



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 09:44 PM UTC

PDB ID : 6W6E / pdb_00006w6e
EMDB ID : EMD-21553
Title : The Mycobacterium tuberculosis ClpB disaggregase hexamer structure with a locally refined ClpB middle domain and a DnaK nucleotide binding domain
Authors : Yin, Y.; Li, H.
Deposited on : 2020-03-16
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

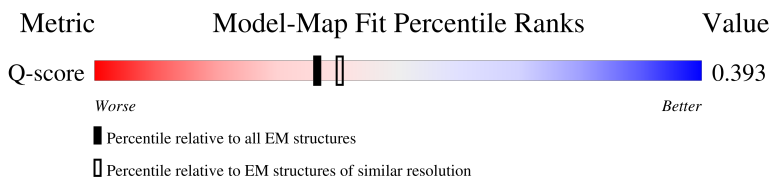
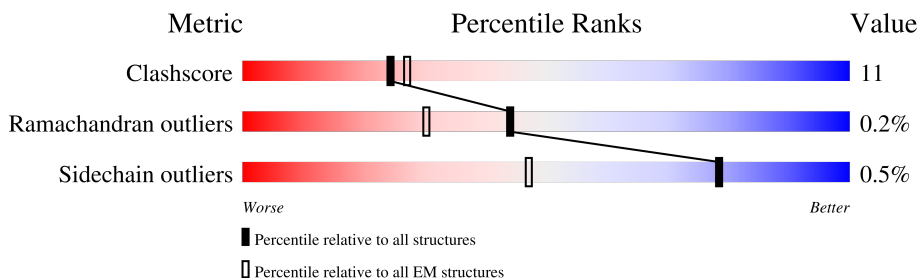
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	848	
1	B	848	
1	C	848	
1	D	848	

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Mol	Chain	Length	Quality of chain
1	E	848	6% 44% 50%
1	F	848	6% 44% 50%
2	I	625	35% 45% 20%
3	N	33	73% 6% 21%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30805 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	674	Total	C	N	O	S	0	0
			5222	3253	954	1004	11		
1	B	621	Total	C	N	O	S	0	0
			4804	2994	877	923	10		
1	C	624	Total	C	N	O	S	0	0
			4821	3004	880	927	10		
1	D	562	Total	C	N	O	S	0	0
			4321	2701	790	821	9		
1	E	548	Total	C	N	O	S	0	0
			4230	2647	772	802	9		
1	F	546	Total	C	N	O	S	0	0
			4219	2641	770	799	9		

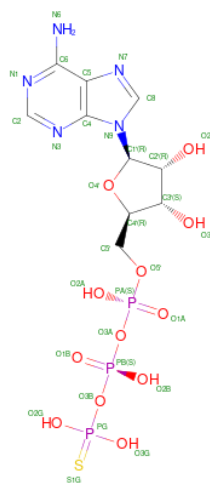
- Molecule 2 is a protein called Chaperone protein DnaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	357	Total	C	N	O	S	0	0
			2694	1675	474	539	6		

- Molecule 3 is a protein called Substrate.

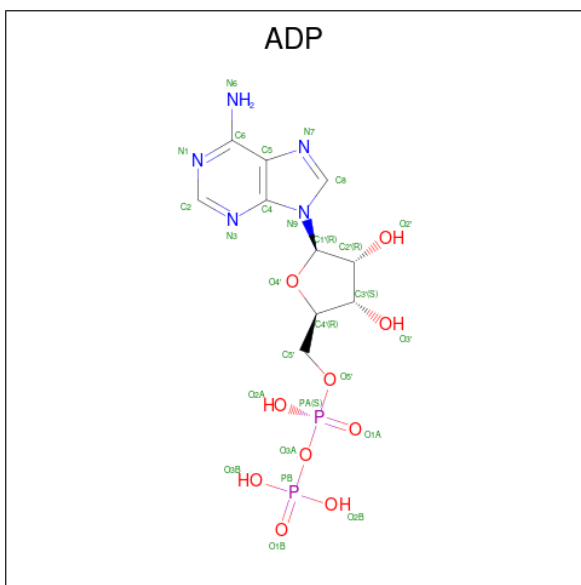
Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



4	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

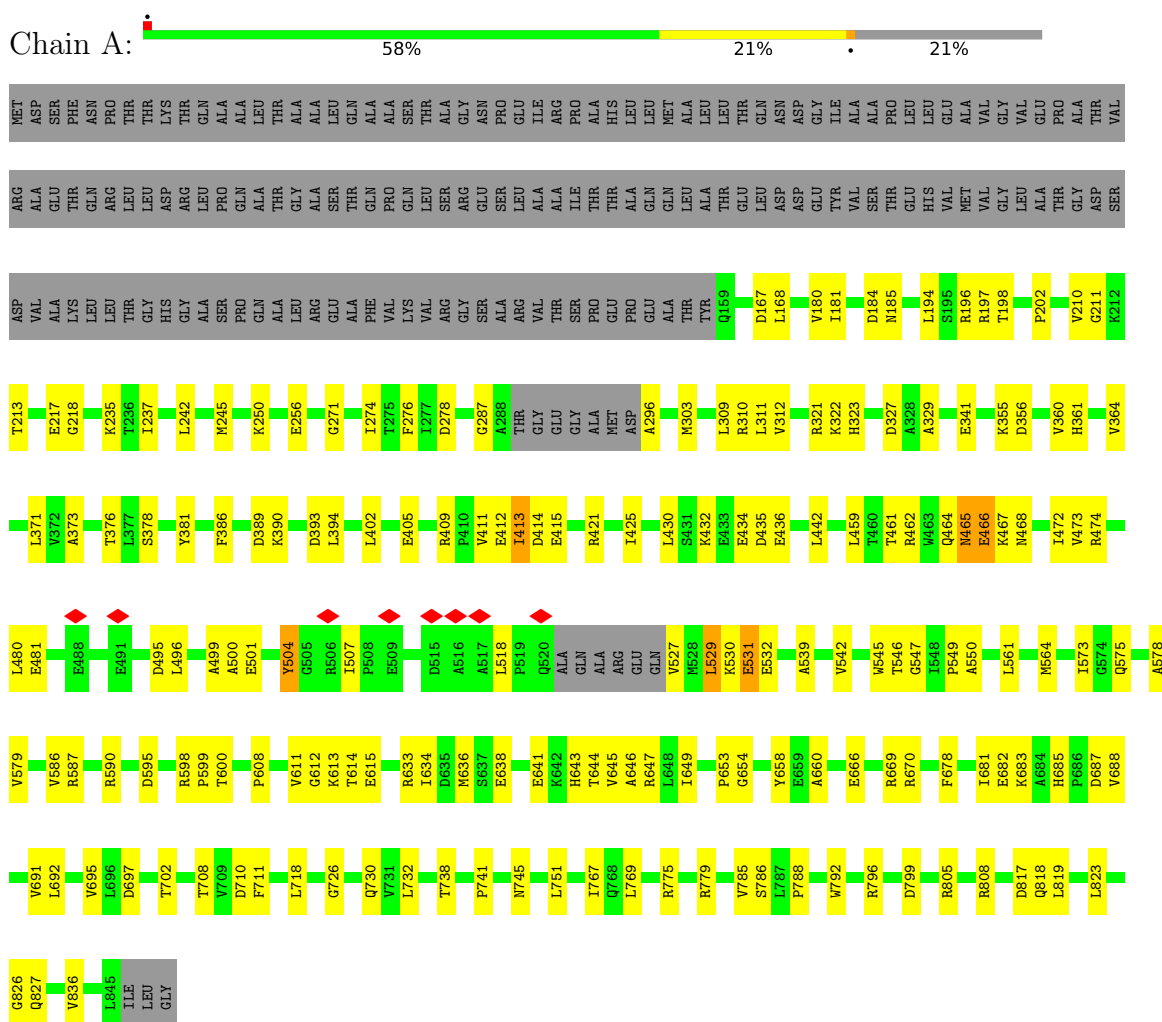


Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total 27	C 10	N 5	O 10	P 2	0
5	F	1	Total 27	C 10	N 5	O 10	P 2	0

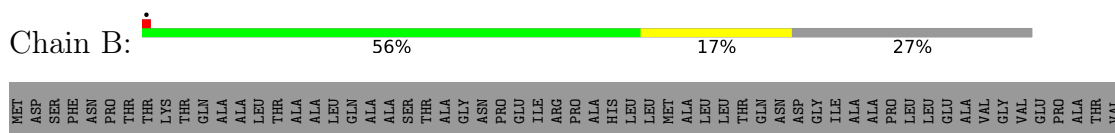
3 Residue-property plots

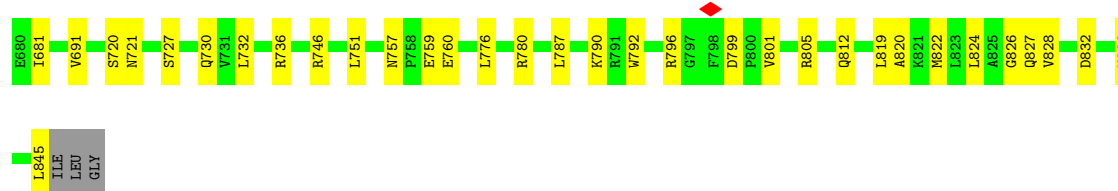
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Chaperone protein ClpB



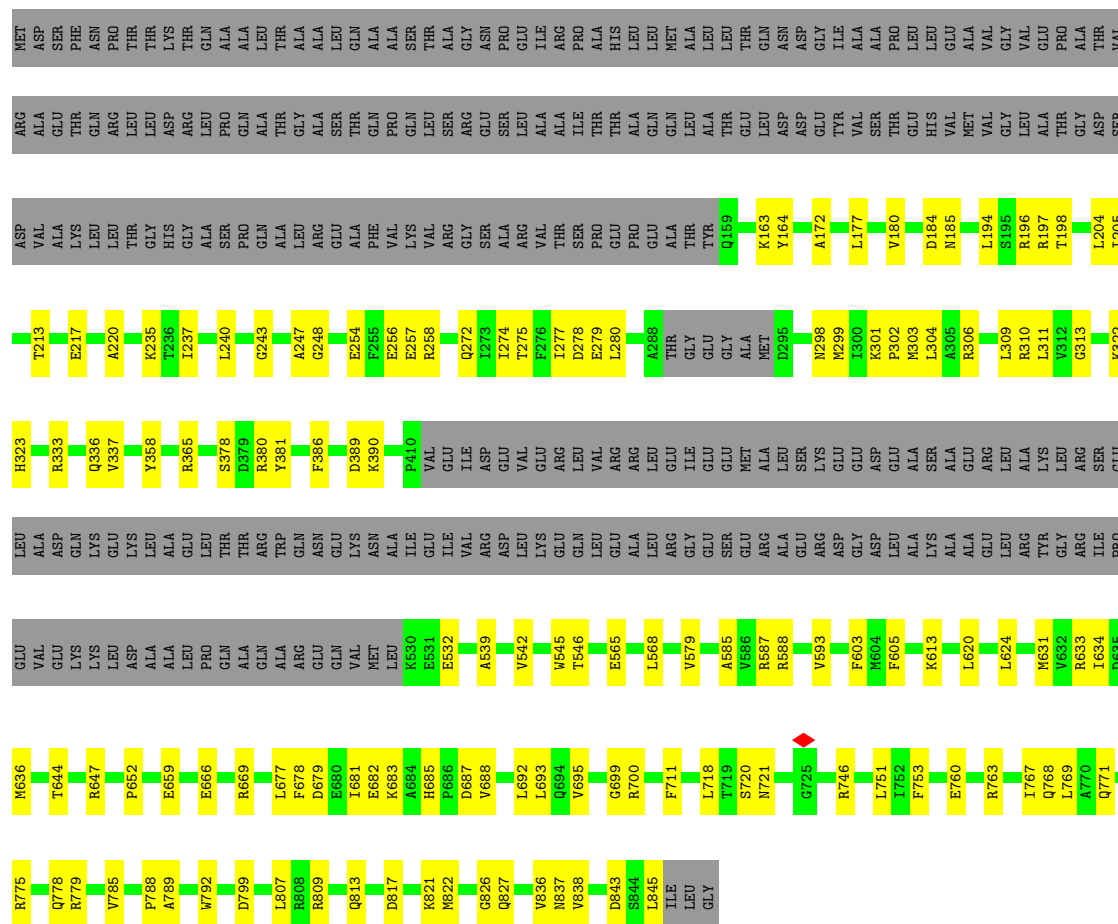
• Molecule 1: Chaperone protein ClpB





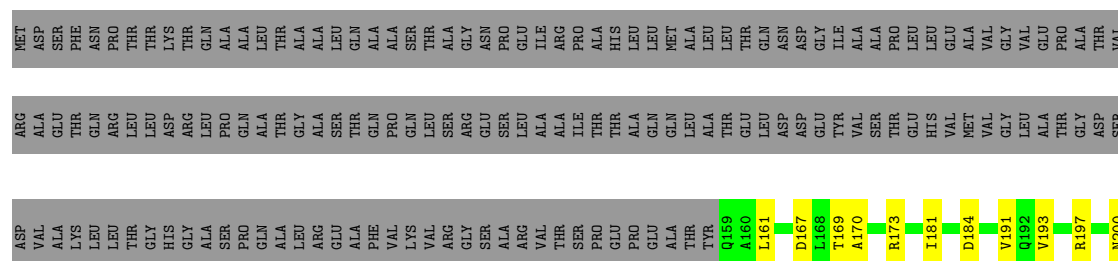
• Molecule 1: Chaperone protein ClpB

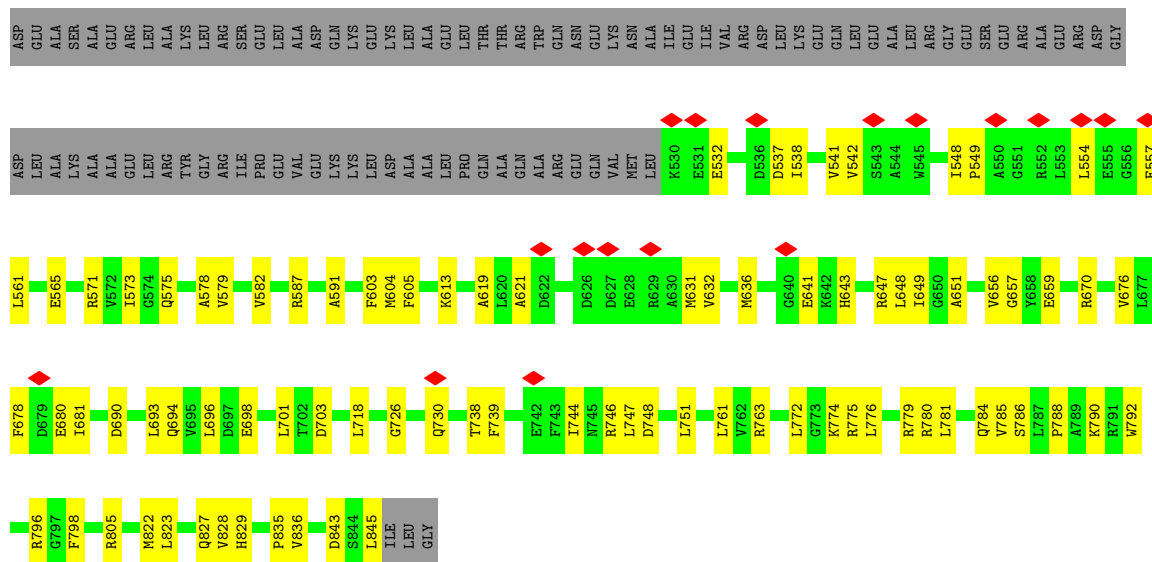
Chain D: 51% 16% 34%



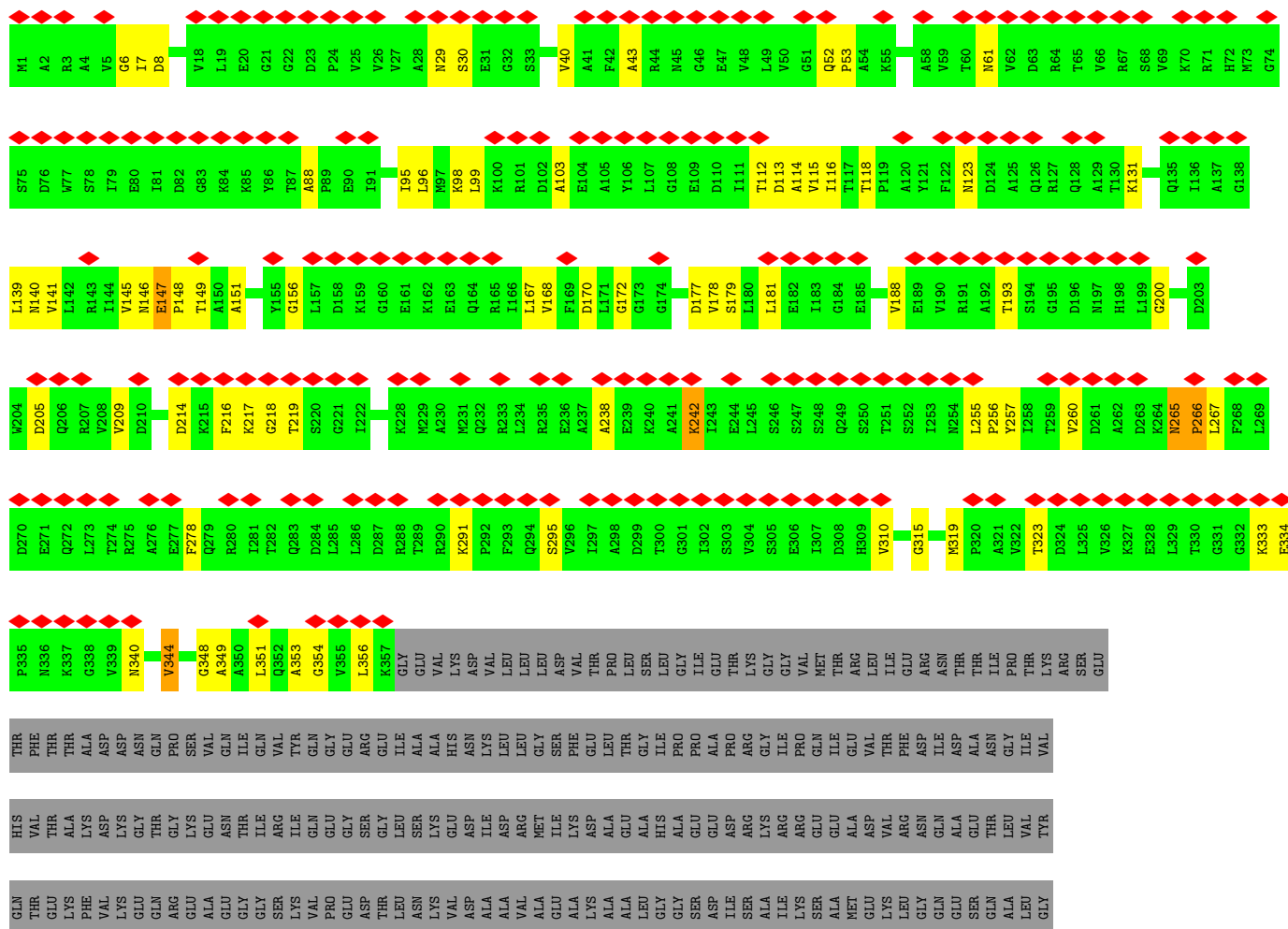
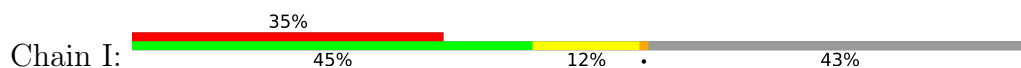
• Molecule 1: Chaperone protein ClpB

Chain E: 44% 21% 35%





• Molecule 2: Chaperone protein DnaK



GLN	ALA	ILE	TYR	GLU	ALA	ALA	GLN	ALA	ALA	SER	GLN	ALA	THR	GLY	ALA	ALA	HIS	PRO	GLY	GLY	GLU	PRO	GLY	GLY	ALA	ALA	HIS	PRO	GLY	SER	ALA	ASP	ASP	VAL	VAL	ASP	ALA	GLU	VAL	VAL	ASP	ASP	GLY	ARG	GLU	ALA	LYS
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● Molecule 3: Substrate



