



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:57 PM UTC

PDB ID : 6M2W / pdb_00006m2w
EMDB ID : EMD-30067
Title : Structure of RyR1 (Ca²⁺/Caffeine/ATP/CaM1234/CHL)
Authors : Ma, R.; Haji-Ghassemi, O.; Ma, D.; Lin, L.; Samurkas, A.; Van Petegem, F.; Yuchi, Z.
Deposited on : 2020-03-01
Resolution : 3.80 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:

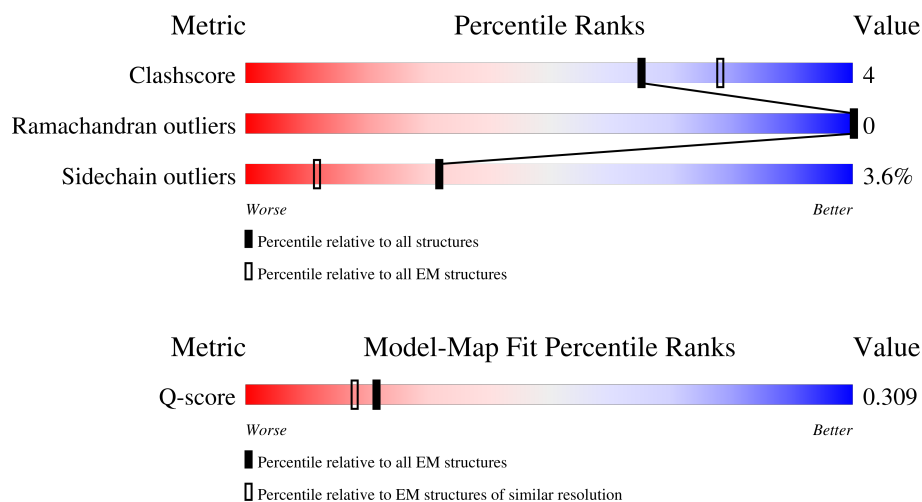
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



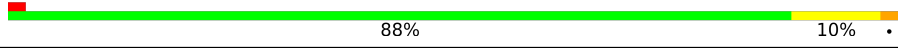
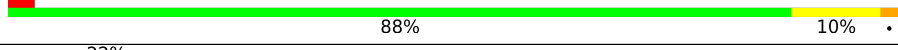
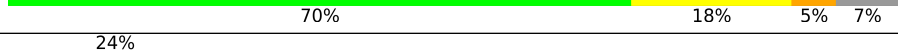
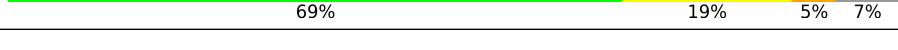
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	A	5037	9% 70% 8% 22%
1	D	5037	9% 70% 8% 22%
1	G	5037	9% 70% 8% 22%
1	J	5037	9% 70% 8% 22%

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Mol	Chain	Length	Quality of chain
2	B	107	
2	E	107	
2	H	107	
2	K	107	
3	C	149	
3	F	149	
3	I	149	
3	L	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	A	5101	-	X	-	-
4	CFF	D	5101	-	X	-	-
4	CFF	G	5101	-	X	-	-
4	CFF	J	5101	-	X	-	-
6	ATP	D	5103	-	-	X	-
6	ATP	G	5103	-	-	X	-
6	ATP	J	5103	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 120452 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 Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	D	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	G	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	J	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	K	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

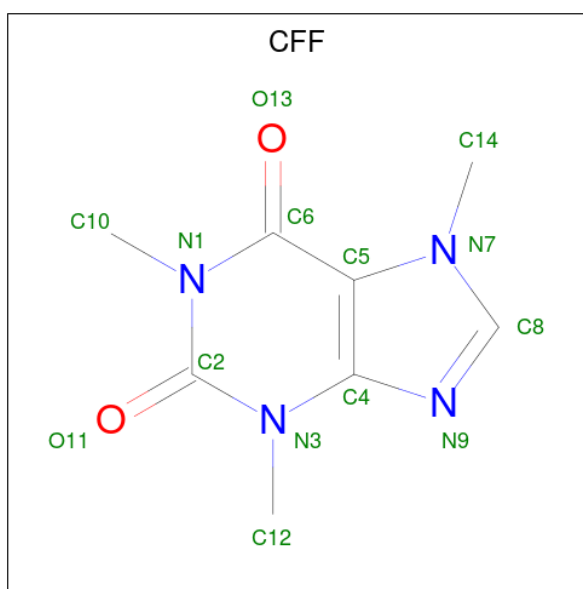
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
3	F	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
3	I	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		
3	L	139	Total	C	N	O	S	0	0
			1042	646	174	212	10		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	D	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

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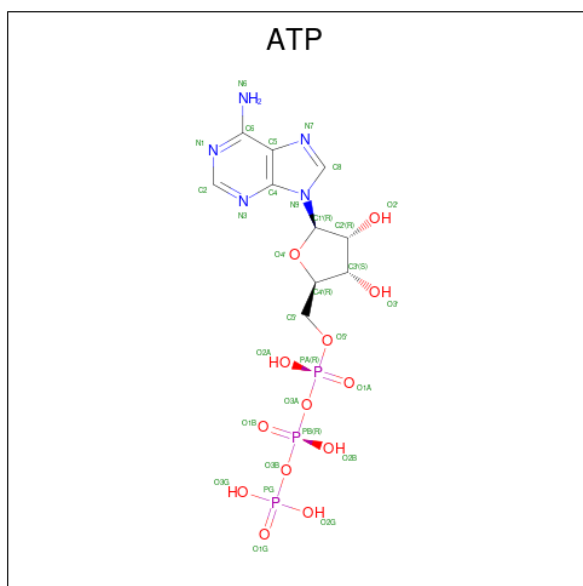
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Mol	Chain	Residues	Atoms				AltConf
4	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	
5	G	1	Total	Ca	0
			1	1	
5	J	1	Total	Ca	0
			1	1	

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

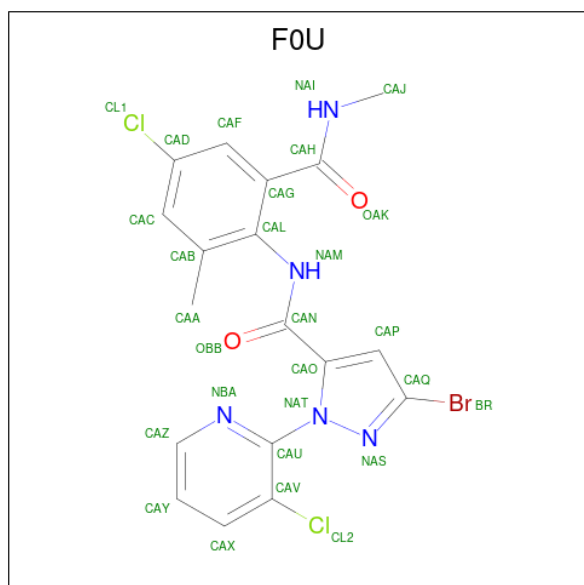


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	
7	D	1	Total	Zn	0
			1	1	
7	G	1	Total	Zn	0
			1	1	
7	J	1	Total	Zn	0
			1	1	

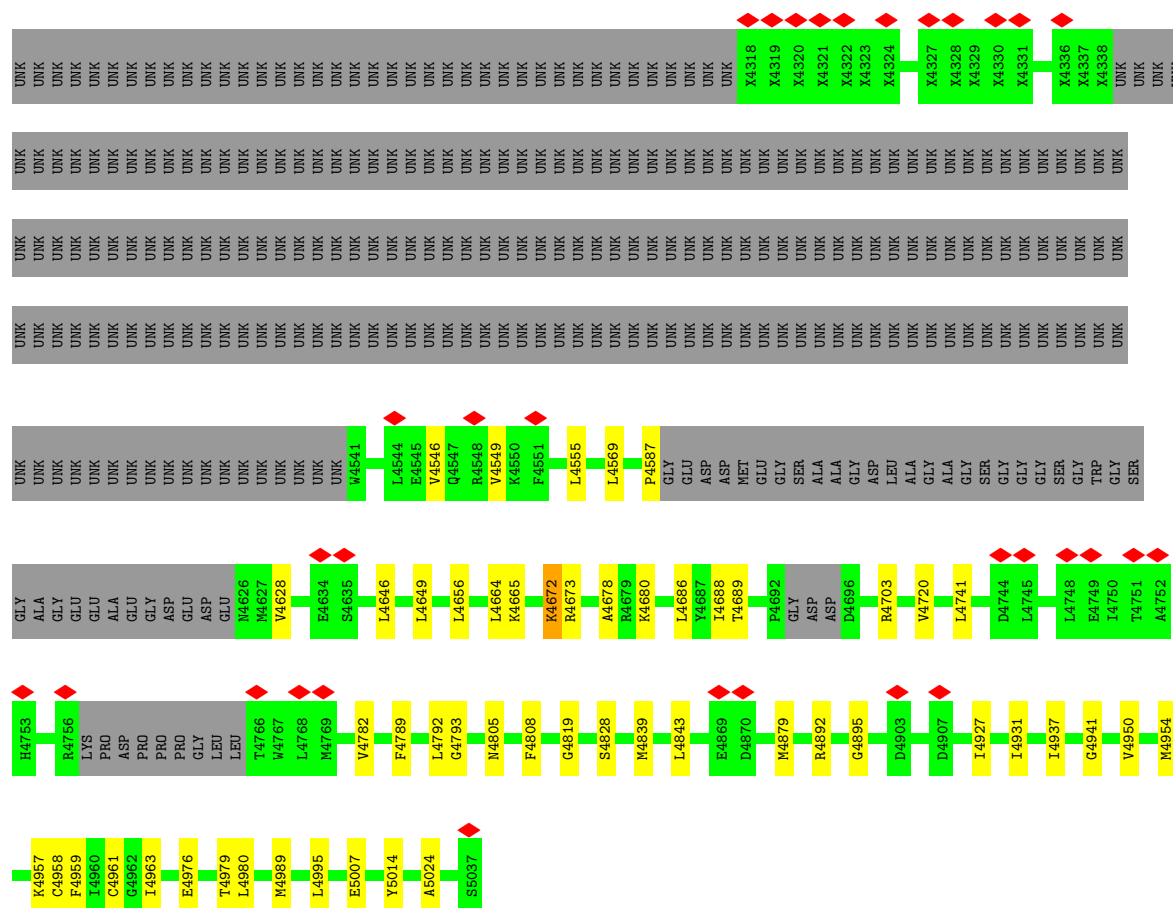
- Molecule 8 is 5-bromanyl-N-[4-chloranyl-2-methyl-6-(methylcarbamoyl)phenyl]-2-(3-chloranylpyridin-2-yl)pyrazole-3-carboxamide (CCD ID: F0U) (formula: C₁₈H₁₄BrCl₂N₅O₂) (labeled as "Ligand of Interest" by depositor).



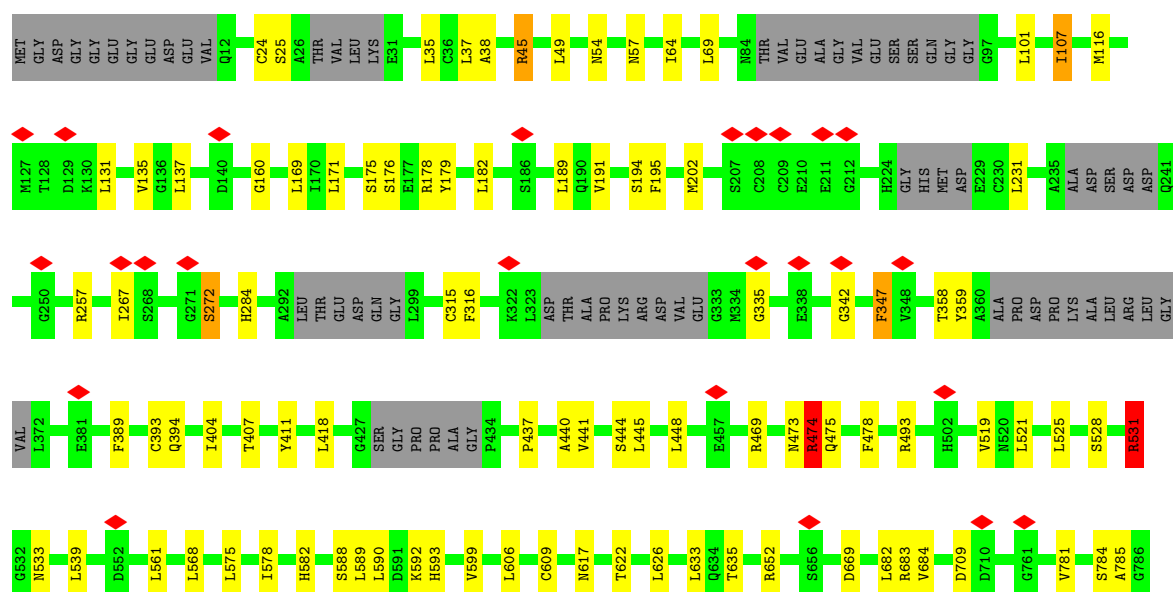
Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
8	D	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
8	G	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
8	J	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	

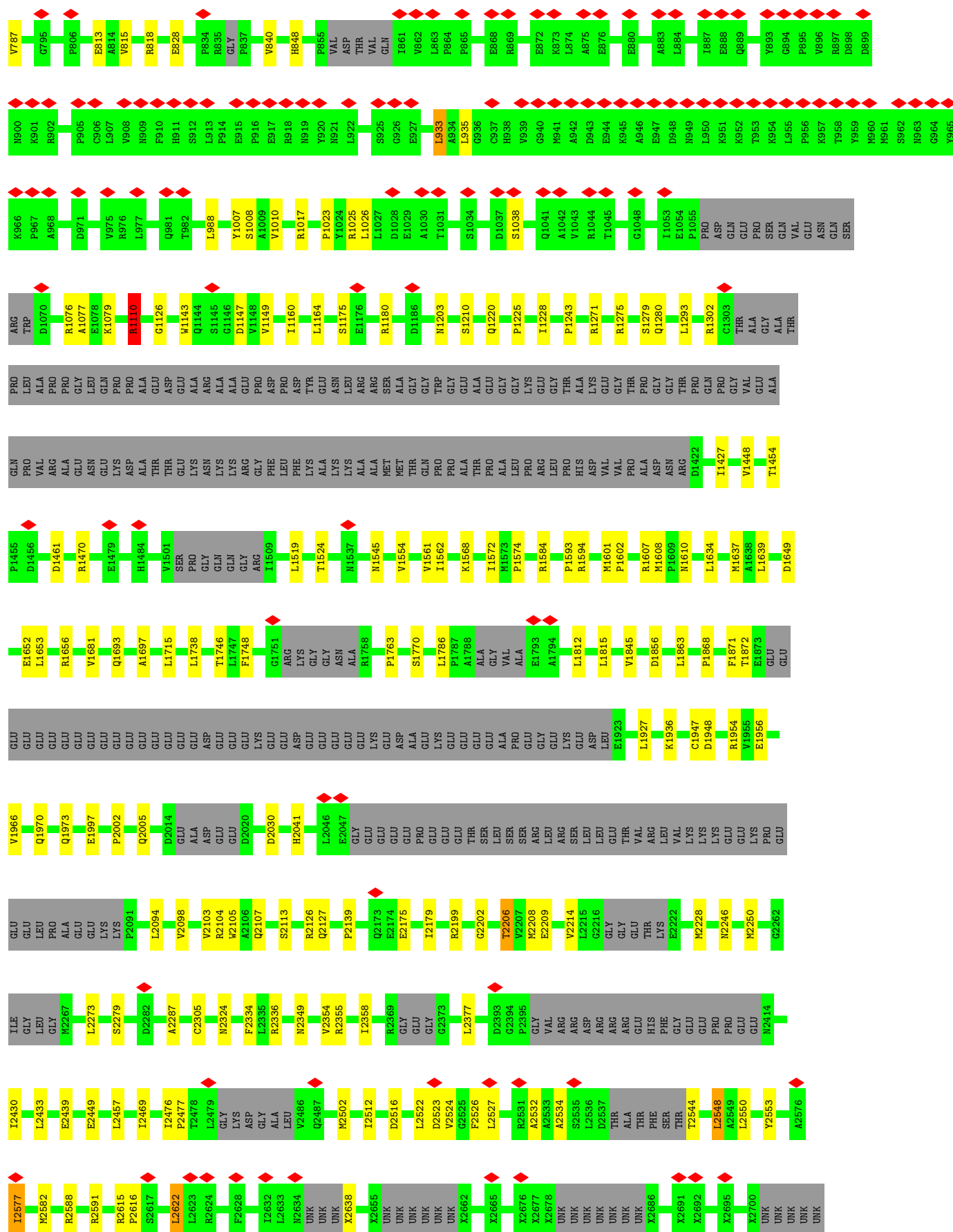




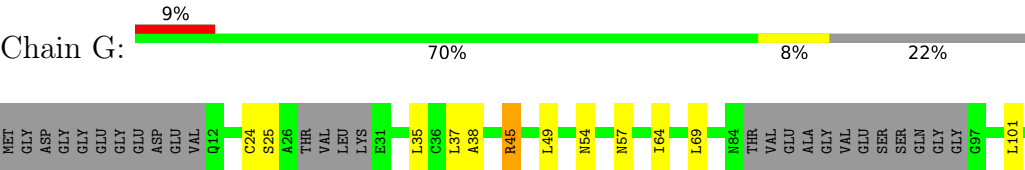
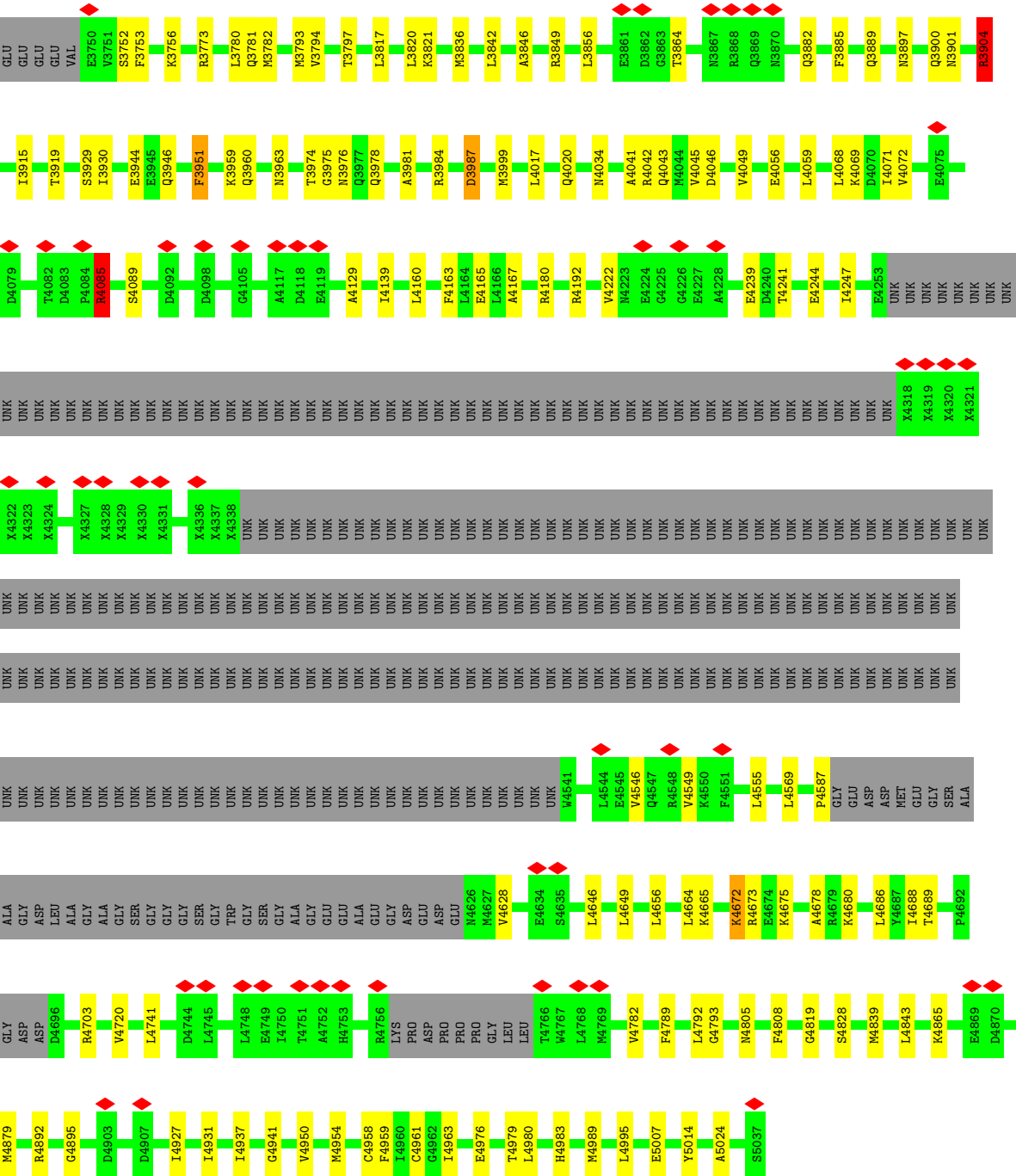


- Molecule 1: Ryanodine receptor 1, Ryanodine receptor 1, Ryanodine receptor 1, Ryanodine receptor 1, Ryanodine receptor 1, Ryanodine receptor 1, Ryanodine receptor 1





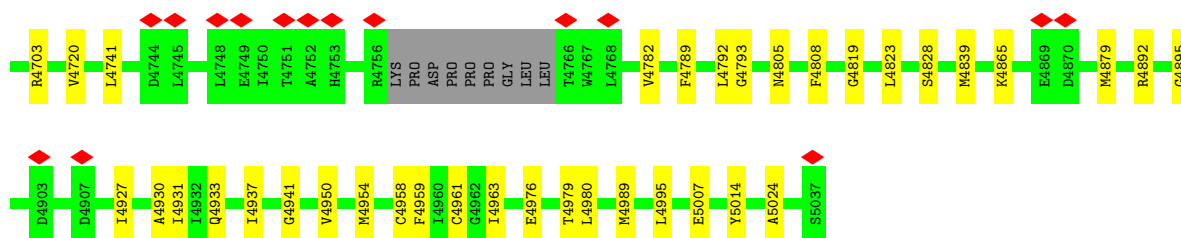




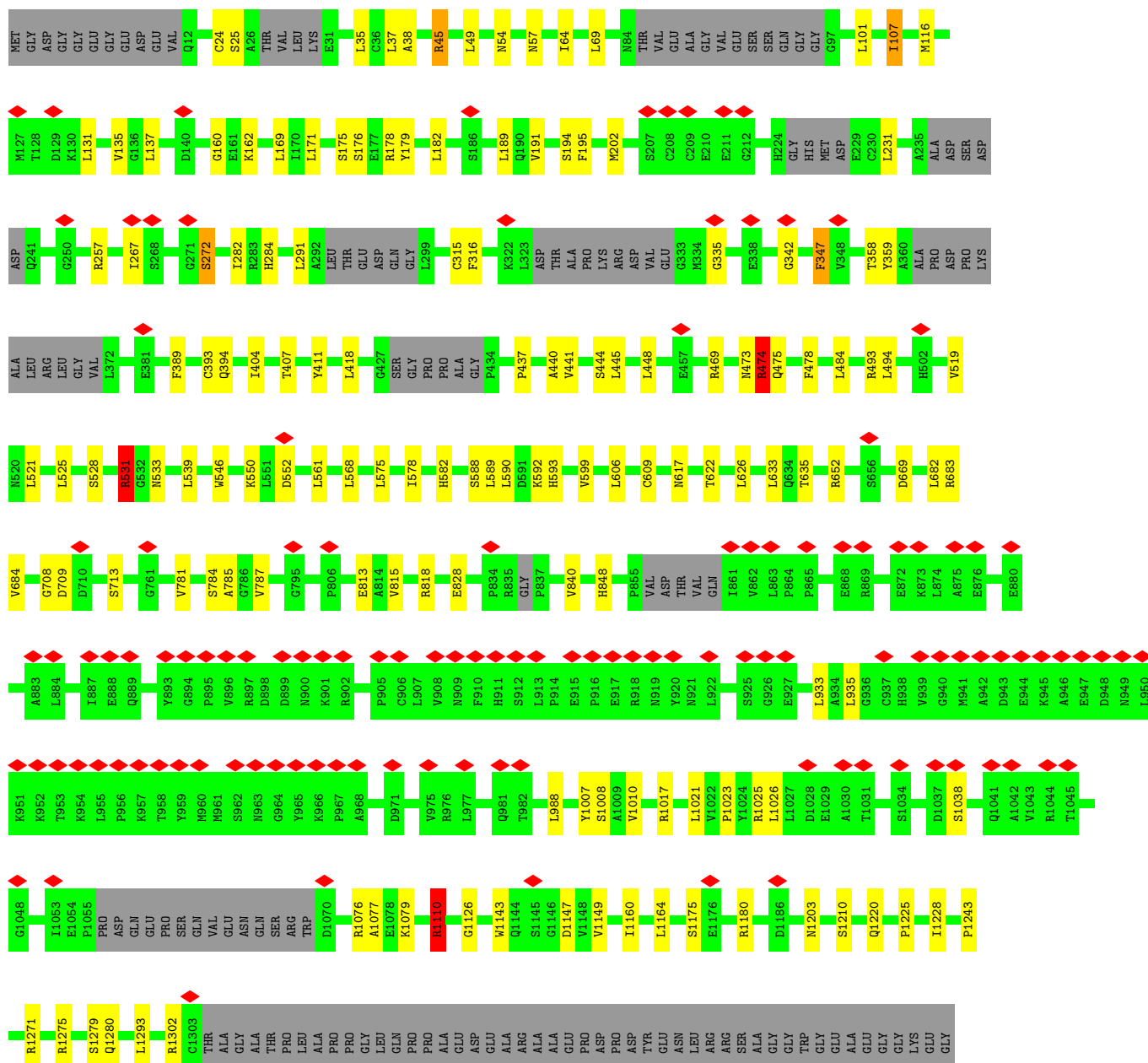








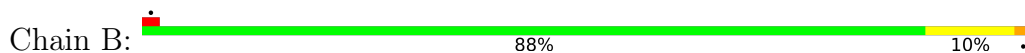
• Molecule 1: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1



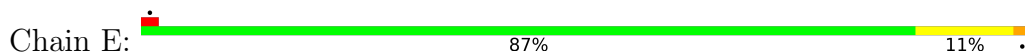




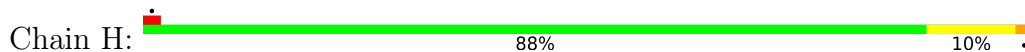
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



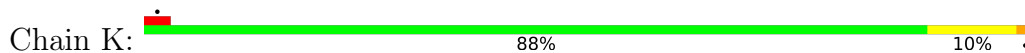
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

