



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:58 AM UTC

PDB ID : 8W0F / pdb_00008w0f
EMDB ID : EMD-43708
Title : Cryo-EM structure of a human MCM2-7 double hexamer on dsDNA
Authors : Hunker, O.; Yang, R.; Bleichert, F.
Deposited on : 2024-02-13
Resolution : 2.80 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:

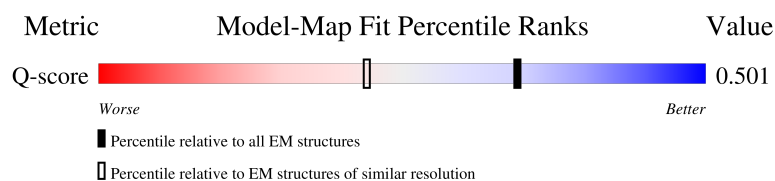
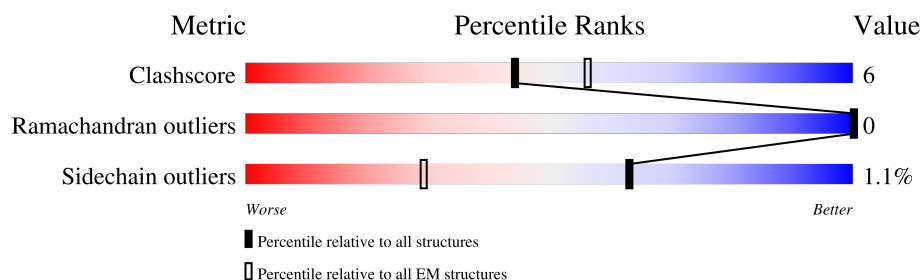
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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.



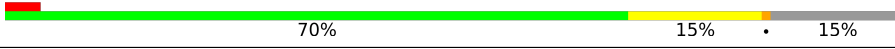
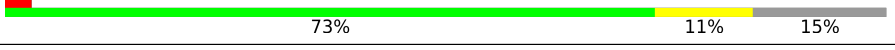
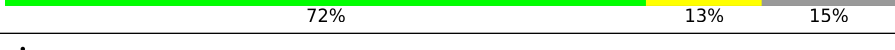
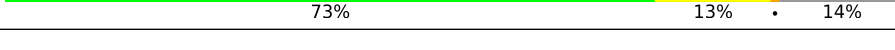
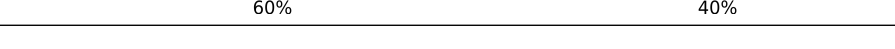
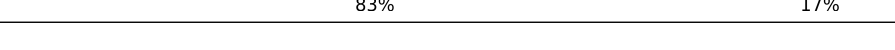
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	2	904	5% 62% 9% 28%
1	A	904	7% 63% 11% 26%
2	3	810	65% 13% 21%
2	B	810	8% 73% 7% 20%

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Mol	Chain	Length	Quality of chain
3	4	866	
3	C	866	
4	5	734	
4	D	734	
5	6	821	
5	E	821	
6	7	719	
6	F	719	
7	O	47	
8	S	47	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 126041 atoms, of which 62720 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	649	Total	C	H	N	O	S	0	0
			10277	3228	5143	917	959	30		
1	A	669	Total	C	H	N	O	S	0	0
			10605	3336	5302	948	989	30		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	638	Total	C	H	N	O	S	0	0
			10019	3126	5018	879	970	26		
2	B	651	Total	C	H	N	O	S	0	0
			10230	3189	5130	896	989	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-1	SER	-	expression tag	UNP P25205
3	0	ASN	-	expression tag	UNP P25205
3	1	ALA	-	expression tag	UNP P25205
B	-1	SER	-	expression tag	UNP P25205
B	0	ASN	-	expression tag	UNP P25205
B	1	ALA	-	expression tag	UNP P25205

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	648	Total	C	H	N	O	S	0	0
			10367	3246	5206	921	967	27		
3	C	646	Total	C	H	N	O	S	0	0
			10337	3237	5190	919	964	27		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-2	SER	-	expression tag	UNP P33991
4	-1	ASN	-	expression tag	UNP P33991
4	0	ALA	-	expression tag	UNP P33991
4	650	MET	LEU	variant	UNP P33991
C	-2	SER	-	expression tag	UNP P33991
C	-1	ASN	-	expression tag	UNP P33991
C	0	ALA	-	expression tag	UNP P33991
C	650	MET	LEU	variant	UNP P33991

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	627	Total	C	H	N	O	S	0	0
			9855	3073	4950	873	924	35		
4	D	625	Total	C	H	N	O	S	0	0
			9814	3061	4932	868	918	35		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	637	Total	C	H	N	O	S	0	0
			10175	3187	5099	903	960	26		
5	E	696	Total	C	H	N	O	S	0	0
			11209	3510	5631	986	1055	27		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	614	Total	C	H	N	O	S	0	0
			9804	3057	4928	865	922	32		
6	F	621	Total	C	H	N	O	S	0	0
			9921	3091	4988	878	932	32		

- Molecule 7 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	47	Total	C	H	N	O	P	0	0
			1505	470	542	163	283	47		

- Molecule 8 is a DNA chain called DNA (47-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	S	47	Total	C	H	N	O	P	0	0
			1505	470	541	166	281	47		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	2	1	Total	Zn	0
			1	1	
9	4	1	Total	Zn	0
			1	1	
9	5	1	Total	Zn	0
			1	1	
9	6	1	Total	Zn	0
			1	1	
9	7	1	Total	Zn	0
			1	1	
9	A	1	Total	Zn	0
			1	1	
9	C	1	Total	Zn	0
			1	1	
9	D	1	Total	Zn	0
			1	1	
9	E	1	Total	Zn	0
			1	1	
9	F	1	Total	Zn	0
			1	1	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

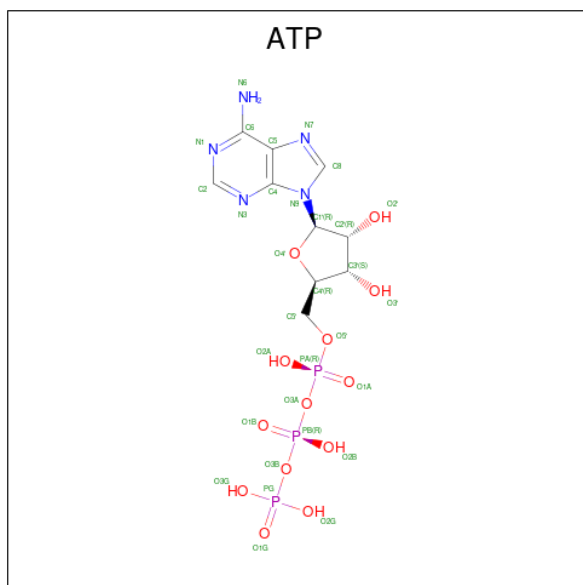
Mol	Chain	Residues	Atoms		AltConf
10	2	1	Total	Mg	0
			1	1	
10	3	1	Total	Mg	0
			1	1	
10	5	1	Total	Mg	0
			1	1	
10	6	1	Total	Mg	0
			1	1	
10	7	1	Total	Mg	0
			1	1	
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	

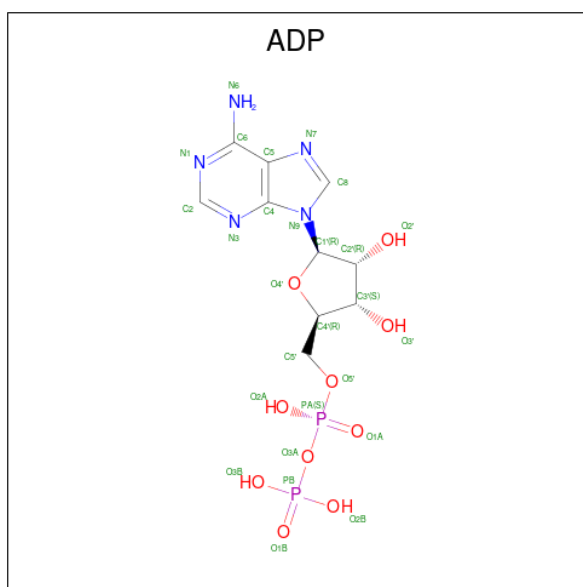
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Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



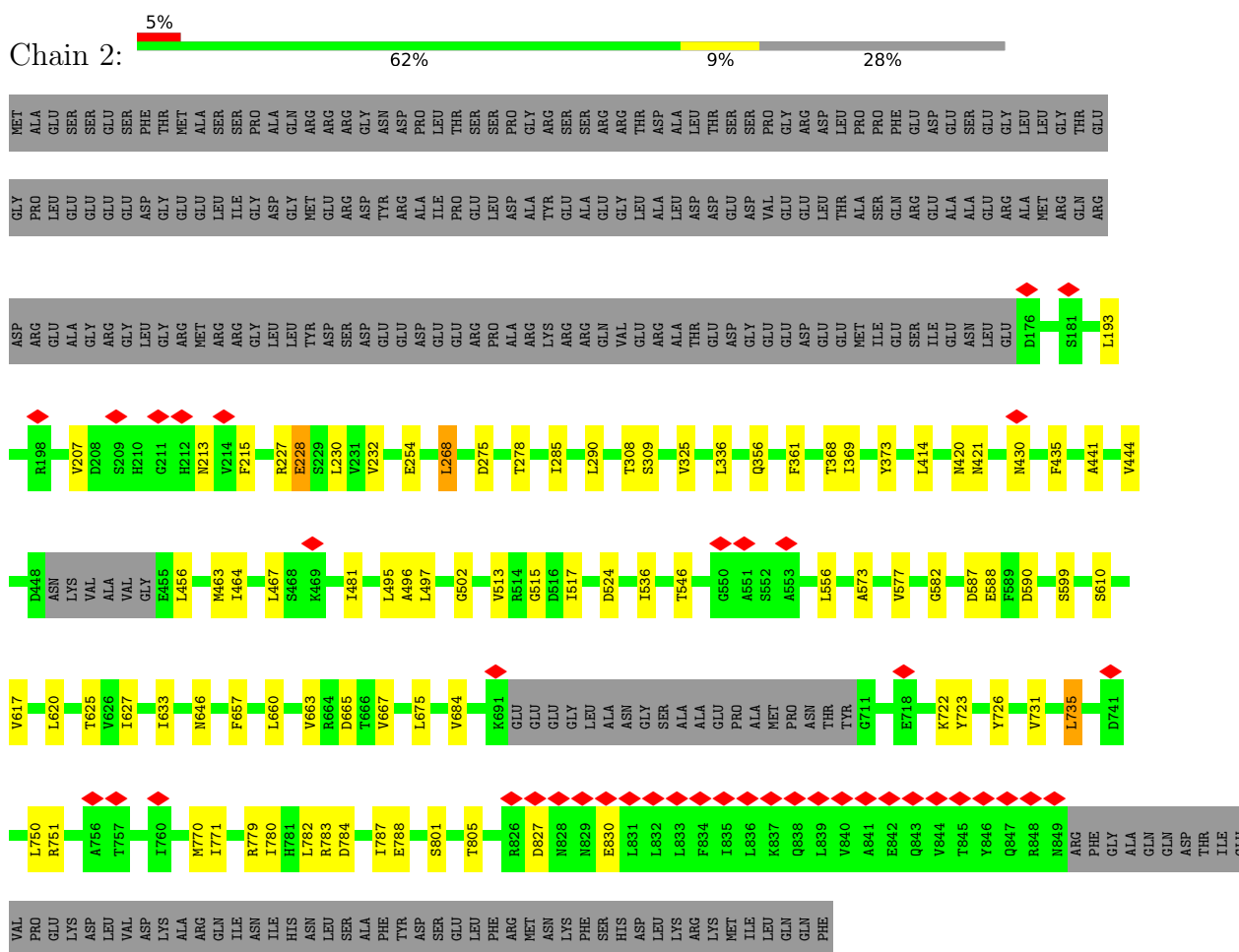


Mol	Chain	Residues	Atoms						AltConf
12	3	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	5	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	6	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	7	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
12	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

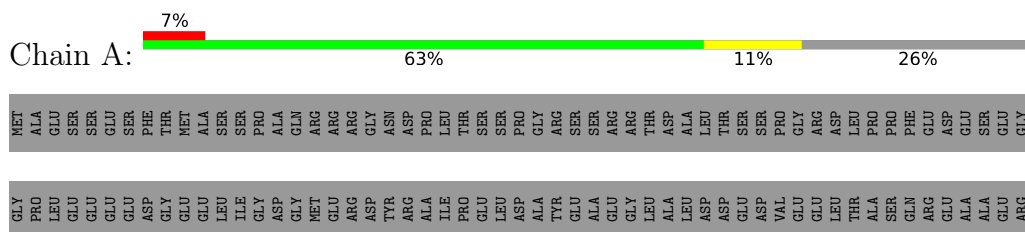
3 Residue-property plots

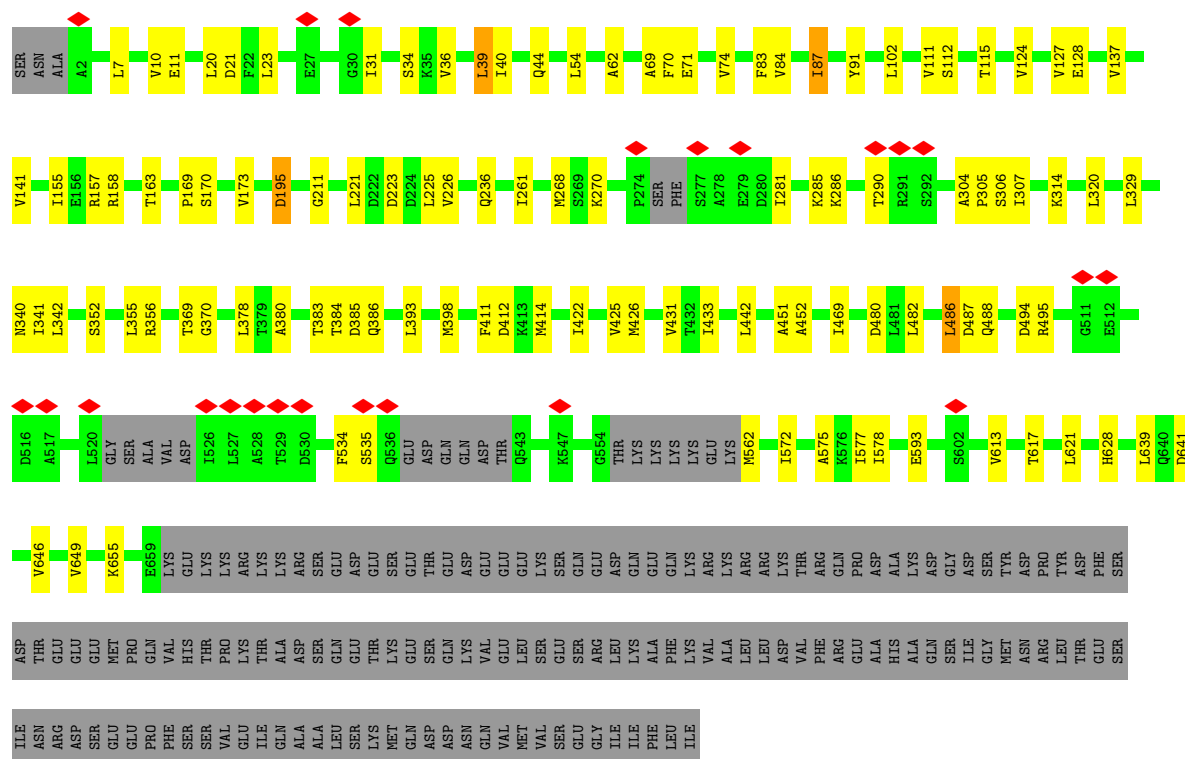
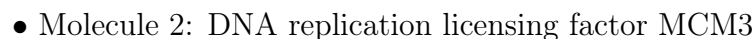
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA replication licensing factor MCM2



• Molecule 1: DNA replication licensing factor MCM2

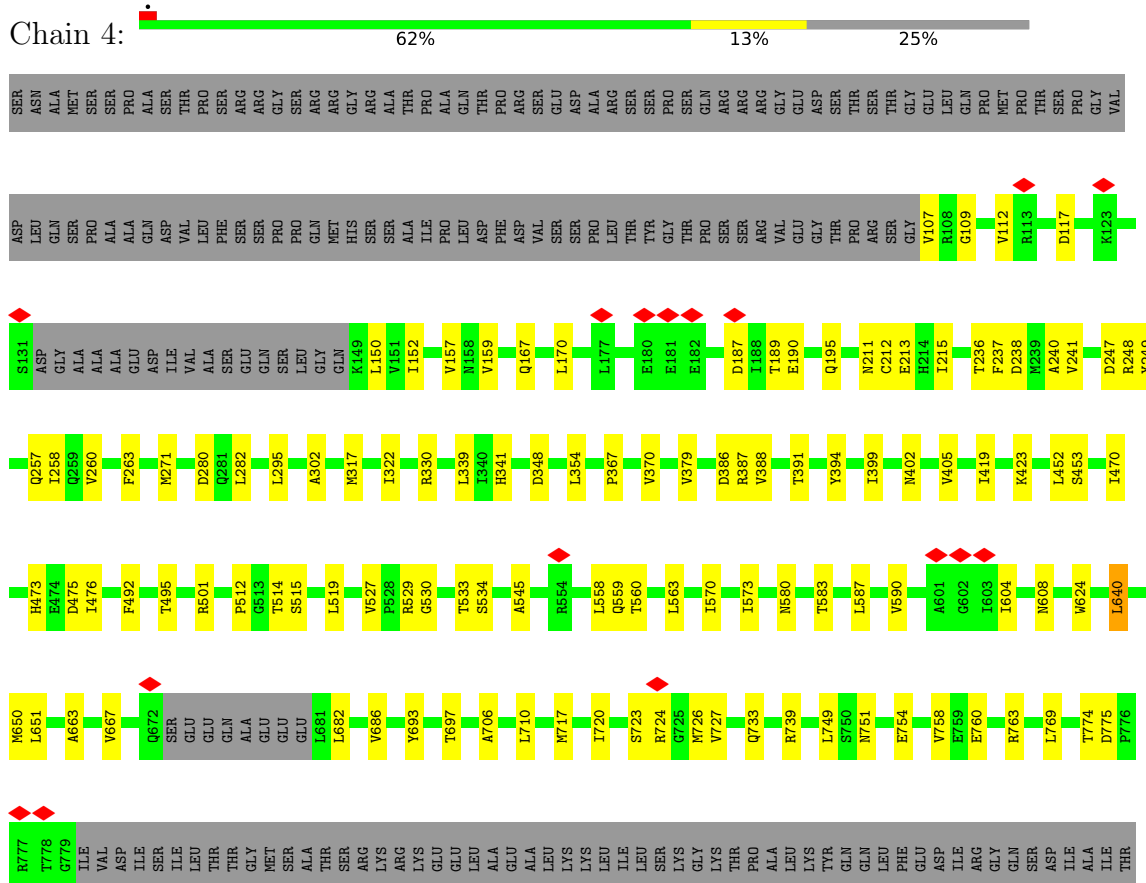




Chain B:



Chain 4:



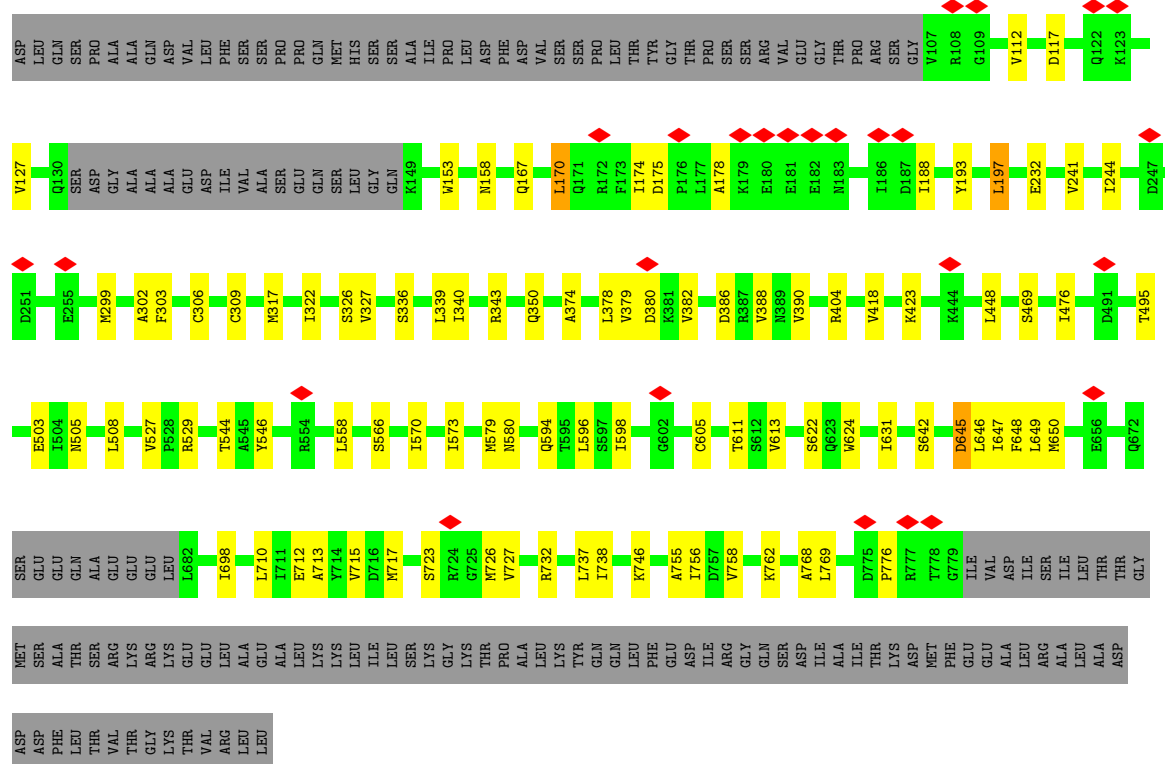
LYS
ASP
MET
PHE
GLU
GLU
ALA
ALA
LEU
ARG
ALA
LEU
LEU
ASP
ASP
PHE
PHE
LEU
THR
THR
THR
GLY
LEU
VAL
ARG
LEU
LEU

• Molecule 3: DNA replication licensing factor MCM4

Chain C:

