A:726:CYS:SG	3.06	0.43
3:C:71:ASP:O	3:C:75:GLU:HB2	2.18	0.43
3:C:421:LYS:HE3	3:C:479:PHE:CE1	2.54	0.43
3:C:647:VAL:O	3:C:651:GLU:HB2	2.18	0.43
3:C:683:ARG:NE	3:C:683:ARG:HA	2.32	0.43
5:E:412:SER:CB	5:E:413:LEU:HA	2.47	0.43
2:B:319:LYS:HE3	2:B:423:SER:HB2	2.00	0.43
2:B:347:SER:N	2:B:350:SER:OG	2.49	0.43
2:B:400:LEU:HD22	2:B:409:ILE:CD1	2.48	0.43
3:C:43:ARG:O	3:C:46:THR:OG1	2.35	0.43
3:C:419:LEU:HD22	3:C:567:TYR:CE1	2.53	0.43
3:C:425:SER:OG	3:C:471:ILE:HD13	2.18	0.43
3:C:646:LEU:HD12	3:C:702:ASP:HB3	2.00	0.43
3:C:461:ARG:HG2	3:C:552:LEU:HD21	2.01	0.43
4:D:223:PHE:HB3	4:D:224:PRO:HD3	2.01	0.43
1:A:794:THR:HA	1:A:843:LEU:O	2.19	0.43
2:B:339:ILE:CD1	2:B:351:VAL:HG13	2.49	0.43
2:B:377:VAL:HG13	2:B:381:LYS:HG3	2.01	0.43
2:B:379:LYS:O	2:B:383:ASP:HB2	2.18	0.43
3:C:74:ILE:O	3:C:78:GLN:HB2	2.18	0.43
3:C:354:ARG:O	3:C:358:LEU:HG	2.19	0.43
3:C:478:VAL:HA	3:C:481:SER:HB3	2.01	0.43
3:C:497:PHE:CE1	3:C:557:VAL:HG13	2.53	0.43
1:A:566:ILE:HG23	1:A:586:LYS:HG3	2.00	0.43
2:B:311:ILE:CG1	2:B:421:ILE:HG12	2.45	0.43
3:C:427:PRO:C	3:C:429:TYR:H	2.22	0.43
3:C:564:VAL:O	3:C:568:LEU:HD21	2.18	0.43
3:C:100:ILE:HD11	3:C:237:SER:CB	2.48	0.43
3:C:150:LYS:O	3:C:154:GLN:CG	2.66	0.43
3:C:371:SER:O	3:C:575:PRO:HA	2.19	0.43
3:C:476:PHE:CD1	3:C:480:LYS:HE3	2.53	0.43
2:B:362:HIS:HB3	2:B:379:LYS:NZ	2.34	0.43
2:B:427:LEU:HD21	3:C:693:PHE:CZ	2.53	0.43
3:C:191:VAL:HG12	3:C:191:VAL:O	2.19	0.43
3:C:355:ILE:O	3:C:395:LYS:HE3	2.19	0.43
3:C:569:LEU:HB3	3:C:570:PRO:HD2	2.01	0.43
3:C:632:ILE:O	3:C:636:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:GLN:OE1	4:D:43:GLN:N	2.42	0.43
3:C:467:GLU:HG2	3:C:471:ILE:HD12	2.00	0.42
2:B:331:LEU:O	2:B:336:HIS:NE2	2.52	0.42
3:C:238:SER:HA	3:C:241:LEU:CD1	2.49	0.42
3:C:372:PHE:CE2	3:C:376:VAL:HG21	2.54	0.42
4:D:203:GLU:OE2	4:D:205:ARG:NH1	2.44	0.42
2:B:327:ARG:HA	2:B:331:LEU:HD12	2.00	0.42
3:C:234:ILE:HD13	3:C:267:VAL:CG1	2.50	0.42
3:C:312:ASN:O	3:C:316:TYR:HB2	2.18	0.42
3:C:421:LYS:HZ3	3:C:478:VAL:HB	1.85	0.42
3:C:562:CYS:HB3	3:C:567:TYR:CE2	2.54	0.42
3:C:649:TRP:HZ3	3:C:704:VAL:HB	1.84	0.42
5:E:311:ILE:HG23	5:E:419:ILE:HG21	1.99	0.42
2:B:318:SER:HB2	2:B:457:GLU:OE1	2.19	0.42
2:B:390:LEU:CD2	2:B:418:ILE:HD12	2.50	0.42
3:C:202:LYS:HE3	3:C:215:VAL:HG21	2.01	0.42
3:C:263:LEU:CD1	3:C:271:LEU:HD11	2.50	0.42
3:C:319:PHE:CZ	5:E:303:PRO:HA	2.41	0.42
3:C:370:PRO:C	3:C:372:PHE:H	2.23	0.42
3:C:563:LEU:HA	3:C:567:TYR:CD2	2.54	0.42
3:C:44:PHE:HZ	3:C:337:TYR:CZ	2.38	0.42
3:C:557:VAL:O	3:C:561:ASP:HB2	2.19	0.42
4:D:111:LEU:HD21	4:D:135:ASN:ND2	2.35	0.42
4:D:418:TYR:HB3	4:D:421:CYS:HB2	2.00	0.42
2:B:373:LEU:CD2	2:B:412:LEU:HD21	2.47	0.42
3:C:43:ARG:HH11	3:C:336:PHE:C	2.23	0.42
3:C:363:CYS:SG	3:C:391:GLU:CD	2.98	0.42
3:C:474:LYS:O	3:C:478:VAL:HG23	2.20	0.42
3:C:41:LYS:HD2	3:C:44:PHE:HE2	1.85	0.42
3:C:310:LEU:O	3:C:313:ILE:N	2.52	0.42
3:C:367:ARG:NE	3:C:388:LEU:O	2.52	0.42
3:C:379:GLN:HB3	3:C:380:ALA:H	1.61	0.42
3:C:416:LEU:HD12	3:C:567:TYR:CD1	2.53	0.42
3:C:570:PRO:O	3:C:573:THR:OG1	2.26	0.42
1:A:582:GLN:O	1:A:586:LYS:HG2	2.19	0.42
1:A:817:SER:OG	5:E:163:GLU:OE2	2.32	0.42
2:B:398:GLN:CG	2:B:401:ARG:HG3	2.49	0.42
3:C:151:LEU:CG	3:C:198:LYS:HD2	2.47	0.42
3:C:202:LYS:CE	3:C:215:VAL:CG2	2.98	0.42
3:C:202:LYS:C	3:C:206:THR:O	2.58	0.42
3:C:332:LEU:HD23	3:C:336:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:416:LEU:HA	3:C:567:TYR:HE1	1.84	0.42
3:C:418:CYS:O	3:C:422:PHE:HD2	2.02	0.42
3:C:456:VAL:HA	3:C:459:LEU:HD12	2.02	0.42
5:E:311:ILE:HG21	5:E:419:ILE:CG2	2.49	0.42
5:E:311:ILE:HG21	5:E:419:ILE:HG21	2.02	0.42
1:A:499:ALA:HB3	1:A:727:ARG:HD3	2.02	0.42
3:C:305:LYS:O	3:C:309:VAL:HG23	2.20	0.42
3:C:314:PHE:HD2	3:C:324:PHE:HB2	1.85	0.42
3:C:342:SER:CB	3:C:579:VAL:CG1	2.98	0.42
3:C:387:LEU:HD23	3:C:394:LEU:HA	2.01	0.42
3:C:548:LYS:O	3:C:552:LEU:HG	2.20	0.42
1:A:714:ALA:O	1:A:715:LEU:HD23	2.19	0.42
2:B:355:ILE:O	2:B:359:VAL:HG23	2.20	0.42
3:C:81:HIS:NE2	3:C:214:PRO:HB3	2.35	0.42
3:C:386:ALA:HB1	3:C:393:TYR:CB	2.50	0.42
3:C:453:TYR:OH	3:C:563:LEU:HD13	2.19	0.42
4:D:51:LEU:HB3	4:D:84:LEU:HD22	2.02	0.42
2:B:336:HIS:HA	2:B:389:PHE:O	2.21	0.41
2:B:356:THR:OG1	2:B:365:THR:CG2	2.68	0.41
3:C:107:LEU:HD23	3:C:278:SER:HB2	2.00	0.41
3:C:219:LEU:HD13	3:C:222:MET:SD	2.59	0.41
3:C:420:HIS:CE1	3:C:435:ILE:HG23	2.55	0.41
2:B:397:SER:CB	2:B:400:LEU:H	2.32	0.41
3:C:62:GLN:O	3:C:66:ASN:CG	2.58	0.41
3:C:147:PHE:CE2	3:C:229:VAL:CG1	3.03	0.41
3:C:367:ARG:CZ	3:C:388:LEU:O	2.68	0.41
3:C:370:PRO:HA	3:C:373:ARG:HB2	2.02	0.41
3:C:408:TYR:HB3	3:C:412:TYR:HE2	1.84	0.41
3:C:75:GLU:O	3:C:79:LYS:HG3	2.20	0.41
3:C:448:TRP:CH2	3:C:559:PHE:HB3	2.55	0.41
3:C:686:SER:O	3:C:690:LEU:HG	2.20	0.41
2:B:304:GLN:OE1	2:B:446:TYR:OH	2.30	0.41
2:B:319:LYS:HE3	2:B:423:SER:CB	2.50	0.41
2:B:427:LEU:HD21	3:C:693:PHE:CE2	2.54	0.41
3:C:51:TRP:CH2	3:C:55:LYS:HE3	2.56	0.41
3:C:122:THR:HA	3:C:133:VAL:HG21	2.02	0.41
3:C:152:ILE:HD13	3:C:197:PRO:HD2	2.02	0.41
3:C:153:SER:O	3:C:157:ASP:CG	2.59	0.41
3:C:255:SER:CB	3:C:256:PRO:CD	2.99	0.41
3:C:501:PHE:CD1	3:C:554:GLU:OE2	2.73	0.41
3:C:569:LEU:CB	3:C:571:PRO:HD2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:604:LEU:CD1	3:C:693:PHE:CZ	3.03	0.41
1:A:830:ARG:HG3	4:D:197:ASP:HB3	2.01	0.41
2:B:388:LEU:O	2:B:418:ILE:HA	2.21	0.41
3:C:106:VAL:HG13	3:C:253:ALA:O	2.20	0.41
3:C:162:ILE:HG22	3:C:162:ILE:O	2.21	0.41
3:C:367:ARG:NH2	3:C:391:GLU:HG2	2.36	0.41
2:B:295:GLU:HA	2:B:298:PHE:CG	2.55	0.41
2:B:318:SER:HA	2:B:319:LYS:NZ	2.35	0.41
2:B:388:LEU:HB3	2:B:418:ILE:HG22	2.02	0.41
2:B:395:LEU:HD12	2:B:400:LEU:HD13	2.02	0.41
3:C:97:LEU:HA	3:C:242:HIS:CG	2.55	0.41
3:C:402:LEU:HD21	3:C:576:LEU:HD13	2.02	0.41
3:C:578:GLU:O	3:C:579:VAL:HB	2.21	0.41
2:B:320:ARG:NH2	2:B:342:PHE:CZ	2.85	0.41
2:B:331:LEU:HD11	2:B:391:LEU:CG	2.51	0.41
2:B:552:ASP:N	2:B:552:ASP:OD1	2.47	0.41
3:C:106:VAL:O	3:C:278:SER:HB2	2.20	0.41
3:C:152:ILE:CD1	3:C:195:THR:C	2.88	0.41
3:C:222:MET:HG3	3:C:250:PHE:HD1	1.84	0.41
3:C:342:SER:O	3:C:345:CYS:CB	2.68	0.41
3:C:352:LYS:HG2	3:C:355:ILE:HD12	2.02	0.41
5:E:103:VAL:O	5:E:107:LYS:N	2.42	0.41
1:A:721:ARG:HH12	4:D:213:ARG:NH1	2.19	0.41
2:B:300:LYS:HE3	3:C:337:TYR:CD1	2.56	0.41
2:B:397:SER:HB3	2:B:400:LEU:HD12	2.02	0.41
3:C:100:ILE:HD11	3:C:237:SER:HB2	2.02	0.41
3:C:135:SER:HB2	3:C:220:LYS:HE3	2.02	0.41
3:C:152:ILE:HD12	3:C:194:LYS:O	2.20	0.41
3:C:209:GLN:OE1	3:C:211:GLN:O	2.39	0.41
3:C:497:PHE:O	3:C:500:GLN:HB2	2.21	0.41
3:C:555:ASN:O	3:C:558:ASN:N	2.54	0.41
3:C:694:ILE:CD1	3:C:704:VAL:HG13	2.48	0.41
1:A:504:LEU:HB3	1:A:505:PRO:CD	2.51	0.41
1:A:849:VAL:HG12	1:A:853:ASP:HB2	2.03	0.41
2:B:318:SER:HB2	2:B:454:TYR:H	1.86	0.41
2:B:320:ARG:NE	2:B:456:GLU:HB2	2.36	0.41
2:B:332:GLN:O	2:B:336:HIS:HD2	2.03	0.41
2:B:420:LEU:HD21	2:B:443:TRP:HH2	1.86	0.41
2:B:445:TRP:CE2	3:C:594:ALA:HB2	2.55	0.41
3:C:59:GLU:O	3:C:63:GLU:HG3	2.20	0.41
3:C:100:ILE:CG1	3:C:241:LEU:HD11	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:GLN:HB3	3:C:162:ILE:CD1	2.51	0.41
3:C:152:ILE:CG1	3:C:198:LYS:H	2.34	0.41
3:C:199:MET:CE	3:C:243:GLU:OE1	2.69	0.41
3:C:199:MET:HG2	3:C:244:PHE:HE2	1.85	0.41
3:C:266:ALA:O	3:C:270:LEU:HG	2.21	0.41
3:C:421:LYS:HB2	3:C:479:PHE:CZ	2.56	0.41
3:C:552:LEU:O	3:C:556:VAL:CG2	2.69	0.41
3:C:641:SER:OG	3:C:642:ARG:N	2.51	0.41
3:C:695:LYS:O	3:C:697:THR:HG23	2.21	0.41
3:C:700:LYS:HB3	3:C:703:HIS:CE1	2.56	0.41
4:D:163:LEU:O	4:D:167:HIS:CE1	2.74	0.41
4:D:326:ILE:HD11	4:D:418:TYR:CE1	2.56	0.41
5:E:45:TYR:HB2	6:E:501:ATP:H5'2	2.03	0.41
5:E:51:LEU:O	5:E:55:GLU:HG3	2.21	0.41
5:E:124:LEU:HD12	5:E:156:PHE:CE1	2.56	0.41
5:E:308:PHE:CE1	5:E:423:VAL:HG11	2.55	0.41
1:A:535:VAL:CG1	1:A:536:PRO:HD2	2.51	0.41
3:C:76:PHE:HE2	3:C:103:ALA:HB2	1.86	0.41
3:C:155:LEU:HD12	3:C:198:LYS:HD3	2.03	0.41
3:C:199:MET:HE1	3:C:243:GLU:OE1	2.21	0.41
3:C:283:GLU:O	3:C:287:THR:HG23	2.20	0.41
3:C:370:PRO:O	3:C:371:SER:OG	2.35	0.41
3:C:426:LEU:HD21	3:C:460:LEU:HG	2.02	0.41
3:C:476:PHE:CE2	3:C:501:PHE:CG	3.09	0.41
3:C:685:VAL:O	3:C:689:GLU:HG3	2.21	0.41
1:A:580:TYR:HE2	1:A:632:ILE:HG22	1.86	0.40
2:B:390:LEU:HD23	2:B:418:ILE:HD12	2.03	0.40
3:C:69:LEU:HD22	3:C:277:GLN:O	2.20	0.40
3:C:257:ILE:HG22	3:C:261:ARG:NE	2.36	0.40
3:C:306:VAL:O	3:C:310:LEU:HB2	2.21	0.40
3:C:394:LEU:O	3:C:395:LYS:C	2.60	0.40
3:C:419:LEU:HB2	3:C:567:TYR:OH	2.21	0.40
3:C:589:ARG:O	3:C:593:ASN:HB2	2.21	0.40
1:A:621:GLU:HG2	4:D:205:ARG:HE	1.86	0.40
2:B:478:THR:HG21	3:C:701:THR:CG2	2.51	0.40
3:C:69:LEU:HD13	3:C:278:SER:HA	2.03	0.40
3:C:144:MET:HE3	3:C:233:PHE:CZ	2.55	0.40
3:C:282:LYS:O	3:C:286:THR:HG23	2.21	0.40
3:C:341:LEU:HD21	3:C:365:ASN:HB2	2.03	0.40
3:C:564:VAL:O	3:C:568:LEU:HD11	2.21	0.40
3:C:695:LYS:HG3	3:C:696:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:8:VAL:HG22	5:E:45:TYR:CE2	2.56	0.40
5:E:45:TYR:HB2	6:E:501:ATP:C5'	2.52	0.40
5:E:222:LEU:HD23	6:E:501:ATP:C8	2.56	0.40
2:B:420:LEU:HD21	2:B:443:TRP:CH2	2.56	0.40
3:C:147:PHE:CE1	3:C:225:PHE:CZ	3.07	0.40
3:C:203:LYS:HA	3:C:207:SER:HA	2.03	0.40
3:C:332:LEU:HD23	3:C:336:PHE:HD2	1.86	0.40
3:C:371:SER:OG	3:C:576:LEU:N	2.53	0.40
3:C:494:ILE:HA	3:C:497:PHE:CD2	2.55	0.40
1:A:500:VAL:CB	1:A:501:PRO:HD3	2.50	0.40
2:B:310:ASN:HB3	2:B:420:LEU:O	2.22	0.40
2:B:320:ARG:NH2	2:B:457:GLU:HG3	2.36	0.40
2:B:326:PHE:CE2	2:B:421:ILE:CD1	3.04	0.40
3:C:97:LEU:HD23	3:C:242:HIS:CG	2.56	0.40
3:C:118:PHE:HB3	3:C:220:LYS:HE2	2.02	0.40
3:C:238:SER:HA	3:C:241:LEU:HG	2.02	0.40
3:C:313:ILE:HG12	3:C:318:ASP:OD1	2.22	0.40
3:C:418:CYS:CA	3:C:479:PHE:CZ	3.03	0.40
3:C:419:LEU:HB2	3:C:567:TYR:CZ	2.57	0.40
3:C:570:PRO:CD	3:C:571:PRO:HD3	2.52	0.40
3:C:128:ASN:C	3:C:130:THR:H	2.25	0.40
3:C:423:THR:CG2	3:C:438:LEU:HD21	2.51	0.40
3:C:657:VAL:HG12	3:C:677:ILE:HD11	2.03	0.40
5:E:416:ILE:HG23	5:E:417:ARG:N	2.37	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	327/522 (63%)	315 (96%)	12 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	287/347 (83%)	266 (93%)	21 (7%)	0	100	100
3	C	541/712 (76%)	462 (85%)	70 (13%)	9 (2%)	9	42
4	D	386/436 (88%)	372 (96%)	14 (4%)	0	100	100
5	E	347/435 (80%)	320 (92%)	22 (6%)	5 (1%)	11	46
All	All	1888/2452 (77%)	1735 (92%)	139 (7%)	14 (1%)	26	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	129	VAL
3	C	130	THR
3	C	382	GLU
5	E	320	PRO
5	E	412	SER
3	C	190	THR
3	C	579	VAL
3	C	640	CYS
3	C	131	PRO
5	E	407	TYR
5	E	424	ASN
3	C	379	GLN
5	E	405	PRO
3	C	570	PRO

