



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:42 AM UTC

PDB ID : 7ABR / pdb_00007abr
EMDB ID : EMD-11707
Title : Cryo-EM structure of B. subtilis ClpC (DWB mutant) hexamer bound to a substrate polypeptide
Authors : Morreale, F.E.; Meinhart, A.; Haselbach, D.; Clausen, T.
Deposited on : 2020-09-08
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

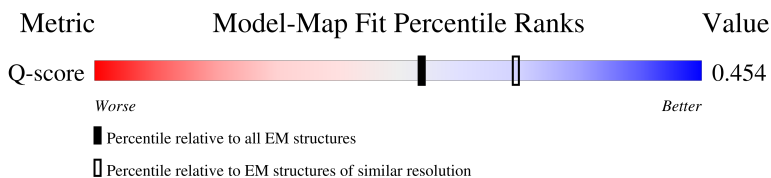
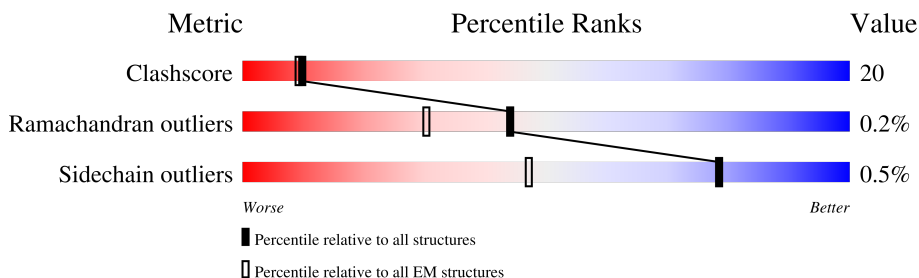
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



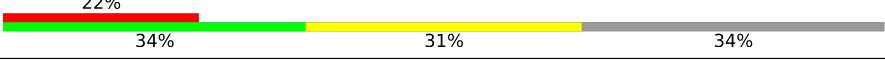
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	818	
1	B	818	
1	C	818	
1	D	818	

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Mol	Chain	Length	Quality of chain
1	E	818	
1	F	818	
2	S	26	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27209 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 Negative regulator of genetic competence ClpC/MecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	574	Total	C	N	O	S	0	0
			4482	2801	799	869	13		
1	B	574	Total	C	N	O	S	0	0
			4488	2803	801	871	13		
1	C	578	Total	C	N	O	S	0	0
			4513	2817	804	879	13		
1	D	586	Total	C	N	O	S	0	0
			4582	2859	821	889	13		
1	E	571	Total	C	N	O	S	0	0
			4476	2796	799	868	13		
1	F	536	Total	C	N	O	S	0	0
			4213	2634	756	810	13		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ALA	GLU	engineered mutation	UNP P37571
A	618	ALA	GLU	engineered mutation	UNP P37571
A	811	LEU	-	expression tag	UNP P37571
A	812	GLU	-	expression tag	UNP P37571
A	813	HIS	-	expression tag	UNP P37571
A	814	HIS	-	expression tag	UNP P37571
A	815	HIS	-	expression tag	UNP P37571
A	816	HIS	-	expression tag	UNP P37571
A	817	HIS	-	expression tag	UNP P37571
A	818	HIS	-	expression tag	UNP P37571
B	280	ALA	GLU	engineered mutation	UNP P37571
B	618	ALA	GLU	engineered mutation	UNP P37571
B	811	LEU	-	expression tag	UNP P37571
B	812	GLU	-	expression tag	UNP P37571
B	813	HIS	-	expression tag	UNP P37571
B	814	HIS	-	expression tag	UNP P37571
B	815	HIS	-	expression tag	UNP P37571
B	816	HIS	-	expression tag	UNP P37571

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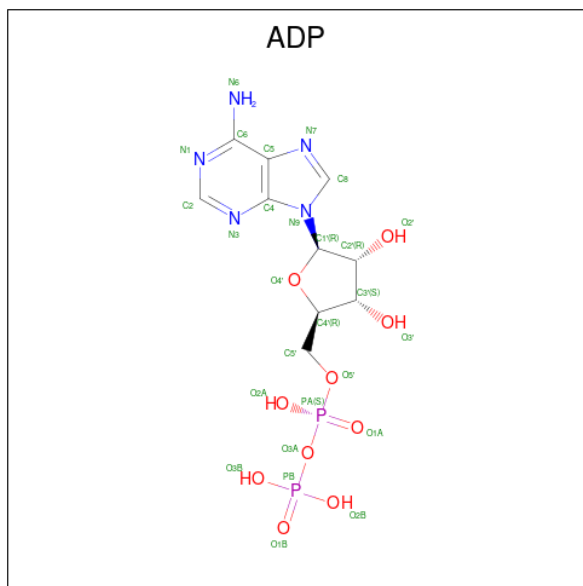
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Chain	Residue	Modelled	Actual	Comment	Reference
B	817	HIS	-	expression tag	UNP P37571
B	818	HIS	-	expression tag	UNP P37571
C	280	ALA	GLU	engineered mutation	UNP P37571
C	618	ALA	GLU	engineered mutation	UNP P37571
C	811	LEU	-	expression tag	UNP P37571
C	812	GLU	-	expression tag	UNP P37571
C	813	HIS	-	expression tag	UNP P37571
C	814	HIS	-	expression tag	UNP P37571
C	815	HIS	-	expression tag	UNP P37571
C	816	HIS	-	expression tag	UNP P37571
C	817	HIS	-	expression tag	UNP P37571
C	818	HIS	-	expression tag	UNP P37571
D	280	ALA	GLU	engineered mutation	UNP P37571
D	618	ALA	GLU	engineered mutation	UNP P37571
D	811	LEU	-	expression tag	UNP P37571
D	812	GLU	-	expression tag	UNP P37571
D	813	HIS	-	expression tag	UNP P37571
D	814	HIS	-	expression tag	UNP P37571
D	815	HIS	-	expression tag	UNP P37571
D	816	HIS	-	expression tag	UNP P37571
D	817	HIS	-	expression tag	UNP P37571
D	818	HIS	-	expression tag	UNP P37571
E	280	ALA	GLU	engineered mutation	UNP P37571
E	618	ALA	GLU	engineered mutation	UNP P37571
E	811	LEU	-	expression tag	UNP P37571
E	812	GLU	-	expression tag	UNP P37571
E	813	HIS	-	expression tag	UNP P37571
E	814	HIS	-	expression tag	UNP P37571
E	815	HIS	-	expression tag	UNP P37571
E	816	HIS	-	expression tag	UNP P37571
E	817	HIS	-	expression tag	UNP P37571
E	818	HIS	-	expression tag	UNP P37571
F	280	ALA	GLU	engineered mutation	UNP P37571
F	618	ALA	GLU	engineered mutation	UNP P37571
F	811	LEU	-	expression tag	UNP P37571
F	812	GLU	-	expression tag	UNP P37571
F	813	HIS	-	expression tag	UNP P37571
F	814	HIS	-	expression tag	UNP P37571
F	815	HIS	-	expression tag	UNP P37571
F	816	HIS	-	expression tag	UNP P37571
F	817	HIS	-	expression tag	UNP P37571
F	818	HIS	-	expression tag	UNP P37571

- Molecule 2 is a protein called substrate polypeptide.

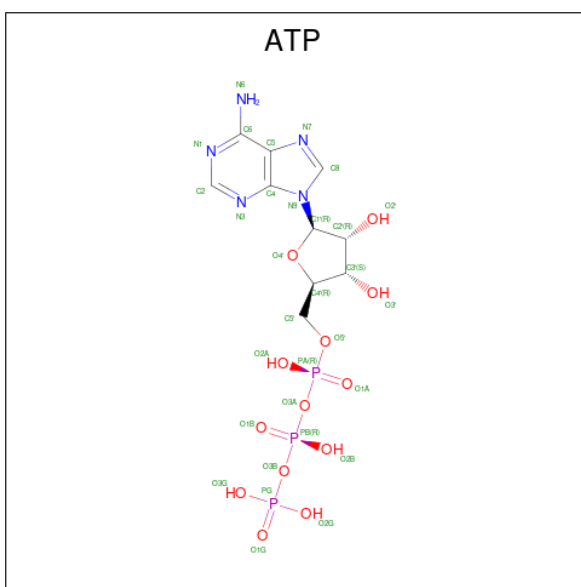
Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	26	Total	C	N	O	0	0
			130	78	26	26		

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

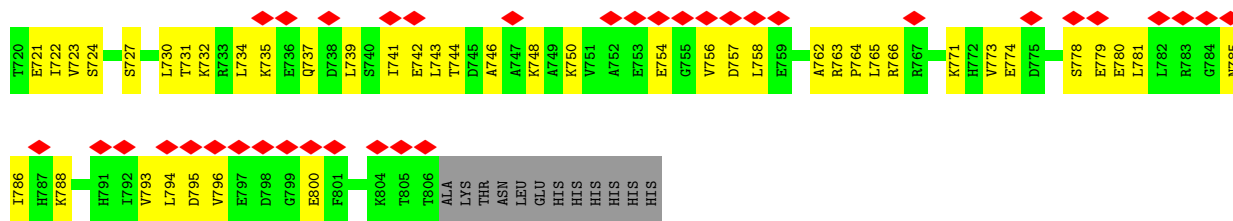


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

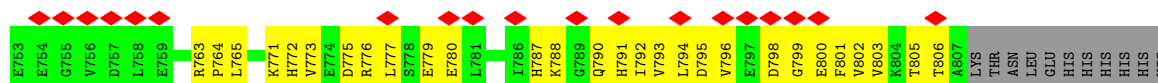
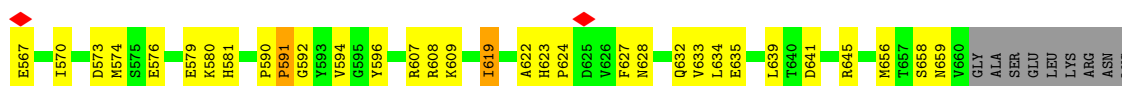
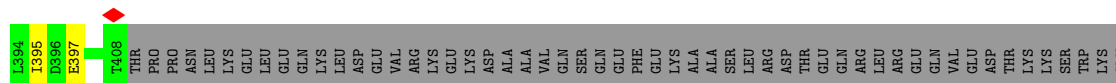
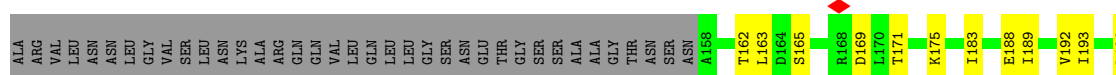
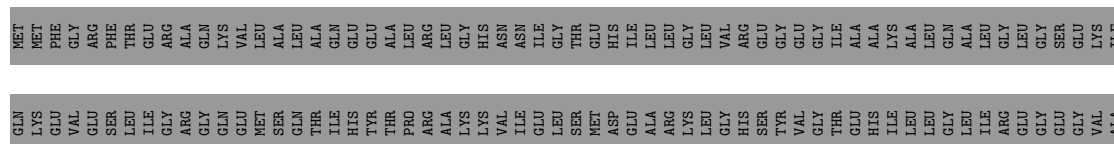
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



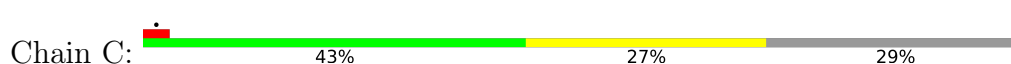
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	C	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0



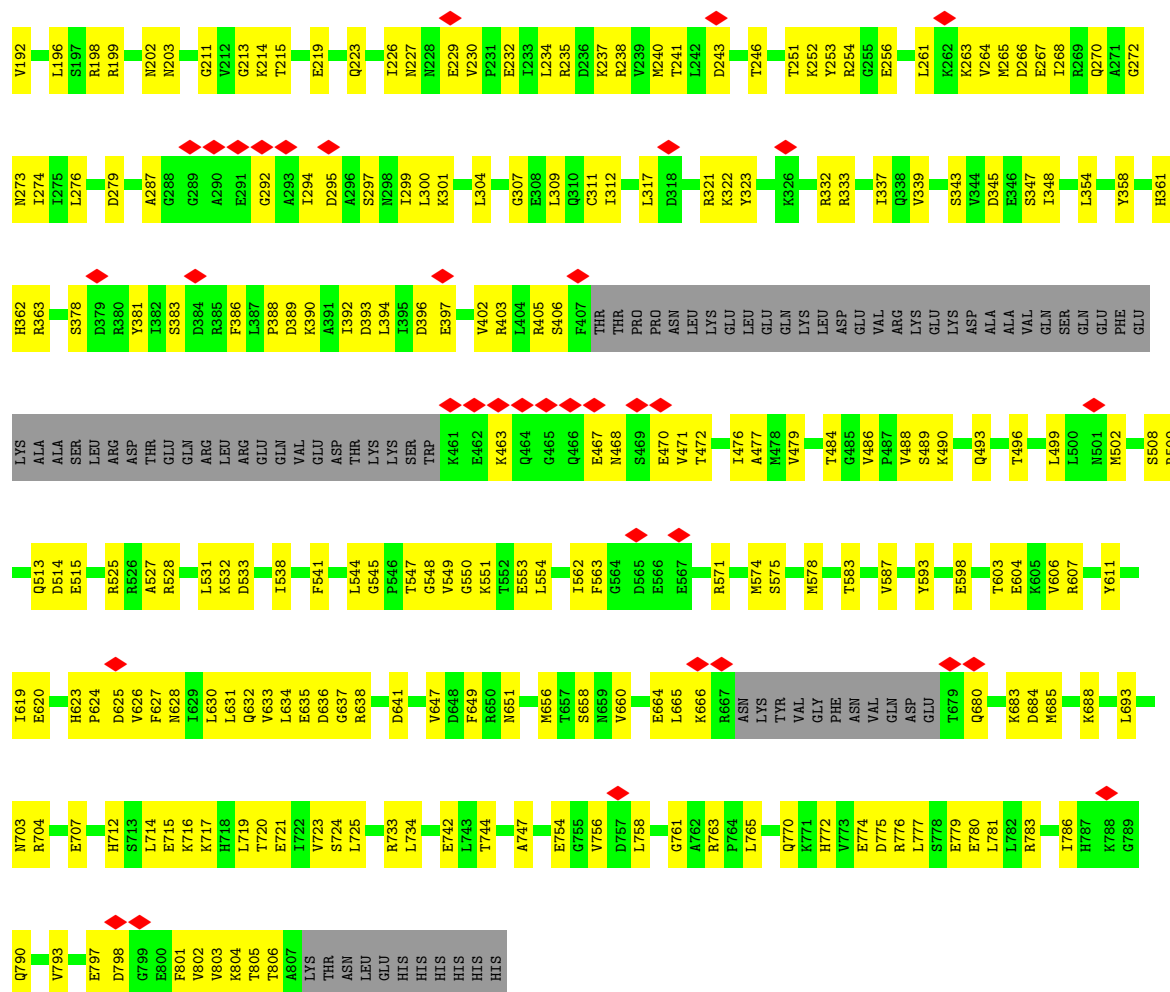
• Molecule 1: Negative regulator of genetic competence ClpC/MecB



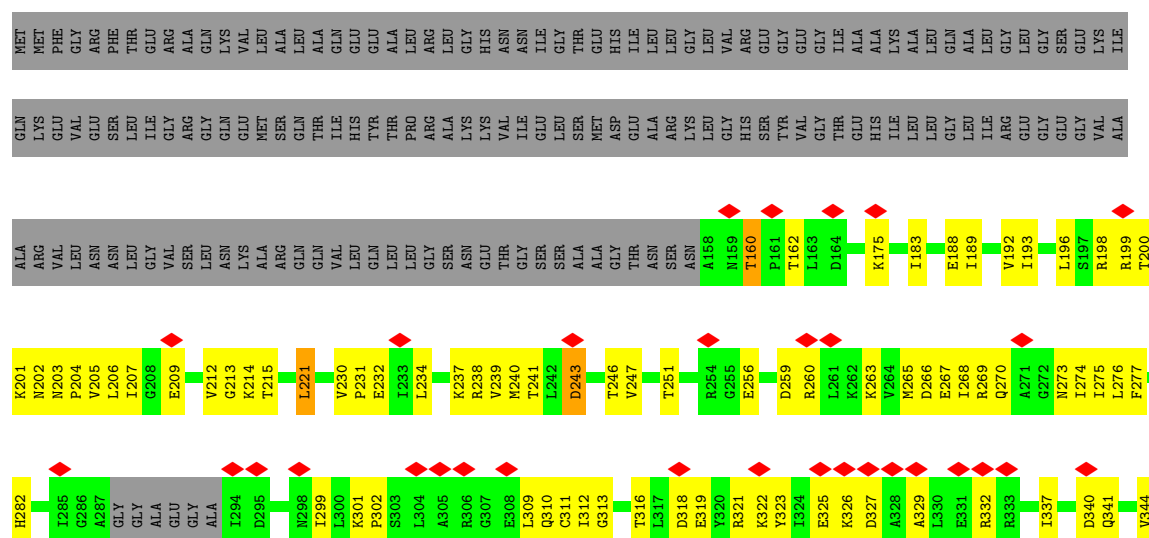
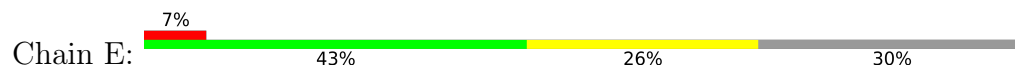
• Molecule 1: Negative regulator of genetic competence ClpC/MecB

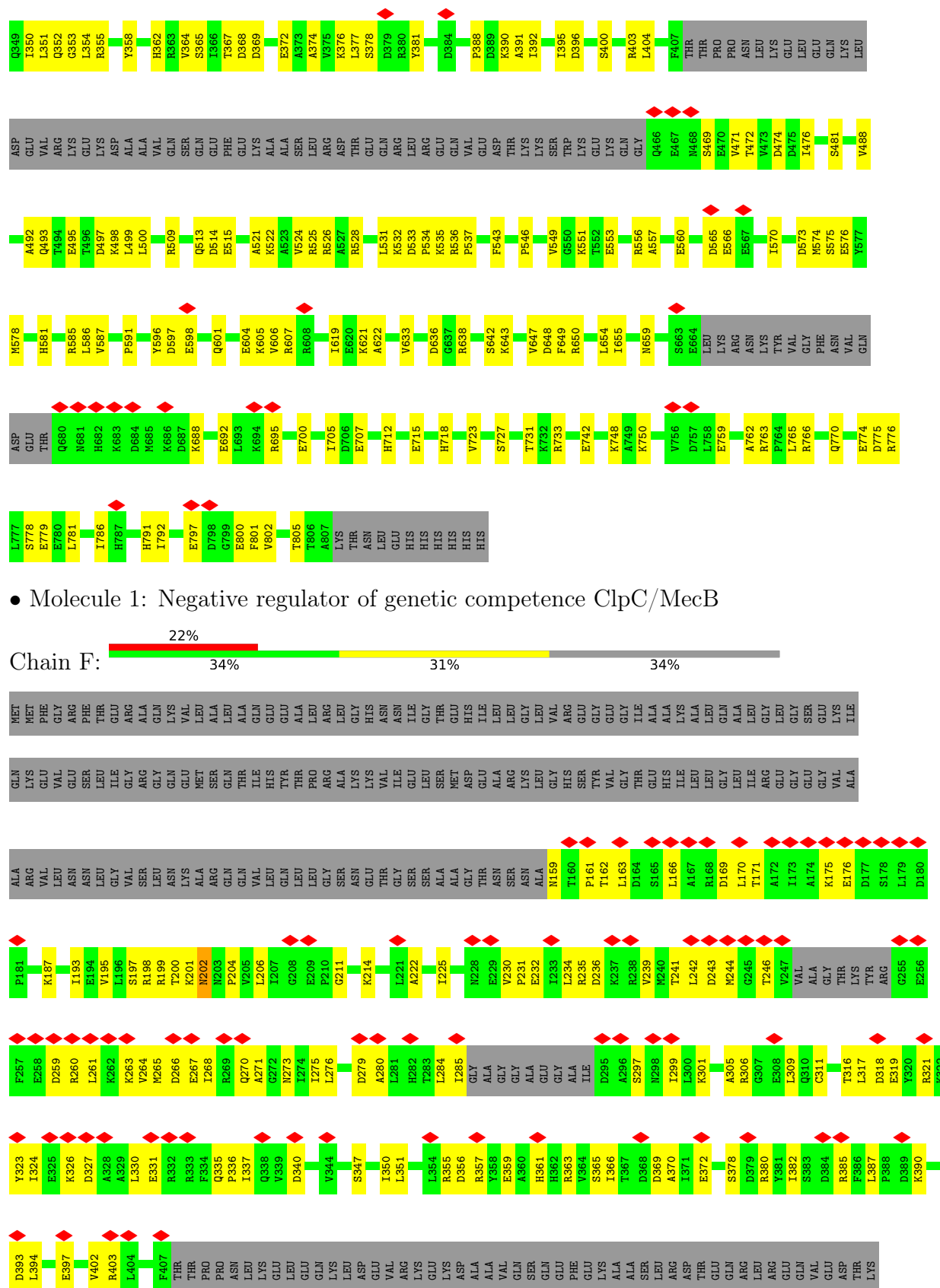


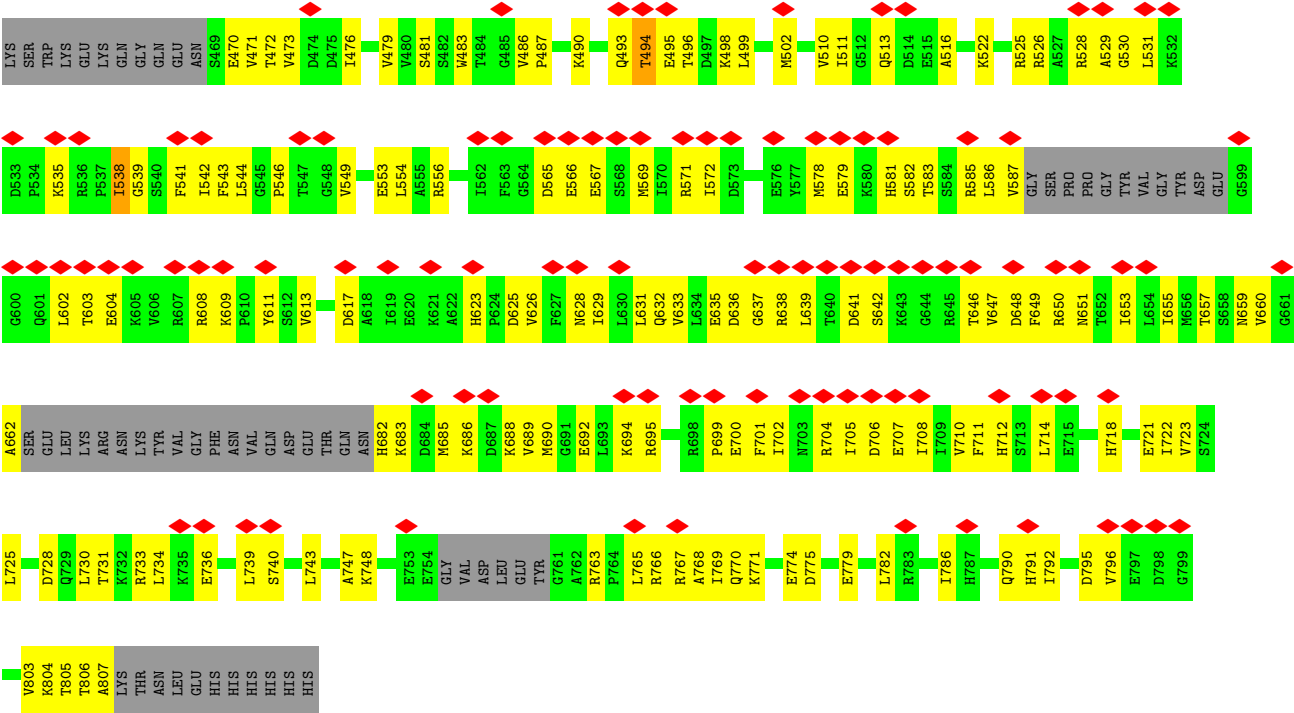




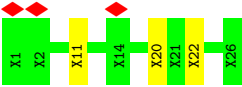
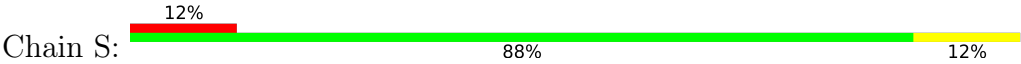
● Molecule 1: Negative regulator of genetic competence ClpC/MecB







● Molecule 2: substrate polypeptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212314	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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: ADP, 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	0.38	0/4536	0.52	0/6113
1	B	0.48	0/4542	0.55	1/6122 (0.0%)
1	C	0.53	0/4566	0.57	0/6151
1	D	0.51	0/4636	0.55	0/6243
1	E	0.43	0/4529	0.51	1/6102 (0.0%)
1	F	0.31	0/4257	0.49	0/5727
All	All	0.45	0/27066	0.53	2/36458 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	586	LEU	N-CA-C	-7.10	105.24	114.04
1	B	324	ILE	N-CA-C	-6.44	107.59	113.71

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	4482	0	4582	208	0
1	B	4488	0	4585	172	0
1	C	4513	0	4609	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4582	0	4683	200	0
1	E	4476	0	4572	176	0
1	F	4213	0	4334	205	0
2	S	130	0	30	3	0
3	A	54	0	23	2	0
3	B	27	0	12	2	0
3	F	27	0	12	1	0
4	A	31	0	12	2	0
4	C	62	0	24	7	0
4	D	93	0	36	9	0
4	E	31	0	12	6	0
All	All	27209	0	27526	1073	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 20.