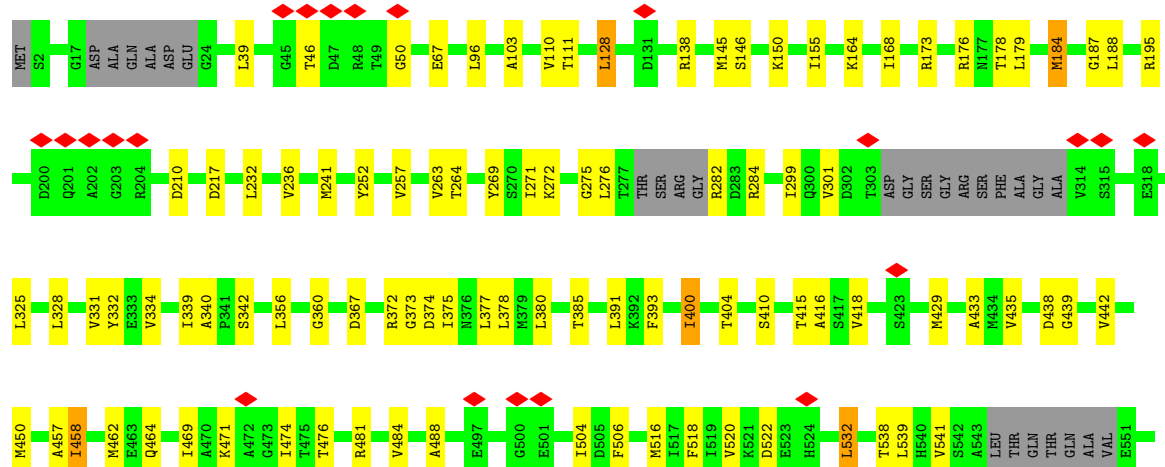


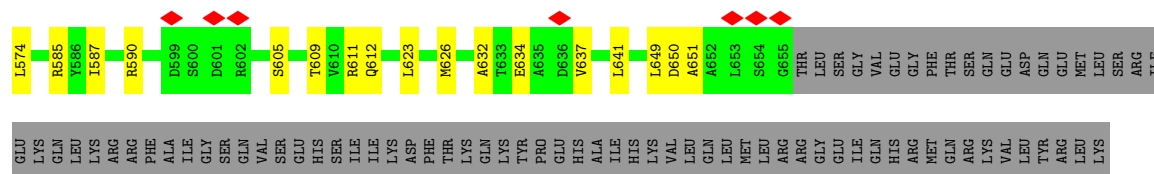
SER
ASN
ALA
MET
SER
SER
PRO
ALA
ALA
SER
THR
PRO
SER
PHE
SER
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SER
PHE
ARG
GLY
THR
THR
ALA
THR
LEU
VAL
GLN
THR
PRO
ASP
PHE
VAL
ASP
THR
SER
SER
GLN
ARG
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ARG
GLY
GLY
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LEU
GLN
PRO
MET
PRO
THR
SER
PRO
GLY
VAL



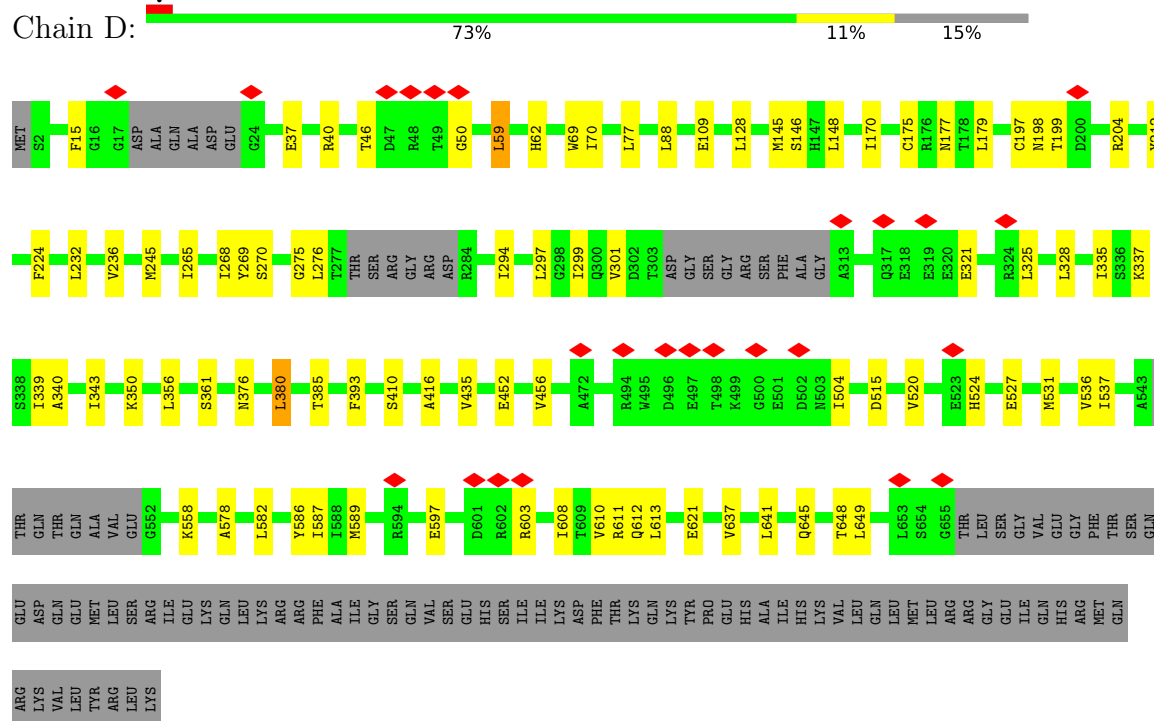
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:

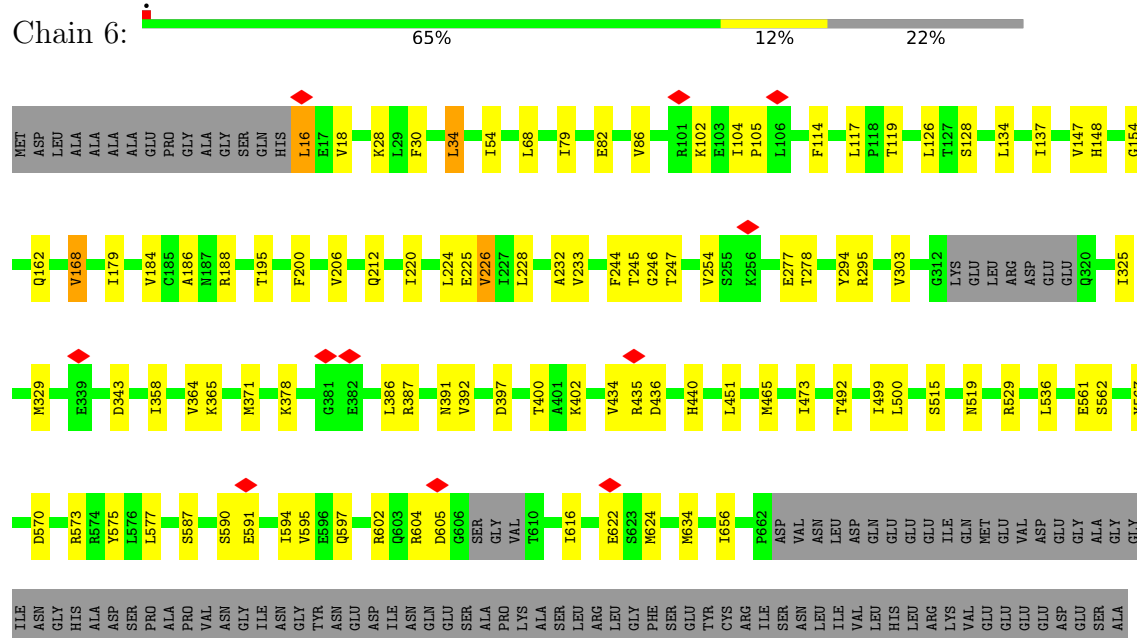




• Molecule 4: DNA replication licensing factor MCM5



• Molecule 5: DNA replication licensing factor MCM6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100748	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 ($e^-/\text{\AA}^2$)	50.96, 49.86	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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, ZN, ATP, MG

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	2	0.12	0/5229	0.28	0/7065
1	A	0.12	0/5401	0.28	0/7295
2	3	0.12	0/5076	0.26	0/6854
2	B	0.12	0/5179	0.28	0/6993
3	4	0.12	0/5252	0.28	0/7098
3	C	0.12	0/5238	0.28	0/7079
4	5	0.13	0/4982	0.28	0/6699
4	D	0.12	0/4959	0.27	0/6669
5	6	0.12	0/5159	0.26	0/6961
5	E	0.12	0/5663	0.25	0/7634
6	7	0.12	0/4950	0.26	0/6677
6	F	0.12	0/5008	0.27	0/6757
7	O	0.19	0/1079	0.47	0/1663
8	S	0.19	0/1081	0.47	0/1666
All	All	0.12	0/64256	0.28	0/87110