X1	X11	X25	X26	UNK	UNK	UNK	UNK	UNK	UNK
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0126	Depositor
Map size ($\text{\AA}$)	386.64, 386.64, 386.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	9/5286 (0.2%)	0.55	3/7126 (0.0%)
1	B	0.23	0/4865	0.48	1/6562 (0.0%)
1	C	0.23	0/4882	0.45	0/6586
1	D	0.22	0/4380	0.46	0/5914
1	E	0.17	0/4286	0.45	0/5786
1	F	0.17	0/4276	0.46	0/5774
2	I	1.71	67/2727 (2.5%)	1.14	21/3695 (0.6%)
All	All	0.58	76/30702 (0.2%)	0.57	25/41443 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	I	0	1
All	All	0	2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	115	VAL	CA-C	-14.29	1.35	1.52
1	A	473	VAL	CA-C	-9.23	1.41	1.52
2	I	167	LEU	CA-C	-9.19	1.41	1.52
2	I	95	ILE	CA-C	-9.14	1.41	1.52
2	I	8	ASP	N-CA	-8.93	1.35	1.46
2	I	145	VAL	CA-C	-8.49	1.42	1.52
2	I	40	VAL	CA-C	8.46	1.63	1.52
2	I	216	PHE	CA-C	-8.11	1.42	1.52
2	I	349	ALA	CA-C	-7.99	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	ALA	CA-C	-7.76	1.43	1.52
2	I	344	VAL	CA-C	-7.76	1.43	1.52
2	I	267	LEU	CA-C	-7.61	1.43	1.53
2	I	200	GLY	CA-C	7.51	1.61	1.51
2	I	310	VAL	CA-C	-7.51	1.43	1.52
2	I	205	ASP	CA-C	-7.47	1.43	1.52
2	I	98	LYS	C-N	-7.39	1.23	1.33
2	I	170	ASP	CA-C	7.38	1.62	1.53
2	I	8	ASP	CA-C	-7.29	1.43	1.52
2	I	256	PRO	CA-C	-7.19	1.43	1.52
2	I	266	PRO	N-CA	-7.09	1.38	1.47
1	A	472	ILE	CA-C	-6.96	1.44	1.52
2	I	114	ALA	N-CA	6.93	1.54	1.46
2	I	351	LEU	N-CA	-6.75	1.38	1.46
2	I	168	VAL	N-CA	-6.72	1.38	1.46
2	I	131	LYS	CA-C	-6.70	1.44	1.52
2	I	7	ILE	CA-C	-6.70	1.43	1.52
2	I	6	GLY	CA-C	-6.69	1.47	1.52
2	I	7	ILE	N-CA	-6.68	1.37	1.46
2	I	99	LEU	N-CA	-6.67	1.38	1.46
2	I	141	VAL	CA-C	-6.64	1.45	1.53
2	I	349	ALA	N-CA	-6.61	1.38	1.46
2	I	118	THR	C-N	-6.58	1.24	1.33
2	I	177	ASP	C-N	-6.54	1.23	1.33
2	I	139	LEU	CA-C	-6.47	1.44	1.52
1	A	518	LEU	N-CA	-6.46	1.39	1.46
2	I	218	GLY	N-CA	-6.38	1.37	1.45
2	I	323	THR	CA-C	-6.36	1.44	1.52
2	I	43	ALA	CA-C	-6.32	1.44	1.52
2	I	257	TYR	CA-C	-6.25	1.44	1.53
2	I	356	LEU	N-CA	-6.24	1.39	1.46
2	I	178	VAL	N-CA	-6.09	1.38	1.46
2	I	348	GLY	CA-C	-6.09	1.44	1.51
2	I	278	PHE	N-CA	-6.07	1.39	1.46
2	I	103	ALA	CA-C	-6.01	1.45	1.52
1	A	473	VAL	N-CA	-5.96	1.39	1.46
2	I	96	LEU	CA-C	-5.93	1.44	1.52
2	I	146	ASN	N-CA	-5.75	1.39	1.46
2	I	315	GLY	C-N	-5.71	1.26	1.33
2	I	179	SER	CA-C	5.66	1.59	1.52
1	A	480	LEU	CA-C	-5.59	1.45	1.52
2	I	116	ILE	N-CA	-5.55	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	156	GLY	CA-C	-5.55	1.45	1.51
2	I	113	ASP	CA-C	5.51	1.59	1.52
1	A	481	GLU	N-CA	-5.51	1.39	1.46
1	A	474	ARG	N-CA	-5.48	1.39	1.46
2	I	123	ASN	CA-C	-5.34	1.46	1.53
2	I	181	LEU	CA-C	5.34	1.59	1.52
2	I	238	ALA	CA-C	-5.34	1.46	1.52
2	I	209	VAL	CA-C	-5.32	1.46	1.52
2	I	112	THR	C-N	-5.31	1.25	1.33
2	I	219	THR	CA-C	5.30	1.59	1.52
2	I	214	ASP	N-CA	-5.27	1.40	1.46
2	I	217	LYS	CA-C	-5.22	1.46	1.52
2	I	315	GLY	CA-C	-5.21	1.44	1.51
2	I	353	ALA	CA-C	5.21	1.59	1.52
2	I	140	ASN	N-CA	-5.17	1.39	1.46
2	I	354	GLY	N-CA	5.15	1.52	1.45
1	A	507	ILE	CA-C	-5.13	1.47	1.52
2	I	295	SER	CA-C	5.13	1.59	1.52
2	I	95	ILE	N-CA	-5.13	1.40	1.46
2	I	242	LYS	CA-C	-5.10	1.46	1.52
2	I	61	ASN	CA-C	-5.10	1.46	1.53
2	I	193	THR	CA-C	-5.09	1.46	1.52
2	I	172	GLY	N-CA	-5.05	1.39	1.45
2	I	354	GLY	CA-C	5.05	1.57	1.52
2	I	260	VAL	CA-C	5.03	1.59	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	319	MET	CA-C-N	8.98	128.63	119.56
2	I	319	MET	C-N-CA	8.98	128.63	119.56
1	B	413	ILE	N-CA-C	-8.54	104.85	113.47
2	I	340	ASN	CA-C-N	8.07	128.84	119.47
2	I	340	ASN	C-N-CA	8.07	128.84	119.47
2	I	255	LEU	CA-C-N	7.21	127.13	119.85
2	I	255	LEU	C-N-CA	7.21	127.13	119.85
2	I	334	GLU	CA-C-N	6.41	126.17	119.76
2	I	334	GLU	C-N-CA	6.41	126.17	119.76
2	I	88	ALA	CA-C-N	6.24	125.73	119.24
2	I	88	ALA	C-N-CA	6.24	125.73	119.24
2	I	147	GLU	CA-C-N	6.22	125.95	119.05
2	I	147	GLU	C-N-CA	6.22	125.95	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ILE	N-CA-C	-6.08	106.98	111.90
2	I	291	LYS	CA-C-N	5.92	125.79	119.28
2	I	291	LYS	C-N-CA	5.92	125.79	119.28
2	I	118	THR	CA-C-N	5.91	125.87	119.78
2	I	118	THR	C-N-CA	5.91	125.87	119.78
2	I	7	ILE	N-CA-C	5.70	116.07	107.75
1	A	518	LEU	CA-C-N	5.61	126.85	119.84
1	A	518	LEU	C-N-CA	5.61	126.85	119.84
2	I	344	VAL	N-CA-C	5.20	115.82	110.36
2	I	260	VAL	N-CA-C	5.12	115.23	107.80
2	I	265	ASN	CA-C-N	5.04	126.14	119.84
2	I	265	ASN	C-N-CA	5.04	126.14	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	387	LEU	Peptide
2	I	333	LYS	Mainchain

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	5222	0	5286	136	0
1	B	4804	0	4857	104	0
1	C	4821	0	4871	100	0
1	D	4321	0	4377	87	0
1	E	4230	0	4291	131	0
1	F	4219	0	4283	129	0
2	I	2694	0	2721	6	0
3	N	130	0	31	2	0
4	A	62	0	24	7	0
4	B	62	0	24	7	0
4	C	31	0	12	6	0
4	D	93	0	35	10	0
4	E	31	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	31	0	12	3	0
5	E	27	0	12	4	0
5	F	27	0	12	2	0
All	All	30805	0	30860	658	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 11.