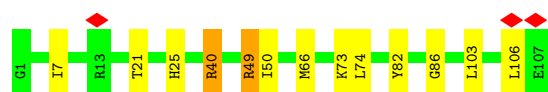


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

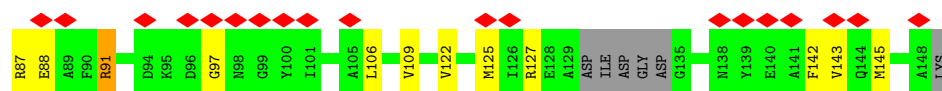
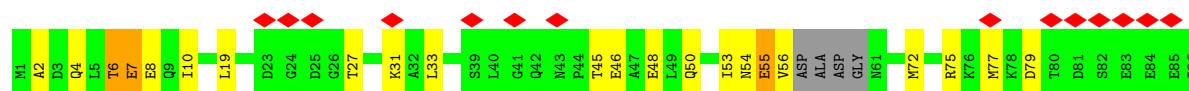


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

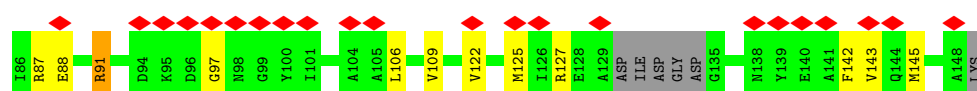




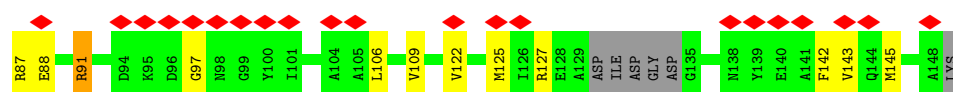
• Molecule 3: Calmodulin-1



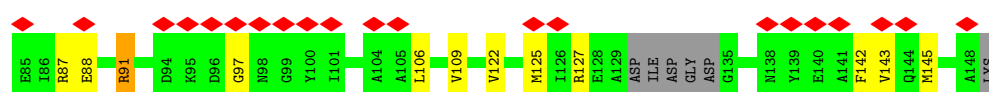
• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.322	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0302	Depositor
Map size ($\text{\AA}$)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CFF, CA, FOU, 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	0.24	0/26486	0.59	19/36018 (0.1%)
1	D	0.24	0/26486	0.59	19/36018 (0.1%)
1	G	0.24	0/26486	0.59	19/36018 (0.1%)
1	J	0.24	0/26486	0.59	19/36018 (0.1%)
2	B	0.26	0/820	0.65	0/1105
2	E	0.26	0/820	0.66	0/1105
2	H	0.26	0/820	0.66	0/1105
2	K	0.26	0/820	0.65	0/1105
3	C	0.33	0/1052	0.84	2/1416 (0.1%)
3	F	0.33	0/1052	0.84	2/1416 (0.1%)
3	I	0.33	0/1052	0.83	2/1416 (0.1%)
3	L	0.33	0/1052	0.83	2/1416 (0.1%)
All	All	0.24	0/113432	0.61	84/154156 (0.1%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4085	ARG	CG-CD-NE	9.72	133.38	112.00
1	D	4085	ARG	CG-CD-NE	9.72	133.38	112.00
1	G	4085	ARG	CG-CD-NE	9.72	133.38	112.00
1	J	4085	ARG	CG-CD-NE	9.72	133.38	112.00
1	A	474	ARG	CG-CD-NE	9.56	133.04	112.00
1	D	474	ARG	CG-CD-NE	9.56	133.04	112.00
1	G	474	ARG	CG-CD-NE	9.56	133.04	112.00
1	J	474	ARG	CG-CD-NE	9.56	133.04	112.00
1	A	531	ARG	CG-CD-NE	8.56	130.84	112.00
1	D	531	ARG	CG-CD-NE	8.56	130.84	112.00
1	G	531	ARG	CG-CD-NE	8.56	130.84	112.00
1	J	531	ARG	CG-CD-NE	8.56	130.84	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1110	ARG	CG-CD-NE	8.02	129.65	112.00
1	D	1110	ARG	CG-CD-NE	8.02	129.65	112.00
1	G	1110	ARG	CG-CD-NE	8.02	129.65	112.00
1	J	1110	ARG	CG-CD-NE	8.02	129.65	112.00
1	A	474	ARG	CB-CG-CD	7.49	128.52	111.30
1	D	474	ARG	CB-CG-CD	7.49	128.52	111.30
1	G	474	ARG	CB-CG-CD	7.49	128.52	111.30
1	J	474	ARG	CB-CG-CD	7.49	128.52	111.30
1	A	3904	ARG	CG-CD-NE	6.75	126.85	112.00
1	D	3904	ARG	CG-CD-NE	6.75	126.85	112.00
1	G	3904	ARG	CG-CD-NE	6.75	126.85	112.00
1	J	3904	ARG	CG-CD-NE	6.75	126.85	112.00
1	A	4085	ARG	CB-CG-CD	6.65	126.60	111.30
1	D	4085	ARG	CB-CG-CD	6.65	126.60	111.30
1	G	4085	ARG	CB-CG-CD	6.65	126.60	111.30
1	J	4085	ARG	CB-CG-CD	6.65	126.60	111.30
1	A	474	ARG	CD-NE-CZ	6.56	133.58	124.40
1	D	474	ARG	CD-NE-CZ	6.56	133.58	124.40
1	G	474	ARG	CD-NE-CZ	6.56	133.58	124.40
1	J	474	ARG	CD-NE-CZ	6.56	133.58	124.40
1	A	4085	ARG	CD-NE-CZ	6.38	133.33	124.40
1	D	4085	ARG	CD-NE-CZ	6.38	133.33	124.40
1	G	4085	ARG	CD-NE-CZ	6.38	133.33	124.40
1	J	4085	ARG	CD-NE-CZ	6.38	133.33	124.40
3	C	55	GLU	CA-CB-CG	6.38	126.85	114.10
3	F	55	GLU	CA-CB-CG	6.37	126.84	114.10
1	A	531	ARG	CB-CG-CD	6.14	125.41	111.30
1	D	531	ARG	CB-CG-CD	6.14	125.41	111.30
1	G	531	ARG	CB-CG-CD	6.14	125.41	111.30
1	J	531	ARG	CB-CG-CD	6.14	125.41	111.30
1	A	3904	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	D	3904	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	G	3904	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	J	3904	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	A	1110	ARG	CD-NE-CZ	5.94	132.71	124.40
1	D	1110	ARG	CD-NE-CZ	5.94	132.71	124.40
1	G	1110	ARG	CD-NE-CZ	5.94	132.71	124.40
1	J	1110	ARG	CD-NE-CZ	5.94	132.71	124.40
1	A	4672	LYS	CG-CD-CE	5.88	124.81	111.30
1	D	4672	LYS	CG-CD-CE	5.88	124.81	111.30
1	G	4672	LYS	CG-CD-CE	5.88	124.81	111.30
1	J	4672	LYS	CG-CD-CE	5.88	124.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4672	LYS	CD-CE-NZ	5.69	130.10	111.90
1	D	4672	LYS	CD-CE-NZ	5.69	130.10	111.90
1	G	4672	LYS	CD-CE-NZ	5.69	130.10	111.90
1	J	4672	LYS	CD-CE-NZ	5.69	130.10	111.90
1	A	3904	ARG	CD-NE-CZ	5.51	132.11	124.40
1	D	3904	ARG	CD-NE-CZ	5.51	132.11	124.40
1	G	3904	ARG	CD-NE-CZ	5.51	132.11	124.40
1	J	3904	ARG	CD-NE-CZ	5.51	132.11	124.40
1	A	45	ARG	CG-CD-NE	5.48	124.05	112.00
1	D	45	ARG	CG-CD-NE	5.48	124.05	112.00
1	G	45	ARG	CG-CD-NE	5.48	124.05	112.00
1	J	45	ARG	CG-CD-NE	5.48	124.05	112.00
3	I	54	ASN	N-CA-C	-5.40	105.55	111.82
1	A	45	ARG	CD-NE-CZ	5.39	131.95	124.40
1	D	45	ARG	CD-NE-CZ	5.39	131.95	124.40
1	G	45	ARG	CD-NE-CZ	5.39	131.95	124.40
1	J	45	ARG	CD-NE-CZ	5.39	131.95	124.40
3	L	54	ASN	N-CA-C	-5.25	105.73	111.82
3	C	91	ARG	CD-NE-CZ	5.11	131.56	124.40
3	I	91	ARG	CD-NE-CZ	5.09	131.53	124.40
3	F	91	ARG	CD-NE-CZ	5.07	131.50	124.40
3	L	91	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	1271	ARG	CG-CD-NE	5.06	123.14	112.00
1	D	1271	ARG	CG-CD-NE	5.06	123.14	112.00
1	G	1271	ARG	CG-CD-NE	5.06	123.14	112.00
1	J	1271	ARG	CG-CD-NE	5.06	123.14	112.00
1	A	531	ARG	CD-NE-CZ	5.01	131.42	124.40
1	D	531	ARG	CD-NE-CZ	5.01	131.42	124.40
1	G	531	ARG	CD-NE-CZ	5.01	131.42	124.40
1	J	531	ARG	CD-NE-CZ	5.01	131.42	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	28192	0	24931	217	0
1	D	28192	0	24931	216	0
1	G	28192	0	24931	216	0
1	J	28192	0	24931	217	0
2	B	804	0	812	4	0
2	E	804	0	812	5	0
2	H	804	0	812	4	0
2	K	804	0	812	4	0
3	C	1042	0	972	11	0
3	F	1042	0	972	10	0
3	I	1042	0	972	10	0
3	L	1042	0	972	13	0
4	A	14	0	10	0	0
4	D	14	0	10	0	0
4	G	14	0	10	0	0
4	J	14	0	10	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	31	0	12	8	0
6	D	31	0	12	10	0
6	G	31	0	12	9	0
6	J	31	0	12	9	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
8	A	28	0	0	2	0
8	D	28	0	0	2	0
8	G	28	0	0	2	0
8	J	28	0	0	2	0
All	All	120452	0	106948	908	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 4.