All (1073) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:THR:HG23	1:B:256:GLU:HB2	1.43	0.97
4:D:1003:ATP:O2B	1:E:551:LYS:NZ	2.03	0.91
1:C:700:GLU:OE2	1:C:704:ARG:NE	2.08	0.86
1:D:550:GLY:O	1:D:554:LEU:N	2.08	0.86
1:C:635:GLU:OE1	1:D:763:ARG:NH2	2.09	0.85
1:F:791:HIS:H	1:F:807:ALA:H	1.26	0.84
1:C:770:GLN:O	1:C:774:GLU:HB3	1.78	0.83
1:F:631:LEU:HD13	1:F:701:PHE:HD1	1.45	0.82
1:B:742:GLU:HB3	1:B:793:VAL:HG12	1.63	0.81
1:D:406:SER:HB2	1:D:468:ASN:HD21	1.43	0.81
1:F:261:LEU:HG	1:F:299:ILE:HD11	1.61	0.81
1:F:633:VAL:O	1:F:637:GLY:N	2.12	0.80
1:F:543:PHE:HB2	1:F:657:THR:HG22	1.63	0.80
1:A:397:GLU:OE2	1:F:198:ARG:NH2	2.14	0.80
1:D:664:GLU:HB2	1:D:688:LYS:HE3	1.63	0.80
1:C:198:ARG:NH2	1:C:335:GLN:OE1	2.14	0.80
1:B:332:ARG:HH21	4:C:1001:ATP:H5'2	1.46	0.79
1:C:571:ARG:NH2	1:C:617:ASP:OD2	2.15	0.79
1:C:261:LEU:HD23	1:C:299:ILE:HD11	1.63	0.79
1:A:238:ARG:N	1:A:273:ASN:O	2.15	0.79
1:A:778:SER:HB2	1:F:526:ARG:HG2	1.63	0.79
1:F:791:HIS:HB3	1:F:806:THR:HB	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:PRO:HG2	1:C:581:HIS:HD2	1.47	0.78
1:C:208:GLY:O	1:C:214:LYS:NZ	2.14	0.77
1:C:629:ILE:HG23	1:C:639:LEU:HD21	1.64	0.77
1:F:513:GLN:HE22	1:F:554:LEU:HB2	1.50	0.76
1:C:251:THR:HG21	1:C:257:PHE:HB2	1.67	0.76
1:A:543:PHE:HD2	1:A:709:ILE:HB	1.50	0.76
1:A:306:ARG:NH2	4:A:1003:ATP:O1A	2.19	0.76
1:D:587:VAL:HG13	1:D:641:ASP:HA	1.67	0.75
1:B:570:ILE:HD11	1:B:609:LYS:HD2	1.68	0.75
1:D:574:MET:HG3	1:D:619:ILE:HD12	1.67	0.75
1:C:203:ASN:HD22	1:C:311:CYS:H	1.33	0.75
1:F:583:THR:HB	1:F:626:VAL:HG12	1.69	0.74
1:D:232:GLU:HA	1:D:235:ARG:HB2	1.69	0.74
1:D:363:ARG:HD2	1:D:403:ARG:HH22	1.54	0.73
1:C:743:LEU:O	1:C:748:LYS:NZ	2.22	0.73
1:B:171:THR:HG21	1:B:238:ARG:HA	1.70	0.72
1:A:543:PHE:O	1:A:658:SER:OG	2.07	0.72
1:E:509:ARG:NH1	1:E:553:GLU:OE2	2.22	0.72
1:B:619:ILE:HD12	1:B:656:MET:HB3	1.71	0.72
1:B:744:THR:HG23	1:B:747:ALA:H	1.54	0.72
1:A:660:VAL:HG22	1:A:662:ALA:H	1.53	0.72
1:E:205:VAL:HA	1:E:313:GLY:O	1.89	0.72
1:B:500:LEU:HD21	1:C:783:ARG:HG2	1.72	0.72
1:B:574:MET:HB3	1:B:622:ALA:HB2	1.72	0.72
1:B:204:PRO:HD2	1:B:312:ILE:HA	1.71	0.71
1:D:531:LEU:HD21	1:E:778:SER:HB3	1.72	0.71
1:A:638:ARG:HA	1:A:648:ASP:HA	1.71	0.71
1:C:525:ARG:NE	1:D:779:GLU:OE2	2.23	0.71
1:E:574:MET:HG3	1:E:622:ALA:HB2	1.72	0.71
1:D:238:ARG:N	1:D:273:ASN:O	2.22	0.71
1:C:332:ARG:NH1	1:D:389:ASP:OD1	2.24	0.71
1:D:199:ARG:HE	1:E:358:TYR:HE1	1.39	0.71
1:C:405:ARG:NH2	1:C:478:MET:SD	2.64	0.70
1:F:387:LEU:HD22	1:F:390:LYS:HE3	1.72	0.70
1:B:244:MET:HE3	1:B:284:LEU:HD23	1.74	0.70
1:C:198:ARG:NH1	1:D:393:ASP:OD1	2.24	0.70
1:A:574:MET:HE2	1:A:616:LEU:HD11	1.72	0.70
1:B:723:VAL:HG21	1:B:752:ALA:HB2	1.72	0.70
1:A:568:SER:HB3	1:A:612:SER:HB2	1.73	0.70
1:A:351:LEU:HD11	1:A:391:ALA:HB1	1.74	0.70
1:F:795:ASP:OD2	1:F:804:LYS:NZ	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:743:LEU:O	1:F:748:LYS:NZ	2.25	0.69
1:A:536:ARG:NH1	1:A:634:LEU:O	2.25	0.69
1:F:637:GLY:HA3	1:F:649:PHE:HB2	1.73	0.69
1:D:704:ARG:NH1	1:E:763:ARG:HH22	1.91	0.69
1:E:364:VAL:HG23	1:E:469:SER:HA	1.73	0.69
1:A:332:ARG:NE	1:B:389:ASP:OD2	2.22	0.69
1:F:528:ARG:HH11	1:F:538:ILE:HG13	1.58	0.69
1:A:497:ASP:HA	1:A:500:LEU:HD13	1.73	0.69
1:D:321:ARG:HH11	1:E:598:GLU:HA	1.58	0.69
1:F:685:MET:HG3	1:F:688:LYS:HD3	1.75	0.69
1:D:754:GLU:OE1	1:D:772:HIS:NE2	2.25	0.69
1:C:638:ARG:HH21	1:D:571:ARG:HD2	1.58	0.69
1:A:548:GLY:N	3:A:1002:ADP:O2B	2.25	0.68
1:E:321:ARG:O	1:E:325:GLU:HB3	1.93	0.68
4:A:1003:ATP:O1A	1:B:215:THR:OG1	2.10	0.68
1:E:362:HIS:HA	1:E:403:ARG:HD2	1.75	0.68
1:D:362:HIS:NE2	1:D:396:ASP:OD1	2.16	0.68
1:D:402:VAL:HG21	1:D:471:VAL:HG22	1.75	0.68
1:F:162:THR:OG1	1:F:267:GLU:OE1	2.11	0.68
1:A:515:GLU:OE2	1:A:712:HIS:ND1	2.27	0.68
1:A:617:ASP:HA	1:A:657:THR:HB	1.76	0.68
1:E:162:THR:O	1:E:263:LYS:NZ	2.26	0.67
1:F:510:VAL:HG22	1:F:553:GLU:HG3	1.76	0.67
1:F:765:LEU:HD12	1:F:768:ALA:HB3	1.76	0.67
1:C:380:ARG:HH21	1:C:534:PRO:HB3	1.58	0.67
1:F:169:ASP:OD1	1:F:171:THR:N	2.26	0.67
1:D:163:LEU:HD12	1:D:264:VAL:HG13	1.77	0.67
1:E:535:LYS:O	1:E:650:ARG:HG2	1.94	0.67
1:E:797:GLU:HB2	1:E:802:VAL:HG21	1.77	0.67
1:A:780:GLU:HB3	1:A:786:ILE:HG12	1.77	0.67
1:E:576:GLU:OE2	1:E:585:ARG:NH1	2.27	0.67
1:B:732:LYS:HA	1:B:735:LYS:HD2	1.77	0.67
1:C:721:GLU:O	1:C:724:SER:OG	2.11	0.67
1:D:514:ASP:OD1	1:D:515:GLU:N	2.27	0.67
1:E:365:SER:OG	1:E:469:SER:O	2.12	0.67
1:B:591:PRO:HA	1:B:596:TYR:CD1	2.30	0.66
1:E:321:ARG:O	1:E:325:GLU:CB	2.44	0.66
1:A:237:LYS:NZ	1:A:272:GLY:O	2.29	0.66
1:D:719:LEU:HD22	1:D:765:LEU:HD11	1.78	0.66
1:C:345:ASP:O	1:C:349:GLN:NE2	2.30	0.65
1:E:513:GLN:NE2	1:E:712:HIS:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:635:GLU:OE1	1:F:704:ARG:NE	2.29	0.65
1:A:165:SER:O	1:F:306:ARG:NH1	2.30	0.65
1:B:332:ARG:NH2	4:C:1001:ATP:H5'2	2.10	0.65
1:B:311:CYS:SG	1:B:312:ILE:N	2.69	0.65
1:C:405:ARG:O	1:C:463:LYS:NZ	2.28	0.65
1:C:776:ARG:NE	1:C:780:GLU:OE2	2.30	0.65
1:D:333:ARG:NH2	4:E:1001:ATP:O3G	2.30	0.65
1:A:355:ARG:NH2	1:A:366:ILE:O	2.30	0.65
1:D:549:VAL:HG12	1:D:550:GLY:H	1.62	0.65
1:D:721:GLU:O	1:D:724:SER:OG	2.13	0.64
1:A:540:SER:HB2	1:A:705:ILE:HD12	1.80	0.64
1:D:397:GLU:HB3	1:D:479:VAL:HG21	1.77	0.64
1:F:626:VAL:HA	1:F:629:ILE:HD12	1.80	0.64
1:E:351:LEU:HD11	1:E:391:ALA:HB1	1.79	0.64
1:E:560:GLU:HB2	1:E:566:GLU:HB3	1.79	0.64
1:A:200:THR:HG23	1:A:201:LYS:HG3	1.79	0.64
1:A:321:ARG:HH12	1:B:608:ARG:HD2	1.63	0.64
1:C:203:ASN:ND2	1:C:311:CYS:H	1.95	0.64
1:A:201:LYS:NZ	1:B:393:ASP:OD2	2.30	0.64
1:B:183:ILE:HB	1:B:350:ILE:HD13	1.78	0.64
1:B:201:LYS:NZ	1:B:332:ARG:O	2.30	0.63
1:B:679:THR:OG1	1:B:680:GLN:N	2.29	0.63
1:A:545:GLY:HA3	1:A:711:PHE:HB2	1.79	0.63
1:C:620:GLU:OE2	1:C:621:LYS:NZ	2.31	0.63
1:F:347:SER:HA	1:F:350:ILE:HD12	1.80	0.63
1:F:587:VAL:HG23	1:F:642:SER:H	1.64	0.63
1:D:551:LYS:NZ	4:D:1002:ATP:O1B	2.32	0.63
1:F:206:LEU:O	1:F:214:LYS:NZ	2.32	0.63
1:D:203:ASN:HB3	1:D:311:CYS:H	1.63	0.63
1:D:405:ARG:NH1	1:D:467:GLU:OE1	2.32	0.63
1:F:318:ASP:HA	1:F:321:ARG:HG2	1.81	0.63
1:A:494:THR:HB	1:A:498:LYS:HB3	1.80	0.62
1:B:317:LEU:HD11	1:C:608:ARG:HD2	1.81	0.62
1:B:633:VAL:HG22	1:B:639:LEU:HG	1.81	0.62
1:A:719:LEU:O	1:A:723:VAL:HG23	1.99	0.62
1:B:516:ALA:HB2	1:B:709:ILE:HG21	1.81	0.62
1:D:378:SER:OG	1:D:390:LYS:HB3	1.99	0.62
1:F:578:MET:O	1:F:623:HIS:NE2	2.31	0.62
1:C:335:GLN:NE2	1:D:397:GLU:OE2	2.33	0.62
1:D:179:LEU:HD11	1:D:219:GLU:HB2	1.81	0.62
1:A:654:LEU:HD21	1:A:656:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:LEU:O	1:F:733:ARG:NE	2.33	0.61
1:B:635:GLU:OE2	1:B:704:ARG:NH2	2.34	0.61
1:E:364:VAL:HG21	1:E:471:VAL:HG23	1.82	0.61
1:C:498:LYS:O	1:C:502:MET:HB2	1.99	0.61
1:A:640:THR:HA	1:A:646:THR:HA	1.81	0.61
1:A:730:LEU:HD21	1:A:773:VAL:HG21	1.82	0.61
1:D:513:GLN:NE2	1:D:712:HIS:O	2.34	0.61
1:F:685:MET:HA	1:F:688:LYS:HG2	1.83	0.61
1:E:372:GLU:O	1:E:376:LYS:HG2	2.01	0.61
1:E:522:LYS:HG2	1:E:525:ARG:HH11	1.66	0.61
1:B:590:PRO:HG2	1:C:581:HIS:CD2	2.32	0.61
1:F:211:GLY:N	3:F:1001:ADP:O3B	2.29	0.61
1:B:521:ALA:HB1	1:B:525:ARG:HH21	1.66	0.60
1:E:193:ILE:HD11	1:E:221:LEU:HD11	1.82	0.60
1:F:629:ILE:HA	1:F:632:GLN:HE21	1.64	0.60
1:A:328:ALA:HA	1:B:210:PRO:HG3	1.83	0.60
1:B:332:ARG:HH11	1:B:333:ARG:HE	1.47	0.60
1:C:351:LEU:HD11	1:C:391:ALA:HB1	1.83	0.60
1:D:772:HIS:HD2	1:D:801:PHE:HE2	1.48	0.60
1:A:261:LEU:HD23	1:A:299:ILE:HD11	1.83	0.60
1:D:311:CYS:SG	1:D:312:ILE:N	2.74	0.60
1:E:160:THR:OG1	1:E:162:THR:OG1	2.19	0.60
1:E:232:GLU:OE1	1:E:232:GLU:N	2.28	0.60
1:B:254:ARG:HD2	1:C:251:THR:OG1	2.02	0.60
1:B:773:VAL:O	1:B:777:LEU:HG	2.02	0.60
1:C:243:ASP:HB2	1:C:246:THR:HG22	1.83	0.60
1:E:575:SER:HA	1:E:621:LYS:HB2	1.83	0.60
1:E:781:LEU:HB2	1:E:786:ILE:HD11	1.82	0.60
1:B:721:GLU:O	1:B:724:SER:OG	2.16	0.60
1:F:629:ILE:O	1:F:633:VAL:HG23	2.01	0.60
1:B:719:LEU:O	1:B:723:VAL:HG23	2.02	0.60
1:B:787:HIS:H	1:B:790:GLN:NE2	1.99	0.60
1:E:198:ARG:HH12	1:F:393:ASP:CG	2.09	0.60
1:A:543:PHE:CD2	1:A:709:ILE:HB	2.34	0.59
1:A:693:LEU:HD23	1:A:702:ILE:HG21	1.84	0.59
1:B:203:ASN:HD22	1:B:311:CYS:H	1.50	0.59
1:A:295:ASP:OD2	1:A:297:SER:N	2.35	0.59
1:C:551:LYS:HZ1	4:C:1002:ATP:PG	2.25	0.59
1:E:509:ARG:HG2	1:E:557:ALA:HB2	1.84	0.59
1:F:380:ARG:HH21	1:F:611:TYR:HB2	1.66	0.59
1:D:192:VAL:O	1:D:196:LEU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:THR:OG1	4:E:1001:ATP:O3A	2.18	0.59
1:E:243:ASP:HB2	1:E:246:THR:OG1	2.03	0.59
1:E:316:THR:HB	1:E:319:GLU:HB2	1.83	0.59
1:A:715:GLU:HB3	1:A:718:HIS:HB2	1.83	0.59
1:F:301:LYS:HE3	1:F:330:LEU:HD11	1.85	0.59
1:B:203:ASN:ND2	1:B:311:CYS:H	2.00	0.59
1:D:214:LYS:HG2	1:D:339:VAL:HG21	1.84	0.59
1:E:727:SER:O	1:E:731:THR:HG23	2.03	0.59
1:F:734:LEU:HD22	1:F:739:LEU:HB2	1.83	0.59
1:F:544:LEU:HB2	1:F:710:VAL:HG13	1.85	0.59
1:F:790:GLN:HB3	1:F:805:THR:HB	1.84	0.59
1:A:660:VAL:HG13	1:A:661:GLY:H	1.67	0.59
1:C:362:HIS:NE2	1:C:396:ASP:OD1	2.34	0.59
1:B:320:TYR:HA	1:B:324:ILE:HG22	1.85	0.59
1:D:786:ILE:HD11	1:D:803:VAL:HG11	1.85	0.59
1:A:474:ASP:OD1	1:A:474:ASP:N	2.35	0.58
1:D:797:GLU:HB2	1:D:802:VAL:HG11	1.85	0.58
1:F:260:ARG:O	1:F:264:VAL:HG23	2.03	0.58
1:A:735:LYS:HA	1:A:739:LEU:O	2.02	0.58
1:D:804:LYS:HE2	1:D:806:THR:HG22	1.85	0.58
1:E:347:SER:HA	1:E:350:ILE:HD12	1.84	0.58
1:F:511:ILE:HG22	1:F:718:HIS:HB3	1.83	0.58
1:B:502:MET:HA	1:B:505:ILE:HD12	1.85	0.58
1:A:490:LYS:O	1:A:494:THR:OG1	2.21	0.58
1:A:505:ILE:O	1:A:508:SER:OG	2.20	0.58
1:B:511:ILE:H	3:B:901:ADP:HN62	1.51	0.58
1:A:198:ARG:NH1	1:B:393:ASP:OD1	2.36	0.58
1:A:781:LEU:HD13	1:F:530:GLY:HA2	1.84	0.58
1:C:546:PRO:HD2	1:C:549:VAL:HG21	1.84	0.58
1:F:316:THR:HG22	1:F:317:LEU:H	1.69	0.58
1:E:378:SER:HB3	1:E:390:LYS:HG3	1.85	0.58
1:F:541:PHE:HB2	1:F:655:ILE:HG22	1.86	0.58
1:B:282:HIS:CD2	1:B:323:TYR:HE2	2.21	0.58
1:E:199:ARG:HD3	1:F:361:HIS:CD2	2.39	0.58
1:F:786:ILE:HD13	1:F:792:ILE:HD13	1.84	0.58
1:B:723:VAL:HG22	1:B:765:LEU:HD21	1.86	0.57
1:C:342:PRO:HB2	1:C:346:GLU:HG3	1.83	0.57
1:F:499:LEU:HD12	1:F:499:LEU:H	1.69	0.57
1:F:771:LYS:HA	1:F:775:ASP:OD1	2.04	0.57
1:D:276:LEU:O	1:D:311:CYS:HA	2.04	0.57
1:D:509:ARG:NH1	1:D:553:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ASN:N	1:A:684:ASP:OD2	2.37	0.57
1:C:551:LYS:NZ	4:C:1002:ATP:O3B	2.33	0.57
1:F:613:VAL:HG13	1:F:653:ILE:HB	1.85	0.57
1:E:533:ASP:HB3	1:F:733:ARG:HD3	1.85	0.57
1:B:251:THR:HG22	1:B:253:TYR:H	1.70	0.57
1:D:628:ASN:O	1:D:631:LEU:HG	2.04	0.57
1:F:193:ILE:O	1:F:197:SER:OG	2.18	0.57
1:A:191:ARG:NH1	1:B:397:GLU:OE1	2.34	0.57
1:B:546:PRO:HD2	1:B:549:VAL:HG21	1.85	0.57
1:D:723:VAL:HG23	1:D:765:LEU:HD13	1.86	0.57
1:C:160:THR:HB	1:C:163:LEU:HB3	1.86	0.57
1:C:199:ARG:HB3	1:D:361:HIS:CD2	2.39	0.57
1:C:365:SER:N	1:C:468:ASN:O	2.37	0.57
1:D:213:GLY:HA2	4:D:1001:ATP:O2A	2.04	0.57
1:D:641:ASP:OD1	1:D:641:ASP:N	2.38	0.57
1:E:354:LEU:HD21	4:E:1001:ATP:H2	1.70	0.57
1:C:328:ALA:C	1:C:330:LEU:H	2.12	0.57
1:C:761:GLY:O	1:C:763:ARG:N	2.36	0.57
1:D:548:GLY:O	1:D:761:GLY:HA3	2.05	0.57
1:D:634:LEU:HD11	1:D:656:MET:HE1	1.86	0.57
1:B:351:LEU:HD23	1:B:371:ILE:HG23	1.87	0.57
1:D:533:ASP:HB2	1:E:766:ARG:HH21	1.70	0.57
1:D:541:PHE:HD1	1:D:707:GLU:HB3	1.70	0.57
1:E:378:SER:O	1:E:390:LYS:NZ	2.27	0.57
1:E:587:VAL:O	1:E:642:SER:OG	2.14	0.57
1:B:345:ASP:O	1:B:349:GLN:NE2	2.38	0.56
1:F:690:MET:HB3	1:F:694:LYS:HE2	1.87	0.56
1:C:251:THR:OG1	1:C:252:LYS:N	2.37	0.56
1:E:196:LEU:O	1:E:310:GLN:NE2	2.38	0.56
1:A:328:ALA:HB1	1:B:210:PRO:HB3	1.86	0.56
1:B:592:GLY:N	1:C:589:SER:OG	2.38	0.56
1:C:743:LEU:HD12	1:C:794:LEU:HB3	1.87	0.56
1:D:169:ASP:HB2	1:D:240:MET:HE2	1.87	0.56
1:D:301:LYS:O	1:D:333:ARG:NH1	2.38	0.56
1:D:363:ARG:HB2	1:D:403:ARG:NH2	2.20	0.56
1:D:544:LEU:HD22	1:D:660:VAL:HG22	1.86	0.56
1:B:514:ASP:N	1:B:514:ASP:OD1	2.38	0.56
1:C:466:GLN:O	1:C:470:GLU:HG2	2.04	0.56
1:D:486:VAL:HG11	1:D:651:ASN:OD1	2.05	0.56
1:E:546:PRO:HD2	1:E:549:VAL:HG21	1.86	0.56
1:F:659:ASN:OD1	1:F:662:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:722:ILE:HG21	1:F:763:ARG:NH1	2.19	0.56
1:A:566:GLU:N	1:A:566:GLU:OE1	2.38	0.56
1:A:546:PRO:HD2	1:A:549:VAL:HG21	1.86	0.56
1:E:570:ILE:HD12	1:E:605:LYS:HB3	1.86	0.56
1:A:573:ASP:HA	1:A:617:ASP:HB2	1.88	0.56
1:B:700:GLU:O	1:B:704:ARG:NH1	2.38	0.56
1:C:719:LEU:O	1:C:723:VAL:HG23	2.06	0.56
1:A:756:VAL:HG11	1:A:762:ALA:HA	1.87	0.56
1:A:780:GLU:OE1	1:A:785:ASN:HB2	2.05	0.56
1:C:266:ASP:OD1	1:C:269:ARG:NH2	2.38	0.56
1:D:620:GLU:HB2	1:D:658:SER:OG	2.06	0.56
1:B:230:VAL:HB	1:B:234:LEU:HD23	1.88	0.56
1:B:632:GLN:NE2	1:C:573:ASP:OD2	2.39	0.56
1:B:750:LYS:NZ	1:B:799:GLY:O	2.39	0.56
1:D:499:LEU:HD11	1:D:528:ARG:HG2	1.87	0.56
1:E:574:MET:HG2	1:E:619:ILE:HD12	1.87	0.56
1:E:596:TYR:CE1	1:E:643:LYS:HG2	2.41	0.56
1:B:573:ASP:O	1:B:576:GLU:HG2	2.07	0.55
1:B:794:LEU:HD21	1:B:801:PHE:HD1	1.71	0.55
1:C:351:LEU:HD22	1:C:395:ILE:HD12	1.88	0.55
1:E:497:ASP:OD1	1:E:498:LYS:N	2.39	0.55
1:F:241:THR:HG22	1:F:242:LEU:H	1.72	0.55
1:F:513:GLN:NE2	1:F:554:LEU:HB2	2.20	0.55
1:F:522:LYS:O	1:F:526:ARG:HG3	2.06	0.55
1:F:495:GLU:HG2	1:F:496:THR:N	2.22	0.55
1:F:786:ILE:HD11	1:F:803:VAL:HG21	1.89	0.55
1:B:205:VAL:HG12	1:B:207:ILE:HG23	1.87	0.55
1:E:351:LEU:HD13	1:E:395:ILE:HD11	1.87	0.55
1:B:544:LEU:HD23	1:B:689:VAL:HG12	1.89	0.55
1:D:345:ASP:HA	1:D:348:ILE:HD12	1.89	0.55
1:F:631:LEU:HD13	1:F:701:PHE:CD1	2.35	0.55
1:A:284:LEU:HD21	1:A:300:LEU:HD12	1.88	0.55
1:B:243:ASP:OD1	1:B:244:MET:N	2.40	0.55
1:C:326:LYS:NZ	1:C:327:ASP:OD2	2.34	0.55
1:D:174:ALA:HB3	1:D:226:ILE:HD12	1.87	0.55
1:B:355:ARG:HG3	1:B:371:ILE:HD11	1.89	0.55
1:F:323:TYR:HA	1:F:326:LYS:NZ	2.21	0.55
1:F:609:LYS:HD2	1:F:611:TYR:HB3	1.88	0.55
1:C:327:ASP:N	1:C:327:ASP:OD1	2.40	0.55
1:C:584:SER:O	1:C:588:GLY:N	2.37	0.55
1:F:685:MET:HB3	1:F:712:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:ASP:O	1:F:273:ASN:HB2	2.07	0.54
1:F:351:LEU:O	1:F:355:ARG:N	2.38	0.54
1:A:160:THR:HG22	1:A:267:GLU:HB3	1.88	0.54
1:C:372:GLU:HB2	1:C:376:LYS:HZ1	1.72	0.54
1:E:531:LEU:HD12	1:F:774:GLU:HG3	1.88	0.54
1:A:335:GLN:N	1:A:335:GLN:OE1	2.41	0.54
1:A:569:MET:HE3	1:A:571:ARG:HB2	1.89	0.54
1:D:470:GLU:O	1:D:472:THR:HG23	2.07	0.54
1:A:690:MET:O	1:A:694:LYS:HG2	2.07	0.54
1:D:171:THR:O	1:D:226:ILE:HD11	2.08	0.54
1:A:254:ARG:HH11	1:B:251:THR:HG21	1.72	0.54
1:B:382:ILE:O	1:B:384:ASP:N	2.41	0.54
1:B:550:GLY:HA2	3:B:901:ADP:H5'2	1.89	0.54
1:B:658:SER:OG	1:B:659:ASN:N	2.39	0.54
1:C:571:ARG:NH1	1:C:573:ASP:OD1	2.41	0.54
1:E:266:ASP:O	1:E:269:ARG:HB3	2.08	0.54
1:F:499:LEU:HA	1:F:502:MET:HE3	1.90	0.54
1:D:175:LYS:HG3	1:D:226:ILE:HD13	1.90	0.54
1:C:293:ALA:O	1:C:295:ASP:N	2.39	0.54
1:D:251:THR:OG1	1:D:252:LYS:N	2.38	0.54
1:E:188:GLU:OE2	1:E:188:GLU:N	2.41	0.54
1:A:743:LEU:HD23	1:A:743:LEU:H	1.73	0.54
1:C:594:VAL:HG23	2:S:20:UNK:O	2.08	0.54
1:E:256:GLU:O	1:E:259:ASP:HB3	2.07	0.54
1:E:742:GLU:OE2	1:E:791:HIS:NE2	2.40	0.54
1:F:579:GLU:CD	1:F:581:HIS:HB3	2.33	0.54
1:A:393:ASP:OD2	1:F:198:ARG:NH1	2.41	0.54
1:C:176:GLU:OE1	1:C:178:SER:OG	2.19	0.54
1:C:563:PHE:HZ	1:C:611:TYR:O	1.91	0.54
1:C:498:LYS:O	1:C:502:MET:CB	2.56	0.54
1:F:326:LYS:HB2	1:F:330:LEU:HD12	1.89	0.54
1:F:380:ARG:HH12	1:F:650:ARG:HD2	1.72	0.54
1:B:330:LEU:C	1:B:332:ARG:H	2.16	0.53
1:B:731:THR:HG22	1:B:741:ILE:HG23	1.91	0.53
1:C:366:ILE:HG12	1:C:471:VAL:HG21	1.89	0.53
1:A:659:ASN:OD1	1:A:661:GLY:N	2.41	0.53
1:D:790:GLN:OE1	1:D:805:THR:OG1	2.16	0.53
1:A:721:GLU:O	1:A:724:SER:OG	2.18	0.53
1:C:544:LEU:HD23	1:C:660:VAL:HG22	1.90	0.53
1:D:332:ARG:NH2	4:E:1001:ATP:O2A	2.41	0.53
1:E:322:LYS:HG3	1:E:323:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:MET:HG3	1:A:274:ILE:HG23	1.90	0.53
1:A:510:VAL:HG22	1:A:553:GLU:HG3	1.89	0.53
1:C:661:GLY:HA3	1:C:689:VAL:HG22	1.91	0.53
1:F:494:THR:HG22	1:F:498:LYS:HB2	1.90	0.53
1:F:723:VAL:HG13	1:F:769:ILE:HD11	1.90	0.53
1:A:511:ILE:O	3:A:1002:ADP:N6	2.42	0.53
1:D:742:GLU:HB3	1:D:793:VAL:HG12	1.90	0.53
1:D:772:HIS:HD2	1:D:801:PHE:CE2	2.26	0.53
1:E:556:ARG:HB3	1:E:566:GLU:OE1	2.09	0.53
1:F:638:ARG:NH2	1:F:646:THR:OG1	2.42	0.53
1:A:638:ARG:HA	1:A:647:VAL:O	2.07	0.53
1:F:243:ASP:HB2	1:F:246:THR:HG22	1.90	0.53
1:A:613:VAL:HG22	1:A:653:ILE:HB	1.90	0.53
1:B:198:ARG:NH1	1:C:393:ASP:OD1	2.42	0.53
1:E:202:ASN:OD1	1:E:203:ASN:ND2	2.42	0.53
1:D:733:ARG:NH2	1:D:774:GLU:OE2	2.42	0.53
1:A:237:LYS:HG3	1:A:273:ASN:HA	1.90	0.53
1:A:566:GLU:O	1:A:568:SER:OG	2.23	0.53
1:C:351:LEU:HD12	1:C:375:VAL:HG23	1.90	0.53
1:E:543:PHE:HE1	1:E:655:ILE:HG23	1.74	0.53
1:E:648:ASP:HB2	1:E:650:ARG:HD3	1.91	0.53
1:C:343:SER:OG	1:C:346:GLU:OE2	2.21	0.52
1:D:187:LYS:NZ	1:D:190:GLN:OE1	2.34	0.52
1:D:666:LYS:NZ	1:D:758:LEU:O	2.37	0.52
1:E:378:SER:C	1:E:390:LYS:HZ3	2.14	0.52
1:F:369:ASP:OD1	1:F:370:ALA:N	2.42	0.52
1:F:393:ASP:O	1:F:397:GLU:HG2	2.09	0.52
1:A:642:SER:HB3	1:A:645:ARG:HB2	1.91	0.52
1:B:476:ILE:HA	1:B:479:VAL:HG12	1.90	0.52
1:E:543:PHE:CE1	1:E:655:ILE:HG23	2.44	0.52
1:A:796:VAL:HA	1:A:800:GLU:O	2.09	0.52
1:B:619:ILE:HG23	1:B:627:PHE:CZ	2.44	0.52
1:D:402:VAL:HG22	1:D:405:ARG:HH21	1.74	0.52
1:F:639:LEU:O	1:F:647:VAL:HG12	2.10	0.52
1:D:237:LYS:NZ	1:D:272:GLY:O	2.41	0.52
1:A:232:GLU:HA	1:A:235:ARG:HB2	1.91	0.52
1:B:335:GLN:NE2	1:C:393:ASP:OD2	2.42	0.52
1:C:351:LEU:HD21	1:C:392:ILE:HG22	1.91	0.52
1:C:738:ASP:HB2	1:C:788:LYS:HD2	1.91	0.52
1:D:704:ARG:HH11	1:E:763:ARG:HH22	1.57	0.52
1:F:513:GLN:HB2	1:F:516:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASP:OD1	1:A:369:ASP:N	2.43	0.52
1:A:566:GLU:CD	1:A:567:GLU:H	2.17	0.52
1:A:734:LEU:HD22	1:A:741:ILE:HG22	1.92	0.52
1:D:215:THR:OG1	4:D:1001:ATP:O2B	2.25	0.52
1:D:265:MET:HA	1:D:268:ILE:HG22	1.92	0.52
1:B:202:ASN:OD1	1:B:202:ASN:N	2.39	0.52
1:E:352:GLN:O	1:E:355:ARG:HG3	2.10	0.52
1:E:377:LEU:HD12	1:E:476:ILE:HG22	1.92	0.52
1:A:540:SER:OG	1:A:706:ASP:N	2.41	0.52
1:A:723:VAL:HG22	1:A:765:LEU:HD21	1.91	0.52
1:E:201:LYS:HD3	1:E:332:ARG:O	2.10	0.52
1:A:744:THR:HG22	1:A:794:LEU:O	2.09	0.52
1:C:248:VAL:HG12	1:C:248:VAL:O	2.09	0.52
1:C:311:CYS:SG	1:C:312:ILE:N	2.83	0.52
1:C:663:SER:OG	1:C:664:GLU:N	2.42	0.52
1:E:206:LEU:HD23	1:E:337:ILE:HB	1.91	0.52
1:F:195:VAL:HG11	1:F:204:PRO:HB3	1.91	0.52
1:A:199:ARG:HD3	1:B:358:TYR:CZ	2.45	0.52
1:A:321:ARG:NH1	1:B:608:ARG:HD2	2.24	0.52
1:A:400:SER:HB2	1:F:197:SER:HB2	1.91	0.52
1:E:188:GLU:O	1:E:192:VAL:HG23	2.10	0.52
1:E:715:GLU:OE2	1:E:718:HIS:ND1	2.43	0.52
1:C:723:VAL:HG22	1:C:765:LEU:HD13	1.92	0.51
1:D:203:ASN:ND2	1:D:304:LEU:HD22	2.25	0.51
1:A:688:LYS:O	1:A:692:GLU:HG2	2.11	0.51
1:A:732:LYS:HA	1:A:735:LYS:HE3	1.91	0.51
1:D:703:ASN:HD21	1:E:763:ARG:HG3	1.74	0.51
1:E:247:VAL:O	1:E:260:ARG:NH1	2.43	0.51
1:F:222:ALA:HA	1:F:225:ILE:HD12	1.92	0.51
1:C:366:ILE:HA	1:C:471:VAL:CG2	2.41	0.51
1:E:267:GLU:O	1:E:270:GLN:HB3	2.11	0.51
1:E:474:ASP:OD2	1:E:474:ASP:N	2.43	0.51
1:E:607:ARG:HG3	1:E:647:VAL:HG23	1.93	0.51
1:A:619:ILE:HG22	1:A:658:SER:HA	1.93	0.51
1:B:282:HIS:CE1	1:B:319:GLU:HG2	2.45	0.51
1:A:212:VAL:HG13	1:A:341:GLN:HA	1.92	0.51
1:C:631:LEU:O	1:C:704:ARG:NH1	2.44	0.51
1:A:378:SER:HB2	1:A:390:LYS:HE3	1.93	0.51
1:A:743:LEU:O	1:A:748:LYS:NZ	2.44	0.51
1:C:604:GLU:O	1:C:608:ARG:HG3	2.10	0.51
1:D:476:ILE:HA	1:D:479:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:THR:OG1	1:F:201:LYS:N	2.44	0.51
1:F:239:VAL:HA	1:F:275:ILE:O	2.10	0.51
1:F:631:LEU:HD11	1:F:704:ARG:HH11	1.76	0.51
1:A:515:GLU:OE1	1:A:515:GLU:N	2.43	0.51
1:D:167:ALA:HB1	1:D:241:THR:O	2.10	0.51
1:D:531:LEU:HD12	1:E:774:GLU:HG2	1.93	0.51
1:C:171:THR:O	1:C:226:ILE:HD11	2.11	0.51
1:C:345:ASP:OD1	1:C:345:ASP:N	2.43	0.51
1:C:372:GLU:HB2	1:C:376:LYS:NZ	2.26	0.51
1:E:237:LYS:HZ2	1:E:273:ASN:HA	1.75	0.51
1:F:556:ARG:NH1	1:F:566:GLU:HG2	2.26	0.51
1:A:237:LYS:HA	1:A:273:ASN:HB2	1.93	0.51
1:A:401:LYS:HG2	1:A:478:MET:HE1	1.92	0.51
1:B:351:LEU:HD21	1:B:395:ILE:HG13	1.93	0.51
1:D:583:THR:HG22	1:D:626:VAL:HG22	1.91	0.51
1:E:209:GLU:O	1:E:214:LYS:NZ	2.44	0.51
1:B:237:LYS:HG2	1:B:273:ASN:HB2	1.93	0.50
1:C:281:LEU:HD11	1:C:334:PHE:CZ	2.46	0.50
1:D:493:GLN:HA	1:D:496:THR:HB	1.93	0.50
1:D:680:GLN:HA	1:D:683:LYS:HD2	1.92	0.50
1:F:335:GLN:OE1	1:F:336:PRO:HD2	2.11	0.50
1:F:631:LEU:HD11	1:F:704:ARG:NH1	2.27	0.50
1:B:594:VAL:HG23	2:S:22:UNK:O	2.10	0.50
1:A:363:ARG:HB2	1:A:403:ARG:HH12	1.76	0.50
1:A:495:GLU:OE1	1:A:495:GLU:N	2.44	0.50
1:B:542:ILE:HG13	1:B:705:ILE:HG21	1.93	0.50
1:A:203:ASN:HD22	1:A:311:CYS:H	1.60	0.50
1:D:172:ALA:O	1:D:176:GLU:HG2	2.11	0.50
1:D:243:ASP:O	1:D:246:THR:OG1	2.22	0.50
1:D:383:SER:O	1:D:383:SER:OG	2.25	0.50
1:B:502:MET:SD	1:B:524:VAL:HG11	2.52	0.50
1:C:268:ILE:HG23	1:C:274:ILE:CG2	2.42	0.50
1:D:381:TYR:O	1:D:484:THR:HG21	2.12	0.50
1:D:606:VAL:HG11	1:D:649:PHE:HD1	1.75	0.50
1:A:727:SER:HB2	1:A:743:LEU:HD21	1.93	0.50
1:C:324:ILE:HG23	1:C:325:GLU:H	1.77	0.50
1:D:635:GLU:HB2	1:D:704:ARG:NE	2.27	0.50
1:F:301:LYS:HE3	1:F:330:LEU:HD21	1.93	0.50
1:F:617:ASP:HA	1:F:657:THR:OG1	2.12	0.50
1:A:771:LYS:HA	1:A:774:GLU:HG2	1.94	0.50
1:C:168:ARG:O	1:C:241:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LYS:O	1:E:733:ARG:NH2	2.45	0.50
1:D:623:HIS:O	1:D:625:ASP:N	2.45	0.50
1:E:282:HIS:HB2	1:E:323:TYR:CD1	2.46	0.50
1:E:311:CYS:SG	1:E:312:ILE:N	2.84	0.50
1:F:198:ARG:HG2	1:F:199:ARG:H	1.77	0.50
1:B:580:LYS:HG3	1:B:623:HIS:ND1	2.27	0.50
1:B:740:SER:OG	1:B:790:GLN:O	2.24	0.50
1:B:503:GLU:OE1	1:B:503:GLU:N	2.28	0.49
1:C:189:ILE:O	1:C:193:ILE:HG12	2.12	0.49
1:B:264:VAL:O	1:B:268:ILE:HG12	2.11	0.49
1:C:467:GLU:HA	1:C:470:GLU:CG	2.43	0.49
1:C:539:GLY:HA2	1:C:706:ASP:OD1	2.12	0.49
1:F:487:PRO:HG2	1:F:490:LYS:HB2	1.94	0.49
1:F:682:HIS:N	1:F:685:MET:HE2	2.27	0.49
1:A:254:ARG:NH1	1:B:257:PHE:HB3	2.26	0.49
1:B:730:LEU:O	1:B:734:LEU:HG	2.13	0.49
1:E:237:LYS:NZ	1:E:273:ASN:HA	2.27	0.49
1:C:565:ASP:O	1:C:567:GLU:HG2	2.13	0.49
1:E:533:ASP:OD1	1:E:533:ASP:N	2.45	0.49
1:A:795:ASP:OD1	1:A:796:VAL:N	2.39	0.49
1:C:611:TYR:O	1:C:611:TYR:CG	2.65	0.49
1:C:757:ASP:HB2	1:C:764:PRO:HG2	1.93	0.49
1:E:688:LYS:O	1:E:692:GLU:HG2	2.13	0.49
1:F:159:ASN:CG	1:F:161:PRO:HD2	2.37	0.49
1:F:359:GLU:HB3	1:F:366:ILE:HD12	1.94	0.49
1:A:198:ARG:CZ	1:A:335:GLN:HE21	2.25	0.49
1:D:254:ARG:HD2	1:E:251:THR:O	2.12	0.49
1:E:533:ASP:N	1:E:534:PRO:HD2	2.27	0.49
1:A:289:GLY:HA3	1:A:293:ALA:HB3	1.95	0.49
1:A:639:LEU:HD12	1:A:641:ASP:OD2	2.13	0.49
1:C:250:GLY:H	1:C:260:ARG:HH12	1.60	0.49
1:F:369:ASP:O	1:F:372:GLU:HG3	2.11	0.49
1:A:224:GLN:HB3	1:A:229:GLU:HB3	1.94	0.49
1:A:706:ASP:OD2	1:A:707:GLU:HG2	2.11	0.49
1:B:163:LEU:HD22	1:B:268:ILE:HD11	1.94	0.49
1:C:328:ALA:C	1:C:330:LEU:N	2.69	0.49
1:E:183:ILE:HB	1:E:350:ILE:HA	1.95	0.49
1:A:264:VAL:HG12	1:A:265:MET:HE2	1.94	0.49
1:A:627:PHE:HA	1:A:630:LEU:HD12	1.95	0.49
1:A:685:MET:O	1:A:689:VAL:HG22	2.13	0.49
1:F:385:ARG:O	1:F:390:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:625:ASP:OD1	1:F:625:ASP:N	2.45	0.49
1:F:682:HIS:CD2	1:F:683:LYS:HG3	2.48	0.49
1:B:688:LYS:HG2	1:B:692:GLU:OE2	2.12	0.48
1:B:523:ALA:HA	1:B:526:ARG:HE	1.78	0.48
1:C:293:ALA:C	1:C:295:ASP:H	2.21	0.48
1:C:321:ARG:HD2	1:D:604:GLU:OE1	2.13	0.48
1:A:344:VAL:O	1:A:347:SER:OG	2.28	0.48
1:A:756:VAL:HG12	1:A:764:PRO:HD2	1.95	0.48
1:B:209:GLU:HB3	1:B:210:PRO:HD2	1.95	0.48
1:C:237:LYS:HA	1:C:273:ASN:HB2	1.94	0.48
1:C:794:LEU:HD21	1:C:801:PHE:HD1	1.78	0.48
1:B:385:ARG:NH2	1:B:393:ASP:OD2	2.47	0.48
1:C:549:VAL:HG12	1:C:549:VAL:O	2.13	0.48
1:D:562:ILE:HG22	1:D:563:PHE:CD1	2.48	0.48
1:F:650:ARG:HG2	1:F:651:ASN:ND2	2.27	0.48
1:A:577:TYR:CE1	1:A:585:ARG:HG2	2.49	0.48
1:F:276:LEU:O	1:F:311:CYS:HA	2.13	0.48
1:B:776:ARG:HD3	1:B:794:LEU:HD11	1.95	0.48
1:C:511:ILE:O	4:C:1002:ATP:N6	2.45	0.48
1:E:367:THR:OG1	1:E:369:ASP:OD1	2.14	0.48
1:A:327:ASP:O	1:A:328:ALA:C	2.55	0.48
1:C:189:ILE:HG12	1:C:217:ILE:HG23	1.94	0.48
1:C:565:ASP:O	1:C:566:GLU:HG2	2.13	0.48
1:E:362:HIS:HD2	1:E:403:ARG:HD3	1.79	0.48
1:E:770:GLN:HA	1:E:774:GLU:HB2	1.94	0.48
1:F:636:ASP:HB3	1:F:638:ARG:HG2	1.96	0.48
1:A:324:ILE:O	1:A:324:ILE:HG22	2.12	0.48
1:B:171:THR:HG23	1:B:239:VAL:H	1.79	0.48
1:B:295:ASP:OD1	1:B:295:ASP:N	2.43	0.48
1:B:564:GLY:O	1:B:566:GLU:N	2.47	0.48
1:C:229:GLU:N	1:C:229:GLU:OE1	2.46	0.48
1:C:380:ARG:NH2	1:C:534:PRO:HB3	2.27	0.48
1:E:374:ALA:HA	1:E:476:ILE:HG21	1.95	0.48
1:F:700:GLU:HG3	1:F:704:ARG:HH12	1.78	0.48
1:F:728:ASP:O	1:F:731:THR:OG1	2.20	0.48
1:A:381:TYR:CE2	1:A:491:ILE:HG12	2.48	0.48
1:A:694:LYS:HZ2	1:A:699:PRO:HB3	1.78	0.48
1:B:730:LEU:HD12	1:B:733:ARG:HE	1.79	0.48
1:E:388:PRO:O	1:E:392:ILE:HG23	2.13	0.48
1:F:259:ASP:O	1:F:263:LYS:HG3	2.14	0.48
1:F:587:VAL:HG23	1:F:642:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:714:LEU:HD23	1:F:714:LEU:H	1.78	0.48
1:B:369:ASP:OD1	1:B:370:ALA:N	2.47	0.48
1:B:607:ARG:HH12	1:B:645:ARG:HH11	1.62	0.48
1:D:378:SER:HB2	1:D:394:LEU:HD12	1.95	0.48
1:D:268:ILE:HG13	1:D:274:ILE:CG2	2.43	0.47
1:B:213:GLY:O	1:B:217:ILE:HG13	2.13	0.47
1:B:317:LEU:HD22	1:C:608:ARG:HH11	1.79	0.47
1:F:340:ASP:OD1	1:F:340:ASP:N	2.47	0.47
1:F:363:ARG:HB2	1:F:403:ARG:NH2	2.28	0.47
1:F:733:ARG:HD2	1:F:734:LEU:HG	1.94	0.47
1:C:241:THR:HA	1:C:277:PHE:O	2.13	0.47
1:C:332:ARG:HD2	1:D:211:GLY:HA3	1.96	0.47
1:C:663:SER:OG	1:C:688:LYS:NZ	2.23	0.47
1:E:241:THR:HA	1:E:277:PHE:O	2.15	0.47
1:D:489:SER:OG	1:D:490:LYS:N	2.46	0.47
1:D:527:ALA:HB2	1:D:538:ILE:HG23	1.97	0.47
1:D:636:ASP:OD1	1:D:638:ARG:NH2	2.48	0.47
1:E:526:ARG:NE	1:F:770:GLN:HE21	2.11	0.47
1:B:772:HIS:O	1:B:776:ARG:HB2	2.15	0.47
1:D:191:ARG:HH11	1:D:337:ILE:HG12	1.80	0.47
1:D:297:SER:O	1:D:301:LYS:N	2.47	0.47
1:D:630:LEU:HD13	1:D:630:LEU:HA	1.71	0.47
1:E:239:VAL:HA	1:E:275:ILE:O	2.15	0.47
1:B:254:ARG:NH1	1:C:257:PHE:HB3	2.29	0.47
1:B:685:MET:O	1:B:689:VAL:HG23	2.14	0.47
1:C:684:ASP:HA	1:C:687:ASP:OD2	2.15	0.47
1:D:402:VAL:HG22	1:D:405:ARG:NH2	2.29	0.47
1:D:403:ARG:O	1:D:403:ARG:HD3	2.15	0.47
1:E:213:GLY:HA2	4:E:1001:ATP:O1A	2.14	0.47
1:A:209:GLU:O	1:A:214:LYS:NZ	2.47	0.47
1:A:212:VAL:HG22	1:A:341:GLN:HB3	1.97	0.47
1:A:254:ARG:NH1	1:B:251:THR:HG21	2.28	0.47
1:A:531:LEU:HD22	1:B:734:LEU:HD22	1.97	0.47
1:A:560:GLU:O	1:A:564:GLY:HA2	2.15	0.47
1:A:577:TYR:HE1	1:A:585:ARG:HG2	1.79	0.47
1:A:626:VAL:O	1:A:630:LEU:HG	2.14	0.47
1:B:208:GLY:C	1:B:214:LYS:HZ1	2.22	0.47
1:C:198:ARG:HB2	1:D:396:ASP:OD2	2.15	0.47
1:D:214:LYS:N	4:D:1001:ATP:O1B	2.46	0.47
1:D:261:LEU:HD22	1:D:299:ILE:HD11	1.97	0.47
1:D:744:THR:O	1:D:747:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:GLU:HB2	1:D:802:VAL:CG1	2.44	0.47
1:E:532:LYS:C	1:E:534:PRO:HD2	2.39	0.47
1:F:542:ILE:HB	1:F:708:ILE:HD12	1.96	0.47
1:A:238:ARG:HD3	1:A:273:ASN:ND2	2.29	0.47
1:A:563:PHE:CE2	1:A:613:VAL:HG23	2.49	0.47
1:C:761:GLY:C	1:C:763:ARG:H	2.21	0.47
1:D:603:THR:HG23	1:D:647:VAL:HG11	1.97	0.47
1:F:230:VAL:HG13	1:F:235:ARG:HD3	1.96	0.47
1:F:685:MET:O	1:F:689:VAL:HG13	2.14	0.47
1:A:694:LYS:NZ	1:A:702:ILE:HD11	2.30	0.47
1:A:702:ILE:HA	1:A:705:ILE:HG22	1.97	0.47
1:C:752:ALA:O	1:C:756:VAL:HG13	2.14	0.47
1:D:798:ASP:OD2	1:D:798:ASP:N	2.45	0.47
1:C:316:THR:HG22	1:C:318:ASP:H	1.79	0.47
1:C:556:ARG:HG3	1:C:569:MET:HE1	1.96	0.47
1:D:684:ASP:OD1	1:D:685:MET:N	2.47	0.47
1:D:553:GLU:HB2	4:D:1002:ATP:O2A	2.15	0.46
1:E:525:ARG:NH1	1:F:779:GLU:OE2	2.49	0.46
1:F:265:MET:HG3	1:F:299:ILE:HD12	1.97	0.46
1:F:271:ALA:HB1	1:F:273:ASN:ND2	2.30	0.46
1:F:385:ARG:HH22	1:F:483:TRP:HH2	1.62	0.46
1:F:791:HIS:H	1:F:807:ALA:N	2.05	0.46
1:B:378:SER:OG	1:B:390:LYS:HG3	2.15	0.46
1:B:796:VAL:HG13	1:B:800:GLU:N	2.29	0.46
1:C:371:ILE:HG12	1:C:395:ILE:HD11	1.97	0.46
1:D:169:ASP:CG	1:D:172:ALA:H	2.23	0.46
1:E:604:GLU:OE2	1:E:607:ARG:NH2	2.49	0.46
1:F:355:ARG:NH2	1:F:366:ILE:O	2.48	0.46
1:A:563:PHE:HE2	1:A:613:VAL:HG23	1.80	0.46
1:B:243:ASP:OD1	1:B:245:GLY:N	2.46	0.46
1:B:591:PRO:HB2	1:C:589:SER:OG	2.15	0.46
1:C:238:ARG:HD3	1:C:240:MET:HE2	1.96	0.46
1:C:630:LEU:O	1:C:634:LEU:HG	2.15	0.46
1:D:253:TYR:HB2	1:D:256:GLU:HG3	1.98	0.46
1:D:268:ILE:HG13	1:D:274:ILE:HG23	1.96	0.46
1:D:363:ARG:HD2	1:D:403:ARG:NH2	2.27	0.46
1:D:715:GLU:HG2	1:D:717:LYS:HZ3	1.79	0.46
1:C:199:ARG:HD3	1:D:358:TYR:CD2	2.50	0.46
1:C:237:LYS:HZ2	1:C:273:ASN:HA	1.80	0.46
1:D:253:TYR:HB2	1:D:256:GLU:CG	2.46	0.46
1:D:719:LEU:HA	1:D:719:LEU:HD23	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:HG11	1:A:711:PHE:HB3	1.97	0.46
1:B:192:VAL:O	1:B:196:LEU:HB2	2.15	0.46
1:B:634:LEU:HB3	1:B:704:ARG:HB3	1.98	0.46
1:D:575:SER:O	1:D:578:MET:HG3	2.16	0.46
1:E:196:LEU:HD12	1:E:196:LEU:HA	1.78	0.46
1:E:326:LYS:HG3	1:E:327:ASP:OD2	2.16	0.46
1:F:763:ARG:O	1:F:765:LEU:N	2.49	0.46
1:D:486:VAL:HG12	1:D:611:TYR:HB2	1.98	0.46
1:E:204:PRO:HD2	1:E:311:CYS:O	2.15	0.46
1:F:546:PRO:HG2	1:F:549:VAL:HG21	1.97	0.46
1:F:549:VAL:HB	1:F:711:PHE:HE2	1.81	0.46
1:B:240:MET:HB2	1:B:276:LEU:HD12	1.96	0.46
1:B:486:VAL:HG12	1:B:488:VAL:HG13	1.97	0.46
1:D:499:LEU:O	1:D:502:MET:HB3	2.15	0.46
1:D:562:ILE:HD13	1:D:562:ILE:HA	1.81	0.46
1:D:684:ASP:O	1:D:688:LYS:HE2	2.16	0.46
1:F:683:LYS:HA	1:F:686:LYS:HB2	1.98	0.46
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.72	0.46
1:A:275:ILE:HG22	1:A:310:GLN:HB3	1.98	0.46
1:A:346:GLU:O	1:A:350:ILE:HG12	2.15	0.46
1:A:750:LYS:O	1:A:754:GLU:HG3	2.15	0.46
1:C:628:ASN:O	1:C:631:LEU:HG	2.15	0.46
1:D:716:LYS:O	1:D:720:THR:HG23	2.16	0.46
1:F:319:GLU:OE2	1:F:319:GLU:N	2.48	0.46
1:F:747:ALA:HA	1:F:796:VAL:HG23	1.97	0.46
1:A:543:PHE:CE1	1:A:655:ILE:HG21	2.50	0.46
1:D:545:GLY:HA2	1:D:665:LEU:HD13	1.97	0.46
1:E:321:ARG:O	1:E:325:GLU:HB2	2.16	0.46
1:F:206:LEU:HD23	1:F:337:ILE:HB	1.98	0.46
1:F:365:SER:HB2	1:F:470:GLU:OE1	2.16	0.46
1:A:577:TYR:CD1	1:A:586:LEU:HG	2.51	0.46
1:C:191:ARG:NH1	1:C:337:ILE:HG12	2.31	0.46
1:D:525:ARG:NH1	1:E:779:GLU:OE2	2.49	0.46
1:D:633:VAL:HG13	1:D:649:PHE:HE2	1.81	0.46
4:D:1003:ATP:C8	1:E:762:ALA:HB3	2.50	0.46
1:E:481:SER:OG	1:E:488:VAL:N	2.49	0.46
1:E:521:ALA:HA	1:E:524:VAL:HG12	1.97	0.46
1:F:309:LEU:O	1:F:309:LEU:HD23	2.16	0.46
1:F:472:THR:OG1	1:F:473:VAL:N	2.49	0.46
1:F:525:ARG:O	1:F:529:ALA:HB3	2.16	0.46
1:F:549:VAL:HB	1:F:711:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:582:SER:O	1:F:585:ARG:HG2	2.15	0.46
1:F:583:THR:O	1:F:586:LEU:HB2	2.16	0.46
1:A:514:ASP:O	1:A:518:VAL:HG13	2.15	0.45
1:A:757:ASP:OD2	1:A:758:LEU:N	2.47	0.45
1:B:198:ARG:NH2	1:B:201:LYS:O	2.49	0.45
1:C:290:ALA:O	1:C:292:GLY:N	2.49	0.45
1:C:507:HIS:NE2	1:C:514:ASP:OD1	2.48	0.45
1:D:633:VAL:CG1	1:D:649:PHE:HE2	2.29	0.45
1:E:522:LYS:O	1:E:526:ARG:HG2	2.15	0.45
1:E:659:ASN:OD1	1:E:659:ASN:N	2.47	0.45
1:F:264:VAL:O	1:F:268:ILE:HG12	2.16	0.45
1:F:481:SER:OG	1:F:486:VAL:O	2.20	0.45
1:E:742:GLU:N	1:E:742:GLU:OE1	2.49	0.45
1:F:327:ASP:HA	1:F:331:GLU:HB2	1.98	0.45
1:F:792:ILE:HA	1:F:804:LYS:O	2.16	0.45
1:C:715:GLU:OE1	1:C:717:LYS:N	2.35	0.45
1:E:362:HIS:HE1	1:E:396:ASP:OD2	1.99	0.45
1:E:759:GLU:H	1:E:759:GLU:CD	2.24	0.45
1:F:266:ASP:O	1:F:270:GLN:HG2	2.17	0.45
1:F:535:LYS:HA	1:F:535:LYS:HD2	1.67	0.45
1:A:213:GLY:O	1:A:217:ILE:HG13	2.17	0.45
1:B:798:ASP:OD1	1:B:798:ASP:N	2.48	0.45
1:D:227:ASN:HB2	1:D:229:GLU:OE1	2.17	0.45
1:E:340:ASP:OD1	1:E:341:GLN:N	2.49	0.45
1:E:492:ALA:O	1:E:495:GLU:HB2	2.15	0.45
1:A:766:ARG:HA	1:A:766:ARG:HD2	1.83	0.45
1:C:345:ASP:HA	1:C:348:ILE:HD12	1.98	0.45
1:F:356:ASP:HA	1:F:359:GLU:OE2	2.17	0.45
1:F:739:LEU:HD23	1:F:739:LEU:HA	1.80	0.45
1:A:628:ASN:O	1:A:631:LEU:HG	2.17	0.45
1:D:266:ASP:O	1:D:270:GLN:HG2	2.16	0.45
1:D:378:SER:HB2	1:D:394:LEU:CD1	2.46	0.45
1:E:183:ILE:HD11	1:E:353:GLY:HA3	1.97	0.45
1:C:351:LEU:HA	1:C:351:LEU:HD23	1.58	0.45
1:E:499:LEU:HD11	1:E:528:ARG:HG2	1.99	0.45
1:F:613:VAL:HG22	1:F:653:ILE:HG13	1.97	0.45
1:A:533:ASP:N	1:B:733:ARG:HH22	2.15	0.45
1:A:718:HIS:HA	1:A:721:GLU:CD	2.41	0.45
1:A:774:GLU:O	1:A:778:SER:HB3	2.17	0.45
1:C:213:GLY:H	4:C:1001:ATP:PB	2.40	0.45
1:C:268:ILE:HG23	1:C:274:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ALA:C	1:C:292:GLY:H	2.24	0.45
1:C:491:ILE:HD12	1:C:496:THR:HG22	1.98	0.45
1:C:623:HIS:O	1:C:625:ASP:N	2.50	0.45
1:C:703:ASN:HD21	1:D:763:ARG:HB2	1.82	0.45
1:D:633:VAL:O	1:D:637:GLY:N	2.35	0.45
1:E:344:VAL:HG23	1:E:345:ASP:OD1	2.16	0.45
1:E:400:SER:O	1:E:404:LEU:HG	2.16	0.45
1:A:566:GLU:CG	1:A:567:GLU:N	2.80	0.45
1:B:511:ILE:HD11	1:B:725:LEU:HD22	1.98	0.45
1:B:635:GLU:HB2	1:B:704:ARG:HE	1.81	0.45
1:C:580:LYS:HB2	1:C:623:HIS:ND1	2.32	0.45
1:D:343:SER:O	1:D:347:SER:OG	2.21	0.45
1:E:514:ASP:OD2	1:E:515:GLU:N	2.49	0.45
1:F:734:LEU:HA	1:F:734:LEU:HD23	1.70	0.45
1:F:766:ARG:HA	1:F:769:ILE:HD12	1.99	0.45
1:B:169:ASP:OD1	1:B:169:ASP:N	2.47	0.45
1:B:384:ASP:OD2	1:B:385:ARG:N	2.50	0.45
1:C:532:LYS:HE3	1:C:538:ILE:HD13	1.98	0.45
1:C:562:ILE:HG22	1:C:563:PHE:CD1	2.52	0.45
1:C:641:ASP:N	1:C:641:ASP:OD1	2.43	0.45
1:D:202:ASN:ND2	1:D:307:GLY:O	2.49	0.45
1:D:531:LEU:HD23	1:D:531:LEU:H	1.81	0.45
1:A:323:TYR:O	1:A:324:ILE:HD13	2.17	0.44
1:D:309:LEU:H	1:D:309:LEU:HD23	1.82	0.44
1:E:700:GLU:H	1:E:700:GLU:CD	2.22	0.44
1:F:162:THR:OG1	1:F:163:LEU:N	2.50	0.44
1:F:230:VAL:CG2	1:F:234:LEU:HB2	2.47	0.44
1:F:356:ASP:O	1:F:359:GLU:HG2	2.18	0.44
1:F:740:SER:OG	1:F:791:HIS:HA	2.17	0.44
1:B:382:ILE:O	1:B:382:ILE:HG22	2.18	0.44
1:D:292:GLY:O	1:D:294:ILE:N	2.51	0.44
1:D:388:PRO:O	1:D:392:ILE:HG23	2.17	0.44
1:D:625:ASP:HB3	1:E:578:MET:SD	2.57	0.44
1:E:260:ARG:O	1:E:263:LYS:HB3	2.17	0.44
1:E:318:ASP:O	1:E:322:LYS:HG2	2.18	0.44
1:B:775:ASP:O	1:B:779:GLU:HG2	2.18	0.44
1:C:191:ARG:O	1:C:195:VAL:HG12	2.17	0.44
1:D:214:LYS:HE2	1:D:214:LYS:HB2	1.71	0.44
1:E:240:MET:O	1:E:276:LEU:HD12	2.17	0.44
1:A:372:GLU:O	1:A:376:LYS:HG2	2.17	0.44
1:C:174:ALA:HB3	1:C:226:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LYS:HG2	1:D:533:ASP:H	1.83	0.44
1:E:259:ASP:O	1:E:260:ARG:C	2.60	0.44
1:F:510:VAL:HG11	1:F:513:GLN:NE2	2.32	0.44
1:F:733:ARG:O	1:F:736:GLU:HB2	2.17	0.44
1:A:619:ILE:HD11	1:A:630:LEU:HD13	2.00	0.44
1:A:660:VAL:HG13	1:A:661:GLY:N	2.30	0.44
1:C:175:LYS:HD3	1:C:226:ILE:HD13	1.99	0.44
1:C:544:LEU:HD21	1:C:693:LEU:HD13	1.99	0.44
1:D:304:LEU:HD23	1:D:309:LEU:HD21	1.99	0.44
1:D:551:LYS:HZ3	4:D:1002:ATP:PG	2.39	0.44
1:C:526:ARG:HD3	1:D:775:ASP:OD1	2.18	0.44
1:D:716:LYS:HA	1:D:719:LEU:HB2	2.00	0.44
1:E:275:ILE:HD13	1:E:275:ILE:HA	1.86	0.44
1:F:284:LEU:HG	1:F:285:ILE:HG23	2.00	0.44
1:A:231:PRO:C	1:A:233:ILE:H	2.26	0.44
1:C:792:ILE:HG23	1:C:803:VAL:HG23	2.00	0.44
1:E:775:ASP:O	1:E:776:ARG:C	2.58	0.44
1:F:169:ASP:OD1	1:F:170:LEU:N	2.51	0.44
1:F:279:ASP:OD2	1:F:280:ALA:N	2.51	0.44
1:A:742:GLU:O	1:A:793:VAL:HA	2.18	0.44
1:C:292:GLY:HA3	1:D:323:TYR:CE1	2.53	0.44
1:E:509:ARG:HG2	1:E:557:ALA:CB	2.46	0.44
1:A:169:ASP:OD2	1:A:172:ALA:N	2.38	0.43
1:A:325:GLU:C	1:A:327:ASP:H	2.25	0.43
1:A:525:ARG:HA	1:A:528:ARG:HB3	1.99	0.43
1:B:162:THR:O	1:B:165:SER:OG	2.35	0.43
1:B:499:LEU:HD11	1:B:528:ARG:HD3	2.00	0.43
1:B:719:LEU:O	1:B:722:ILE:HG22	2.18	0.43
1:C:470:GLU:C	1:C:472:THR:H	2.25	0.43
1:D:549:VAL:HG13	1:D:714:LEU:HD21	1.99	0.43
1:D:684:ASP:HB2	1:D:688:LYS:NZ	2.33	0.43
1:E:654:LEU:HD12	1:E:654:LEU:HA	1.87	0.43
1:A:499:LEU:HG	1:A:500:LEU:HD12	2.01	0.43
1:A:778:SER:OG	1:A:779:GLU:N	2.50	0.43
1:D:354:LEU:HB3	1:D:358:TYR:CE1	2.53	0.43
1:E:199:ARG:HB2	1:F:361:HIS:CE1	2.54	0.43
1:F:490:LYS:O	1:F:494:THR:OG1	2.35	0.43
1:C:355:ARG:HB2	1:C:371:ILE:HD11	2.00	0.43
1:D:203:ASN:HD22	1:D:304:LEU:HD22	1.83	0.43
1:B:776:ARG:O	1:B:780:GLU:HG2	2.18	0.43
1:C:160:THR:O	1:C:160:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:LEU:O	1:C:502:MET:HB3	2.19	0.43
1:C:787:HIS:HB3	1:C:790:GLN:NE2	2.32	0.43
1:D:263:LYS:O	1:D:267:GLU:HG2	2.19	0.43
1:E:565:ASP:O	1:E:566:GLU:HG2	2.18	0.43
1:E:750:LYS:HG2	1:E:801:PHE:CZ	2.53	0.43
1:A:238:ARG:HE	1:A:274:ILE:HD11	1.84	0.43
1:B:229:GLU:H	1:B:229:GLU:HG3	1.67	0.43
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.81	0.43
1:D:354:LEU:HB3	1:D:358:TYR:HE1	1.83	0.43
1:D:403:ARG:O	1:D:406:SER:HB3	2.18	0.43
1:E:268:ILE:HG21	1:E:309:LEU:HB2	2.00	0.43
1:E:606:VAL:HG21	1:E:649:PHE:CE2	2.53	0.43
1:A:198:ARG:NH2	1:A:335:GLN:HE21	2.17	0.43
1:A:533:ASP:H	1:B:733:ARG:HH22	1.65	0.43
1:C:619:ILE:HG12	1:C:658:SER:HB3	1.99	0.43
1:D:322:LYS:HG2	1:E:597:ASP:HB3	2.00	0.43
1:E:202:ASN:HB2	1:E:310:GLN:NE2	2.33	0.43
1:E:578:MET:HE3	1:E:578:MET:HB2	1.73	0.43
1:A:246:THR:HG22	1:F:301:LYS:HE2	2.00	0.43
1:A:601:GLN:O	1:A:605:LYS:HB2	2.18	0.43
1:A:746:ALA:HB1	1:A:796:VAL:HG12	2.01	0.43
1:B:261:LEU:HD23	1:B:261:LEU:HA	1.76	0.43
1:C:321:ARG:HD3	1:D:598:GLU:OE2	2.18	0.43
1:C:743:LEU:HD12	1:C:743:LEU:HA	1.87	0.43
1:D:467:GLU:O	1:D:470:GLU:HB2	2.18	0.43
1:E:500:LEU:HD13	1:E:500:LEU:HA	1.86	0.43
1:E:727:SER:OG	1:E:748:LYS:HE2	2.19	0.43
1:F:323:TYR:CZ	1:F:330:LEU:HD13	2.54	0.43
1:A:481:SER:HB2	1:A:486:VAL:O	2.19	0.43
1:A:623:HIS:CG	1:A:624:PRO:HD2	2.54	0.43
1:B:169:ASP:HB3	1:B:240:MET:HE1	2.01	0.43
1:C:237:LYS:NZ	1:C:273:ASN:HA	2.33	0.43
1:C:700:GLU:O	1:C:704:ARG:HD2	2.19	0.43
1:D:593:TYR:CZ	1:E:581:HIS:HB2	2.53	0.43
1:D:716:LYS:NZ	1:D:756:VAL:HG21	2.33	0.43
1:D:734:LEU:HD23	1:D:734:LEU:HA	1.76	0.43
1:E:265:MET:HE2	1:E:265:MET:HA	2.00	0.43
1:E:692:GLU:OE1	1:E:695:ARG:NH2	2.50	0.43
1:F:263:LYS:HA	1:F:266:ASP:OD2	2.19	0.43
1:A:160:THR:HA	1:A:267:GLU:HG2	2.00	0.43
1:A:202:ASN:O	1:A:204:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HD11	1:A:320:TYR:CD1	2.54	0.43
1:E:585:ARG:O	1:E:601:GLN:HB3	2.19	0.43
1:E:750:LYS:HE2	1:E:800:GLU:HA	2.00	0.43
1:A:549:VAL:HB	1:A:711:PHE:HD2	1.83	0.43
1:A:788:LYS:HE3	1:A:788:LYS:HB3	1.77	0.43
1:B:193:ILE:HG23	1:B:234:LEU:HD22	2.01	0.43
1:C:214:LYS:N	4:C:1001:ATP:O1B	2.48	0.43
1:C:472:THR:OG1	1:C:473:VAL:N	2.52	0.43
1:C:616:LEU:HD12	1:C:656:MET:HG2	2.00	0.43
1:C:620:GLU:HG3	1:C:621:LYS:N	2.34	0.43
1:D:477:ALA:HB1	1:D:488:VAL:O	2.19	0.43
1:D:632:GLN:NE2	1:E:573:ASP:OD1	2.52	0.43
1:F:321:ARG:HA	1:F:324:ILE:HG12	1.99	0.43
1:A:377:LEU:HD11	1:A:491:ILE:HG23	2.01	0.42
1:B:544:LEU:HD23	1:B:689:VAL:CG1	2.49	0.42
1:B:715:GLU:O	1:B:719:LEU:N	2.50	0.42
1:C:340:ASP:OD1	1:C:340:ASP:N	2.43	0.42
1:D:772:HIS:O	1:D:776:ARG:HB2	2.19	0.42
1:E:309:LEU:HD12	1:E:310:GLN:N	2.34	0.42
1:F:378:SER:O	1:F:382:ILE:HG22	2.19	0.42
1:A:284:LEU:O	1:A:296:ALA:HB3	2.19	0.42
1:A:520:VAL:O	1:A:524:VAL:HG12	2.20	0.42
1:B:607:ARG:HE	1:B:608:ARG:HH11	1.67	0.42
1:C:346:GLU:HA	1:C:349:GLN:HE21	1.84	0.42
1:D:175:LYS:HE2	1:D:226:ILE:HG12	2.01	0.42
1:D:386:PHE:O	1:D:390:LYS:HG3	2.19	0.42
1:E:269:ARG:NH1	1:E:270:GLN:HA	2.33	0.42
1:E:301:LYS:HE3	1:E:329:ALA:HB3	2.00	0.42
1:E:493:GLN:C	1:E:495:GLU:H	2.27	0.42
1:F:539:GLY:HA3	1:F:706:ASP:HB2	2.02	0.42
1:A:199:ARG:HD3	1:B:358:TYR:CE1	2.54	0.42
1:B:641:ASP:OD1	1:B:645:ARG:HB2	2.19	0.42
1:C:315:THR:OG1	1:C:320:TYR:HB2	2.19	0.42
1:C:366:ILE:HA	1:C:471:VAL:HG21	2.02	0.42
1:C:483:TRP:CD1	1:C:483:TRP:C	2.96	0.42
1:D:279:ASP:OD2	1:D:279:ASP:N	2.52	0.42
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.82	0.42
1:D:463:LYS:HE3	1:D:463:LYS:HB2	1.80	0.42
1:A:543:PHE:HA	1:A:709:ILE:O	2.20	0.42
1:A:580:LYS:O	1:A:583:THR:HG22	2.19	0.42
1:A:737:GLN:OE1	1:F:531:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ILE:HD12	1:B:792:ILE:O	2.19	0.42
1:B:771:LYS:HA	1:B:775:ASP:OD1	2.19	0.42
1:E:534:PRO:HB2	1:E:536:ARG:HG2	2.01	0.42
1:F:655:ILE:HG13	1:F:655:ILE:O	2.18	0.42
1:A:558:LEU:O	1:A:562:ILE:N	2.48	0.42
1:B:200:THR:OG1	1:B:201:LYS:N	2.53	0.42
1:B:282:HIS:CG	1:B:323:TYR:HE2	2.37	0.42
1:C:585:ARG:HB3	1:C:601:GLN:HG3	2.01	0.42
1:D:541:PHE:CD1	1:D:707:GLU:HB3	2.53	0.42
1:F:356:ASP:OD1	1:F:357:ARG:N	2.52	0.42
1:F:565:ASP:C	1:F:567:GLU:H	2.27	0.42
1:F:572:ILE:HG12	1:F:602:LEU:HB3	2.02	0.42
1:A:686:LYS:HD3	1:A:686:LYS:HA	1.81	0.42
1:B:199:ARG:HB2	1:C:361:HIS:CD2	2.55	0.42
1:B:484:THR:C	1:B:486:VAL:H	2.27	0.42
1:B:624:PRO:HA	1:B:627:PHE:CD2	2.54	0.42
1:B:787:HIS:CG	1:B:788:LYS:H	2.38	0.42
1:B:791:HIS:CE1	1:B:793:VAL:HG13	2.54	0.42
1:C:204:PRO:HD2	1:C:311:CYS:O	2.18	0.42
1:C:205:VAL:HG13	1:C:336:PRO:HA	2.01	0.42
1:C:544:LEU:HD12	1:C:544:LEU:H	1.85	0.42
1:C:620:GLU:HB3	1:C:658:SER:HB2	2.02	0.42
1:C:755:GLY:HA3	1:C:765:LEU:HD23	2.02	0.42
1:D:476:ILE:HG13	1:D:477:ALA:N	2.34	0.42
1:D:693:LEU:HD12	1:D:693:LEU:HA	1.86	0.42
1:E:241:THR:HG22	1:E:277:PHE:HD1	1.84	0.42
1:E:381:TYR:CE2	1:E:488:VAL:HG11	2.54	0.42
1:E:705:ILE:HD13	1:E:705:ILE:HA	1.90	0.42
1:E:707:GLU:OE2	1:F:767:ARG:NH1	2.39	0.42
1:F:244:MET:HE2	1:F:284:LEU:HD13	2.01	0.42
1:F:363:ARG:HB2	1:F:403:ARG:HH22	1.84	0.42
1:F:700:GLU:HG3	1:F:704:ARG:NH1	2.33	0.42
1:F:721:GLU:O	1:F:725:LEU:HG	2.19	0.42
1:A:574:MET:HG2	1:A:622:ALA:HB2	2.01	0.42
1:B:333:ARG:N	1:B:333:ARG:HD2	2.34	0.42
1:E:536:ARG:HB2	1:E:537:PRO:HD2	2.01	0.42
1:F:166:LEU:HD21	1:F:242:LEU:HA	2.02	0.42
1:F:402:VAL:HG21	1:F:471:VAL:HG12	2.02	0.42
1:A:363:ARG:NH2	1:F:232:GLU:OE1	2.32	0.42
1:C:159:ASN:O	1:C:161:PRO:HD3	2.19	0.42
1:E:193:ILE:HG23	1:E:234:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ASP:OD2	1:E:369:ASP:N	2.53	0.42
1:F:202:ASN:OD1	1:F:202:ASN:N	2.36	0.42
1:A:361:HIS:HD2	1:A:362:HIS:CD2	2.38	0.42
1:A:763:ARG:HG2	1:A:764:PRO:HD3	2.02	0.42
1:C:533:ASP:OD1	1:C:533:ASP:N	2.52	0.42
1:D:165:SER:O	1:D:166:LEU:HD23	2.19	0.42
1:D:624:PRO:O	1:D:627:PHE:HB2	2.19	0.42
1:D:717:LYS:H	1:D:717:LYS:HG3	1.59	0.42
1:F:176:GLU:H	1:F:176:GLU:CD	2.27	0.42
1:A:214:LYS:HG2	1:A:339:VAL:HG11	2.01	0.42
1:A:363:ARG:HB2	1:A:403:ARG:NH1	2.34	0.42
1:A:503:GLU:HG2	1:A:504:ASN:N	2.34	0.42
1:A:719:LEU:O	1:A:722:ILE:HG12	2.20	0.42
1:C:228:ASN:HB3	1:C:235:ARG:NH1	2.34	0.42
1:C:346:GLU:H	1:C:346:GLU:HG2	1.56	0.42
1:E:238:ARG:O	1:E:274:ILE:HD12	2.19	0.42
1:F:603:THR:HG21	1:F:641:ASP:HB2	2.02	0.42
1:F:653:ILE:HG22	1:F:655:ILE:HG23	2.02	0.42
1:A:168:ARG:HD3	1:F:305:ALA:HB1	2.01	0.41
1:A:499:LEU:HD23	1:A:499:LEU:H	1.85	0.41
1:C:591:PRO:HA	1:C:596:TYR:CD2	2.55	0.41
1:D:294:ILE:HD12	1:D:294:ILE:HA	1.92	0.41
1:D:300:LEU:HD12	1:D:300:LEU:HA	1.85	0.41
1:E:209:GLU:HB2	1:E:212:VAL:HG23	2.01	0.41
1:E:212:VAL:HG22	1:E:341:GLN:HB3	2.03	0.41
1:E:344:VAL:O	1:E:348:ILE:HG13	2.20	0.41
1:F:326:LYS:HD2	1:F:330:LEU:HD12	2.02	0.41
1:F:351:LEU:HD23	1:F:351:LEU:HA	1.80	0.41
1:F:628:ASN:O	1:F:632:GLN:HG2	2.19	0.41
1:C:526:ARG:NH2	1:D:770:GLN:OE1	2.53	0.41
1:D:169:ASP:O	1:D:173:ILE:HG12	2.20	0.41
1:F:159:ASN:HD21	1:F:162:THR:HG23	1.84	0.41
1:F:692:GLU:HG3	1:F:695:ARG:HE	1.84	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.80	0.41
1:A:275:ILE:O	1:A:275:ILE:HG13	2.20	0.41
1:A:294:ILE:H	1:A:294:ILE:HD12	1.84	0.41
1:B:607:ARG:NH1	1:B:645:ARG:HH11	2.19	0.41
1:C:577:TYR:CD2	1:C:577:TYR:N	2.89	0.41
1:C:658:SER:O	1:C:658:SER:OG	2.38	0.41
1:D:179:LEU:HD23	1:D:223:GLN:HG3	2.01	0.41
1:E:189:ILE:O	1:E:193:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:VAL:HG13	1:E:341:GLN:HA	2.03	0.41
1:E:282:HIS:HB2	1:E:323:TYR:HD1	1.85	0.41
1:E:351:LEU:CD2	1:E:392:ILE:HG22	2.50	0.41
1:E:723:VAL:HG23	1:E:765:LEU:HD13	2.02	0.41
1:E:792:ILE:HG12	1:E:805:THR:HG22	2.02	0.41
1:F:175:LYS:HA	1:F:175:LYS:HD2	1.83	0.41
1:F:569:MET:HE3	1:F:571:ARG:NH2	2.35	0.41
1:F:604:GLU:O	1:F:608:ARG:HG2	2.20	0.41
1:F:629:ILE:HG23	1:F:639:LEU:HD11	2.02	0.41
1:B:628:ASN:O	1:C:575:SER:HB2	2.20	0.41
1:B:724:SER:HA	1:B:748:LYS:HE3	2.02	0.41
1:B:763:ARG:HB2	1:B:764:PRO:HD3	2.02	0.41
1:C:700:GLU:HA	1:D:547:THR:HG23	2.02	0.41
1:D:252:LYS:O	1:D:252:LYS:HG2	2.19	0.41
1:D:490:LYS:HD2	1:D:490:LYS:HA	1.77	0.41
1:D:777:LEU:O	1:D:781:LEU:N	2.53	0.41
1:F:493:GLN:NE2	1:F:494:THR:HG23	2.35	0.41
1:A:244:MET:O	1:A:248:VAL:HG23	2.21	0.41
1:A:566:GLU:HG2	1:A:567:GLU:N	2.35	0.41
1:A:648:ASP:C	1:A:649:PHE:HD1	2.29	0.41
1:B:189:ILE:O	1:B:193:ILE:HG12	2.20	0.41
1:B:242:LEU:HB2	1:B:276:LEU:HD11	2.02	0.41
1:C:169:ASP:HB3	1:C:240:MET:SD	2.60	0.41
1:C:540:SER:HB3	1:C:634:LEU:HD22	2.01	0.41
1:E:200:THR:HG22	1:E:201:LYS:HG2	2.02	0.41
1:E:276:LEU:HD12	1:E:276:LEU:HA	1.83	0.41
1:B:291:GLU:HG3	2:S:11:UNK:O	2.20	0.41
1:B:607:ARG:NE	1:B:608:ARG:HH11	2.19	0.41
1:C:282:HIS:CE1	1:C:319:GLU:HG2	2.55	0.41
1:F:394:LEU:HD23	1:F:394:LEU:HA	1.89	0.41
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.63	0.41
1:A:407:PHE:CD1	1:F:231:PRO:HA	2.56	0.41
1:A:502:MET:HE2	1:A:502:MET:HB2	1.94	0.41
1:B:395:ILE:HD13	1:B:395:ILE:HA	1.85	0.41
1:B:791:HIS:ND1	1:B:806:THR:HB	2.36	0.41
1:C:243:ASP:O	1:C:246:THR:HG22	2.20	0.41
1:D:551:LYS:NZ	4:D:1002:ATP:O2G	2.30	0.41
4:E:1001:ATP:N3	4:E:1001:ATP:H2'	2.35	0.41
1:F:541:PHE:HA	1:F:707:GLU:O	2.20	0.41
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.92	0.41
1:A:524:VAL:O	1:A:528:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:PRO:HA	1:A:596:TYR:CD1	2.56	0.41
1:A:639:LEU:HD12	1:A:641:ASP:CG	2.46	0.41
1:C:221:LEU:HD12	1:C:221:LEU:HA	1.77	0.41
1:C:242:LEU:HA	1:C:242:LEU:HD12	1.73	0.41
1:C:344:VAL:O	1:C:348:ILE:HG13	2.21	0.41
1:C:533:ASP:HB3	1:D:733:ARG:NH2	2.36	0.41
1:C:763:ARG:O	1:C:766:ARG:N	2.54	0.41
1:C:765:LEU:HD23	1:C:765:LEU:HA	1.79	0.41
1:D:198:ARG:HB2	1:E:396:ASP:OD2	2.21	0.41
1:D:268:ILE:HD13	1:D:309:LEU:HB2	2.03	0.41
1:E:175:LYS:HA	1:E:175:LYS:HD3	1.78	0.41
1:E:207:ILE:O	1:E:207:ILE:HG13	2.21	0.41
1:E:531:LEU:HD13	1:F:733:ARG:HH12	1.85	0.41
1:E:531:LEU:HD13	1:E:531:LEU:HA	1.96	0.41
1:E:638:ARG:HB3	1:E:648:ASP:HA	2.02	0.41
1:F:187:LYS:H	1:F:187:LYS:HG2	1.70	0.41
1:F:366:ILE:HA	1:F:471:VAL:HG22	2.03	0.41
1:F:378:SER:HB3	1:F:390:LYS:HB3	2.03	0.41
1:F:544:LEU:HD22	1:F:660:VAL:HG22	2.03	0.41
1:F:705:ILE:CD1	1:F:708:ILE:HG12	2.51	0.41
1:B:332:ARG:NH1	1:B:333:ARG:HE	2.16	0.41
1:B:565:ASP:C	1:B:567:GLU:H	2.28	0.41
1:C:562:ILE:HD13	1:C:562:ILE:HA	1.92	0.41
1:D:287:ALA:HB3	1:D:295:ASP:HA	2.03	0.41
1:E:591:PRO:HA	1:E:596:TYR:CD1	2.56	0.41
1:F:476:ILE:HA	1:F:479:VAL:HG12	2.03	0.41
1:F:690:MET:O	1:F:694:LYS:HG3	2.21	0.41
1:A:514:ASP:O	1:A:517:VAL:HG22	2.21	0.40
1:A:569:MET:HE1	1:A:571:ARG:HH21	1.86	0.40
1:B:188:GLU:HG2	1:B:339:VAL:HG22	2.01	0.40
1:B:273:ASN:OD1	1:B:273:ASN:N	2.55	0.40
1:B:532:LYS:HD2	1:B:533:ASP:O	2.22	0.40
1:C:160:THR:HG22	1:C:267:GLU:OE2	2.21	0.40
1:C:716:LYS:O	1:C:720:THR:HG23	2.21	0.40
1:D:508:SER:OG	1:D:509:ARG:N	2.54	0.40
1:D:780:GLU:HA	1:D:783:ARG:HH21	1.86	0.40
1:A:238:ARG:HE	1:A:274:ILE:CD1	2.34	0.40
1:A:609:LYS:HD2	1:A:611:TYR:HB3	2.03	0.40
1:A:731:THR:HG22	1:A:741:ILE:HG23	2.01	0.40
1:B:579:GLU:C	1:B:581:HIS:H	2.28	0.40
1:D:606:VAL:HG11	1:D:649:PHE:CD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:LEU:HD12	1:D:725:LEU:HA	1.81	0.40
1:F:648:ASP:C	1:F:649:PHE:HD1	2.29	0.40
1:F:699:PRO:HA	1:F:702:ILE:HD12	2.04	0.40
1:A:385:ARG:HE	1:A:385:ARG:HB2	1.58	0.40
1:A:555:ALA:O	1:A:558:LEU:HG	2.21	0.40
1:A:702:ILE:O	1:A:705:ILE:HG22	2.20	0.40
1:B:171:THR:O	1:B:175:LYS:HE3	2.21	0.40
1:B:750:LYS:HE2	1:B:800:GLU:HA	2.02	0.40
1:B:803:VAL:HG12	1:B:805:THR:OG1	2.21	0.40
1:C:565:ASP:O	1:C:567:GLU:N	2.55	0.40
1:C:607:ARG:HG3	1:C:647:VAL:HG23	2.04	0.40
1:D:230:VAL:HG21	1:D:234:LEU:HB2	2.04	0.40
1:E:299:ILE:O	1:E:302:PRO:HD2	2.22	0.40
1:F:782:LEU:HA	1:F:782:LEU:HD23	1.81	0.40
1:A:237:LYS:HE2	1:A:237:LYS:HB2	1.95	0.40
1:B:478:MET:HE3	1:B:478:MET:HB3	1.90	0.40
1:B:495:GLU:O	1:B:499:LEU:HG	2.21	0.40
1:C:477:ALA:HB1	1:C:488:VAL:O	2.21	0.40
1:A:541:PHE:CD1	1:A:707:GLU:HB2	2.57	0.40
1:A:587:VAL:HA	1:A:603:THR:HG21	2.04	0.40
1:A:634:LEU:HD13	1:A:704:ARG:HB3	2.03	0.40
1:B:382:ILE:HD12	1:B:483:TRP:CE3	2.56	0.40
1:B:795:ASP:O	1:B:802:VAL:HG12	2.22	0.40
1:D:607:ARG:HE	1:D:607:ARG:HB3	1.63	0.40
1:E:230:VAL:HB	1:E:231:PRO:HD2	2.02	0.40
1:F:285:ILE:HA	1:F:297:SER:HB3	2.02	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	568/818 (69%)	511 (90%)	56 (10%)	1 (0%)	43	72
1	B	568/818 (69%)	510 (90%)	54 (10%)	4 (1%)	18	50
1	C	572/818 (70%)	510 (89%)	60 (10%)	2 (0%)	36	65
1	D	580/818 (71%)	519 (90%)	61 (10%)	0	100	100
1	E	563/818 (69%)	519 (92%)	44 (8%)	0	100	100
1	F	522/818 (64%)	471 (90%)	50 (10%)	1 (0%)	43	72
All	All	3373/4908 (69%)	3040 (90%)	325 (10%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	ILE
1	B	383	SER
1	A	567	GLU
1	B	252	LYS
1	B	565	ASP
1	F	494	THR
1	B	591	PRO
1	C	471	VAL