All (658) 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:A:530:LYS:O	1:A:531:GLU:CG	1.72	1.35
1:A:530:LYS:O	1:A:531:GLU:HG3	0.88	1.05
1:A:405:GLU:OE1	1:A:529:LEU:CD2	2.08	1.02
1:A:405:GLU:OE1	1:A:529:LEU:HD21	1.64	0.96
1:A:530:LYS:C	1:A:531:GLU:HG3	1.92	0.93
1:E:573:ILE:H	5:E:902:ADP:HN62	1.25	0.85
1:B:280:LEU:HD23	1:B:313:GLY:HA3	1.59	0.82
1:F:605:PHE:HB3	1:F:751:LEU:HB2	1.62	0.81
1:B:389:ASP:OD2	1:C:332:ARG:NH1	2.16	0.79
1:E:757:ASN:HB3	1:E:760:GLU:HB2	1.65	0.79
1:C:280:LEU:HD23	1:C:313:GLY:HA3	1.65	0.78
1:E:610:GLY:HA3	1:E:803:GLY:HA3	1.65	0.77
1:A:405:GLU:OE1	1:A:529:LEU:HD23	1.85	0.77
1:A:465:ASN:O	1:A:467:LYS:N	2.18	0.76
4:D:902:AGS:S1G	1:E:332:ARG:NH1	2.59	0.76
1:A:465:ASN:O	1:A:468:ASN:N	2.18	0.75
4:B:902:AGS:S1G	1:C:746:ARG:NH2	2.60	0.75
4:C:901:AGS:S1G	1:D:746:ARG:NH2	2.61	0.73
1:C:547:GLY:H	1:C:671:ARG:HH21	1.35	0.73
1:E:283:ILE:HG22	1:E:284:VAL:HG13	1.70	0.73
1:F:681:ILE:HG12	1:F:718:LEU:HD23	1.70	0.72
1:F:236:THR:OG1	1:F:272:GLN:O	2.07	0.72
1:D:545:TRP:HD1	1:D:546:THR:HG23	1.53	0.71
1:F:212:LYS:HD3	1:F:314:ALA:HB1	1.72	0.71
1:C:822:MET:HB3	1:C:828:VAL:HG21	1.72	0.71
1:F:573:ILE:H	4:F:901:AGS:HN62	1.39	0.70
1:D:775:ARG:NH1	1:E:593:VAL:O	2.25	0.69
4:B:901:AGS:S1G	1:C:333:ARG:NH1	2.62	0.69
1:E:613:LYS:HA	1:E:753:PHE:HE2	1.57	0.69
1:A:561:LEU:O	1:A:587:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:784:GLN:HE22	1:E:786:SER:HB3	1.58	0.69
1:E:228:VAL:O	1:E:233:ARG:NH2	2.26	0.68
1:F:693:LEU:O	1:F:746:ARG:NH1	2.27	0.68
1:A:194:LEU:O	1:A:310:ARG:NH1	2.27	0.68
1:A:287:GLY:O	1:B:252:ARG:NH2	2.27	0.67
1:C:199:LYS:HD2	1:C:333:ARG:HA	1.76	0.67
1:C:566:ASP:O	1:C:570:LYS:NZ	2.27	0.67
1:F:267:LYS:NZ	1:F:308:GLU:OE2	2.26	0.67
1:E:669:ARG:HB3	1:E:709:VAL:HG12	1.76	0.67
1:F:575:GLN:HB3	1:F:578:ALA:HB3	1.76	0.67
1:F:302:PRO:O	1:F:306:ARG:NH1	2.28	0.67
1:A:775:ARG:NH2	1:B:595:ASP:OD1	2.29	0.66
1:B:604:MET:HB2	1:B:718:LEU:HB2	1.77	0.66
1:F:394:LEU:HD21	1:F:538:ILE:HG23	1.78	0.66
1:B:566:ASP:O	1:B:570:LYS:NZ	2.28	0.66
1:A:167:ASP:OD1	1:A:168:LEU:N	2.30	0.65
1:F:220:ALA:HB2	1:F:237:ILE:HD11	1.79	0.65
1:C:836:VAL:HG12	1:C:845:LEU:HG	1.78	0.65
1:F:229:PRO:HG2	1:F:232:LEU:HD13	1.77	0.65
1:E:362:HIS:O	1:E:403:ARG:NH1	2.29	0.65
1:A:702:THR:HG22	1:A:708:THR:HG22	1.78	0.64
1:E:284:VAL:HG12	1:E:297:GLY:HA2	1.78	0.64
1:E:639:TYR:OH	1:E:663:GLN:OE1	2.14	0.64
1:D:631:MET:HE3	1:D:633:ARG:HB3	1.78	0.64
1:C:727:SER:HB3	1:C:730:GLN:HE21	1.62	0.64
1:F:280:LEU:HD22	1:F:313:GLY:HA3	1.80	0.64
1:F:565:GLU:OE2	1:F:587:ARG:NH2	2.30	0.64
1:E:386:PHE:O	1:E:390:LYS:CB	2.45	0.64
1:B:605:PHE:HB3	1:B:751:LEU:HB2	1.78	0.64
1:F:696:LEU:O	1:F:746:ARG:NH1	2.31	0.64
1:A:647:ARG:NH2	1:B:702:THR:O	2.31	0.63
1:A:638:GLU:OE1	1:A:647:ARG:NH2	2.31	0.63
1:B:805:ARG:NH1	4:B:902:AGS:S1G	2.70	0.63
1:C:536:ASP:OD2	1:C:552:ARG:NH2	2.31	0.63
1:A:256:GLU:OE1	1:A:256:GLU:N	2.26	0.63
1:E:252:ARG:HH12	3:N:11:UNK:HA	1.62	0.63
1:E:666:GLU:OE2	1:E:669:ARG:NH2	2.32	0.63
4:D:901:AGS:O2G	4:D:901:AGS:O1B	2.16	0.63
1:D:568:LEU:HD23	1:D:579:VAL:HG13	1.79	0.63
1:F:263:LEU:HB3	1:F:303:MET:HE1	1.80	0.63
4:B:901:AGS:O2G	4:B:901:AGS:O1B	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:769:LEU:HA	1:E:772:LEU:HG	1.80	0.62
1:B:665:THR:HG23	1:B:709:VAL:HG21	1.81	0.62
4:D:902:AGS:O2B	4:D:902:AGS:O2A	2.18	0.62
1:C:197:ARG:HG2	1:C:198:THR:HG23	1.80	0.62
1:C:605:PHE:HB3	1:C:751:LEU:HB2	1.81	0.62
1:F:316:THR:OG1	1:F:318:ASP:OD1	2.14	0.62
1:A:210:VAL:HG13	1:A:341:GLU:HA	1.82	0.62
1:E:211:GLY:H	4:E:901:AGS:PB	2.23	0.62
1:E:184:ASP:OD1	1:E:222:ARG:NH1	2.33	0.61
1:A:608:PRO:O	1:A:613:LYS:NZ	2.33	0.61
1:A:378:SER:OG	1:A:390:LYS:HG3	2.01	0.61
1:A:409:ARG:NH2	1:A:414:ASP:OD1	2.32	0.61
1:F:603:PHE:HB3	1:F:748:ASP:HB2	1.82	0.61
1:C:393:ASP:OD1	1:D:196:ARG:NH2	2.28	0.61
1:D:788:PRO:HB2	1:D:838:VAL:HG21	1.82	0.61
1:E:374:ALA:HB2	1:E:538:ILE:HD13	1.82	0.61
1:C:167:ASP:OD1	1:C:168:LEU:N	2.34	0.60
1:E:563:ARG:HH21	1:E:567:GLU:HB2	1.66	0.60
4:B:902:AGS:O1B	4:B:902:AGS:O2G	2.18	0.60
1:E:281:HIS:O	1:E:323:HIS:ND1	2.26	0.60
1:A:435:ASP:OD1	1:A:436:GLU:N	2.34	0.60
1:E:659:GLU:OE1	1:E:659:GLU:N	2.33	0.60
1:E:818:GLN:HE21	1:E:845:LEU:HD12	1.66	0.60
1:E:386:PHE:O	1:E:390:LYS:HB2	2.01	0.60
4:A:901:AGS:O2G	4:A:901:AGS:O1B	2.18	0.60
1:C:608:PRO:HG2	1:C:611:VAL:HG21	1.84	0.60
1:D:380:ARG:NH1	1:D:381:TYR:OH	2.35	0.60
1:E:546:THR:HG23	1:E:548:ILE:H	1.67	0.59
1:F:548:ILE:HD12	1:F:549:PRO:HD2	1.83	0.59
1:A:465:ASN:C	1:A:467:LYS:N	2.58	0.59
1:F:538:ILE:O	1:F:542:VAL:HG23	2.02	0.59
4:C:901:AGS:O1B	4:C:901:AGS:O2G	2.20	0.59
4:D:903:AGS:O2G	4:D:903:AGS:O1B	2.19	0.59
1:B:387:LEU:O	1:B:389:ASP:N	2.36	0.59
1:F:621:ALA:HB2	1:F:631:MET:HE3	1.84	0.59
1:B:411:VAL:O	1:B:412:GLU:HG2	2.01	0.59
1:F:779:ARG:HH21	1:F:823:LEU:HG	1.66	0.59
1:B:242:LEU:HD11	1:B:283:ILE:HG13	1.85	0.59
4:B:902:AGS:O2A	4:B:902:AGS:O2B	2.20	0.59
1:C:414:ASP:OD2	1:C:418:ARG:NH1	2.36	0.59
1:A:654:GLY:HA2	1:F:656:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:GLY:HA3	1:B:730:GLN:HB2	1.85	0.59
1:E:698:GLU:OE2	1:E:700:ARG:NH1	2.35	0.59
1:F:344:VAL:HG13	1:F:375:ALA:HB1	1.85	0.59
1:E:765:VAL:O	1:E:769:LEU:HG	2.03	0.58
1:F:345:GLU:HA	1:F:348:ILE:HD12	1.85	0.58
1:A:702:THR:O	1:F:647:ARG:NH2	2.36	0.58
1:A:545:TRP:CD1	1:A:546:THR:HG23	2.38	0.58
1:A:196:ARG:NH2	1:F:397:GLU:OE2	2.36	0.58
1:E:221:GLN:HA	1:E:224:VAL:HG12	1.85	0.58
1:A:785:VAL:HA	1:A:836:VAL:HG22	1.84	0.58
1:B:645:VAL:HG11	1:B:691:VAL:HG21	1.85	0.58
1:B:808:ARG:HH22	1:C:598:ARG:HD2	1.68	0.58
1:E:263:LEU:HD23	1:E:303:MET:HG3	1.85	0.58
1:F:189:ARG:NH1	1:F:192:GLN:OE1	2.36	0.58
4:C:901:AGS:O2A	4:C:901:AGS:O2B	2.19	0.58
1:A:670:ARG:HD3	1:B:317:LEU:HD21	1.84	0.58
1:A:779:ARG:HH22	1:A:823:LEU:HD21	1.69	0.58
1:A:666:GLU:O	1:A:670:ARG:NH1	2.36	0.58
1:A:415:GLU:OE2	1:B:188:ARG:NH2	2.36	0.57
1:A:250:LYS:NZ	1:B:254:GLU:OE1	2.32	0.57
1:A:321:ARG:HB3	1:F:670:ARG:HH22	1.70	0.57
1:A:653:PRO:HA	1:A:658:TYR:CZ	2.40	0.57
1:E:571:ARG:NH2	1:E:628:GLU:OE1	2.32	0.57
1:C:274:ILE:HG12	1:C:310:ARG:HD3	1.85	0.57
1:D:769:LEU:HD13	1:D:785:VAL:HG21	1.87	0.57
1:F:279:GLU:HB3	1:F:281:HIS:NE2	2.20	0.57
1:A:411:VAL:O	1:A:412:GLU:HG2	2.05	0.57
1:B:161:LEU:O	1:B:165:SER:OG	2.19	0.57
1:C:757:ASN:HB2	1:C:760:GLU:HG3	1.87	0.57
1:A:378:SER:HB2	1:A:394:LEU:HD11	1.87	0.56
1:E:691:VAL:O	1:E:695:VAL:HG23	2.04	0.56
1:A:669:ARG:NH2	1:B:325:GLU:OE1	2.30	0.56
1:F:604:MET:HB2	1:F:718:LEU:HB2	1.87	0.56
1:A:202:PRO:HG2	1:A:312:VAL:HG23	1.88	0.56
1:E:772:LEU:HA	1:E:775:ARG:HG2	1.88	0.56
1:A:549:PRO:HB2	1:A:590:ARG:HH12	1.71	0.56
1:F:603:PHE:HA	1:F:747:LEU:HD22	1.87	0.56
1:A:769:LEU:HD13	1:A:785:VAL:HG21	1.88	0.56
1:B:608:PRO:O	1:B:613:LYS:NZ	2.39	0.56
1:C:326:LYS:NZ	1:C:327:ASP:OD1	2.35	0.56
1:E:726:GLY:HA3	1:E:730:GLN:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:786:SER:HB2	1:F:788:PRO:HD2	1.88	0.56
1:A:235:LYS:NZ	1:A:271:GLY:O	2.30	0.55
1:C:635:ASP:OD2	1:D:700:ARG:NH1	2.35	0.55
1:E:167:ASP:OD1	1:E:170:ALA:N	2.31	0.55
1:E:720:SER:OG	1:E:721:ASN:N	2.39	0.55
1:A:595:ASP:OD1	1:F:775:ARG:NH2	2.39	0.55
1:B:267:LYS:HB2	1:B:303:MET:HE1	1.88	0.55
1:A:386:PHE:C	1:A:390:LYS:HD2	2.32	0.55
1:A:561:LEU:HD21	1:A:590:ARG:HG3	1.89	0.55
1:D:767:ILE:O	1:D:771:GLN:HG3	2.07	0.55
1:E:275:THR:OG1	1:E:276:PHE:N	2.37	0.55
1:B:703:ASP:OD1	1:B:703:ASP:N	2.39	0.55
1:E:656:VAL:HG22	3:N:25:UNK:HA	1.89	0.55
1:E:814:ALA:O	1:E:818:GLN:HB3	2.06	0.55
1:A:287:GLY:HA2	1:A:296:ALA:HB3	1.87	0.55
1:E:566:ASP:O	1:E:570:LYS:N	2.39	0.55
1:E:726:GLY:H	1:E:730:GLN:HE21	1.55	0.55
1:A:276:PHE:HD1	1:A:312:VAL:HG13	1.71	0.54
1:A:181:ILE:HD12	1:A:181:ILE:H	1.72	0.54
1:A:808:ARG:NH1	4:A:902:AGS:O3'	2.40	0.54
1:B:545:TRP:HB2	1:C:189:ARG:NH2	2.22	0.54
1:E:191:VAL:HG23	1:E:232:LEU:HD13	1.89	0.54
1:B:557:GLU:OE1	1:B:590:ARG:NH2	2.41	0.54
1:C:263:LEU:HD11	1:C:300:ILE:HG22	1.88	0.54
1:D:163:LYS:NZ	1:D:164:TYR:OH	2.41	0.54
4:D:902:AGS:O1B	4:D:902:AGS:O2G	2.26	0.54
1:E:809:ARG:HA	1:E:812:GLN:HG2	1.89	0.54
1:A:614:THR:OG1	4:A:902:AGS:O1B	2.24	0.54
1:C:298:ASN:HB2	1:C:301:LYS:HE3	1.90	0.54
1:D:565:GLU:OE2	1:D:587:ARG:NH2	2.31	0.54
1:D:685:HIS:O	1:D:687:ASP:N	2.34	0.54
1:F:613:LYS:NZ	4:F:901:AGS:O3G	2.37	0.54
4:A:902:AGS:O1B	4:A:902:AGS:O2G	2.24	0.53
1:B:799:ASP:O	1:B:801:VAL:N	2.33	0.53
1:D:799:ASP:N	1:D:799:ASP:OD1	2.42	0.53
1:E:342:PRO:HG2	1:E:388:PRO:HG3	1.89	0.53
1:A:465:ASN:O	1:A:466:GLU:C	2.51	0.53
1:E:805:ARG:HG2	5:E:902:ADP:H5'2	1.90	0.53
1:C:194:LEU:HD21	1:C:274:ILE:HG21	1.90	0.53
1:A:741:PRO:O	1:A:745:ASN:HB2	2.09	0.53
1:F:318:ASP:O	1:F:322:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ILE:HD11	1:A:678:PHE:HE1	1.73	0.53
1:A:786:SER:OG	1:A:788:PRO:HD2	2.09	0.53
1:E:819:LEU:O	1:E:823:LEU:HG	2.08	0.53
1:F:222:ARG:HH22	1:F:228:VAL:HG12	1.72	0.53
1:A:726:GLY:HA3	1:A:730:GLN:HB2	1.91	0.53
1:B:300:ILE:HD11	1:B:309:LEU:HD11	1.90	0.53
1:C:826:GLY:O	1:C:827:GLN:HG2	2.08	0.53
1:D:386:PHE:O	1:D:390:LYS:HB3	2.09	0.53
1:D:539:ALA:HA	1:D:542:VAL:HG12	1.91	0.53
1:E:242:LEU:HD11	1:E:283:ILE:HD11	1.91	0.53
1:E:740:LYS:HG3	1:E:742:GLU:HG3	1.90	0.53
1:F:234:ASP:O	1:F:236:THR:N	2.42	0.53
1:F:843:ASP:N	1:F:843:ASP:OD1	2.42	0.53
1:A:196:ARG:HG2	1:A:197:ARG:H	1.74	0.52
1:C:381:TYR:HE2	1:C:550:ALA:HB2	1.72	0.52
1:C:430:LEU:HD22	1:C:442:LEU:HD13	1.91	0.52
1:D:681:ILE:HG21	1:D:718:LEU:HD12	1.89	0.52
1:E:301:LYS:HE2	1:E:330:LEU:HD13	1.91	0.52
1:F:210:VAL:HG11	1:F:339:VAL:HG21	1.92	0.52
1:B:646:ALA:HA	1:B:649:ILE:HG22	1.91	0.52
1:E:181:ILE:H	1:E:181:ILE:HD12	1.74	0.52
1:D:826:GLY:O	1:D:827:GLN:HG2	2.10	0.52
1:D:256:GLU:HG3	1:D:299:MET:HE1	1.92	0.52
1:C:720:SER:OG	1:C:721:ASN:N	2.40	0.52
1:F:319:GLU:O	1:F:323:HIS:HB2	2.10	0.52
1:A:710:ASP:OD1	1:A:710:ASP:N	2.40	0.52
4:A:902:AGS:S1G	1:B:746:ARG:NH2	2.75	0.52
1:D:692:LEU:HA	1:D:695:VAL:HB	1.92	0.52
4:E:901:AGS:O1A	1:F:332:ARG:NH1	2.43	0.52
1:F:350:ILE:HG12	5:F:902:ADP:N1	2.24	0.52
1:F:352:ARG:O	1:F:355:LYS:NZ	2.33	0.52
1:F:308:GLU:N	1:F:308:GLU:OE1	2.43	0.51
1:F:403:ARG:HA	1:F:406:ILE:HD12	1.91	0.51
1:F:785:VAL:HA	1:F:836:VAL:HG12	1.92	0.51
1:A:361:HIS:CD2	1:B:197:ARG:HB2	2.45	0.51
1:E:710:ASP:OD1	1:E:710:ASP:N	2.42	0.51
1:A:213:THR:O	1:A:217:GLU:HG2	2.10	0.51
1:E:167:ASP:OD1	1:E:169:THR:N	2.43	0.51
1:C:546:THR:O	1:C:548:ILE:N	2.43	0.51
1:C:732:LEU:O	1:C:736:ARG:NH2	2.43	0.51
1:D:763:ARG:O	1:D:767:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:614:THR:O	1:E:618:LYS:HG3	2.11	0.51
1:F:579:VAL:HA	1:F:582:VAL:HG12	1.93	0.51
1:A:745:ASN:ND2	1:F:805:ARG:HD2	2.25	0.51
1:E:609:THR:OG1	5:E:902:ADP:O3B	2.29	0.51
1:D:633:ARG:NH2	1:D:679:ASP:OD1	2.44	0.51
1:E:318:ASP:OD1	1:E:319:GLU:N	2.42	0.51
1:B:434:GLU:OE1	1:B:434:GLU:N	2.43	0.51
1:D:205:ILE:HD12	1:D:336:GLN:HB3	1.93	0.51
1:A:194:LEU:HD11	1:A:310:ARG:HB3	1.93	0.51
1:A:666:GLU:HB3	1:A:670:ARG:HH12	1.75	0.51
1:B:441:ARG:NH2	1:C:368:ASP:OD2	2.44	0.51
1:D:277:ILE:HD12	1:D:311:LEU:HD11	1.92	0.51
1:C:643:HIS:HD2	1:D:652:PRO:HG3	1.76	0.50
1:E:386:PHE:O	1:E:390:LYS:HB3	2.11	0.50
1:F:232:LEU:O	1:F:234:ASP:N	2.42	0.50
1:A:421:ARG:O	1:A:425:ILE:HG13	2.11	0.50
1:C:427:GLU:O	1:C:431:SER:OG	2.29	0.50
1:C:799:ASP:O	1:C:801:VAL:N	2.38	0.50
1:E:355:LYS:HG3	1:E:366:ILE:HG13	1.92	0.50
1:F:234:ASP:C	1:F:236:THR:H	2.19	0.50
1:D:322:LYS:HE3	1:D:323:HIS:CD2	2.46	0.50
1:D:785:VAL:HA	1:D:836:VAL:HG22	1.94	0.50
1:E:563:ARG:NH2	1:E:567:GLU:HB2	2.25	0.50
1:A:643:HIS:HB2	1:B:655:TYR:CZ	2.47	0.50
1:F:222:ARG:HH11	1:F:227:ASP:HB2	1.77	0.50
1:A:692:LEU:HA	1:A:695:VAL:HB	1.94	0.50
1:B:659:GLU:CD	1:B:659:GLU:H	2.19	0.50
1:A:321:ARG:HB3	1:F:670:ARG:NH2	2.25	0.50
1:C:242:LEU:HD11	1:C:283:ILE:HG13	1.93	0.50
1:E:650:GLY:O	1:E:704:GLY:HA3	2.12	0.50
1:F:779:ARG:HE	1:F:823:LEU:HD21	1.76	0.50
1:C:822:MET:HG2	1:C:827:GLN:HE21	1.77	0.50
1:E:534:GLY:H	1:E:537:ASP:HB3	1.77	0.50
1:B:812:GLN:HE22	1:C:594:SER:HA	1.77	0.49
1:C:460:THR:O	1:C:464:GLN:HG2	2.12	0.49
1:C:554:LEU:HD23	1:C:554:LEU:H	1.77	0.49
1:C:812:GLN:HB3	1:D:588:ARG:NH1	2.27	0.49
1:D:172:ALA:HB2	1:D:177:LEU:HD12	1.93	0.49
1:F:537:ASP:O	1:F:541:VAL:HG23	2.12	0.49
1:D:194:LEU:HD11	1:D:310:ARG:HB3	1.94	0.49
1:D:605:PHE:HB3	1:D:751:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:820:ALA:HA	1:E:823:LEU:HD12	1.94	0.49
1:B:423:LEU:HD22	1:B:445:LEU:HD11	1.94	0.49
1:C:407:ASP:CG	1:C:408:SER:H	2.20	0.49
1:F:183:ARG:NH1	1:F:340:GLY:O	2.41	0.49
1:C:436:GLU:OE2	1:C:780:ARG:NH1	2.44	0.49
1:E:784:GLN:NE2	1:E:785:VAL:O	2.45	0.49
1:D:720:SER:OG	1:D:721:ASN:N	2.46	0.49
1:E:365:ARG:HH11	1:E:532:GLU:HB3	1.77	0.49
1:E:681:ILE:HG12	1:E:718:LEU:HD23	1.93	0.49
1:E:761:LEU:HD12	1:E:794:ALA:HB1	1.94	0.49
1:C:573:ILE:H	4:C:901:AGS:HN62	1.60	0.49
1:C:645:VAL:HG21	1:C:691:VAL:HG21	1.95	0.49
1:F:387:LEU:HA	1:F:390:LYS:HE2	1.95	0.49
1:A:608:PRO:HG2	1:A:611:VAL:HG21	1.94	0.49
1:B:539:ALA:HA	1:B:542:VAL:HG12	1.94	0.49
1:A:646:ALA:HA	1:A:649:ILE:HG22	1.95	0.49
1:C:355:LYS:HD3	1:C:371:LEU:HD11	1.95	0.49
1:E:837:ASN:N	1:E:845:LEU:O	2.43	0.49
1:D:304:LEU:HD21	1:D:311:LEU:HD22	1.95	0.48
1:E:365:ARG:NH1	1:E:531:GLU:O	2.46	0.48
1:F:571:ARG:HG2	1:F:619:ALA:HB2	1.95	0.48
1:B:685:HIS:O	1:B:687:ASP:N	2.44	0.48
1:B:539:ALA:HB1	1:B:550:ALA:O	2.13	0.48
1:C:414:ASP:O	1:C:417:GLU:HG3	2.14	0.48
1:D:278:ASP:OD1	1:D:279:GLU:N	2.46	0.48
1:A:180:VAL:HG11	1:A:218:GLY:HA3	1.94	0.48
1:B:355:LYS:HD3	1:B:371:LEU:HD11	1.95	0.48
1:B:362:HIS:O	1:B:364:VAL:N	2.46	0.48
1:D:248:GLY:O	1:D:258:ARG:NH2	2.39	0.48
1:D:301:LYS:HB3	1:D:333:ARG:NH2	2.28	0.48
1:A:564:MET:HE1	1:A:586:VAL:HG21	1.95	0.48
1:C:203:VAL:HG22	1:C:280:LEU:HD21	1.96	0.48
1:C:260:LYS:HA	1:C:260:LYS:HD3	1.70	0.48
1:D:613:LYS:HG2	1:D:753:PHE:CD2	2.48	0.48
1:D:778:GLN:HG2	1:D:779:ARG:HD2	1.94	0.48
1:F:792:TRP:HE1	1:F:796:ARG:HH11	1.62	0.48
1:B:678:PHE:HB2	1:B:718:LEU:HD23	1.94	0.48
1:F:350:ILE:HG23	5:F:902:ADP:C2	2.48	0.48
1:A:430:LEU:HG	1:A:442:LEU:HD13	1.96	0.48
1:C:259:LEU:HD23	1:C:299:MET:HE3	1.96	0.48
1:E:575:GLN:NE2	1:E:754:GLU:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ILE:CD1	1:C:353:GLY:HA3	2.44	0.48
1:D:768:GLN:HG3	1:D:807:LEU:HD22	1.96	0.48
1:D:817:ASP:O	1:D:821:LYS:HG2	2.14	0.48
1:E:193:VAL:HG11	1:E:202:PRO:HB3	1.95	0.48
1:E:213:THR:HA	1:E:216:VAL:HG12	1.95	0.48
1:E:582:VAL:O	1:E:586:VAL:HG23	2.13	0.48
4:A:901:AGS:O2A	4:A:901:AGS:O2B	2.32	0.48
1:F:222:ARG:HD2	1:F:227:ASP:HB2	1.96	0.48
1:B:799:ASP:C	1:B:801:VAL:H	2.22	0.47
1:D:386:PHE:O	1:D:390:LYS:CB	2.62	0.47
1:F:648:LEU:HD12	1:F:649:ILE:HG12	1.96	0.47
1:E:684:ALA:HB1	1:E:688:VAL:HG11	1.96	0.47
1:F:389:ASP:OD1	1:F:390:LYS:N	2.47	0.47
1:A:381:TYR:HD2	1:A:542:VAL:HG11	1.80	0.47
1:A:669:ARG:HH22	1:B:325:GLU:CD	2.19	0.47
1:A:678:PHE:HB2	1:A:718:LEU:HG	1.96	0.47
1:B:727:SER:OG	1:B:728:ALA:N	2.47	0.47
1:D:235:LYS:HE2	1:D:272:GLN:HA	1.95	0.47
1:F:303:MET:HE2	1:F:303:MET:HB3	1.70	0.47
1:F:822:MET:HE3	1:F:828:VAL:HG21	1.96	0.47
1:B:695:VAL:HG13	1:B:711:PHE:HD2	1.79	0.47
1:F:207:GLU:O	1:F:210:VAL:HG23	2.14	0.47
1:E:648:LEU:HA	1:E:663:GLN:H	1.79	0.47
1:E:749:ASP:OD1	1:E:749:ASP:N	2.47	0.47
1:A:184:ASP:OD1	1:A:185:ASN:N	2.47	0.47