All (908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4958:CYS:HA	6:D:5103:ATP:H2	1.09	1.16
1:G:4958:CYS:HA	6:G:5103:ATP:H2	1.09	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4958:CYS:HA	6:J:5103:ATP:H2	1.09	1.12
1:A:4958:CYS:HA	6:A:5103:ATP:H2	1.09	1.12
1:G:4958:CYS:CA	6:G:5103:ATP:H2	1.80	0.94
1:A:4958:CYS:CA	6:A:5103:ATP:H2	1.80	0.93
1:J:4958:CYS:CA	6:J:5103:ATP:H2	1.80	0.93
1:D:4958:CYS:CA	6:D:5103:ATP:H2	1.80	0.93
1:G:4958:CYS:HA	6:G:5103:ATP:C2	2.05	0.91
1:J:4958:CYS:HA	6:J:5103:ATP:C2	2.05	0.91
1:D:4958:CYS:HA	6:D:5103:ATP:C2	2.05	0.91
1:A:4958:CYS:HA	6:A:5103:ATP:C2	2.05	0.90
1:J:4958:CYS:O	6:J:5103:ATP:N1	2.07	0.87
1:D:4958:CYS:O	6:D:5103:ATP:N1	2.07	0.87
1:G:4958:CYS:O	6:G:5103:ATP:N1	2.07	0.87
1:A:4958:CYS:O	6:A:5103:ATP:N1	2.07	0.86
3:L:50:GLN:NE2	3:L:50:GLN:HA	1.95	0.80
1:J:2548:LEU:HD12	1:J:2548:LEU:O	1.87	0.75
1:D:4958:CYS:C	6:D:5103:ATP:C2	2.65	0.75
1:J:4958:CYS:C	6:J:5103:ATP:C2	2.65	0.75
1:A:2536:LEU:HD13	1:A:2547:ALA:HB2	1.66	0.74
1:A:4958:CYS:C	6:A:5103:ATP:C2	2.65	0.74
1:G:4958:CYS:C	6:G:5103:ATP:C2	2.65	0.74
1:D:4954:MET:HE1	1:D:4959:PHE:HB2	1.71	0.72
1:G:4954:MET:HE1	1:G:4959:PHE:HB2	1.71	0.72
1:A:4954:MET:HE1	1:A:4959:PHE:HB2	1.71	0.71
1:J:4954:MET:HE1	1:J:4959:PHE:HB2	1.71	0.70
1:G:1008:SER:HB3	1:G:1017:ARG:HE	1.58	0.69
1:A:1008:SER:HB3	1:A:1017:ARG:HE	1.58	0.69
1:J:2548:LEU:HD12	1:J:2548:LEU:C	2.17	0.69
2:K:21:THR:HG22	2:K:49:ARG:HD3	1.75	0.69
1:D:1008:SER:HB3	1:D:1017:ARG:HE	1.58	0.68
1:J:1008:SER:HB3	1:J:1017:ARG:HE	1.58	0.67
2:B:21:THR:HG22	2:B:49:ARG:HD3	1.75	0.67
3:F:50:GLN:OE1	3:F:50:GLN:HA	1.94	0.67
2:E:21:THR:HG22	2:E:49:ARG:HD3	1.75	0.67
1:G:4085:ARG:HH11	1:G:4085:ARG:HB3	1.59	0.67
1:A:3900:GLN:HB3	1:A:3976:ASN:HD21	1.59	0.66
1:J:4085:ARG:HH11	1:J:4085:ARG:HB3	1.59	0.66
1:G:3900:GLN:HB3	1:G:3976:ASN:HD21	1.59	0.66
1:A:4085:ARG:HH11	1:A:4085:ARG:HB3	1.59	0.66
1:J:3900:GLN:HB3	1:J:3976:ASN:HD21	1.59	0.66
3:I:50:GLN:HA	3:I:50:GLN:OE1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2523:ASP:HA	1:G:2527:LEU:HD12	1.78	0.65
2:H:21:THR:HG22	2:H:49:ARG:HD3	1.75	0.65
1:D:3900:GLN:HB3	1:D:3976:ASN:HD21	1.59	0.65
1:J:4958:CYS:CA	6:J:5103:ATP:C2	2.75	0.65
1:D:2523:ASP:HA	1:D:2527:LEU:HD12	1.78	0.65
1:A:2523:ASP:HA	1:A:2527:LEU:HD12	1.78	0.65
1:J:2523:ASP:HA	1:J:2527:LEU:HD12	1.78	0.65
1:G:474:ARG:HH11	1:G:474:ARG:HB2	1.62	0.65
1:D:4958:CYS:C	6:D:5103:ATP:H2	2.04	0.65
1:D:4085:ARG:HB3	1:D:4085:ARG:HH11	1.59	0.65
1:J:474:ARG:HH11	1:J:474:ARG:HB2	1.62	0.64
2:B:82:TYR:HB3	2:B:86:GLY:HA2	1.80	0.64
3:L:6:THR:OG1	3:L:7:GLU:N	2.30	0.64
1:A:4958:CYS:C	6:A:5103:ATP:H2	2.04	0.64
2:K:82:TYR:HB3	2:K:86:GLY:HA2	1.80	0.64
2:H:82:TYR:HB3	2:H:86:GLY:HA2	1.80	0.64
1:J:4958:CYS:C	6:J:5103:ATP:H2	2.04	0.64
2:E:82:TYR:HB3	2:E:86:GLY:HA2	1.80	0.64
1:G:4958:CYS:C	6:G:5103:ATP:H2	2.04	0.63
3:F:6:THR:OG1	3:F:7:GLU:N	2.30	0.63
3:C:6:THR:OG1	3:C:7:GLU:N	2.30	0.63
3:C:33:LEU:HD11	3:C:72:MET:HE1	1.81	0.63
1:J:4958:CYS:O	6:J:5103:ATP:C2	2.52	0.63
1:G:1293:LEU:HD11	1:G:1594:ARG:HG2	1.81	0.63
3:C:50:GLN:OE1	3:C:50:GLN:HA	1.99	0.63
3:I:33:LEU:HD11	3:I:72:MET:HE1	1.81	0.63
1:J:1293:LEU:HD11	1:J:1594:ARG:HG2	1.81	0.62
1:J:4241:THR:OG1	1:J:4989:MET:SD	2.57	0.62
1:A:1293:LEU:HD11	1:A:1594:ARG:HG2	1.81	0.62
1:D:474:ARG:HH11	1:D:474:ARG:HB2	1.62	0.62
3:L:33:LEU:HD11	3:L:72:MET:HE1	1.81	0.62
1:D:1293:LEU:HD11	1:D:1594:ARG:HG2	1.81	0.62
3:F:33:LEU:HD11	3:F:72:MET:HE1	1.81	0.62
1:A:474:ARG:HH11	1:A:474:ARG:HB2	1.62	0.62
1:D:4958:CYS:O	6:D:5103:ATP:C2	2.52	0.62
3:I:6:THR:OG1	3:I:7:GLU:N	2.30	0.62
1:A:4958:CYS:O	6:A:5103:ATP:C2	2.52	0.62
1:D:2544:THR:O	1:D:2548:LEU:HG	1.99	0.61
1:G:4958:CYS:O	6:G:5103:ATP:C2	2.52	0.61
1:A:393:CYS:SG	1:A:394:GLN:N	2.74	0.61
1:A:3889:GLN:OE1	1:A:3960:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:393:CYS:SG	1:J:394:GLN:N	2.74	0.61
1:D:2273:LEU:HD21	1:D:2334:PHE:HB2	1.83	0.60
1:J:2305:CYS:HB2	1:J:2324:ASN:HB3	1.84	0.60
1:A:2305:CYS:HB2	1:A:2324:ASN:HB3	1.84	0.60
1:G:54:ASN:HB3	1:G:57:ASN:HD21	1.67	0.60
1:D:69:LEU:HB3	1:D:107:ILE:HD11	1.84	0.60
1:D:1607:ARG:HH11	1:D:1610:ASN:HD21	1.50	0.60
1:D:2305:CYS:HB2	1:D:2324:ASN:HB3	1.84	0.60
1:A:2273:LEU:HD21	1:A:2334:PHE:HB2	1.83	0.59
1:D:54:ASN:HB3	1:D:57:ASN:HD21	1.67	0.59
1:G:3889:GLN:OE1	1:G:3960:GLN:NE2	2.34	0.59
1:A:4046:ASP:HA	1:A:4049:VAL:HG22	1.85	0.59
1:D:4241:THR:OG1	1:D:4989:MET:SD	2.57	0.59
1:G:1607:ARG:HH11	1:G:1610:ASN:HD21	1.50	0.59
1:G:2273:LEU:HD21	1:G:2334:PHE:HB2	1.83	0.59
1:G:2305:CYS:HB2	1:G:2324:ASN:HB3	1.84	0.59
1:A:54:ASN:HB3	1:A:57:ASN:HD21	1.67	0.59
1:A:69:LEU:HB3	1:A:107:ILE:HD11	1.84	0.59
1:G:4046:ASP:HA	1:G:4049:VAL:HG22	1.85	0.59
1:J:69:LEU:HB3	1:J:107:ILE:HD11	1.84	0.59
1:A:828:GLU:HG3	1:A:840:VAL:HG21	1.84	0.59
1:D:3981:ALA:HB1	1:D:4043:GLN:HE22	1.67	0.59
1:D:4020:GLN:HE21	1:D:4139:ILE:HG12	1.68	0.59
1:G:393:CYS:SG	1:G:394:GLN:N	2.74	0.59
1:J:54:ASN:HB3	1:J:57:ASN:HD21	1.67	0.59
3:L:50:GLN:HA	3:L:50:GLN:HE21	1.64	0.59
1:A:4020:GLN:HE21	1:A:4139:ILE:HG12	1.68	0.59
1:D:393:CYS:SG	1:D:394:GLN:N	2.74	0.59
1:J:1607:ARG:HH11	1:J:1610:ASN:HD21	1.50	0.59
1:D:4046:ASP:HA	1:D:4049:VAL:HG22	1.85	0.59
1:G:828:GLU:HG3	1:G:840:VAL:HG21	1.84	0.59
1:A:1607:ARG:HH11	1:A:1610:ASN:HD21	1.50	0.59
1:J:4046:ASP:HA	1:J:4049:VAL:HG22	1.85	0.59
1:A:1243:PRO:HB3	1:A:1602:PRO:HA	1.85	0.58
1:A:2242:ILE:HA	3:C:2:ALA:HB3	1.85	0.58
1:D:828:GLU:HG3	1:D:840:VAL:HG21	1.84	0.58
1:D:3889:GLN:OE1	1:D:3960:GLN:NE2	2.34	0.58
1:G:4020:GLN:HE21	1:G:4139:ILE:HG12	1.68	0.58
1:J:4020:GLN:HE21	1:J:4139:ILE:HG12	1.68	0.58
1:G:69:LEU:HB3	1:G:107:ILE:HD11	1.84	0.58
3:C:87:ARG:NH2	3:C:97:GLY:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:828:GLU:HG3	1:J:840:VAL:HG21	1.84	0.58
3:F:87:ARG:NH2	3:F:97:GLY:O	2.37	0.58
1:G:3981:ALA:HB1	1:G:4043:GLN:HE22	1.67	0.58
3:I:87:ARG:NH2	3:I:97:GLY:O	2.37	0.58
1:J:2273:LEU:HD21	1:J:2334:PHE:HB2	1.83	0.58
1:J:3889:GLN:OE1	1:J:3960:GLN:NE2	2.34	0.58
1:J:3981:ALA:HB1	1:J:4043:GLN:HE22	1.67	0.58
1:D:1243:PRO:HB3	1:D:1602:PRO:HA	1.85	0.58
1:A:3981:ALA:HB1	1:A:4043:GLN:HE22	1.67	0.58
1:J:1243:PRO:HB3	1:J:1602:PRO:HA	1.85	0.58
1:A:411:TYR:HH	1:A:444:SER:HG	1.52	0.57
1:A:4241:THR:OG1	1:A:4989:MET:SD	2.57	0.57
3:L:87:ARG:NH2	3:L:97:GLY:O	2.37	0.57
1:D:2103:VAL:HG12	1:D:2107:GLN:HE21	1.69	0.57
1:J:2103:VAL:HG12	1:J:2107:GLN:HE21	1.69	0.57
1:D:182:LEU:HD21	1:D:189:LEU:HD13	1.86	0.57
1:D:445:LEU:HD23	1:D:521:LEU:HB2	1.87	0.57
1:A:4688:ILE:HG13	1:A:4689:THR:HG23	1.87	0.57
1:G:1243:PRO:HB3	1:G:1602:PRO:HA	1.85	0.57
1:A:445:LEU:HD23	1:A:521:LEU:HB2	1.87	0.57
1:D:315:CYS:SG	1:D:316:PHE:N	2.78	0.57
1:D:3897:ASN:O	1:D:3901:ASN:ND2	2.38	0.57
1:G:445:LEU:HD23	1:G:521:LEU:HB2	1.87	0.57
1:J:3897:ASN:O	1:J:3901:ASN:ND2	2.38	0.57
1:J:4688:ILE:HG13	1:J:4689:THR:HG23	1.87	0.57
1:A:3897:ASN:O	1:A:3901:ASN:ND2	2.38	0.56
1:D:4688:ILE:HG13	1:D:4689:THR:HG23	1.87	0.56
1:G:3897:ASN:O	1:G:3901:ASN:ND2	2.38	0.56
1:A:182:LEU:HD21	1:A:189:LEU:HD13	1.86	0.56
1:G:315:CYS:SG	1:G:316:PHE:N	2.78	0.56
1:J:1948:ASP:OD1	1:J:2126:ARG:NH2	2.38	0.56
1:G:24:CYS:SG	1:G:25:SER:N	2.79	0.56
1:G:182:LEU:HD21	1:G:189:LEU:HD13	1.86	0.56
1:G:2103:VAL:HG12	1:G:2107:GLN:HE21	1.69	0.56
1:G:2179:ILE:HD11	1:G:2228:MET:HA	1.87	0.56
1:A:315:CYS:SG	1:A:316:PHE:N	2.78	0.56
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.38	0.56
1:G:1948:ASP:OD1	1:G:2126:ARG:NH2	2.38	0.56
1:J:445:LEU:HD23	1:J:521:LEU:HB2	1.87	0.56
1:A:24:CYS:SG	1:A:25:SER:N	2.79	0.56
1:A:2179:ILE:HD11	1:A:2228:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:GLY:HA2	1:G:389:PHE:HB2	1.88	0.56
1:G:1076:ARG:NH2	1:G:1077:ALA:O	2.39	0.56
1:J:652:ARG:O	1:J:848:HIS:NE2	2.38	0.56
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.38	0.56
1:D:2179:ILE:HD11	1:D:2228:MET:HA	1.87	0.56
1:G:4241:THR:OG1	1:G:4989:MET:SD	2.57	0.56
1:A:2103:VAL:HG12	1:A:2107:GLN:HE21	1.69	0.56
1:D:24:CYS:SG	1:D:25:SER:N	2.79	0.56
1:G:4688:ILE:HG13	1:G:4689:THR:HG23	1.87	0.56
1:A:1076:ARG:NH2	1:A:1077:ALA:O	2.39	0.56
1:J:24:CYS:SG	1:J:25:SER:N	2.79	0.56
1:J:1076:ARG:NH2	1:J:1077:ALA:O	2.39	0.56
1:J:2179:ILE:HD11	1:J:2228:MET:HA	1.87	0.56
1:D:1076:ARG:NH2	1:D:1077:ALA:O	2.39	0.55
1:J:315:CYS:SG	1:J:316:PHE:N	2.78	0.55
1:G:4241:THR:HA	1:G:4244:GLU:HG2	1.88	0.55
1:G:4895:GLY:O	1:J:4892:ARG:NH2	2.37	0.55
1:A:342:GLY:HA2	1:A:389:PHE:HB2	1.88	0.55
1:J:3731:LYS:HA	1:J:3734:HIS:HB2	1.89	0.55
1:A:4241:THR:HA	1:A:4244:GLU:HG2	1.88	0.55
1:A:4892:ARG:NH2	1:J:4895:GLY:O	2.37	0.55
1:G:2199:ARG:NH1	1:G:2246:ASN:OD1	2.40	0.55
1:G:3731:LYS:HA	1:G:3734:HIS:HB2	1.89	0.55
1:J:182:LEU:HD21	1:J:189:LEU:HD13	1.86	0.55
1:J:2199:ARG:NH1	1:J:2246:ASN:OD1	2.40	0.55
1:A:3731:LYS:HA	1:A:3734:HIS:HB2	1.89	0.55
1:D:2199:ARG:NH1	1:D:2246:ASN:OD1	2.40	0.55
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.89	0.55
1:A:2199:ARG:NH1	1:A:2246:ASN:OD1	2.40	0.55
1:D:342:GLY:HA2	1:D:389:PHE:HB2	1.88	0.55
1:J:342:GLY:HA2	1:J:389:PHE:HB2	1.88	0.55
1:D:3731:LYS:HA	1:D:3734:HIS:HB2	1.89	0.55
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.89	0.55
1:D:2002:PRO:HA	1:D:2005:GLN:HG3	1.88	0.55
1:J:1561:VAL:HG12	1:J:1562:ILE:HG23	1.89	0.55
1:J:2287:ALA:O	1:J:2349:ASN:ND2	2.37	0.55
1:J:4241:THR:HA	1:J:4244:GLU:HG2	1.88	0.55
1:J:2002:PRO:HA	1:J:2005:GLN:HG3	1.88	0.54
1:D:4241:THR:HA	1:D:4244:GLU:HG2	1.88	0.54
1:D:469:ARG:O	1:D:473:ASN:ND2	2.41	0.54
1:G:4017:LEU:HD22	1:G:4139:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4569:LEU:HD11	1:G:4646:LEU:HD22	1.89	0.54
1:A:588:SER:O	1:A:592:LYS:NZ	2.38	0.54
1:A:4569:LEU:HD11	1:A:4646:LEU:HD22	1.89	0.54
1:A:4895:GLY:O	1:D:4892:ARG:NH2	2.37	0.54
1:G:469:ARG:O	1:G:473:ASN:ND2	2.41	0.54
1:G:1561:VAL:HG12	1:G:1562:ILE:HG23	1.89	0.54
1:J:4017:LEU:HD22	1:J:4139:ILE:HG21	1.90	0.54
1:G:4054:ASN:OD1	1:G:4054:ASN:N	2.37	0.54
1:A:469:ARG:O	1:A:473:ASN:ND2	2.41	0.54
1:A:2002:PRO:HA	1:A:2005:GLN:HG3	1.88	0.54
1:G:3780:LEU:HD23	1:G:3820:LEU:HD21	1.90	0.54
1:G:652:ARG:O	1:G:848:HIS:NE2	2.38	0.54
1:D:4569:LEU:HD11	1:D:4646:LEU:HD22	1.89	0.53
1:A:2287:ALA:O	1:A:2349:ASN:ND2	2.37	0.53
1:A:3780:LEU:HD23	1:A:3820:LEU:HD21	1.90	0.53
1:G:2002:PRO:HA	1:G:2005:GLN:HG3	1.88	0.53
1:D:437:PRO:HB2	1:D:440:ALA:HB3	1.91	0.53
1:D:4680:LYS:HD2	1:D:4686:LEU:HD22	1.90	0.53
1:D:4958:CYS:CA	6:D:5103:ATP:C2	2.75	0.53
1:A:3752:SER:OG	1:A:3753:PHE:N	2.42	0.53
1:J:4569:LEU:HD11	1:J:4646:LEU:HD22	1.89	0.53
1:D:652:ARG:O	1:D:848:HIS:NE2	2.38	0.53
1:D:3710:LEU:HD21	1:D:3781:GLN:HG2	1.91	0.53
1:D:4017:LEU:HD22	1:D:4139:ILE:HG21	1.90	0.53
1:D:4895:GLY:O	1:G:4892:ARG:NH2	2.37	0.53
1:G:1653:LEU:HA	1:G:1656:ARG:HB2	1.91	0.53
1:G:3710:LEU:HD21	1:G:3781:GLN:HG2	1.91	0.53
1:J:2214:VAL:HG21	1:J:2228:MET:HE2	1.91	0.53
1:J:469:ARG:O	1:J:473:ASN:ND2	2.41	0.53
1:A:437:PRO:HB2	1:A:440:ALA:HB3	1.91	0.53
1:A:4017:LEU:HD22	1:A:4139:ILE:HG21	1.90	0.53
1:G:2214:VAL:HG21	1:G:2228:MET:HE2	1.91	0.53
1:J:3752:SER:OG	1:J:3753:PHE:N	2.42	0.53
1:A:633:LEU:HD13	1:A:1639:LEU:HD13	1.91	0.53
1:G:437:PRO:HB2	1:G:440:ALA:HB3	1.91	0.53
1:J:3780:LEU:HD23	1:J:3820:LEU:HD21	1.90	0.53
1:D:2214:VAL:HG21	1:D:2228:MET:HE2	1.91	0.53
1:D:4664:LEU:HG	1:D:4665:LYS:HD3	1.91	0.53
1:J:633:LEU:HD13	1:J:1639:LEU:HD13	1.91	0.53
1:J:1023:PRO:HG2	1:J:1026:LEU:HD13	1.91	0.53
1:J:4664:LEU:HG	1:J:4665:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3780:LEU:HD23	1:D:3820:LEU:HD21	1.90	0.52
1:G:3723:MET:HE2	1:G:3793:MET:HG3	1.91	0.52
1:D:1653:LEU:HA	1:D:1656:ARG:HB2	1.91	0.52
1:J:437:PRO:HB2	1:J:440:ALA:HB3	1.91	0.52
1:J:4680:LYS:HD2	1:J:4686:LEU:HD22	1.90	0.52
1:G:3951:PHE:HE2	1:G:3999:MET:HE2	1.75	0.52
1:A:1653:LEU:HA	1:A:1656:ARG:HB2	1.91	0.52
1:A:4664:LEU:HG	1:A:4665:LYS:HD3	1.91	0.52
1:D:682:LEU:HD13	1:D:787:VAL:HG11	1.91	0.52
1:D:3723:MET:HE2	1:D:3793:MET:HG3	1.91	0.52
1:D:3951:PHE:HE2	1:D:3999:MET:HE2	1.75	0.52
1:G:4680:LYS:HD2	1:G:4686:LEU:HD22	1.90	0.52
1:A:652:ARG:O	1:A:848:HIS:NE2	2.38	0.52
1:D:1023:PRO:HG2	1:D:1026:LEU:HD13	1.91	0.52
1:G:682:LEU:HD13	1:G:787:VAL:HG11	1.91	0.52
1:J:3723:MET:HE2	1:J:3793:MET:HG3	1.91	0.52
1:J:3951:PHE:HE2	1:J:3999:MET:HE2	1.75	0.52
1:A:2214:VAL:HG21	1:A:2228:MET:HE2	1.91	0.52
1:A:3710:LEU:HD21	1:A:3781:GLN:HG2	1.91	0.52
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.90	0.52
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.92	0.52
1:J:682:LEU:HD13	1:J:787:VAL:HG11	1.91	0.52
1:A:2534:ALA:HB1	1:A:2588:ARG:HD2	1.91	0.52
1:A:2548:LEU:HD11	3:C:50:GLN:HG2	1.91	0.52
1:G:3836:MET:HE1	1:G:3915:ILE:HG23	1.92	0.52
1:G:4664:LEU:HG	1:G:4665:LYS:HD3	1.91	0.52
1:J:1653:LEU:HA	1:J:1656:ARG:HB2	1.91	0.52
1:D:3846:ALA:HA	1:D:3849:ARG:HD2	1.93	0.51
1:G:633:LEU:HD13	1:G:1639:LEU:HD13	1.91	0.51
1:G:2534:ALA:HB1	1:G:2588:ARG:HD2	1.91	0.51
1:G:3846:ALA:HA	1:G:3849:ARG:HD2	1.93	0.51
1:A:1023:PRO:HG2	1:A:1026:LEU:HD13	1.91	0.51
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.92	0.51
1:G:1023:PRO:HG2	1:G:1026:LEU:HD13	1.91	0.51
1:A:682:LEU:HD13	1:A:787:VAL:HG11	1.91	0.51
1:D:2534:ALA:HB1	1:D:2588:ARG:HD2	1.91	0.51
1:D:633:LEU:HD13	1:D:1639:LEU:HD13	1.91	0.51
1:J:3710:LEU:HD21	1:J:3781:GLN:HG2	1.91	0.51
1:A:257:ARG:O	1:A:284:HIS:NE2	2.35	0.51
1:A:3951:PHE:HE2	1:A:3999:MET:HE2	1.75	0.51
1:D:3836:MET:HE1	1:D:3915:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2534:ALA:HB1	1:J:2588:ARG:HD2	1.91	0.51
1:J:3836:MET:HE1	1:J:3915:ILE:HG23	1.92	0.51
1:A:3836:MET:HE1	1:A:3915:ILE:HG23	1.92	0.51
1:D:3752:SER:OG	1:D:3753:PHE:N	2.42	0.51
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.92	0.51
1:A:3723:MET:HE2	1:A:3793:MET:HG3	1.91	0.51
1:D:3885:PHE:HE1	1:D:3919:THR:HG23	1.76	0.51
1:G:683:ARG:NH1	1:G:709:ASP:OD1	2.41	0.51
1:G:3752:SER:OG	1:G:3753:PHE:N	2.42	0.51
3:I:142:PHE:HA	3:I:145:MET:HG2	1.93	0.51
1:J:575:LEU:O	1:J:617:ASN:ND2	2.44	0.51
1:J:683:ARG:NH1	1:J:709:ASP:OD1	2.41	0.51
1:G:3885:PHE:HE1	1:G:3919:THR:HG23	1.76	0.51
1:J:1008:SER:OG	1:J:1010:VAL:O	2.29	0.51
1:D:3695:PRO:HB3	1:D:3699:HIS:HD2	1.76	0.51
1:D:3944:GLU:HG2	1:D:3946:GLN:H	1.76	0.51
1:G:1637:MET:HE1	1:G:1697:ALA:HB2	1.93	0.51
1:G:3695:PRO:HB3	1:G:3699:HIS:HD2	1.76	0.51
1:J:3846:ALA:HA	1:J:3849:ARG:HD2	1.93	0.51
1:J:4673:ARG:HE	1:J:4782:VAL:HG21	1.76	0.51
1:D:4673:ARG:HE	1:D:4782:VAL:HG21	1.76	0.50
1:D:1008:SER:OG	1:D:1010:VAL:O	2.29	0.50
1:G:1966:VAL:O	1:G:1970:GLN:NE2	2.43	0.50
1:J:1637:MET:HE1	1:J:1697:ALA:HB2	1.93	0.50
1:J:3627:GLN:HB3	1:J:3856:LEU:HD22	1.94	0.50
1:A:1637:MET:HE1	1:A:1697:ALA:HB2	1.93	0.50
1:G:3627:GLN:HB3	1:G:3856:LEU:HD22	1.94	0.50
1:A:575:LEU:O	1:A:617:ASN:ND2	2.44	0.50
1:A:3846:ALA:HA	1:A:3849:ARG:HD2	1.93	0.50
1:D:578:ILE:HD12	1:D:606:LEU:HD11	1.94	0.50
1:D:813:GLU:HB3	1:D:1008:SER:HB2	1.93	0.50
1:G:411:TYR:OH	1:G:444:SER:OG	2.29	0.50
1:G:4673:ARG:HE	1:G:4782:VAL:HG21	1.76	0.50
1:J:3944:GLU:HG2	1:J:3946:GLN:H	1.76	0.50
2:K:7:ILE:HD11	2:K:73:LYS:HB2	1.92	0.50
1:A:3944:GLU:HG2	1:A:3946:GLN:H	1.76	0.50
1:A:4555:LEU:HD11	1:A:4656:LEU:HB3	1.94	0.50
1:D:1637:MET:HE1	1:D:1697:ALA:HB2	1.93	0.50
3:F:142:PHE:HA	3:F:145:MET:HG2	1.93	0.50
1:G:818:ARG:NH2	1:G:1025:ARG:O	2.45	0.50
1:G:1008:SER:OG	1:G:1010:VAL:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4555:LEU:HD11	1:J:4656:LEU:HB3	1.94	0.50
1:A:1008:SER:OG	1:A:1010:VAL:O	2.29	0.50
1:A:3885:PHE:HE1	1:A:3919:THR:HG23	1.76	0.50
1:D:575:LEU:O	1:D:617:ASN:ND2	2.44	0.50
1:G:1927:LEU:O	1:G:2104:ARG:NH2	2.45	0.50
3:L:142:PHE:HA	3:L:145:MET:HG2	1.93	0.50
1:A:3695:PRO:HB3	1:A:3699:HIS:HD2	1.76	0.50
1:J:257:ARG:O	1:J:284:HIS:NE2	2.35	0.50
1:J:3885:PHE:HE1	1:J:3919:THR:HG23	1.76	0.50
1:A:578:ILE:HD12	1:A:606:LEU:HD11	1.94	0.50
1:A:684:VAL:HG22	1:A:781:VAL:HG23	1.94	0.50
1:A:3627:GLN:HB3	1:A:3856:LEU:HD22	1.94	0.50
1:D:3627:GLN:HB3	1:D:3856:LEU:HD22	1.94	0.50
1:G:2591:ARG:NH2	1:G:2638:UNK:O	2.45	0.50
1:J:684:VAL:HG22	1:J:781:VAL:HG23	1.94	0.50
1:J:818:ARG:NH2	1:J:1025:ARG:O	2.45	0.50
1:J:1225:PRO:HG2	1:J:1228:ILE:HB	1.94	0.50
1:A:575:LEU:HD22	1:A:609:CYS:HB3	1.94	0.49
1:A:4673:ARG:HE	1:A:4782:VAL:HG21	1.76	0.49
1:D:2591:ARG:NH2	1:D:2638:UNK:O	2.45	0.49
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.94	0.49
1:A:1856:ASP:N	1:A:1856:ASP:OD1	2.45	0.49
1:G:3944:GLU:HG2	1:G:3946:GLN:H	1.76	0.49
1:J:3695:PRO:HB3	1:J:3699:HIS:HD2	1.76	0.49
1:A:813:GLU:HB3	1:A:1008:SER:HB2	1.93	0.49
1:A:4069:LYS:HA	1:A:4072:VAL:HG12	1.94	0.49
1:D:1856:ASP:OD1	1:D:1856:ASP:N	2.45	0.49
1:D:4069:LYS:HA	1:D:4072:VAL:HG12	1.94	0.49
1:G:575:LEU:O	1:G:617:ASN:ND2	2.44	0.49
1:G:1225:PRO:HG2	1:G:1228:ILE:HB	1.94	0.49
1:D:588:SER:O	1:D:592:LYS:NZ	2.38	0.49
1:D:683:ARG:NH1	1:D:709:ASP:OD1	2.41	0.49
1:D:1927:LEU:O	1:D:2104:ARG:NH2	2.45	0.49
1:G:684:VAL:HG22	1:G:781:VAL:HG23	1.94	0.49
1:G:4034:ASN:HD21	1:G:4041:ALA:HB2	1.78	0.49
1:J:813:GLU:HB3	1:J:1008:SER:HB2	1.93	0.49
1:A:131:LEU:HG	1:A:178:ARG:HH11	1.78	0.49
1:D:575:LEU:HD22	1:D:609:CYS:HB3	1.94	0.49
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.45	0.49
1:G:131:LEU:HG	1:G:178:ARG:HH11	1.78	0.49
1:G:578:ILE:HD12	1:G:606:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:588:SER:O	1:J:592:LYS:NZ	2.38	0.49
1:A:1225:PRO:HG2	1:A:1228:ILE:HB	1.94	0.49
1:D:131:LEU:HG	1:D:178:ARG:HH11	1.78	0.49
1:D:4034:ASN:HD21	1:D:4041:ALA:HB2	1.78	0.49
1:A:418:LEU:HD23	1:A:493:ARG:HB3	1.94	0.49
1:D:4555:LEU:HD11	1:D:4656:LEU:HB3	1.94	0.49
1:G:418:LEU:HD23	1:G:493:ARG:HB3	1.94	0.49
1:J:131:LEU:HG	1:J:178:ARG:HH11	1.78	0.49
1:J:4678:ALA:HB1	1:J:4720:VAL:HG21	1.94	0.49
1:A:3753:PHE:HA	1:A:3756:LYS:HE2	1.94	0.49
3:C:142:PHE:HA	3:C:145:MET:HG2	1.93	0.49
1:G:1856:ASP:OD1	1:G:1856:ASP:N	2.45	0.49
1:J:1856:ASP:N	1:J:1856:ASP:OD1	2.45	0.49
1:J:1966:VAL:O	1:J:1970:GLN:NE2	2.43	0.49
1:A:4034:ASN:HD21	1:A:4041:ALA:HB2	1.78	0.49
1:G:4555:LEU:HD11	1:G:4656:LEU:HB3	1.94	0.49
1:J:1927:LEU:O	1:J:2104:ARG:NH2	2.45	0.49
1:J:4034:ASN:HD21	1:J:4041:ALA:HB2	1.78	0.49
1:J:4069:LYS:HA	1:J:4072:VAL:HG12	1.94	0.49
1:A:2591:ARG:NH2	1:A:2638:UNK:O	2.45	0.49
1:A:4085:ARG:HB3	1:A:4085:ARG:NH1	2.27	0.49
1:G:813:GLU:HB3	1:G:1008:SER:HB2	1.93	0.49
1:G:3753:PHE:HA	1:G:3756:LYS:HE2	1.94	0.49
1:J:815:VAL:O	1:J:1007:TYR:OH	2.28	0.49
1:D:418:LEU:HD23	1:D:493:ARG:HB3	1.94	0.48
1:D:684:VAL:HG22	1:D:781:VAL:HG23	1.94	0.48
1:D:2577:ILE:H	1:D:2577:ILE:HG12	1.45	0.48
1:G:4069:LYS:HA	1:G:4072:VAL:HG12	1.94	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.45	0.48
1:A:1954:ARG:HH11	1:A:2041:HIS:HD2	1.61	0.48
1:A:4244:GLU:HA	1:A:4247:ILE:HG22	1.95	0.48
1:A:1927:LEU:O	1:A:2104:ARG:NH2	2.45	0.48
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.94	0.48
1:D:2202:GLY:O	1:D:2206:THR:OG1	2.31	0.48
3:I:53:ILE:HA	3:I:56:VAL:HG22	1.95	0.48
1:J:578:ILE:HD12	1:J:606:LEU:HD11	1.94	0.48
1:J:2202:GLY:O	1:J:2206:THR:OG1	2.31	0.48
1:J:2591:ARG:NH2	1:J:2638:UNK:O	2.45	0.48
1:J:4244:GLU:HA	1:J:4247:ILE:HG22	1.95	0.48
1:D:1225:PRO:HG2	1:D:1228:ILE:HB	1.94	0.48
1:D:1954:ARG:HH11	1:D:2041:HIS:HD2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2287:ALA:O	1:G:2349:ASN:ND2	2.37	0.48
1:G:3676:ASP:HA	1:G:3679:LYS:HG2	1.95	0.48
1:J:575:LEU:HD22	1:J:609:CYS:HB3	1.94	0.48
1:J:3753:PHE:HA	1:J:3756:LYS:HE2	1.94	0.48
3:C:53:ILE:HA	3:C:56:VAL:HG22	1.95	0.48
1:G:575:LEU:HD22	1:G:609:CYS:HB3	1.94	0.48
1:J:1954:ARG:HH11	1:J:2041:HIS:HD2	1.61	0.48
1:A:3987:ASP:OD1	1:A:3987:ASP:N	2.46	0.48
1:D:4244:GLU:HA	1:D:4247:ILE:HG22	1.95	0.48
1:D:2287:ALA:O	1:D:2349:ASN:ND2	2.37	0.48
1:J:418:LEU:HD23	1:J:493:ARG:HB3	1.94	0.48
1:J:3987:ASP:OD1	1:J:3987:ASP:N	2.46	0.48
1:J:4085:ARG:HB3	1:J:4085:ARG:NH1	2.27	0.48
1:D:1966:VAL:O	1:D:1970:GLN:NE2	2.43	0.48
1:G:1868:PRO:O	1:G:1872:THR:OG1	2.31	0.48
1:G:2202:GLY:O	1:G:2206:THR:OG1	2.31	0.48
1:J:2139:PRO:HG3	1:J:3658:LYS:HE2	1.96	0.48
1:J:4937:ILE:O	1:J:4941:GLY:N	2.47	0.48
1:G:4678:ALA:HB1	1:G:4720:VAL:HG21	1.94	0.48
1:G:588:SER:O	1:G:592:LYS:NZ	2.38	0.48
1:G:3987:ASP:OD1	1:G:3987:ASP:N	2.46	0.48
1:J:3676:ASP:HA	1:J:3679:LYS:HG2	1.95	0.48
1:A:2202:GLY:O	1:A:2206:THR:OG1	2.31	0.47
1:D:2139:PRO:HG3	1:D:3658:LYS:HE2	1.96	0.47
3:F:53:ILE:HA	3:F:56:VAL:HG22	1.95	0.47
1:G:1954:ARG:HH11	1:G:2041:HIS:HD2	1.61	0.47
1:D:3676:ASP:HA	1:D:3679:LYS:HG2	1.95	0.47
1:G:2355:ARG:HE	1:G:2355:ARG:HB2	1.46	0.47
1:J:1601:MET:HE3	1:J:1601:MET:HB2	1.85	0.47
1:D:3753:PHE:HA	1:D:3756:LYS:HE2	1.94	0.47
1:D:4085:ARG:HB3	1:D:4085:ARG:NH1	2.27	0.47
1:D:4937:ILE:O	1:D:4941:GLY:N	2.47	0.47
1:G:2139:PRO:HG3	1:G:3658:LYS:HE2	1.96	0.47
3:L:46:GLU:O	3:L:50:GLN:HB2	2.15	0.47
1:A:2139:PRO:HG3	1:A:3658:LYS:HE2	1.96	0.47
1:D:622:THR:HG23	1:D:626:LEU:HD12	1.97	0.47
1:D:1770:SER:OG	1:D:1956:GLU:OE2	2.31	0.47
1:G:257:ARG:O	1:G:284:HIS:NE2	2.35	0.47
1:G:4244:GLU:HA	1:G:4247:ILE:HG22	1.95	0.47
1:A:4819:GLY:HA3	8:A:5105:F0U:BR	2.70	0.47
1:D:4222:VAL:HG23	1:D:4950:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1461:ASP:N	1:G:1461:ASP:OD1	2.48	0.47
1:G:4085:ARG:HB3	1:G:4085:ARG:NH1	2.27	0.47
1:G:4239:GLU:OE2	1:G:5014:TYR:OH	2.30	0.47
1:G:4819:GLY:HA3	8:G:5105:F0U:BR	2.70	0.47
1:A:1601:MET:HE3	1:A:1601:MET:HB2	1.85	0.47
1:D:4239:GLU:OE2	1:D:5014:TYR:OH	2.30	0.47
3:L:53:ILE:HA	3:L:56:VAL:HG22	1.95	0.47
1:D:4819:GLY:HA3	8:D:5105:F0U:BR	2.70	0.47
1:J:4819:GLY:HA3	8:J:5105:F0U:BR	2.70	0.47
1:A:2548:LEU:CD1	3:C:50:GLN:HG2	2.45	0.47
1:A:3676:ASP:HA	1:A:3679:LYS:HG2	1.95	0.47
1:D:3987:ASP:OD1	1:D:3987:ASP:N	2.46	0.47
1:G:4937:ILE:O	1:G:4941:GLY:N	2.47	0.47
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.97	0.46