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	490/693 (71%)	487 (99%)	3 (1%)	78	79
1	B	491/693 (71%)	489 (100%)	2 (0%)	84	81
1	C	493/693 (71%)	491 (100%)	2 (0%)	84	81
1	D	500/693 (72%)	500 (100%)	0	100	100
1	E	491/693 (71%)	485 (99%)	6 (1%)	63	72
1	F	465/693 (67%)	463 (100%)	2 (0%)	84	81
All	All	2930/4158 (70%)	2915 (100%)	15 (0%)	78	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	531	LEU
1	A	542	ILE
1	A	648	ASP
1	B	381	TYR
1	B	619	ILE
1	C	488	VAL
1	C	705	ILE
1	E	160	THR
1	E	221	LEU
1	E	243	ASP
1	E	472	THR
1	E	633	VAL
1	E	636	ASP
1	F	202	ASN
1	F	538	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	203	ASN
1	A	270	GLN
1	A	338	GLN
1	A	352	GLN
1	A	361	HIS
1	A	682	HIS
1	A	785	ASN
1	B	203	ASN
1	B	282	HIS
1	B	349	GLN
1	B	352	GLN
1	B	737	GLN
1	B	787	HIS
1	B	790	GLN
1	C	203	ASN
1	C	227	ASN
1	C	228	ASN
1	C	349	GLN
1	C	352	GLN
1	C	361	HIS
1	C	581	HIS