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5134	5143	5143	69	0
1	A	5303	5302	5302	76	0
2	3	5001	5018	5018	87	0
2	B	5100	5130	5130	45	0
3	4	5161	5206	5206	75	0
3	C	5147	5190	5190	71	0
4	5	4905	4950	4950	82	0
4	D	4882	4932	4932	64	0
5	6	5076	5099	5099	75	0
5	E	5578	5631	5631	78	0
6	7	4876	4928	4928	60	0
6	F	4933	4988	4988	72	0
7	O	963	542	542	19	0
8	S	964	541	541	6	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0
9	6	1	0	0	0	0
9	7	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
10	2	1	0	0	0	0
10	3	1	0	0	0	0
10	5	1	0	0	0	0
10	6	1	0	0	0	0
10	7	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
11	2	31	12	12	3	0
11	A	31	12	12	1	0
12	3	27	12	12	1	0
12	5	27	12	12	2	0
12	6	27	12	12	1	0
12	7	27	12	12	0	0
12	B	27	12	12	1	0
12	D	27	12	12	0	0
12	E	27	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	F	27	12	12	1	0
All	All	63321	62720	62720	806	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (806) 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)
2:3:378:LEU:HD21	2:3:422:ILE:HD11	1.47	0.94
6:7:340:ILE:HD11	6:7:394:ILE:HD11	1.50	0.93
3:C:170:LEU:HD21	3:C:241:VAL:HG12	1.56	0.87
6:F:588:MET:HE1	6:F:609:ILE:HD11	1.63	0.81
12:3:1002:ADP:O3A	4:5:611:ARG:NH2	2.17	0.77
3:C:476:ILE:HD13	3:C:650:MET:HE2	1.68	0.76
1:2:573:ALA:HB1	1:2:577:VAL:HG21	1.66	0.75
6:F:588:MET:CE	6:F:609:ILE:HD11	2.17	0.75
5:E:575:TYR:OH	5:E:634:MET:O	2.04	0.75
3:4:302:ALA:HB2	3:4:322:ILE:HD13	1.69	0.74
1:A:203:LEU:HD12	1:A:266:VAL:HG11	1.69	0.74
3:C:642:SER:OG	3:C:732:ARG:NH1	2.21	0.74
1:2:502:GLY:O	1:2:779:ARG:NH1	2.20	0.74
1:A:302:LEU:HD22	1:A:420:ASN:HB2	1.71	0.73
3:4:238:ASP:OD1	3:4:260:VAL:HG12	1.88	0.72
3:C:232:GLU:OE1	3:C:232:GLU:N	2.22	0.71
4:5:609:THR:N	4:5:612:GLN:OE1	2.23	0.71
3:C:127:VAL:HG21	3:C:153:TRP:HE3	1.55	0.71
3:C:503:GLU:OE1	3:C:594:GLN:NE2	2.24	0.71
6:7:585:TYR:HB2	6:7:606:LEU:HD23	1.73	0.70
3:4:187:ASP:N	3:4:195:GLN:OE1	2.23	0.70
3:4:545:ALA:HB1	3:4:558:LEU:HD21	1.73	0.70
4:D:335:ILE:O	4:D:339:ILE:HG23	1.90	0.70
1:A:801:SER:O	1:A:805:THR:HG23	1.92	0.69
2:B:40:ILE:HD11	2:B:84:VAL:HG13	1.74	0.69
2:3:414:MET:HE1	2:3:422:ILE:CD1	2.23	0.69
4:5:46:THR:O	4:5:50:GLY:N	2.25	0.69
6:F:356:LEU:HD13	6:F:612:LEU:HD22	1.75	0.69
5:E:54:ILE:HD13	5:E:102:LYS:HZ3	1.56	0.68
4:5:145:MET:O	4:5:146:SER:OG	2.07	0.68
4:5:415:THR:HG21	4:5:457:ALA:HB3	1.74	0.68
1:A:456:LEU:O	1:A:456:LEU:HD23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:241:VAL:HG11	3:4:258:ILE:HG21	1.77	0.67
1:A:248:LEU:HD21	1:A:285:ILE:HG13	1.76	0.67
3:C:174:ILE:HD12	3:C:174:ILE:O	1.93	0.67
1:2:675:LEU:HD11	11:2:1002:ATP:C6	2.30	0.67
3:4:387:ARG:NH2	3:4:530:GLY:O	2.27	0.67
4:5:504:ILE:HD12	4:5:504:ILE:O	1.95	0.67
2:B:287:PHE:CE2	2:B:295:ILE:HD11	2.30	0.66
2:B:384:THR:OG1	8:S:-38:DA:OP1	2.13	0.66
2:3:281:ILE:HG22	2:3:285:LYS:NZ	2.11	0.66
3:4:271:MET:SD	3:4:370:VAL:HG11	2.36	0.66
1:2:723:TYR:OH	1:2:780:ILE:O	2.10	0.66
6:7:581:ILE:HG22	6:7:606:LEU:HD21	1.79	0.65
6:7:36:GLN:O	6:7:40:LEU:HD12	1.97	0.65
4:D:612:GLN:N	4:D:612:GLN:OE1	2.30	0.65
4:D:46:THR:O	4:D:50:GLY:N	2.30	0.65
2:3:575:ALA:O	2:3:578:ILE:HG22	1.97	0.65
5:6:68:LEU:HD21	5:6:79:ILE:HD12	1.79	0.65
4:5:385:THR:HG21	4:5:520:VAL:HG12	1.78	0.65
2:3:69:ALA:HB2	2:3:124:VAL:HG23	1.78	0.64
3:4:706:ALA:HB2	3:4:754:GLU:HA	1.79	0.64
5:6:16:LEU:O	5:6:16:LEU:HD13	1.98	0.64
6:F:343:GLU:O	6:F:536:HIS:NE2	2.31	0.64
4:5:439:GLY:N	4:5:481:ARG:O	2.31	0.64
7:O:40:DT:H2'	7:O:41:DT:H72	1.80	0.64
3:4:470:ILE:HD13	3:4:519:LEU:HD22	1.79	0.64
5:E:147:VAL:HG13	5:E:233:VAL:HG21	1.79	0.64
6:F:56:ALA:HB2	6:F:63:VAL:HG21	1.80	0.64
7:O:31:DT:H2''	7:O:32:DT:H72	1.78	0.64
6:F:276:ILE:HD13	6:F:299:GLU:OE2	1.98	0.63
1:2:620:LEU:HD23	1:2:620:LEU:H	1.63	0.63
5:6:54:ILE:HG21	5:6:102:LYS:HG2	1.81	0.63
4:D:77:LEU:CD2	4:D:88:LEU:HD12	2.28	0.63
6:F:256:LEU:HD12	6:F:297:TYR:CD2	2.32	0.63
2:3:304:ALA:O	2:3:314:LYS:NZ	2.27	0.63
4:5:385:THR:HG21	4:5:520:VAL:CG1	2.28	0.63
4:5:415:THR:HG21	4:5:457:ALA:CB	2.28	0.63
4:5:332:TYR:CD1	4:5:626:MET:HE1	2.34	0.62
5:6:114:PHE:O	5:6:245:THR:HG21	1.99	0.62
4:D:128:LEU:HD12	4:D:128:LEU:O	1.99	0.62
2:3:380:ALA:HB2	2:3:442:LEU:HD12	1.81	0.62
3:C:302:ALA:HB2	3:C:322:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:527:VAL:HG11	3:C:570:ILE:HD12	1.80	0.62
6:F:416:ALA:HB2	6:F:478:LEU:HD21	1.79	0.62
6:F:415:THR:HG23	6:F:467:ILE:HG21	1.80	0.62
1:A:177:LEU:O	1:A:177:LEU:HD12	1.99	0.62
6:7:337:ALA:O	6:7:340:ILE:HG22	2.00	0.62
3:4:580:ASN:OD1	3:4:583:THR:HG22	1.98	0.62
5:6:597:GLN:HB2	5:6:624:MET:HE1	1.80	0.62
3:C:386:ASP:OD1	3:C:529:ARG:NH1	2.33	0.61
2:3:102:LEU:HD12	2:3:124:VAL:HG11	1.82	0.61
4:5:462:MET:SD	4:5:484:VAL:HG21	2.40	0.61
12:B:1002:ADP:O1B	4:D:611:ARG:NH2	2.33	0.61
2:3:340:ASN:N	2:3:480:ASP:OD2	2.28	0.61
3:C:546:TYR:O	3:C:558:LEU:HD12	1.99	0.60
6:7:581:ILE:CG2	6:7:606:LEU:HD21	2.31	0.60
3:4:341:HIS:ND1	5:6:294:TYR:OH	2.34	0.60
1:A:288:LEU:HD12	1:A:415:THR:HG23	1.84	0.60
1:A:516:ASP:HB3	1:A:625:THR:HG22	1.84	0.60
3:4:560:THR:CG2	5:6:220:ILE:HD11	2.31	0.60
4:5:377:LEU:HD23	4:5:378:LEU:N	2.17	0.60
5:6:587:SER:O	5:6:590:SER:OG	2.20	0.60
6:7:146:PRO:HA	6:7:162:THR:HG23	1.84	0.59
3:4:280:ASP:N	3:4:394:TYR:O	2.32	0.59
5:6:591:GLU:O	5:6:595:VAL:HG13	2.01	0.59
2:3:195:ASP:HB3	2:3:226:VAL:HG11	1.83	0.59
3:4:388:VAL:HG12	3:4:423:LYS:HD2	1.84	0.59
3:C:544:THR:HA	3:C:596:LEU:HD21	1.83	0.59
1:2:582:GLY:O	1:2:625:THR:HG22	2.03	0.59
1:A:422:TYR:OH	1:A:436:ALA:O	2.16	0.59
2:B:25:ASP:OD1	2:B:31:ILE:N	2.35	0.59
7:O:32:DT:H2'	7:O:33:DT:H72	1.83	0.59
2:3:342:LEU:HD23	2:3:482:LEU:HD13	1.83	0.59
1:A:325:VAL:HA	1:A:368:THR:HG23	1.85	0.59
6:F:256:LEU:HD12	6:F:297:TYR:CE2	2.37	0.59
8:S:-14:DT:H2'	8:S:-13:DT:H72	1.85	0.59
3:4:558:LEU:HD23	3:4:559:GLN:N	2.18	0.59
6:7:223:GLN:O	6:7:227:SER:OG	2.17	0.59
1:A:222:MET:CE	1:A:281:ILE:HD12	2.32	0.59
6:7:374:ASN:OD1	6:7:465:GLN:NE2	2.34	0.58
6:F:362:VAL:HG22	6:F:614:THR:HG21	1.84	0.58
2:3:378:LEU:CD2	2:3:422:ILE:HD11	2.26	0.58
4:5:623:LEU:HA	4:5:626:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:404:THR:HG21	4:5:433:ALA:HB2	1.85	0.58
1:2:633:ILE:HG22	1:2:646:ASN:O	2.03	0.58
2:3:398:MET:SD	2:3:425:VAL:HG11	2.43	0.58
2:3:221:LEU:HD13	2:3:225:LEU:O	2.04	0.58
6:7:452:GLU:O	6:7:456:THR:HG23	2.04	0.58
2:3:383:THR:HG22	2:3:384:THR:H	1.69	0.57
4:5:168:ILE:HD13	4:5:184:MET:HE1	1.85	0.57
3:C:756:ILE:HD12	3:C:756:ILE:H	1.69	0.57
3:4:563:LEU:HD13	3:4:590:VAL:HG21	1.87	0.57
2:3:137:VAL:HG23	2:3:137:VAL:O	2.05	0.57
3:4:170:LEU:CD1	3:4:241:VAL:HG22	2.33	0.57
1:A:667:VAL:HG13	1:A:667:VAL:O	2.04	0.57
3:C:505:ASN:N	3:C:645:ASP:OD1	2.33	0.57
3:4:604:ILE:HD11	5:6:451:LEU:HD12	1.87	0.57
1:A:476:LYS:HE3	1:A:715:LEU:HD21	1.86	0.57
1:2:684:VAL:HG21	5:6:591:GLU:OE2	2.04	0.57
4:D:589:MET:CE	4:D:648:THR:HG21	2.35	0.57
5:E:726:LEU:HD11	5:E:776:VAL:HG21	1.87	0.57
1:2:232:VAL:HG13	1:2:285:ILE:HD13	1.87	0.57
1:2:573:ALA:HB1	1:2:577:VAL:CG2	2.34	0.57
4:5:188:LEU:HD13	4:5:272:LYS:HE2	1.87	0.57
1:A:222:MET:HE3	1:A:281:ILE:HD12	1.87	0.57
1:A:481:ILE:HD12	1:A:496:ALA:HB2	1.85	0.56
1:A:432:PHE:CZ	5:E:227:ILE:HD11	2.39	0.56
5:6:30:PHE:O	5:6:34:LEU:HD12	2.06	0.56
1:A:604:MET:HE1	1:A:657:PHE:CZ	2.40	0.56
3:C:350:GLN:OE1	3:C:380:ASP:N	2.35	0.56
4:5:275:GLY:C	4:5:276:LEU:HD23	2.30	0.56
3:C:167:GLN:CG	3:C:244:ILE:HD11	2.36	0.56
3:C:647:ILE:O	3:C:768:ALA:HB1	2.05	0.56
5:E:117:LEU:HD11	5:E:134:LEU:HG	1.87	0.56
5:6:364:VAL:HG21	5:6:536:LEU:HD21	1.86	0.56
6:F:417:ALA:O	6:F:429:LEU:HD12	2.06	0.56
8:S:-10:DT:H2'	8:S:-9:DT:H72	1.87	0.56
2:3:163:THR:HG23	6:7:289:VAL:HG23	1.87	0.56
4:5:380:LEU:HD21	4:5:506:PHE:HE2	1.70	0.56
6:F:182:TYR:OH	6:F:193:GLN:OE1	2.17	0.56
2:3:378:LEU:HD21	2:3:422:ILE:CD1	2.31	0.55
1:A:426:LEU:HD23	1:A:432:PHE:O	2.06	0.55
4:D:265:ILE:HD13	4:D:294:ILE:HG21	1.88	0.55
5:E:239:GLY:HA3	5:E:451:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:135:GLU:OE2	6:F:137:TYR:OH	2.23	0.55
2:3:378:LEU:HD11	2:3:398:MET:HE3	1.88	0.55
5:6:602:ARG:NH2	5:6:616:ILE:O	2.39	0.55
1:A:849:ASN:CB	5:E:727:ILE:HD11	2.36	0.55
1:2:325:VAL:HA	1:2:368:THR:HG23	1.86	0.55
3:4:187:ASP:O	3:4:195:GLN:NE2	2.38	0.55
1:A:577:VAL:HG21	1:A:620:LEU:CD1	2.36	0.55
5:6:186:ALA:O	1:A:356:GLN:NE2	2.37	0.55
2:3:355:LEU:HD11	2:3:451:ALA:HB2	1.88	0.55
1:A:650:THR:HG22	1:A:652:PRO:HD2	1.88	0.55
4:D:452:GLU:O	4:D:456:VAL:HG23	2.05	0.55
2:3:7:LEU:HD12	2:B:154:THR:HG22	1.87	0.55
1:2:731:VAL:HG21	1:2:782:LEU:HG	1.89	0.55
2:3:307:ILE:O	2:3:314:LYS:NZ	2.31	0.55
2:B:128:GLU:OE2	2:B:236:GLN:NE2	2.40	0.55
4:D:268:ILE:O	4:D:270:SER:OG	2.20	0.55
3:4:527:VAL:HG11	3:4:570:ILE:HD12	1.87	0.55
4:5:257:VAL:HG11	4:5:299:ILE:HG21	1.89	0.54
3:4:727:VAL:HB	3:4:769:LEU:HD21	1.88	0.54
4:D:170:ILE:HD11	4:D:179:LEU:HD23	1.88	0.54
5:E:450:MET:HE1	5:E:493:LEU:CB	2.36	0.54
5:E:605:ASP:HB2	5:E:616:ILE:HD13	1.90	0.54
4:D:385:THR:HG21	4:D:520:VAL:HG11	1.90	0.54
2:3:83:PHE:O	2:3:87:ILE:HD12	2.07	0.54
6:7:617:ALA:N	6:7:629:ASP:OD2	2.41	0.54
1:A:203:LEU:CD1	1:A:266:VAL:HG11	2.37	0.54
1:A:764:VAL:HG13	4:D:536:VAL:HG21	1.90	0.54
5:E:284:LEU:HD22	5:E:289:VAL:HG21	1.90	0.54
2:3:355:LEU:HD11	2:3:451:ALA:CB	2.38	0.54
5:6:594:ILE:HG23	5:6:624:MET:HE2	1.90	0.54
1:A:759:SER:HB3	1:A:810:VAL:HG11	1.90	0.54
2:3:628:HIS:ND1	2:3:641:ASP:OD1	2.40	0.54
3:4:501:ARG:O	3:4:739:ARG:NE	2.36	0.54
5:6:30:PHE:CE2	5:6:34:LEU:HD11	2.43	0.54
5:6:278:THR:HG23	5:6:278:THR:O	2.07	0.54
1:A:803:ILE:HD12	1:A:814:MET:HB3	1.89	0.54
2:B:614:THR:O	2:B:617:THR:N	2.41	0.54
4:D:380:LEU:HD13	4:D:504:ILE:HG22	1.90	0.54
5:E:254:VAL:O	5:E:254:VAL:HG13	2.06	0.54
3:C:388:VAL:HG12	3:C:423:LYS:HD2	1.90	0.53
6:F:356:LEU:HD21	6:F:616:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:342:SER:O	4:5:539:LEU:HD11	2.07	0.53
2:B:336:ARG:NH2	2:B:480:ASP:OD1	2.41	0.53
2:3:31:ILE:O	2:3:34:SER:OG	2.26	0.53
2:3:128:GLU:N	2:3:128:GLU:OE1	2.39	0.53
2:3:495:ARG:HA	4:5:587:ILE:HD11	1.90	0.53
6:F:421:ASP:OD1	6:F:422:SER:N	2.40	0.53
1:2:587:ASP:OD1	1:2:588:GLU:N	2.41	0.53
2:3:431:VAL:HG12	2:3:433:ILE:HG23	1.89	0.53
4:5:145:MET:CE	4:5:271:ILE:HG23	2.38	0.53
4:5:257:VAL:CG1	4:5:299:ILE:HG21	2.38	0.53
4:D:339:ILE:O	4:D:393:PHE:CZ	2.62	0.53
4:D:339:ILE:HD12	4:D:340:ALA:CB	2.39	0.53
6:F:387:LYS:NZ	12:F:1002:ADP:O2B	2.42	0.53
6:7:18:GLN:CD	6:7:84:LEU:HD21	2.34	0.53
6:F:206:CYS:SG	6:F:208:SER:OG	2.62	0.53
1:A:414:LEU:HD11	1:A:441:ALA:CB	2.39	0.53
1:A:764:VAL:CG1	4:D:536:VAL:HG21	2.39	0.53
4:D:148:LEU:HD13	4:D:297:LEU:HD12	1.91	0.53
1:A:347:VAL:O	1:A:347:VAL:HG13	2.08	0.52
2:B:614:THR:HG22	2:B:615:ALA:N	2.23	0.52
5:E:565:ARG:NH2	5:E:569:LEU:HD13	2.24	0.52
1:2:801:SER:O	1:2:805:THR:HG23	2.09	0.52
1:2:751:ARG:NH2	4:5:522:ASP:O	2.39	0.52
4:D:416:ALA:HB2	4:D:435:VAL:HG11	1.90	0.52
2:3:414:MET:HE1	2:3:422:ILE:HD12	1.91	0.52
3:4:237:PHE:CB	3:4:260:VAL:HG11	2.38	0.52
3:4:726:MET:HE1	3:4:774:THR:OG1	2.08	0.52
3:4:693:TYR:HE1	3:4:697:THR:HG21	1.74	0.52
5:E:494:ASN:OD1	5:E:496:ARG:NH2	2.42	0.52
5:6:184:VAL:O	5:6:184:VAL:HG13	2.08	0.52
3:C:326:SER:O	3:C:327:VAL:HG23	2.10	0.52
4:D:170:ILE:HD12	4:D:212:TYR:CG	2.45	0.52
1:A:288:LEU:HD12	1:A:415:THR:CG2	2.39	0.52
3:C:566:SER:O	3:C:611:THR:HG22	2.10	0.52
2:3:155:ILE:HG23	2:B:4:THR:HG23	1.92	0.52
6:7:574:PRO:HG3	6:7:624:VAL:HG13	1.91	0.52
4:D:265:ILE:HD12	4:D:265:ILE:O	2.10	0.52
3:4:152:ILE:HD12	3:4:157:VAL:HG21	1.92	0.52
2:B:526:ILE:HD12	2:B:526:ILE:H	1.75	0.52
3:C:112:VAL:O	3:C:112:VAL:HG13	2.10	0.52
6:F:187:CYS:SG	6:F:188:GLY:N	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:751:ARG:NH2	4:5:522:ASP:OD1	2.43	0.52
2:B:380:ALA:HB3	2:B:433:ILE:HD13	1.92	0.52
3:C:768:ALA:O	3:C:769:LEU:HD12	2.10	0.52
4:D:578:ALA:HB1	4:D:637:VAL:HG21	1.92	0.52
4:5:418:VAL:HG12	4:5:429:MET:HG2	1.92	0.51
3:C:127:VAL:HG13	6:F:109:MET:HE1	1.91	0.51
4:5:380:LEU:HD21	4:5:506:PHE:CE2	2.45	0.51
3:4:237:PHE:HB2	3:4:260:VAL:HG11	1.92	0.51
4:5:372:ARG:NH1	4:5:374:ASP:O	2.41	0.51
5:6:604:ARG:NH2	5:6:656:ILE:O	2.43	0.51
6:7:281:LEU:HG	6:7:283:THR:HG23	1.92	0.51
6:7:400:ARG:NH2	6:7:436:LEU:O	2.43	0.51
1:A:585:LEU:HD23	1:A:627:ILE:HB	1.92	0.51
3:C:558:LEU:HD23	5:E:220:ILE:HD13	1.92	0.51
6:F:450:MET:HE1	6:F:458:ILE:HG13	1.92	0.51
5:E:726:LEU:HD11	5:E:776:VAL:CG2	2.40	0.51
1:2:495:LEU:HD12	1:2:536:ILE:HG13	1.93	0.51
3:4:211:ASN:OD1	3:4:213:GLU:N	2.40	0.51
5:E:168:VAL:HG23	5:E:168:VAL:O	2.11	0.51
5:6:134:LEU:HD12	5:6:246:GLY:O	2.10	0.51
5:E:586:ILE:HA	5:E:640:VAL:HG12	1.93	0.51
3:C:170:LEU:HD21	3:C:241:VAL:CG1	2.35	0.51
3:4:212:CYS:HA	3:4:215:ILE:HD12	1.93	0.51
3:4:706:ALA:HB2	3:4:754:GLU:CA	2.41	0.51
4:5:649:LEU:HD12	4:5:649:LEU:O	2.11	0.51
5:E:68:LEU:HD21	5:E:79:ILE:CD1	2.40	0.51
5:E:616:ILE:HD12	5:E:616:ILE:N	2.26	0.51
6:F:234:GLU:OE2	6:F:254:THR:HG23	2.11	0.51
4:5:325:LEU:HD12	4:5:328:LEU:HD12	1.93	0.50
5:6:278:THR:HG21	6:7:205:MET:HE3	1.92	0.50
1:2:193:LEU:HD23	1:2:193:LEU:C	2.36	0.50
2:3:195:ASP:OD1	6:7:154:ALA:N	2.38	0.50
3:4:367:PRO:CD	6:7:478:LEU:HD13	2.41	0.50
4:D:645:GLN:HA	4:D:648:THR:HG22	1.93	0.50
2:3:173:VAL:HG22	4:D:204:ARG:CZ	2.42	0.50
3:C:476:ILE:HD13	3:C:650:MET:CE	2.39	0.50
1:2:464:ILE:HG23	1:2:723:TYR:CD2	2.46	0.50
1:2:495:LEU:HD13	1:2:627:ILE:HD13	1.91	0.50
4:5:110:VAL:HG23	4:5:111:THR:HG23	1.92	0.50
3:C:386:ASP:OD2	5:E:217:ARG:NH2	2.44	0.50
3:C:193:TYR:O	3:C:197:LEU:HD22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:265:ILE:HG22	4:D:299:ILE:HD13	1.94	0.50
5:E:68:LEU:HD21	5:E:79:ILE:HD12	1.94	0.50
6:F:374:ASN:OD1	6:F:465:GLN:NE2	2.44	0.50
2:3:157:ARG:NH1	2:3:158:ARG:O	2.45	0.50
6:7:18:GLN:OE1	6:7:84:LEU:HD21	2.12	0.50
1:2:779:ARG:O	1:2:782:LEU:HD12	2.12	0.50
2:3:286:LYS:O	2:3:290:THR:HG23	2.11	0.50
7:O:44:DT:H2'	7:O:45:DT:H72	1.94	0.50
3:C:598:ILE:O	3:C:598:ILE:HD12	2.11	0.50
3:4:476:ILE:CD1	3:4:650:MET:HE3	2.41	0.50
3:4:560:THR:HG23	5:6:220:ILE:HD11	1.94	0.50
1:A:203:LEU:HD11	1:A:219:ILE:HD11	1.93	0.50
6:F:276:ILE:HD12	6:F:276:ILE:N	2.26	0.50
5:6:104:ILE:HD12	5:6:105:PRO:O	2.12	0.49
5:6:188:ARG:NH1	1:A:353:PRO:O	2.41	0.49
4:D:339:ILE:HD12	4:D:340:ALA:N	2.27	0.49
7:O:36:DT:H2'	7:O:37:DT:H72	1.94	0.49
5:6:225:GLU:OE2	5:6:295:ARG:NH1	2.44	0.49
6:7:280:ILE:HD11	6:7:297:TYR:CD2	2.47	0.49
6:7:403:TYR:HE1	6:7:405:THR:HG1	1.59	0.49
1:A:862:GLU:OE1	1:A:881:TYR:OH	2.19	0.49
2:B:497:ILE:O	2:B:501:VAL:HG23	2.12	0.49
1:2:502:GLY:N	1:2:515:GLY:O	2.41	0.49
2:B:336:ARG:NH1	2:B:338:ASP:O	2.44	0.49
3:C:727:VAL:HG21	3:C:769:LEU:CD2	2.42	0.49
7:O:39:DT:H2'	7:O:40:DT:H71	1.93	0.49
2:3:422:ILE:O	2:3:422:ILE:HG22	2.11	0.49
2:B:223:ASP:N	2:B:223:ASP:OD1	2.45	0.49
2:B:585:GLU:OE1	2:B:585:GLU:N	2.41	0.49
4:D:275:GLY:C	4:D:276:LEU:HD23	2.38	0.49
4:D:597:GLU:OE1	4:D:603:ARG:NH1	2.45	0.49
7:O:45:DT:H2'	7:O:46:DT:H72	1.94	0.49
3:4:282:LEU:CD1	3:4:419:ILE:HD12	2.42	0.49
4:5:360:GLY:N	4:5:373:GLY:O	2.45	0.49
6:7:93:VAL:HG12	6:7:95:ASN:H	1.76	0.49
6:F:405:THR:HG22	6:F:406:GLY:H	1.78	0.49
4:5:138:ARG:NH2	4:5:241:MET:O	2.45	0.49
1:A:676:ALA:HB3	5:E:595:VAL:HG23	1.95	0.49
5:E:450:MET:HE1	5:E:493:LEU:HB2	1.95	0.49
6:F:344:ILE:O	6:F:351:LYS:NZ	2.40	0.49
1:2:787:ILE:HG22	1:2:788:GLU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:362:VAL:HG11	6:7:571:PRO:HD2	1.94	0.49
1:2:481:ILE:HD12	1:2:496:ALA:HB2	1.94	0.49
2:3:40:ILE:HD11	2:3:84:VAL:HG13	1.95	0.49
1:A:203:LEU:C	1:A:203:LEU:HD13	2.38	0.49
4:D:197:CYS:SG	4:D:199:THR:HG22	2.53	0.49
7:O:46:DT:H2'	7:O:47:DT:H72	1.95	0.49
1:2:467:LEU:HD11	1:2:723:TYR:CD2	2.47	0.48
4:5:39:LEU:HD23	4:5:103:ALA:HA	1.95	0.48
4:5:418:VAL:HG23	4:5:471:LYS:HG3	1.95	0.48
2:B:375:GLY:O	2:B:378:LEU:N	2.45	0.48
3:C:167:GLN:HG2	3:C:244:ILE:HD11	1.95	0.48
7:O:43:DT:H2'	7:O:44:DT:H72	1.95	0.48
1:A:674:MET:HA	1:A:674:MET:HE2	1.95	0.48
2:B:51:VAL:HG22	2:B:103:GLU:O	2.13	0.48
2:B:513:GLN:N	2:B:513:GLN:OE1	2.46	0.48
5:6:224:LEU:C	5:6:224:LEU:HD12	2.39	0.48
3:C:309:CYS:O	5:E:18:VAL:HG22	2.12	0.48
4:D:582:LEU:HD13	4:D:582:LEU:C	2.39	0.48
1:2:675:LEU:HD11	11:2:1002:ATP:N6	2.27	0.48
6:F:429:LEU:HD11	6:F:474:ILE:CD1	2.43	0.48
6:F:516:ASP:OD2	6:F:611:ARG:NH1	2.44	0.48
1:A:516:ASP:CB	1:A:625:THR:HG22	2.44	0.48
1:A:577:VAL:HG22	1:A:622:ALA:HB2	1.94	0.48
6:F:434:LEU:HD12	6:F:467:ILE:HD11	1.95	0.48
2:3:411:PHE:CD1	2:3:414:MET:HE2	2.48	0.48
2:3:639:LEU:HD23	2:3:639:LEU:O	2.13	0.48
3:4:470:ILE:CD1	3:4:519:LEU:HD22	2.44	0.48
1:A:576:LEU:O	1:A:622:ALA:HB1	2.14	0.48
5:E:117:LEU:HD12	5:E:136:ARG:HB2	1.95	0.48
2:3:486:LEU:HD11	2:3:655:LYS:HE2	1.96	0.48
1:2:617:VAL:HG21	2:3:211:GLY:HA2	1.94	0.48
4:5:339:ILE:O	4:5:393:PHE:CZ	2.67	0.48
2:3:44:GLN:O	2:3:91:TYR:OH	2.27	0.48
2:3:422:ILE:HG22	2:3:426:MET:HG3	1.95	0.48
6:7:56:ALA:HB2	6:7:63:VAL:HG21	1.95	0.48
2:B:387:GLU:HG3	2:B:388:THR:HG23	1.96	0.48
5:6:371:MET:HE1	5:6:500:LEU:HD13	1.94	0.48
4:D:59:LEU:HD21	4:D:70:ILE:HD13	1.95	0.48
5:E:446:ALA:HB1	5:E:450:MET:HB2	1.96	0.48
2:3:384:THR:HG23	7:O:12:DA:OP1	2.14	0.47
4:5:173:ARG:O	4:5:176:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.96	0.47
6:7:372:ARG:NH2	6:7:374:ASN:O	2.46	0.47
2:B:84:VAL:HG11	2:B:98:PHE:CZ	2.49	0.47
3:C:573:ILE:CD1	3:C:613:VAL:HG13	2.44	0.47
2:3:340:ASN:C	2:3:341:ILE:HD12	2.39	0.47
2:3:380:ALA:CB	2:3:433:ILE:HD13	2.44	0.47
2:3:393:LEU:HD12	2:3:433:ILE:HD11	1.95	0.47
3:C:469:SER:OG	6:F:369:MET:HE2	2.13	0.47
5:E:535:ILE:HG22	5:E:537:VAL:HG23	1.96	0.47
1:2:731:VAL:HG13	1:2:784:ASP:OD1	2.13	0.47
4:5:464:GLN:OE1	4:5:464:GLN:N	2.47	0.47
3:C:723:SER:OG	3:C:776:PRO:O	2.19	0.47
1:2:524:ASP:OD2	1:2:665:ASP:N	2.39	0.47
1:2:546:THR:HG21	1:2:556:LEU:HD11	1.95	0.47
3:4:760:GLU:OE2	3:4:763:ARG:NH2	2.48	0.47
3:C:732:ARG:NH2	12:E:1002:ADP:O2B	2.44	0.47
1:2:308:THR:HG22	1:2:309:SER:N	2.29	0.47
5:6:228:LEU:HD13	5:6:232:ALA:O	2.15	0.47
2:3:71:GLU:OE1	2:3:71:GLU:N	2.43	0.47
3:4:512:PRO:O	6:7:604:ARG:NE	2.37	0.47
4:5:416:ALA:HB2	4:5:435:VAL:HG21	1.95	0.47
4:5:504:ILE:HD11	4:5:605:SER:HB2	1.95	0.47
5:6:244:PHE:HD2	5:6:303:VAL:HG22	1.79	0.47
2:B:436:ALA:CB	6:F:417:ALA:HB3	2.45	0.47
3:C:303:PHE:O	3:C:339:LEU:HD12	2.14	0.47
5:E:206:VAL:HG22	5:E:226:VAL:HG13	1.95	0.47
6:7:84:LEU:HD22	6:7:88:TYR:HE2	1.80	0.47
6:7:220:LEU:HD23	6:7:220:LEU:H	1.78	0.47
1:A:604:MET:CE	1:A:626:VAL:HG11	2.45	0.47
1:A:799:LEU:O	1:A:800:GLU:C	2.58	0.47
3:C:299:MET:HE3	5:E:292:LEU:HD13	1.97	0.47
4:D:175:CYS:SG	4:D:177:ASN:ND2	2.88	0.47
2:3:613:VAL:HA	2:3:617:THR:HG21	1.97	0.47
5:E:652:LEU:HD13	5:E:652:LEU:O	2.14	0.47
6:F:458:ILE:CG2	6:F:462:MET:HE3	2.45	0.47
2:3:383:THR:HG22	2:3:384:THR:N	2.29	0.47
1:A:759:SER:CB	1:A:810:VAL:HG11	2.45	0.47
4:D:62:HIS:ND1	4:D:69:TRP:O	2.48	0.47
11:2:1002:ATP:O3'	5:6:622:GLU:OE2	2.31	0.46
2:B:5:VAL:HG23	2:B:5:VAL:O	2.15	0.46
6:F:397:LEU:C	6:F:397:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:723:TYR:OH	1:2:782:LEU:HD13	2.15	0.46
2:3:305:PRO:HB3	2:3:562:MET:HE1	1.98	0.46
2:B:287:PHE:CZ	2:B:295:ILE:HD11	2.49	0.46