1:G:101:LEU:HD13	1:G:107:ILE:HD13	1.97	0.46
1:A:1966:VAL:O	1:A:1970:GLN:NE2	2.43	0.46
1:A:4961:CYS:HA	1:A:5024:ALA:HA	1.97	0.46
1:D:475:GLN:HE21	1:D:533:ASN:HB2	1.81	0.46
1:D:4961:CYS:HA	1:D:5024:ALA:HA	1.97	0.46
1:J:784:SER:OG	1:J:785:ALA:N	2.48	0.46
1:G:194:SER:OG	1:G:195:PHE:N	2.49	0.46
1:G:4069:LYS:HD2	1:G:4129:ALA:HB1	1.97	0.46
1:A:1868:PRO:O	1:A:1872:THR:OG1	2.31	0.46
1:G:4961:CYS:HA	1:G:5024:ALA:HA	1.97	0.46
1:A:1461:ASP:OD1	1:A:1461:ASP:N	2.48	0.46
1:D:101:LEU:HD13	1:D:107:ILE:HD13	1.97	0.46
1:G:4222:VAL:HG23	1:G:4950:VAL:HG22	1.97	0.46
1:A:475:GLN:HE21	1:A:533:ASN:HB2	1.81	0.46
3:F:79:ASP:OD1	3:F:79:ASP:N	2.48	0.46
1:A:194:SER:OG	1:A:195:PHE:N	2.49	0.46
1:A:358:THR:OG1	1:A:359:TYR:N	2.49	0.46
1:A:635:THR:OG1	1:A:1693:GLN:NE2	2.46	0.46
1:A:1770:SER:OG	1:A:1956:GLU:OE2	2.31	0.46
1:D:176:SER:OG	1:D:178:ARG:NH2	2.49	0.46
1:J:475:GLN:HE21	1:J:533:ASN:HB2	1.81	0.46
1:J:622:THR:HG23	1:J:626:LEU:HD12	1.97	0.46
1:J:4069:LYS:HD2	1:J:4129:ALA:HB1	1.97	0.46
1:A:176:SER:OG	1:A:178:ARG:NH2	2.49	0.46
1:D:622:THR:HG21	1:D:1681:VAL:HG23	1.98	0.46
3:L:52:MET:O	3:L:55:GLU:HB3	2.16	0.46
1:A:4069:LYS:HD2	1:A:4129:ALA:HB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4979:THR:HG21	6:D:5103:ATP:H2'	1.98	0.46
1:G:622:THR:HG21	1:G:1681:VAL:HG23	1.98	0.46
1:G:4958:CYS:CA	6:G:5103:ATP:C2	2.75	0.46
3:I:52:MET:O	3:I:55:GLU:HB3	2.16	0.46
1:J:358:THR:OG1	1:J:359:TYR:N	2.49	0.46
1:J:4961:CYS:HA	1:J:5024:ALA:HA	1.97	0.46
1:A:4239:GLU:OE2	1:A:5014:TYR:OH	2.30	0.45
1:D:407:THR:HG21	1:D:448:LEU:HD11	1.98	0.45
1:G:407:THR:HG21	1:G:448:LEU:HD11	1.98	0.45
1:G:475:GLN:HE21	1:G:533:ASN:HB2	1.81	0.45
3:I:46:GLU:O	3:I:50:GLN:HB2	2.16	0.45
1:J:407:THR:HG21	1:J:448:LEU:HD11	1.98	0.45
1:J:708:GLY:N	1:J:713:SER:OG	2.36	0.45
1:J:1279:SER:OG	1:J:1280:GLN:N	2.49	0.45
1:J:3817:LEU:HG	1:J:3821:LYS:HD2	1.98	0.45
1:A:407:THR:HG21	1:A:448:LEU:HD11	1.98	0.45
1:G:622:THR:HG23	1:G:626:LEU:HD12	1.97	0.45
1:G:1279:SER:OG	1:G:1280:GLN:N	2.49	0.45
1:G:4995:LEU:HD21	1:G:5007:GLU:HB3	1.98	0.45
3:I:79:ASP:N	3:I:79:ASP:OD1	2.48	0.45
1:A:2208:MET:HE3	1:A:2208:MET:HB2	1.75	0.45
1:J:194:SER:OG	1:J:195:PHE:N	2.49	0.45
1:J:1461:ASP:OD1	1:J:1461:ASP:N	2.48	0.45
1:J:4222:VAL:HG23	1:J:4950:VAL:HG22	1.97	0.45
1:J:4789:PHE:O	1:J:4793:GLY:N	2.46	0.45
1:A:4937:ILE:O	1:A:4941:GLY:N	2.47	0.45
1:D:257:ARG:O	1:D:284:HIS:NE2	2.35	0.45
1:D:411:TYR:OH	1:D:444:SER:OG	2.29	0.45
1:D:2476:ILE:HD12	1:D:2477:PRO:HD2	1.98	0.45
1:G:411:TYR:HH	1:G:444:SER:HG	1.61	0.45
1:G:2577:ILE:H	1:G:2577:ILE:HG12	1.45	0.45
1:G:3699:HIS:HB2	1:G:3773:ARG:HG3	1.99	0.45
1:J:38:ALA:HB1	1:J:64:ILE:HG13	1.98	0.45
1:J:1868:PRO:O	1:J:1872:THR:OG1	2.31	0.45
1:J:2476:ILE:HD12	1:J:2477:PRO:HD2	1.98	0.45
1:J:4979:THR:HG21	6:J:5103:ATP:H2'	1.98	0.45
1:J:4995:LEU:HD21	1:J:5007:GLU:HB3	1.98	0.45
1:A:4979:THR:HG21	6:A:5103:ATP:H2'	1.98	0.45
1:D:4069:LYS:HD2	1:D:4129:ALA:HB1	1.97	0.45
1:G:38:ALA:HB1	1:G:64:ILE:HG13	1.98	0.45
1:J:4239:GLU:OE2	1:J:5014:TYR:OH	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:VAL:HG22	1:A:1164:LEU:HD13	1.99	0.45
1:A:2577:ILE:H	1:A:2577:ILE:HG12	1.45	0.45
3:C:79:ASP:OD1	3:C:79:ASP:N	2.48	0.45
1:D:358:THR:OG1	1:D:359:TYR:N	2.49	0.45
1:D:3699:HIS:HB2	1:D:3773:ARG:HG3	1.99	0.45
1:J:1947:CYS:SG	1:J:2127:GLN:NE2	2.90	0.45
1:A:622:THR:HG21	1:A:1681:VAL:HG23	1.98	0.45
1:A:784:SER:OG	1:A:785:ALA:N	2.48	0.45
1:D:1601:MET:HE3	1:D:1601:MET:HB2	1.85	0.45
1:J:3699:HIS:HB2	1:J:3773:ARG:HG3	1.99	0.45
1:A:101:LEU:HD13	1:A:107:ILE:HD13	1.97	0.45
1:A:683:ARG:NH1	1:A:709:ASP:OD1	2.41	0.45
1:A:3699:HIS:HB2	1:A:3773:ARG:HG3	1.99	0.45
1:A:3817:LEU:HG	1:A:3821:LYS:HD2	1.98	0.45
1:D:194:SER:OG	1:D:195:PHE:N	2.49	0.45
1:D:1149:VAL:HG22	1:D:1164:LEU:HD13	1.99	0.45
1:G:176:SER:OG	1:G:178:ARG:NH2	2.49	0.45
1:G:1601:MET:HE3	1:G:1601:MET:HB2	1.85	0.45
1:G:3817:LEU:HG	1:G:3821:LYS:HD2	1.98	0.45
1:J:552:ASP:OD2	1:J:552:ASP:N	2.45	0.45
1:G:404:ILE:HD11	1:G:478:PHE:HA	1.99	0.45
1:G:2098:VAL:HG11	1:G:2127:GLN:HE21	1.82	0.45
1:G:2476:ILE:HD12	1:G:2477:PRO:HD2	1.98	0.45
1:G:4979:THR:HG21	6:G:5103:ATP:H2'	1.98	0.45
1:J:622:THR:HG21	1:J:1681:VAL:HG23	1.98	0.45
1:A:669:ASP:OD1	1:A:669:ASP:N	2.50	0.45
1:A:815:VAL:O	1:A:1007:TYR:OH	2.28	0.45
1:D:3817:LEU:HG	1:D:3821:LYS:HD2	1.98	0.45
1:J:2355:ARG:HE	1:J:2355:ARG:HB2	1.46	0.45
1:D:635:THR:OG1	1:D:1693:GLN:NE2	2.46	0.44
1:G:1149:VAL:HG22	1:G:1164:LEU:HD13	1.99	0.44
1:G:1947:CYS:SG	1:G:2127:GLN:NE2	2.90	0.44
1:J:590:LEU:HB2	1:J:599:VAL:HG11	1.99	0.44
1:J:1076:ARG:HH22	1:J:1079:LYS:HG3	1.82	0.44
1:J:3658:LYS:HA	1:J:3662:ILE:HD12	2.00	0.44
1:A:590:LEU:HB2	1:A:599:VAL:HG11	1.99	0.44
1:A:1076:ARG:HH22	1:A:1079:LYS:HG3	1.82	0.44
1:A:3904:ARG:HE	1:A:3975:GLY:HA3	1.83	0.44
1:D:1868:PRO:O	1:D:1872:THR:OG1	2.31	0.44
1:D:4675:LYS:HB3	1:D:4675:LYS:HE3	1.80	0.44
1:G:1770:SER:OG	1:G:1956:GLU:OE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:101:LEU:HD13	1:J:107:ILE:HD13	1.97	0.44
1:J:2577:ILE:H	1:J:2577:ILE:HG12	1.45	0.44
1:A:2476:ILE:HD12	1:A:2477:PRO:HD2	1.98	0.44
1:D:404:ILE:HD11	1:D:478:PHE:HA	1.99	0.44
1:D:528:SER:HA	1:D:531:ARG:HH12	1.83	0.44
1:D:1076:ARG:HH22	1:D:1079:LYS:HG3	1.82	0.44
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.90	0.44
3:F:46:GLU:O	3:F:50:GLN:HB2	2.17	0.44
1:G:1110:ARG:HH11	1:G:1110:ARG:HB3	1.83	0.44
1:A:4222:VAL:HG23	1:A:4950:VAL:HG22	1.97	0.44
1:D:38:ALA:HB1	1:D:64:ILE:HG13	1.98	0.44
1:D:474:ARG:HH11	1:D:474:ARG:CB	2.30	0.44
1:G:1076:ARG:HH22	1:G:1079:LYS:HG3	1.82	0.44
1:D:4995:LEU:HD21	1:D:5007:GLU:HB3	1.98	0.44
1:G:528:SER:HA	1:G:531:ARG:HH12	1.83	0.44
1:G:669:ASP:N	1:G:669:ASP:OD1	2.50	0.44
1:J:528:SER:HA	1:J:531:ARG:HH12	1.83	0.44
1:J:1149:VAL:HG22	1:J:1164:LEU:HD13	1.99	0.44
1:J:1649:ASP:HB3	1:J:1652:GLU:HG3	1.99	0.44
1:A:404:ILE:HD11	1:A:478:PHE:HA	1.99	0.44
1:A:578:ILE:HG23	1:A:582:HIS:HB2	1.99	0.44
1:A:2098:VAL:HG11	1:A:2127:GLN:HE21	1.82	0.44
1:A:3984:ARG:NH1	1:J:160:GLY:O	2.51	0.44
1:D:815:VAL:O	1:D:1007:TYR:OH	2.28	0.44
1:D:4059:LEU:HD13	1:D:4167:ALA:HB2	1.99	0.44
1:G:561:LEU:HD13	1:G:589:LEU:HD21	1.99	0.44
1:G:3658:LYS:HA	1:G:3662:ILE:HD12	2.00	0.44
1:G:3904:ARG:HE	1:G:3975:GLY:HA3	1.83	0.44
1:J:561:LEU:HD13	1:J:589:LEU:HD21	1.99	0.44
1:A:38:ALA:HB1	1:A:64:ILE:HG13	1.98	0.44
1:A:1147:ASP:OD1	1:A:1147:ASP:N	2.49	0.44
1:G:35:LEU:HB3	1:G:49:LEU:HB3	2.00	0.44
1:J:176:SER:OG	1:J:178:ARG:NH2	2.49	0.44
1:J:578:ILE:HG23	1:J:582:HIS:HB2	1.99	0.44
1:J:4059:LEU:HD13	1:J:4167:ALA:HB2	1.99	0.44
1:A:1203:ASN:ND2	1:A:1210:SER:OG	2.51	0.44
1:A:1649:ASP:HB3	1:A:1652:GLU:HG3	1.99	0.44
1:A:4995:LEU:HD21	1:A:5007:GLU:HB3	1.98	0.44
1:D:35:LEU:HB3	1:D:49:LEU:HB3	2.00	0.44
1:D:1461:ASP:N	1:D:1461:ASP:OD1	2.48	0.44
1:J:1147:ASP:OD1	1:J:1147:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2098:VAL:HG11	1:J:2127:GLN:HE21	1.82	0.44
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.90	0.44
1:A:2544:THR:HB	1:A:2547:ALA:HB3	1.99	0.44
1:D:347:PHE:H	1:D:347:PHE:HD2	1.66	0.44
1:D:1110:ARG:HH11	1:D:1110:ARG:HB3	1.83	0.44
1:G:358:THR:OG1	1:G:359:TYR:N	2.49	0.44
1:G:815:VAL:O	1:G:1007:TYR:OH	2.28	0.44
1:J:3904:ARG:HE	1:J:3975:GLY:HA3	1.83	0.44
1:D:561:LEU:HD13	1:D:589:LEU:HD21	1.99	0.43
1:D:2098:VAL:HG11	1:D:2127:GLN:HE21	1.82	0.43
1:G:160:GLY:O	1:J:3984:ARG:NH1	2.51	0.43
1:G:708:GLY:N	1:G:713:SER:OG	2.36	0.43
1:J:1203:ASN:ND2	1:J:1210:SER:OG	2.51	0.43
1:J:4792:LEU:HG	8:J:5105:F0U:CL1	2.55	0.43
1:J:4805:ASN:HB3	1:J:4808:PHE:HD2	1.84	0.43
1:A:528:SER:HA	1:A:531:ARG:HH12	1.83	0.43
1:A:3658:LYS:HA	1:A:3662:ILE:HD12	2.00	0.43
1:D:590:LEU:HB2	1:D:599:VAL:HG11	1.99	0.43
1:D:1746:THR:OG1	1:D:1748:PHE:O	2.36	0.43
1:J:404:ILE:HD11	1:J:478:PHE:HA	1.99	0.43
1:J:1126:GLY:HA3	1:J:1143:TRP:CE2	2.54	0.43
1:A:4587:PRO:HD3	1:A:4628:VAL:HG21	2.00	0.43
1:D:160:GLY:O	1:G:3984:ARG:NH1	2.51	0.43
1:D:1649:ASP:HB3	1:D:1652:GLU:HG3	1.99	0.43
1:D:4792:LEU:HG	8:D:5105:F0U:CL1	2.55	0.43
1:D:4865:LYS:HB3	1:D:4865:LYS:HE3	1.84	0.43
1:G:347:PHE:H	1:G:347:PHE:HD2	1.66	0.43
1:G:1126:GLY:HA3	1:G:1143:TRP:CE2	2.54	0.43
1:G:4789:PHE:O	1:G:4793:GLY:N	2.46	0.43
1:G:4792:LEU:HG	8:G:5105:F0U:CL1	2.55	0.43
1:J:35:LEU:HB3	1:J:49:LEU:HB3	2.00	0.43
1:A:35:LEU:HB3	1:A:49:LEU:HB3	2.00	0.43
1:A:160:GLY:O	1:D:3984:ARG:NH1	2.51	0.43
1:A:347:PHE:H	1:A:347:PHE:HD2	1.66	0.43
1:A:1279:SER:OG	1:A:1280:GLN:N	2.49	0.43
1:A:2030:ASP:OD1	1:A:2030:ASP:N	2.52	0.43
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	2.00	0.43
1:D:1973:GLN:NE2	1:D:1997:GLU:OE1	2.49	0.43
1:G:578:ILE:HG23	1:G:582:HIS:HB2	1.99	0.43
3:L:70:LEU:HD12	3:L:70:LEU:HA	1.88	0.43
1:A:2548:LEU:HA	1:A:2548:LEU:HD23	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:ILE:HG23	1:D:582:HIS:HB2	1.99	0.43
1:D:2476:ILE:HD13	1:D:2532:ALA:HB1	2.01	0.43
1:G:474:ARG:H	1:G:474:ARG:HG3	1.67	0.43
1:G:784:SER:OG	1:G:785:ALA:N	2.48	0.43
1:G:1649:ASP:HB3	1:G:1652:GLU:HG3	1.99	0.43
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	2.00	0.43
1:J:2550:LEU:HA	1:J:2553:TYR:HB3	2.00	0.43
3:L:79:ASP:OD1	3:L:79:ASP:N	2.48	0.43
1:A:1110:ARG:HB3	1:A:1110:ARG:HH11	1.83	0.43
1:A:1126:GLY:HA3	1:A:1143:TRP:CE2	2.54	0.43
1:A:4927:ILE:O	1:A:4931:ILE:N	2.52	0.43
1:D:2550:LEU:HA	1:D:2553:TYR:HB3	2.00	0.43
1:D:3794:VAL:HA	1:D:3797:THR:HG22	2.00	0.43
1:G:590:LEU:HB2	1:G:599:VAL:HG11	1.99	0.43
1:G:2550:LEU:HA	1:G:2553:TYR:HB3	2.00	0.43
1:G:3882:GLN:HG3	1:G:3960:GLN:HG2	2.01	0.43
1:G:4805:ASN:HB3	1:G:4808:PHE:HD2	1.84	0.43
1:J:635:THR:OG1	1:J:1693:GLN:NE2	2.46	0.43
1:A:1573:MET:HE2	1:A:1573:MET:HB3	1.88	0.43
1:A:4976:GLU:HG2	1:A:4980:LEU:HD23	2.01	0.43
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.99	0.43
1:J:669:ASP:OD1	1:J:669:ASP:N	2.50	0.43
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	2.00	0.43
1:A:3794:VAL:HA	1:A:3797:THR:HG22	2.00	0.43
1:D:4587:PRO:HD3	1:D:4628:VAL:HG21	2.00	0.43
1:J:1770:SER:OG	1:J:1956:GLU:OE2	2.31	0.43
1:J:3882:GLN:HG3	1:J:3960:GLN:HG2	2.01	0.43
1:J:4976:GLU:HG2	1:J:4980:LEU:HD23	2.01	0.43
1:A:37:LEU:HD13	1:A:191:VAL:HG11	2.01	0.43
1:A:2355:ARG:HE	1:A:2355:ARG:HB2	1.46	0.43
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.99	0.43
1:D:37:LEU:HD13	1:D:191:VAL:HG11	2.01	0.43
1:D:2469:ILE:HG21	1:D:2502:MET:HE3	2.01	0.43
1:D:3658:LYS:HA	1:D:3662:ILE:HD12	2.00	0.43
1:A:4805:ASN:HB3	1:A:4808:PHE:HD2	1.84	0.43
1:D:1126:GLY:HA3	1:D:1143:TRP:CE2	2.54	0.43
1:D:3882:GLN:HG3	1:D:3960:GLN:HG2	2.01	0.43
1:D:3904:ARG:HE	1:D:3975:GLY:HA3	1.83	0.43
1:G:272:SER:HB3	1:G:335:GLY:H	1.84	0.43
1:G:474:ARG:HH11	1:G:474:ARG:CB	2.30	0.43
1:G:593:HIS:HD2	1:G:1593:PRO:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:25:HIS:CE1	2:H:40:ARG:HG2	2.54	0.43
1:J:272:SER:HB3	1:J:335:GLY:H	1.84	0.43
1:J:1110:ARG:HH11	1:J:1110:ARG:HB3	1.83	0.43
1:A:593:HIS:HD2	1:A:1593:PRO:HD2	1.84	0.42
1:A:2550:LEU:HA	1:A:2553:TYR:HB3	2.00	0.42
1:A:3882:GLN:HG3	1:A:3960:GLN:HG2	2.01	0.42
1:J:593:HIS:HD2	1:J:1593:PRO:HD2	1.84	0.42
2:E:25:HIS:CE1	2:E:40:ARG:HG2	2.54	0.42
1:G:552:ASP:OD2	1:G:552:ASP:N	2.45	0.42
1:G:3794:VAL:HA	1:G:3797:THR:HG22	2.00	0.42
1:J:2250:MET:HE2	1:J:2250:MET:HB2	1.86	0.42
1:J:4587:PRO:HD3	1:J:4628:VAL:HG21	2.00	0.42
1:J:4927:ILE:O	1:J:4931:ILE:N	2.52	0.42
2:K:25:HIS:CE1	2:K:40:ARG:HG2	2.54	0.42
1:A:708:GLY:N	1:A:713:SER:OG	2.36	0.42
1:A:1763:PRO:HG3	1:A:2094:LEU:HD22	2.02	0.42
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	2.01	0.42
1:A:2433:LEU:HD22	1:A:2457:LEU:HD22	2.02	0.42
1:A:2469:ILE:HG21	1:A:2502:MET:HE3	2.01	0.42
1:A:4792:LEU:HG	8:A:5105:F0U:CL1	2.55	0.42
1:D:593:HIS:HD2	1:D:1593:PRO:HD2	1.84	0.42
1:D:1545:ASN:HD21	2:E:32:ASN:HA	1.85	0.42
1:D:2433:LEU:HD22	1:D:2457:LEU:HD22	2.02	0.42
1:G:484:LEU:HD12	1:G:484:LEU:HA	1.84	0.42
1:G:4675:LYS:HB3	1:G:4675:LYS:HE3	1.80	0.42
1:G:4976:GLU:HG2	1:G:4980:LEU:HD23	2.01	0.42
1:J:411:TYR:OH	1:J:444:SER:OG	2.29	0.42
1:J:546:TRP:O	1:J:550:LYS:NZ	2.48	0.42
1:J:1863:LEU:HB3	1:J:1871:PHE:CG	2.55	0.42
1:J:2175:GLU:HG3	1:J:2228:MET:HB2	2.01	0.42
1:J:3794:VAL:HA	1:J:3797:THR:HG22	2.00	0.42
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.02	0.42
1:D:1203:ASN:ND2	1:D:1210:SER:OG	2.51	0.42
1:D:4042:ARG:HA	1:D:4045:VAL:HG12	2.01	0.42
1:D:4805:ASN:HB3	1:D:4808:PHE:HD2	1.84	0.42
1:J:2186:MET:O	1:J:2192:TYR:OH	2.28	0.42
1:A:272:SER:HB3	1:A:335:GLY:H	1.84	0.42
1:A:561:LEU:HD13	1:A:589:LEU:HD21	1.99	0.42
1:A:606:LEU:HD12	1:A:606:LEU:HA	1.90	0.42
1:A:1302:ARG:HH21	1:A:1524:THR:HG23	1.85	0.42
1:A:2476:ILE:HD13	1:A:2532:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1147:ASP:OD1	1:D:1147:ASP:N	2.49	0.42
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	2.01	0.42
1:G:1973:GLN:NE2	1:G:1997:GLU:OE1	2.49	0.42
1:G:4587:PRO:HD3	1:G:4628:VAL:HG21	2.00	0.42
1:J:2476:ILE:HD13	1:J:2532:ALA:HB1	2.01	0.42
1:A:116:MET:HG3	1:A:137:LEU:HD23	2.01	0.42
1:A:1863:LEU:HB3	1:A:1871:PHE:CG	2.55	0.42
1:D:272:SER:HB3	1:D:335:GLY:H	1.84	0.42
1:G:1746:THR:OG1	1:G:1748:PHE:O	2.36	0.42
1:G:1863:LEU:HB3	1:G:1871:PHE:CG	2.55	0.42
1:G:2175:GLU:HG3	1:G:2228:MET:HB2	2.01	0.42
1:J:1815:LEU:HD22	1:J:1845:VAL:HG21	2.00	0.42
2:B:25:HIS:CE1	2:B:40:ARG:HG2	2.54	0.42
1:D:116:MET:HG3	1:D:137:LEU:HD23	2.01	0.42
1:D:1812:LEU:HD23	1:D:1812:LEU:HA	1.92	0.42
1:D:4976:GLU:HG2	1:D:4980:LEU:HD23	2.01	0.42
1:G:1203:ASN:ND2	1:G:1210:SER:OG	2.51	0.42
1:G:1763:PRO:HG3	1:G:2094:LEU:HD22	2.02	0.42
1:G:2433:LEU:HD22	1:G:2457:LEU:HD22	2.02	0.42
1:J:282:ILE:HB	1:J:291:LEU:HB3	2.02	0.42
1:J:1763:PRO:HG3	1:J:2094:LEU:HD22	2.02	0.42
1:A:1220:GLN:HE21	1:D:3528:UNK:HA	1.85	0.42
1:A:4042:ARG:HA	1:A:4045:VAL:HG12	2.01	0.42
1:G:2476:ILE:HD13	1:G:2532:ALA:HB1	2.01	0.42
1:D:606:LEU:HD12	1:D:606:LEU:HA	1.90	0.42
1:G:2469:ILE:HG21	1:G:2502:MET:HE3	2.01	0.42
1:J:1632:ASP:OD2	1:J:1632:ASP:N	2.53	0.42
1:J:2469:ILE:HG21	1:J:2502:MET:HE3	2.01	0.42
1:A:3528:UNK:HA	1:J:1220:GLN:HE21	1.85	0.42
1:G:1448:VAL:HG22	1:G:1554:VAL:HG23	2.02	0.42
1:G:2186:MET:O	1:G:2192:TYR:OH	2.28	0.42
1:J:484:LEU:HD12	1:J:484:LEU:HA	1.84	0.42
1:J:2433:LEU:HD22	1:J:2457:LEU:HD22	2.02	0.42
1:A:4248:ALA:O	1:A:4252:SER:OG	2.38	0.41
1:D:1175:SER:HB2	1:D:1180:ARG:HH12	1.85	0.41
1:D:1863:LEU:HB3	1:D:1871:PHE:CG	2.55	0.41
1:D:4068:LEU:HA	1:D:4071:ILE:HB	2.02	0.41
1:G:37:LEU:HD13	1:G:191:VAL:HG11	2.01	0.41
1:G:116:MET:HG3	1:G:137:LEU:HD23	2.01	0.41
1:G:1175:SER:HB2	1:G:1180:ARG:HH12	1.85	0.41
1:J:37:LEU:HD13	1:J:191:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2192:TYR:HB2	3:C:10:ILE:HG21	2.01	0.41
1:D:669:ASP:N	1:D:669:ASP:OD1	2.50	0.41
1:D:933:LEU:H	1:D:933:LEU:HG	1.75	0.41
1:D:4927:ILE:O	1:D:4931:ILE:N	2.52	0.41
1:G:3842:LEU:O	1:G:3929:SER:OG	2.39	0.41
1:G:4042:ARG:HA	1:G:4045:VAL:HG12	2.01	0.41
1:G:4865:LYS:HB3	1:G:4865:LYS:HE3	1.84	0.41
1:J:1746:THR:OG1	1:J:1748:PHE:O	2.36	0.41
1:J:4180:ARG:HD3	1:J:4192:ARG:HH11	1.85	0.41
1:A:1470:ARG:HH11	1:A:1470:ARG:HD2	1.71	0.41
1:D:1279:SER:OG	1:D:1280:GLN:N	2.49	0.41
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	2.02	0.41
1:D:1608:MET:HE2	1:D:1608:MET:HB3	1.91	0.41
1:D:1763:PRO:HG3	1:D:2094:LEU:HD22	2.02	0.41
1:G:2030:ASP:N	1:G:2030:ASP:OD1	2.52	0.41
1:G:4927:ILE:O	1:G:4931:ILE:N	2.52	0.41
1:J:347:PHE:H	1:J:347:PHE:HD2	1.66	0.41
1:J:4042:ARG:HA	1:J:4045:VAL:HG12	2.01	0.41
1:D:1519:LEU:HD21	1:D:1572:ILE:HD12	2.02	0.41
1:J:1302:ARG:HH21	1:J:1524:THR:HG23	1.85	0.41
1:J:1448:VAL:HG22	1:J:1554:VAL:HG23	2.02	0.41
1:J:4150:LEU:HD12	1:J:4150:LEU:HA	1.89	0.41
1:J:4675:LYS:HE3	1:J:4675:LYS:HB3	1.80	0.41
1:A:169:LEU:HD12	1:A:202:MET:HE2	2.02	0.41
1:A:1568:LYS:HB3	1:A:1574:PRO:HD3	2.03	0.41
1:D:1302:ARG:HH21	1:D:1524:THR:HG23	1.85	0.41
1:D:1568:LYS:HB3	1:D:1574:PRO:HD3	2.03	0.41
1:D:2522:LEU:HA	1:D:2526:PHE:HD1	1.86	0.41
1:D:3842:LEU:O	1:D:3929:SER:OG	2.39	0.41
1:G:2250:MET:HE2	1:G:2250:MET:HB2	1.86	0.41
1:G:4546:VAL:HA	1:G:4549:VAL:HG22	2.03	0.41
1:D:784:SER:OG	1:D:785:ALA:N	2.48	0.41
1:D:1220:GLN:HE21	1:G:3528:UNK:HA	1.85	0.41
1:G:162:LYS:HB2	1:G:162:LYS:HE3	1.90	0.41
1:G:1302:ARG:HH21	1:G:1524:THR:HG23	1.85	0.41
1:G:4068:LEU:HA	1:G:4071:ILE:HB	2.02	0.41
1:J:116:MET:HG3	1:J:137:LEU:HD23	2.01	0.41
1:J:2030:ASP:N	1:J:2030:ASP:OD1	2.52	0.41
1:D:169:LEU:HD12	1:D:202:MET:HE2	2.02	0.41
1:D:4180:ARG:HD3	1:D:4192:ARG:HH11	1.85	0.41
1:G:282:ILE:HB	1:G:291:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1021:LEU:HD23	1:J:1021:LEU:HA	1.91	0.41
1:J:3727:ASP:O	1:J:3731:LYS:NZ	2.54	0.41
1:J:3842:LEU:O	1:J:3929:SER:OG	2.39	0.41
1:J:4546:VAL:HA	1:J:4549:VAL:HG22	2.03	0.41
1:A:282:ILE:HB	1:A:291:LEU:HB3	2.02	0.41
1:A:4546:VAL:HA	1:A:4549:VAL:HG22	2.03	0.41
1:A:4789:PHE:O	1:A:4793:GLY:N	2.46	0.41
1:D:4546:VAL:HA	1:D:4549:VAL:HG22	2.03	0.41
1:D:4839:MET:HB3	1:G:4823:LEU:HD21	2.03	0.41
1:G:341:TYR:HD1	1:G:341:TYR:HA	1.79	0.41
1:G:1220:GLN:HE21	1:J:3528:UNK:HA	1.85	0.41
1:J:474:ARG:HH11	1:J:474:ARG:CB	2.30	0.41
1:J:1175:SER:HB2	1:J:1180:ARG:HH12	1.85	0.41
1:J:1519:LEU:HD21	1:J:1572:ILE:HD12	2.02	0.41
3:L:76:LYS:HE2	3:L:76:LYS:HB2	1.98	0.41
1:A:568:LEU:HD13	1:A:606:LEU:HD13	2.03	0.41
1:A:794:GLY:HA3	1:A:812:HIS:HB3	2.03	0.41
1:A:1519:LEU:HD23	1:A:1519:LEU:HA	1.88	0.41
1:A:1936:LYS:HD3	1:A:2105:TRP:CD2	2.56	0.41
1:A:3959:LYS:O	1:A:3963:ASN:ND2	2.54	0.41
1:D:2030:ASP:OD1	1:D:2030:ASP:N	2.52	0.41
1:D:2615:ARG:HA	1:D:2616:PRO:HD3	1.97	0.41
1:D:3727:ASP:O	1:D:3731:LYS:NZ	2.54	0.41
1:G:169:LEU:HD12	1:G:202:MET:HE2	2.02	0.41
1:G:2208:MET:HE3	1:G:2208:MET:HB2	1.75	0.41
1:G:4930:ALA:HA	1:G:4933:GLN:HG2	2.03	0.41
3:I:43:ASN:OD1	3:I:43:ASN:N	2.54	0.41
1:J:162:LYS:HE3	1:J:162:LYS:HB2	1.90	0.41
1:J:1568:LYS:HB3	1:J:1574:PRO:HD3	2.03	0.41
1:J:4865:LYS:HB3	1:J:4865:LYS:HE3	1.84	0.41
1:A:1175:SER:HB2	1:A:1180:ARG:HH12	1.85	0.41
1:A:4180:ARG:HD3	1:A:4192:ARG:HH11	1.85	0.41
1:D:1786:LEU:HD23	1:D:1786:LEU:HA	1.96	0.41
1:D:1936:LYS:HD3	1:D:2105:TRP:CD2	2.56	0.41
1:D:3959:LYS:O	1:D:3963:ASN:ND2	2.54	0.41
1:D:4789:PHE:O	1:D:4793:GLY:N	2.46	0.41
1:G:1936:LYS:HD3	1:G:2105:TRP:CD2	2.56	0.41
1:G:2522:LEU:HA	1:G:2526:PHE:HD1	1.86	0.41
1:J:4068:LEU:HA	1:J:4071:ILE:HB	2.02	0.41
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.50	0.40
1:A:3842:LEU:O	1:A:3929:SER:OG	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2622:LEU:HD13	1:D:2622:LEU:HA	1.77	0.40
1:G:606:LEU:HD12	1:G:606:LEU:HA	1.90	0.40
1:G:4839:MET:HB3	1:J:4823:LEU:HD21	2.03	0.40
1:J:2548:LEU:C	1:J:2548:LEU:CD1	2.86	0.40
1:A:1632:ASP:OD2	1:A:1632:ASP:N	2.53	0.40
1:A:4839:MET:O	1:A:4843:LEU:N	2.53	0.40
1:A:4957:LYS:HE3	1:A:4957:LYS:HB3	1.87	0.40
1:D:2208:MET:HE3	1:D:2208:MET:HB2	1.75	0.40
1:D:3974:THR:O	1:D:3978:GLN:HG2	2.21	0.40
3:F:43:ASN:OD1	3:F:43:ASN:N	2.54	0.40
1:G:635:THR:OG1	1:G:1693:GLN:NE2	2.46	0.40
1:G:1018:ASN:HA	1:G:1019:PRO:HD3	1.92	0.40
1:G:1568:LYS:HB3	1:G:1574:PRO:HD3	2.03	0.40
1:G:2622:LEU:HD13	1:G:2622:LEU:HA	1.77	0.40
1:G:4150:LEU:HA	1:G:4150:LEU:HD12	1.89	0.40
3:L:43:ASN:OD1	3:L:43:ASN:N	2.54	0.40
1:A:341:TYR:HD1	1:A:341:TYR:HA	1.79	0.40
1:A:3940:LYS:HE2	1:A:3940:LYS:HB3	1.88	0.40
1:D:4839:MET:O	1:D:4843:LEU:N	2.53	0.40
3:F:70:LEU:HD12	3:F:70:LEU:HA	1.88	0.40
1:G:1519:LEU:HD21	1:G:1572:ILE:HD12	2.02	0.40
1:G:4180:ARG:HD3	1:G:4192:ARG:HH11	1.85	0.40
1:J:169:LEU:HD12	1:J:202:MET:HE2	2.02	0.40
1:J:1778:SER:HB3	1:J:1798:LEU:HB2	2.03	0.40
1:J:1936:LYS:HD3	1:J:2105:TRP:CD2	2.56	0.40
1:A:1731:LEU:HD23	1:A:1772:ARG:HH21	1.86	0.40
1:A:4150:LEU:HA	1:A:4150:LEU:HD12	1.89	0.40
1:G:1731:LEU:HD23	1:G:1772:ARG:HE	1.87	0.40
1:J:494:LEU:HD23	1:J:494:LEU:HA	1.96	0.40
1:J:568:LEU:HD13	1:J:606:LEU:HD13	2.03	0.40
1:J:3959:LYS:O	1:J:3963:ASN:ND2	2.54	0.40
1:J:4160:LEU:HD23	1:J:4163:PHE:HD2	1.86	0.40
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.93	0.40
1:A:1778:SER:HB3	1:A:1798:LEU:HB2	2.03	0.40
1:A:2522:LEU:HA	1:A:2526:PHE:HD1	1.86	0.40
1:A:4068:LEU:HA	1:A:4071:ILE:HB	2.02	0.40
1:D:568:LEU:HD13	1:D:606:LEU:HD13	2.03	0.40
1:D:2250:MET:HE2	1:D:2250:MET:HB2	1.86	0.40
1:D:2354:VAL:O	1:D:2358:ILE:HG12	2.22	0.40
1:D:2430:ILE:HD13	1:D:2430:ILE:HA	1.97	0.40
1:D:4160:LEU:HD23	1:D:4163:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4983:HIS:O	6:D:5103:ATP:N6	2.55	0.40
1:G:4160:LEU:HD23	1:G:4163:PHE:HD2	1.86	0.40
1:J:2522:LEU:HA	1:J:2526:PHE:HD1	1.86	0.40
1:J:4930:ALA:HA	1:J:4933:GLN:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3427/5037 (68%)	3321 (97%)	106 (3%)	0	100	100
1	D	3427/5037 (68%)	3321 (97%)	106 (3%)	0	100	100
1	G	3427/5037 (68%)	3321 (97%)	106 (3%)	0	100	100
1	J	3427/5037 (68%)	3321 (97%)	106 (3%)	0	100	100
2	B	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	K	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	C	133/149 (89%)	133 (100%)	0	0	100	100
3	F	133/149 (89%)	133 (100%)	0	0	100	100
3	I	133/149 (89%)	133 (100%)	0	0	100	100
3	L	133/149 (89%)	133 (100%)	0	0	100	100
All	All	14660/21172 (69%)	14208 (97%)	452 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2495/3416 (73%)	2429 (97%)	66 (3%)	40	60
1	D	2495/3416 (73%)	2428 (97%)	67 (3%)	39	59
1	G	2495/3416 (73%)	2428 (97%)	67 (3%)	39	59
1	J	2495/3416 (73%)	2428 (97%)	67 (3%)	39	59
2	B	84/88 (96%)	77 (92%)	7 (8%)	10	34
2	E	84/88 (96%)	77 (92%)	7 (8%)	10	34
2	H	84/88 (96%)	77 (92%)	7 (8%)	10	34
2	K	84/88 (96%)	77 (92%)	7 (8%)	10	34
3	C	104/123 (85%)	82 (79%)	22 (21%)	1	6
3	F	104/123 (85%)	82 (79%)	22 (21%)	1	6
3	I	104/123 (85%)	81 (78%)	23 (22%)	1	6
3	L	104/123 (85%)	81 (78%)	23 (22%)	1	6
All	All	10732/14508 (74%)	10347 (96%)	385 (4%)	32	54