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Mol	Chain	Res	Type
1	C	790	GLN
1	D	228	ASN
1	D	352	GLN
1	D	361	HIS
1	D	468	ASN
1	D	504	ASN
1	D	628	ASN
1	D	712	HIS
1	E	203	ASN
1	E	362	HIS
1	E	501	ASN
1	E	623	HIS
1	E	682	HIS
1	E	772	HIS
1	F	159	ASN
1	F	228	ASN
1	F	352	GLN
1	F	513	GLN
1	F	632	GLN
1	F	682	HIS
1	F	712	HIS
1	F	718	HIS
1	F	770	GLN
1	F	787	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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
4	ATP	D	1003	-	32,33,33	1.32	3 (9%)	48,52,52	1.80	9 (18%)
3	ADP	B	901	-	28,29,29	0.45	0	43,45,45	0.59	0
4	ATP	C	1001	-	32,33,33	1.34	4 (12%)	48,52,52	1.78	10 (20%)
4	ATP	D	1001	-	32,33,33	1.34	4 (12%)	48,52,52	1.77	11 (22%)
3	ADP	A	1002	-	28,29,29	1.34	5 (17%)	43,45,45	1.88	9 (20%)
3	ADP	F	1001	-	28,29,29	1.34	4 (14%)	43,45,45	1.87	9 (20%)
4	ATP	C	1002	-	32,33,33	1.30	4 (12%)	48,52,52	1.73	9 (18%)
4	ATP	D	1002	-	32,33,33	1.29	4 (12%)	48,52,52	1.79	9 (18%)
4	ATP	A	1003	-	32,33,33	1.32	4 (12%)	48,52,52	1.76	9 (18%)
3	ADP	A	1001	-	28,29,29	1.32	4 (14%)	43,45,45	2.01	10 (23%)
4	ATP	E	1001	-	32,33,33	1.31	3 (9%)	48,52,52	1.91	9 (18%)