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	298/454 (66%)	295 (99%)	3 (1%)	76	86
2	B	266/323 (82%)	258 (97%)	8 (3%)	41	63
3	C	517/659 (78%)	504 (98%)	13 (2%)	47	68
4	D	363/403 (90%)	359 (99%)	4 (1%)	73	84
5	E	289/399 (72%)	283 (98%)	6 (2%)	53	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1733/2238 (77%)	1699 (98%)	34 (2%)	57 74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	SER
1	A	622	LEU
1	A	683	TYR
2	B	388	LEU
2	B	418	ILE
2	B	423	SER
2	B	442	ASN
2	B	457	GLU
2	B	509	ILE
2	B	526	VAL
2	B	541	ASP
3	C	199	MET
3	C	225	PHE
3	C	248	LEU
3	C	272	CYS
3	C	325	ILE
3	C	342	SER
3	C	381	SER
3	C	394	LEU
3	C	457	LEU
3	C	570	PRO
3	C	683	ARG
3	C	704	VAL
3	C	706	ARG
4	D	167	HIS
4	D	245	PHE
4	D	358	GLN
4	D	362	HIS
5	E	356	PRO
5	E	358	PRO
5	E	376	PRO
5	E	387	LEU
5	E	396	VAL
5	E	405	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	239	GLN
4	D	347	GLN
4	D	351	ASN
5	E	383	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
6	ATP	A	901	7	26,33,33	0.95	2 (7%)	31,52,52	1.72	6 (19%)
6	ATP	E	501	-	26,33,33	0.95	1 (3%)	31,52,52	1.69	6 (19%)
6	ATP	D	901	7	26,33,33	0.93	1 (3%)	31,52,52	1.64	4 (12%)