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	107	ILE
1	A	135	VAL
1	A	171	LEU
1	A	175	SER
1	A	179	TYR
1	A	231	LEU
1	A	267	ILE
1	A	272	SER
1	A	347	PHE
1	A	441	VAL
1	A	474	ARG
1	A	519	VAL
1	A	525	LEU

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Mol	Chain	Res	Type
1	A	531	ARG
1	A	539	LEU
1	A	933	LEU
1	A	935	LEU
1	A	988	LEU
1	A	1038	SER
1	A	1110	ARG
1	A	1160	ILE
1	A	1275	ARG
1	A	1427	ILE
1	A	1454	THR
1	A	1470	ARG
1	A	1584	ARG
1	A	1634	LEU
1	A	1715	LEU
1	A	1738	LEU
1	A	2113	SER
1	A	2206	THR
1	A	2209	GLU
1	A	2279	SER
1	A	2336	ARG
1	A	2355	ARG
1	A	2377	LEU
1	A	2439	GLU
1	A	2449	GLU
1	A	2512	ILE
1	A	2516	ASP
1	A	2524	VAL
1	A	2577	ILE
1	A	2582	MET
1	A	2622	LEU
1	A	3648	ARG
1	A	3714	SER
1	A	3731	LYS
1	A	3732	SER
1	A	3782	MET
1	A	3864	THR
1	A	3904	ARG
1	A	3930	ILE
1	A	3951	PHE
1	A	3987	ASP
1	A	4056	GLU

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Mol	Chain	Res	Type
1	A	4085	ARG
1	A	4089	SER
1	A	4165	GLU
1	A	4649	LEU
1	A	4672	LYS
1	A	4703	ARG
1	A	4741	LEU
1	A	4828	SER
1	A	4879	MET
1	A	4963	ILE
2	B	40	ARG
2	B	49	ARG
2	B	50	ILE
2	B	66	MET
2	B	74	LEU
2	B	103	LEU
2	B	106	LEU
3	C	4	GLN
3	C	6	THR
3	C	7	GLU
3	C	8	GLU
3	C	19	LEU
3	C	27	THR
3	C	31	LYS
3	C	45	THR
3	C	46	GLU
3	C	48	GLU
3	C	54	ASN
3	C	55	GLU
3	C	75	ARG
3	C	77	MET
3	C	88	GLU
3	C	91	ARG
3	C	106	LEU
3	C	109	VAL
3	C	122	VAL
3	C	125	MET
3	C	127	ARG
3	C	143	VAL
1	D	45	ARG
1	D	107	ILE
1	D	135	VAL

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Mol	Chain	Res	Type
1	D	171	LEU
1	D	175	SER
1	D	179	TYR
1	D	231	LEU
1	D	267	ILE
1	D	272	SER
1	D	347	PHE
1	D	441	VAL
1	D	474	ARG
1	D	519	VAL
1	D	525	LEU
1	D	531	ARG
1	D	539	LEU
1	D	933	LEU
1	D	935	LEU
1	D	988	LEU
1	D	1038	SER
1	D	1110	ARG
1	D	1160	ILE
1	D	1275	ARG
1	D	1427	ILE
1	D	1454	THR
1	D	1470	ARG
1	D	1584	ARG
1	D	1634	LEU
1	D	1715	LEU
1	D	1738	LEU
1	D	2113	SER
1	D	2206	THR
1	D	2209	GLU
1	D	2279	SER
1	D	2336	ARG
1	D	2355	ARG
1	D	2377	LEU
1	D	2439	GLU
1	D	2449	GLU
1	D	2512	ILE
1	D	2516	ASP
1	D	2524	VAL
1	D	2548	LEU
1	D	2577	ILE
1	D	2582	MET

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Mol	Chain	Res	Type
1	D	2622	LEU
1	D	3648	ARG
1	D	3714	SER
1	D	3731	LYS
1	D	3732	SER
1	D	3782	MET
1	D	3864	THR
1	D	3904	ARG
1	D	3930	ILE
1	D	3951	PHE
1	D	3987	ASP
1	D	4056	GLU
1	D	4085	ARG
1	D	4089	SER
1	D	4165	GLU
1	D	4649	LEU
1	D	4672	LYS
1	D	4703	ARG
1	D	4741	LEU
1	D	4828	SER
1	D	4879	MET
1	D	4963	ILE
2	E	40	ARG
2	E	49	ARG
2	E	50	ILE
2	E	66	MET
2	E	74	LEU
2	E	103	LEU
2	E	106	LEU
3	F	4	GLN
3	F	6	THR
3	F	7	GLU
3	F	8	GLU
3	F	19	LEU
3	F	27	THR
3	F	31	LYS
3	F	45	THR
3	F	46	GLU
3	F	48	GLU
3	F	50	GLN
3	F	55	GLU
3	F	75	ARG

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Mol	Chain	Res	Type
3	F	77	MET
3	F	88	GLU
3	F	91	ARG
3	F	106	LEU
3	F	109	VAL
3	F	122	VAL
3	F	125	MET
3	F	127	ARG
3	F	143	VAL
1	G	45	ARG
1	G	107	ILE
1	G	135	VAL
1	G	171	LEU
1	G	175	SER
1	G	179	TYR
1	G	231	LEU
1	G	267	ILE
1	G	272	SER
1	G	347	PHE
1	G	441	VAL
1	G	474	ARG
1	G	519	VAL
1	G	525	LEU
1	G	531	ARG
1	G	539	LEU
1	G	933	LEU
1	G	935	LEU
1	G	988	LEU
1	G	1038	SER
1	G	1110	ARG
1	G	1160	ILE
1	G	1275	ARG
1	G	1427	ILE
1	G	1454	THR
1	G	1470	ARG
1	G	1584	ARG
1	G	1634	LEU
1	G	1715	LEU
1	G	1738	LEU
1	G	2113	SER
1	G	2206	THR
1	G	2209	GLU

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Mol	Chain	Res	Type
1	G	2279	SER
1	G	2336	ARG
1	G	2355	ARG
1	G	2377	LEU
1	G	2439	GLU
1	G	2449	GLU
1	G	2512	ILE
1	G	2516	ASP
1	G	2524	VAL
1	G	2548	LEU
1	G	2577	ILE
1	G	2582	MET
1	G	2622	LEU
1	G	3648	ARG
1	G	3714	SER
1	G	3731	LYS
1	G	3732	SER
1	G	3782	MET
1	G	3864	THR
1	G	3904	ARG
1	G	3930	ILE
1	G	3951	PHE
1	G	3987	ASP
1	G	4056	GLU
1	G	4085	ARG
1	G	4089	SER
1	G	4165	GLU
1	G	4649	LEU
1	G	4672	LYS
1	G	4703	ARG
1	G	4741	LEU
1	G	4828	SER
1	G	4879	MET
1	G	4963	ILE
2	H	40	ARG
2	H	49	ARG
2	H	50	ILE
2	H	66	MET
2	H	74	LEU
2	H	103	LEU
2	H	106	LEU
3	I	4	GLN

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Mol	Chain	Res	Type
3	I	6	THR
3	I	7	GLU
3	I	8	GLU
3	I	19	LEU
3	I	27	THR
3	I	31	LYS
3	I	45	THR
3	I	46	GLU
3	I	48	GLU
3	I	50	GLN
3	I	54	ASN
3	I	55	GLU
3	I	75	ARG
3	I	77	MET
3	I	88	GLU
3	I	91	ARG
3	I	106	LEU
3	I	109	VAL
3	I	122	VAL
3	I	125	MET
3	I	127	ARG
3	I	143	VAL
1	J	45	ARG
1	J	107	ILE
1	J	135	VAL
1	J	171	LEU
1	J	175	SER
1	J	179	TYR
1	J	231	LEU
1	J	267	ILE
1	J	272	SER
1	J	347	PHE
1	J	441	VAL
1	J	474	ARG
1	J	519	VAL
1	J	525	LEU
1	J	531	ARG
1	J	539	LEU
1	J	933	LEU
1	J	935	LEU
1	J	988	LEU
1	J	1038	SER

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Mol	Chain	Res	Type
1	J	1110	ARG
1	J	1160	ILE
1	J	1275	ARG
1	J	1427	ILE
1	J	1454	THR
1	J	1470	ARG
1	J	1584	ARG
1	J	1634	LEU
1	J	1715	LEU
1	J	1738	LEU
1	J	2113	SER
1	J	2206	THR
1	J	2209	GLU
1	J	2279	SER
1	J	2336	ARG
1	J	2355	ARG
1	J	2377	LEU
1	J	2439	GLU
1	J	2449	GLU
1	J	2512	ILE
1	J	2516	ASP
1	J	2524	VAL
1	J	2548	LEU
1	J	2577	ILE
1	J	2582	MET
1	J	2622	LEU
1	J	3648	ARG
1	J	3714	SER
1	J	3731	LYS
1	J	3732	SER
1	J	3782	MET
1	J	3864	THR
1	J	3904	ARG
1	J	3930	ILE
1	J	3951	PHE
1	J	3987	ASP
1	J	4056	GLU
1	J	4085	ARG
1	J	4089	SER
1	J	4165	GLU
1	J	4649	LEU
1	J	4672	LYS

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Mol	Chain	Res	Type
1	J	4703	ARG
1	J	4741	LEU
1	J	4828	SER
1	J	4879	MET
1	J	4963	ILE
2	K	40	ARG
2	K	49	ARG
2	K	50	ILE
2	K	66	MET
2	K	74	LEU
2	K	103	LEU
2	K	106	LEU
3	L	4	GLN
3	L	6	THR
3	L	7	GLU
3	L	8	GLU
3	L	19	LEU
3	L	27	THR
3	L	31	LYS
3	L	45	THR
3	L	46	GLU
3	L	48	GLU
3	L	50	GLN
3	L	54	ASN
3	L	55	GLU
3	L	75	ARG
3	L	77	MET
3	L	88	GLU
3	L	91	ARG
3	L	106	LEU
3	L	109	VAL
3	L	122	VAL
3	L	125	MET
3	L	127	ARG
3	L	143	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	224	HIS
1	A	413	GLN
1	A	473	ASN
1	A	475	GLN
1	A	610	ASN
1	A	617	ASN
1	A	838	HIS
1	A	994	ASN
1	A	1041	GLN
1	A	1084	GLN
1	A	1203	ASN
1	A	1229	ASN
1	A	1281	ASN
1	A	1429	ASN
1	A	1560	ASN
1	A	1611	HIS
1	A	1660	GLN
1	A	1691	GLN
1	A	1861	GLN
1	A	1938	GLN
1	A	1949	GLN
1	A	1952	GLN
1	A	1953	HIS
1	A	2041	HIS
1	A	2107	GLN
1	A	2127	GLN
1	A	2213	ASN
1	A	2247	GLN
1	A	2283	ASN
1	A	2515	GLN
1	A	2520	HIS
1	A	2584	HIS
1	A	3627	GLN
1	A	3734	HIS
1	A	3767	GLN
1	A	3837	GLN
1	A	3851	ASN
1	A	3882	GLN
1	A	3897	ASN
1	A	3909	ASN
1	A	3946	GLN
1	A	3963	ASN

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Mol	Chain	Res	Type
1	A	3970	GLN
1	A	3976	ASN
1	A	3977	GLN
1	A	4020	GLN
1	A	4043	GLN
1	A	4162	ASN
1	A	4204	GLN
1	A	4216	GLN
1	A	4250	GLN
1	A	4574	ASN
1	A	4626	ASN
1	A	4947	GLN
2	B	20	GLN
2	B	43	ASN
2	B	53	GLN
2	B	94	ASN
3	C	9	GLN
1	D	23	GLN
1	D	57	ASN
1	D	71	GLN
1	D	224	HIS
1	D	394	GLN
1	D	473	ASN
1	D	475	GLN
1	D	593	HIS
1	D	617	ASN
1	D	838	HIS
1	D	994	ASN
1	D	1041	GLN
1	D	1084	GLN
1	D	1203	ASN
1	D	1229	ASN
1	D	1281	ASN
1	D	1299	GLN
1	D	1429	ASN
1	D	1560	ASN
1	D	1611	HIS
1	D	1660	GLN
1	D	1691	GLN
1	D	1861	GLN
1	D	1938	GLN
1	D	1952	GLN

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Mol	Chain	Res	Type
1	D	1953	HIS
1	D	2041	HIS
1	D	2107	GLN
1	D	2193	GLN
1	D	2213	ASN
1	D	2283	ASN
1	D	2515	GLN
1	D	2520	HIS
1	D	2584	HIS
1	D	3627	GLN
1	D	3734	HIS
1	D	3767	GLN
1	D	3837	GLN
1	D	3851	ASN
1	D	3882	GLN
1	D	3897	ASN
1	D	3909	ASN
1	D	3963	ASN
1	D	3970	GLN
1	D	3976	ASN
1	D	3977	GLN
1	D	3994	HIS
1	D	4020	GLN
1	D	4043	GLN
1	D	4162	ASN
1	D	4204	GLN
1	D	4216	GLN
1	D	4250	GLN
1	D	4626	ASN
1	D	4947	GLN
2	E	20	GLN
2	E	43	ASN
2	E	53	GLN
2	E	94	ASN
3	F	9	GLN
1	G	23	GLN
1	G	57	ASN
1	G	71	GLN
1	G	224	HIS
1	G	473	ASN
1	G	475	GLN
1	G	593	HIS

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Mol	Chain	Res	Type
1	G	838	HIS
1	G	866	HIS
1	G	1041	GLN
1	G	1158	ASN
1	G	1203	ASN
1	G	1229	ASN
1	G	1244	GLN
1	G	1281	ASN
1	G	1299	GLN
1	G	1429	ASN
1	G	1560	ASN
1	G	1611	HIS
1	G	1660	GLN
1	G	1691	GLN
1	G	1861	GLN
1	G	1938	GLN
1	G	1949	GLN
1	G	1952	GLN
1	G	1953	HIS
1	G	2041	HIS
1	G	2107	GLN
1	G	2127	GLN
1	G	2193	GLN
1	G	2213	ASN
1	G	2283	ASN
1	G	2515	GLN
1	G	2520	HIS
1	G	2584	HIS
1	G	3627	GLN
1	G	3734	HIS
1	G	3767	GLN
1	G	3837	GLN
1	G	3851	ASN
1	G	3882	GLN
1	G	3897	ASN
1	G	3909	ASN
1	G	3946	GLN
1	G	3963	ASN
1	G	3970	GLN
1	G	3976	ASN
1	G	3977	GLN
1	G	4020	GLN

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Mol	Chain	Res	Type
1	G	4043	GLN
1	G	4162	ASN
1	G	4204	GLN
1	G	4216	GLN
1	G	4250	GLN
1	G	4574	ASN
1	G	4626	ASN
1	G	4947	GLN
2	H	20	GLN
2	H	43	ASN
2	H	53	GLN
2	H	94	ASN
3	I	9	GLN
1	J	23	GLN
1	J	57	ASN
1	J	71	GLN
1	J	224	HIS
1	J	473	ASN
1	J	475	GLN
1	J	593	HIS
1	J	838	HIS
1	J	866	HIS
1	J	919	ASN
1	J	1041	GLN
1	J	1084	GLN
1	J	1158	ASN
1	J	1203	ASN
1	J	1229	ASN
1	J	1244	GLN
1	J	1281	ASN
1	J	1429	ASN
1	J	1560	ASN
1	J	1611	HIS
1	J	1660	GLN
1	J	1691	GLN
1	J	1861	GLN
1	J	1938	GLN
1	J	1949	GLN
1	J	1952	GLN
1	J	1953	HIS
1	J	2041	HIS
1	J	2107	GLN

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Mol	Chain	Res	Type
1	J	2193	GLN
1	J	2194	HIS
1	J	2213	ASN
1	J	2283	ASN
1	J	2515	GLN
1	J	2520	HIS
1	J	2584	HIS
1	J	3627	GLN
1	J	3734	HIS
1	J	3767	GLN
1	J	3837	GLN
1	J	3851	ASN
1	J	3882	GLN
1	J	3897	ASN
1	J	3909	ASN
1	J	3946	GLN
1	J	3963	ASN
1	J	3970	GLN
1	J	3976	ASN
1	J	3977	GLN
1	J	4020	GLN
1	J	4043	GLN
1	J	4162	ASN
1	J	4204	GLN
1	J	4216	GLN
1	J	4250	GLN
1	J	4574	ASN
1	J	4626	ASN
1	J	4947	GLN
2	K	20	GLN
2	K	43	ASN
2	K	53	GLN
2	K	94	ASN
3	L	9	GLN
3	L	50	GLN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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$
4	CFF	J	5101	-	15,15,15	4.85	10 (66%)	23,23,23	2.70	8 (34%)
6	ATP	A	5103	-	32,33,33	0.54	0	48,52,52	0.53	0
6	ATP	G	5103	-	32,33,33	0.54	0	48,52,52	0.53	0
6	ATP	D	5103	-	32,33,33	0.54	0	48,52,52	0.53	0
6	ATP	J	5103	-	32,33,33	0.54	0	48,52,52	0.53	0
8	F0U	A	5105	-	30,30,30	2.36	7 (23%)	43,43,43	2.63	13 (30%)
4	CFF	A	5101	-	15,15,15	4.85	10 (66%)	23,23,23	2.70	8 (34%)
8	F0U	D	5105	-	30,30,30	2.36	7 (23%)	43,43,43	2.63	13 (30%)
8	F0U	G	5105	-	30,30,30	2.36	7 (23%)	43,43,43	2.63	13 (30%)
8	F0U	J	5105	-	30,30,30	2.36	7 (23%)	43,43,43	2.63	13 (30%)
4	CFF	D	5101	-	15,15,15	4.85	10 (66%)	23,23,23	2.70	8 (34%)
4	CFF	G	5101	-	15,15,15	4.85	10 (66%)	23,23,23	2.70	8 (34%)