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
4	ATP	D	1003	-	-	6/22/38/38	0/3/3/3
3	ADP	B	901	-	-	5/16/32/32	0/3/3/3
4	ATP	C	1001	-	-	6/22/38/38	0/3/3/3
4	ATP	D	1001	-	-	6/22/38/38	0/3/3/3
3	ADP	A	1002	-	-	5/16/32/32	0/3/3/3
3	ADP	F	1001	-	-	4/16/32/32	0/3/3/3
4	ATP	C	1002	-	-	0/22/38/38	0/3/3/3
4	ATP	D	1002	-	-	4/22/38/38	0/3/3/3
4	ATP	A	1003	-	-	2/22/38/38	0/3/3/3
3	ADP	A	1001	-	-	2/16/32/32	0/3/3/3
4	ATP	E	1001	-	-	8/22/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1001	ADP	C5-C4	4.21	1.46	1.39
3	A	1002	ADP	C5-C4	4.14	1.46	1.39
4	E	1001	ATP	C5-C4	4.10	1.46	1.39
4	A	1003	ATP	C5-C4	4.01	1.46	1.39
4	D	1003	ATP	C5-C4	4.01	1.46	1.39
3	A	1001	ADP	C5-C4	3.98	1.46	1.39
4	C	1002	ATP	C5-C4	3.72	1.45	1.39
4	D	1001	ATP	C5-C4	3.60	1.45	1.39
4	C	1001	ATP	C5-C4	3.47	1.45	1.39
4	D	1002	ATP	C5-C4	3.32	1.45	1.39
4	D	1002	ATP	C5-N7	-3.30	1.33	1.39
4	C	1001	ATP	C5-N7	-3.19	1.33	1.39
4	E	1001	ATP	C5-N7	-3.10	1.33	1.39
4	C	1002	ATP	C5-N7	-3.05	1.33	1.39
4	A	1003	ATP	C5-N7	-3.03	1.33	1.39
4	D	1003	ATP	C5-N7	-3.01	1.33	1.39
4	D	1001	ATP	C5-N7	-2.98	1.33	1.39
4	D	1002	ATP	C4-N9	-2.97	1.31	1.37
4	C	1001	ATP	C4-N9	-2.80	1.31	1.37
4	C	1002	ATP	C4-N9	-2.79	1.31	1.37
4	D	1001	ATP	C4-N9	-2.67	1.32	1.37
3	A	1002	ADP	C5-N7	-2.66	1.34	1.39
3	A	1001	ADP	C5-N7	-2.66	1.34	1.39
3	F	1001	ADP	C5-N7	-2.62	1.34	1.39
4	A	1003	ATP	C4-N9	-2.56	1.32	1.37
3	A	1001	ADP	C8-N7	2.52	1.36	1.31
4	D	1002	ATP	C8-N9	-2.50	1.33	1.37
3	F	1001	ADP	C5-C6	2.40	1.47	1.41
3	A	1002	ADP	C5-C6	2.37	1.47	1.41
3	A	1001	ADP	C5-C6	2.34	1.47	1.41
4	C	1001	ATP	C8-N9	-2.30	1.33	1.37
4	D	1003	ATP	C4-N9	-2.26	1.33	1.37
3	F	1001	ADP	C8-N7	2.25	1.36	1.31
4	A	1003	ATP	C8-N9	-2.25	1.33	1.37
3	A	1002	ADP	C8-N7	2.20	1.35	1.31
4	D	1001	ATP	C8-N7	2.17	1.35	1.31
3	A	1002	ADP	C4-N9	-2.13	1.33	1.37
4	E	1001	ATP	C8-N7	2.03	1.35	1.31
4	C	1002	ATP	C8-N7	2.01	1.35	1.31