1:A:393:ASP:OD2	1:B:335:GLN:NE2	2.47	0.47
1:A:612:GLY:O	1:A:615:GLU:N	2.48	0.47
1:B:761:LEU:HD12	1:B:764:ILE:HB	1.97	0.47
1:C:646:ALA:HA	1:C:649:ILE:HG22	1.97	0.47
1:D:177:LEU:HD22	1:D:217:GLU:HG2	1.95	0.47
1:D:634:ILE:HD11	1:D:678:PHE:CE1	2.50	0.47
1:E:538:ILE:O	1:E:542:VAL:HG23	2.15	0.47
1:E:727:SER:OG	1:E:728:ALA:N	2.48	0.47
1:E:769:LEU:HD11	1:E:790:LYS:HG2	1.97	0.47
1:F:349:GLY:HA2	1:F:352:ARG:HD2	1.95	0.47
1:A:634:ILE:HD11	1:A:678:PHE:CE1	2.49	0.47
1:B:594:SER:OG	1:B:595:ASP:N	2.47	0.47
1:D:666:GLU:OE2	1:D:669:ARG:NH2	2.48	0.47
1:E:542:VAL:O	1:E:546:THR:HG22	2.15	0.47
1:F:368:ASP:O	1:F:372:VAL:HG22	2.15	0.47
1:B:821:LYS:HB2	1:B:821:LYS:HE3	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HG2	1:D:198:THR:HG23	1.96	0.47
1:A:465:ASN:C	1:A:467:LYS:H	2.23	0.47
1:D:682:GLU:HG2	1:D:683:LYS:HD2	1.97	0.47
1:F:403:ARG:HD2	1:F:406:ILE:HD12	1.97	0.46
1:A:276:PHE:CD1	1:A:312:VAL:HG13	2.50	0.46
1:A:356:ASP:O	1:A:360:VAL:HG23	2.15	0.46
1:C:437:ALA:O	1:C:441:ARG:NH1	2.48	0.46
1:B:229:PRO:O	1:B:233:ARG:HG3	2.15	0.46
1:B:606:LEU:HB3	1:B:720:SER:HB3	1.98	0.46
1:E:613:LYS:HA	1:E:753:PHE:CE2	2.45	0.46
1:A:373:ALA:HA	1:A:376:THR:HG22	1.97	0.46
1:A:695:VAL:HG13	1:A:711:PHE:HD2	1.80	0.46
1:E:786:SER:C	1:E:790:LYS:HE2	2.40	0.46
1:A:685:HIS:O	1:A:687:ASP:N	2.43	0.46
1:B:676:VAL:HB	1:B:716:LEU:HD23	1.98	0.46
1:F:311:LEU:HD12	1:F:311:LEU:O	2.16	0.46
1:D:303:MET:HE2	1:D:309:LEU:HD22	1.97	0.46
1:D:809:ARG:NH1	1:D:813:GLN:HB3	2.31	0.46
4:D:901:AGS:O2A	4:D:901:AGS:O2B	2.34	0.46
1:E:263:LEU:HD21	1:E:300:ILE:HG22	1.96	0.46
1:C:609:THR:OG1	4:C:901:AGS:S1G	2.71	0.46
1:C:792:TRP:HE1	1:C:796:ARG:NH2	2.14	0.46
1:E:792:TRP:HE3	1:E:793:LEU:HD12	1.81	0.46
1:E:798:PHE:CE2	1:E:800:PRO:HB3	2.49	0.46
1:B:785:VAL:HA	1:B:836:VAL:HG22	1.97	0.46
1:C:378:SER:OG	1:C:390:LYS:HG3	2.16	0.46
1:D:789:ALA:HB2	1:D:838:VAL:HG22	1.98	0.46
1:E:573:ILE:N	5:E:902:ADP:HN62	2.05	0.46
2:I:52:GLN:N	2:I:53:PRO:HD2	2.30	0.46
1:A:805:ARG:HD2	1:B:745:ASN:ND2	2.31	0.46
1:F:255:PHE:O	1:F:258:ARG:HG2	2.16	0.46
2:I:149:THR:HG23	2:I:188:VAL:HB	1.98	0.46
1:C:277:ILE:HD12	1:C:311:LEU:HD11	1.97	0.45
1:C:594:SER:OG	1:C:595:ASP:N	2.48	0.45
1:F:786:SER:O	1:F:790:LYS:HG3	2.16	0.45
1:B:358:TYR:HE1	1:C:197:ARG:HH21	1.63	0.45
1:B:380:ARG:NH2	1:B:596:PRO:O	2.49	0.45
1:D:220:ALA:HB2	1:D:237:ILE:HD11	1.97	0.45
1:E:161:LEU:HD22	1:E:261:ALA:HB1	1.97	0.45
1:A:278:ASP:OD1	1:A:278:ASP:N	2.49	0.45
1:A:633:ARG:NH2	1:B:698:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLU:OE2	1:B:669:ARG:NE	2.45	0.45
1:D:699:GLY:HA2	1:D:711:PHE:HB2	1.97	0.45
1:D:822:MET:HG3	1:D:827:GLN:HE21	1.81	0.45
1:F:263:LEU:HD23	1:F:266:ILE:HD12	1.98	0.45
1:F:373:ALA:HB3	1:F:538:ILE:HD12	1.98	0.45
1:A:434:GLU:H	1:A:434:GLU:CD	2.25	0.45
1:A:529:LEU:HD22	1:A:529:LEU:HA	1.77	0.45
1:A:681:ILE:HG12	1:A:718:LEU:HD23	1.98	0.45
1:D:778:GLN:NE2	1:E:592:GLY:O	2.49	0.45
1:F:382:ILE:HD11	1:F:542:VAL:HA	1.99	0.45
1:A:495:ASP:OD1	1:A:495:ASP:C	2.60	0.45
1:B:249:SER:HB2	1:C:252:ARG:HH21	1.82	0.45
1:E:726:GLY:N	1:E:730:GLN:HE21	2.15	0.45
1:E:744:ILE:HA	1:E:747:LEU:HD13	1.98	0.45
1:A:389:ASP:OD1	1:A:390:LYS:N	2.49	0.45
1:A:413:ILE:HG12	1:A:459:LEU:HD23	1.99	0.45
1:E:207:GLU:OE1	1:E:207:GLU:N	2.49	0.45
1:E:304:LEU:HA	1:E:309:LEU:HD21	1.97	0.45
1:F:573:ILE:HG23	1:F:763:ARG:HH21	1.80	0.45
1:A:364:VAL:HG21	1:A:402:LEU:HD23	1.98	0.45
1:D:180:VAL:HA	4:D:902:AGS:N1	2.32	0.45
1:E:200:ASN:OD1	1:E:201:ASN:ND2	2.49	0.45
1:E:322:LYS:O	1:E:326:LYS:HG2	2.16	0.45
1:F:379:ASP:OD1	1:F:380:ARG:N	2.45	0.45
1:C:177:LEU:HD13	1:C:217:GLU:HG2	1.99	0.45
1:F:694:GLN:NE2	1:F:701:LEU:HA	2.32	0.45
1:B:196:ARG:HG3	1:B:200:ASN:HB3	1.98	0.45
1:C:231:SER:O	1:C:231:SER:OG	2.35	0.45
1:D:545:TRP:CD1	1:D:546:THR:HG23	2.43	0.45
1:F:298:ASN:N	1:F:301:LYS:HD3	2.32	0.45
1:C:267:LYS:HB3	1:C:267:LYS:HE2	1.80	0.44
1:E:762:VAL:HA	1:E:765:VAL:HG12	1.99	0.44
1:F:561:LEU:O	1:F:587:ARG:HD3	2.16	0.44
1:F:726:GLY:HA3	1:F:730:GLN:HB2	1.99	0.44
1:A:504:TYR:CD1	1:A:504:TYR:C	2.95	0.44
1:A:769:LEU:HD23	1:A:769:LEU:HA	1.81	0.44
1:C:776:LEU:HD11	1:C:819:LEU:HD21	1.98	0.44
1:C:805:ARG:NH2	4:C:901:AGS:S1G	2.89	0.44
1:F:162:GLN:OE1	1:F:162:GLN:N	2.48	0.44
1:A:799:ASP:OD1	1:A:799:ASP:N	2.48	0.44
1:C:193:VAL:O	1:C:196:ARG:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ASP:OD1	1:F:168:LEU:N	2.51	0.44
1:B:328:ALA:HA	1:B:331:GLU:HG3	1.99	0.44
1:C:805:ARG:NH2	1:D:746:ARG:HH21	2.16	0.44
1:A:303:MET:HB3	1:A:309:LEU:HD13	2.00	0.44
1:A:500:ALA:O	1:A:501:GLU:C	2.59	0.44
1:C:545:TRP:O	1:C:546:THR:OG1	2.36	0.44
1:E:277:ILE:HG22	1:E:280:LEU:HB3	1.99	0.44
1:E:372:VAL:O	1:E:376:THR:HG23	2.17	0.44
1:F:168:LEU:HD12	1:F:168:LEU:HA	1.86	0.44
1:B:808:ARG:HH22	1:C:598:ARG:HH11	1.65	0.44
1:A:598:ARG:HG2	1:A:599:PRO:O	2.18	0.44
1:A:685:HIS:C	1:A:687:ASP:H	2.26	0.44
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.82	0.44
1:D:693:LEU:O	1:D:746:ARG:NH1	2.50	0.44
1:E:575:GLN:O	1:E:579:VAL:HG23	2.18	0.44
1:E:784:GLN:HB2	1:E:833:THR:O	2.18	0.44
1:F:347:THR:HA	1:F:350:ILE:HD12	1.99	0.44
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.82	0.44
1:B:211:GLY:HA2	4:B:901:AGS:O2A	2.17	0.44
1:B:826:GLY:O	1:B:827:GLN:HG2	2.18	0.44
1:D:760:GLU:HG2	1:D:763:ARG:NH2	2.33	0.44
1:E:563:ARG:C	1:E:565:GLU:H	2.26	0.44
1:E:699:GLY:O	1:E:712:ARG:NH2	2.51	0.44
1:E:729:GLU:OE1	1:E:729:GLU:N	2.51	0.44
1:F:307:GLY:N	1:F:308:GLU:OE1	2.51	0.44
1:F:573:ILE:O	4:F:901:AGS:N6	2.50	0.44
1:F:649:ILE:HG23	1:F:703:ASP:HA	2.00	0.44
1:A:237:ILE:HG12	1:A:274:ILE:HB	2.00	0.44
1:C:832:ASP:OD1	1:C:832:ASP:N	2.51	0.44
1:E:349:GLY:HA2	1:E:352:ARG:HG2	2.00	0.44
1:A:819:LEU:O	1:A:823:LEU:HB2	2.18	0.43
1:C:199:LYS:HE3	1:C:335:GLN:HE21	1.82	0.43
1:A:792:TRP:HE1	1:A:796:ARG:CZ	2.31	0.43
1:B:428:MET:HE3	1:B:428:MET:HB3	1.81	0.43
1:C:757:ASN:ND2	1:C:760:GLU:OE2	2.51	0.43
1:F:258:ARG:HG3	1:F:259:LEU:HD22	1.99	0.43
1:F:367:THR:OG1	1:F:369:SER:OG	2.27	0.43
1:A:539:ALA:HB1	1:A:550:ALA:O	2.18	0.43
1:A:817:ASP:OD2	1:A:818:GLN:N	2.51	0.43
1:B:422:ARG:HD2	1:C:181:ILE:HG23	2.01	0.43
1:D:613:LYS:HZ3	4:D:903:AGS:PB	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ARG:HE	1:E:224:VAL:HG23	1.82	0.43
1:E:302:PRO:O	1:E:306:ARG:NH2	2.51	0.43
1:B:808:ARG:NH2	1:C:598:ARG:HD2	2.32	0.43
1:D:647:ARG:NH2	1:E:703:ASP:O	2.52	0.43
4:E:901:AGS:O2A	4:E:901:AGS:O1B	2.35	0.43
1:B:318:ASP:OD1	1:B:321:ARG:NE	2.49	0.43
1:B:455:LYS:HG3	1:B:459:LEU:HD13	1.99	0.43
1:D:792:TRP:CZ3	1:D:843:ASP:HB2	2.53	0.43
1:E:201:ASN:HB2	1:E:311:LEU:O	2.18	0.43
1:F:278:ASP:OD2	1:F:279:GLU:HG2	2.19	0.43
1:F:365:ARG:HB2	1:F:532:GLU:HB2	2.00	0.43
1:B:553:LEU:HD21	1:B:590:ARG:HB3	2.01	0.43
1:B:634:ILE:HD11	1:B:678:PHE:CE1	2.54	0.43
1:D:659:GLU:H	1:D:659:GLU:CD	2.23	0.43
1:E:636:MET:HB3	1:E:684:ALA:HB2	2.00	0.43
1:F:632:VAL:HG12	1:F:676:VAL:HG23	2.01	0.43
1:F:761:LEU:HD23	1:F:761:LEU:HA	1.82	0.43
1:F:827:GLN:H	1:F:829:HIS:CE1	2.37	0.43
1:B:199:LYS:HE3	1:B:332:ARG:O	2.18	0.43
1:C:411:VAL:O	1:C:412:GLU:HG2	2.19	0.43
1:C:423:LEU:HD22	1:C:445:LEU:HD11	2.00	0.43
1:D:240:LEU:HD23	1:D:277:ILE:HD11	2.01	0.43
1:D:389:ASP:OD1	1:D:390:LYS:N	2.51	0.43
1:F:276:PHE:HD1	1:F:312:VAL:HG13	1.83	0.43
1:F:344:VAL:HG22	1:F:387:LEU:HD21	2.00	0.43
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.84	0.43
1:B:631:MET:HE2	1:B:633:ARG:NH1	2.32	0.43
1:C:281:HIS:NE2	1:C:319:GLU:OE1	2.52	0.43
1:F:211:GLY:O	1:F:215:ILE:HG13	2.17	0.43
1:F:235:LYS:HA	1:F:235:LYS:HD3	1.70	0.43
1:F:554:LEU:HB3	1:F:557:GLU:HG2	2.01	0.43
1:C:546:THR:O	1:C:546:THR:OG1	2.36	0.43
1:D:636:MET:HE1	1:D:688:VAL:HG11	2.01	0.43
1:E:783:LEU:HA	1:E:834:VAL:HG22	2.00	0.43
1:A:196:ARG:HD2	1:A:198:THR:O	2.18	0.43
1:A:321:ARG:NH1	1:F:659:GLU:O	2.42	0.43
1:C:790:LYS:HE3	1:C:790:LYS:HB2	1.83	0.43
1:D:213:THR:HG22	1:D:217:GLU:OE1	2.19	0.43
1:F:703:ASP:OD1	1:F:703:ASP:N	2.51	0.43
1:A:211:GLY:HA2	4:A:901:AGS:O2A	2.18	0.42
1:A:242:LEU:HA	1:A:245:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ARG:HA	1:B:325:GLU:HB2	2.00	0.42
1:B:332:ARG:HH21	1:B:333:ARG:NH2	2.17	0.42
1:B:435:ASP:OD2	1:B:436:GLU:N	2.52	0.42
1:C:276:PHE:HA	1:C:312:VAL:O	2.19	0.42
1:C:363:GLY:O	1:C:403:ARG:NH1	2.51	0.42
1:A:180:VAL:HG21	1:A:218:GLY:HA2	2.00	0.42
1:A:573:ILE:HD11	1:A:767:ILE:HD12	2.00	0.42
1:C:211:GLY:HA2	4:D:901:AGS:O2A	2.19	0.42
1:C:642:LYS:HB3	1:C:642:LYS:HE3	1.90	0.42
1:C:677:LEU:HD22	1:C:679:ASP:OD2	2.19	0.42
1:D:204:LEU:HD23	1:D:337:VAL:HB	2.01	0.42
1:B:358:TYR:CD1	1:C:197:ARG:HD3	2.54	0.42
1:C:321:ARG:HA	1:C:325:GLU:HB3	2.01	0.42
1:D:280:LEU:HD23	1:D:313:GLY:HA3	2.00	0.42
1:F:343:SER:O	1:F:347:THR:HG23	2.19	0.42
1:B:226:GLY:O	1:B:233:ARG:NH1	2.52	0.42
1:E:799:ASP:O	1:E:801:VAL:N	2.49	0.42
1:F:387:LEU:HB3	1:F:388:PRO:HD3	2.00	0.42
1:A:545:TRP:O	1:A:547:GLY:N	2.53	0.42
1:A:578:ALA:HA	1:A:751:LEU:HD13	2.01	0.42
1:A:645:VAL:HG22	1:A:688:VAL:HG22	2.01	0.42
1:A:682:GLU:OE2	1:A:683:LYS:NZ	2.51	0.42
1:B:778:GLN:N	1:B:778:GLN:OE1	2.53	0.42
1:F:300:ILE:HD11	1:F:309:LEU:HD11	2.02	0.42
1:F:351:LEU:O	1:F:355:LYS:N	2.47	0.42
1:F:678:PHE:HB2	1:F:718:LEU:HG	2.01	0.42
2:I:147:GLU:HB2	2:I:148:PRO:HD3	2.02	0.42
1:A:530:LYS:C	1:A:531:GLU:CG	2.61	0.42
1:A:660:ALA:HA	1:B:321:ARG:HH22	1.84	0.42
1:A:826:GLY:O	1:A:827:GLN:HG2	2.19	0.42
1:B:411:VAL:C	1:B:413:ILE:H	2.28	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.78	0.42
1:D:322:LYS:HE3	1:D:323:HIS:NE2	2.35	0.42
1:D:585:ALA:HB2	1:D:603:PHE:HZ	1.84	0.42
1:E:554:LEU:HD23	1:E:554:LEU:HA	1.80	0.42
1:F:690:ASP:O	1:F:693:LEU:HB3	2.20	0.42
1:A:311:LEU:O	1:A:311:LEU:HD23	2.19	0.42
1:B:602:ALA:HA	1:B:716:LEU:O	2.20	0.42
1:B:784:GLN:HB2	1:B:835:PRO:HB3	2.01	0.42
1:C:386:PHE:O	1:C:390:LYS:HG2	2.20	0.42
1:F:651:ALA:HB3	1:F:657:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:772:LEU:O	1:F:776:LEU:HG	2.19	0.42
1:F:774:LYS:HE2	1:F:774:LYS:HB3	1.90	0.42
1:A:194:LEU:HD21	1:A:274:ILE:HG21	2.01	0.42
1:A:641:GLU:O	1:A:644:THR:OG1	2.36	0.42
1:B:201:ASN:ND2	1:B:304:LEU:HD22	2.35	0.42
1:B:260:LYS:HE2	1:B:260:LYS:HB2	1.75	0.42
1:D:378:SER:HB2	1:D:390:LYS:HG2	2.01	0.42
1:E:264:ASP:OD2	1:E:268:ASN:ND2	2.53	0.42
1:E:365:ARG:O	1:E:533:VAL:HG12	2.19	0.42
1:F:694:GLN:O	1:F:698:GLU:HB3	2.20	0.42
1:A:355:LYS:HB2	1:A:371:LEU:HD11	2.01	0.42
1:C:366:ILE:HA	1:C:533:VAL:HG22	2.02	0.42
1:E:264:ASP:O	1:E:268:ASN:ND2	2.53	0.42
1:E:834:VAL:HG23	1:E:834:VAL:O	2.19	0.42
1:F:244:SER:HB2	1:F:258:ARG:NH2	2.34	0.42
1:C:194:LEU:HD11	1:C:310:ARG:HB3	2.01	0.41
1:E:400:SER:OG	1:F:192:GLN:HG2	2.19	0.41
2:I:265:ASN:HA	2:I:266:PRO:HD3	1.91	0.41
1:A:702:THR:OG1	1:F:647:ARG:NH2	2.53	0.41
1:B:583:SER:O	1:B:583:SER:OG	2.36	0.41
1:D:837:ASN:ND2	1:D:845:LEU:O	2.53	0.41
1:F:636:MET:HB2	1:F:680:GLU:O	2.20	0.41
1:F:780:ARG:O	1:F:781:LEU:HD23	2.20	0.41
1:B:245:MET:HE1	1:B:259:LEU:HD13	2.03	0.41
1:B:418:ARG:HG2	1:B:421:ARG:NH2	2.35	0.41
1:D:298:ASN:ND2	1:D:301:LYS:HD2	2.36	0.41
1:D:631:MET:HE1	1:D:677:LEU:HD13	2.02	0.41
4:D:903:AGS:O2A	4:D:903:AGS:O2B	2.38	0.41
1:E:260:LYS:HA	1:E:260:LYS:HD2	1.80	0.41
1:E:278:ASP:OD1	1:E:278:ASP:N	2.50	0.41
1:E:400:SER:OG	1:F:192:GLN:O	2.36	0.41
1:E:775:ARG:HA	1:E:775:ARG:HD3	1.82	0.41
1:F:355:LYS:HB2	1:F:366:ILE:HD11	2.02	0.41
1:F:784:GLN:O	1:F:835:PRO:HA	2.20	0.41
1:D:243:GLY:O	1:D:247:ALA:HB2	2.20	0.41
1:D:254:GLU:O	1:D:257:GLU:HG2	2.20	0.41
1:D:620:LEU:O	1:D:624:LEU:HD23	2.19	0.41
1:B:316:THR:HG21	1:C:329:ALA:HB2	2.03	0.41
1:C:681:ILE:HG22	1:C:720:SER:HB2	2.02	0.41
1:D:237:ILE:HA	1:D:274:ILE:O	2.21	0.41
1:D:358:TYR:CE1	1:E:197:ARG:HD3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:836:VAL:HG23	1:F:845:LEU:HD23	2.02	0.41
1:B:412:GLU:O	1:B:413:ILE:HD13	2.20	0.41
1:B:826:GLY:C	1:B:828:VAL:H	2.28	0.41
2:I:29:ASN:OD1	2:I:30:SER:N	2.53	0.41
1:A:636:MET:HG3	1:A:681:ILE:HD12	2.03	0.41
1:B:393:ASP:OD1	1:C:335:GLN:NE2	2.52	0.41
1:D:822:MET:HG3	1:D:827:GLN:NE2	2.35	0.41
1:E:235:LYS:HD2	1:E:272:GLN:HB2	2.03	0.41
1:E:604:MET:HB2	1:E:718:LEU:O	2.21	0.41
1:B:277:ILE:O	1:B:313:GLY:HA2	2.21	0.41
1:B:597:ASN:OD1	1:B:597:ASN:N	2.53	0.41
1:E:779:ARG:O	1:E:830:ASP:HB3	2.20	0.41
1:F:823:LEU:HD12	1:F:823:LEU:HA	1.87	0.41
1:A:532:GLU:N	1:A:532:GLU:OE1	2.54	0.41
1:A:600:THR:O	1:A:600:THR:OG1	2.37	0.41
1:A:643:HIS:HB2	1:B:655:TYR:OH	2.21	0.41
1:A:691:VAL:O	1:A:695:VAL:HG23	2.21	0.41
1:B:675:VAL:HG23	1:B:715:ILE:HB	2.01	0.41
1:C:355:LYS:HE2	1:C:355:LYS:HB3	1.93	0.41
1:C:543:SER:O	1:C:547:GLY:HA2	2.20	0.41
1:C:787:LEU:HD23	1:C:787:LEU:HA	1.88	0.41
1:C:820:ALA:O	1:C:824:LEU:HG	2.21	0.41
1:D:365:ARG:HB2	1:D:532:GLU:HB2	2.02	0.41
1:E:352:ARG:HE	1:E:352:ARG:HB3	1.68	0.41
1:E:613:LYS:HB2	1:E:613:LYS:HE3	1.84	0.41
1:F:575:GLN:O	1:F:579:VAL:HG22	2.21	0.41
1:F:641:GLU:HG3	1:F:643:HIS:CE1	2.56	0.41
1:B:374:ALA:HA	1:B:538:ILE:HG21	2.02	0.41
1:C:545:TRP:CD1	1:C:546:THR:HG23	2.56	0.41
1:E:368:ASP:O	1:E:372:VAL:HG12	2.21	0.41
1:B:752:ILE:HD13	1:B:752:ILE:HA	1.93	0.40
1:D:593:VAL:HG23	1:D:593:VAL:O	2.21	0.40
1:E:253:GLY:C	1:E:255:PHE:H	2.29	0.40
1:E:824:LEU:HD12	1:F:591:ALA:HB2	2.03	0.40
1:A:322:LYS:HB3	1:A:323:HIS:HD2	1.86	0.40
1:A:327:ASP:O	1:A:329:ALA:N	2.54	0.40
1:A:697:ASP:OD1	1:F:805:ARG:NH1	2.54	0.40
1:C:246:VAL:HG12	1:C:246:VAL:O	2.20	0.40
1:C:759:GLU:OE1	1:C:759:GLU:N	2.46	0.40
1:E:212:LYS:NZ	4:E:901:AGS:O3B	2.54	0.40
1:E:609:THR:OG1	1:E:610:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:739:PHE:HB2	1:F:744:ILE:HD11	2.04	0.40
1:E:534:GLY:H	1:E:537:ASP:CB	2.34	0.40
1:F:183:ARG:O	1:F:187:ILE:HG12	2.21	0.40
2:I:151:ALA:HA	2:I:344:VAL:HG12	2.03	0.40
1:B:766:ASP:OD1	1:B:790:LYS:HD3	2.20	0.40
1:D:666:GLU:OE1	1:D:669:ARG:NH1	2.54	0.40
1:A:432:LYS:H	1:A:432:LYS:HG2	1.60	0.40
1:A:575:GLN:O	1:A:579:VAL:HG23	2.22	0.40
1:B:822:MET:SD	1:B:845:LEU:HD12	2.62	0.40
1:D:184:ASP:OD1	1:D:185:ASN:N	2.54	0.40
1:D:302:PRO:O	1:D:306:ARG:NH2	2.54	0.40
1:E:334:PHE:HD1	1:E:334:PHE:HA	1.80	0.40
1:F:761:LEU:HD12	1:F:798:PHE:HD1	1.86	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	668/848 (79%)	586 (88%)	79 (12%)	3 (0%)	30	60
1	B	615/848 (72%)	555 (90%)	58 (9%)	2 (0%)	36	65
1	C	618/848 (73%)	546 (88%)	71 (12%)	1 (0%)	43	72
1	D	556/848 (66%)	483 (87%)	73 (13%)	0	100	100
1	E	540/848 (64%)	477 (88%)	62 (12%)	1 (0%)	43	72
1	F	538/848 (63%)	472 (88%)	65 (12%)	1 (0%)	43	72
2	I	355/625 (57%)	349 (98%)	6 (2%)	0	100	100
All	All	3890/5713 (68%)	3468 (89%)	414 (11%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLU
1	A	531	GLU
1	B	387	LEU
1	B	388	PRO
1	C	547	GLY
1	F	235	LYS
1	E	566	ASP
1	A	465	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	549/682 (80%)	542 (99%)	7 (1%)	61	71
1	B	507/682 (74%)	504 (99%)	3 (1%)	78	79
1	C	508/682 (74%)	506 (100%)	2 (0%)	84	81
1	D	455/682 (67%)	453 (100%)	2 (0%)	84	81
1	E	448/682 (66%)	447 (100%)	1 (0%)	87	86
1	F	448/682 (66%)	447 (100%)	1 (0%)	87	86
2	I	291/500 (58%)	290 (100%)	1 (0%)	86	83
All	All	3206/4592 (70%)	3189 (100%)	17 (0%)	78	80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	THR
1	A	462	ARG
1	A	464	GLN
1	A	504	TYR
1	A	527	VAL
1	A	529	LEU
1	A	738	THR
1	B	461	THR
1	B	600	THR
1	B	674	THR