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	CFF	J	5101	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	5103	-	-	6/22/38/38	0/3/3/3
6	ATP	G	5103	-	-	6/22/38/38	0/3/3/3
6	ATP	D	5103	-	-	6/22/38/38	0/3/3/3
6	ATP	J	5103	-	-	6/22/38/38	0/3/3/3
8	F0U	A	5105	-	-	0/18/18/18	0/3/3/3
8	F0U	D	5105	-	-	0/18/18/18	0/3/3/3
4	CFF	A	5101	-	-	-	0/2/2/2
8	F0U	G	5105	-	-	0/18/18/18	0/3/3/3
8	F0U	J	5105	-	-	0/18/18/18	0/3/3/3
4	CFF	D	5101	-	-	-	0/2/2/2
4	CFF	G	5101	-	-	-	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5101	CFF	O11-C2	9.39	1.40	1.22
4	D	5101	CFF	O11-C2	9.39	1.40	1.22
4	G	5101	CFF	O11-C2	9.39	1.40	1.22
4	J	5101	CFF	O11-C2	9.39	1.40	1.22
4	A	5101	CFF	O13-C6	8.62	1.40	1.23
4	D	5101	CFF	O13-C6	8.62	1.40	1.23
4	G	5101	CFF	O13-C6	8.62	1.40	1.23
4	J	5101	CFF	O13-C6	8.62	1.40	1.23
4	A	5101	CFF	C4-N9	7.89	1.52	1.36
4	D	5101	CFF	C4-N9	7.89	1.52	1.36
4	G	5101	CFF	C4-N9	7.89	1.52	1.36
4	J	5101	CFF	C4-N9	7.89	1.52	1.36
8	A	5105	F0U	CAO-CAN	-7.06	1.35	1.49
8	D	5105	F0U	CAO-CAN	-7.06	1.35	1.49
8	G	5105	F0U	CAO-CAN	-7.06	1.35	1.49
8	J	5105	F0U	CAO-CAN	-7.06	1.35	1.49
4	A	5101	CFF	C2-N3	5.33	1.49	1.39
4	D	5101	CFF	C2-N3	5.33	1.49	1.39
4	G	5101	CFF	C2-N3	5.33	1.49	1.39
4	J	5101	CFF	C2-N3	5.33	1.49	1.39
4	A	5101	CFF	C2-N1	5.27	1.49	1.39
4	D	5101	CFF	C2-N1	5.27	1.49	1.39
4	G	5101	CFF	C2-N1	5.27	1.49	1.39
4	J	5101	CFF	C2-N1	5.27	1.49	1.39
8	A	5105	F0U	CAG-CAH	-5.08	1.40	1.50
8	D	5105	F0U	CAG-CAH	-5.08	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	5105	F0U	CAG-CAH	-5.08	1.40	1.50
8	J	5105	F0U	CAG-CAH	-5.08	1.40	1.50
8	A	5105	F0U	CAP-CAQ	-4.92	1.33	1.39
8	D	5105	F0U	CAP-CAQ	-4.92	1.33	1.39
8	G	5105	F0U	CAP-CAQ	-4.92	1.33	1.39
8	J	5105	F0U	CAP-CAQ	-4.92	1.33	1.39
8	A	5105	F0U	CAL-NAM	-4.89	1.34	1.43
8	D	5105	F0U	CAL-NAM	-4.89	1.34	1.43
8	G	5105	F0U	CAL-NAM	-4.89	1.34	1.43
8	J	5105	F0U	CAL-NAM	-4.89	1.34	1.43
4	A	5101	CFF	C5-N7	-4.85	1.29	1.38
4	D	5101	CFF	C5-N7	-4.85	1.29	1.38
4	G	5101	CFF	C5-N7	-4.85	1.29	1.38
4	J	5101	CFF	C5-N7	-4.85	1.29	1.38
4	A	5101	CFF	C4-N3	4.70	1.45	1.38
4	D	5101	CFF	C4-N3	4.70	1.45	1.38
4	G	5101	CFF	C4-N3	4.70	1.45	1.38
4	J	5101	CFF	C4-N3	4.70	1.45	1.38
8	A	5105	F0U	CAU-NAT	-3.43	1.33	1.42
8	D	5105	F0U	CAU-NAT	-3.43	1.33	1.42
8	G	5105	F0U	CAU-NAT	-3.43	1.33	1.42
8	J	5105	F0U	CAU-NAT	-3.43	1.33	1.42
4	A	5101	CFF	C8-N7	-2.89	1.28	1.35
4	D	5101	CFF	C8-N7	-2.89	1.28	1.35
4	G	5101	CFF	C8-N7	-2.89	1.28	1.35
4	J	5101	CFF	C8-N7	-2.89	1.28	1.35
8	A	5105	F0U	CAZ-NBA	2.88	1.40	1.34
8	D	5105	F0U	CAZ-NBA	2.88	1.40	1.34
8	G	5105	F0U	CAZ-NBA	2.88	1.40	1.34
8	J	5105	F0U	CAZ-NBA	2.88	1.40	1.34
4	A	5101	CFF	C5-C6	2.77	1.50	1.43
4	D	5101	CFF	C5-C6	2.77	1.50	1.43
4	G	5101	CFF	C5-C6	2.77	1.50	1.43
4	J	5101	CFF	C5-C6	2.77	1.50	1.43
8	A	5105	F0U	CAP-CAO	-2.28	1.33	1.39
8	D	5105	F0U	CAP-CAO	-2.28	1.33	1.39
8	G	5105	F0U	CAP-CAO	-2.28	1.33	1.39
8	J	5105	F0U	CAP-CAO	-2.28	1.33	1.39
4	A	5101	CFF	C6-N1	2.24	1.45	1.40
4	D	5101	CFF	C6-N1	2.24	1.45	1.40
4	G	5101	CFF	C6-N1	2.24	1.45	1.40
4	J	5101	CFF	C6-N1	2.24	1.45	1.40

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5101	CFF	C8-N7-C5	7.60	119.86	105.59
4	D	5101	CFF	C8-N7-C5	7.60	119.86	105.59
4	G	5101	CFF	C8-N7-C5	7.60	119.86	105.59
4	J	5101	CFF	C8-N7-C5	7.60	119.86	105.59
8	A	5105	F0U	CAN-CAO-NAT	7.02	129.81	121.32
8	D	5105	F0U	CAN-CAO-NAT	7.02	129.81	121.32
8	G	5105	F0U	CAN-CAO-NAT	7.02	129.81	121.32
8	J	5105	F0U	CAN-CAO-NAT	7.02	129.81	121.32
8	A	5105	F0U	CAQ-NAS-NAT	6.58	107.49	103.09
8	D	5105	F0U	CAQ-NAS-NAT	6.58	107.49	103.09
8	G	5105	F0U	CAQ-NAS-NAT	6.58	107.49	103.09
8	J	5105	F0U	CAQ-NAS-NAT	6.58	107.49	103.09
8	A	5105	F0U	BR-CAQ-NAS	6.33	124.61	119.12
8	D	5105	F0U	BR-CAQ-NAS	6.33	124.61	119.12
8	G	5105	F0U	BR-CAQ-NAS	6.33	124.61	119.12
8	J	5105	F0U	BR-CAQ-NAS	6.33	124.61	119.12
8	A	5105	F0U	CAO-NAT-NAS	-5.63	106.77	111.97
8	D	5105	F0U	CAO-NAT-NAS	-5.63	106.77	111.97
8	G	5105	F0U	CAO-NAT-NAS	-5.63	106.77	111.97
8	J	5105	F0U	CAO-NAT-NAS	-5.63	106.77	111.97
8	A	5105	F0U	CAP-CAQ-NAS	-5.61	110.10	113.98
8	D	5105	F0U	CAP-CAQ-NAS	-5.61	110.10	113.98
8	G	5105	F0U	CAP-CAQ-NAS	-5.61	110.10	113.98
8	J	5105	F0U	CAP-CAQ-NAS	-5.61	110.10	113.98
4	A	5101	CFF	C14-N7-C8	-4.79	117.31	126.28
4	D	5101	CFF	C14-N7-C8	-4.79	117.31	126.28
4	G	5101	CFF	C14-N7-C8	-4.79	117.31	126.28
4	J	5101	CFF	C14-N7-C8	-4.79	117.31	126.28
4	A	5101	CFF	C5-C6-N1	3.99	119.36	112.06
4	D	5101	CFF	C5-C6-N1	3.99	119.36	112.06
4	G	5101	CFF	C5-C6-N1	3.99	119.36	112.06
4	J	5101	CFF	C5-C6-N1	3.99	119.36	112.06
4	A	5101	CFF	C6-C5-N7	3.71	138.55	131.10
4	D	5101	CFF	C6-C5-N7	3.71	138.55	131.10
4	G	5101	CFF	C6-C5-N7	3.71	138.55	131.10
4	J	5101	CFF	C6-C5-N7	3.71	138.55	131.10
4	A	5101	CFF	C6-N1-C2	-3.63	119.76	125.66
4	D	5101	CFF	C6-N1-C2	-3.63	119.76	125.66
4	G	5101	CFF	C6-N1-C2	-3.63	119.76	125.66
4	J	5101	CFF	C6-N1-C2	-3.63	119.76	125.66
8	A	5105	F0U	CAO-CAP-CAQ	3.47	106.47	103.95
8	D	5105	F0U	CAO-CAP-CAQ	3.47	106.47	103.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	5105	F0U	CAO-CAP-CAQ	3.47	106.47	103.95
8	J	5105	F0U	CAO-CAP-CAQ	3.47	106.47	103.95
8	A	5105	F0U	CAP-CAO-CAN	-3.33	121.01	129.54
8	D	5105	F0U	CAP-CAO-CAN	-3.33	121.01	129.54
8	G	5105	F0U	CAP-CAO-CAN	-3.33	121.01	129.54
8	J	5105	F0U	CAP-CAO-CAN	-3.33	121.01	129.54
8	A	5105	F0U	CAU-NAT-NAS	3.14	121.75	118.52
8	D	5105	F0U	CAU-NAT-NAS	3.14	121.75	118.52
8	G	5105	F0U	CAU-NAT-NAS	3.14	121.75	118.52
8	J	5105	F0U	CAU-NAT-NAS	3.14	121.75	118.52
4	A	5101	CFF	C4-C5-N7	-3.01	100.50	105.88
4	D	5101	CFF	C4-C5-N7	-3.01	100.50	105.88
4	G	5101	CFF	C4-C5-N7	-3.01	100.50	105.88
4	J	5101	CFF	C4-C5-N7	-3.01	100.50	105.88
8	A	5105	F0U	CAP-CAO-NAT	2.95	109.17	106.42
8	D	5105	F0U	CAP-CAO-NAT	2.95	109.17	106.42
8	G	5105	F0U	CAP-CAO-NAT	2.95	109.17	106.42
8	J	5105	F0U	CAP-CAO-NAT	2.95	109.17	106.42
8	A	5105	F0U	CAJ-NAI-CAH	-2.65	116.75	121.80
8	D	5105	F0U	CAJ-NAI-CAH	-2.65	116.75	121.80
8	G	5105	F0U	CAJ-NAI-CAH	-2.65	116.75	121.80
8	J	5105	F0U	CAJ-NAI-CAH	-2.65	116.75	121.80
8	A	5105	F0U	CAL-CAG-CAH	2.54	123.42	120.85
8	D	5105	F0U	CAL-CAG-CAH	2.54	123.42	120.85
8	G	5105	F0U	CAL-CAG-CAH	2.54	123.42	120.85
8	J	5105	F0U	CAL-CAG-CAH	2.54	123.42	120.85
8	A	5105	F0U	CAZ-NBA-CAU	2.43	120.54	115.05
8	D	5105	F0U	CAZ-NBA-CAU	2.43	120.54	115.05
8	G	5105	F0U	CAZ-NBA-CAU	2.43	120.54	115.05
8	J	5105	F0U	CAZ-NBA-CAU	2.43	120.54	115.05
8	A	5105	F0U	CAY-CAZ-NBA	-2.19	119.95	123.42
8	D	5105	F0U	CAY-CAZ-NBA	-2.19	119.95	123.42
8	G	5105	F0U	CAY-CAZ-NBA	-2.19	119.95	123.42
8	J	5105	F0U	CAY-CAZ-NBA	-2.19	119.95	123.42
4	A	5101	CFF	N3-C4-N9	2.12	129.61	126.27
4	D	5101	CFF	N3-C4-N9	2.12	129.61	126.27
4	G	5101	CFF	N3-C4-N9	2.12	129.61	126.27
4	J	5101	CFF	N3-C4-N9	2.12	129.61	126.27
4	A	5101	CFF	C14-N7-C5	-2.08	122.83	127.77
4	D	5101	CFF	C14-N7-C5	-2.08	122.83	127.77
4	G	5101	CFF	C14-N7-C5	-2.08	122.83	127.77
4	J	5101	CFF	C14-N7-C5	-2.08	122.83	127.77

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	PB-O3B-PG-O2G
6	A	5103	ATP	PB-O3A-PA-O5'
6	A	5103	ATP	C5'-O5'-PA-O2A
6	A	5103	ATP	C5'-O5'-PA-O3A
6	D	5103	ATP	PB-O3B-PG-O2G
6	D	5103	ATP	PB-O3A-PA-O5'
6	D	5103	ATP	C5'-O5'-PA-O2A
6	D	5103	ATP	C5'-O5'-PA-O3A
6	G	5103	ATP	PB-O3B-PG-O2G
6	G	5103	ATP	PB-O3A-PA-O5'
6	G	5103	ATP	C5'-O5'-PA-O2A
6	G	5103	ATP	C5'-O5'-PA-O3A
6	J	5103	ATP	PB-O3B-PG-O2G
6	J	5103	ATP	PB-O3A-PA-O5'
6	J	5103	ATP	C5'-O5'-PA-O2A
6	J	5103	ATP	C5'-O5'-PA-O3A
6	A	5103	ATP	PB-O3B-PG-O1G
6	D	5103	ATP	PB-O3B-PG-O1G
6	G	5103	ATP	PB-O3B-PG-O1G
6	J	5103	ATP	PB-O3B-PG-O1G
6	A	5103	ATP	PB-O3B-PG-O3G
6	D	5103	ATP	PB-O3B-PG-O3G
6	G	5103	ATP	PB-O3B-PG-O3G
6	J	5103	ATP	PB-O3B-PG-O3G

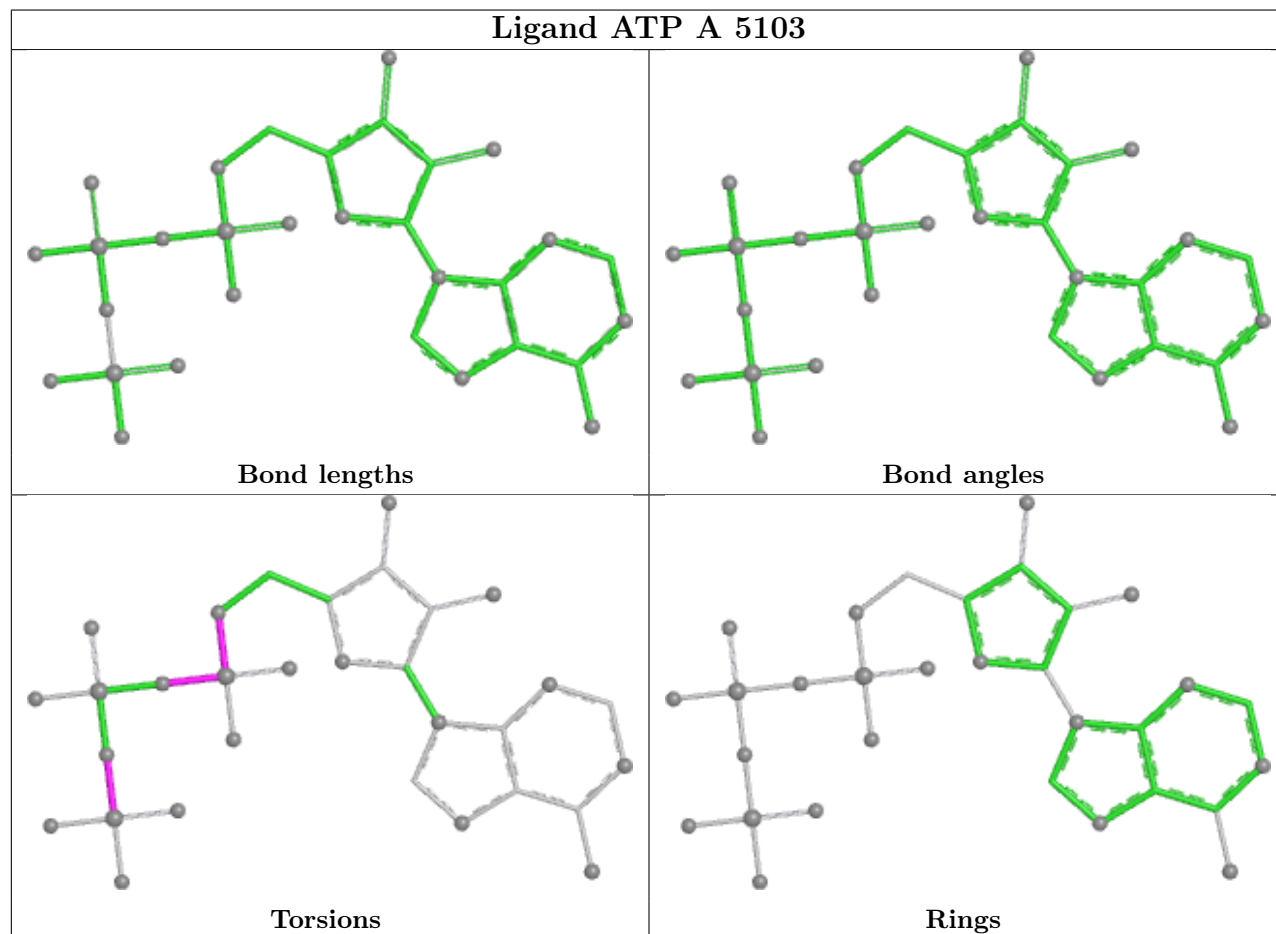
There are no ring outliers.

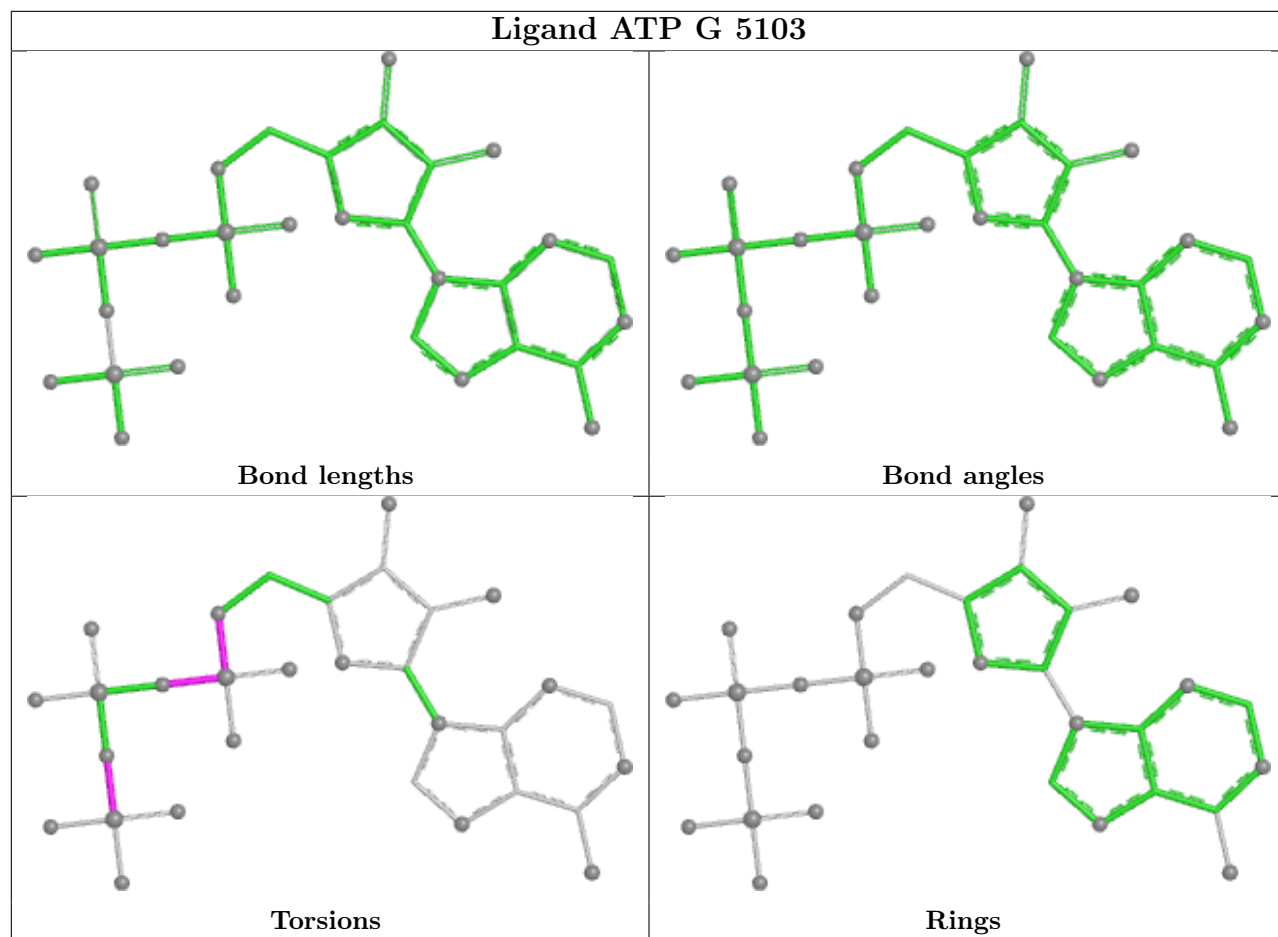
8 monomers are involved in 44 short contacts:

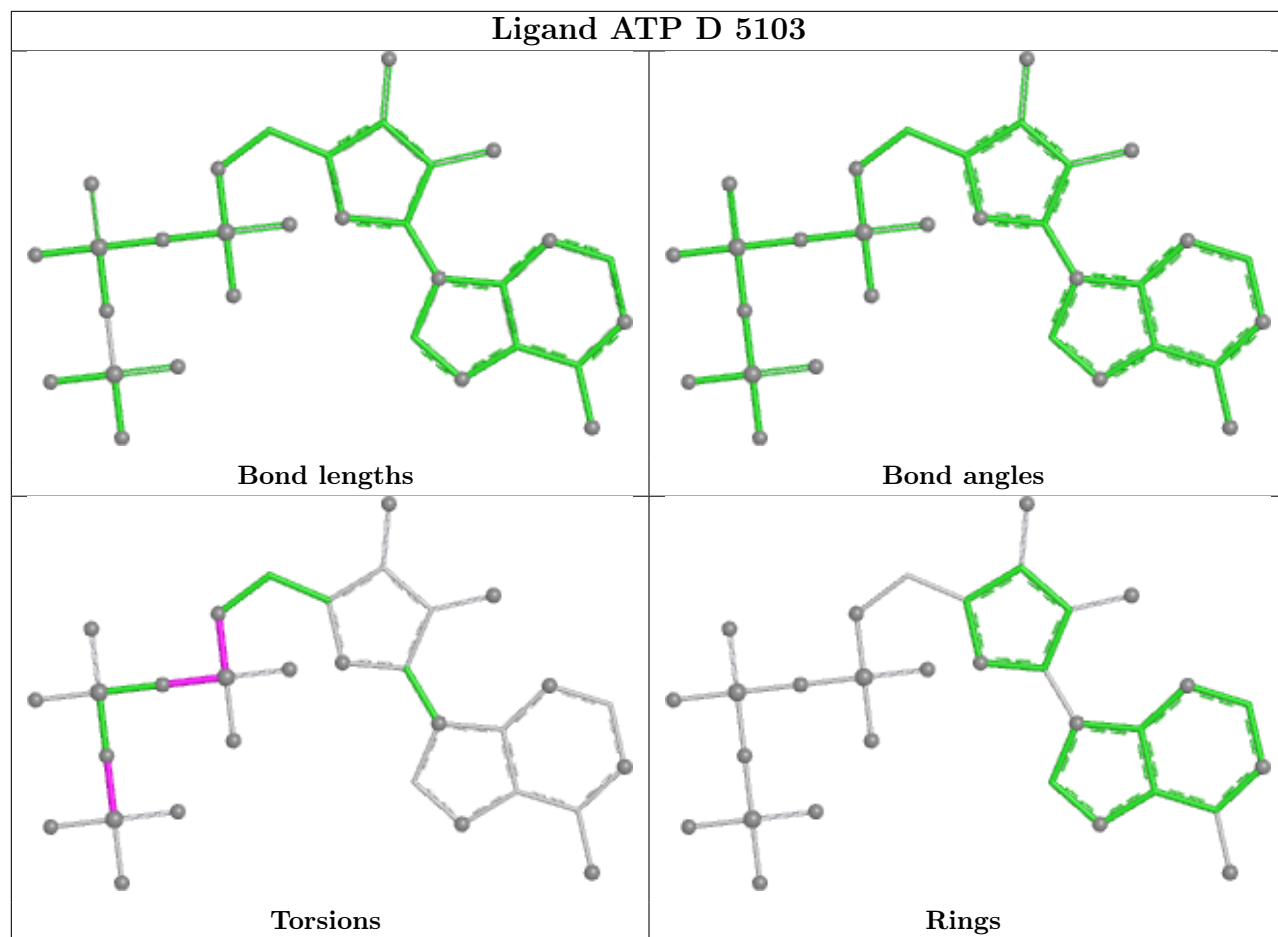
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5103	ATP	8	0
6	G	5103	ATP	9	0
6	D	5103	ATP	10	0
6	J	5103	ATP	9	0
8	A	5105	F0U	2	0
8	D	5105	F0U	2	0
8	G	5105	F0U	2	0
8	J	5105	F0U	2	0

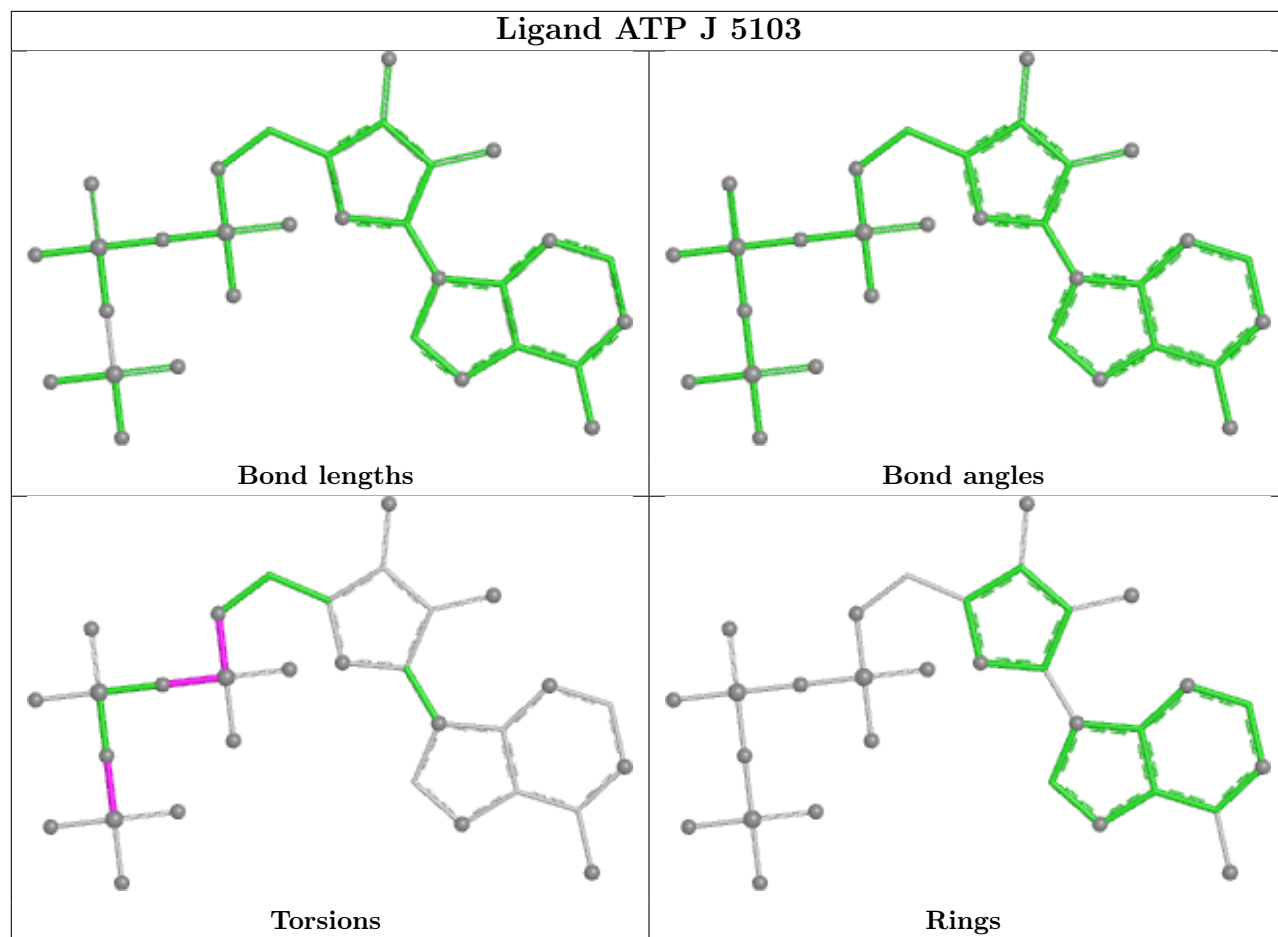
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