3:C:350:GLN:HB2	3:C:379:VAL:HG13	1.98	0.46
4:D:40:ARG:NH1	4:D:109:GLU:OE1	2.48	0.46
1:2:497:LEU:O	1:2:517:ILE:HD12	2.15	0.46
5:6:371:MET:HE2	5:6:392:VAL:HB	1.96	0.46
5:6:575:TYR:OH	5:6:634:MET:O	2.31	0.46
1:A:230:LEU:HD23	1:A:230:LEU:C	2.39	0.46
3:C:158:ASN:OD1	3:C:158:ASN:N	2.43	0.46
5:E:264:ALA:HB2	5:E:292:LEU:HD11	1.97	0.46
5:E:361:ASN:OD1	5:E:536:LEU:HD22	2.15	0.46
6:F:462:MET:HE1	6:F:515:PHE:CE1	2.50	0.46
8:S:-5:DT:H2'	8:S:-4:DT:H72	1.97	0.46
1:2:230:LEU:C	1:2:230:LEU:HD23	2.40	0.46
1:2:463:MET:HE1	1:2:722:LYS:HD2	1.98	0.46
6:7:5:ASP:OD2	6:7:8:LEU:HD23	2.15	0.46
2:B:393:LEU:HD22	2:B:433:ILE:HD11	1.98	0.46
5:E:184:VAL:O	5:E:184:VAL:HG22	2.15	0.46
2:3:329:LEU:N	2:3:329:LEU:HD12	2.30	0.46
2:3:369:THR:HG22	2:3:370:GLY:N	2.31	0.46
4:5:282:ARG:NH2	5:6:440:HIS:O	2.48	0.46
4:5:649:LEU:HD12	4:5:649:LEU:C	2.41	0.46
6:7:570:GLN:OE1	6:7:570:GLN:N	2.41	0.46
3:C:175:ASP:HB3	3:C:178:ALA:HB2	1.98	0.46
5:E:302:CYS:SG	5:E:303:VAL:N	2.88	0.46
1:2:268:LEU:HD11	1:2:275:ASP:HB2	1.98	0.46
2:3:70:PHE:O	2:3:74:VAL:HG23	2.15	0.46
3:4:159:VAL:HG13	3:4:236:THR:HG22	1.96	0.46
5:6:434:VAL:HG12	5:6:435:ARG:N	2.30	0.46
2:B:621:LEU:HD21	2:B:649:VAL:HG11	1.98	0.46
6:F:606:LEU:C	6:F:606:LEU:HD23	2.40	0.46
2:3:261:ILE:N	2:3:261:ILE:HD12	2.30	0.46
4:5:257:VAL:HG12	4:5:301:VAL:CG2	2.46	0.46
1:A:414:LEU:HD11	1:A:441:ALA:HB1	1.98	0.46
1:2:667:VAL:O	1:2:667:VAL:HG23	2.16	0.46
4:5:442:VAL:O	4:5:442:VAL:HG23	2.15	0.46
5:6:402:LYS:NZ	12:6:1002:ADP:O3B	2.44	0.46
3:C:624:TRP:CZ3	3:C:649:LEU:HD22	2.51	0.46
6:F:435:VAL:CG2	6:F:478:LEU:HD23	2.46	0.46
3:4:112:VAL:HG22	3:4:257:GLN:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:NH2	5:E:234:GLU:OE2	2.43	0.46
3:C:755:ALA:HA	3:C:758:VAL:HG22	1.97	0.46
5:E:753:LEU:HD23	5:E:754:LYS:HD2	1.98	0.46
3:4:710:LEU:HD23	3:4:758:VAL:HG13	1.98	0.46
5:6:82:GLU:O	5:6:86:VAL:HG22	2.15	0.46
5:6:391:ASN:OD1	5:6:499:ILE:N	2.47	0.46
3:C:404:ARG:HE	7:O:31:DT:P	2.39	0.46
3:C:508:LEU:HD13	3:C:650:MET:HE3	1.98	0.46
5:E:329:MET:HE1	5:E:337:VAL:HG21	1.98	0.46
6:F:77:PHE:O	6:F:81:VAL:HG23	2.15	0.46
6:F:362:VAL:HG23	6:F:364:GLN:OE1	2.16	0.46
2:3:281:ILE:HG22	2:3:285:LYS:HZ2	1.78	0.45
2:3:380:ALA:CB	2:3:442:LEU:HD12	2.44	0.45
2:3:494:ASP:OD1	4:5:587:ILE:HD13	2.15	0.45
3:4:663:ALA:O	3:4:667:VAL:HG23	2.16	0.45
1:2:278:THR:O	1:2:278:THR:HG22	2.16	0.45
3:4:514:THR:HG22	3:4:515:SER:H	1.81	0.45
4:5:538:THR:O	4:5:541:VAL:HG22	2.15	0.45
6:7:574:PRO:CG	6:7:624:VAL:HG13	2.46	0.45
1:A:491:ILE:HD11	1:A:663:VAL:HG22	1.98	0.45
2:B:482:LEU:C	2:B:482:LEU:HD23	2.42	0.45
5:E:53:LEU:HD21	5:E:110:PHE:CD1	2.52	0.45
5:E:371:MET:HE1	5:E:499:ILE:C	2.42	0.45
4:5:634:GLU:HA	4:5:637:VAL:HG12	1.97	0.45
4:D:637:VAL:O	4:D:641:LEU:HD23	2.16	0.45
4:5:257:VAL:HG12	4:5:301:VAL:HG22	1.99	0.45
5:6:465:MET:SD	5:6:473:ILE:HD12	2.56	0.45
4:D:245:MET:HE3	4:D:245:MET:HA	1.99	0.45
5:E:571:ASP:OD1	5:E:574:ARG:NH2	2.45	0.45
6:F:237:MET:HE3	6:F:271:VAL:HG23	1.98	0.45
7:O:34:DT:H2'	7:O:35:DT:H71	1.99	0.45
2:3:141:VAL:HG12	6:7:292:LEU:HB2	1.97	0.45
5:6:378:LYS:O	5:6:386:LEU:N	2.50	0.45
2:B:288:SER:O	2:B:292:SER:OG	2.33	0.45
3:C:340:ILE:HG21	3:C:343:ARG:HG3	1.98	0.45
5:E:371:MET:HE2	5:E:456:VAL:HG13	1.99	0.45
6:F:415:THR:HG22	6:F:416:ALA:N	2.31	0.45
6:F:563:ILE:O	6:F:567:ARG:HG3	2.17	0.45
1:2:783:ARG:O	1:2:784:ASP:HB2	2.16	0.45
2:B:291:ARG:HB2	2:B:295:ILE:HD13	1.98	0.45
5:E:179:ILE:O	5:E:181:ARG:NH2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:371:MET:HE3	5:E:498:SER:HB2	1.99	0.45
1:2:456:LEU:N	1:2:456:LEU:HD22	2.31	0.45
1:2:783:ARG:HD3	1:2:787:ILE:HD12	1.99	0.45
2:3:621:LEU:HD23	2:3:649:VAL:HG21	1.97	0.45
4:5:232:LEU:O	4:5:236:VAL:HG23	2.17	0.45
4:5:516:MET:HE2	4:5:518:PHE:HE1	1.82	0.45
6:7:369:MET:HA	6:7:369:MET:HE2	1.99	0.45
6:7:429:LEU:HD11	6:7:474:ILE:HD12	1.99	0.45
2:B:291:ARG:O	2:B:295:ILE:HD13	2.16	0.45
3:C:317:MET:HE1	5:E:262:ALA:HA	1.98	0.45
6:F:416:ALA:CB	6:F:478:LEU:HD21	2.46	0.45
4:5:574:LEU:HD23	4:5:632:ALA:HB3	1.99	0.45
1:A:373:TYR:CE1	1:A:397:ILE:HG23	2.51	0.45
2:B:244:LEU:HD21	2:B:259:VAL:HG11	1.99	0.45
4:D:232:LEU:O	4:D:236:VAL:HG23	2.15	0.45
5:E:389:ASP:OD2	5:E:480:GLN:NE2	2.47	0.45
5:E:516:LEU:HD12	5:E:614:TRP:CE3	2.51	0.45
7:O:32:DT:C2'	7:O:33:DT:H72	2.45	0.45
5:6:154:GLY:O	5:6:168:VAL:HG12	2.17	0.45
1:A:684:VAL:HG22	5:E:586:ILE:HB	1.98	0.45
1:A:721:LYS:O	1:A:725:ILE:HG12	2.17	0.45
6:F:119:VAL:HG13	6:F:119:VAL:O	2.16	0.45
6:F:523:ASP:OD1	6:F:523:ASP:N	2.49	0.45
1:2:420:ASN:OD1	1:2:435:PHE:HB3	2.17	0.45
3:4:682:LEU:CD2	3:4:686:VAL:HG13	2.46	0.45
12:5:1002:ADP:O1A	12:5:1002:ADP:O1B	2.35	0.45
1:2:227:ARG:O	1:2:228:GLU:HG2	2.17	0.44
3:4:367:PRO:HD2	6:7:478:LEU:HD13	1.98	0.44
3:4:560:THR:HG22	5:6:220:ILE:HD11	1.98	0.44
5:6:325:ILE:O	5:6:329:MET:HG3	2.17	0.44
1:A:680:VAL:O	1:A:684:VAL:HG23	2.17	0.44
3:C:127:VAL:HG21	3:C:153:TRP:CE3	2.43	0.44
3:C:306:CYS:SG	3:C:336:SER:OG	2.71	0.44
4:D:343:ILE:O	4:D:350:LYS:NZ	2.47	0.44
6:F:609:ILE:HG13	6:F:637:MET:HE1	1.98	0.44
1:2:513:VAL:O	1:2:513:VAL:HG23	2.16	0.44
3:4:187:ASP:OD1	3:4:189:THR:HG22	2.17	0.44
3:4:302:ALA:HB1	3:4:339:LEU:HD13	1.99	0.44
4:5:145:MET:C	4:5:146:SER:HG	2.13	0.44
4:5:418:VAL:HG22	4:5:469:ILE:HG21	1.99	0.44
2:B:303:LEU:O	2:B:357:TYR:OH	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:MET:SD	6:F:407:ARG:NE	2.90	0.44
2:B:495:ARG:HG2	4:D:587:ILE:HD13	1.99	0.44
5:E:35:GLU:O	5:E:44:ILE:HD13	2.17	0.44
5:E:371:MET:HE1	5:E:500:LEU:N	2.31	0.44
6:F:17:LEU:HD21	6:F:81:VAL:HG22	1.98	0.44
3:4:190:GLU:O	3:4:195:GLN:NE2	2.50	0.44
3:4:295:LEU:HD11	3:4:379:VAL:CG1	2.47	0.44
3:4:402:ASN:HB2	3:4:405:VAL:HG22	1.98	0.44
4:5:538:THR:O	4:5:539:LEU:C	2.59	0.44
6:7:182:TYR:HB2	6:7:220:LEU:HD12	1.99	0.44
1:A:647:VAL:HG11	1:A:654:ILE:HD11	1.98	0.44
1:A:848:ARG:NH1	5:E:603:GLN:O	2.50	0.44
3:C:579:MET:O	3:C:580:ASN:C	2.59	0.44
2:3:593:GLU:HG2	2:3:646:VAL:HG22	1.99	0.44
3:4:248:ARG:O	3:4:249:TYR:C	2.60	0.44
4:5:150:LYS:HE2	4:5:264:THR:HG21	1.98	0.44
4:5:178:THR:HG22	4:5:179:LEU:N	2.33	0.44
6:7:148:VAL:O	6:7:151:GLU:N	2.50	0.44
6:F:184:CYS:SG	6:F:185:ASP:N	2.91	0.44
7:O:38:DT:H2''	7:O:39:DT:C7	2.48	0.44
8:S:-4:DT:H2'	8:S:-3:DT:H72	1.99	0.44
5:6:604:ARG:HH21	5:6:656:ILE:HG22	1.83	0.44
1:A:402:LEU:O	1:A:405:SER:OG	2.16	0.44
2:B:6:VAL:HG11	2:B:9:ASP:HB2	1.99	0.44
2:B:614:THR:HG21	6:F:384:GLY:HA3	1.99	0.44
3:C:374:ALA:HB1	3:C:378:LEU:HB2	1.99	0.44
6:F:434:LEU:CD1	6:F:467:ILE:HD11	2.46	0.44
7:O:18:DA:H2''	7:O:19:DA:C8	2.53	0.44
1:2:827:ASP:OD1	1:2:830:GLU:N	2.39	0.44
6:7:616:LEU:O	6:7:616:LEU:HD13	2.18	0.44
1:A:738:MET:HG3	1:A:791:VAL:HG21	2.00	0.44
1:2:356:GLN:NE2	5:E:186:ALA:O	2.48	0.44
4:5:474:ILE:HD12	4:5:476:THR:CG2	2.47	0.44
5:6:573:ARG:O	5:6:577:LEU:HD23	2.16	0.44
6:7:588:MET:SD	6:7:601:THR:OG1	2.64	0.44
2:B:25:ASP:O	2:B:30:GLY:N	2.49	0.44
2:B:223:ASP:O	2:B:224:ASP:OD1	2.35	0.44
3:C:698:ILE:HG21	3:C:746:LYS:HA	2.00	0.44
5:E:123:ILE:HD12	5:E:210:GLU:HA	2.00	0.44
6:F:224:THR:HG22	6:F:229:PHE:HZ	1.81	0.44
1:2:215:PHE:CE1	1:2:230:LEU:HD21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ILE:O	3:C:188:ILE:HG22	2.17	0.44
6:F:215:ARG:HE	6:F:215:ARG:HA	1.83	0.44
7:O:33:DT:H2'	7:O:34:DT:H71	1.99	0.44
1:2:430:ASN:HB2	5:6:254:VAL:HG12	1.99	0.44
2:3:593:GLU:HG2	2:3:646:VAL:HG13	1.99	0.44
4:5:450:MET:SD	4:5:458:ILE:HD12	2.58	0.44
1:A:807:LYS:O	1:A:811:MET:N	2.41	0.44
2:B:614:THR:HG22	2:B:615:ALA:H	1.82	0.44
5:E:30:PHE:HZ	5:E:112:VAL:HG11	1.82	0.44
5:E:99:LYS:NZ	5:E:106:LEU:HD13	2.33	0.44
7:O:31:DT:H2''	7:O:32:DT:C7	2.47	0.44
1:2:207:VAL:O	1:2:213:ASN:N	2.51	0.43
4:D:527:GLU:OE1	4:D:531:MET:HE2	2.18	0.43
6:F:340:ILE:HD12	6:F:355:LEU:HB2	2.00	0.43
6:F:438:ASP:O	6:F:481:ARG:C	2.61	0.43
1:2:336:LEU:HD21	1:2:361:PHE:CE1	2.53	0.43
3:4:473:HIS:ND1	3:4:476:ILE:HD12	2.33	0.43
1:A:203:LEU:HD13	1:A:203:LEU:O	2.18	0.43
5:E:16:LEU:N	5:E:16:LEU:HD23	2.32	0.43
1:2:414:LEU:HD12	1:2:444:VAL:HG22	2.00	0.43
1:2:495:LEU:HD11	1:2:627:ILE:HG21	2.01	0.43
3:4:263:PHE:HA	3:4:391:THR:HG21	2.01	0.43
3:4:624:TRP:CD1	3:4:651:LEU:HD11	2.54	0.43
4:5:380:LEU:HD23	4:5:488:ALA:HB3	2.00	0.43
3:C:622:SER:OG	6:F:510:ALA:N	2.51	0.43
5:E:450:MET:CE	5:E:493:LEU:HD22	2.48	0.43
1:2:735:LEU:CD2	1:2:771:ILE:HG23	2.49	0.43
1:A:849:ASN:HB2	5:E:727:ILE:HD11	1.99	0.43
2:B:502:LEU:HD21	4:D:613:LEU:HD21	1.99	0.43
4:D:589:MET:HE1	4:D:648:THR:HG21	2.01	0.43
5:E:450:MET:SD	5:E:482:ILE:HD12	2.58	0.43
2:3:369:THR:HG22	2:3:370:GLY:H	1.83	0.43
4:5:356:LEU:HD12	4:5:375:ILE:HB	2.01	0.43
6:7:563:ILE:O	6:7:567:ARG:HG2	2.18	0.43
4:D:339:ILE:HD12	4:D:340:ALA:HB2	2.01	0.43
6:F:319:LEU:HD22	6:F:319:LEU:N	2.34	0.43
1:2:657:PHE:HB2	1:2:660:LEU:HD11	1.99	0.43
4:5:146:SER:N	4:5:269:TYR:O	2.36	0.43
8:S:-5:DT:C2'	8:S:-4:DT:H72	2.48	0.43
3:4:604:ILE:HD11	5:6:451:LEU:CD1	2.49	0.43
4:5:650:ASP:OD1	4:5:651:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ILE:HG21	1:A:627:ILE:HD12	2.01	0.43
2:B:597:LEU:CD1	2:B:613:VAL:HG11	2.48	0.43
3:C:598:ILE:HD11	3:C:605:CYS:SG	2.59	0.43
6:F:415:THR:CG2	6:F:469:ILE:HD11	2.47	0.43
5:6:358:ILE:O	5:6:365:LYS:NZ	2.42	0.43
6:7:421:ASP:OD1	6:7:422:SER:N	2.46	0.43
6:7:578:ALA:O	6:7:582:THR:HG23	2.19	0.43
3:C:726:MET:HE2	3:C:726:MET:N	2.34	0.43
6:7:109:MET:HE1	4:D:15:PHE:HA	2.00	0.43
6:7:177:MET:SD	6:7:180:ALA:HB2	2.58	0.43
1:A:787:ILE:HG22	1:A:788:GLU:N	2.34	0.43
3:C:117:ASP:N	3:C:117:ASP:OD1	2.51	0.43
1:2:308:THR:HG22	1:2:309:SER:H	1.83	0.43
4:5:400:ILE:HD13	4:5:438:ASP:O	2.19	0.43
5:6:225:GLU:OE1	5:6:225:GLU:N	2.43	0.43
1:A:292:GLU:O	1:A:308:THR:HG22	2.19	0.43
1:A:458:ASP:OD1	1:A:458:ASP:N	2.50	0.43
3:C:713:ALA:HB2	3:C:762:LYS:HD2	2.00	0.43
5:E:442:PHE:HB2	5:E:489:VAL:HG11	2.01	0.43
6:F:58:ASP:OD1	6:F:58:ASP:N	2.52	0.43
7:O:38:DT:H2''	7:O:39:DT:H72	2.00	0.43
5:6:162:GLN:N	5:6:162:GLN:OE1	2.51	0.42
4:D:325:LEU:HD12	4:D:328:LEU:HD12	2.00	0.42
2:3:469:ILE:HD13	2:3:482:LEU:HD21	2.01	0.42
3:4:717:MET:HA	3:4:720:ILE:HG22	2.00	0.42
4:5:339:ILE:HG13	4:5:340:ALA:H	1.84	0.42
2:B:195:ASP:OD1	2:B:195:ASP:N	2.45	0.42
4:D:524:HIS:CG	4:D:524:HIS:O	2.71	0.42
6:F:458:ILE:HG22	6:F:462:MET:HE3	2.01	0.42
7:O:33:DT:C2'	7:O:34:DT:H71	2.49	0.42
2:3:169:PRO:O	2:3:173:VAL:HG23	2.19	0.42
4:5:128:LEU:HD23	4:5:128:LEU:N	2.33	0.42
5:6:147:VAL:HG13	5:6:233:VAL:HG21	2.01	0.42
5:6:206:VAL:HG22	5:6:226:VAL:HG22	2.01	0.42
6:7:326:GLN:OE1	6:7:562:TYR:OH	2.25	0.42
6:7:404:THR:HG23	6:7:409:SER:OG	2.20	0.42
1:2:546:THR:HG21	1:2:556:LEU:CD1	2.48	0.42
5:6:68:LEU:HD21	5:6:79:ILE:CD1	2.48	0.42
5:6:104:ILE:HD12	5:6:104:ILE:C	2.44	0.42
5:6:117:LEU:HD22	5:6:119:THR:O	2.20	0.42
5:6:277:GLU:OE1	4:D:198:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:343:ASP:OD2	5:6:567:TYR:OH	2.36	0.42
6:7:14:LYS:NZ	6:7:83:GLU:OE1	2.53	0.42
3:C:390:VAL:HG23	3:C:418:VAL:HG13	2.00	0.42
4:D:321:GLU:OE2	4:D:558:LYS:NZ	2.44	0.42
2:3:157:ARG:NH2	2:3:170:SER:O	2.53	0.42
3:4:515:SER:O	3:4:519:LEU:HD23	2.18	0.42
4:5:331:VAL:HA	4:5:334:VAL:HG12	2.01	0.42
1:A:430:ASN:ND2	5:E:437:GLU:O	2.53	0.42
3:C:448:LEU:C	3:C:448:LEU:HD23	2.44	0.42
5:E:452:ALA:O	5:E:455:GLY:N	2.49	0.42
6:F:462:MET:HE1	6:F:515:PHE:CZ	2.55	0.42
1:2:467:LEU:HD12	1:2:467:LEU:C	2.44	0.42
1:2:599:SER:HA	4:5:410:SER:HB2	2.02	0.42
2:3:306:SER:OG	4:5:367:ASP:OD2	2.37	0.42
3:4:241:VAL:CG1	3:4:258:ILE:HG21	2.45	0.42
5:6:387:ARG:NH1	5:6:529:ARG:O	2.45	0.42
5:6:605:ASP:HB2	5:6:616:ILE:HD13	2.02	0.42
3:C:170:LEU:CD2	3:C:241:VAL:HG12	2.38	0.42
3:C:715:VAL:HG21	5:E:546:TYR:CE2	2.55	0.42
4:D:608:ILE:HD12	4:D:608:ILE:N	2.35	0.42
5:E:786:VAL:HG22	5:E:787:LEU:H	1.85	0.42
6:F:458:ILE:O	6:F:461:VAL:HG12	2.19	0.42
4:5:217:ASP:OD1	4:5:217:ASP:N	2.52	0.42
5:6:148:HIS:NE2	5:6:436:ASP:OD2	2.51	0.42
5:6:179:ILE:HD12	5:6:188:ARG:CG	2.50	0.42
2:B:524:VAL:HG13	2:B:525:ASP:N	2.35	0.42
3:4:117:ASP:OD1	3:4:117:ASP:N	2.50	0.42
3:4:386:ASP:OD1	3:4:529:ARG:NH1	2.53	0.42
3:4:723:SER:OG	3:4:724:ARG:N	2.53	0.42
4:D:269:TYR:HA	4:D:294:ILE:HD13	2.01	0.42
6:F:507:LEU:HG	6:F:512:LEU:HD11	2.02	0.42
1:2:735:LEU:HD21	1:2:771:ILE:HG23	2.02	0.42
3:4:237:PHE:HB3	3:4:260:VAL:HG11	2.02	0.42
3:4:492:PHE:O	3:4:495:THR:OG1	2.38	0.42
3:4:608:ASN:OD1	5:6:212:GLN:NE2	2.53	0.42
4:5:155:ILE:HD11	4:5:263:VAL:HG21	2.02	0.41
5:E:460:ASP:OD1	5:E:461:GLU:N	2.51	0.41
6:F:362:VAL:HG13	6:F:614:THR:CG2	2.50	0.41
6:F:420:ARG:NH1	6:F:421:ASP:O	2.53	0.41
1:2:421:ASN:HB3	5:6:195:THR:HG21	2.01	0.41
2:3:236:GLN:HB2	2:3:534:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:385:ASP:O	2:3:386:GLN:HB3	2.20	0.41
3:4:330:ARG:NH1	5:6:18:VAL:HG22	2.35	0.41
4:5:96:LEU:C	4:5:96:LEU:HD13	2.45	0.41
4:5:380:LEU:HD13	4:5:504:ILE:HG22	2.01	0.41
4:5:585:ARG:HG3	4:5:641:LEU:HD13	2.02	0.41
5:6:570:ASP:OD1	5:6:573:ARG:NH1	2.53	0.41
6:7:3:LEU:N	6:7:3:LEU:HD22	2.35	0.41
6:7:627:LYS:HA	6:7:630:VAL:HG12	2.02	0.41
1:A:293:GLU:OE2	1:A:295:ARG:NH2	2.53	0.41
4:D:339:ILE:HD11	4:D:350:LYS:HG2	2.02	0.41
4:D:356:LEU:HD23	4:D:356:LEU:C	2.46	0.41
1:2:590:ASP:N	1:2:590:ASP:OD1	2.53	0.41
4:5:67:GLU:O	4:5:252:TYR:CZ	2.73	0.41
6:7:397:LEU:O	6:7:560:ARG:NE	2.53	0.41
4:D:361:SER:N	4:D:621:GLU:OE1	2.47	0.41
4:D:649:LEU:HD23	4:D:649:LEU:C	2.45	0.41
6:F:447:PHE:HE1	6:F:458:ILE:HG21	1.86	0.41
2:3:393:LEU:N	2:3:393:LEU:HD22	2.35	0.41
3:4:348:ASP:OD1	5:6:128:SER:OG	2.35	0.41
3:4:388:VAL:HG12	3:4:423:LYS:CD	2.49	0.41
5:6:126:LEU:HD11	5:6:137:ILE:HG21	2.02	0.41
5:6:400:THR:HG21	5:6:536:LEU:HB3	2.02	0.41
6:7:163:VAL:HG12	6:7:164:ARG:N	2.35	0.41
6:7:460:GLU:HG2	6:7:466:THR:O	2.20	0.41
1:A:558:ALA:HB3	1:A:611:ILE:HD11	2.02	0.41
3:C:382:VAL:O	3:C:382:VAL:HG23	2.19	0.41
3:C:495:THR:HG22	5:E:563:ILE:HG13	2.02	0.41
3:C:710:LEU:HD13	3:C:738:ILE:HG12	2.02	0.41
1:2:414:LEU:HD11	1:2:441:ALA:CB	2.50	0.41
1:2:464:ILE:HG21	1:2:726:TYR:CD2	2.55	0.41
2:3:39:LEU:HD12	2:3:39:LEU:C	2.45	0.41
3:4:775:ASP:OD1	3:4:775:ASP:N	2.53	0.41
4:5:532:LEU:HD21	12:5:1002:ADP:C6	2.56	0.41
5:6:137:ILE:HD12	5:6:137:ILE:C	2.45	0.41
1:A:391:PRO:CD	5:E:493:LEU:HD23	2.51	0.41
2:B:424:GLU:OE1	6:F:405:THR:HG21	2.20	0.41
3:C:712:GLU:HA	3:C:715:VAL:HG12	2.03	0.41
4:D:198:ASN:O	4:D:199:THR:C	2.63	0.41
5:E:68:LEU:HD22	5:E:114:PHE:CE1	2.56	0.41
1:2:414:LEU:HD11	1:2:441:ALA:HB2	2.01	0.41
2:3:223:ASP:OD1	2:3:223:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:167:GLN:HG3	3:4:240:ALA:HB1	2.02	0.41
5:6:371:MET:HE1	5:6:500:LEU:HB2	2.02	0.41
1:A:414:LEU:CD1	1:A:444:VAL:HG12	2.51	0.41
1:A:560:VAL:O	1:A:560:VAL:HG13	2.20	0.41
3:C:167:GLN:HG3	3:C:244:ILE:HD11	2.03	0.41
6:F:512:LEU:HD12	6:F:518:LEU:HD13	2.01	0.41
2:3:10:VAL:HG13	2:3:11:GLU:N	2.36	0.41
2:3:412:ASP:HB2	2:3:452:ALA:HB1	2.03	0.41
2:3:577:ILE:HD12	2:3:577:ILE:N	2.35	0.41
3:4:717:MET:HE3	3:4:733:GLN:HB3	2.02	0.41
5:6:587:SER:N	5:6:590:SER:OG	2.54	0.41
6:7:172:GLU:OE1	6:7:172:GLU:N	2.43	0.41
1:A:535:TYR:CZ	1:A:539:VAL:HG21	2.56	0.41
1:A:789:ASP:OD1	1:A:790:ASP:N	2.54	0.41
3:C:631:ILE:HD11	3:C:727:VAL:HG22	2.03	0.41
3:C:717:MET:HE1	3:C:737:LEU:HD23	2.03	0.41
4:D:376:ASN:O	4:D:515:ASP:N	2.54	0.41
4:D:582:LEU:HD13	4:D:582:LEU:O	2.21	0.41
1:2:254:GLU:OE1	1:2:254:GLU:N	2.43	0.41
1:2:787:ILE:CG2	1:2:788:GLU:N	2.84	0.41
2:3:20:LEU:C	2:3:20:LEU:HD13	2.46	0.41
2:3:36:VAL:O	2:3:40:ILE:HD13	2.20	0.41
2:3:320:LEU:HD23	2:3:320:LEU:C	2.45	0.41
1:A:609:ILE:HG23	4:D:410:SER:HB3	2.03	0.41
5:E:546:TYR:O	5:E:550:ARG:HG3	2.20	0.41
2:3:54:LEU:HD12	2:3:62:ALA:HA	2.03	0.41
3:4:453:SER:CB	3:4:749:LEU:HD12	2.51	0.41
5:6:186:ALA:HB3	1:A:351:SER:O	2.20	0.41
6:7:432:GLY:O	6:7:436:LEU:HG	2.21	0.41
11:A:1002:ATP:C8	5:E:618:VAL:HG11	2.56	0.41
4:D:145:MET:O	4:D:146:SER:OG	2.23	0.41
4:D:337:LYS:O	4:D:337:LYS:HD3	2.21	0.41
5:E:94:LEU:HD23	5:E:110:PHE:HB3	2.02	0.41
5:E:253:ASP:HB2	5:E:295:ARG:HG3	2.03	0.41
6:F:603:ALA:O	6:F:607:LEU:HD23	2.20	0.41
1:2:373:TYR:OH	4:5:284:ARG:NH2	2.54	0.41
2:3:111:VAL:O	2:3:127:VAL:HA	2.20	0.41
2:3:352:SER:O	2:3:356:ARG:HG2	2.21	0.41
3:4:533:THR:HG22	3:4:534:SER:N	2.36	0.41
5:6:397:ASP:O	5:6:400:THR:OG1	2.28	0.41
6:7:445:ASP:OD1	6:7:446:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ILE:HG21	4:D:610:VAL:HG21	2.03	0.41
5:E:150:GLU:O	5:E:201:VAL:N	2.51	0.41
6:F:337:ALA:HB1	6:F:352:LYS:HG3	2.03	0.41
6:F:395:ASP:HA	6:F:401:SER:HB2	2.02	0.41
6:F:450:MET:HG2	6:F:454:ASP:HB2	2.03	0.41
2:3:112:SER:H	2:3:115:THR:HG1	1.67	0.40
2:3:268:MET:HA	2:3:534:PHE:CE2	2.55	0.40
2:3:270:LYS:HG2	2:3:535:SER:O	2.21	0.40
3:4:640:LEU:HD13	3:4:640:LEU:O	2.20	0.40
6:7:554:LEU:HD22	6:7:558:LEU:HD23	2.04	0.40
1:A:252:PRO:O	1:A:256:LEU:HD13	2.21	0.40
3:C:646:LEU:HD23	3:C:648:PHE:CE2	2.56	0.40
1:2:610:SER:O	4:5:410:SER:O	2.39	0.40
2:3:54:LEU:O	2:3:54:LEU:HD13	2.21	0.40
3:4:573:ILE:HD13	3:4:587:LEU:HD21	2.02	0.40
6:7:448:ASP:OD1	6:7:448:ASP:N	2.52	0.40
4:D:301:VAL:O	4:D:301:VAL:HG13	2.22	0.40
5:E:786:VAL:HG22	5:E:787:LEU:N	2.36	0.40
2:3:488:GLN:O	4:5:590:ARG:NH2	2.54	0.40
4:5:164:LYS:NZ	4:5:187:GLY:O	2.48	0.40
5:6:561:GLU:O	5:6:562:SER:OG	2.36	0.40
1:A:743:VAL:HG21	4:D:537:ILE:HD13	2.03	0.40
1:A:764:VAL:O	1:A:767:ILE:HG12	2.21	0.40
1:2:290:LEU:C	1:2:290:LEU:HD13	2.46	0.40
3:4:107:VAL:HG22	3:4:109:GLY:H	1.86	0.40
4:5:195:ARG:NE	4:5:210:ASP:OD1	2.49	0.40
5:6:515:SER:O	5:6:519:ASN:ND2	2.48	0.40
3:C:717:MET:HE1	3:C:737:LEU:CD2	2.51	0.40
5:E:45:LYS:O	5:E:49:LEU:HD23	2.21	0.40
6:F:93:VAL:HG12	6:F:94:VAL:N	2.36	0.40
2:3:487:ASP:OD1	4:5:590:ARG:NH2	2.43	0.40
6:7:306:MET:HA	6:7:306:MET:HE2	2.02	0.40
1:A:677:ARG:NH2	5:E:592:ASP:OD1	2.50	0.40
4:D:586:TYR:CE2	4:D:613:LEU:HD12	2.57	0.40
5:E:410:GLU:OE2	5:E:458:CYS:HB2	2.22	0.40
5:E:723:ILE:O	5:E:727:ILE:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	643/904 (71%)	598 (93%)	45 (7%)	0	100	100
1	A	659/904 (73%)	628 (95%)	31 (5%)	0	100	100
2	3	628/810 (78%)	599 (95%)	29 (5%)	0	100	100
2	B	647/810 (80%)	622 (96%)	25 (4%)	0	100	100
3	4	642/866 (74%)	608 (95%)	34 (5%)	0	100	100
3	C	640/866 (74%)	604 (94%)	36 (6%)	0	100	100
4	5	617/734 (84%)	579 (94%)	38 (6%)	0	100	100
4	D	615/734 (84%)	585 (95%)	30 (5%)	0	100	100
5	6	631/821 (77%)	609 (96%)	22 (4%)	0	100	100
5	E	684/821 (83%)	659 (96%)	25 (4%)	0	100	100
6	7	604/719 (84%)	575 (95%)	29 (5%)	0	100	100
6	F	613/719 (85%)	577 (94%)	36 (6%)	0	100	100
All	All	7623/9708 (78%)	7243 (95%)	380 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	568/781 (73%)	561 (99%)	7 (1%)	63	87
1	A	586/781 (75%)	580 (99%)	6 (1%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	550/708 (78%)	543 (99%)	7 (1%)	61	86
2	B	561/708 (79%)	557 (99%)	4 (1%)	76	91
3	4	572/755 (76%)	563 (98%)	9 (2%)	55	83
3	C	570/755 (76%)	567 (100%)	3 (0%)	81	93
4	5	533/625 (85%)	527 (99%)	6 (1%)	65	87
4	D	530/625 (85%)	526 (99%)	4 (1%)	73	90
5	6	565/724 (78%)	557 (99%)	8 (1%)	59	85
5	E	624/724 (86%)	621 (100%)	3 (0%)	81	93
6	7	535/619 (86%)	527 (98%)	8 (2%)	57	84
6	F	541/619 (87%)	533 (98%)	8 (2%)	57	84
All	All	6735/8424 (80%)	6662 (99%)	73 (1%)	63	87