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Mol	Chain	Res	Type
1	C	166	THR
1	C	461	THR
1	D	275	THR
1	D	644	THR
1	E	275	THR
1	F	738	THR
2	I	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	ASN
1	A	281	HIS
1	A	323	HIS
1	A	361	HIS
1	A	705	HIS
1	A	784	GLN
1	A	818	GLN
1	B	221	GLN
1	B	361	HIS
1	B	362	HIS
1	B	575	GLN
1	B	685	HIS
1	B	705	HIS
1	B	812	GLN
1	C	221	GLN
1	C	323	HIS
1	C	643	HIS
1	C	685	HIS
1	C	705	HIS
1	C	721	ASN
1	C	730	GLN
1	C	757	ASN
1	C	818	GLN
1	C	827	GLN
1	D	298	ASN
1	D	685	HIS
1	D	782	GLN
1	D	827	GLN
1	E	201	ASN
1	E	272	GLN
1	E	281	HIS

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Mol	Chain	Res	Type
1	E	362	HIS
1	E	685	HIS
1	E	730	GLN
1	E	778	GLN
1	E	784	GLN
1	E	818	GLN
1	E	829	HIS
1	F	268	ASN
1	F	771	GLN
2	I	254	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AGS	A	901	-	32,33,33	0.76	2 (6%)	45,52,52	0.76	1 (2%)
4	AGS	B	901	-	32,33,33	0.85	2 (6%)	45,52,52	0.79	1 (2%)
4	AGS	D	901	-	32,33,33	0.82	3 (9%)	45,52,52	0.78	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	F	902	-	28,29,29	1.40	5 (17%)	43,45,45	1.81	8 (18%)
4	AGS	D	903	-	32,33,33	0.56	1 (3%)	45,52,52	0.72	1 (2%)
4	AGS	B	902	-	32,33,33	0.81	4 (12%)	45,52,52	0.81	1 (2%)
4	AGS	C	901	-	32,33,33	0.74	3 (9%)	45,52,52	0.73	1 (2%)
4	AGS	A	902	-	32,33,33	0.81	3 (9%)	45,52,52	0.80	1 (2%)
4	AGS	F	901	-	32,33,33	0.62	1 (3%)	45,52,52	0.71	1 (2%)
4	AGS	D	902	-	32,33,33	0.75	1 (3%)	45,52,52	0.75	1 (2%)
5	ADP	E	902	-	28,29,29	1.38	4 (14%)	43,45,45	1.87	8 (18%)
4	AGS	E	901	-	32,33,33	0.53	1 (3%)	45,52,52	0.72	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	A	901	-	-	5/21/38/38	0/3/3/3
4	AGS	B	901	-	-	4/21/38/38	0/3/3/3
4	AGS	D	901	-	-	2/21/38/38	0/3/3/3
5	ADP	F	902	-	-	0/16/32/32	0/3/3/3
4	AGS	D	903	-	-	3/21/38/38	0/3/3/3
4	AGS	B	902	-	-	5/21/38/38	0/3/3/3
4	AGS	C	901	-	-	4/21/38/38	0/3/3/3
4	AGS	A	902	-	-	5/21/38/38	0/3/3/3
4	AGS	F	901	-	-	7/21/38/38	0/3/3/3
4	AGS	D	902	-	-	6/21/38/38	0/3/3/3
5	ADP	E	902	-	-	5/16/32/32	0/3/3/3
4	AGS	E	901	-	-	6/21/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	902	ADP	C5-C4	4.66	1.47	1.39
5	E	902	ADP	C5-C4	4.64	1.47	1.39
4	B	901	AGS	PB-O3A	-2.76	1.56	1.59
5	E	902	ADP	C5-C6	2.57	1.48	1.41
5	F	902	ADP	C5-C6	2.57	1.48	1.41
4	D	901	AGS	PB-O3A	-2.43	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	AGS	PB-O3A	-2.43	1.56	1.59
4	B	901	AGS	PA-O3A	-2.41	1.56	1.59
5	F	902	ADP	C5-N7	-2.39	1.34	1.39
5	E	902	ADP	C5-N7	-2.38	1.34	1.39
5	F	902	ADP	C8-N7	2.31	1.36	1.31
4	D	901	AGS	PA-O3A	-2.30	1.57	1.59
4	A	901	AGS	PB-O3A	-2.29	1.57	1.59
5	E	902	ADP	C8-N7	2.20	1.35	1.31
4	A	901	AGS	PA-O3A	-2.14	1.57	1.59
4	D	901	AGS	PG-S1G	2.14	1.95	1.90
4	B	902	AGS	PB-O3A	-2.14	1.57	1.59
4	C	901	AGS	PB-O3A	-2.13	1.57	1.59
4	A	902	AGS	PB-O3B	-2.12	1.57	1.59
4	B	902	AGS	PB-O3B	-2.12	1.57	1.59
4	B	902	AGS	PA-O3A	-2.12	1.57	1.59
4	F	901	AGS	PG-S1G	2.08	1.95	1.90
4	A	902	AGS	PG-S1G	2.07	1.95	1.90
4	D	902	AGS	PB-O3A	-2.07	1.57	1.59
4	C	901	AGS	PA-O3A	-2.04	1.57	1.59
4	E	901	AGS	PG-S1G	2.04	1.95	1.90
4	B	902	AGS	PG-S1G	2.02	1.95	1.90
5	F	902	ADP	C4-N9	-2.01	1.33	1.37
4	C	901	AGS	PG-S1G	2.01	1.95	1.90
4	D	903	AGS	PG-S1G	2.00	1.95	1.90

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	902	ADP	C5-C4-N3	-5.85	118.67	126.72
5	F	902	ADP	C5-C4-N3	-5.67	118.91	126.72
5	E	902	ADP	N3-C4-N9	4.84	135.40	127.17
5	F	902	ADP	N3-C4-N9	4.54	134.88	127.17
4	D	901	AGS	PB-O3B-PG	-4.40	117.08	133.17
4	B	902	AGS	PB-O3B-PG	-4.38	117.13	133.17
4	B	901	AGS	PB-O3B-PG	-4.38	117.15	133.17
4	A	902	AGS	PB-O3B-PG	-4.37	117.17	133.17
4	D	902	AGS	PB-O3B-PG	-4.34	117.30	133.17
4	A	901	AGS	PB-O3B-PG	-4.17	117.89	133.17
4	E	901	AGS	PB-O3B-PG	-4.13	118.07	133.17
4	F	901	AGS	PB-O3B-PG	-4.04	118.38	133.17
4	C	901	AGS	PB-O3B-PG	-3.91	118.86	133.17
4	D	903	AGS	PB-O3B-PG	-3.86	119.05	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	902	ADP	C2-N3-C4	3.73	120.94	111.83
5	F	902	ADP	C2-N3-C4	3.57	120.55	111.83
5	E	902	ADP	N3-C2-N1	-3.32	123.56	128.58
5	F	902	ADP	C4-C5-N7	-3.29	106.82	110.58
5	F	902	ADP	N3-C2-N1	-3.15	123.82	128.58
5	E	902	ADP	C4-C5-N7	-3.11	107.02	110.58
5	E	902	ADP	C4-N9-C8	2.73	108.61	105.74
5	E	902	ADP	C3'-C2'-C1'	2.73	106.62	101.46
5	F	902	ADP	C4-N9-C8	2.68	108.56	105.74
5	F	902	ADP	C5-N7-C8	2.39	107.20	103.45
5	E	902	ADP	C5-N7-C8	2.37	107.17	103.45
5	F	902	ADP	C3'-C2'-C1'	2.32	105.84	101.46

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	AGS	PB-O3B-PG-O2G
4	A	901	AGS	PB-O3B-PG-O3G
4	A	901	AGS	C5'-O5'-PA-O1A
4	A	901	AGS	C5'-O5'-PA-O2A
4	A	901	AGS	C5'-O5'-PA-O3A
4	A	902	AGS	C5'-O5'-PA-O1A
4	A	902	AGS	C5'-O5'-PA-O2A
4	A	902	AGS	C5'-O5'-PA-O3A
4	B	901	AGS	PB-O3B-PG-O2G
4	B	901	AGS	PB-O3B-PG-O3G
4	B	902	AGS	PB-O3B-PG-O2G
4	B	902	AGS	PB-O3B-PG-O3G
4	B	902	AGS	C5'-O5'-PA-O1A
4	C	901	AGS	PB-O3B-PG-O2G
4	C	901	AGS	PB-O3B-PG-O3G
4	D	902	AGS	PB-O3B-PG-O2G
4	D	902	AGS	PB-O3B-PG-O3G
4	D	902	AGS	C5'-O5'-PA-O2A
4	D	903	AGS	PB-O3B-PG-O2G
4	D	903	AGS	PB-O3B-PG-O3G
4	D	903	AGS	C5'-O5'-PA-O1A
4	E	901	AGS	C5'-O5'-PA-O1A
4	E	901	AGS	C5'-O5'-PA-O2A
4	F	901	AGS	PB-O3B-PG-O2G
4	F	901	AGS	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	F	901	AGS	O4'-C4'-C5'-O5'
4	E	901	AGS	O4'-C4'-C5'-O5'
4	B	901	AGS	O4'-C4'-C5'-O5'
4	B	902	AGS	C3'-C4'-C5'-O5'
4	E	901	AGS	C3'-C4'-C5'-O5'
4	F	901	AGS	C3'-C4'-C5'-O5'
4	D	901	AGS	O4'-C4'-C5'-O5'
4	B	902	AGS	O4'-C4'-C5'-O5'
5	E	902	ADP	O4'-C4'-C5'-O5'
5	E	902	ADP	C3'-C4'-C5'-O5'
4	B	901	AGS	C3'-C4'-C5'-O5'
4	D	901	AGS	C3'-C4'-C5'-O5'
4	D	902	AGS	O4'-C4'-C5'-O5'
4	D	902	AGS	C5'-O5'-PA-O1A
4	D	902	AGS	C5'-O5'-PA-O3A
4	E	901	AGS	C5'-O5'-PA-O3A
4	F	901	AGS	C5'-O5'-PA-O1A
4	F	901	AGS	C5'-O5'-PA-O2A
4	F	901	AGS	C5'-O5'-PA-O3A
5	E	902	ADP	C5'-O5'-PA-O1A
5	E	902	ADP	C5'-O5'-PA-O2A
5	E	902	ADP	C5'-O5'-PA-O3A
4	A	902	AGS	PA-O3A-PB-O2B
4	C	901	AGS	PB-O3A-PA-O2A
4	A	902	AGS	PA-O3A-PB-O1B
4	C	901	AGS	PB-O3A-PA-O1A
4	E	901	AGS	PA-O3A-PB-O2B

There are no ring outliers.

12 monomers are involved in 43 short contacts:

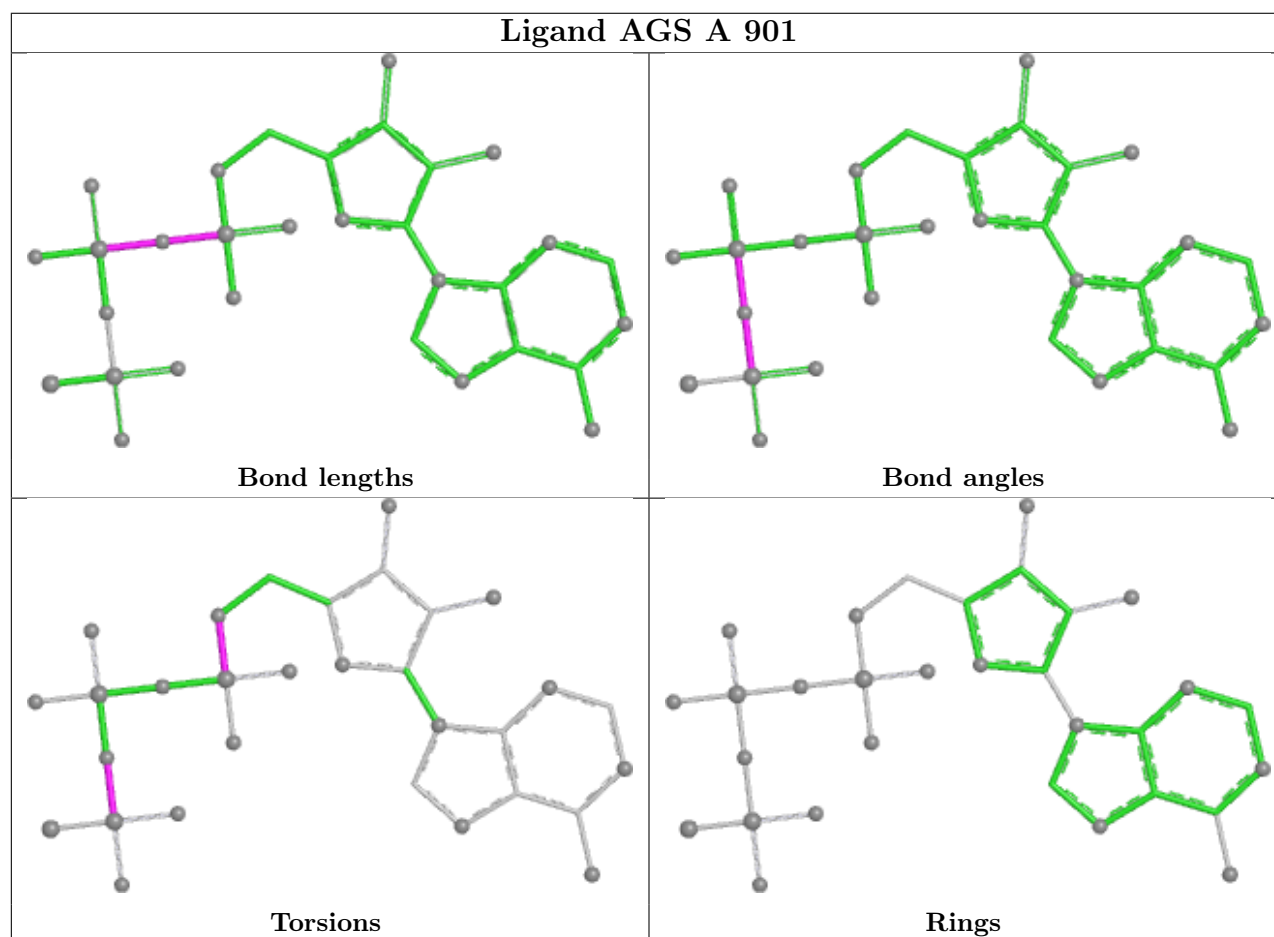
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	AGS	3	0
4	B	901	AGS	3	0
4	D	901	AGS	3	0
5	F	902	ADP	2	0
4	D	903	AGS	3	0
4	B	902	AGS	4	0
4	C	901	AGS	6	0
4	A	902	AGS	4	0
4	F	901	AGS	3	0
4	D	902	AGS	4	0