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
6	ATP	A	901	7	-	6/18/38/38	0/3/3/3
6	ATP	E	501	-	-	3/18/38/38	0/3/3/3
6	ATP	D	901	7	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	501	ATP	C5-C4	2.50	1.47	1.40
6	D	901	ATP	C5-C4	2.40	1.47	1.40
6	A	901	ATP	C5-C4	2.34	1.47	1.40
6	A	901	ATP	O4'-C1'	2.03	1.43	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	901	ATP	PA-O3A-PB	-4.27	118.18	132.83
6	A	901	ATP	PB-O3B-PG	-4.24	118.28	132.83
6	E	501	ATP	PA-O3A-PB	-4.07	118.86	132.83
6	D	901	ATP	PB-O3B-PG	-4.00	119.11	132.83
6	A	901	ATP	N3-C2-N1	-3.95	122.51	128.68
6	E	501	ATP	N3-C2-N1	-3.90	122.58	128.68
6	D	901	ATP	N3-C2-N1	-3.84	122.67	128.68
6	A	901	ATP	C3'-C2'-C1'	3.40	106.09	100.98
6	E	501	ATP	PB-O3B-PG	-3.31	121.46	132.83
6	A	901	ATP	PA-O3A-PB	-3.29	121.55	132.83
6	D	901	ATP	C3'-C2'-C1'	2.58	104.86	100.98
6	E	501	ATP	C3'-C2'-C1'	2.47	104.70	100.98
6	E	501	ATP	C4-C5-N7	-2.45	106.85	109.40
6	A	901	ATP	C2'-C3'-C4'	2.21	106.94	102.64
6	A	901	ATP	O3G-PG-O2G	2.14	115.80	107.64
6	E	501	ATP	C2-N1-C6	2.01	122.18	118.75