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	228	GLU
1	2	268	LEU
1	2	369	ILE
1	2	663	VAL
1	2	735	LEU
1	2	750	LEU
1	2	770	MET
2	3	21	ASP
2	3	23	LEU
2	3	39	LEU
2	3	87	ILE
2	3	195	ASP
2	3	486	LEU
2	3	572	ILE
3	4	150	LEU
3	4	247	ASP
3	4	317	MET
3	4	354	LEU
3	4	399	ILE
3	4	452	LEU
3	4	475	ASP
3	4	640	LEU
3	4	751	ASN

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Mol	Chain	Res	Type
4	5	128	LEU
4	5	184	MET
4	5	391	LEU
4	5	400	ILE
4	5	458	ILE
4	5	532	LEU
5	6	16	LEU
5	6	28	LYS
5	6	34	LEU
5	6	168	VAL
5	6	200	PHE
5	6	226	VAL
5	6	247	THR
5	6	492	THR
6	7	40	LEU
6	7	161	VAL
6	7	287	GLN
6	7	296	THR
6	7	331	ASP
6	7	520	LEU
6	7	588	MET
6	7	609	ILE
1	A	177	LEU
1	A	210	HIS
1	A	395	ASP
1	A	620	LEU
1	A	650	THR
1	A	755	MET
2	B	4	THR
2	B	70	PHE
2	B	224	ASP
2	B	478	ARG
3	C	170	LEU
3	C	197	LEU
3	C	645	ASP
4	D	37	GLU
4	D	59	LEU
4	D	224	PHE
4	D	380	LEU
5	E	133	LEU
5	E	245	THR
5	E	440	HIS

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Mol	Chain	Res	Type
6	F	108	MET
6	F	203	LEU
6	F	206	CYS
6	F	220	LEU
6	F	301	HIS
6	F	364	GLN
6	F	405	THR
6	F	461	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	196	HIS
1	2	212	HIS
1	2	280	HIS
1	2	518	ASN
1	2	601	HIS
1	2	766	HIS
1	2	777	HIS
2	3	439	HIS
2	3	513	GLN
3	4	257	GLN
3	4	300	GLN
3	4	307	GLN
3	4	521	GLN
3	4	531	GLN
3	4	593	GLN
3	4	664	HIS
3	4	733	GLN
4	5	30	GLN
5	6	121	HIS
5	6	404	GLN
6	7	212	GLN
6	7	270	HIS
6	7	307	ASN
6	7	464	GLN
6	7	489	ASN
6	7	631	ASN
1	A	213	ASN
1	A	549	GLN
1	A	690	ASN
1	A	876	ASN

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Mol	Chain	Res	Type
2	B	94	GLN
2	B	584	GLN
3	C	242	ASN
3	C	257	GLN
3	C	311	HIS
3	C	420	HIS
3	C	531	GLN
3	C	568	ASN
3	C	638	HIS
4	D	171	GLN
4	D	244	HIS
4	D	246	GLN
5	E	237	GLN
5	E	327	ASN
5	E	342	GLN
5	E	635	HIS
6	F	186	GLN
6	F	209	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 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	$\# Z > 2$
12	ADP	7	1002	10	28,29,29	1.37	4 (14%)	43,45,45	1.92	9 (20%)
12	ADP	6	1002	10	28,29,29	1.38	4 (14%)	43,45,45	1.93	8 (18%)
12	ADP	F	1002	10	28,29,29	1.36	4 (14%)	43,45,45	1.92	9 (20%)
11	ATP	A	1002	10	32,33,33	1.12	2 (6%)	48,52,52	0.80	1 (2%)
12	ADP	E	1002	10	28,29,29	1.37	4 (14%)	43,45,45	1.91	10 (23%)
12	ADP	3	1002	-	28,29,29	1.37	4 (14%)	43,45,45	1.89	11 (25%)
12	ADP	B	1002	10	28,29,29	1.38	4 (14%)	43,45,45	1.90	12 (27%)
11	ATP	2	1002	10	32,33,33	0.46	0	48,52,52	0.74	0
12	ADP	5	1002	10	28,29,29	1.39	4 (14%)	43,45,45	1.90	9 (20%)
12	ADP	D	1002	10	28,29,29	1.39	4 (14%)	43,45,45	1.89	11 (25%)

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
12	ADP	7	1002	10	-	1/16/32/32	0/3/3/3
12	ADP	6	1002	10	-	2/16/32/32	0/3/3/3
12	ADP	F	1002	10	-	3/16/32/32	0/3/3/3
11	ATP	A	1002	10	-	2/22/38/38	0/3/3/3
12	ADP	E	1002	10	-	2/16/32/32	0/3/3/3
12	ADP	3	1002	-	-	2/16/32/32	0/3/3/3
12	ADP	B	1002	10	-	6/16/32/32	0/3/3/3
11	ATP	2	1002	10	-	7/22/38/38	0/3/3/3
12	ADP	5	1002	10	-	10/16/32/32	0/3/3/3
12	ADP	D	1002	10	-	2/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1002	ATP	PB-O3B	-5.45	1.53	1.59
12	5	1002	ADP	C5-C4	4.52	1.47	1.39
12	6	1002	ADP	C5-C4	4.50	1.47	1.39
12	F	1002	ADP	C5-C4	4.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1002	ADP	C5-C4	4.47	1.47	1.39
12	7	1002	ADP	C5-C4	4.47	1.47	1.39
12	B	1002	ADP	C5-C4	4.47	1.47	1.39
12	3	1002	ADP	C5-C4	4.46	1.47	1.39
12	E	1002	ADP	C5-C4	4.41	1.47	1.39
12	6	1002	ADP	C5-C6	2.63	1.48	1.41
12	D	1002	ADP	C5-C6	2.61	1.48	1.41
12	B	1002	ADP	C5-C6	2.60	1.48	1.41
12	F	1002	ADP	C5-C6	2.59	1.48	1.41
12	E	1002	ADP	C5-C6	2.56	1.48	1.41
12	3	1002	ADP	C5-C6	2.55	1.48	1.41
12	7	1002	ADP	C5-C6	2.53	1.48	1.41
12	5	1002	ADP	C5-C6	2.49	1.47	1.41
12	7	1002	ADP	C5-N7	-2.47	1.34	1.39
12	D	1002	ADP	C5-N7	-2.40	1.34	1.39
12	6	1002	ADP	C5-N7	-2.40	1.34	1.39
12	5	1002	ADP	C5-N7	-2.40	1.34	1.39
12	3	1002	ADP	C5-N7	-2.38	1.34	1.39
12	B	1002	ADP	C8-N7	2.36	1.36	1.31
12	E	1002	ADP	C5-N7	-2.35	1.34	1.39
12	F	1002	ADP	C5-N7	-2.34	1.34	1.39
12	D	1002	ADP	C8-N7	2.33	1.36	1.31
12	B	1002	ADP	C5-N7	-2.32	1.34	1.39
12	3	1002	ADP	C8-N7	2.32	1.36	1.31
12	6	1002	ADP	C8-N7	2.27	1.36	1.31
12	F	1002	ADP	C8-N7	2.22	1.35	1.31
12	7	1002	ADP	C8-N7	2.21	1.35	1.31
12	E	1002	ADP	C8-N7	2.21	1.35	1.31
11	A	1002	ATP	PA-O3A	-2.20	1.57	1.59
12	5	1002	ADP	C8-N7	2.13	1.35	1.31

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	6	1002	ADP	C5-C4-N3	-6.25	118.11	126.72
12	7	1002	ADP	C5-C4-N3	-6.06	118.37	126.72
12	F	1002	ADP	C5-C4-N3	-5.98	118.48	126.72
12	5	1002	ADP	C5-C4-N3	-5.94	118.54	126.72
12	D	1002	ADP	C5-C4-N3	-5.87	118.63	126.72
12	3	1002	ADP	C5-C4-N3	-5.81	118.72	126.72
12	E	1002	ADP	C5-C4-N3	-5.72	118.84	126.72
12	B	1002	ADP	C5-C4-N3	-5.55	119.07	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	1002	ADP	N3-C4-N9	5.05	135.76	127.17
12	5	1002	ADP	N3-C4-N9	5.05	135.75	127.17
12	6	1002	ADP	N3-C4-N9	5.02	135.71	127.17
12	7	1002	ADP	N3-C4-N9	4.97	135.62	127.17
12	E	1002	ADP	N3-C4-N9	4.84	135.41	127.17
12	D	1002	ADP	N3-C4-N9	4.73	135.21	127.17
12	3	1002	ADP	N3-C4-N9	4.68	135.12	127.17
12	B	1002	ADP	N3-C4-N9	4.53	134.86	127.17
12	F	1002	ADP	C2-N3-C4	3.94	121.44	111.83
12	6	1002	ADP	C2-N3-C4	3.91	121.38	111.83
12	7	1002	ADP	C2-N3-C4	3.87	121.29	111.83
12	D	1002	ADP	C2-N3-C4	3.87	121.28	111.83
12	3	1002	ADP	C2-N3-C4	3.86	121.26	111.83
12	5	1002	ADP	C2-N3-C4	3.84	121.21	111.83
12	E	1002	ADP	C2-N3-C4	3.83	121.19	111.83
12	B	1002	ADP	C2-N3-C4	3.81	121.13	111.83
12	F	1002	ADP	N3-C2-N1	-3.78	122.85	128.58
12	B	1002	ADP	N3-C2-N1	-3.77	122.88	128.58
12	E	1002	ADP	N3-C2-N1	-3.76	122.90	128.58
12	3	1002	ADP	N3-C2-N1	-3.69	122.99	128.58
12	D	1002	ADP	N3-C2-N1	-3.69	123.00	128.58
12	5	1002	ADP	N3-C2-N1	-3.66	123.04	128.58
12	7	1002	ADP	N3-C2-N1	-3.60	123.14	128.58
12	6	1002	ADP	C4-C5-N7	-3.59	106.48	110.58
12	6	1002	ADP	N3-C2-N1	-3.45	123.36	128.58
12	B	1002	ADP	C4-C5-N7	-3.44	106.65	110.58
12	D	1002	ADP	C4-C5-N7	-3.44	106.65	110.58
12	7	1002	ADP	C4-C5-N7	-3.42	106.67	110.58
12	3	1002	ADP	C4-C5-N7	-3.41	106.69	110.58
12	E	1002	ADP	C4-N9-C8	3.30	109.20	105.74
12	F	1002	ADP	C4-C5-N7	-3.25	106.86	110.58
12	B	1002	ADP	C4-N9-C8	3.22	109.12	105.74
12	F	1002	ADP	C4-N9-C8	3.22	109.12	105.74
12	5	1002	ADP	C4-N9-C8	3.22	109.12	105.74
12	E	1002	ADP	C4-C5-N7	-3.21	106.91	110.58
12	5	1002	ADP	C4-C5-N7	-3.18	106.94	110.58
12	7	1002	ADP	C4-N9-C8	3.07	108.96	105.74
12	D	1002	ADP	C4-N9-C8	2.97	108.86	105.74
12	3	1002	ADP	C4-N9-C8	2.96	108.85	105.74
12	6	1002	ADP	C4-N9-C8	2.90	108.79	105.74
12	6	1002	ADP	C5-N7-C8	2.82	107.88	103.45
12	7	1002	ADP	C5-N7-C8	2.74	107.75	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1002	ADP	C5-N7-C8	2.70	107.69	103.45
12	D	1002	ADP	C5-N7-C8	2.69	107.67	103.45
12	F	1002	ADP	C5-N7-C8	2.68	107.66	103.45
12	3	1002	ADP	C5-N7-C8	2.67	107.64	103.45
12	5	1002	ADP	C5-N7-C8	2.63	107.58	103.45
12	E	1002	ADP	C5-N7-C8	2.60	107.54	103.45
12	B	1002	ADP	N9-C8-N7	-2.44	110.47	113.94
12	3	1002	ADP	C3'-C2'-C1'	2.42	106.04	101.46
12	F	1002	ADP	N9-C8-N7	-2.36	110.59	113.94
12	E	1002	ADP	N9-C8-N7	-2.35	110.59	113.94
12	7	1002	ADP	N9-C8-N7	-2.35	110.60	113.94
12	5	1002	ADP	N9-C8-N7	-2.31	110.66	113.94
12	D	1002	ADP	N9-C8-N7	-2.31	110.66	113.94
12	3	1002	ADP	N9-C8-N7	-2.30	110.67	113.94
12	6	1002	ADP	N9-C8-N7	-2.30	110.67	113.94
11	A	1002	ATP	O3A-PA-O1A	-2.27	103.89	110.70
12	B	1002	ADP	C6-C5-N7	2.26	136.46	132.09
12	B	1002	ADP	O4'-C1'-N9	2.25	112.41	108.09
12	D	1002	ADP	C3'-C2'-C1'	2.23	105.69	101.46
12	7	1002	ADP	C3'-C2'-C1'	2.16	105.55	101.46
12	B	1002	ADP	C2-N1-C6	2.12	122.21	118.73
12	3	1002	ADP	C6-C5-N7	2.11	136.16	132.09
12	D	1002	ADP	C6-C5-N7	2.08	136.10	132.09
12	E	1002	ADP	C2-N1-C6	2.07	122.13	118.73
12	E	1002	ADP	C3'-C2'-C1'	2.06	105.37	101.46
12	5	1002	ADP	C3'-C2'-C1'	2.04	105.33	101.46
12	F	1002	ADP	C2-N1-C6	2.02	122.04	118.73
12	D	1002	ADP	C2-N1-C6	2.02	122.04	118.73
12	3	1002	ADP	C2-N1-C6	2.01	122.03	118.73
12	B	1002	ADP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	2	1002	ATP	C5'-O5'-PA-O1A
12	5	1002	ADP	C5'-O5'-PA-O2A
12	5	1002	ADP	C5'-O5'-PA-O3A
12	B	1002	ADP	C5'-O5'-PA-O3A
12	D	1002	ADP	C5'-O5'-PA-O2A
12	D	1002	ADP	C5'-O5'-PA-O3A
12	E	1002	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
12	F	1002	ADP	C5'-O5'-PA-O2A
12	F	1002	ADP	C5'-O5'-PA-O3A
11	2	1002	ATP	O4'-C4'-C5'-O5'
11	2	1002	ATP	C3'-C4'-C5'-O5'
12	6	1002	ADP	O4'-C4'-C5'-O5'
12	6	1002	ADP	C3'-C4'-C5'-O5'
12	5	1002	ADP	O4'-C4'-C5'-O5'
11	A	1002	ATP	C3'-C4'-C5'-O5'
12	5	1002	ADP	C3'-C4'-C5'-O5'
12	B	1002	ADP	O4'-C4'-C5'-O5'
12	5	1002	ADP	PA-O3A-PB-O1B
11	2	1002	ATP	PG-O3B-PB-O2B
12	3	1002	ADP	PB-O3A-PA-O2A
12	5	1002	ADP	PB-O3A-PA-O1A
11	A	1002	ATP	O4'-C4'-C5'-O5'
12	B	1002	ADP	C5'-O5'-PA-O1A
12	E	1002	ADP	C5'-O5'-PA-O1A
12	F	1002	ADP	C5'-O5'-PA-O1A
12	5	1002	ADP	C4'-C5'-O5'-PA
12	5	1002	ADP	PA-O3A-PB-O2B
12	5	1002	ADP	PA-O3A-PB-O3B
12	B	1002	ADP	C3'-C4'-C5'-O5'
11	2	1002	ATP	PG-O3B-PB-O1B
11	2	1002	ATP	PB-O3A-PA-O1A
11	2	1002	ATP	PB-O3A-PA-O2A
12	3	1002	ADP	PB-O3A-PA-O1A
12	B	1002	ADP	PB-O3A-PA-O1A
12	7	1002	ADP	O4'-C4'-C5'-O5'
12	5	1002	ADP	PB-O3A-PA-O2A
12	B	1002	ADP	PB-O3A-PA-O2A

There are no ring outliers.