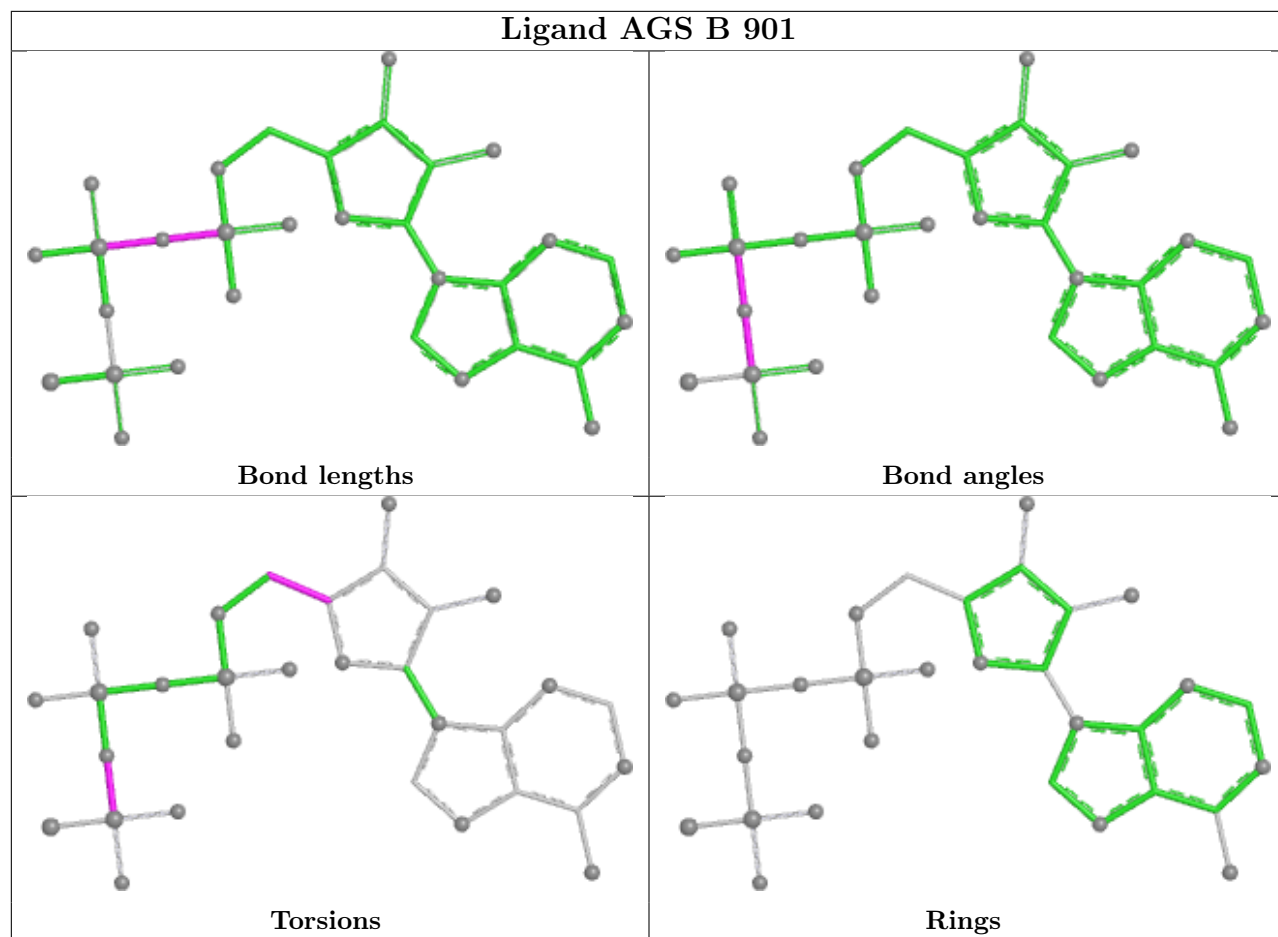
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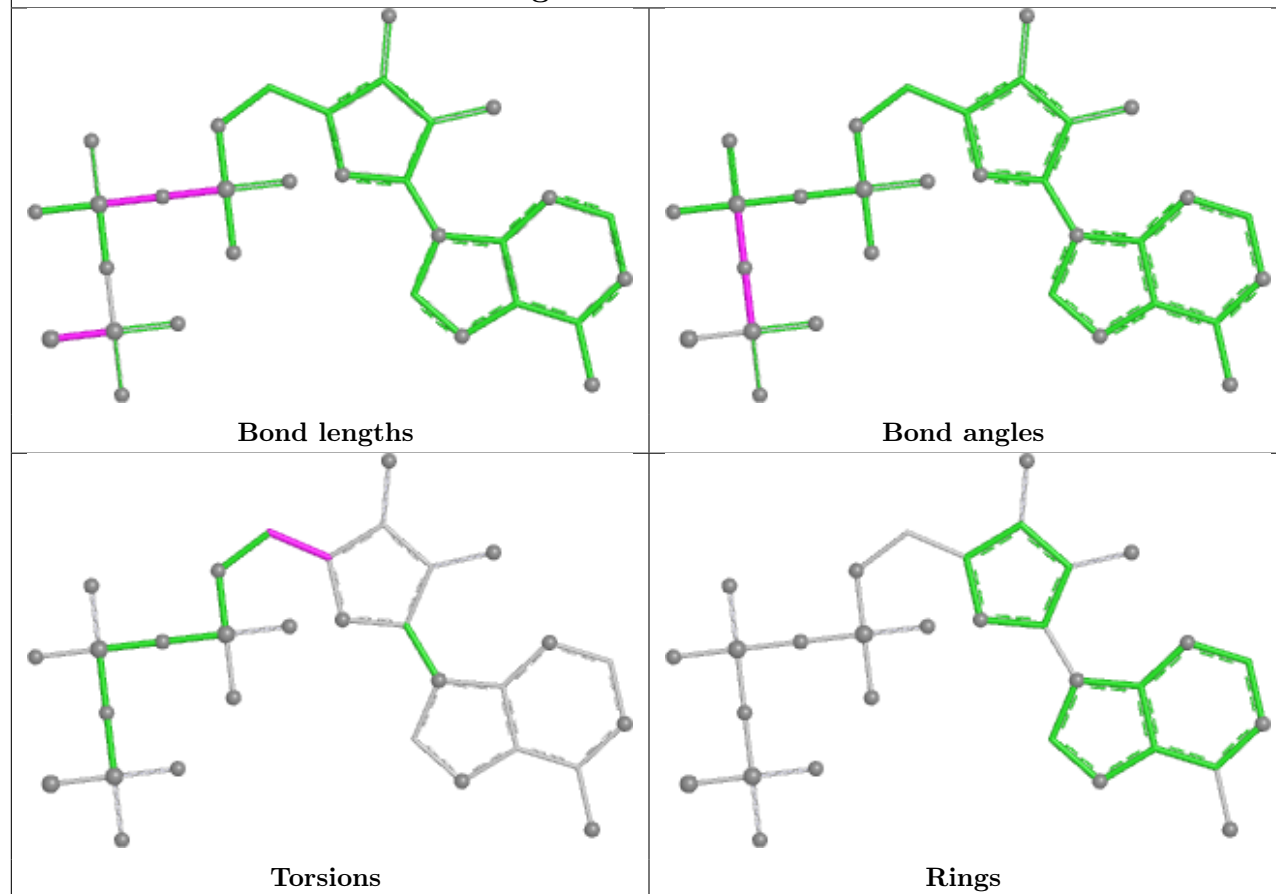
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	902	ADP	4	0
4	E	901	AGS	4	0

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.