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	901	ATP	PB-O3B-PG-O2G
6	D	901	ATP	C5'-O5'-PA-O3A
6	E	501	ATP	C5'-O5'-PA-O3A
6	A	901	ATP	C3'-C4'-C5'-O5'
6	D	901	ATP	O4'-C4'-C5'-O5'

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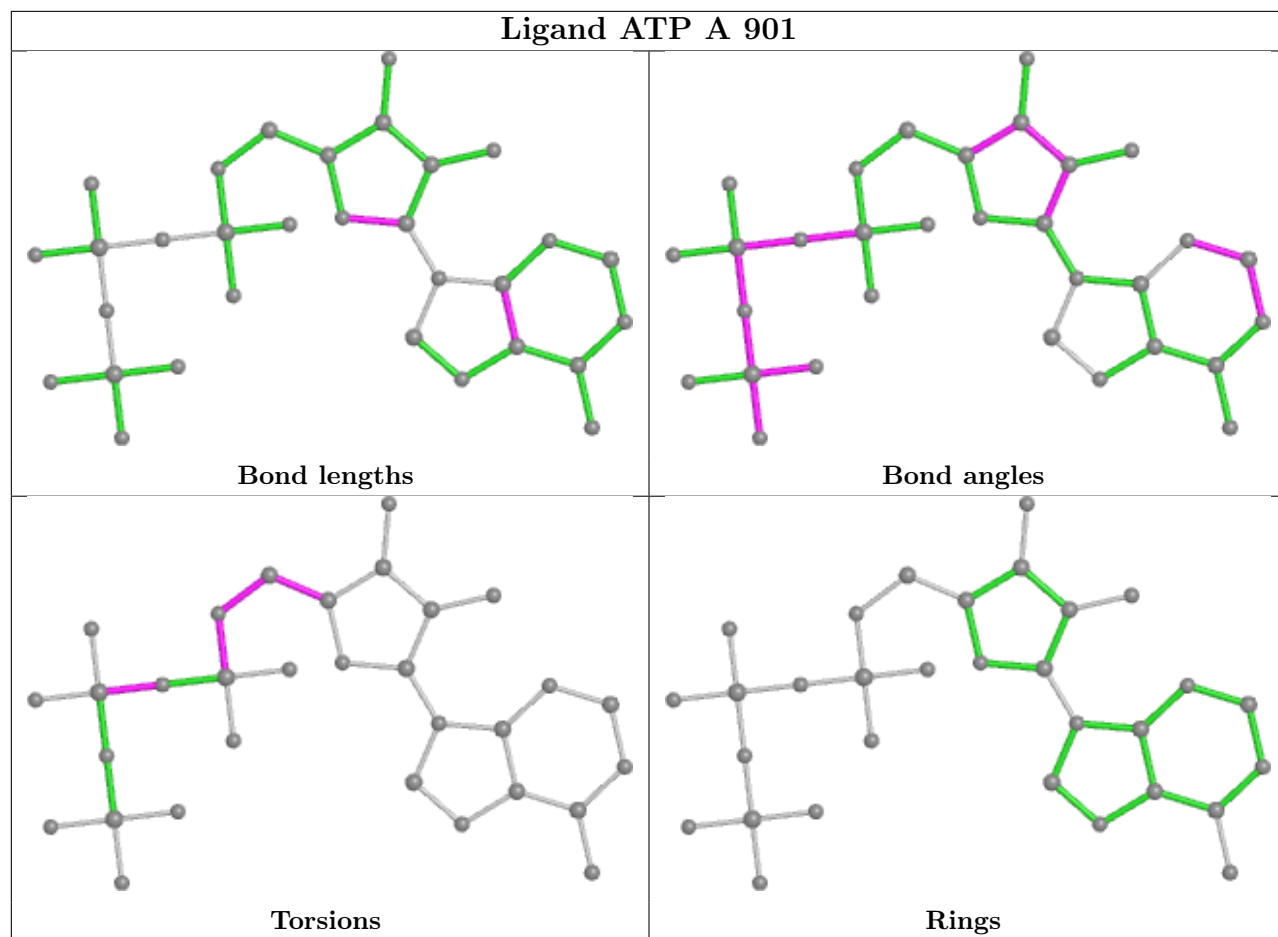
Mol	Chain	Res	Type	Atoms
6	E	501	ATP	C3'-C4'-C5'-O5'
6	A	901	ATP	C5'-O5'-PA-O2A
6	D	901	ATP	C5'-O5'-PA-O1A
6	D	901	ATP	C5'-O5'-PA-O2A
6	E	501	ATP	C5'-O5'-PA-O1A
6	A	901	ATP	O4'-C4'-C5'-O5'
6	A	901	ATP	PA-O3A-PB-O2B
6	D	901	ATP	PB-O3B-PG-O3G
6	A	901	ATP	C5'-O5'-PA-O3A
6	A	901	ATP	C4'-C5'-O5'-PA