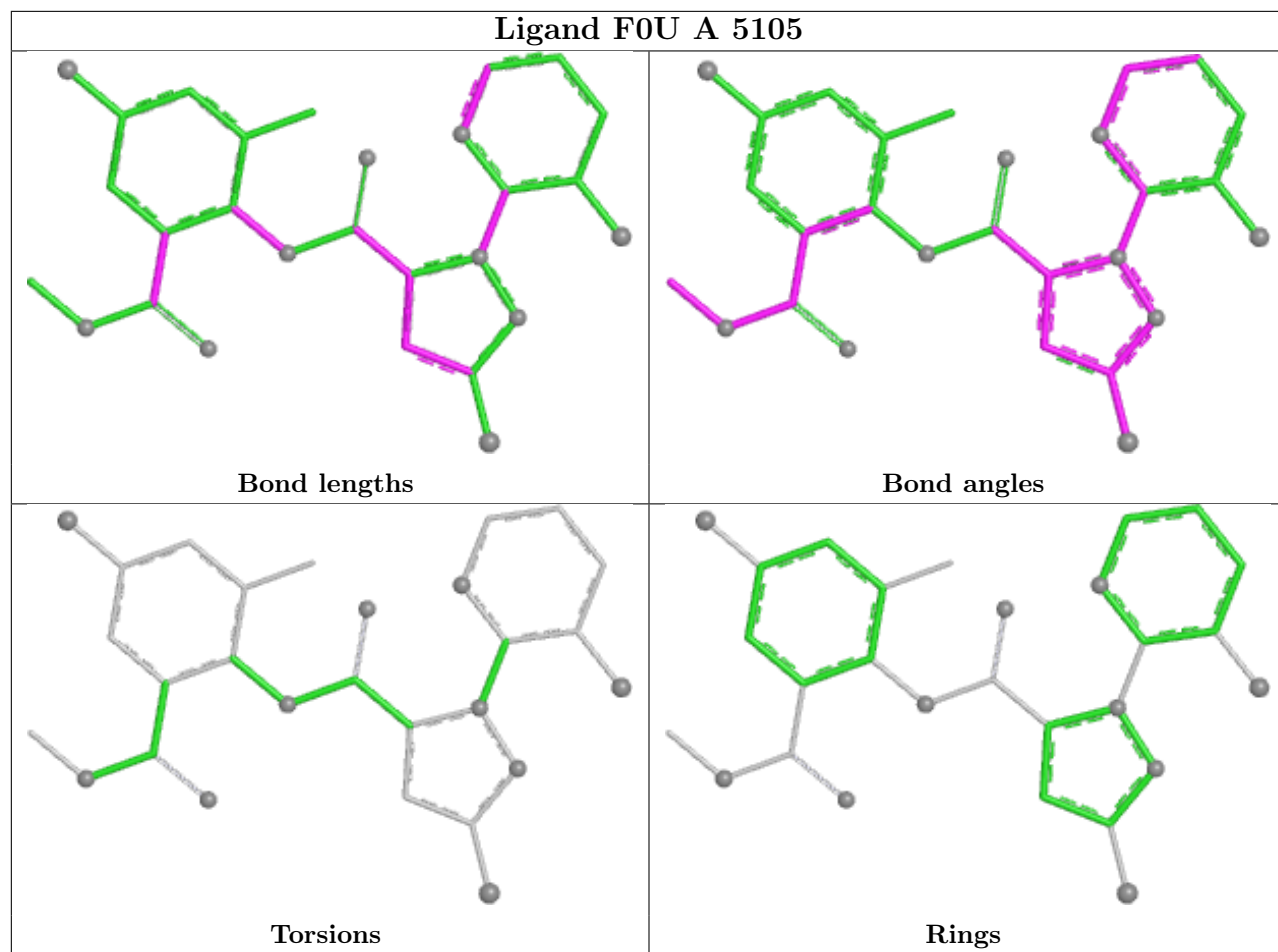
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

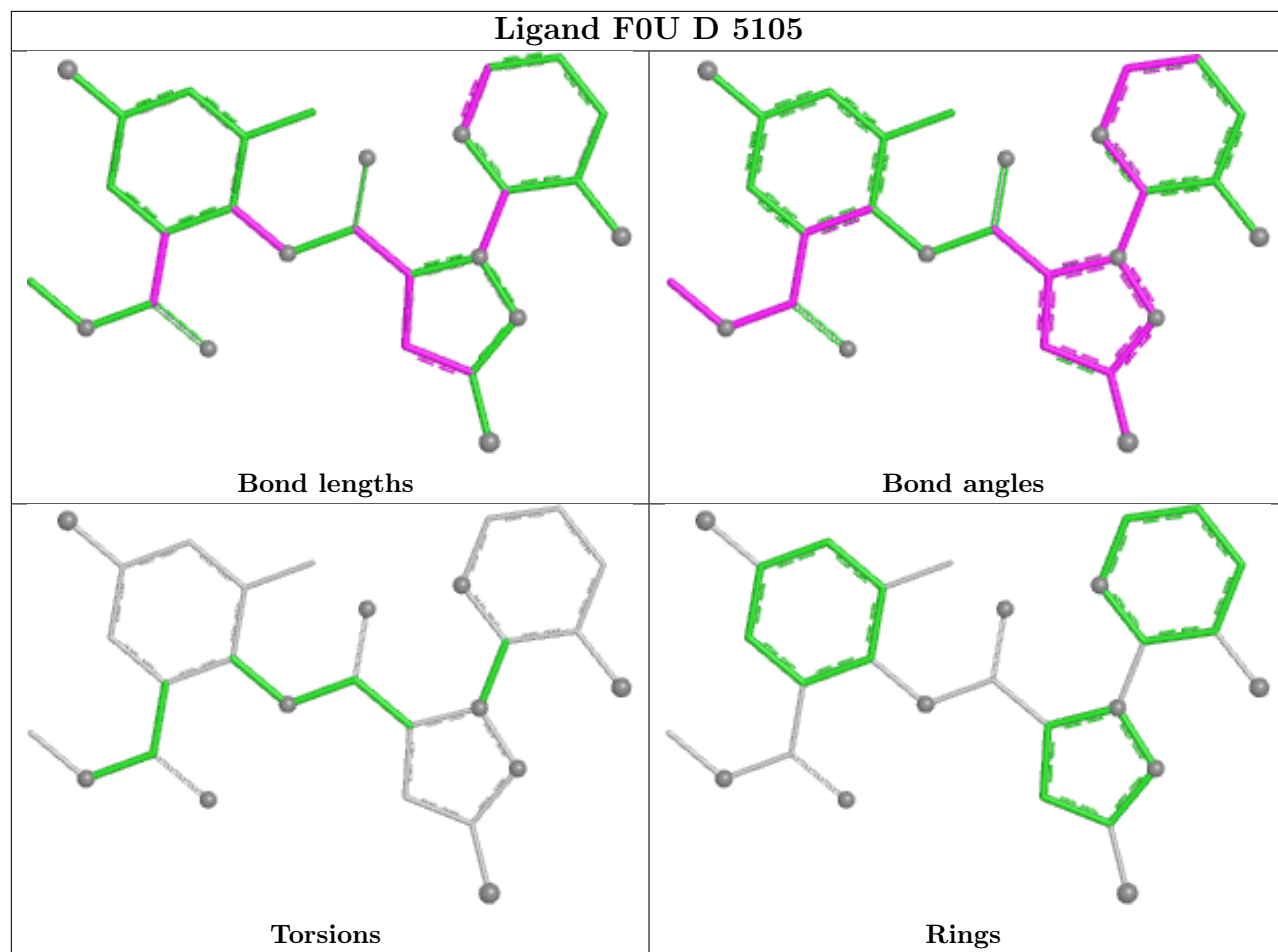


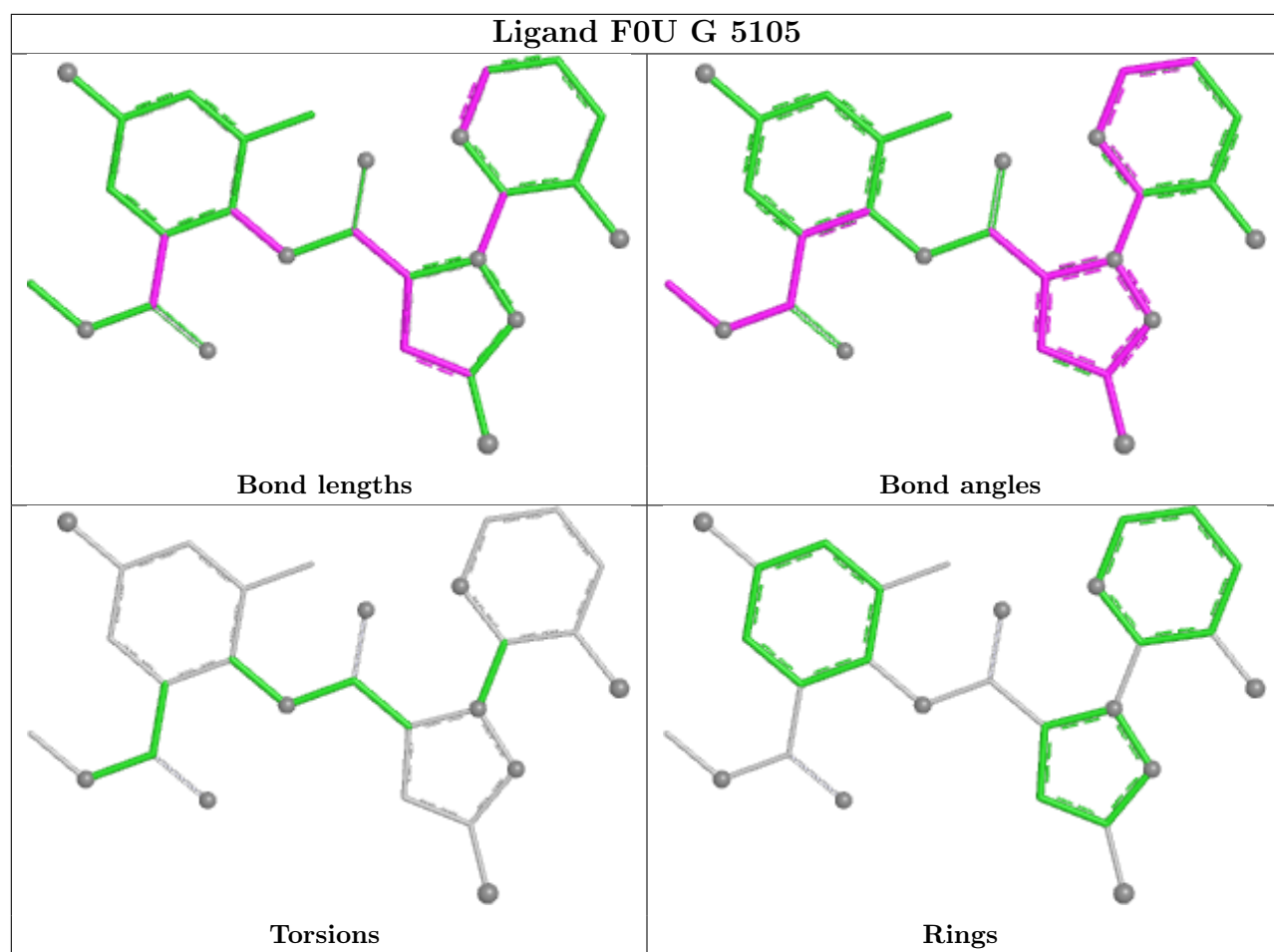


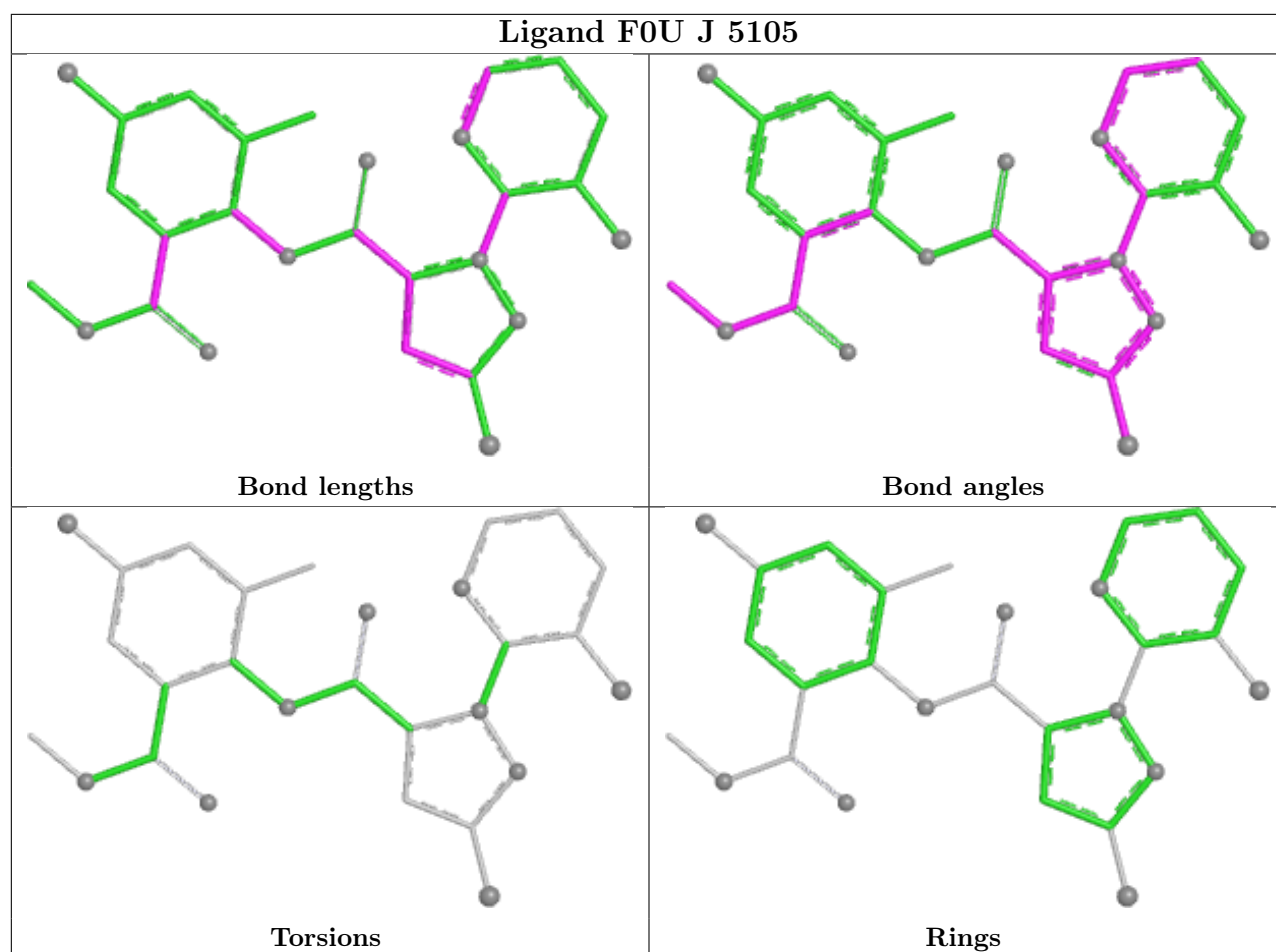












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

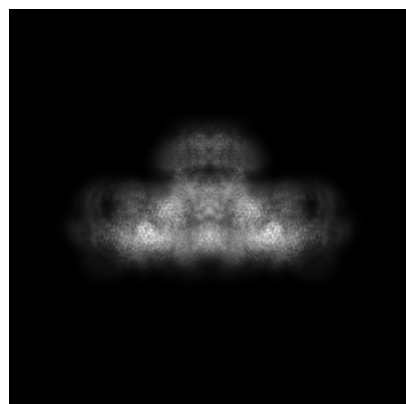
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30067. These allow visual inspection of the internal detail of the map and identification of artifacts.

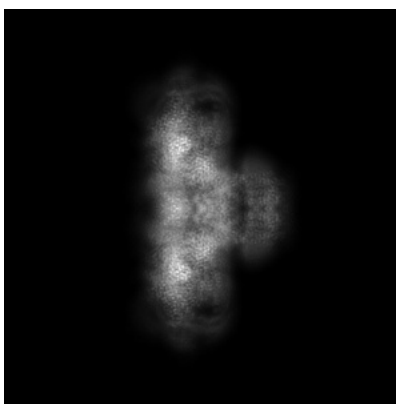
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

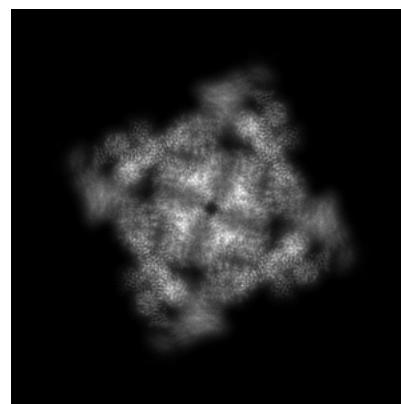
6.1.1 Primary map



X

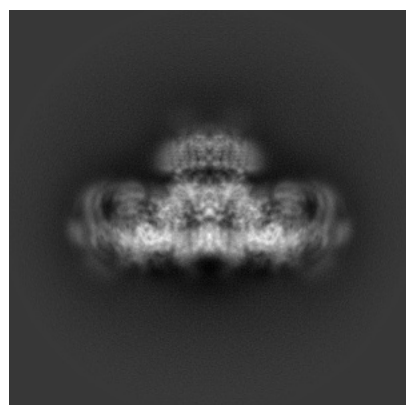


Y

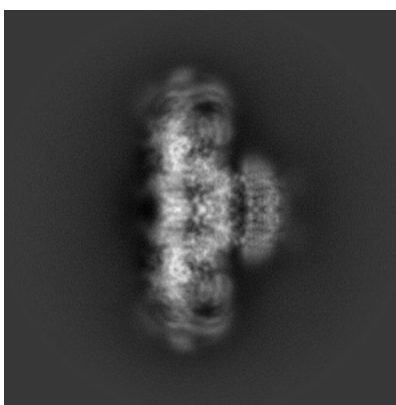


Z

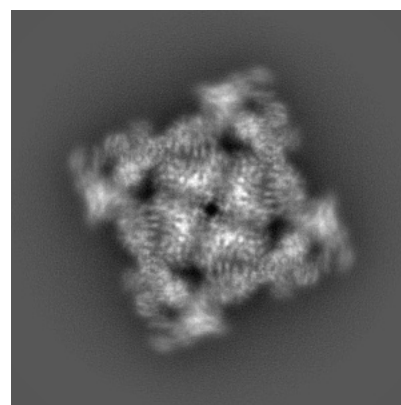
6.1.2 Raw map



X



Y

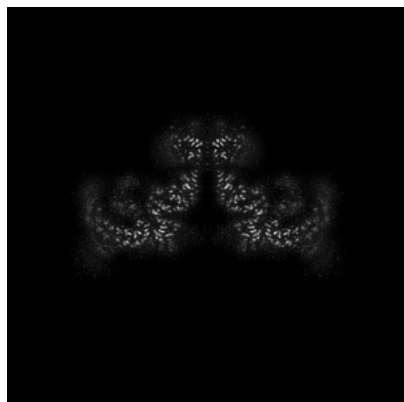


Z

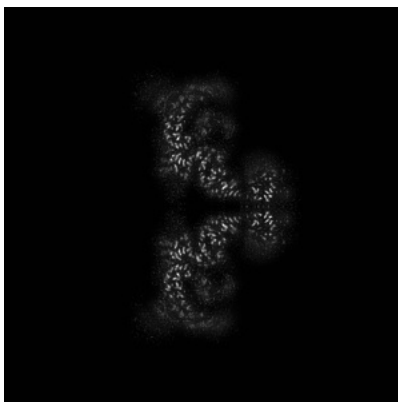
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

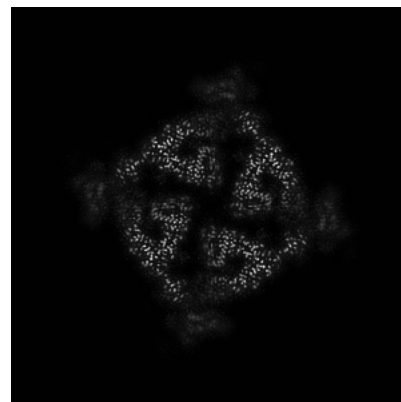
6.2.1 Primary map



X Index: 224

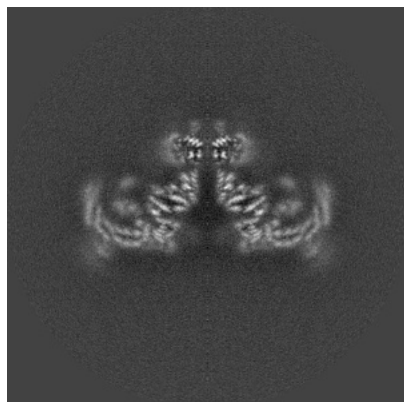


Y Index: 224

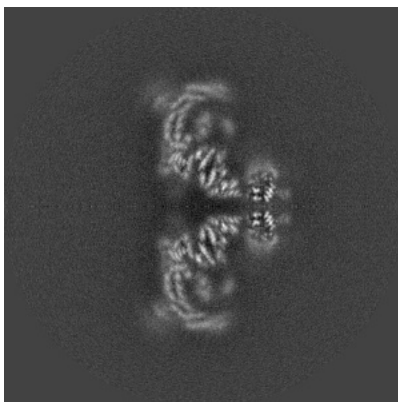


Z Index: 224

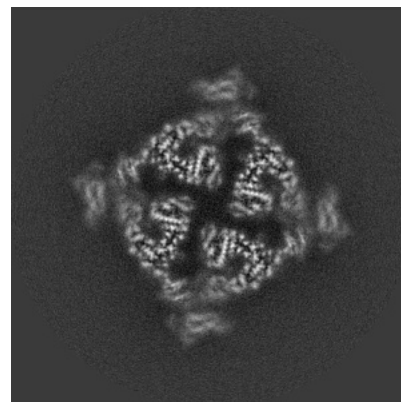
6.2.2 Raw map



X Index: 224



Y Index: 224

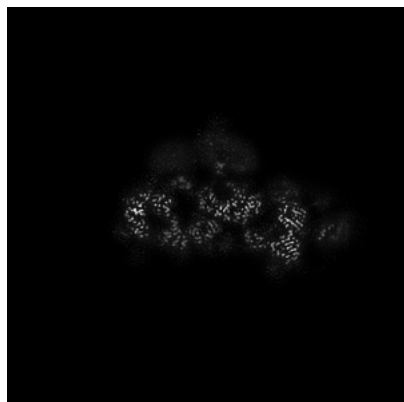


Z Index: 224

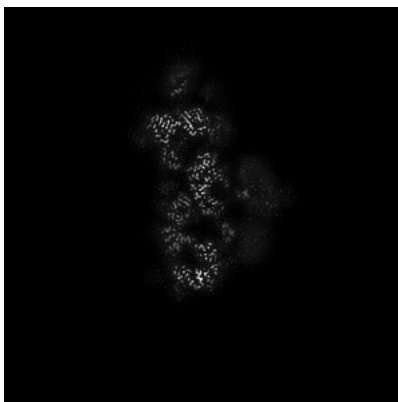
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

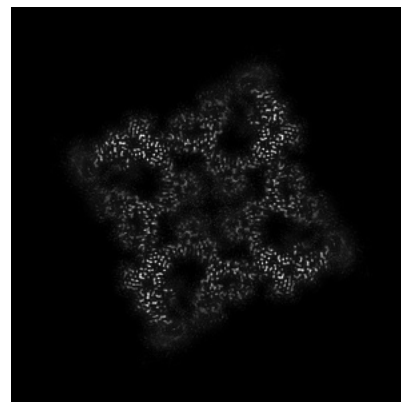
6.3.1 Primary map



X Index: 269

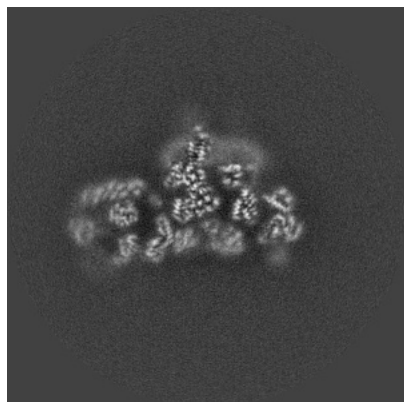


Y Index: 179

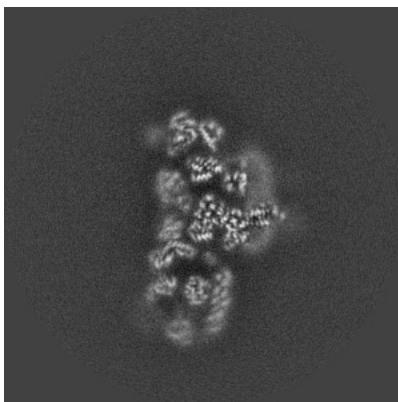


Z Index: 194

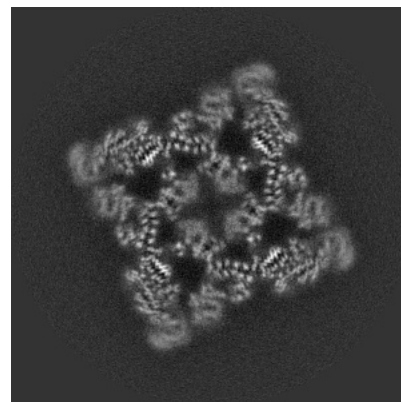
6.3.2 Raw map



X Index: 190



Y Index: 258

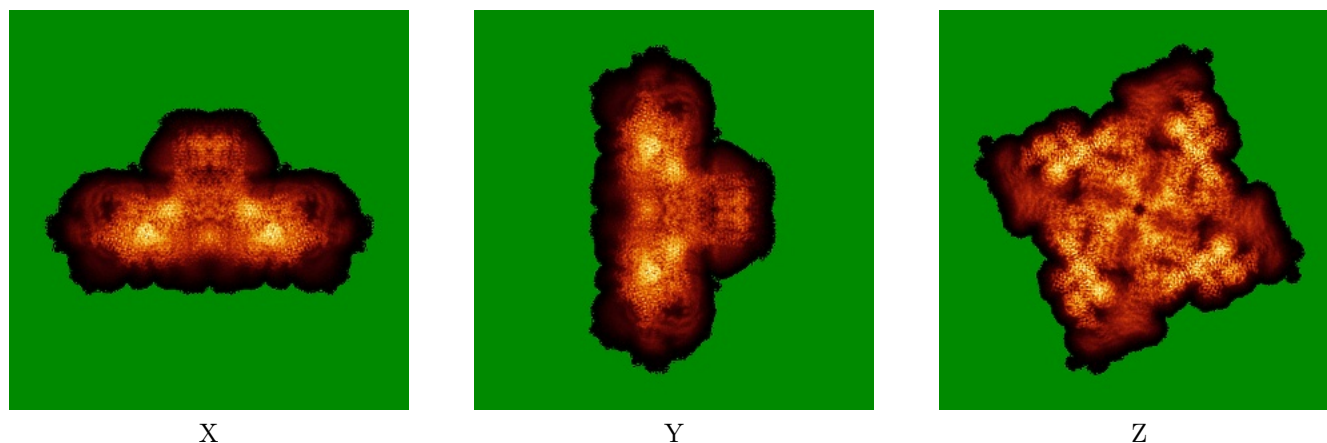


Z Index: 198

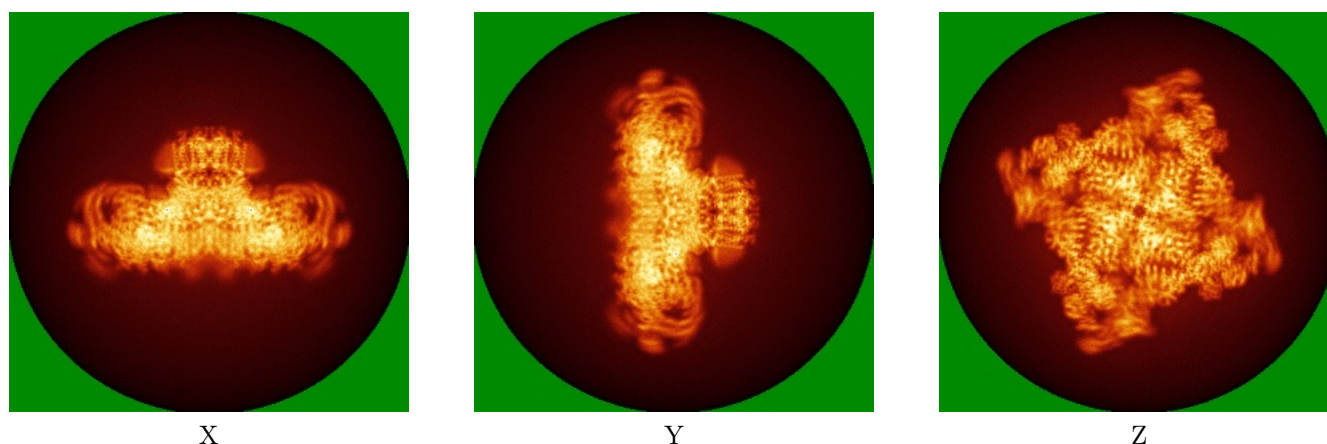
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