8 monomers are involved in 11 short contacts:

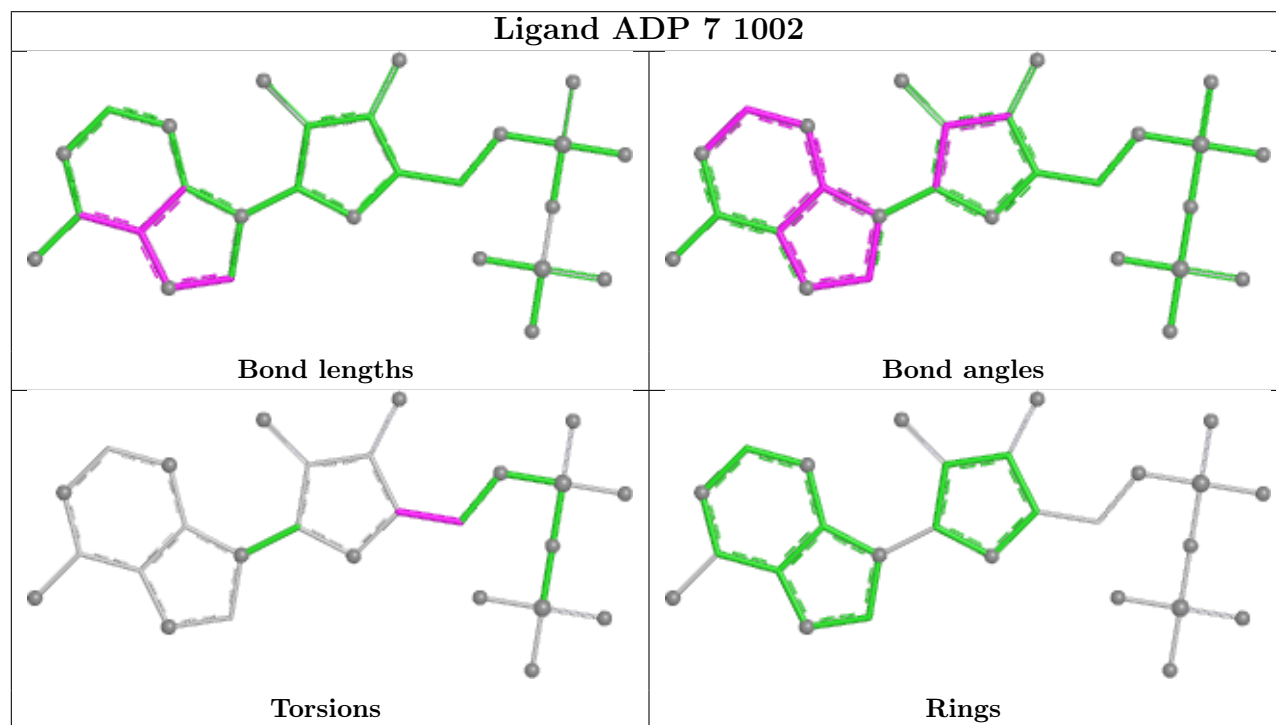
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	6	1002	ADP	1	0
12	F	1002	ADP	1	0
11	A	1002	ATP	1	0
12	E	1002	ADP	1	0
12	3	1002	ADP	1	0
12	B	1002	ADP	1	0
11	2	1002	ATP	3	0

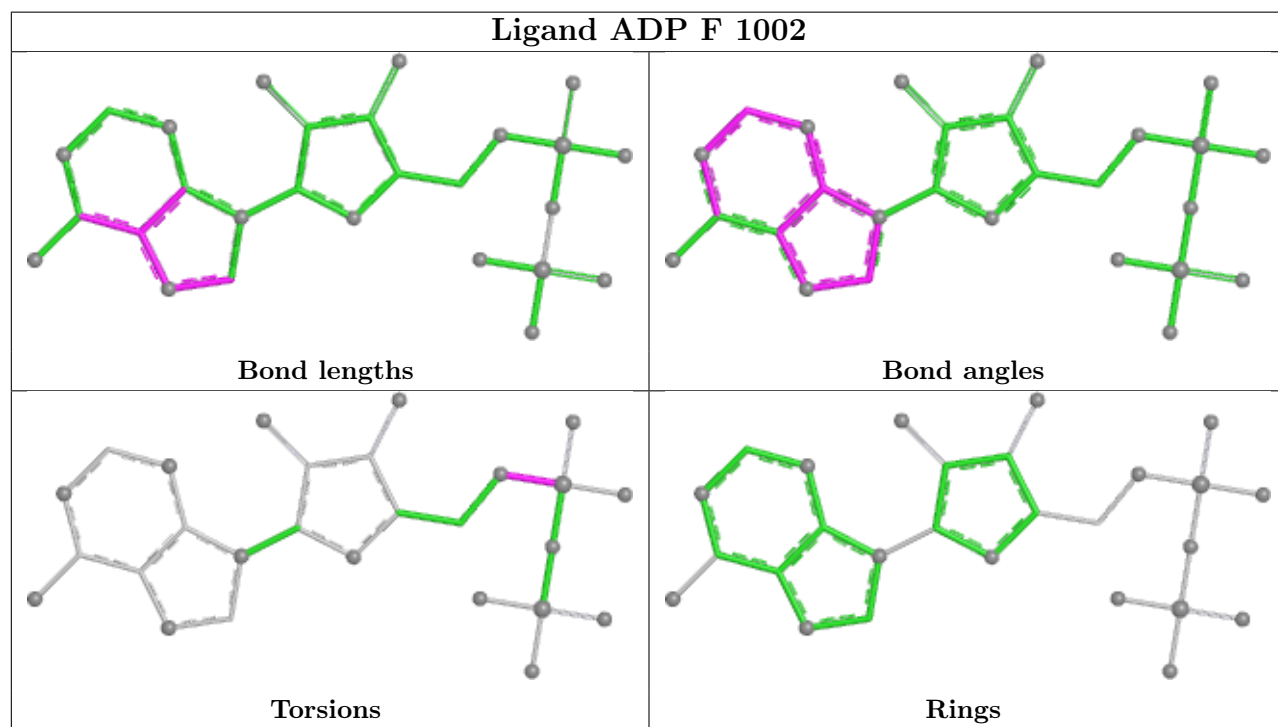
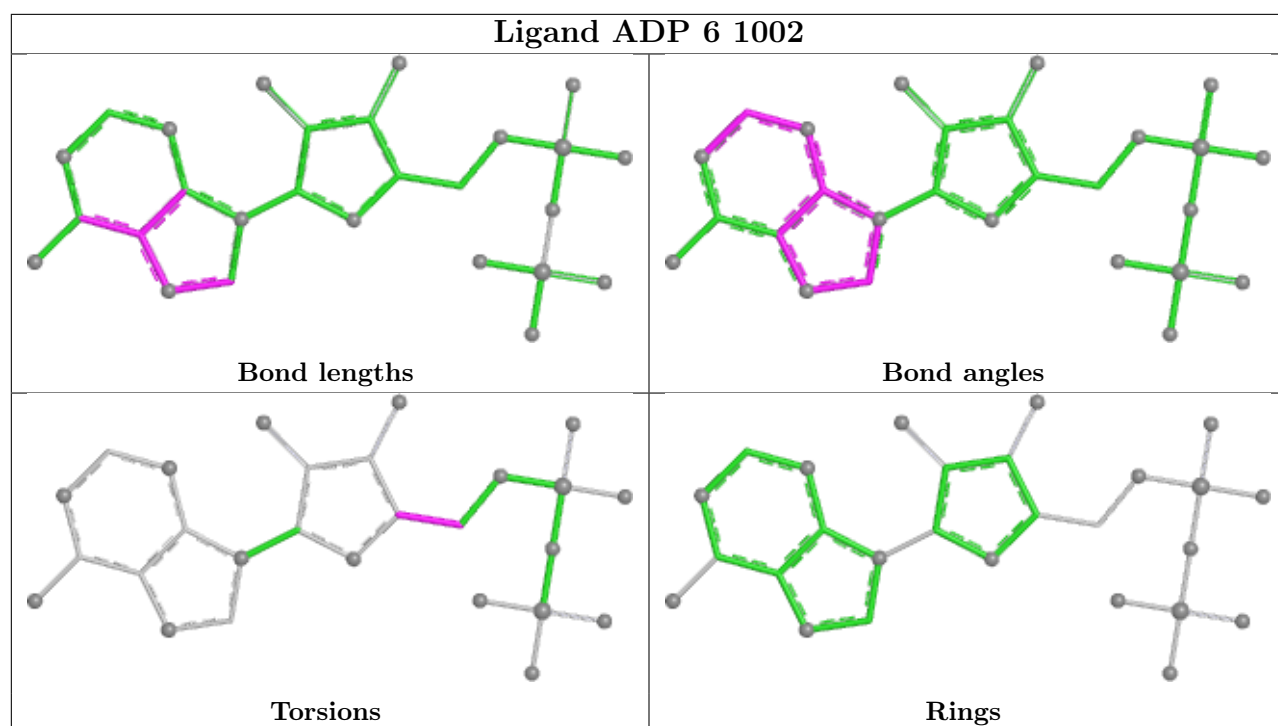
Continued on next page...

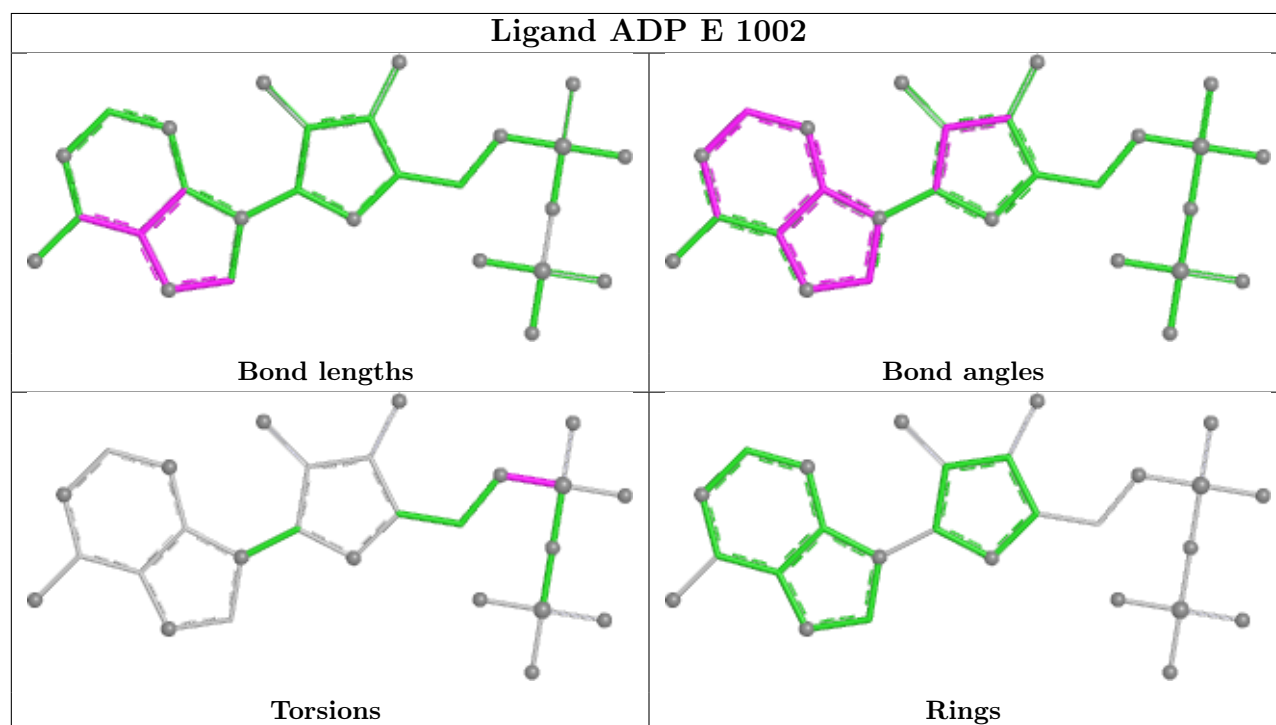
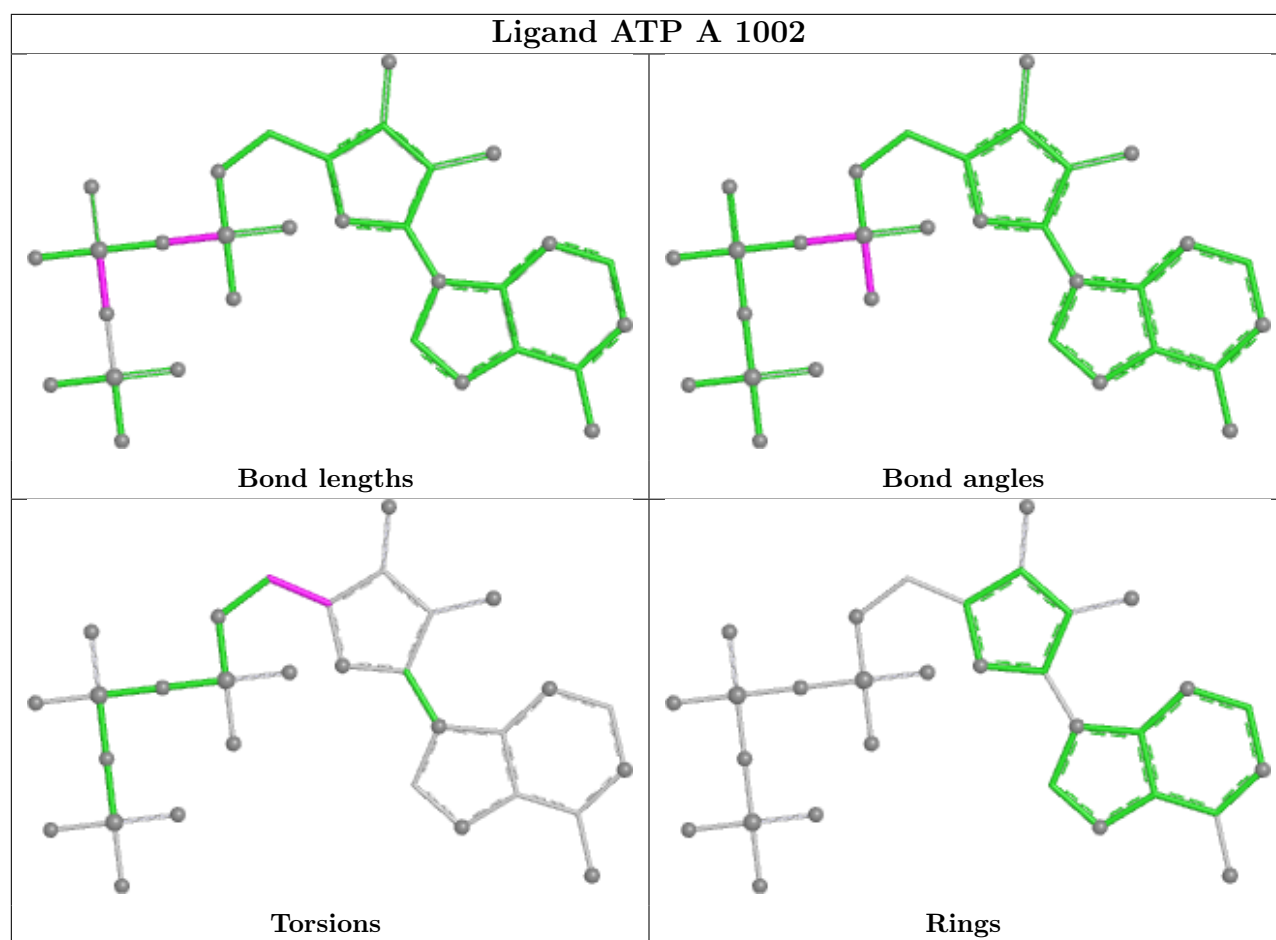
Continued from previous page...

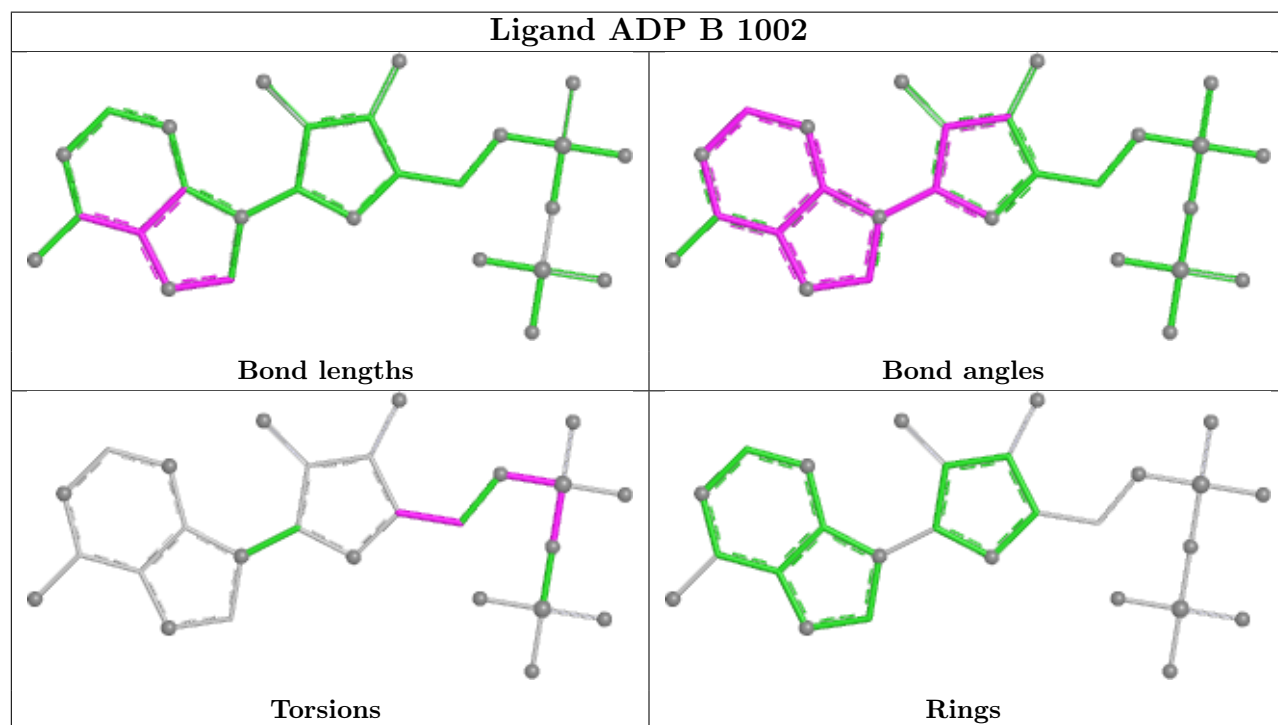
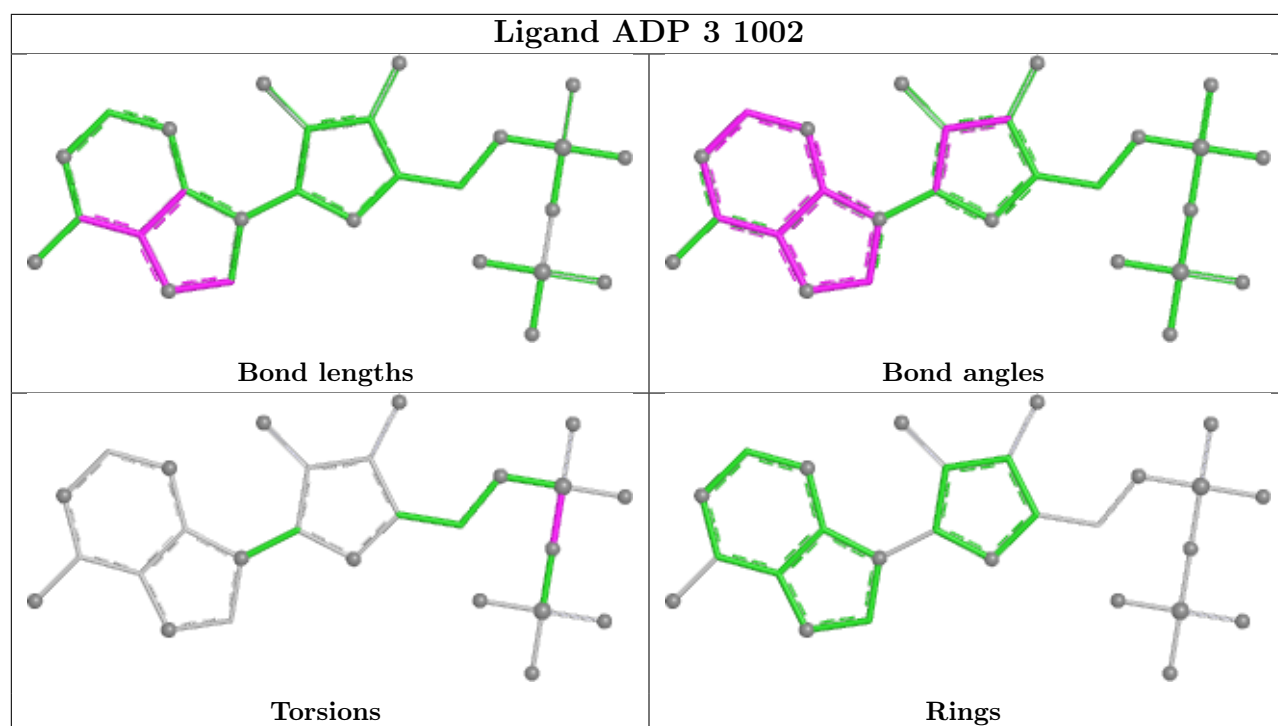
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	5	1002	ADP	2	0