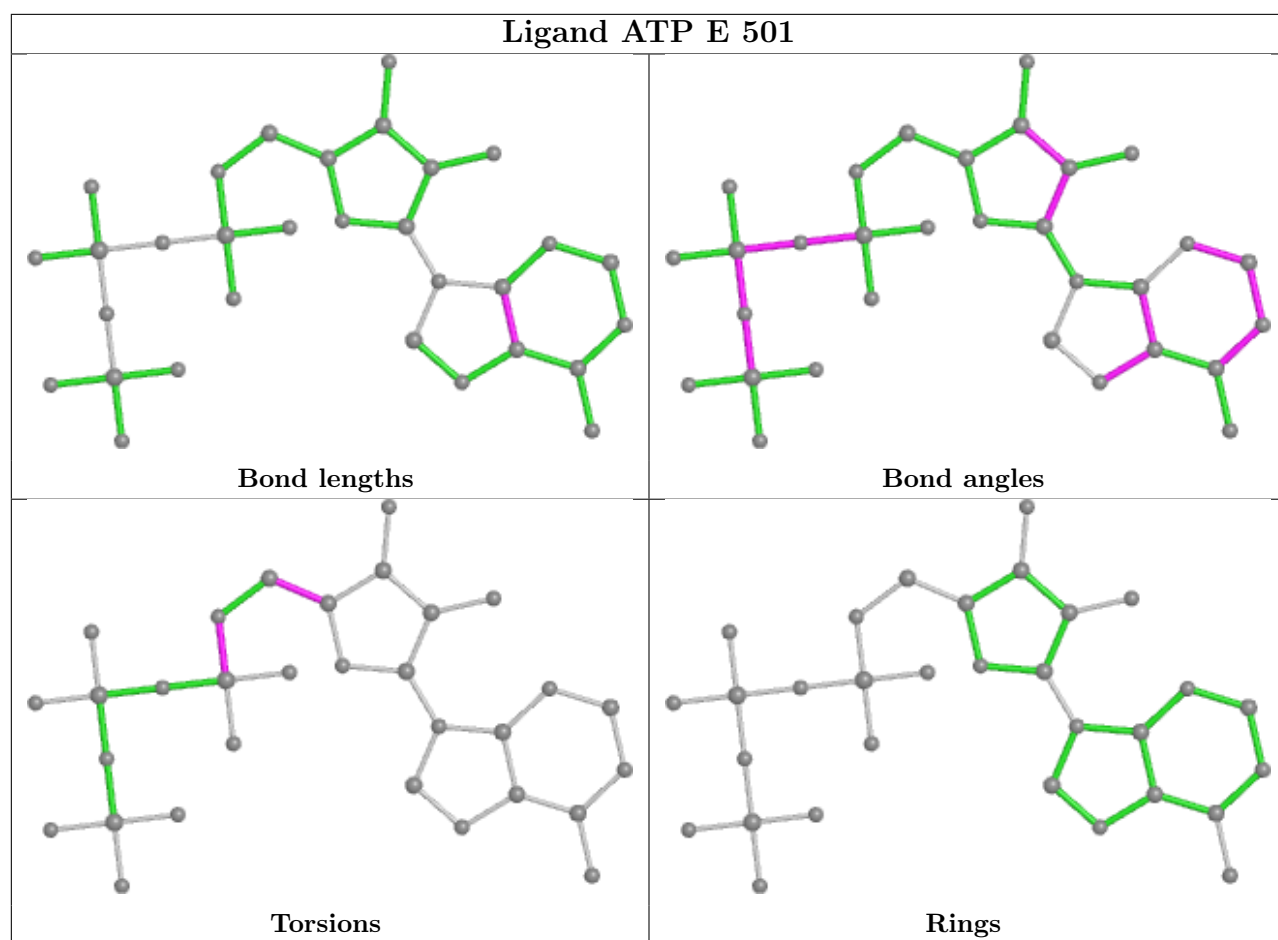
There are no ring outliers.

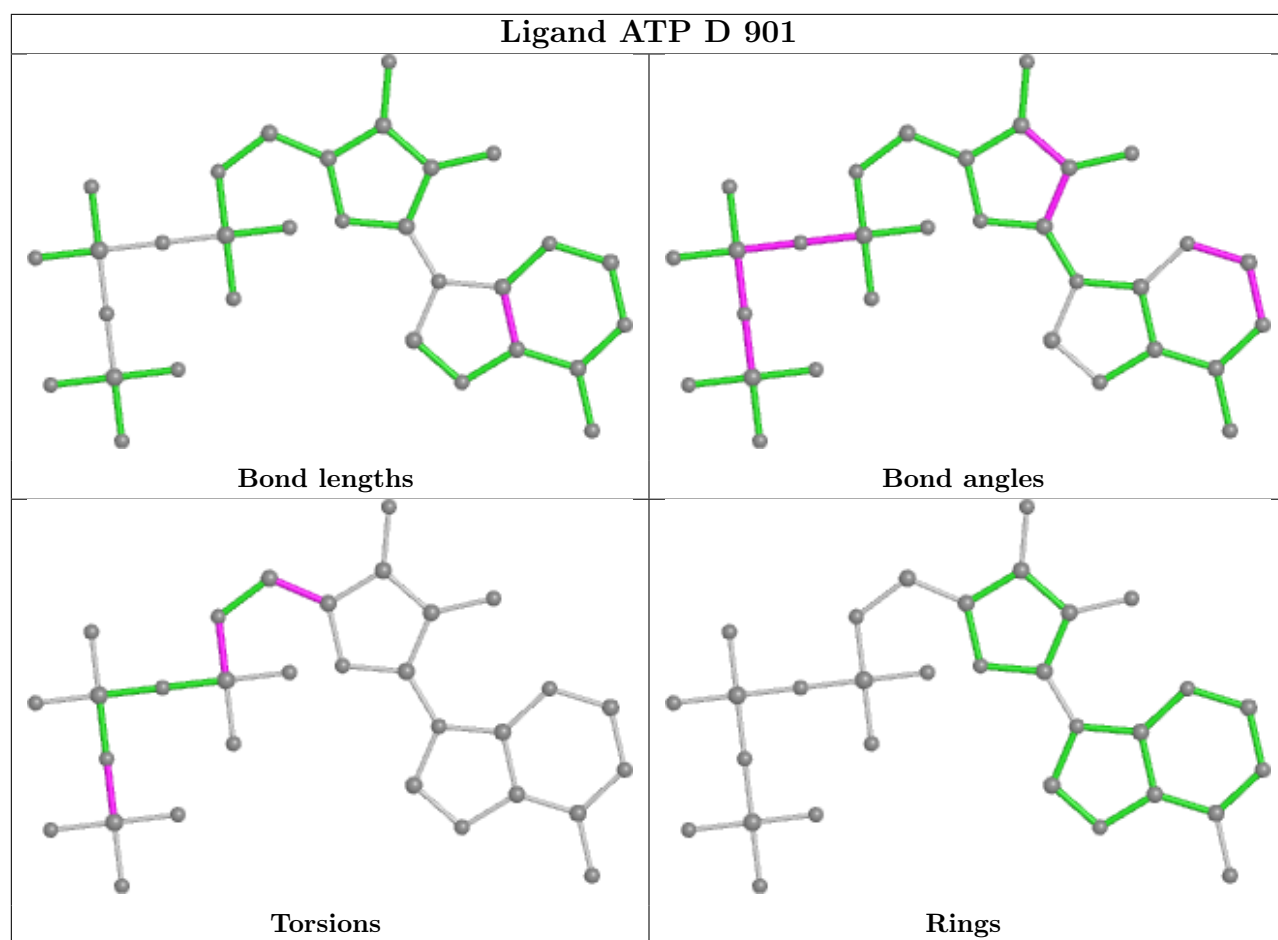
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	901	ATP	2	0
6	E	501	ATP	4	0
6	D	901	ATP	3	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.