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1001	ATP	C5-C4-N3	-6.60	117.62	126.72
3	A	1002	ADP	C5-C4-N3	-6.28	118.07	126.72
3	A	1001	ADP	C5-C4-N3	-6.16	118.23	126.72
3	F	1001	ADP	C5-C4-N3	-6.11	118.30	126.72
4	A	1003	ATP	C5-C4-N3	-5.61	119.00	126.72
4	D	1003	ATP	C5-C4-N3	-5.42	119.25	126.72
4	E	1001	ATP	N3-C4-N9	5.27	136.13	127.17
4	C	1001	ATP	C5-C4-N3	-5.22	119.53	126.72
4	D	1002	ATP	C5-C4-N3	-5.12	119.66	126.72
4	D	1001	ATP	C5-C4-N3	-5.12	119.66	126.72
4	C	1002	ATP	C5-C4-N3	-5.08	119.72	126.72
3	A	1001	ADP	N3-C4-N9	4.88	135.47	127.17
3	A	1002	ADP	N3-C4-N9	4.88	135.47	127.17
4	D	1003	ATP	N3-C4-N9	4.75	135.24	127.17
3	F	1001	ADP	N3-C4-N9	4.73	135.21	127.17
4	A	1003	ATP	N3-C4-N9	4.59	134.98	127.17
4	D	1002	ATP	N3-C4-N9	4.40	134.65	127.17
4	C	1001	ATP	N3-C4-N9	4.33	134.54	127.17
4	C	1002	ATP	N3-C4-N9	4.01	133.99	127.17
4	D	1001	ATP	N3-C4-N9	4.01	133.98	127.17
4	E	1001	ATP	C2-N3-C4	4.01	121.61	111.83
3	A	1002	ADP	C2-N3-C4	3.96	121.51	111.83
3	A	1001	ADP	C2-N3-C4	3.94	121.44	111.83
3	F	1001	ADP	C2-N3-C4	3.90	121.36	111.83
4	D	1002	ATP	C4-N9-C8	3.57	109.49	105.74
4	D	1001	ATP	N3-C2-N1	-3.50	123.28	128.58
4	D	1001	ATP	C2-N3-C4	3.50	120.37	111.83
4	D	1003	ATP	C2-N3-C4	3.43	120.21	111.83
4	D	1003	ATP	C4-N9-C8	3.41	109.32	105.74
3	A	1001	ADP	C4-C5-N7	-3.40	106.69	110.58
4	C	1002	ATP	C2-N3-C4	3.38	120.09	111.83
4	C	1001	ATP	C2-N3-C4	3.37	120.05	111.83
3	A	1002	ADP	C4-C5-N7	-3.35	106.75	110.58
3	F	1001	ADP	N3-C2-N1	-3.34	123.52	128.58
4	E	1001	ATP	N3-C2-N1	-3.33	123.54	128.58
3	F	1001	ADP	C4-C5-N7	-3.32	106.79	110.58
4	C	1002	ATP	N3-C2-N1	-3.30	123.59	128.58
3	A	1002	ADP	N3-C2-N1	-3.28	123.61	128.58
4	D	1002	ATP	C2-N3-C4	3.28	119.85	111.83
3	A	1001	ADP	N3-C2-N1	-3.28	123.62	128.58
4	A	1003	ATP	C2-N3-C4	3.26	119.80	111.83
4	D	1003	ATP	N3-C2-N1	-3.26	123.65	128.58
3	A	1001	ADP	C4-N9-C8	3.22	109.12	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	ATP	C4-N9-C8	3.21	109.11	105.74
4	D	1002	ATP	N3-C2-N1	-3.17	123.79	128.58
4	C	1001	ATP	N3-C2-N1	-3.16	123.80	128.58
3	A	1001	ADP	N9-C8-N7	-3.11	109.52	113.94
3	A	1001	ADP	C5-N7-C8	3.10	108.32	103.45
4	A	1003	ATP	C4-C5-N7	-3.05	107.09	110.58
4	E	1001	ATP	C3'-C2'-C1'	2.99	107.13	101.46
4	D	1003	ATP	C4-C5-N7	-2.97	107.19	110.58
4	D	1001	ATP	C4-C5-N7	-2.95	107.21	110.58
4	C	1001	ATP	C4-C5-N7	-2.91	107.25	110.58
4	D	1001	ATP	C4-N9-C8	2.84	108.72	105.74
4	C	1002	ATP	C4-C5-N7	-2.82	107.36	110.58
4	A	1003	ATP	C4-N9-C8	2.81	108.69	105.74
4	D	1002	ATP	C4-C5-N7	-2.81	107.37	110.58
4	D	1003	ATP	O3G-PG-O2G	2.77	118.19	107.80
4	D	1001	ATP	O4'-C1'-N9	2.77	113.41	108.09
4	C	1001	ATP	O2B-PB-O3B	2.74	114.68	107.27
4	E	1001	ATP	C4-C5-N7	-2.70	107.50	110.58
4	A	1003	ATP	N3-C2-N1	-2.67	124.54	128.58
4	C	1002	ATP	C4-N9-C8	2.67	108.54	105.74
4	D	1003	ATP	C5-N7-C8	2.62	107.57	103.45
3	A	1002	ADP	C4-N9-C8	2.53	108.39	105.74
4	D	1002	ATP	N9-C8-N7	-2.51	110.37	113.94
4	C	1002	ATP	C3'-C2'-C1'	2.51	106.21	101.46
4	D	1003	ATP	N9-C8-N7	-2.49	110.41	113.94
3	A	1002	ADP	C5-N7-C8	2.45	107.30	103.45
3	F	1001	ADP	C5-N7-C8	2.40	107.23	103.45
4	C	1001	ATP	N9-C8-N7	-2.34	110.61	113.94
3	F	1001	ADP	C4-N9-C8	2.32	108.17	105.74
4	C	1001	ATP	C5-N7-C8	2.32	107.09	103.45
4	D	1002	ATP	C5-N7-C8	2.31	107.08	103.45
4	D	1002	ATP	C3'-C2'-C1'	2.30	105.81	101.46
4	E	1001	ATP	O2B-PB-O1B	2.28	123.06	112.44
4	D	1001	ATP	C2'-C1'-N9	-2.24	107.73	113.30
4	A	1003	ATP	C5-N7-C8	2.21	106.93	103.45
3	A	1001	ADP	C3'-C2'-C1'	2.21	105.64	101.46
4	D	1001	ATP	N9-C8-N7	-2.21	110.81	113.94
4	C	1001	ATP	O2B-PB-O1B	2.21	122.71	112.44
4	D	1001	ATP	C5-N7-C8	2.21	106.92	103.45
4	A	1003	ATP	C2'-C1'-N9	-2.17	107.92	113.30
3	A	1001	ADP	C6-C5-N7	2.16	136.25	132.09
4	E	1001	ATP	C5-N7-C8	2.16	106.84	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	ATP	O3G-PG-O2G	2.12	115.75	107.80
4	D	1001	ATP	C5'-C4'-C3'	-2.11	107.63	115.21
3	F	1001	ADP	C5'-C4'-C3'	-2.07	107.76	115.21
4	E	1001	ATP	O3G-PG-O2G	2.07	115.55	107.80
4	C	1002	ATP	C5-N7-C8	2.06	106.68	103.45
4	C	1002	ATP	C2'-C1'-N9	-2.03	108.27	113.30
3	A	1002	ADP	C6-C5-N7	2.01	135.96	132.09
3	A	1002	ADP	N9-C8-N7	-2.00	111.09	113.94
3	F	1001	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	ADP	C5'-O5'-PA-O1A
3	A	1002	ADP	C5'-O5'-PA-O2A
3	A	1002	ADP	C5'-O5'-PA-O3A
3	B	901	ADP	PA-O3A-PB-O3B
3	F	1001	ADP	C5'-O5'-PA-O3A
3	F	1001	ADP	O4'-C4'-C5'-O5'
3	F	1001	ADP	C3'-C4'-C5'-O5'
4	C	1001	ATP	C5'-O5'-PA-O1A
4	C	1001	ATP	C5'-O5'-PA-O2A
4	D	1001	ATP	C5'-O5'-PA-O1A
4	D	1001	ATP	C5'-O5'-PA-O2A
4	D	1001	ATP	C5'-O5'-PA-O3A
4	D	1001	ATP	O4'-C4'-C5'-O5'
4	D	1002	ATP	C5'-O5'-PA-O1A
4	D	1002	ATP	C5'-O5'-PA-O2A
4	D	1002	ATP	C5'-O5'-PA-O3A
4	D	1003	ATP	C5'-O5'-PA-O2A
4	D	1003	ATP	C5'-O5'-PA-O3A
4	D	1003	ATP	O4'-C4'-C5'-O5'
4	D	1003	ATP	C3'-C4'-C5'-O5'
4	E	1001	ATP	C5'-O5'-PA-O1A
4	E	1001	ATP	C5'-O5'-PA-O2A
4	E	1001	ATP	C5'-O5'-PA-O3A
4	E	1001	ATP	C3'-C4'-C5'-O5'
3	A	1002	ADP	C3'-C4'-C5'-O5'
3	B	901	ADP	C3'-C4'-C5'-O5'
4	E	1001	ATP	O4'-C4'-C5'-O5'
4	D	1001	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	C	1001	ATP	C3'-C4'-C5'-O5'
3	A	1002	ADP	O4'-C4'-C5'-O5'
3	B	901	ADP	O4'-C4'-C5'-O5'
4	A	1003	ATP	O4'-C4'-C5'-O5'
4	C	1001	ATP	O4'-C4'-C5'-O5'
4	A	1003	ATP	C3'-C4'-C5'-O5'
4	E	1001	ATP	C2'-C1'-N9-C4
4	E	1001	ATP	C2'-C1'-N9-C8
4	E	1001	ATP	C4'-C5'-O5'-PA
4	D	1003	ATP	PA-O3A-PB-O1B
3	B	901	ADP	C5'-O5'-PA-O1A
3	F	1001	ADP	C5'-O5'-PA-O1A
4	C	1001	ATP	C5'-O5'-PA-O3A
4	C	1001	ATP	PB-O3B-PG-O1G
3	A	1001	ADP	C2'-C1'-N9-C8
3	A	1001	ADP	C2'-C1'-N9-C4
3	B	901	ADP	PA-O3A-PB-O1B
4	D	1001	ATP	PB-O3A-PA-O1A
4	D	1003	ATP	PA-O3A-PB-O2B
4	D	1002	ATP	PG-O3B-PB-O2B

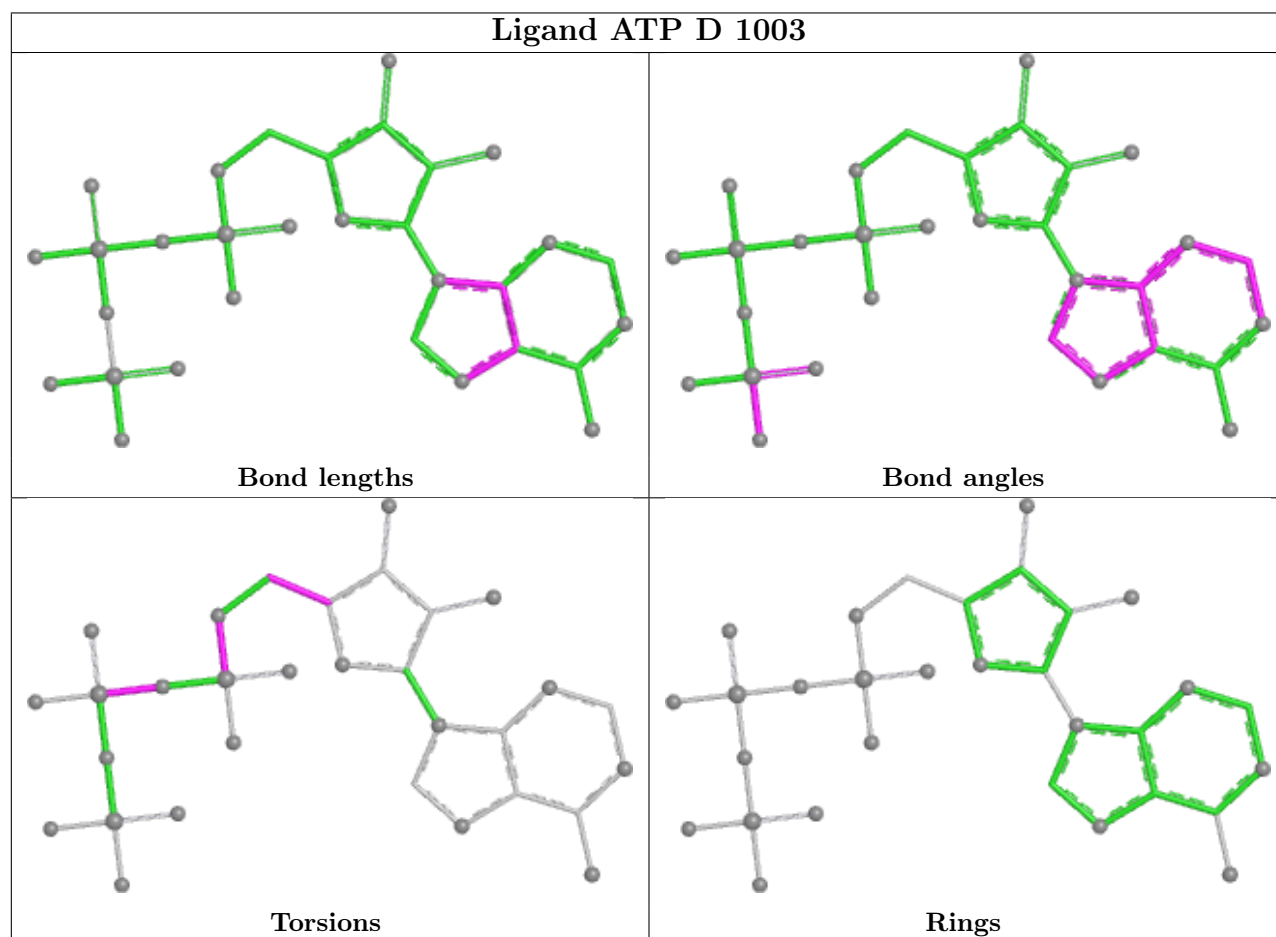
There are no ring outliers.

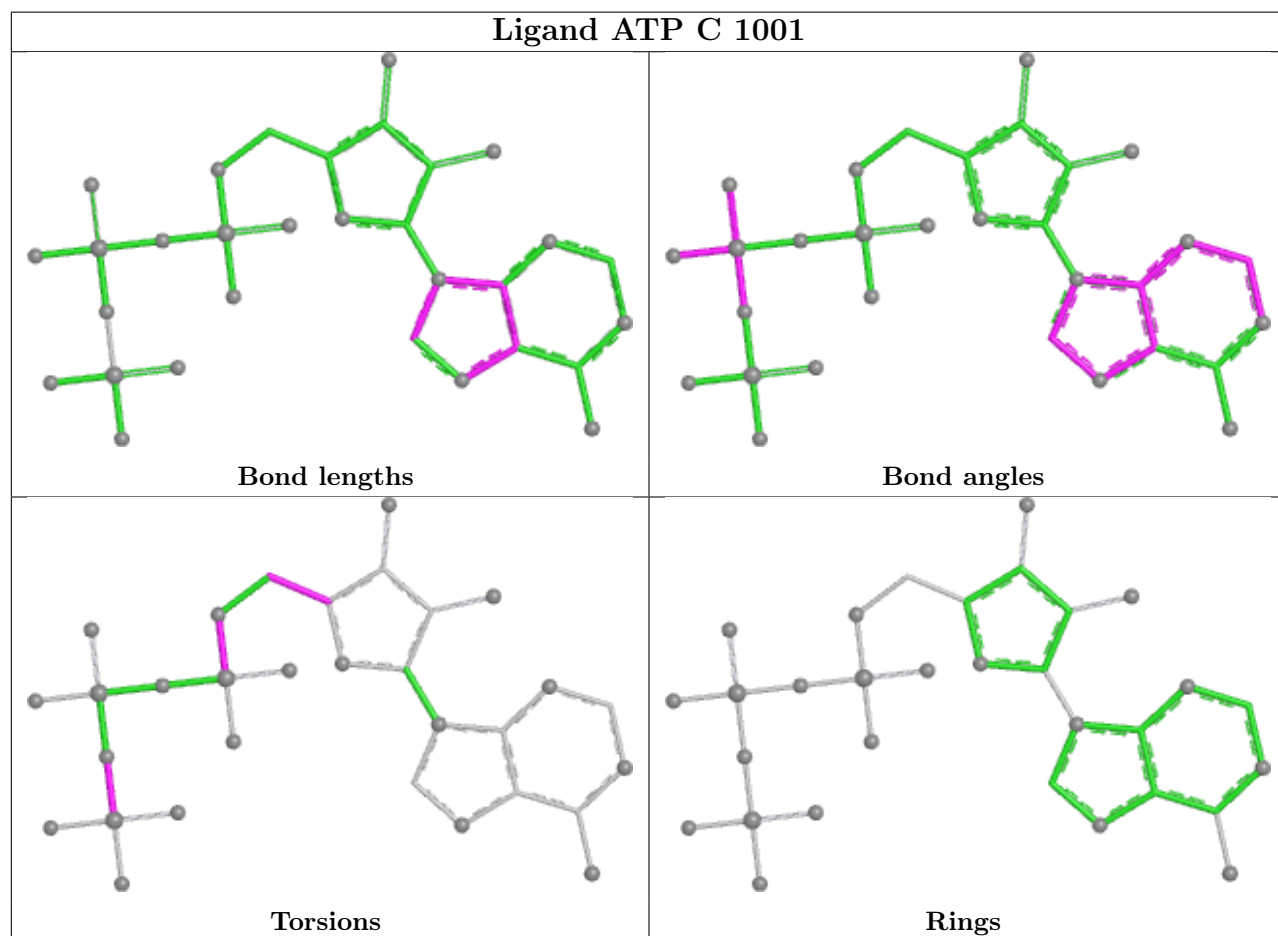
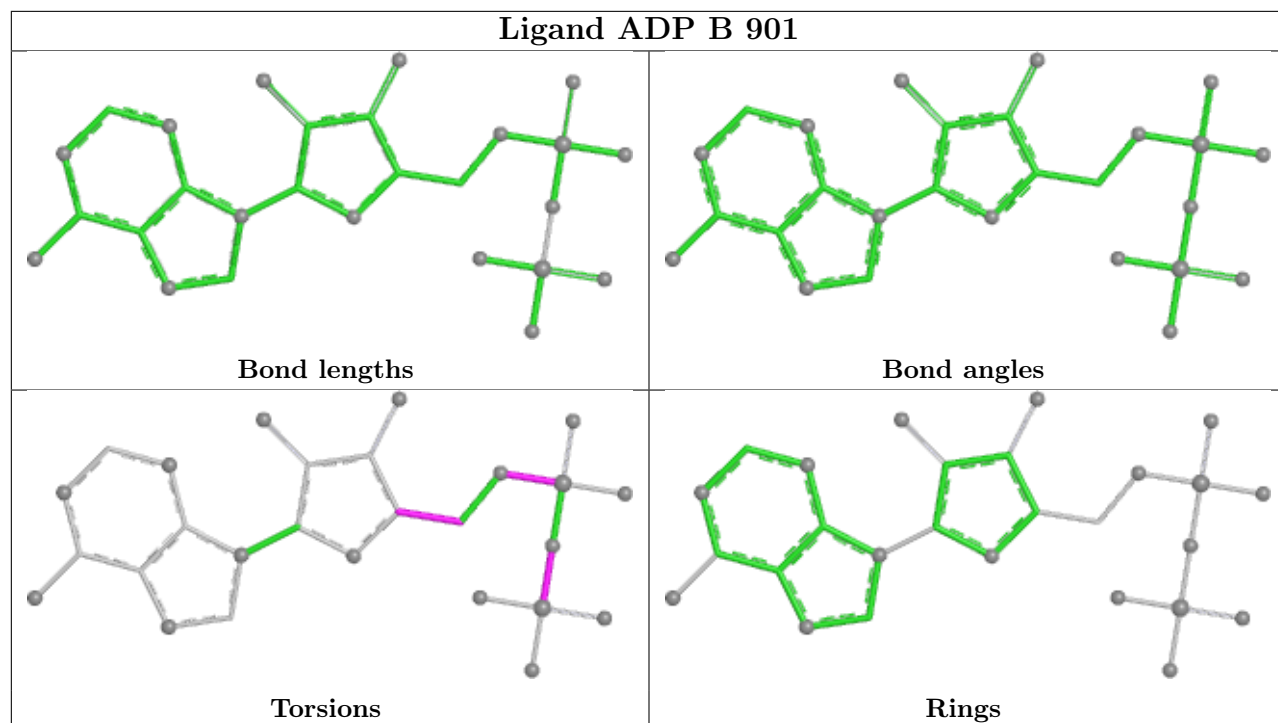
10 monomers are involved in 29 short contacts:

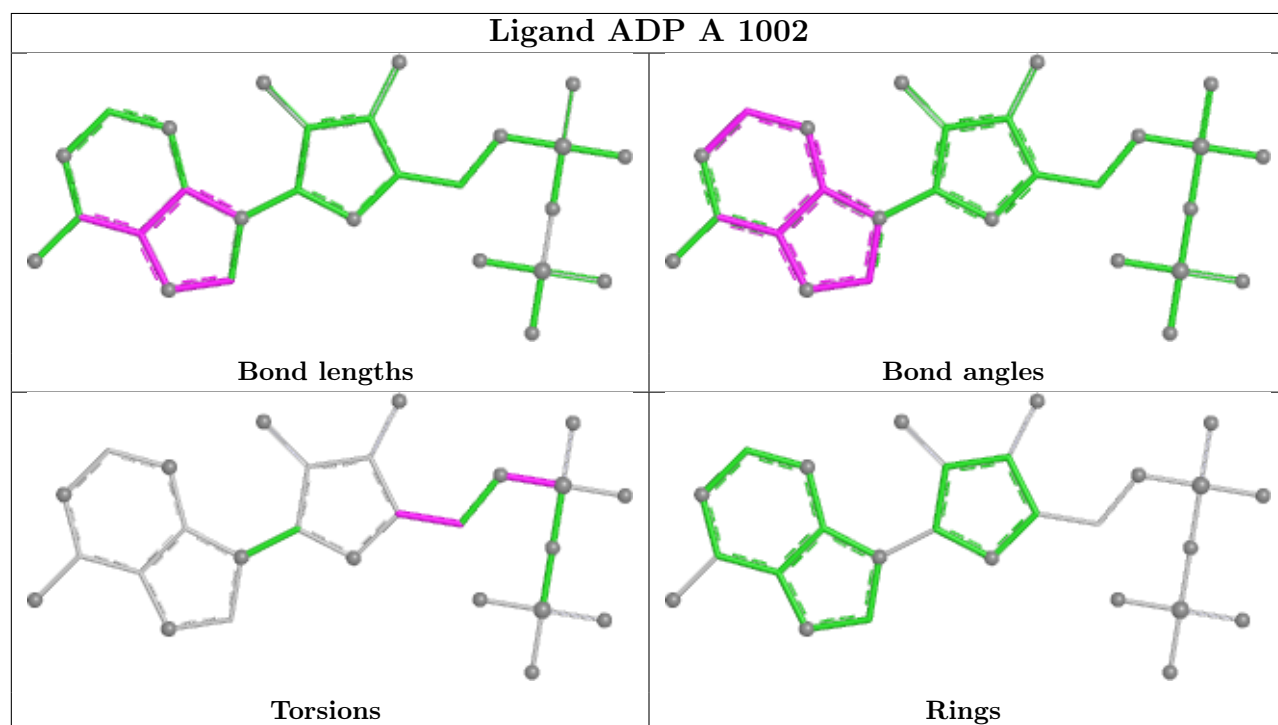
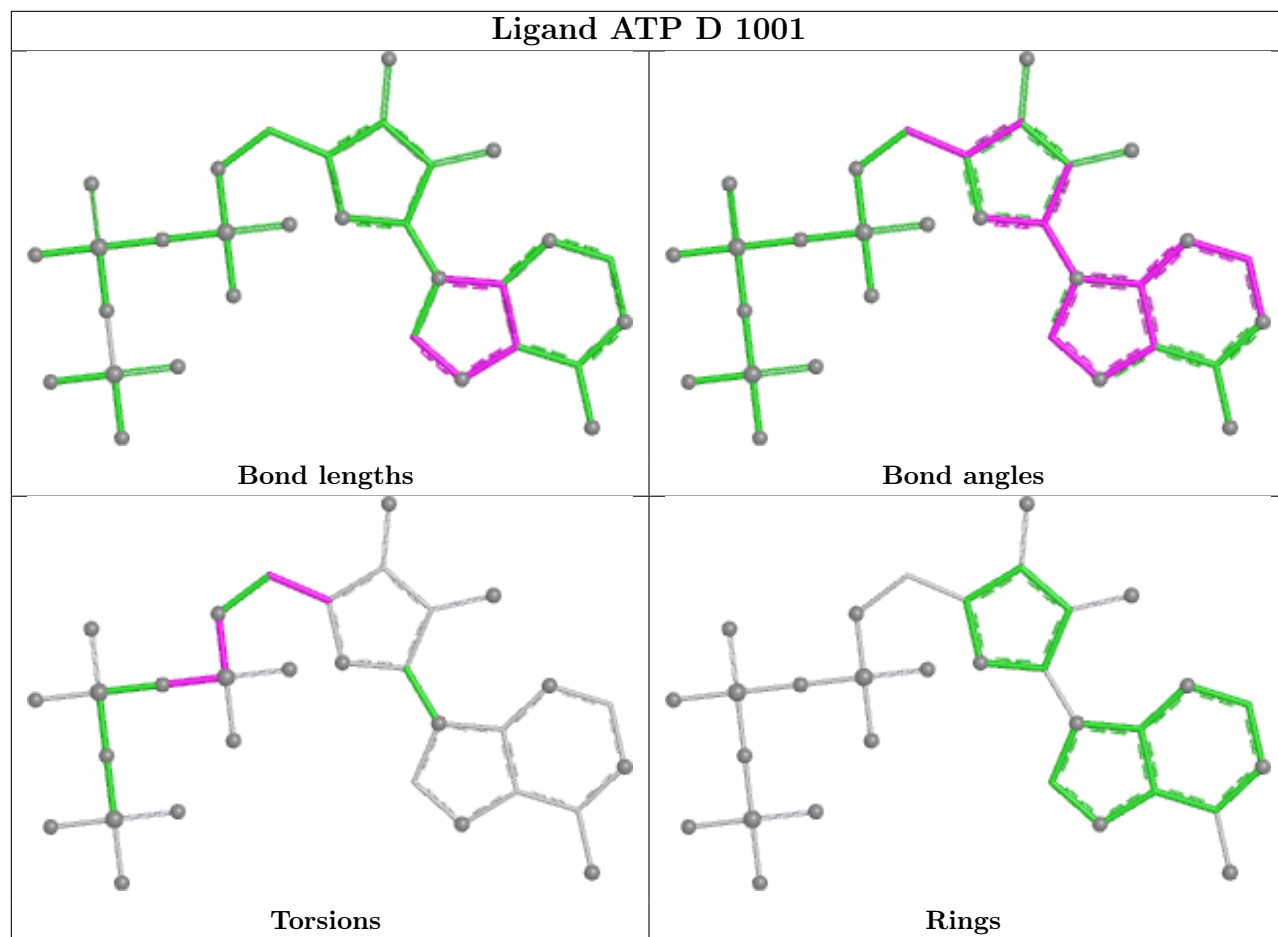
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1003	ATP	2	0
3	B	901	ADP	2	0
4	C	1001	ATP	4	0
4	D	1001	ATP	3	0
3	A	1002	ADP	2	0
3	F	1001	ADP	1	0
4	C	1002	ATP	3	0
4	D	1002	ATP	4	0
4	A	1003	ATP	2	0
4	E	1001	ATP	6	0