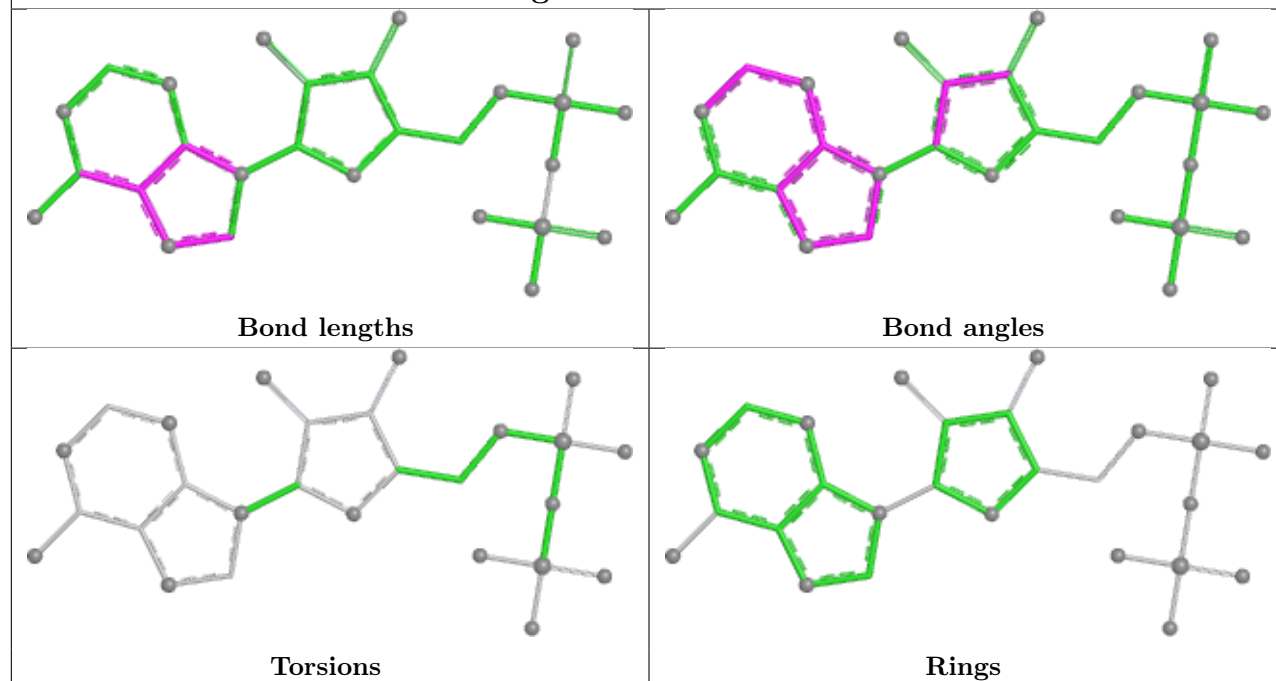


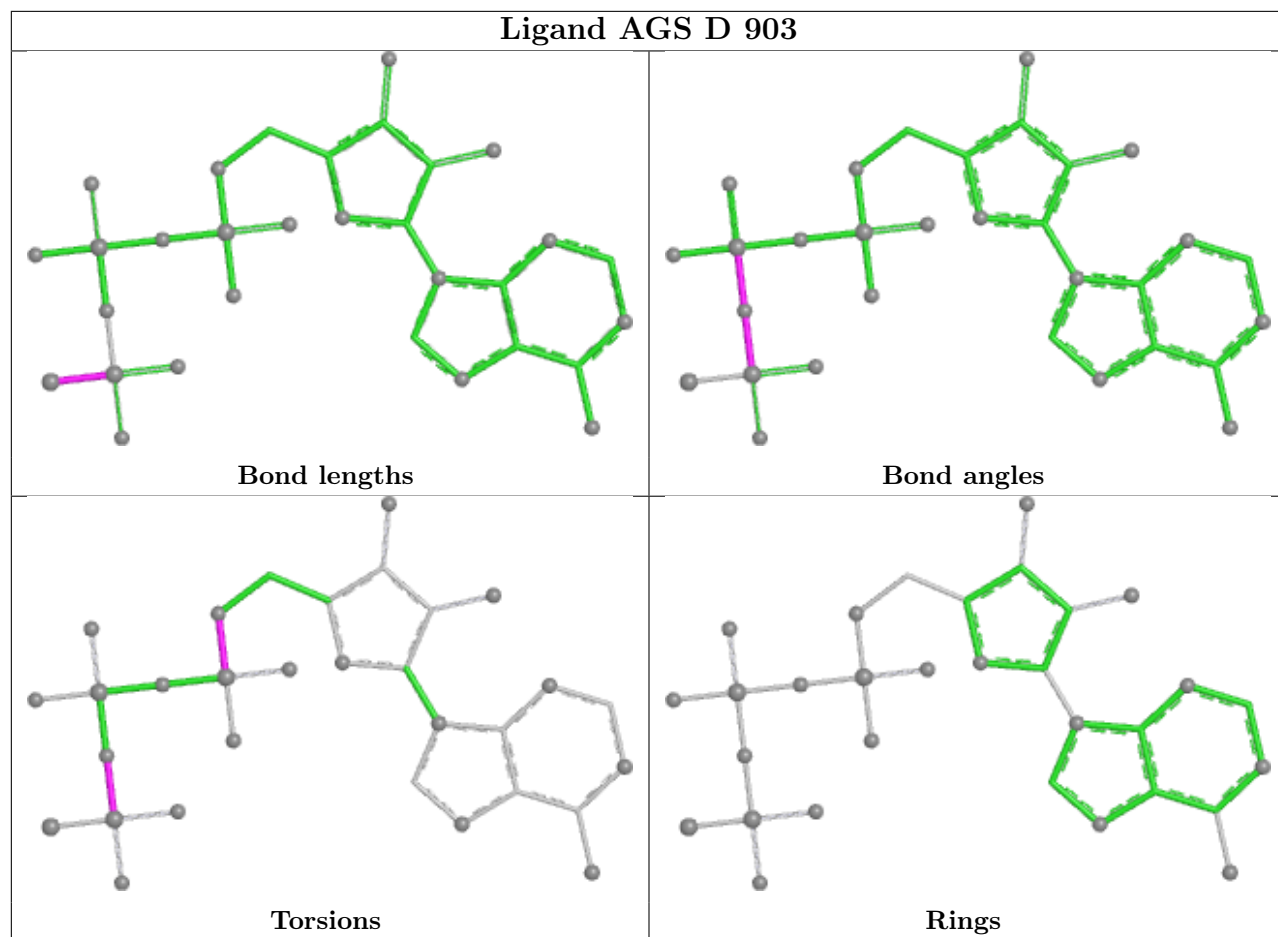


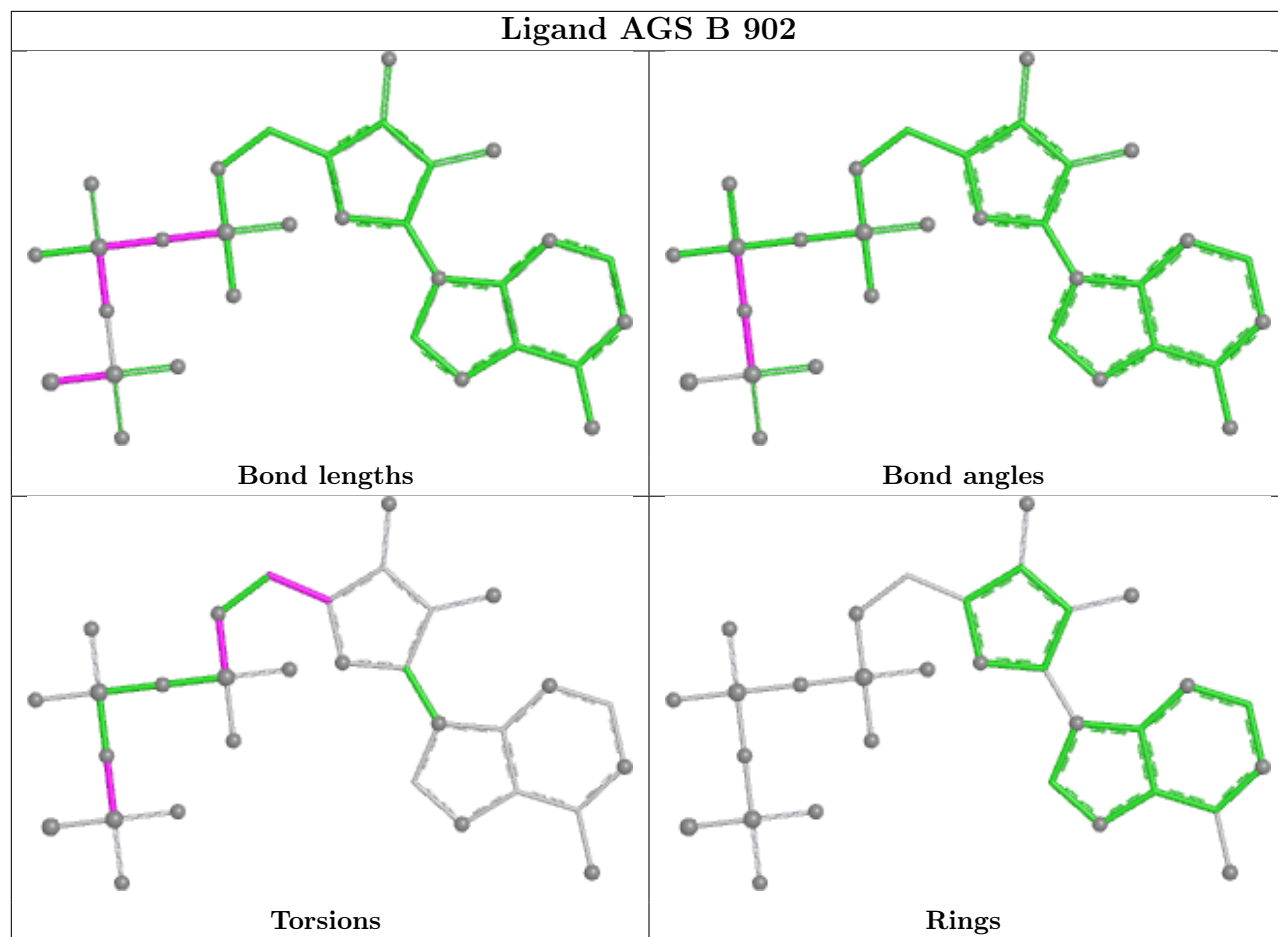
Ligand AGS D 901

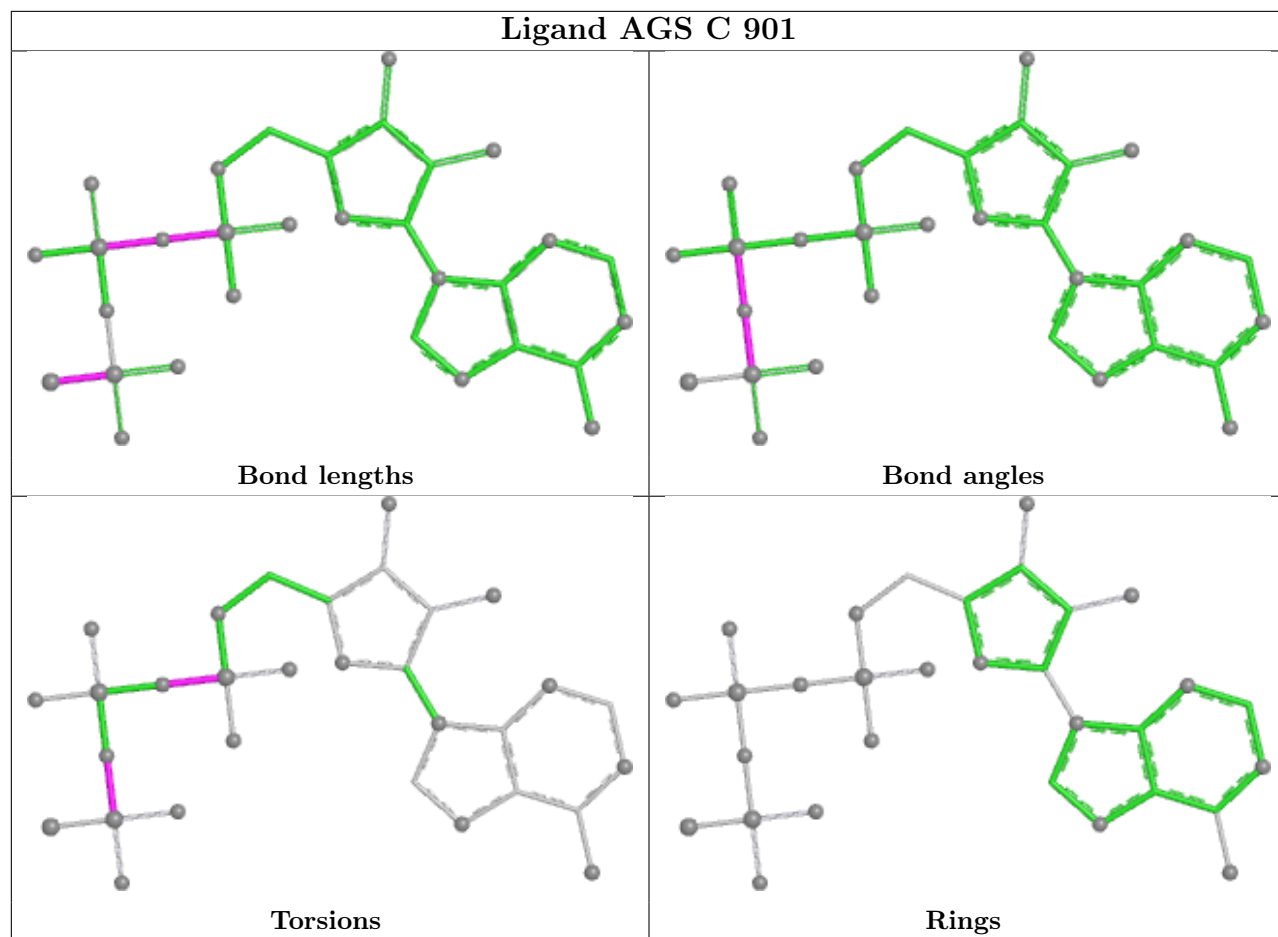


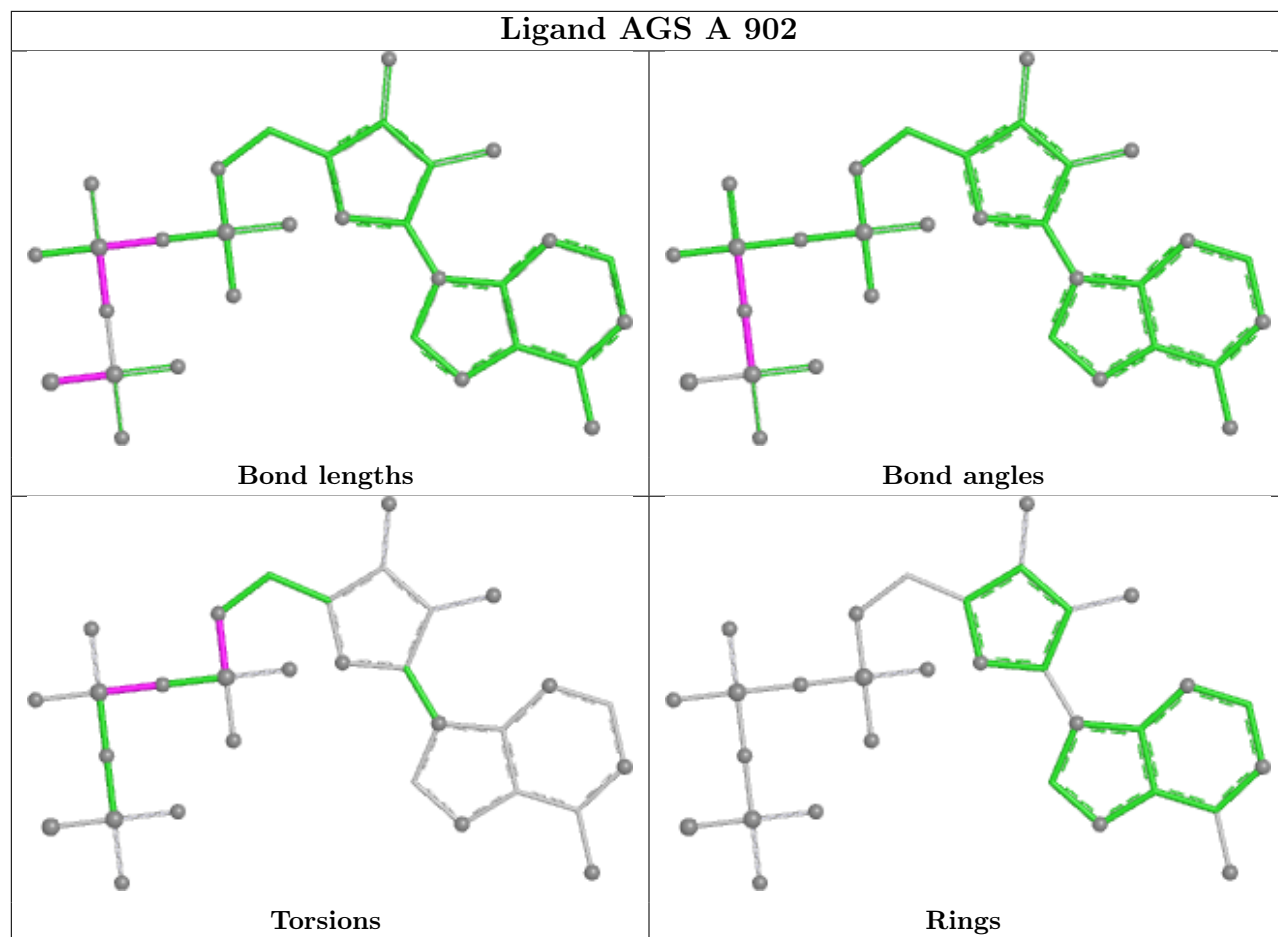
Ligand ADP F 902

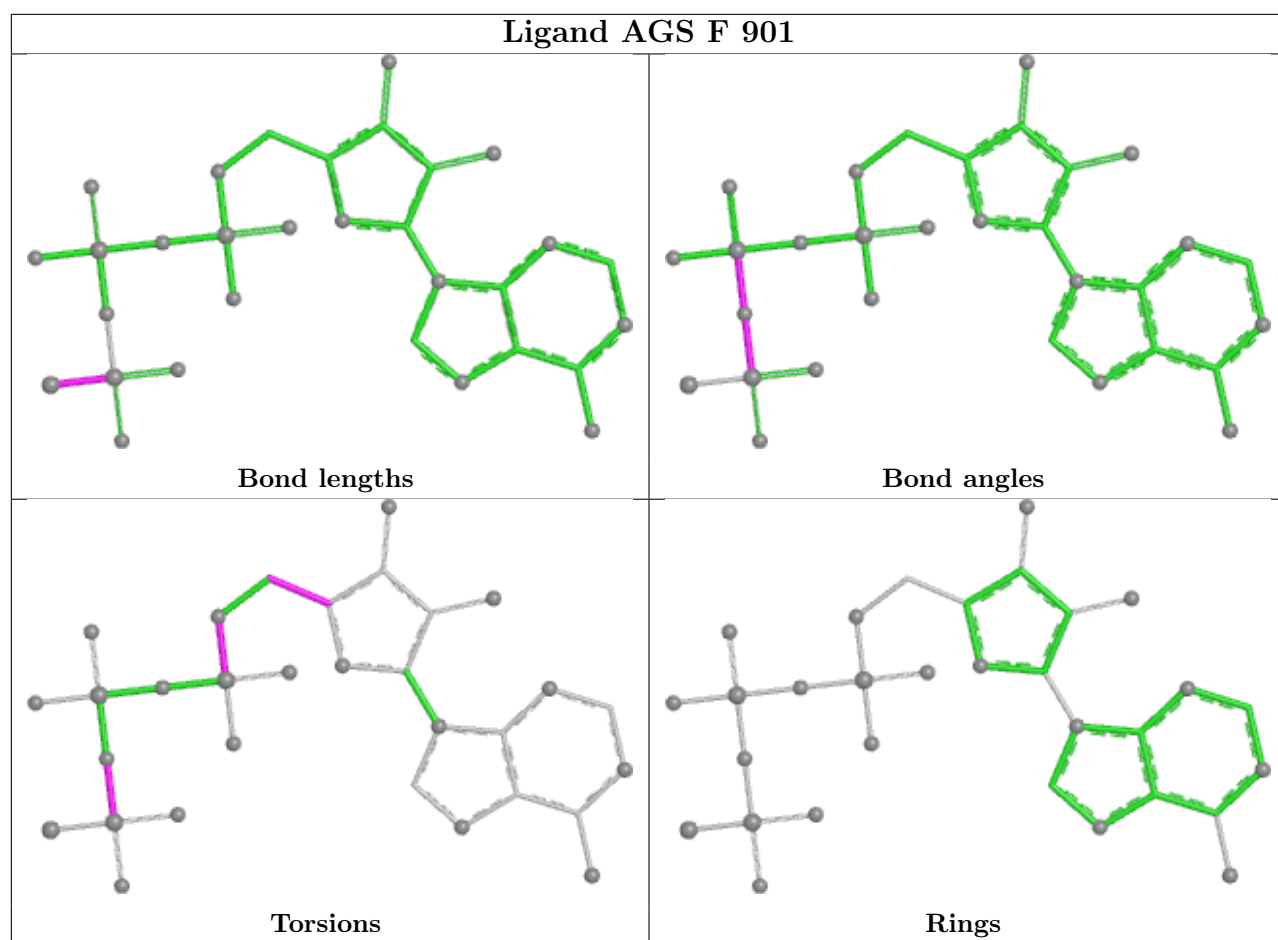




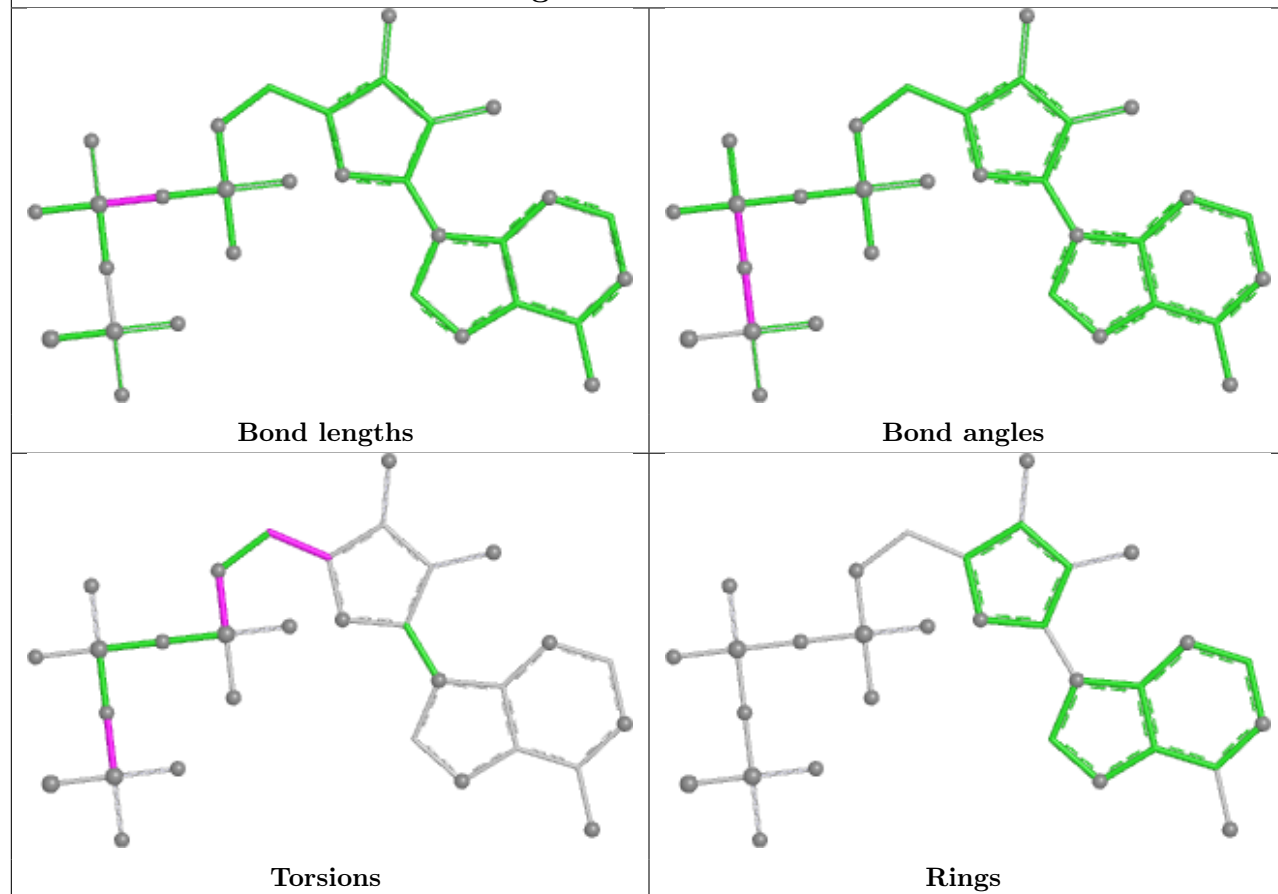




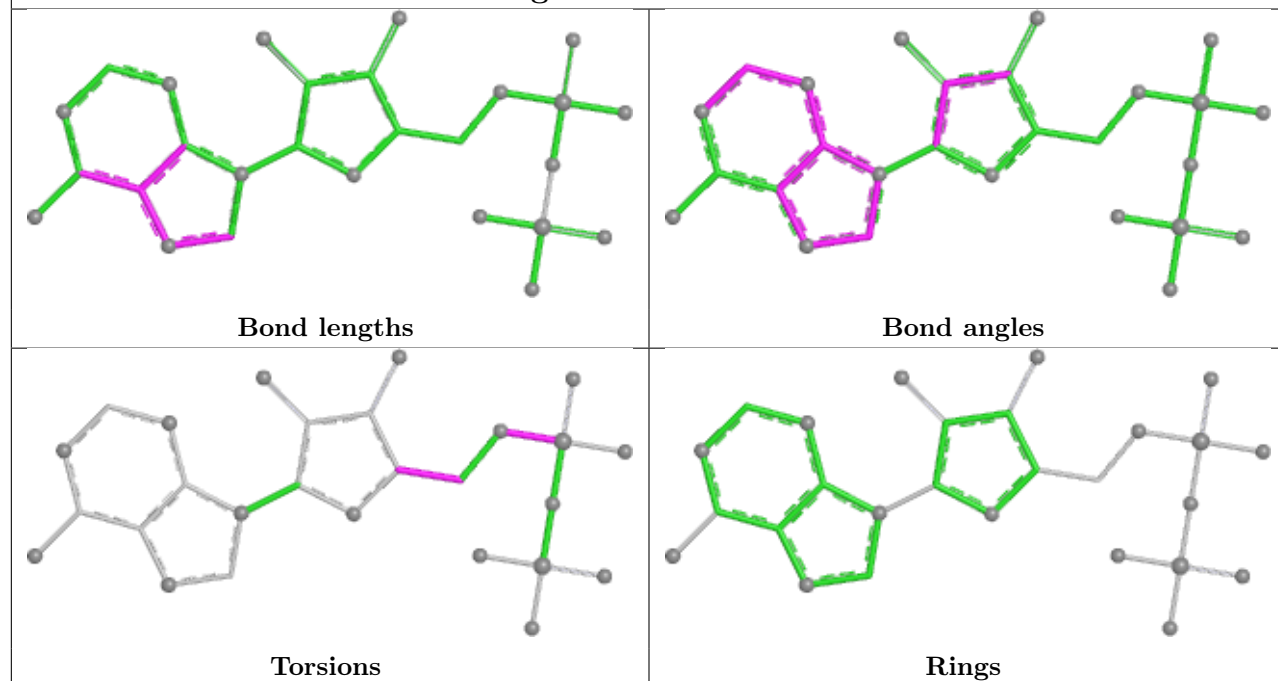


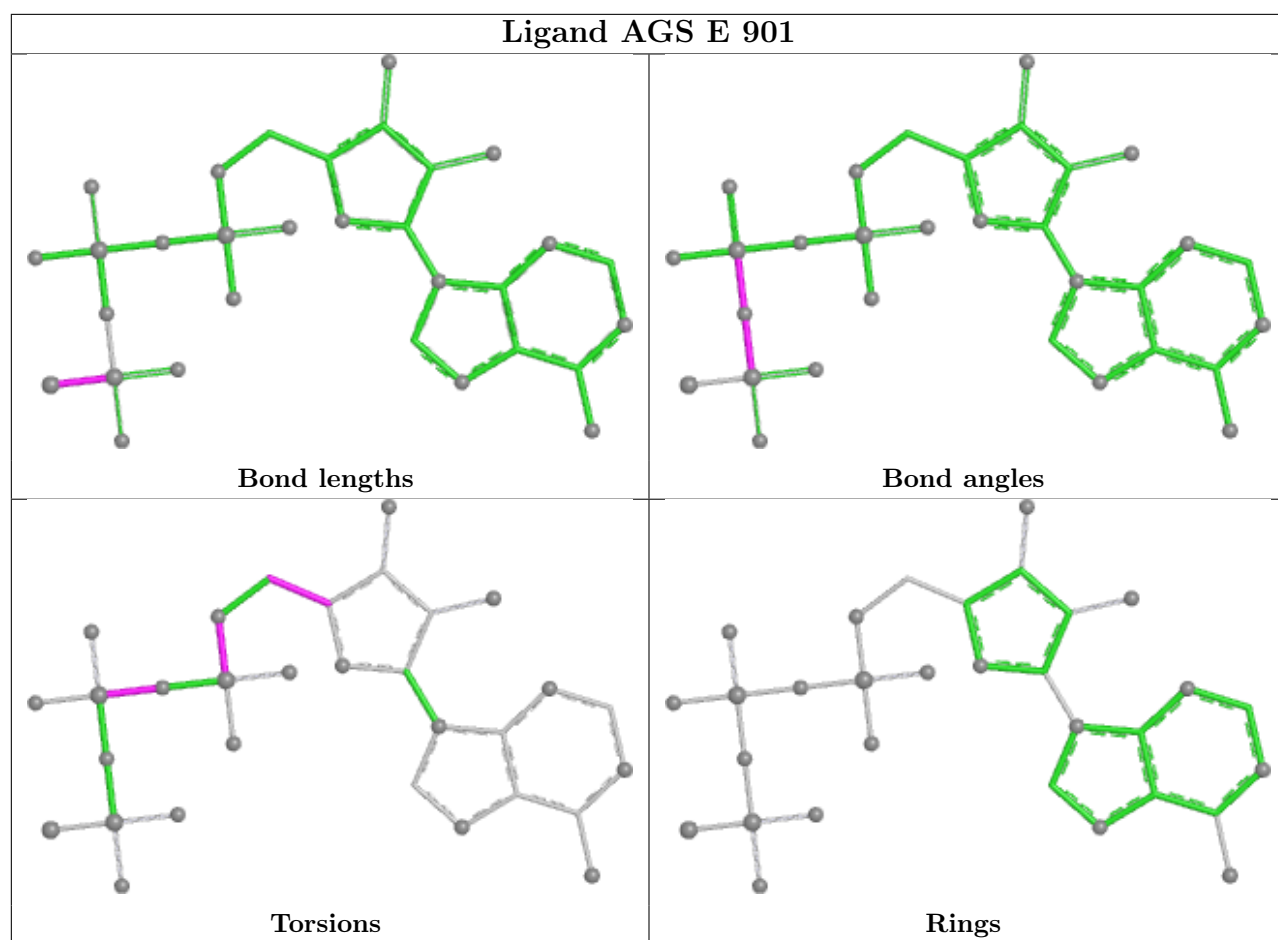


Ligand AGS D 902



Ligand ADP E 902





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.

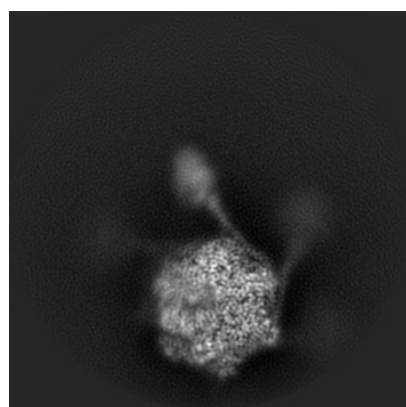
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21553. These allow visual inspection of the internal detail of the map and identification of artifacts.