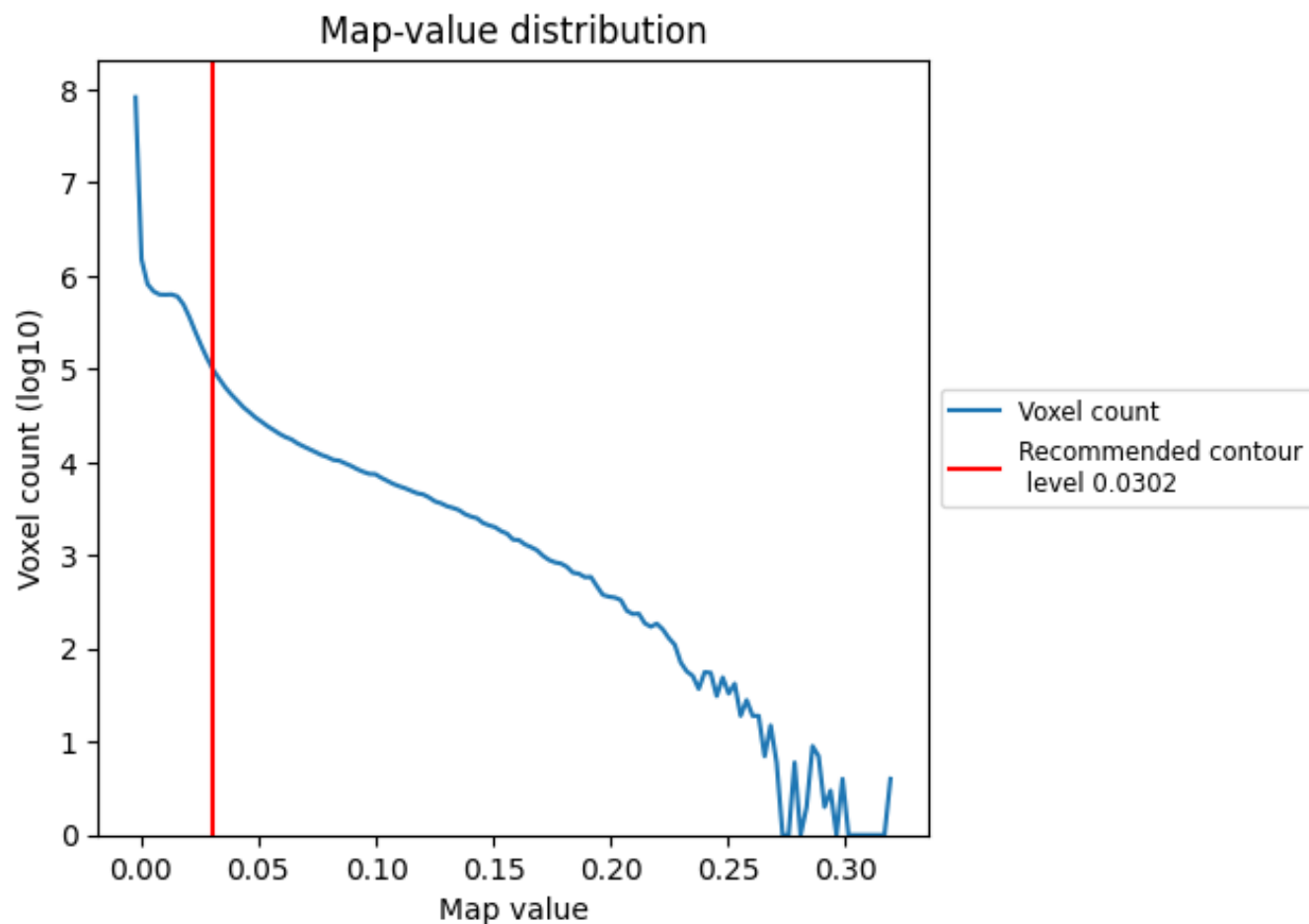
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

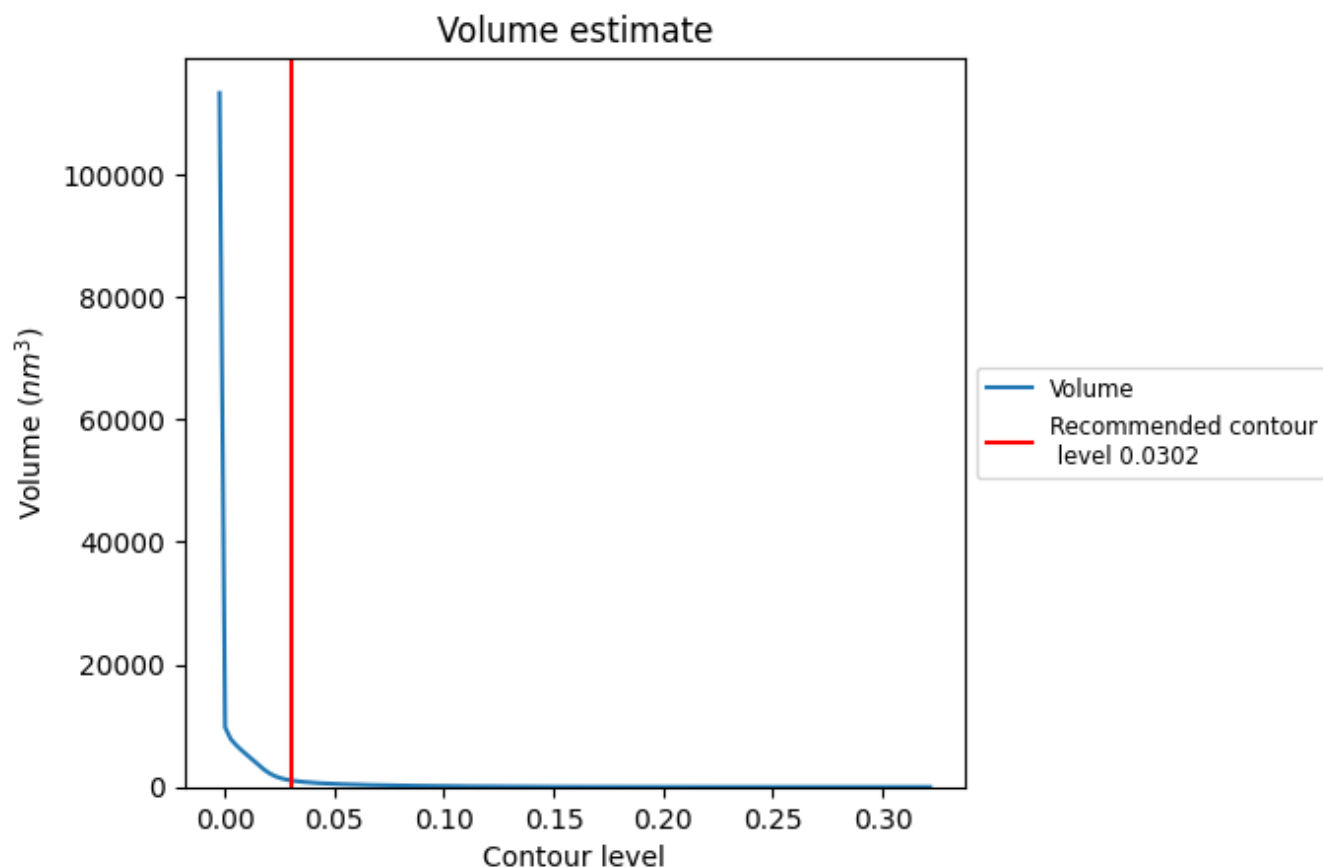
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

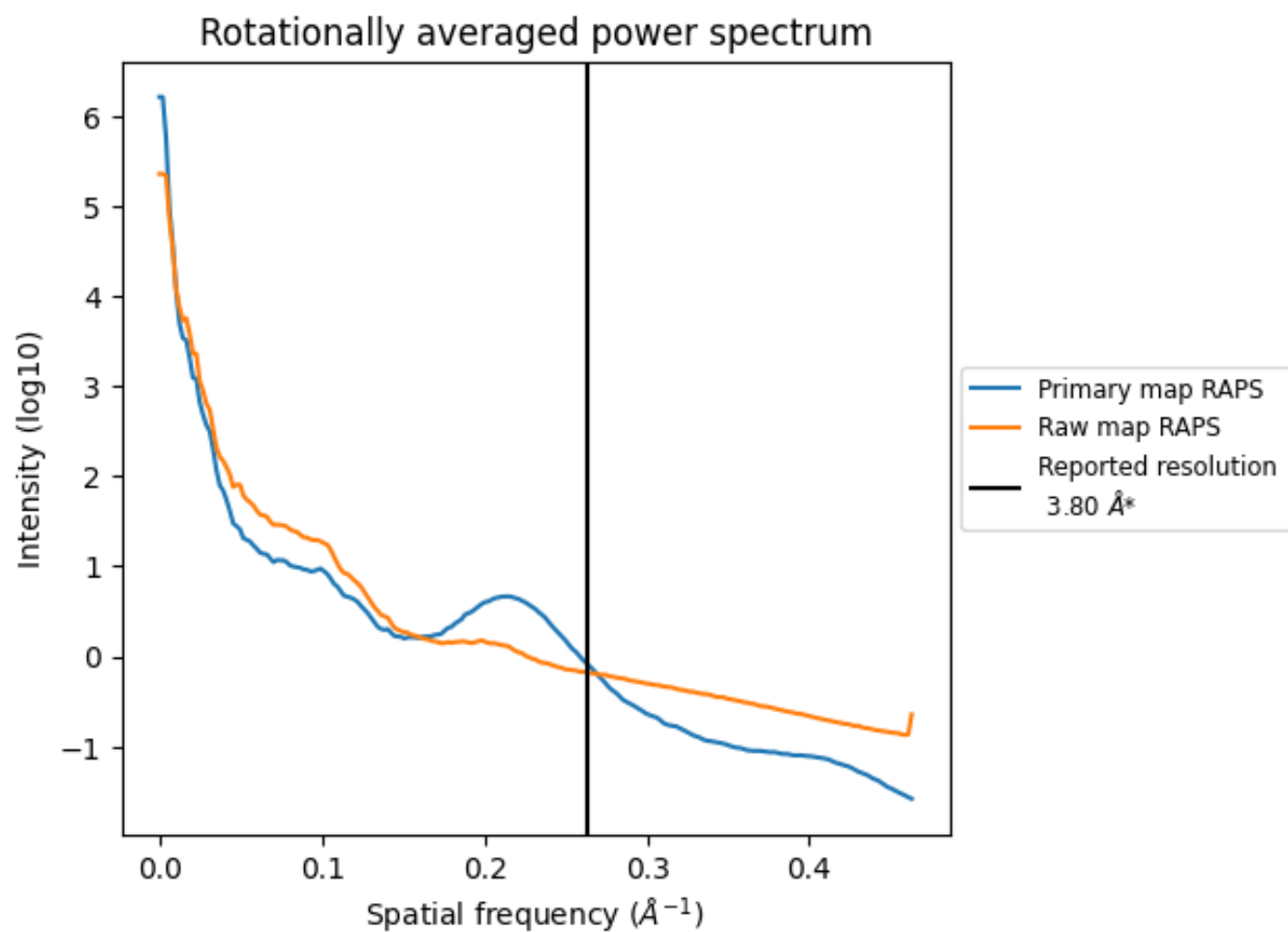
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1077 nm^3 ; this corresponds to an approximate mass of 973 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 ⓘ

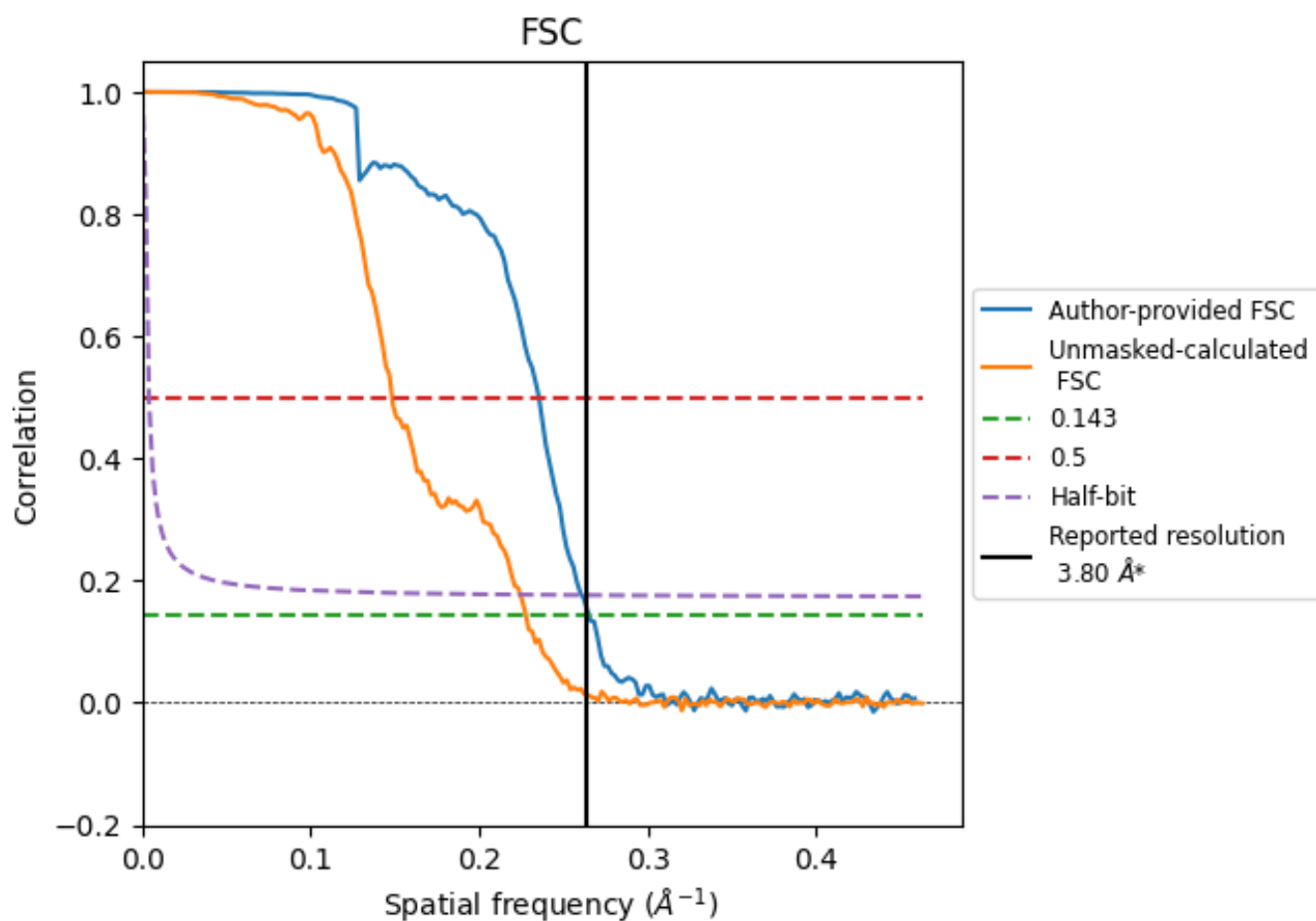


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

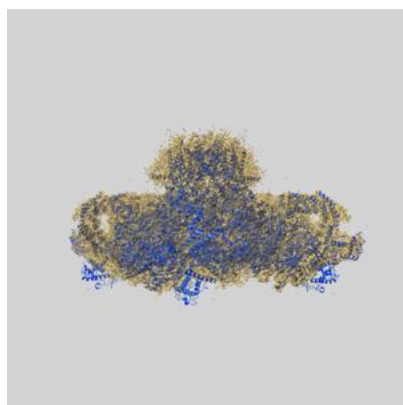
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.25	3.83
Unmasked-calculated*	4.39	6.74	4.45

*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 4.39 differs from the reported value 3.8 by more than 10 %

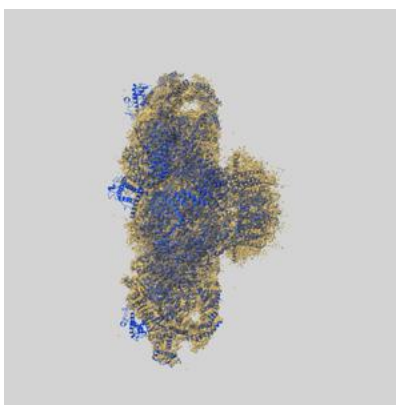
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30067 and PDB model 6M2W. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

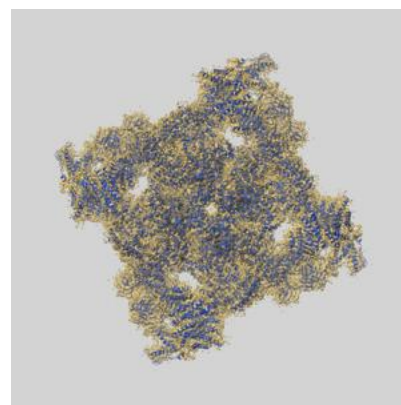
9.1 Map-model overlay [i](#)



X



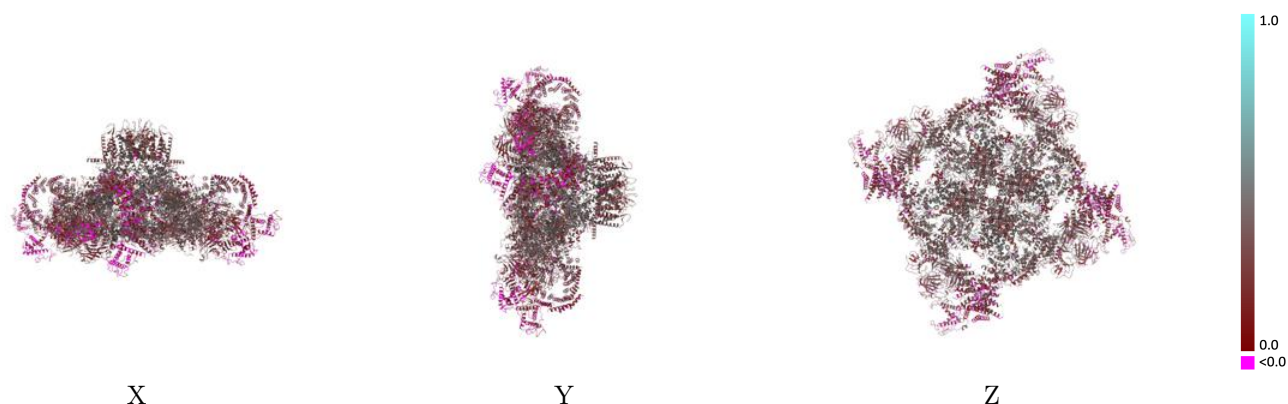
Y



Z

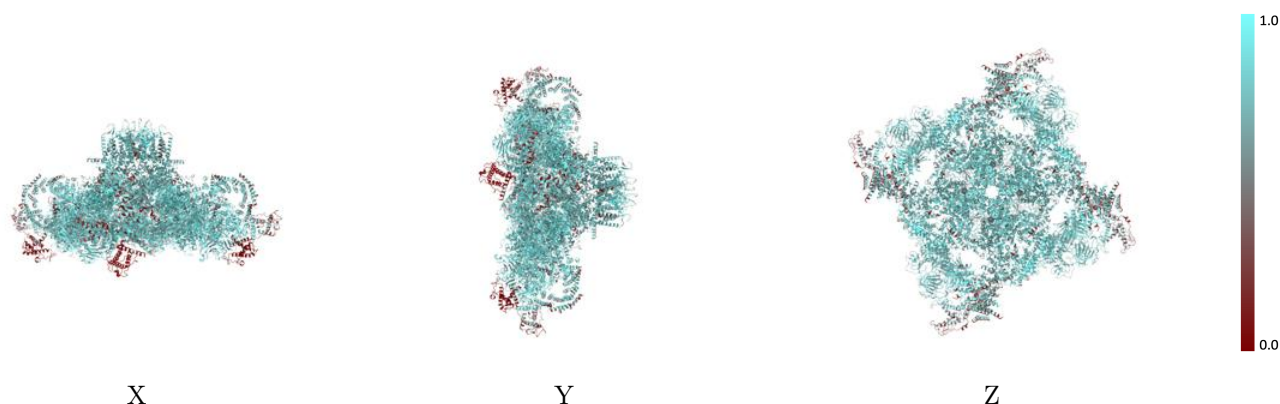
The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



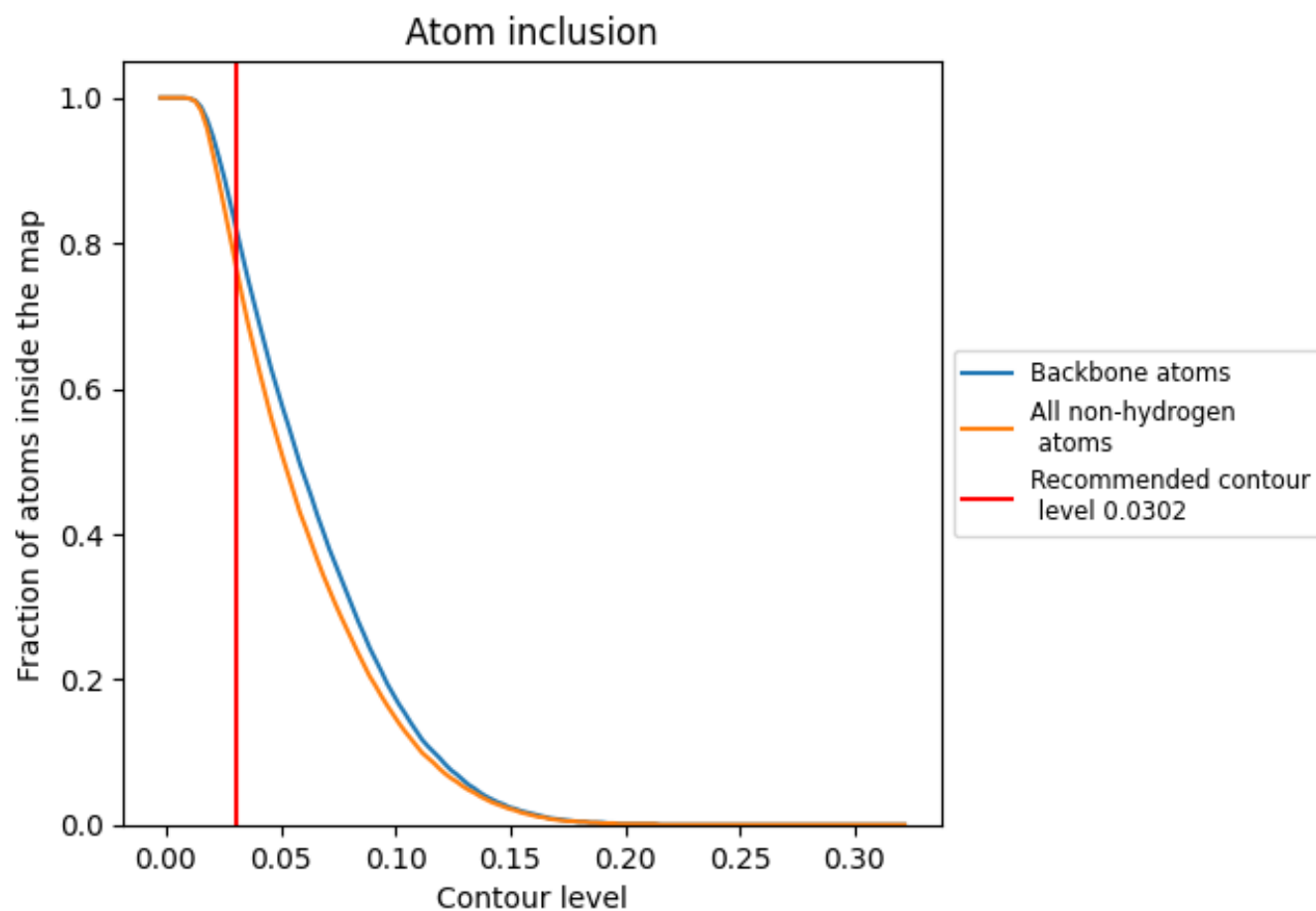
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0302).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.0302) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7730	0.3090
A	0.7800	0.3140
B	0.7710	0.2130
C	0.6120	0.2450
D	0.7790	0.3130
E	0.7840	0.2240
F	0.5780	0.1900
G	0.7790	0.3140
H	0.7830	0.2180
I	0.5810	0.1930
J	0.7800	0.3180
K	0.7760	0.2210
L	0.5770	0.1980

1.0

0.0

<0.0