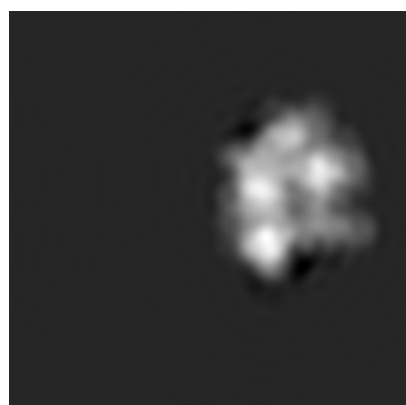
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8541. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

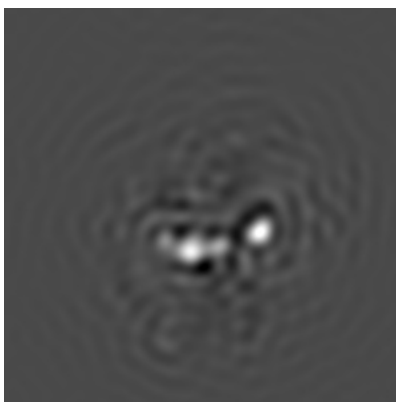
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

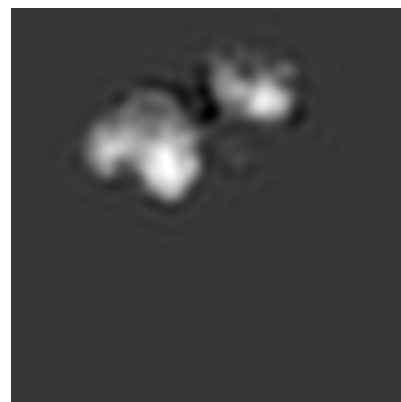
6.2.1 Primary map



X Index: 32



Y Index: 32



Z Index: 32

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: 26



Y Index: 41



Z Index: 38

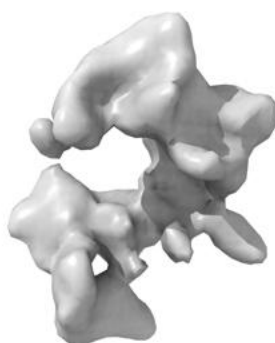
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

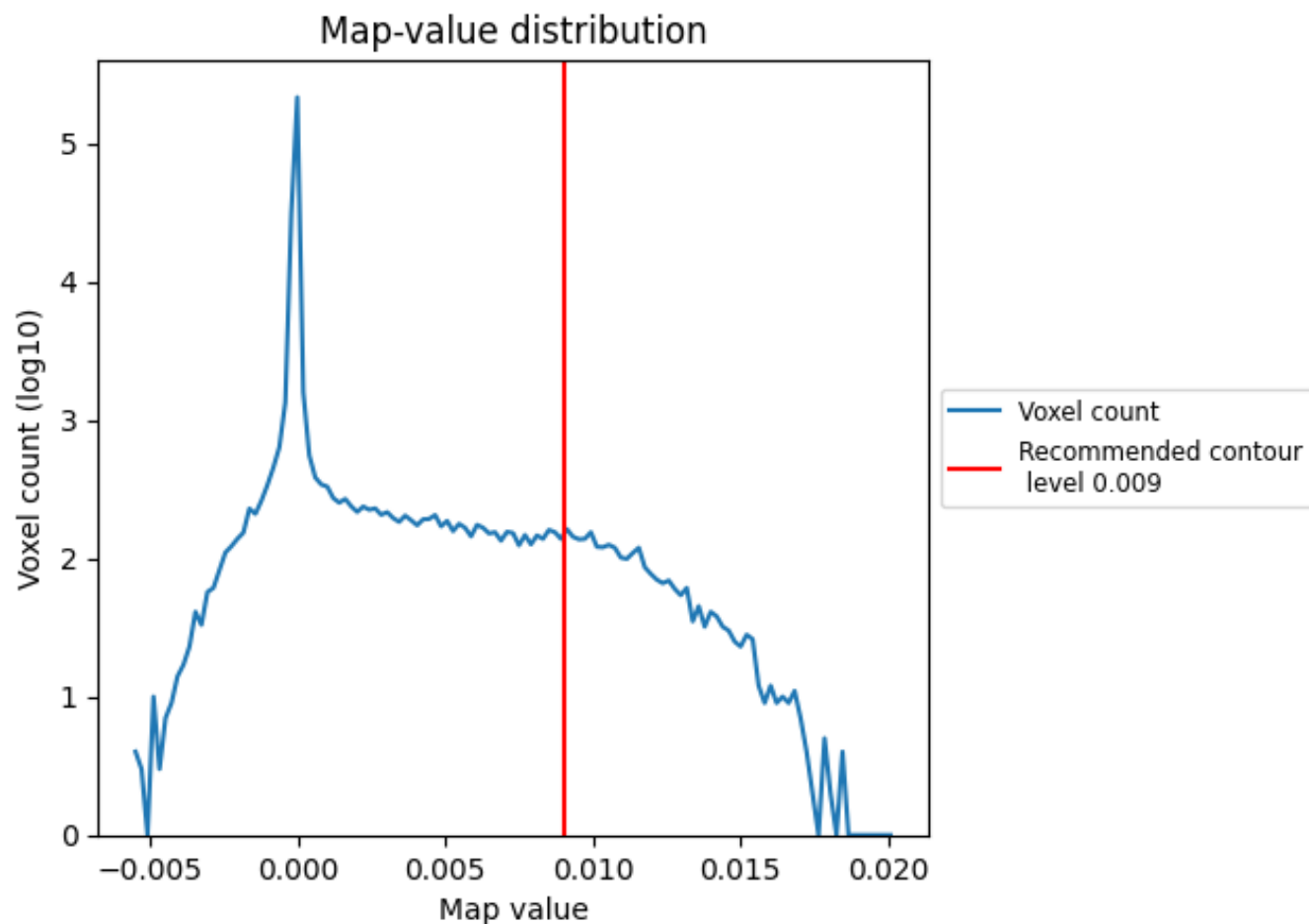
6.5 Mask visualisation

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

7 Map analysis [i](#)

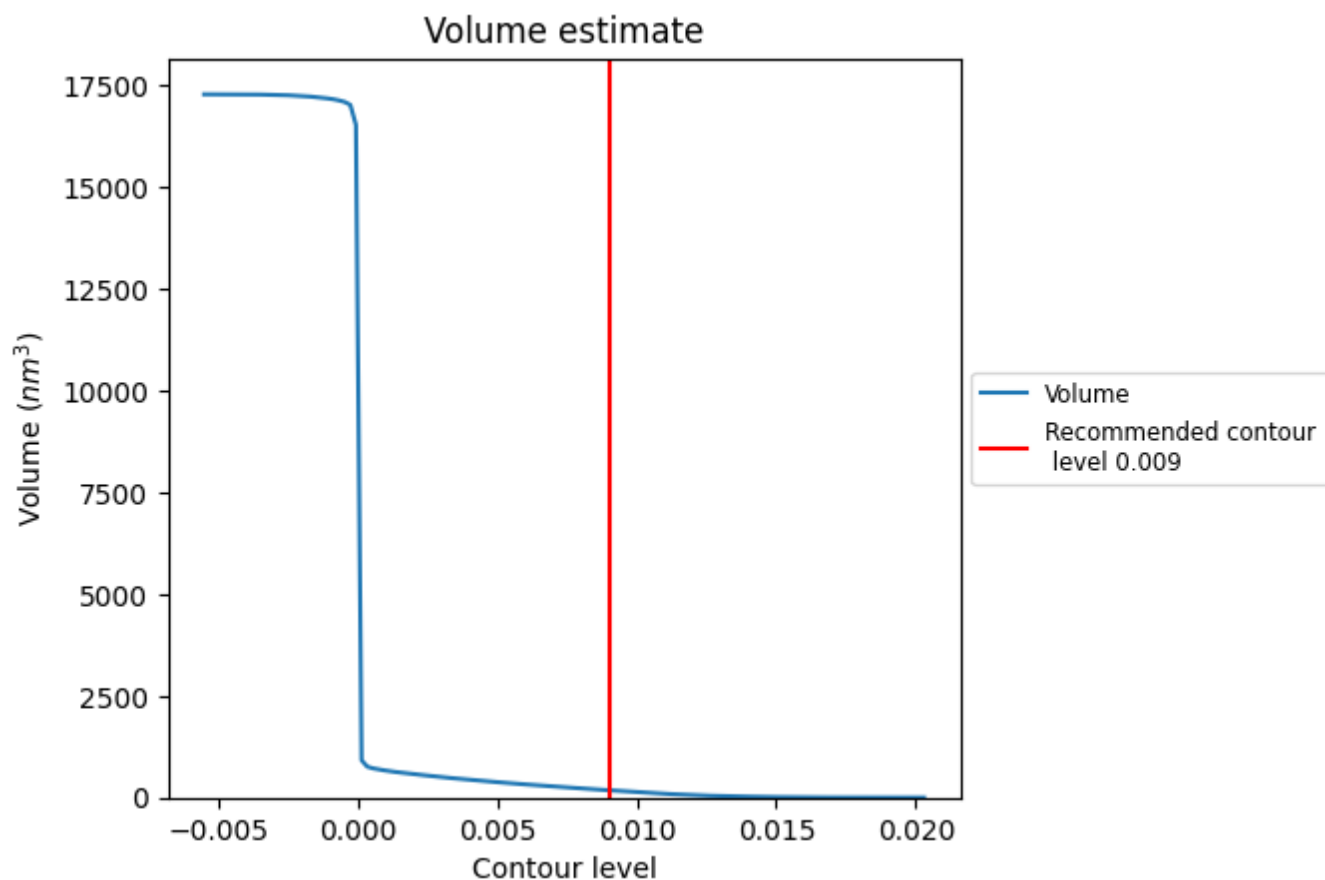
This section contains the results of statistical analysis of the map.