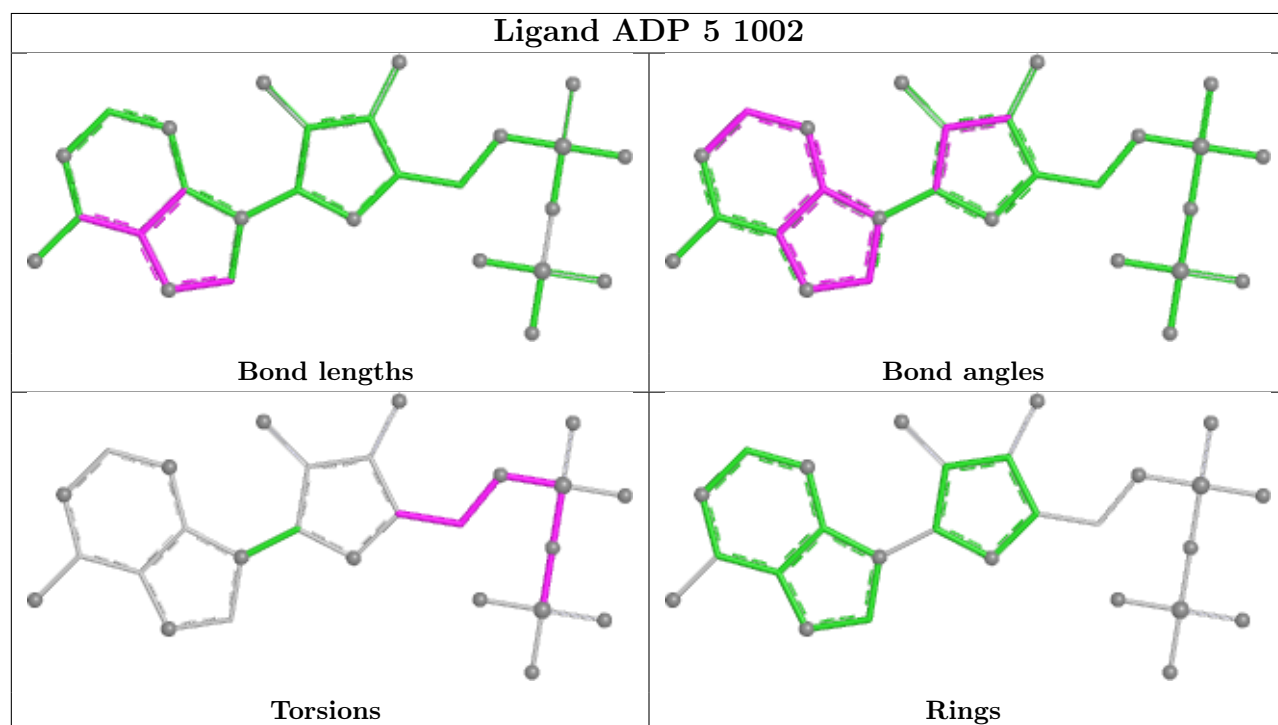
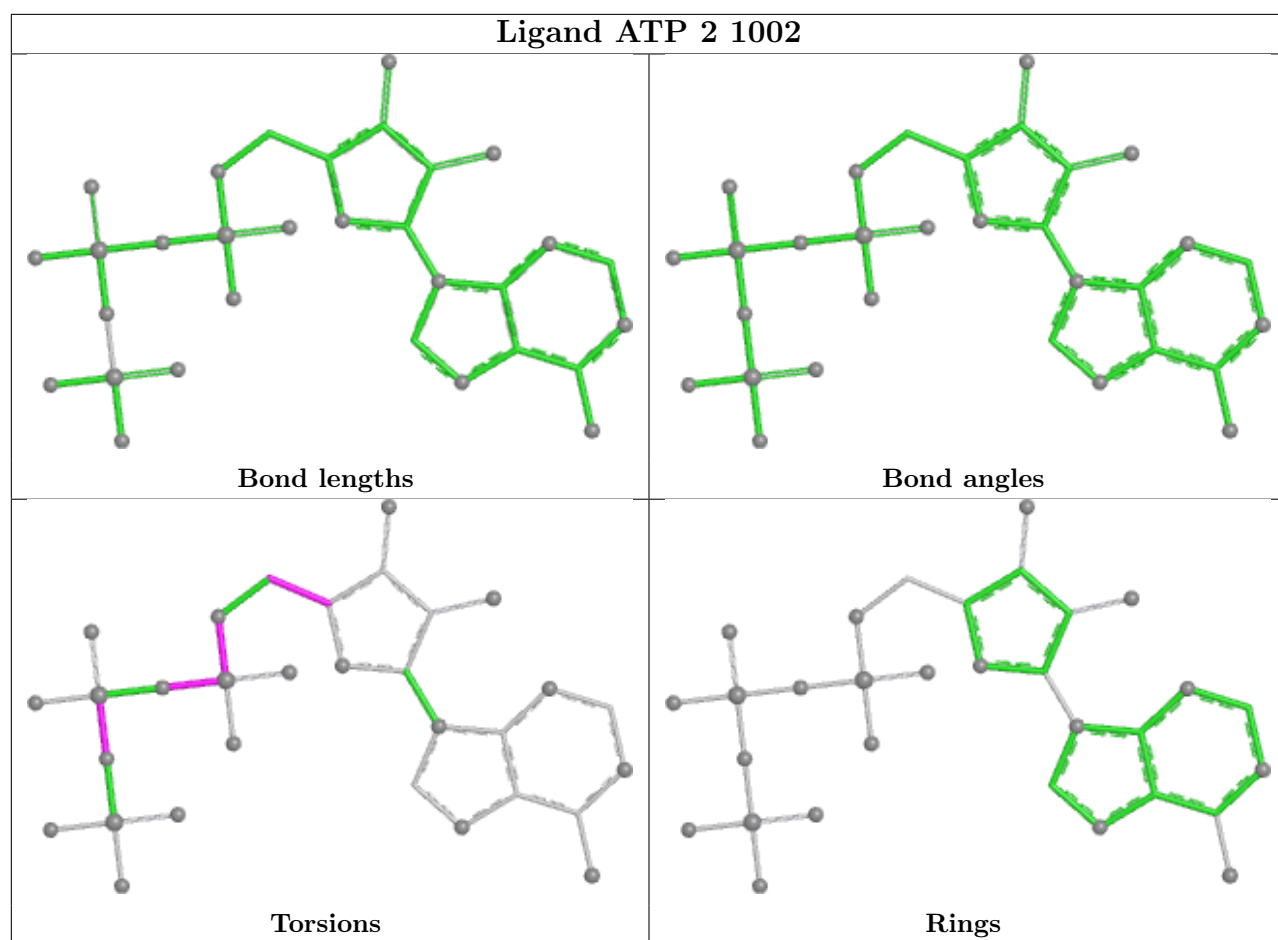
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

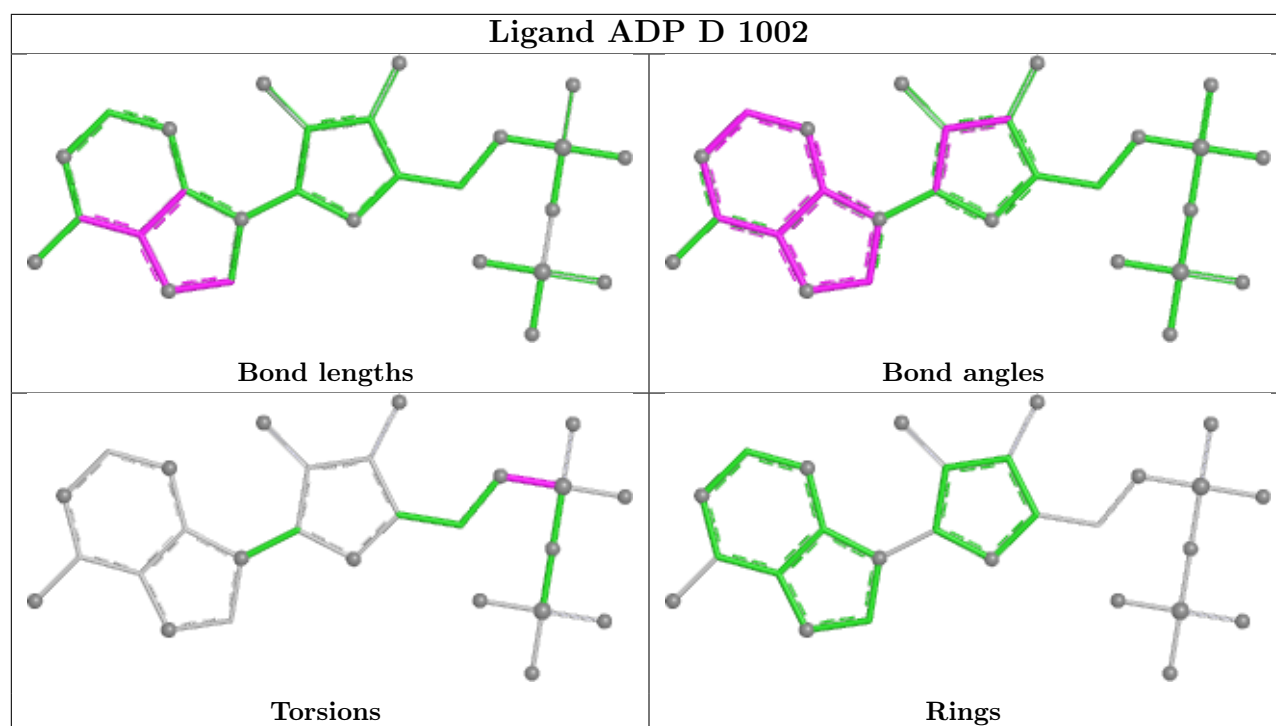












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

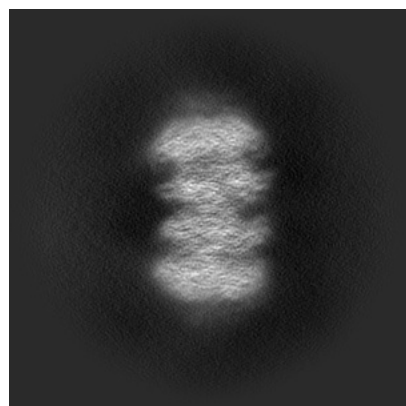
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43708. These allow visual inspection of the internal detail of the map and identification of artifacts.

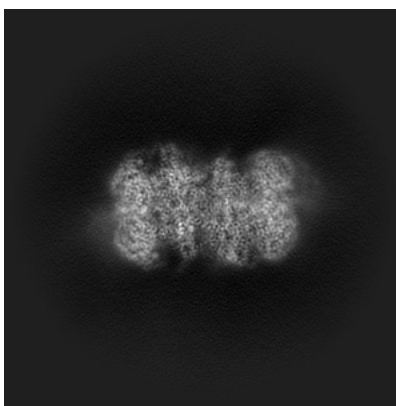
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

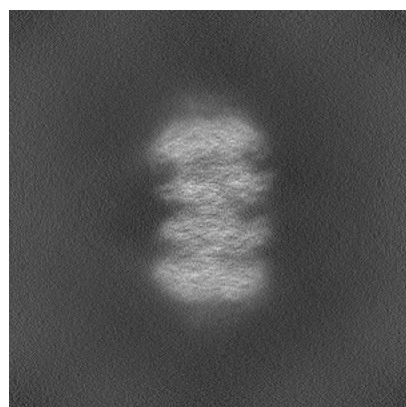


Y

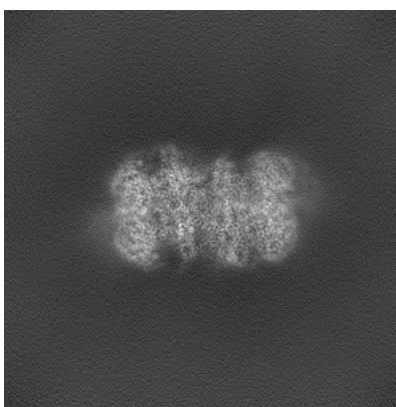


Z

6.1.2 Raw map



X



Y

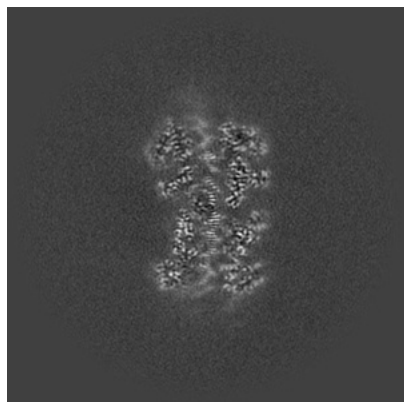


Z

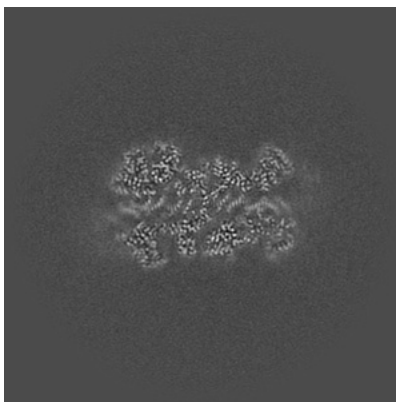
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

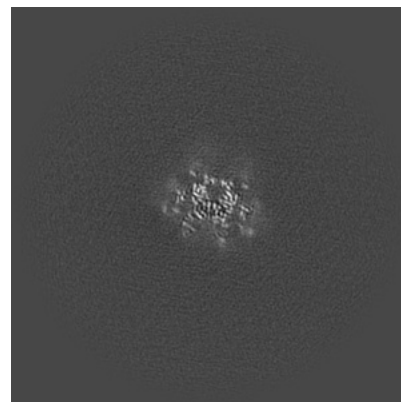
6.2.1 Primary map



X Index: 250

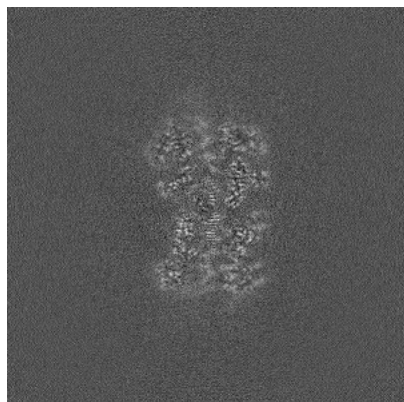


Y Index: 250

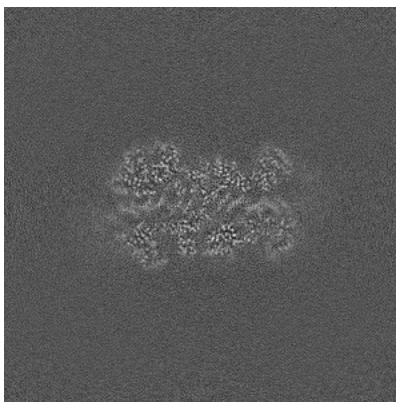


Z Index: 250

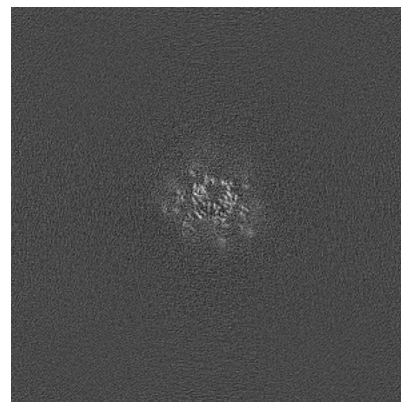
6.2.2 Raw map



X Index: 250



Y Index: 250

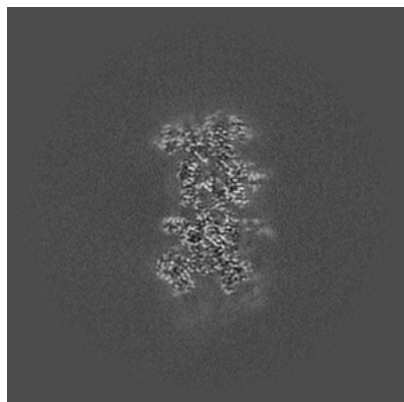


Z Index: 250

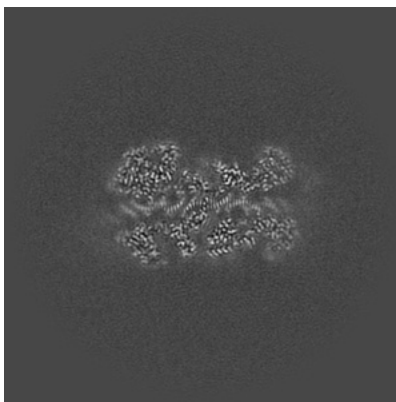
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

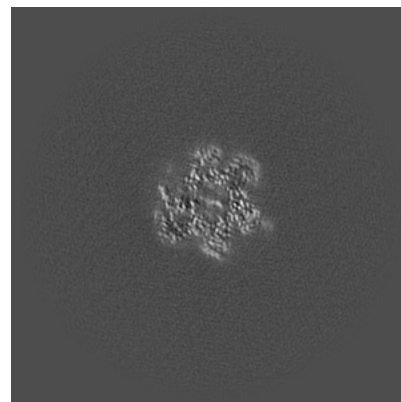
6.3.1 Primary map



X Index: 226

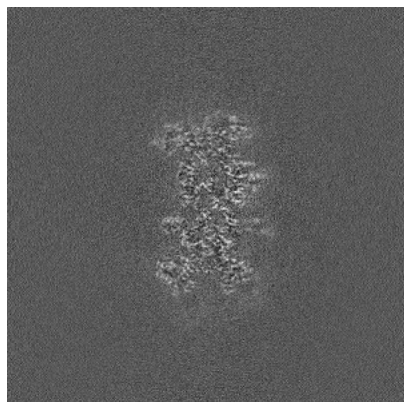


Y Index: 253

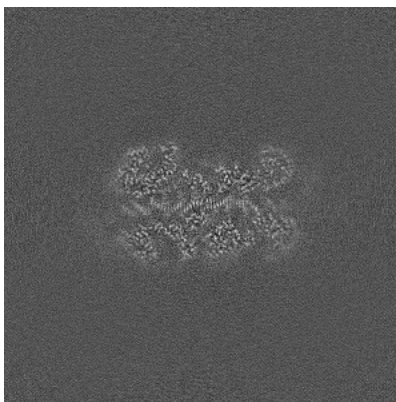


Z Index: 278

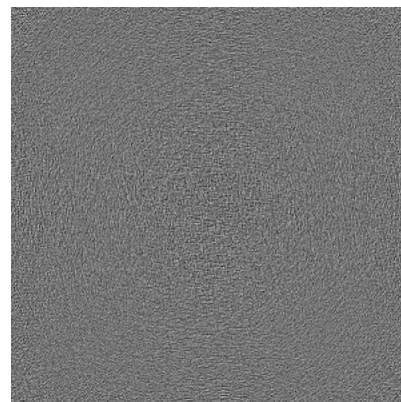
6.3.2 Raw map



X Index: 227



Y Index: 255

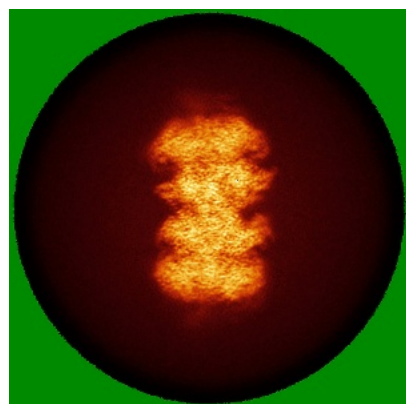


Z Index: 0

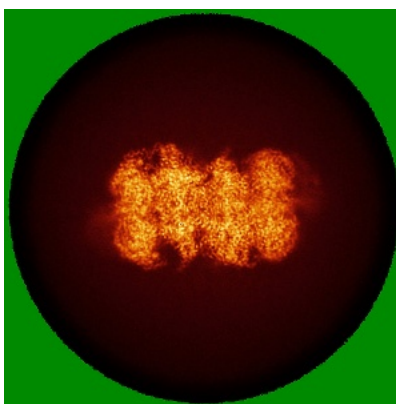
The images above show the largest variance slices of the map in three orthogonal directions.

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

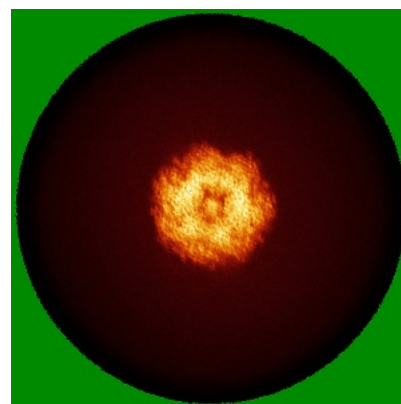
6.4.1 Primary map



X

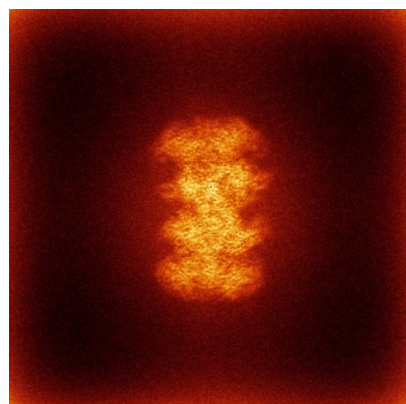


Y

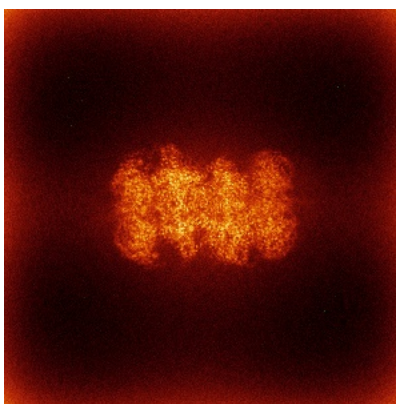


Z

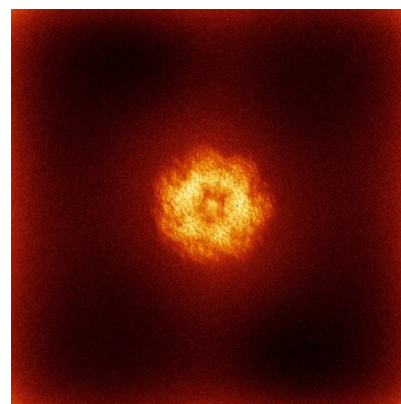
6.4.2 Raw map



X



Y

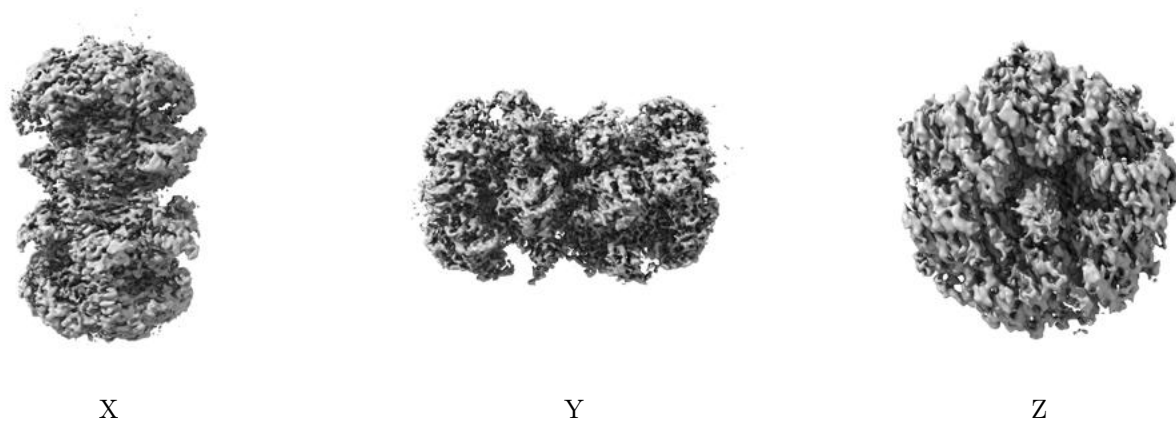


Z

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

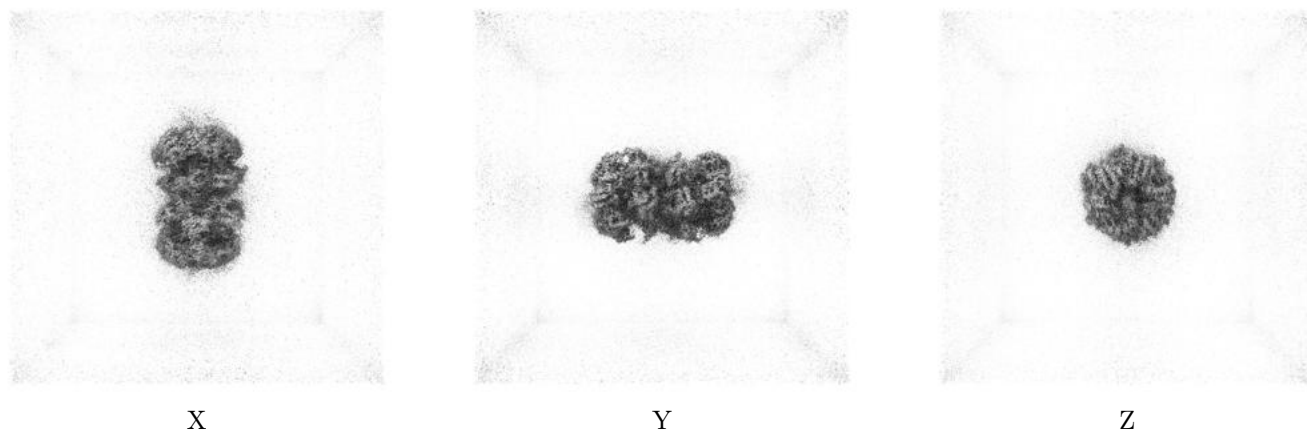
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