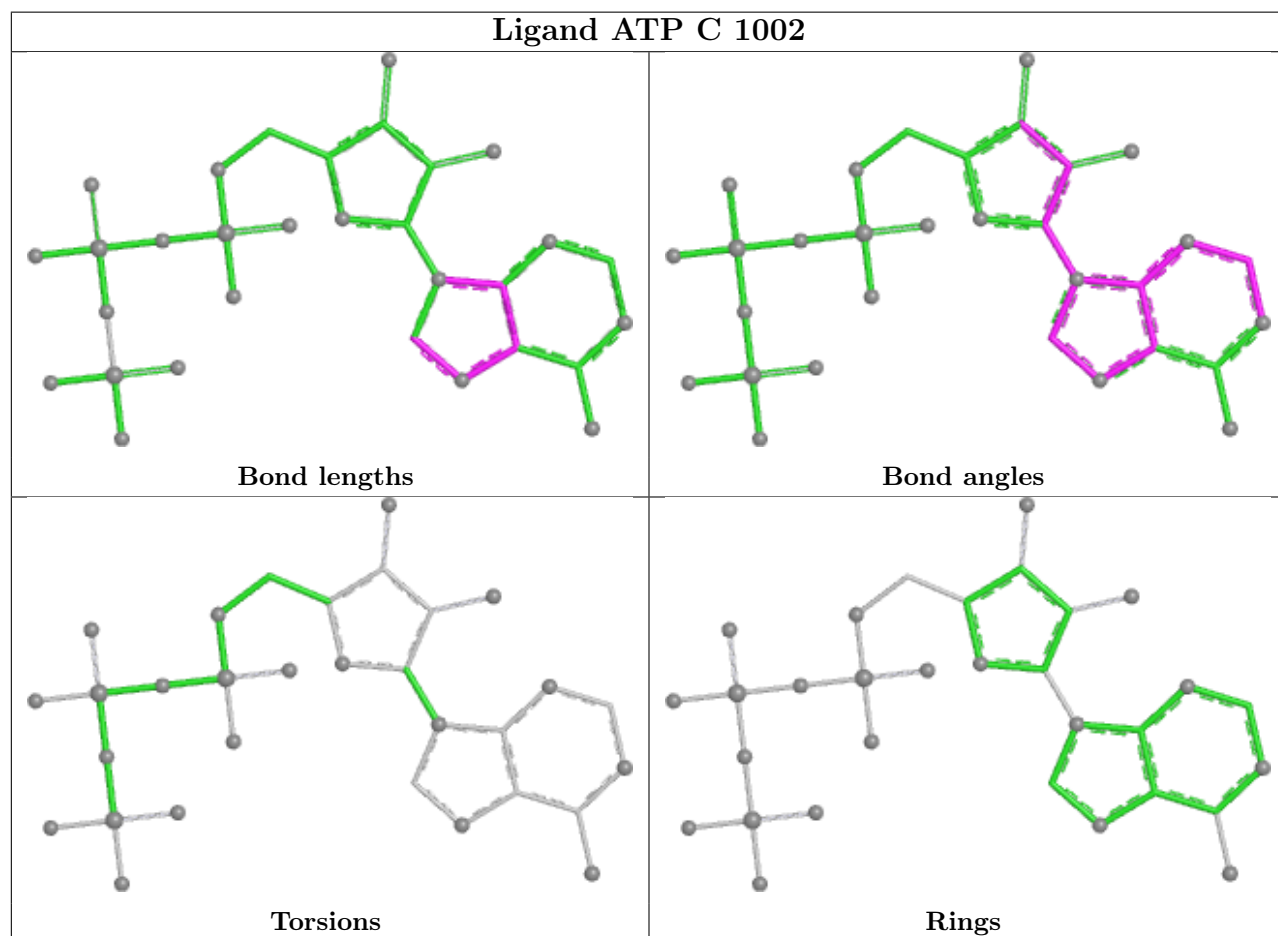
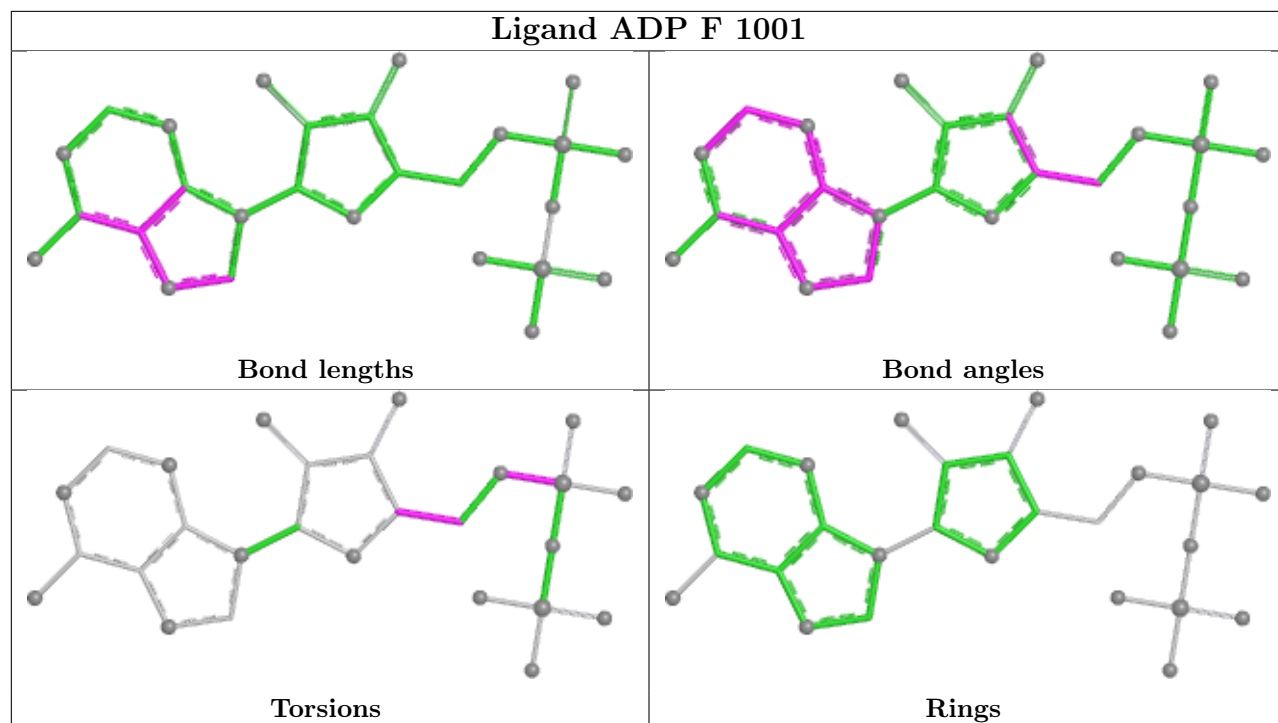
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

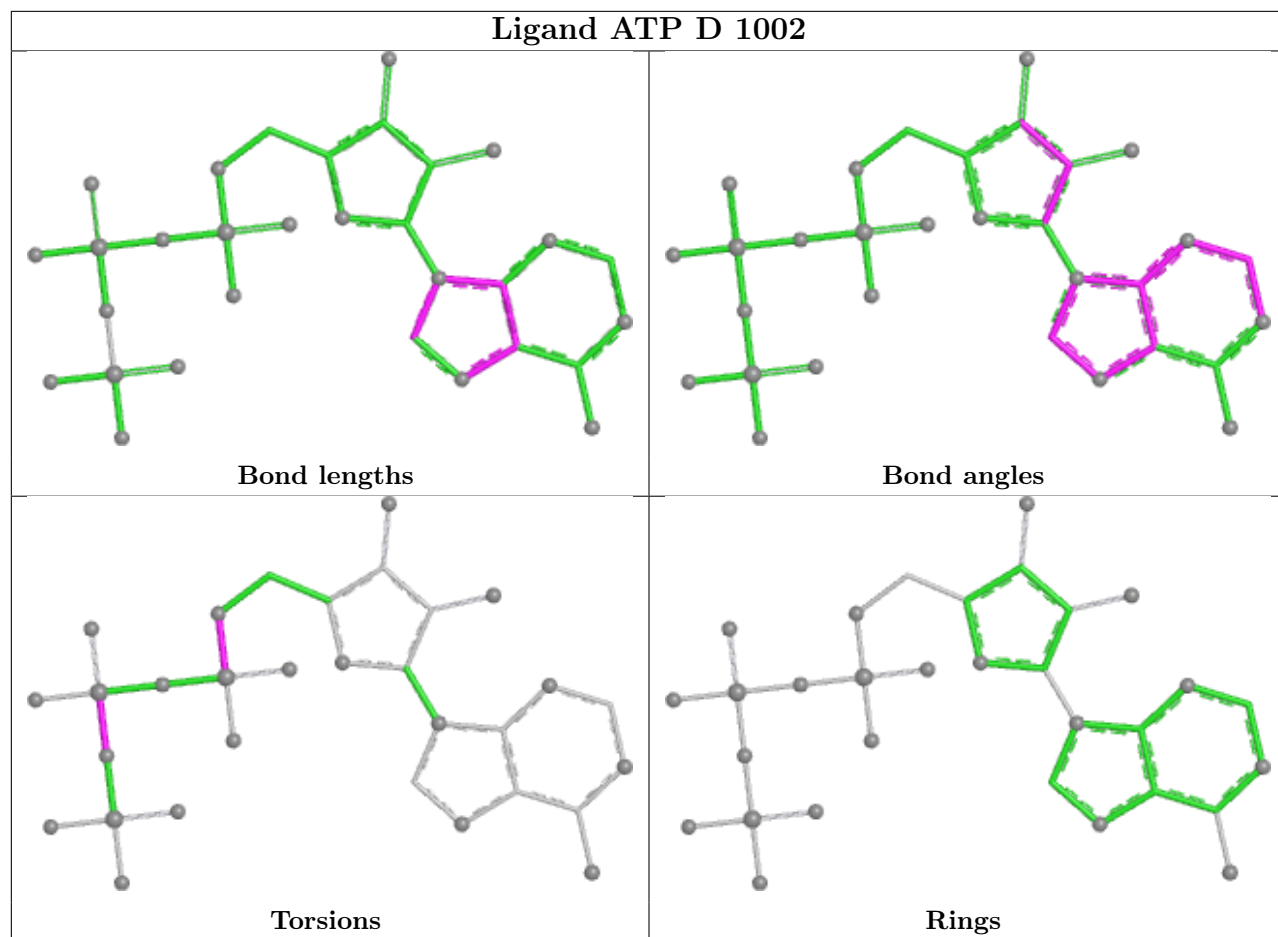
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

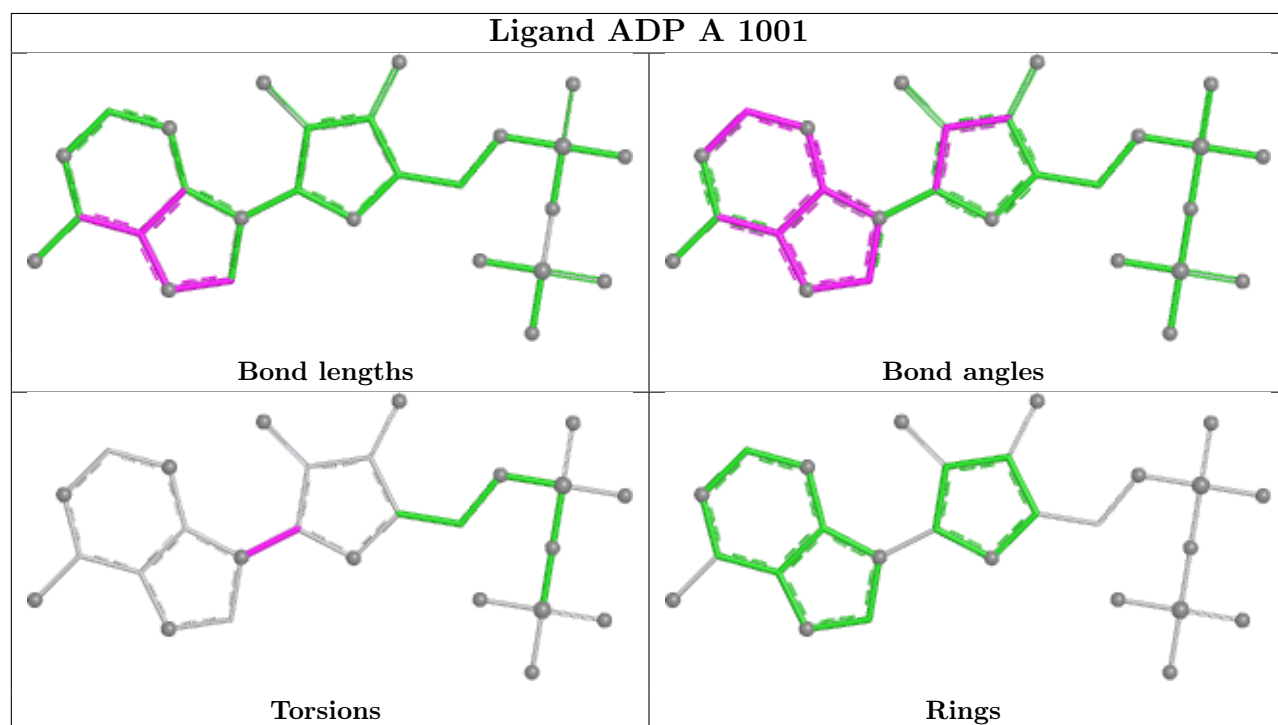
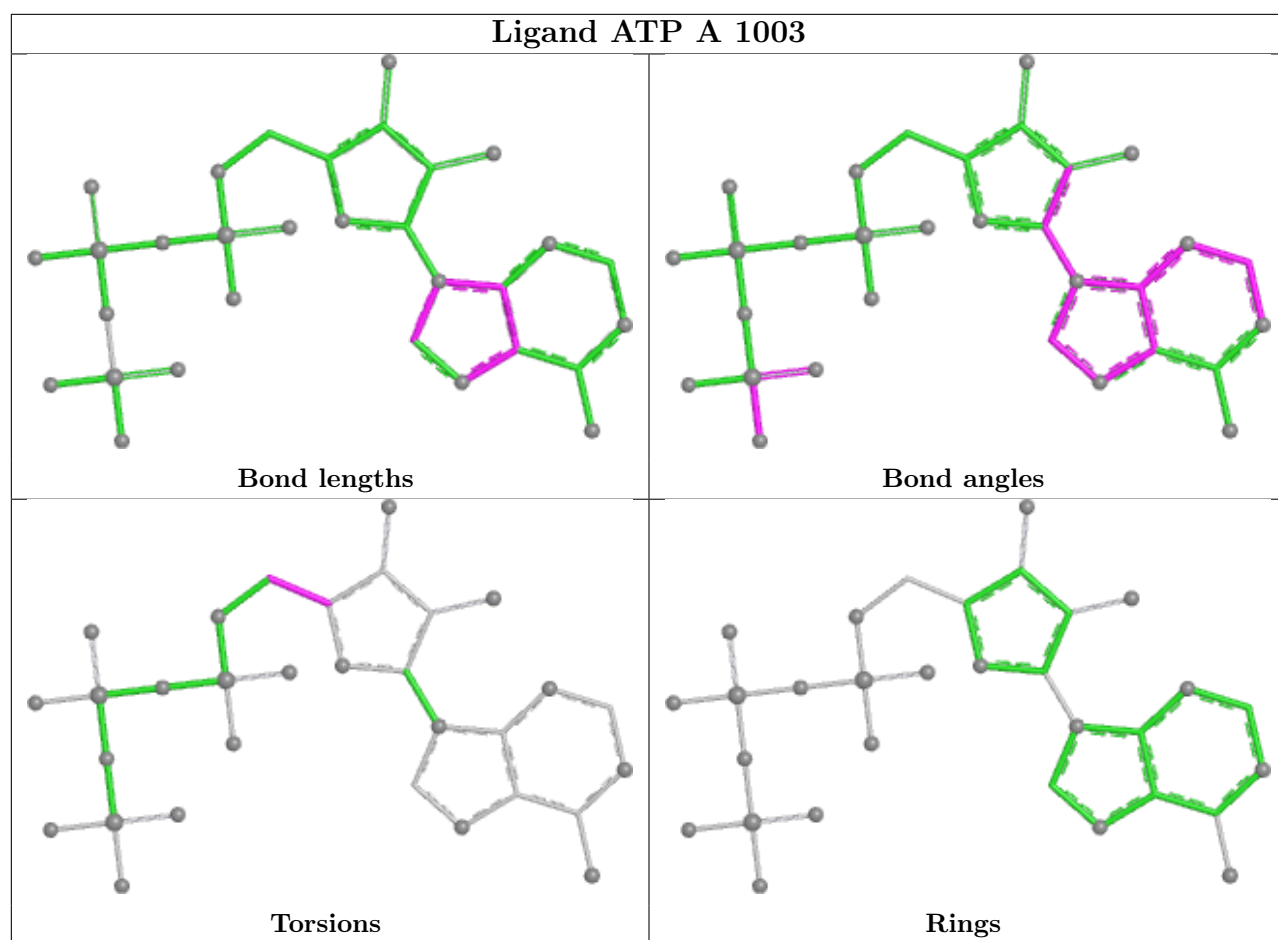


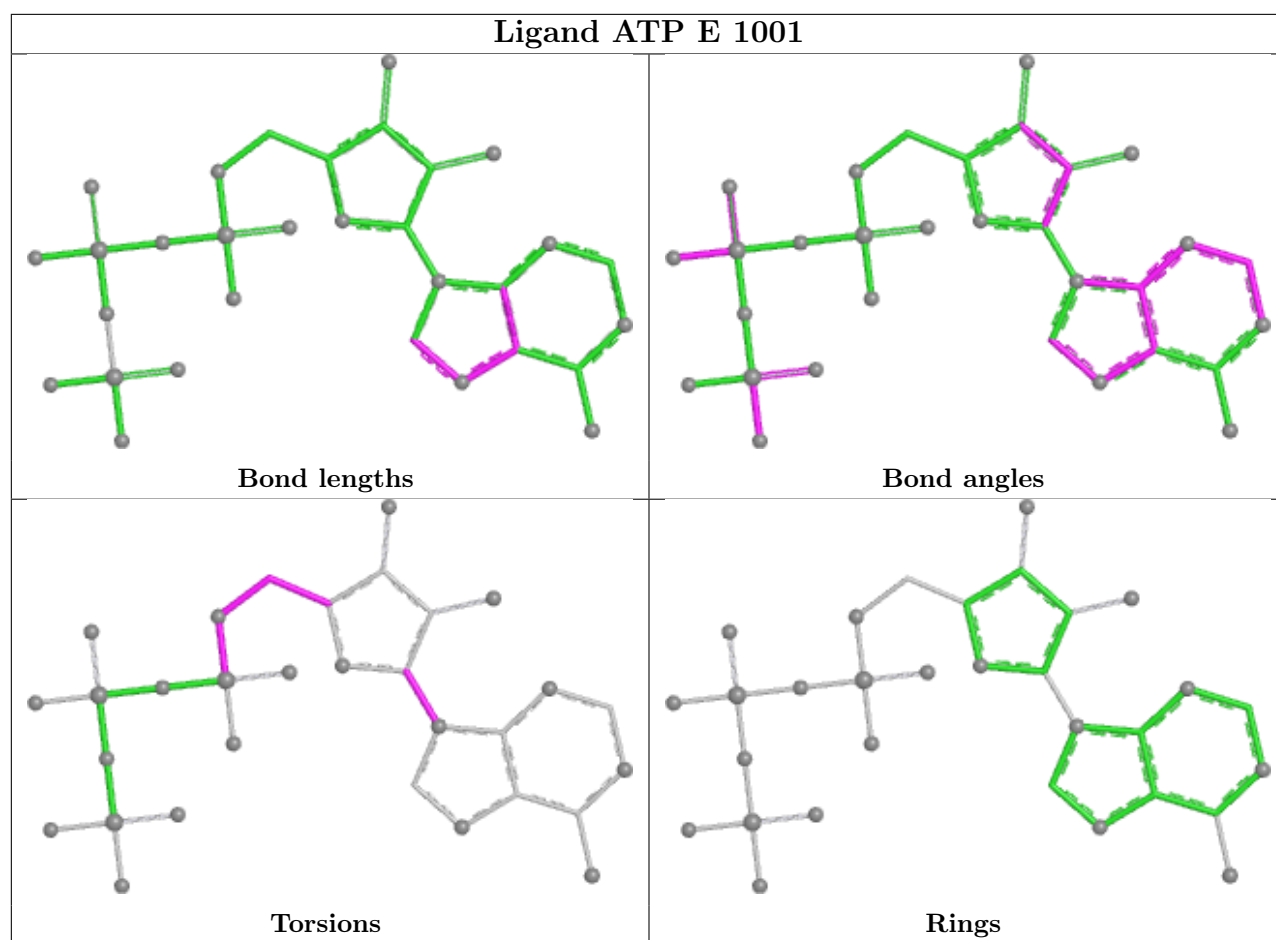












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

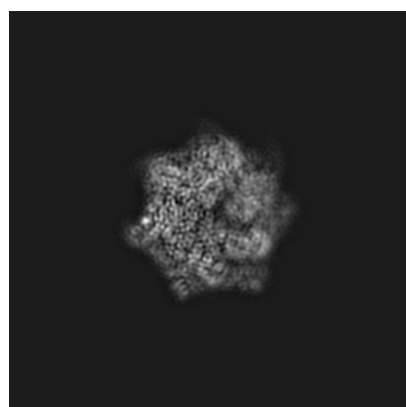
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11707. These allow visual inspection of the internal detail of the map and identification of artifacts.

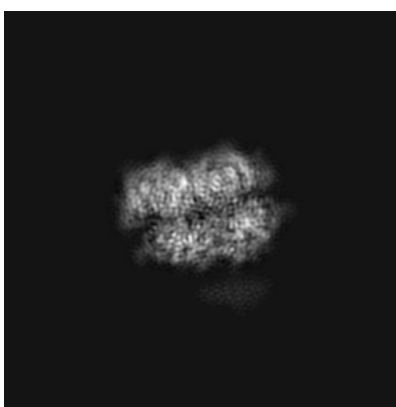
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

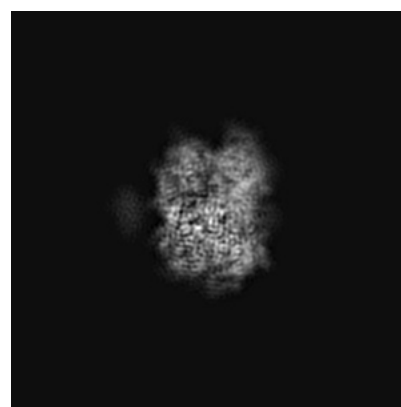
6.1.1 Primary map



X



Y

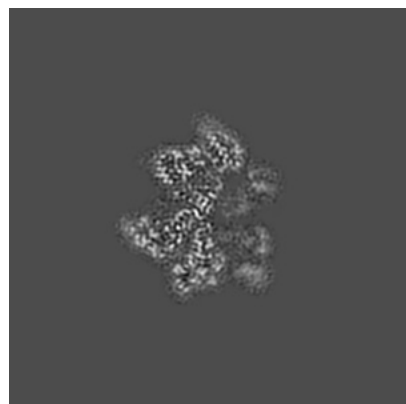


Z

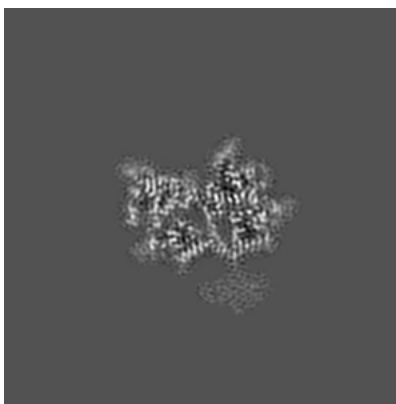
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

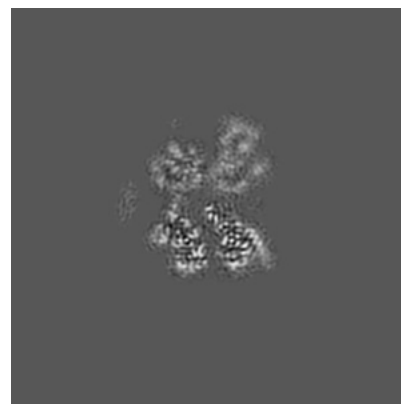
6.2.1 Primary map



X Index: 150



Y Index: 150

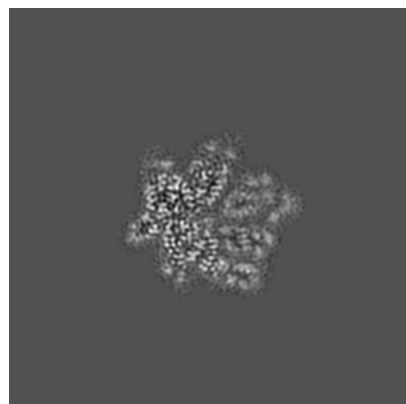


Z Index: 150

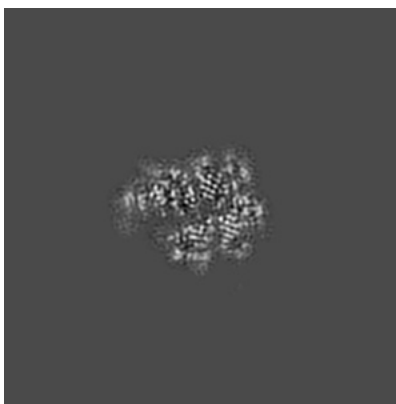
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 166



Y Index: 124

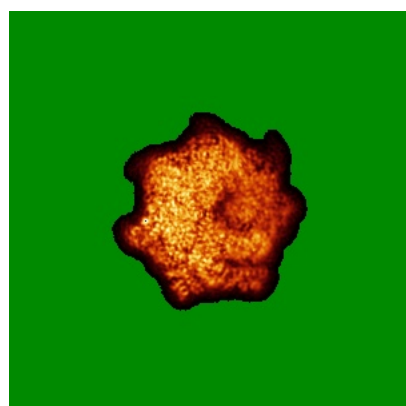


Z Index: 131

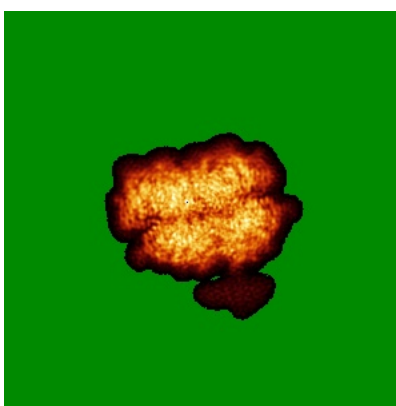
The images above show the largest variance slices of the map in three orthogonal directions.