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.

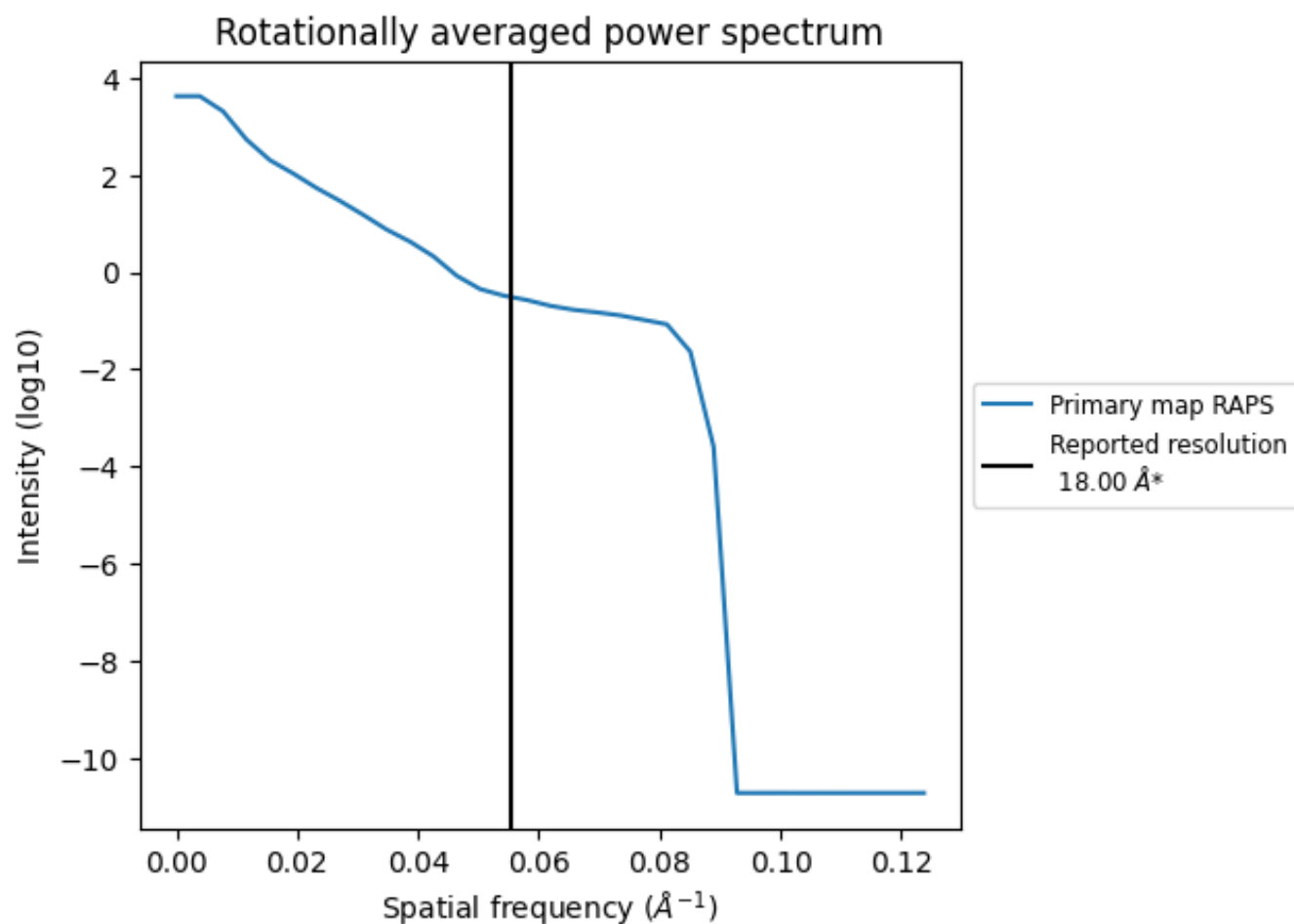
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 180 nm³; this corresponds to an approximate mass of 163 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 0.056 Å⁻¹

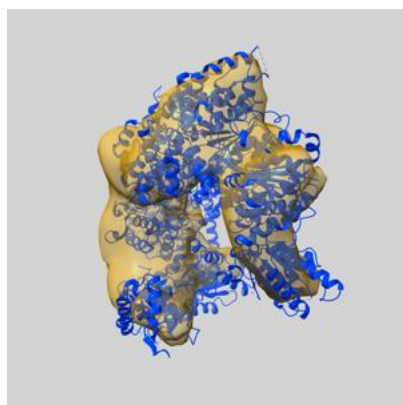
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

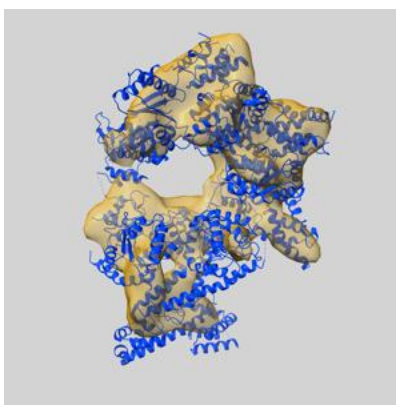
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8541 and PDB model 5UJM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

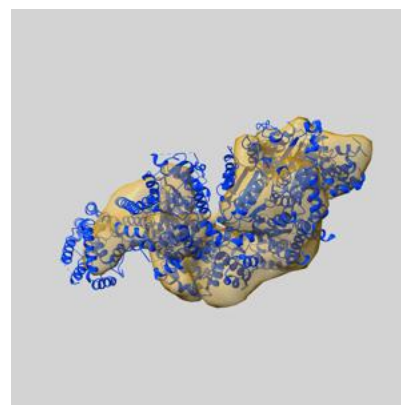
9.1 Map-model overlay [i](#)