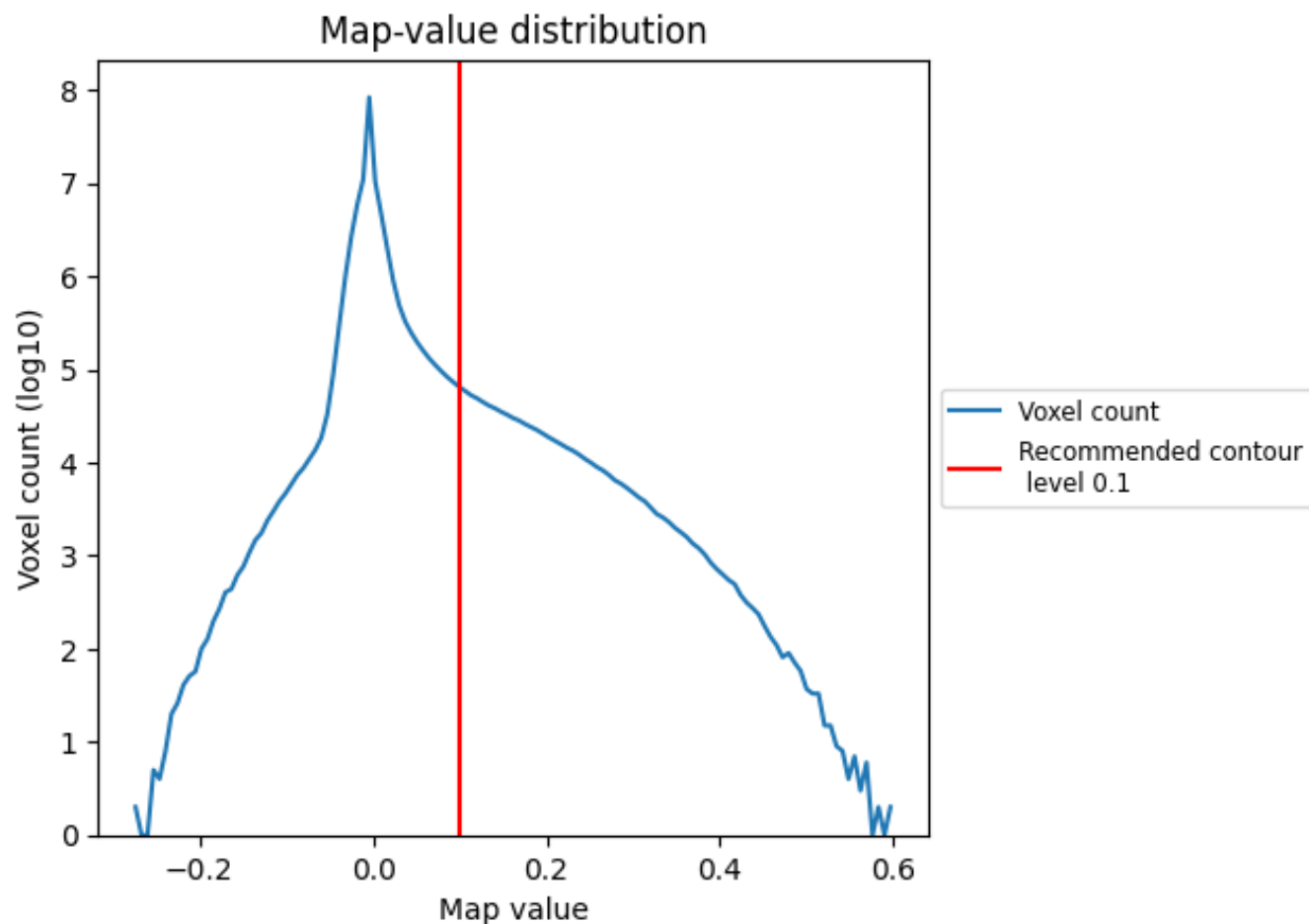
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

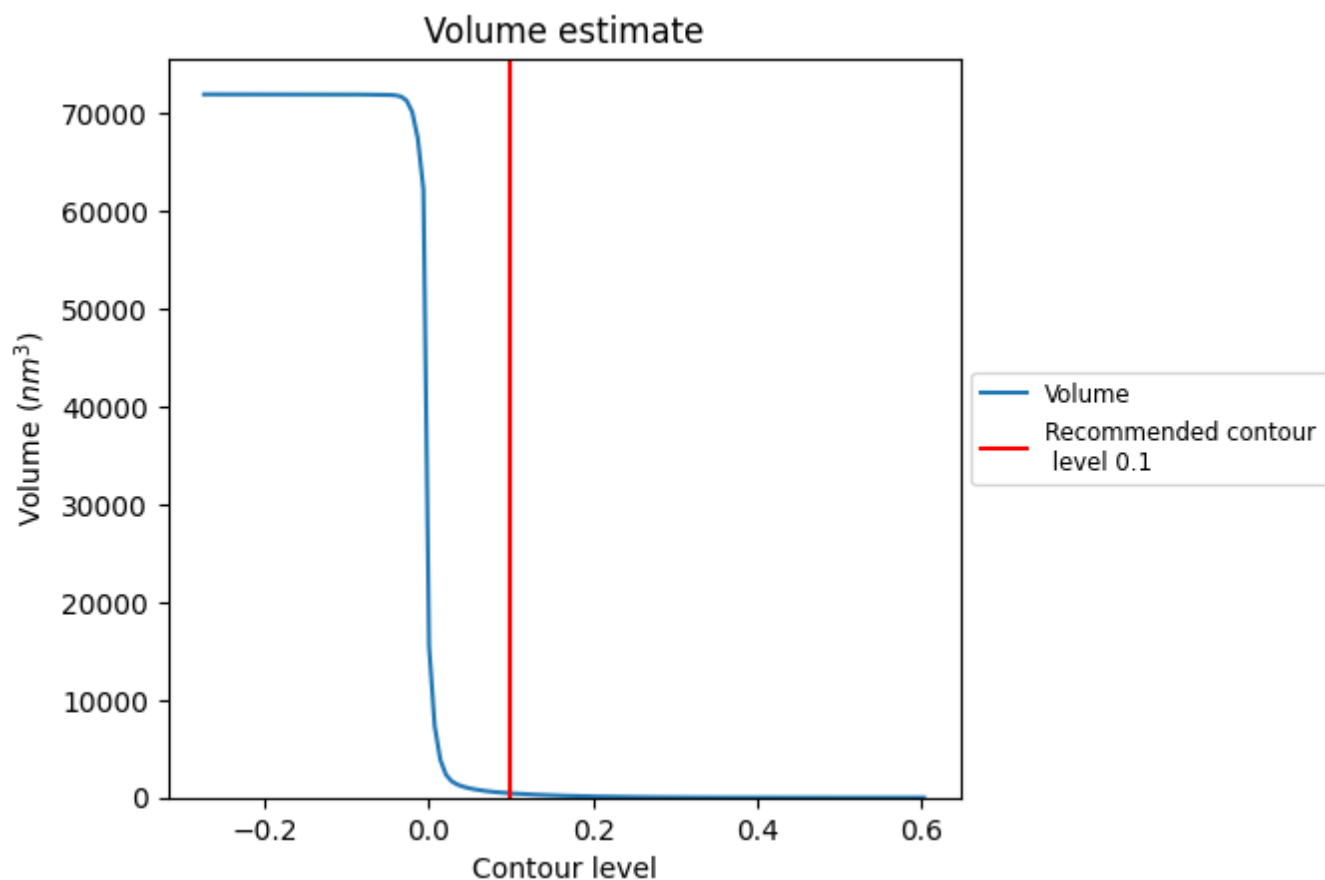
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

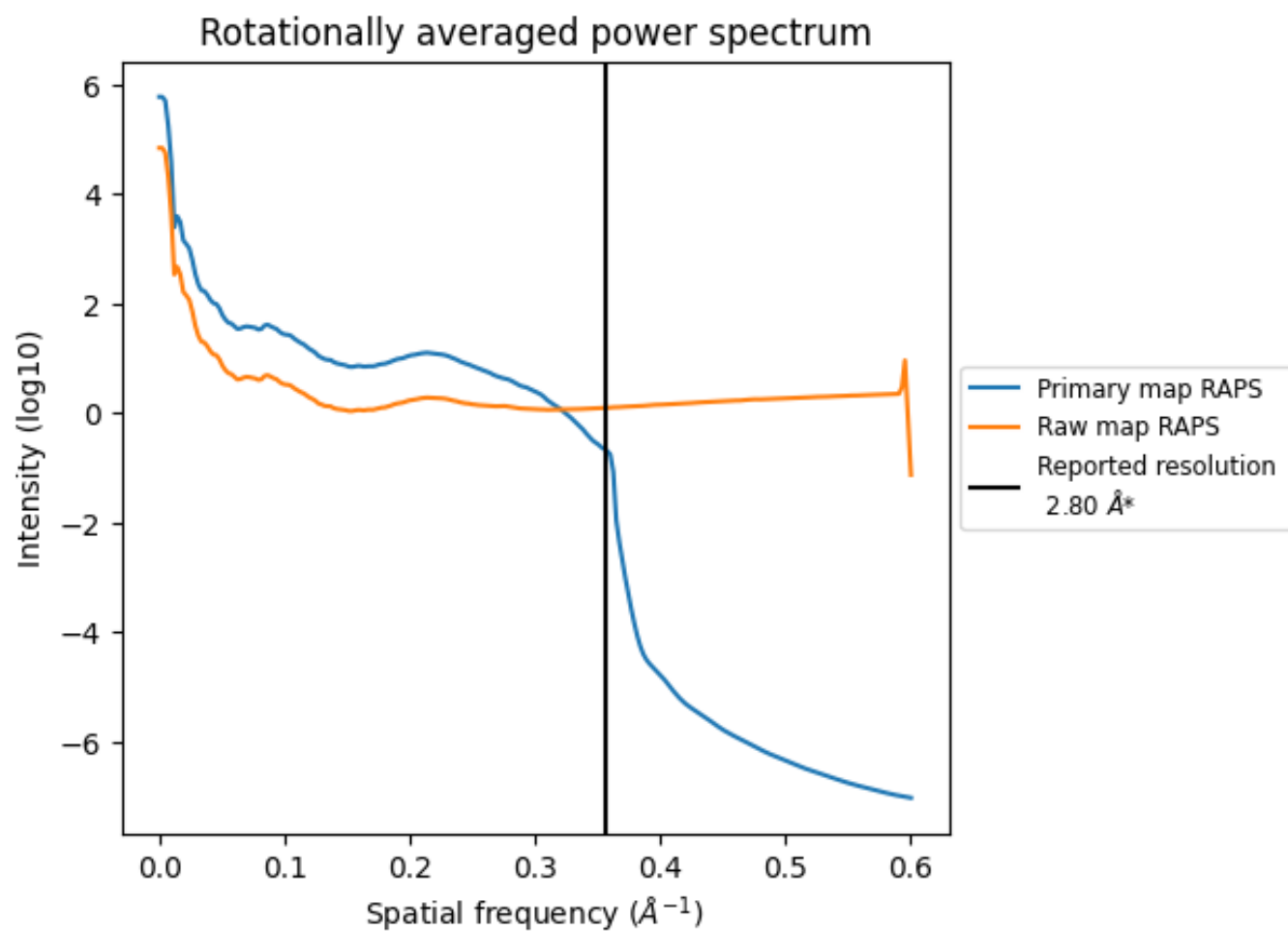
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm^3 ; this corresponds to an approximate mass of 392 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 ⓘ

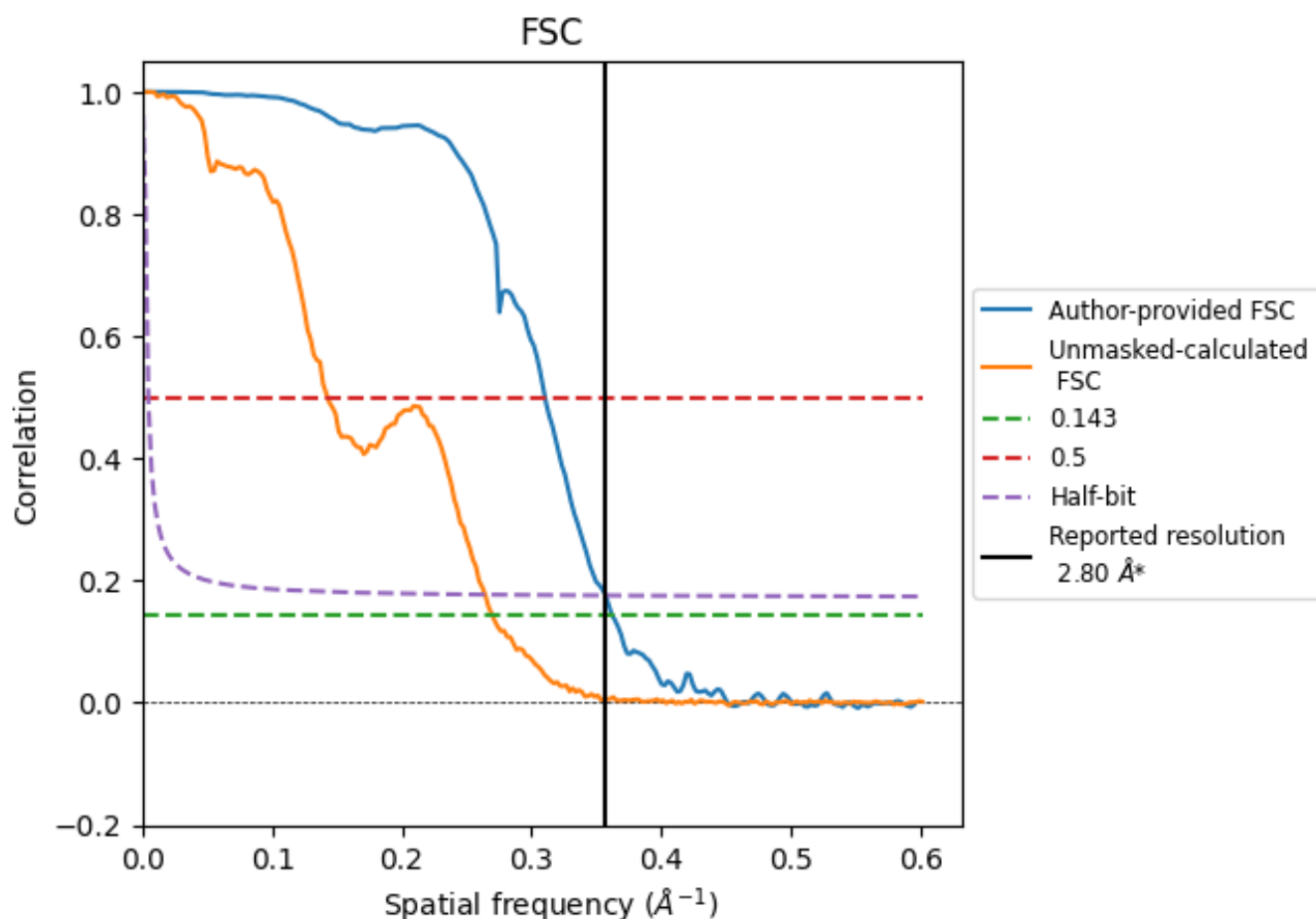


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

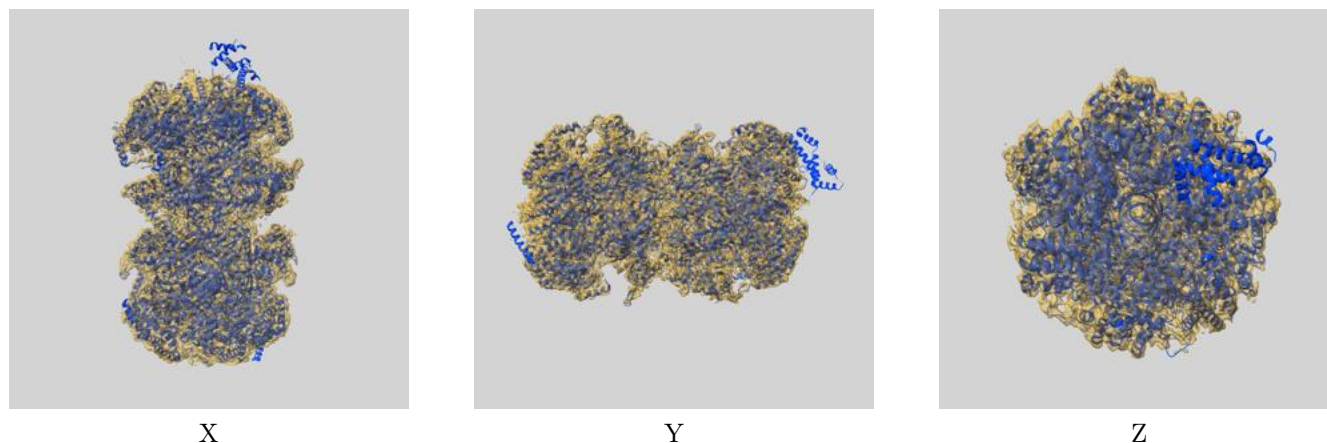
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.22	2.80
Unmasked-calculated*	3.71	7.00	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

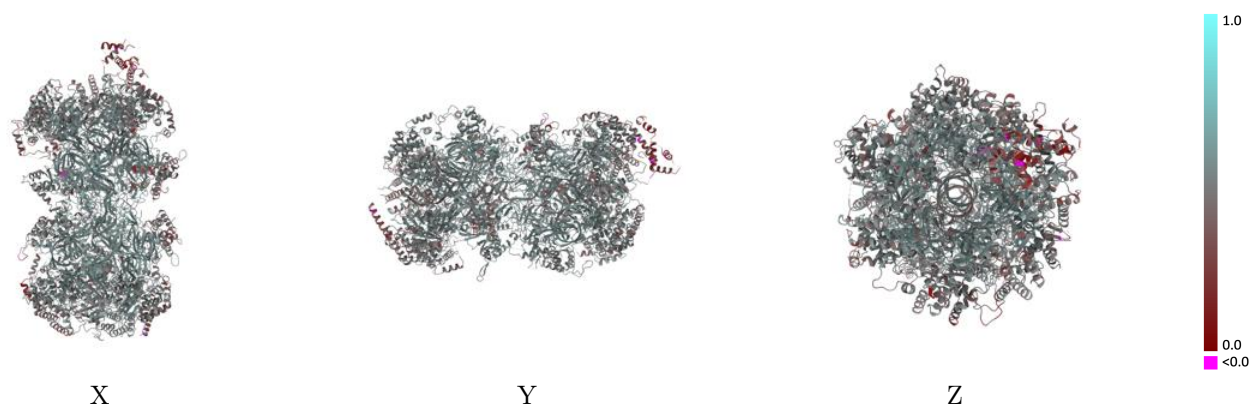
This section contains information regarding the fit between EMDB map EMD-43708 and PDB model 8W0F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



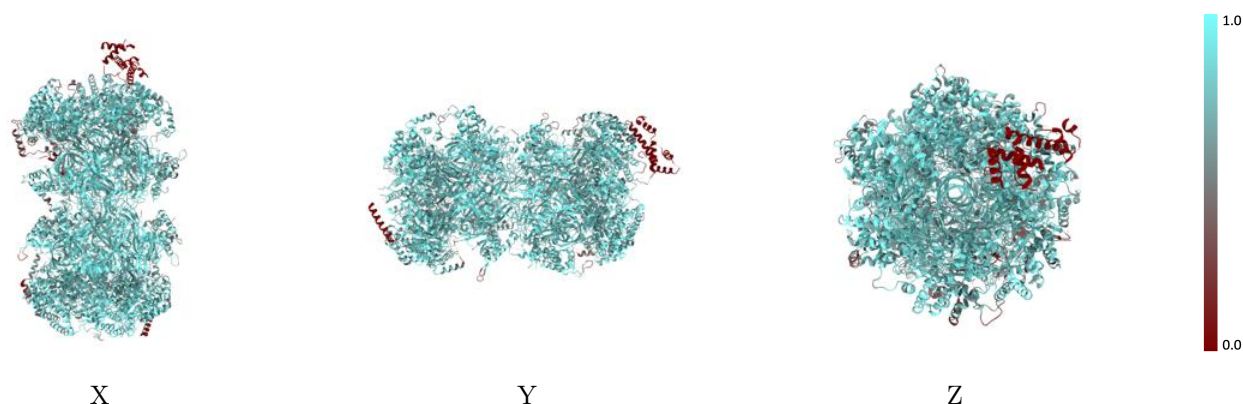
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



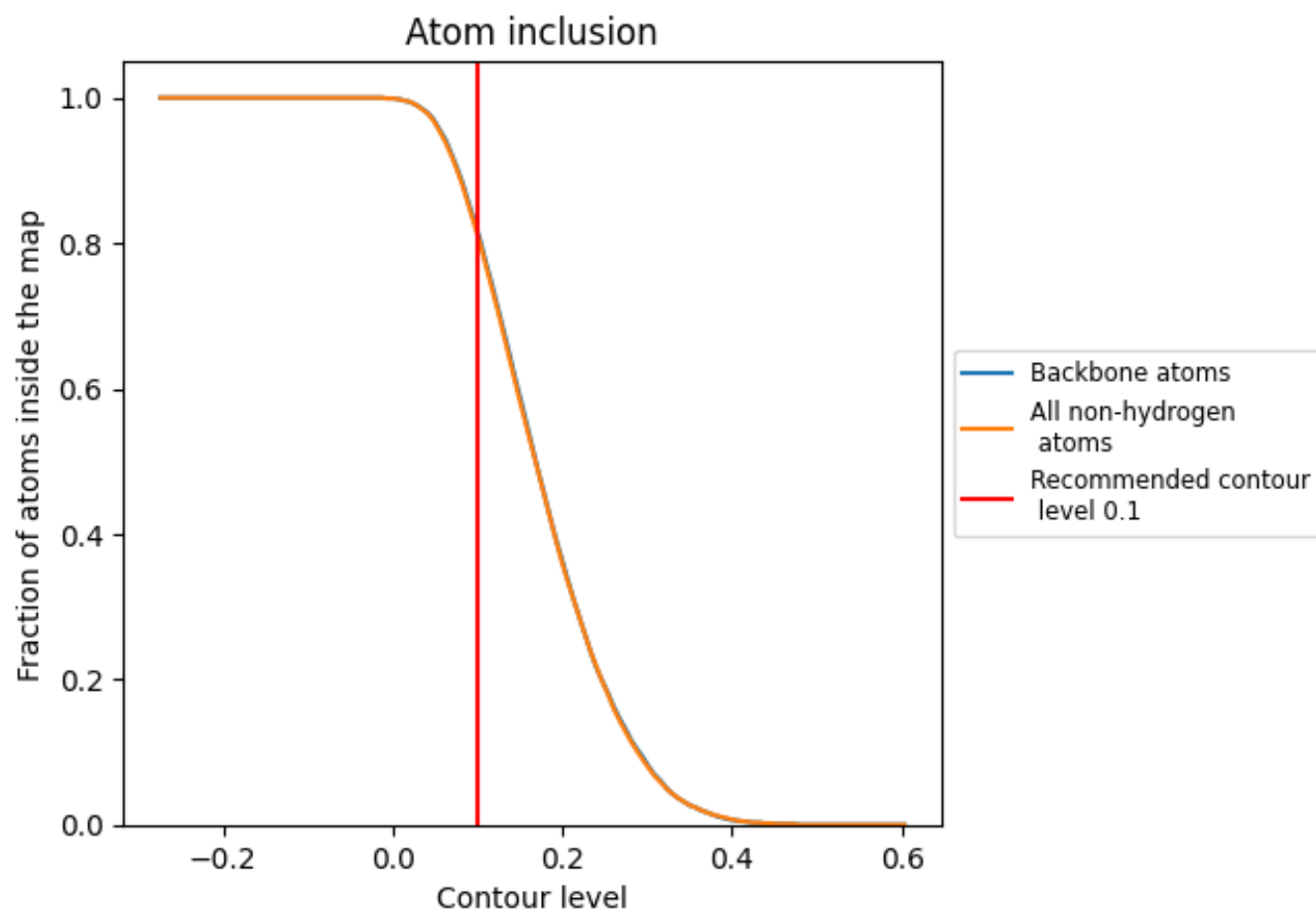
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.5010
2	0.7980	0.4760
3	0.8210	0.5010
4	0.8500	0.5210
5	0.8440	0.5070
6	0.8510	0.5130
7	0.8410	0.5030
A	0.7610	0.4850
B	0.7810	0.4910
C	0.8380	0.5090
D	0.8310	0.5150
E	0.7580	0.4840
F	0.8320	0.5080
O	0.9010	0.4930
S	0.9100	0.4990

1.0

0.0

<0.0