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

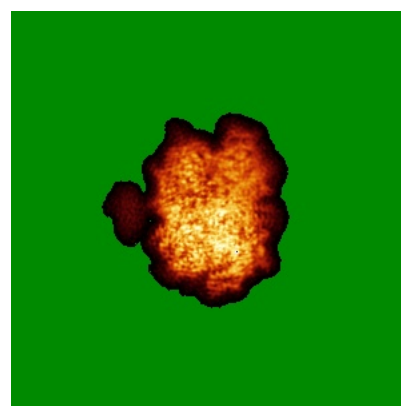
6.4.1 Primary map



X



Y

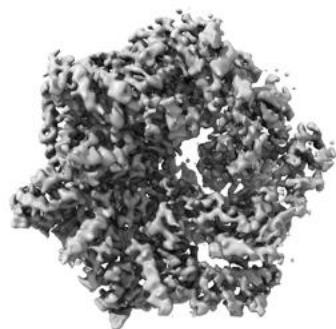


Z

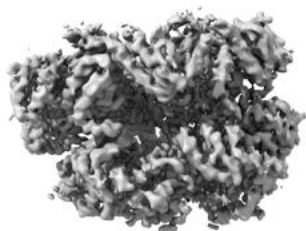
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

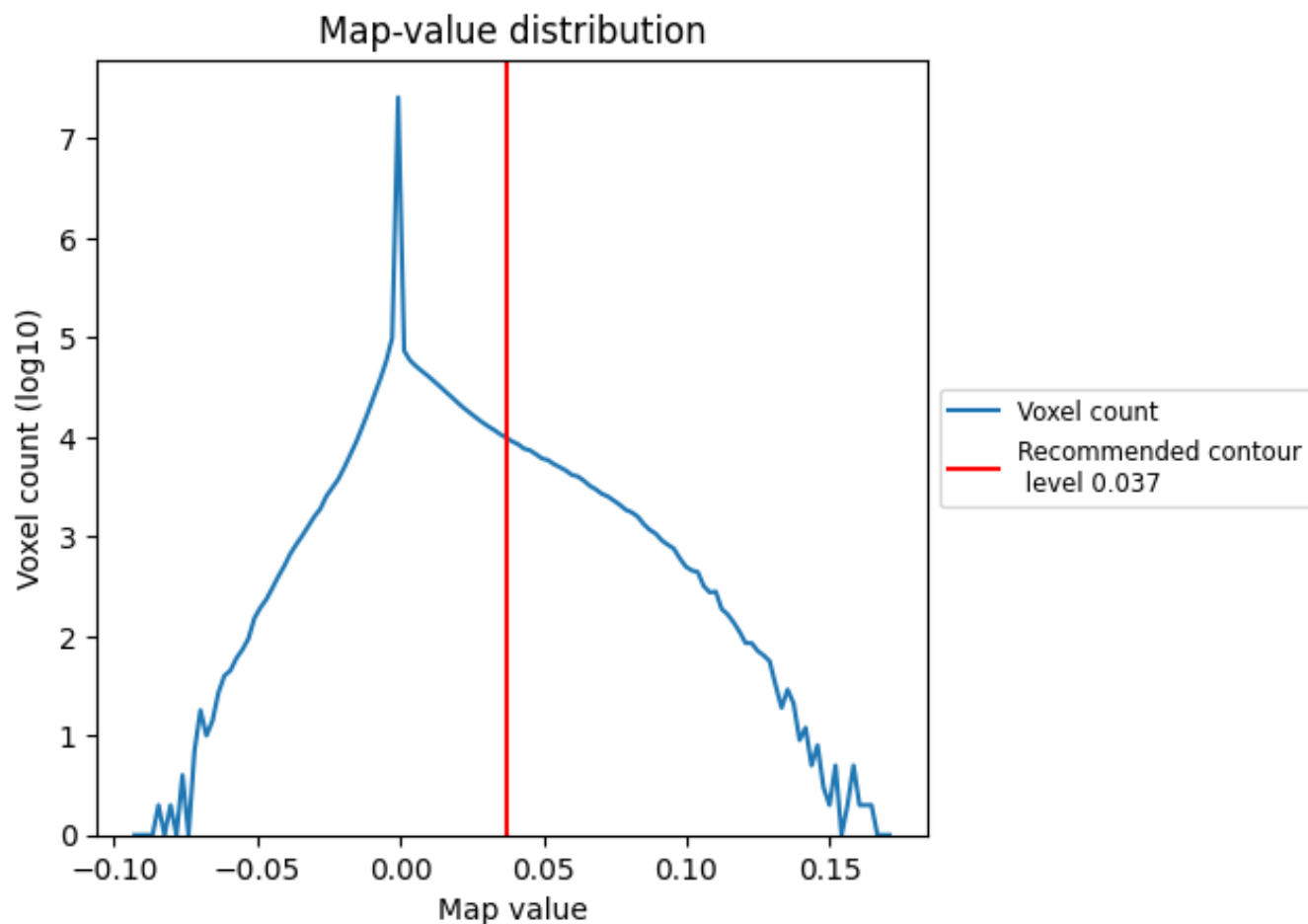
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

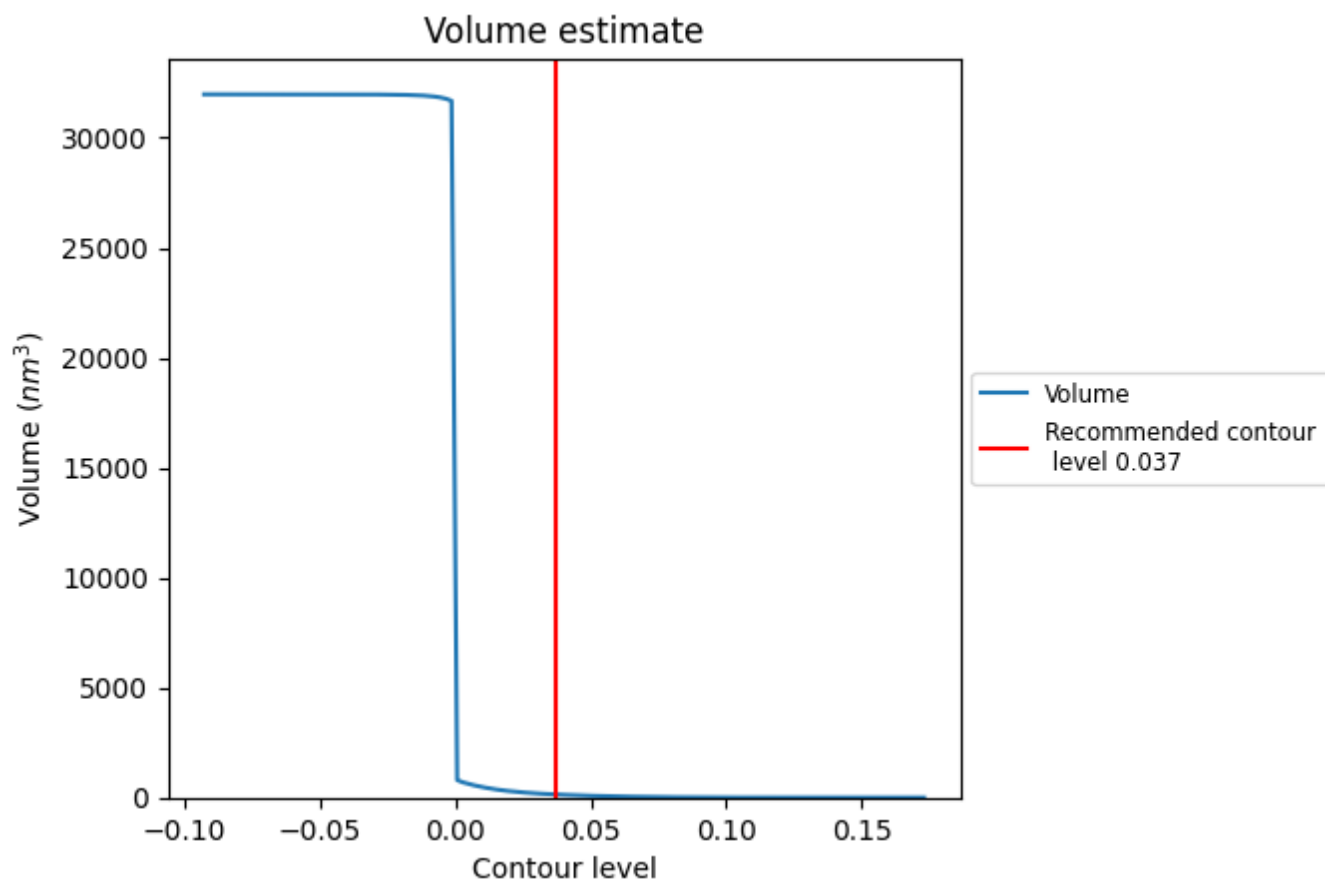
This section contains the results of statistical analysis of the map.

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.

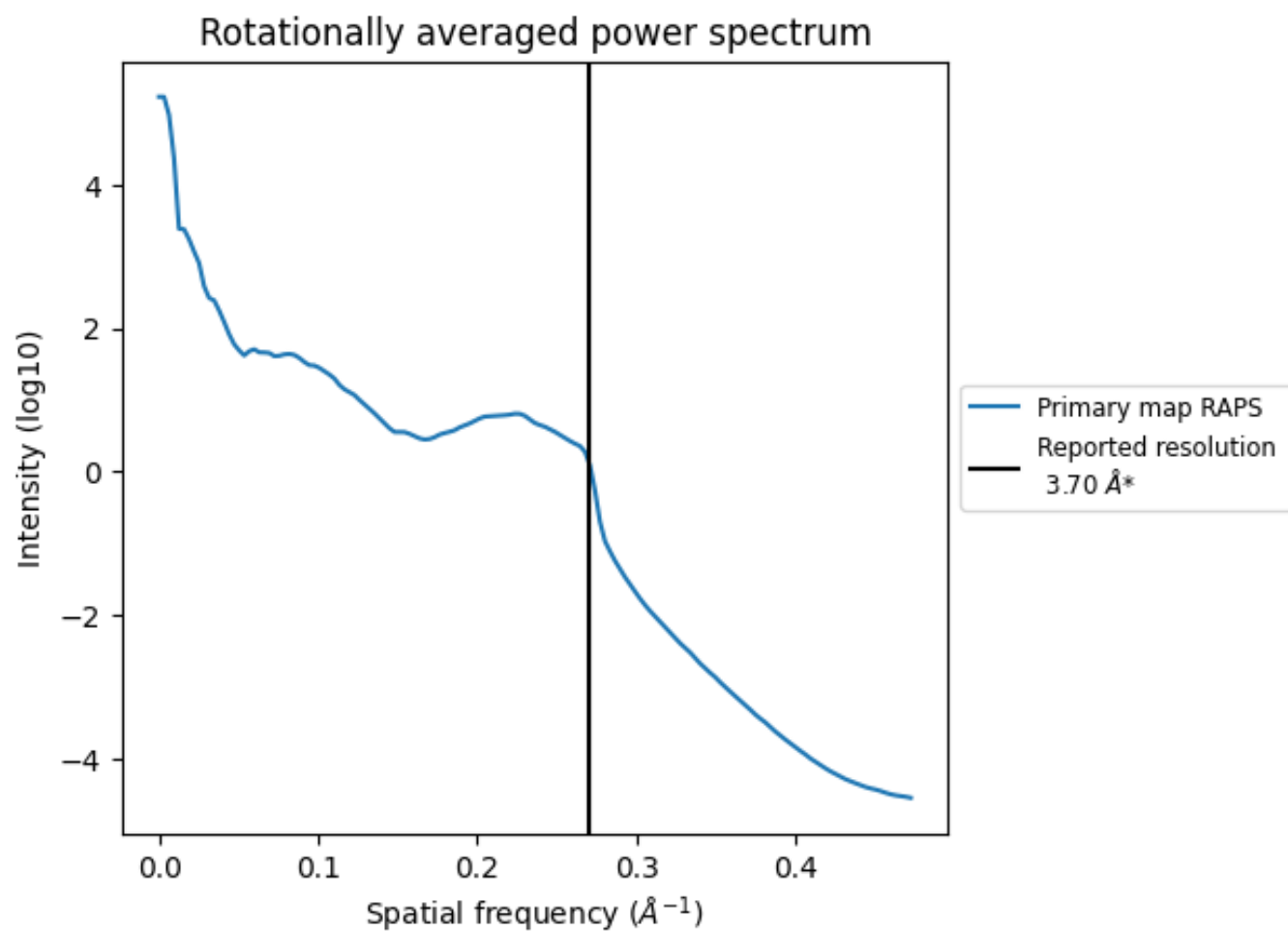
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 127 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 ⓘ

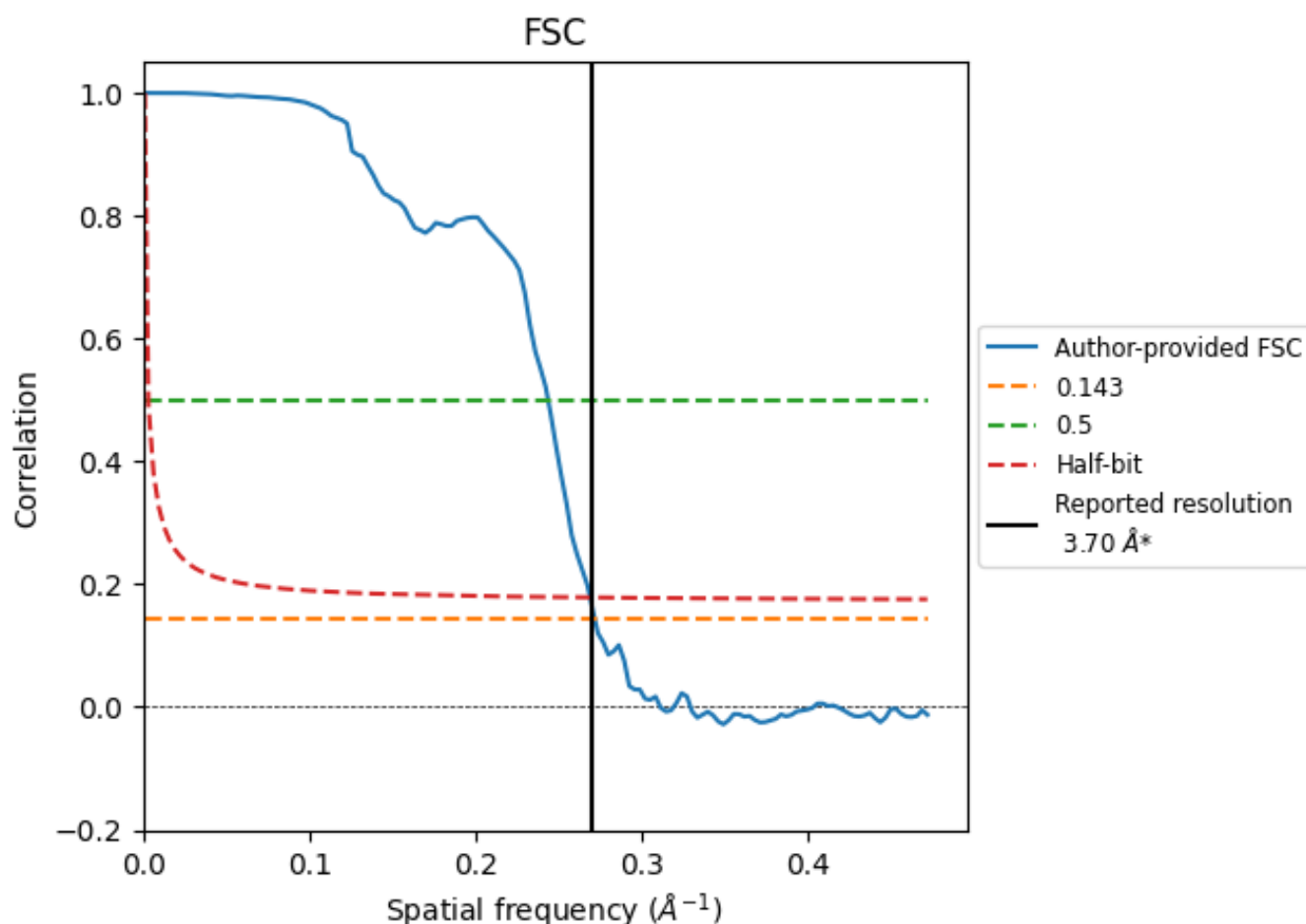


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.10	3.71
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

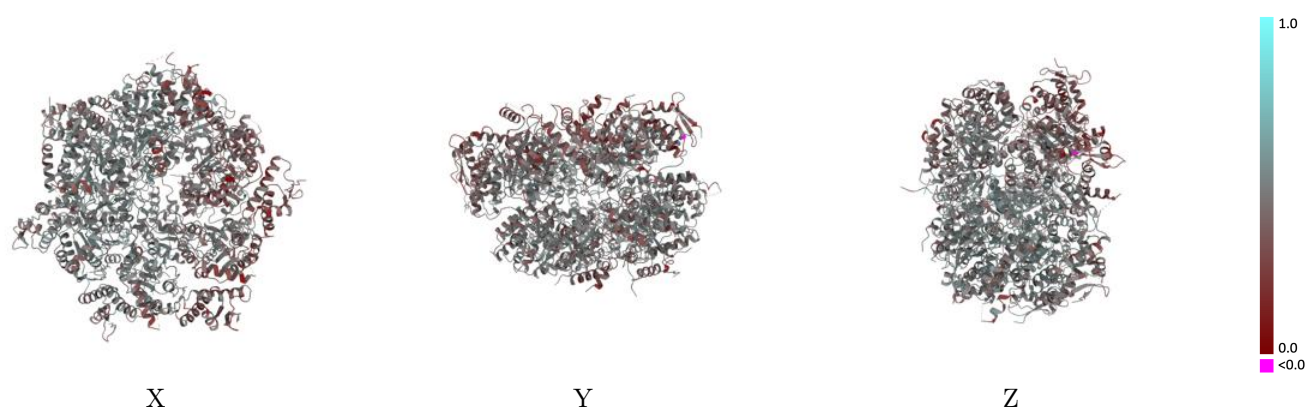
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11707 and PDB model 7ABR. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

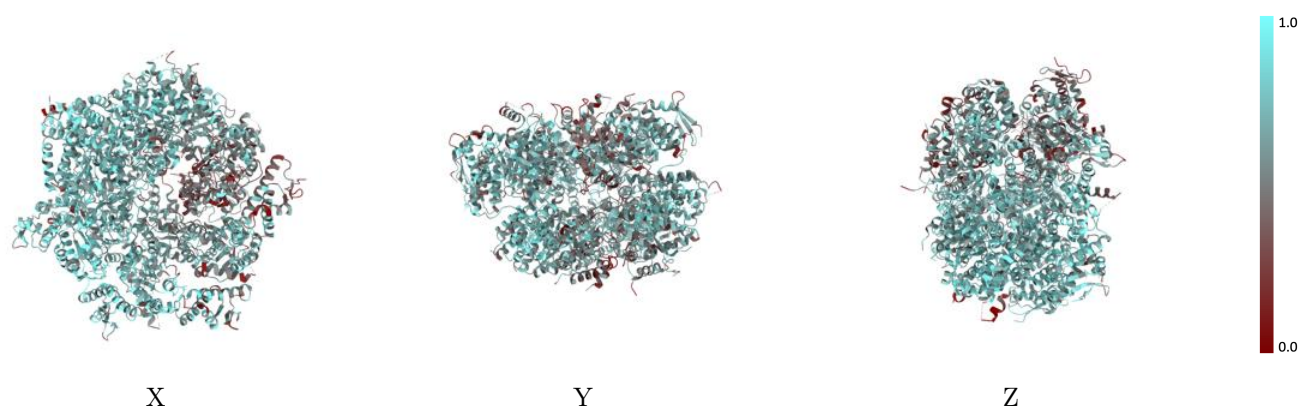
This section was not generated.

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



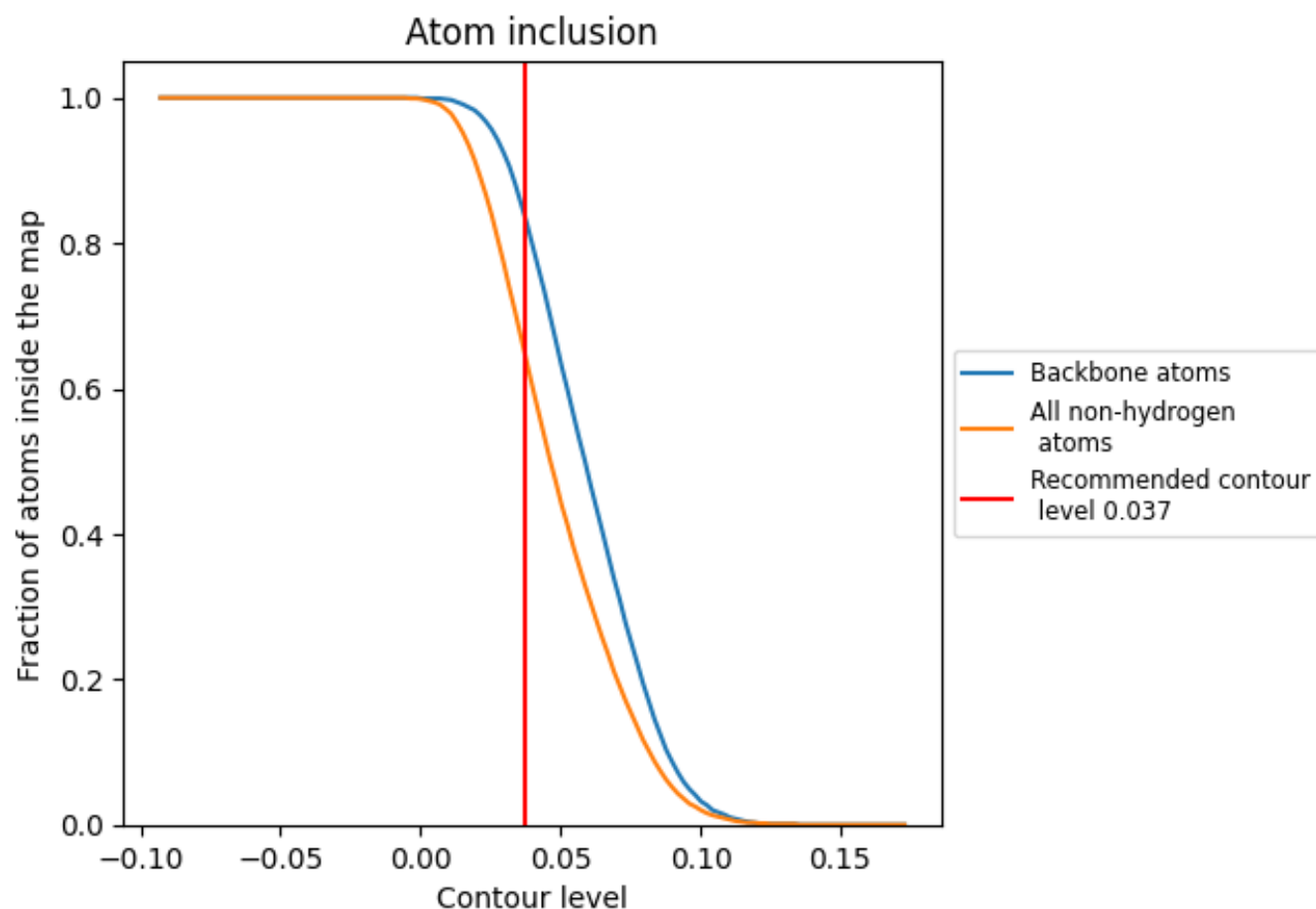
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.037).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.4540
A	0.5960	0.4260
B	0.6930	0.4630
C	0.7400	0.4900
D	0.7270	0.4850
E	0.6630	0.4630
F	0.4840	0.3940
S	0.7610	0.5120

1.0

0.0

<0.0