X



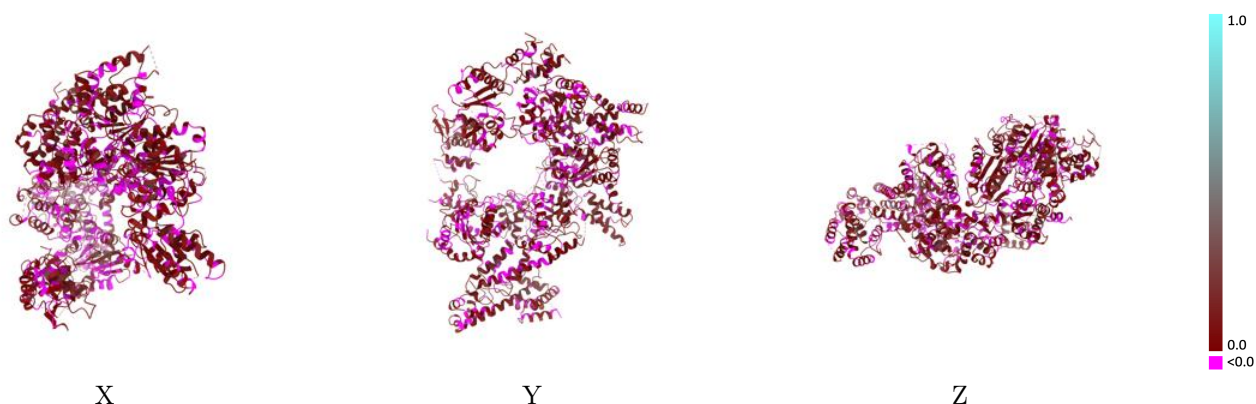
Y



Z

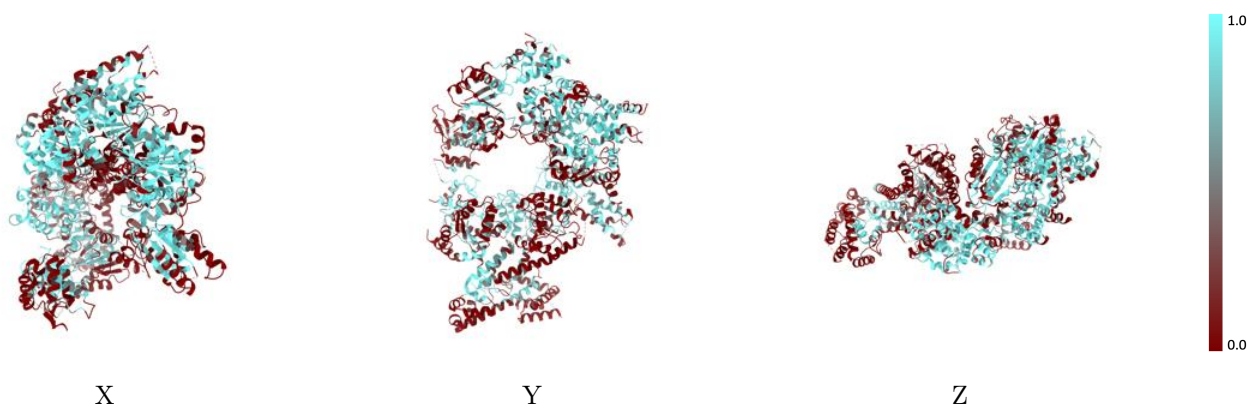
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



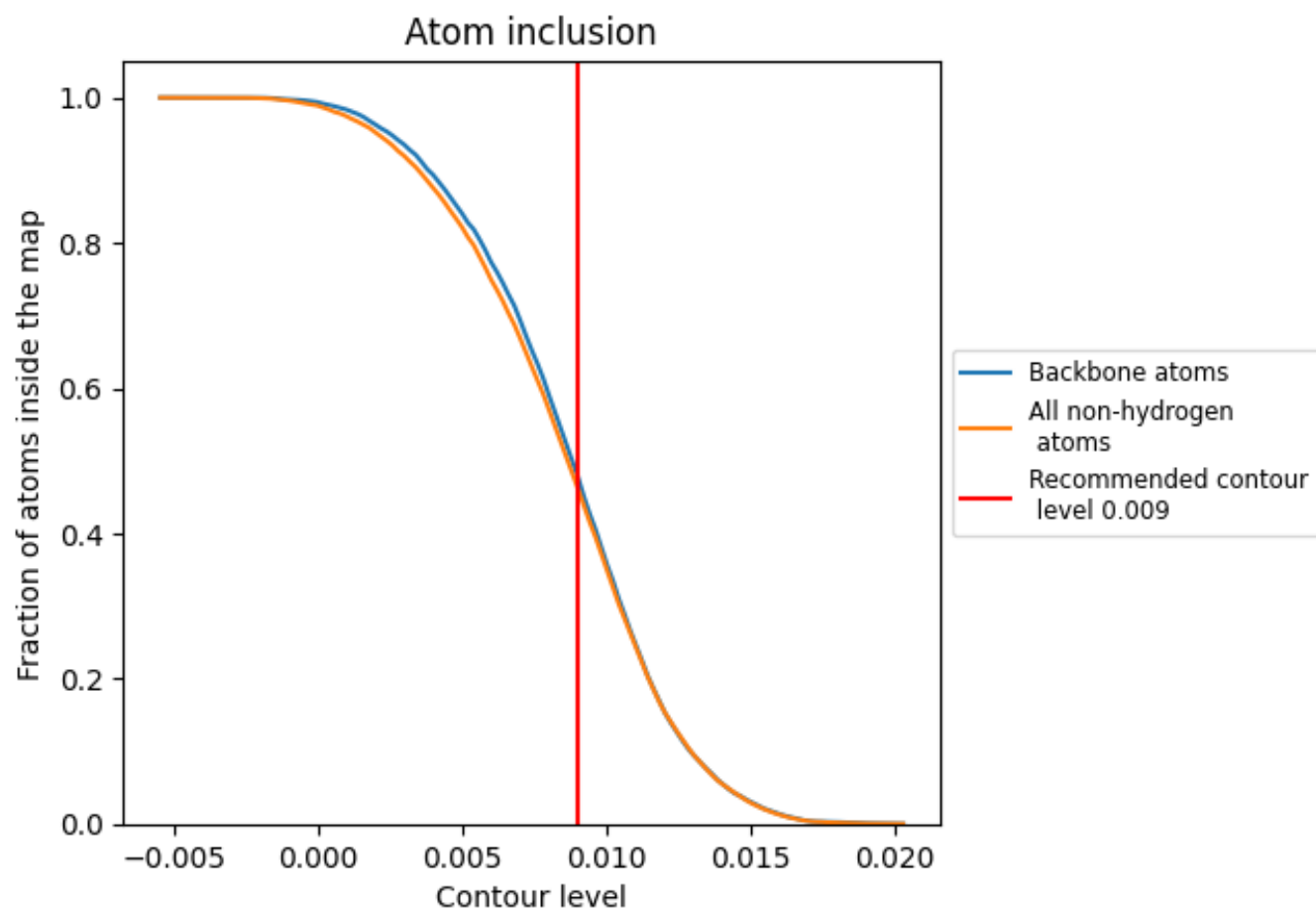
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion ⓘ



At the recommended contour level, 48% of all backbone atoms, 46% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4624	<div></div> 0.0480
A	<div></div> 0.5297	<div></div> 0.0520
B	<div></div> 0.3064	<div></div> 0.0430
C	<div></div> 0.3011	<div></div> 0.0450
D	<div></div> 0.6731	<div></div> 0.0480
E	<div></div> 0.5430	<div></div> 0.0520