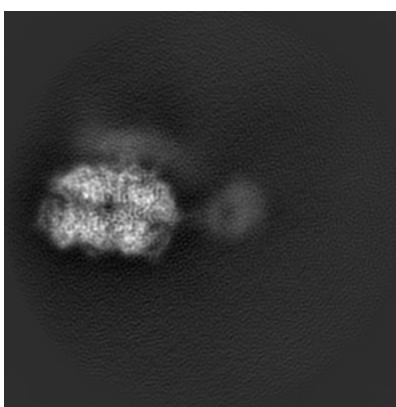
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

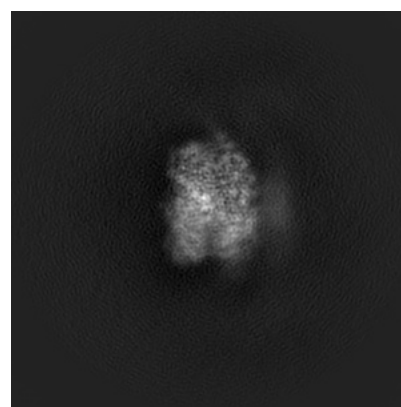
6.1.1 Primary map



X



Y

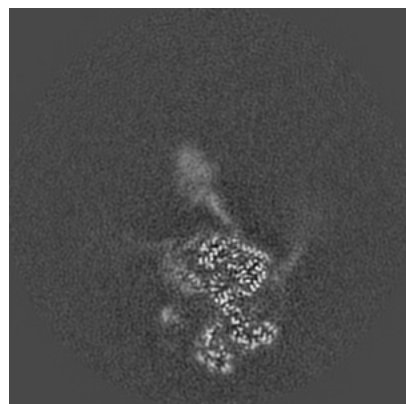


Z

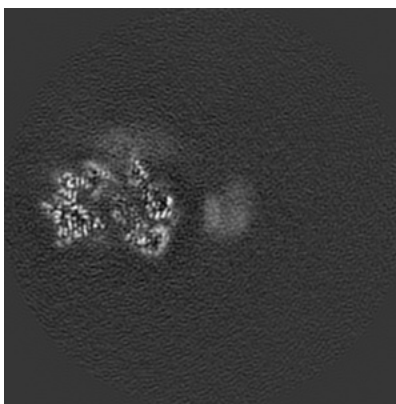
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

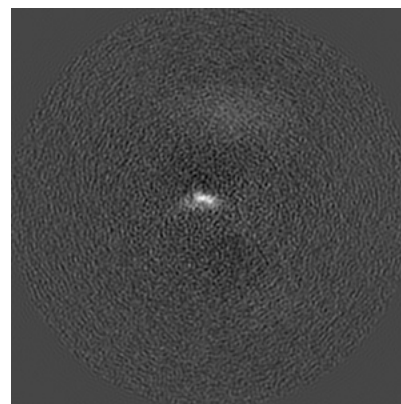
6.2.1 Primary map



X Index: 180



Y Index: 180

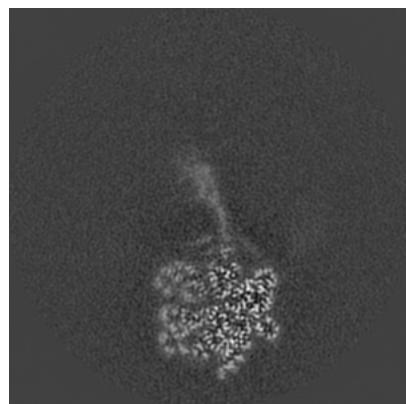


Z Index: 180

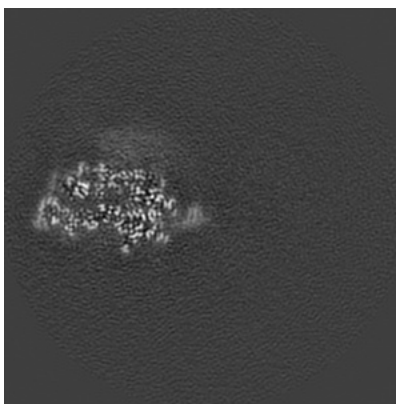
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

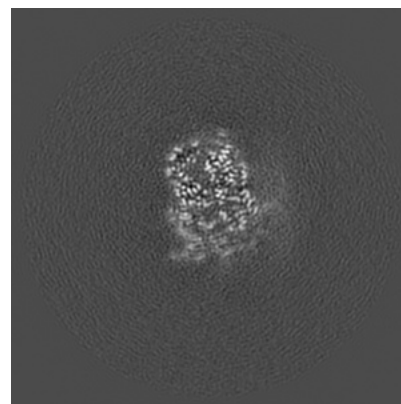
6.3.1 Primary map



X Index: 165



Y Index: 193

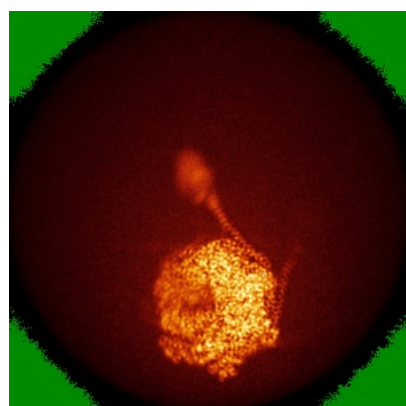


Z Index: 118

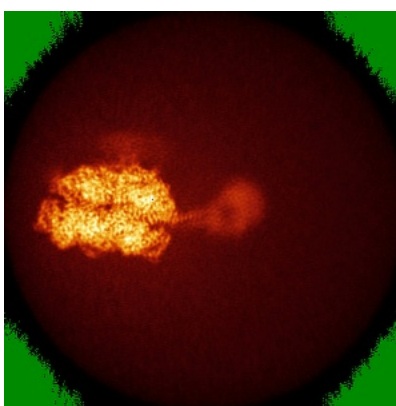
The images above show the largest variance slices of the map in three orthogonal directions.

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

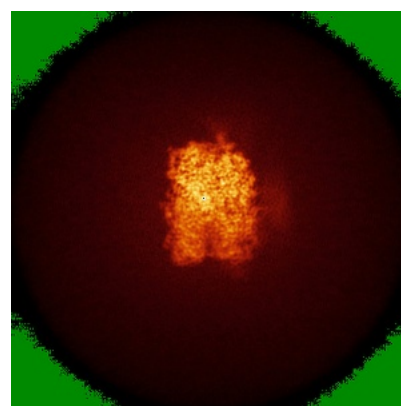
6.4.1 Primary map



X



Y

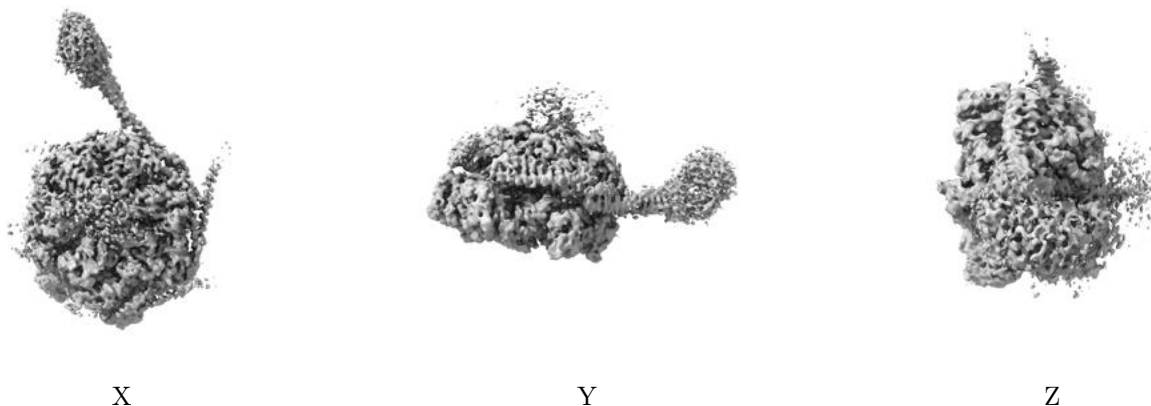


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

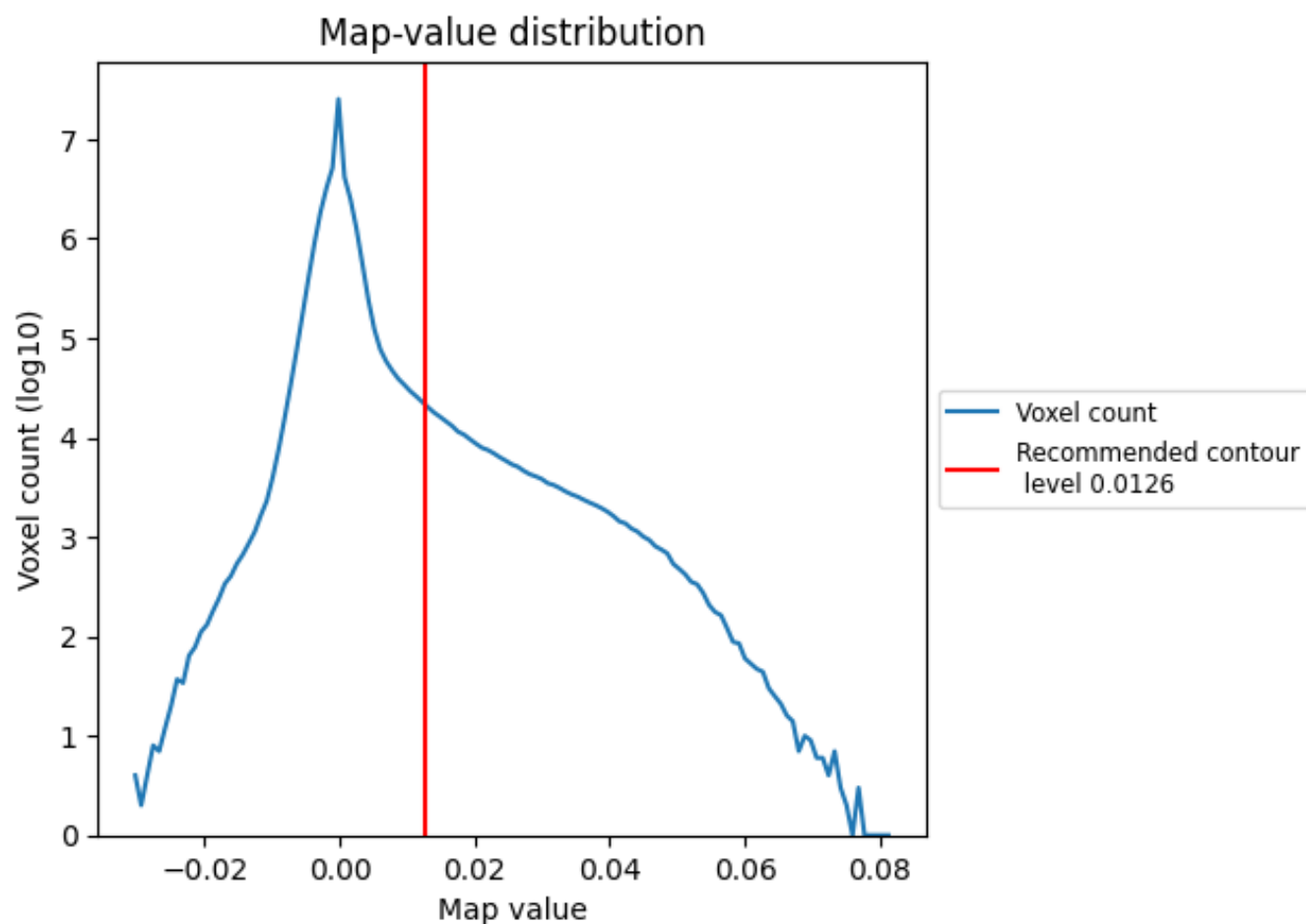
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

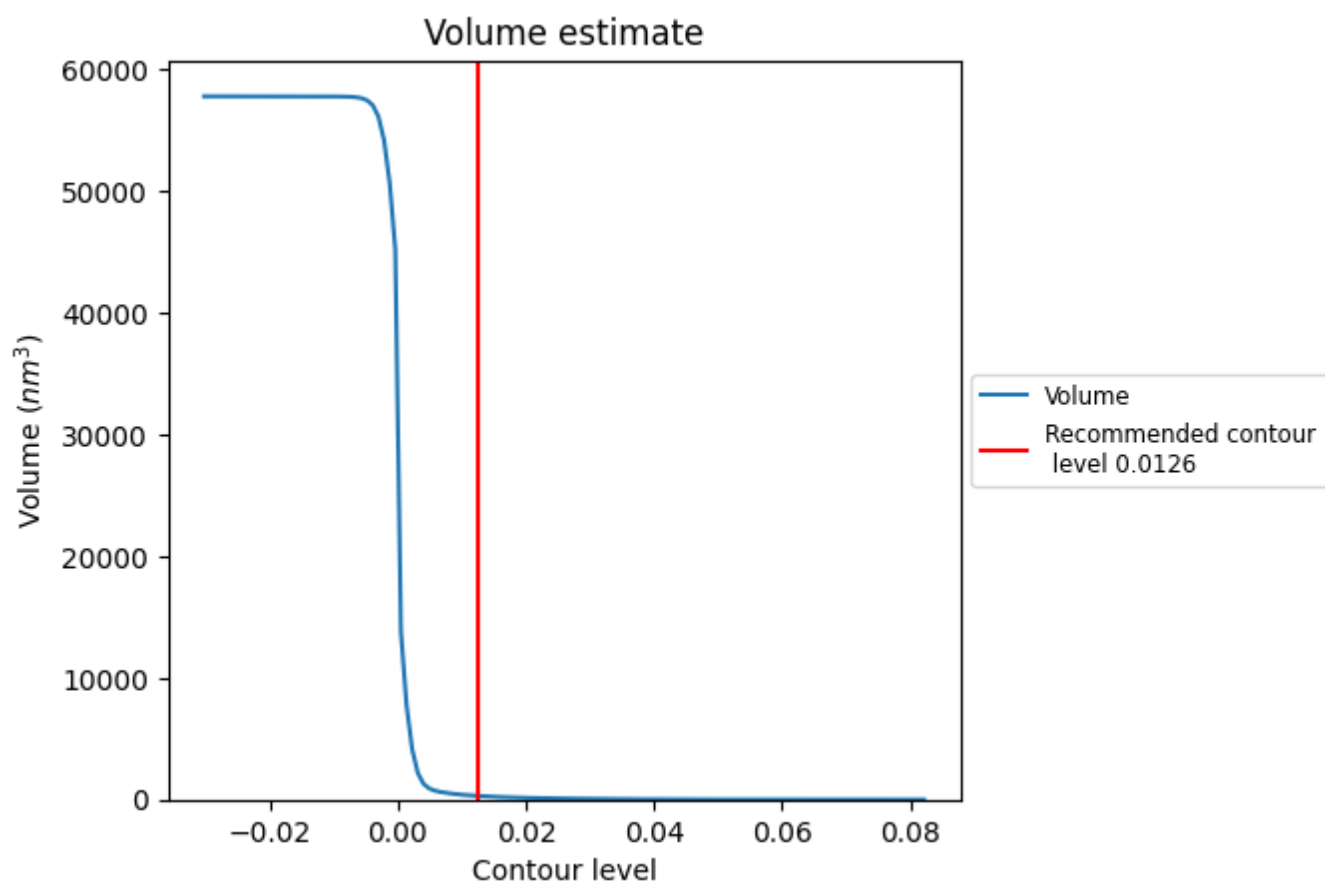
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

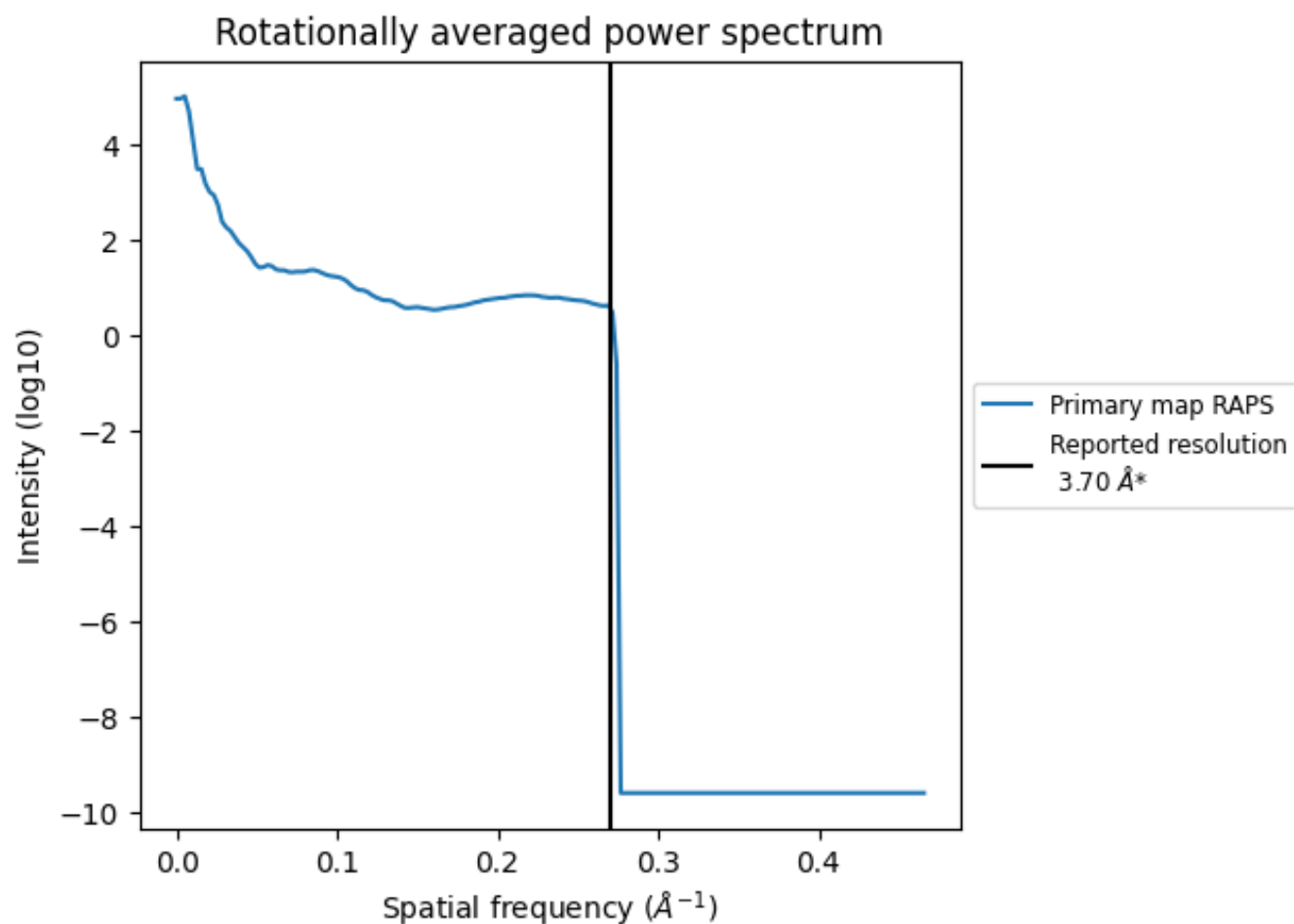
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 268 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

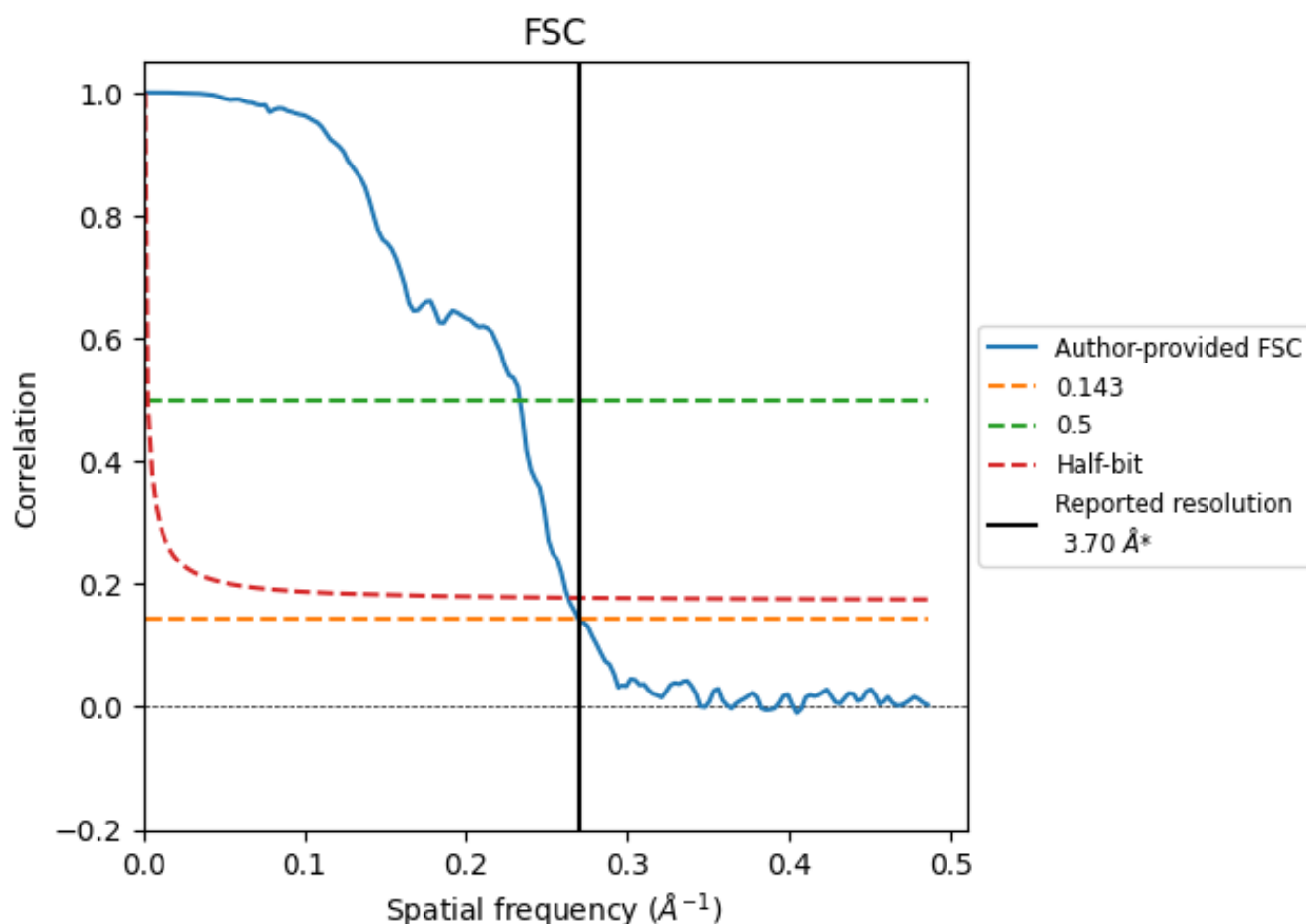


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

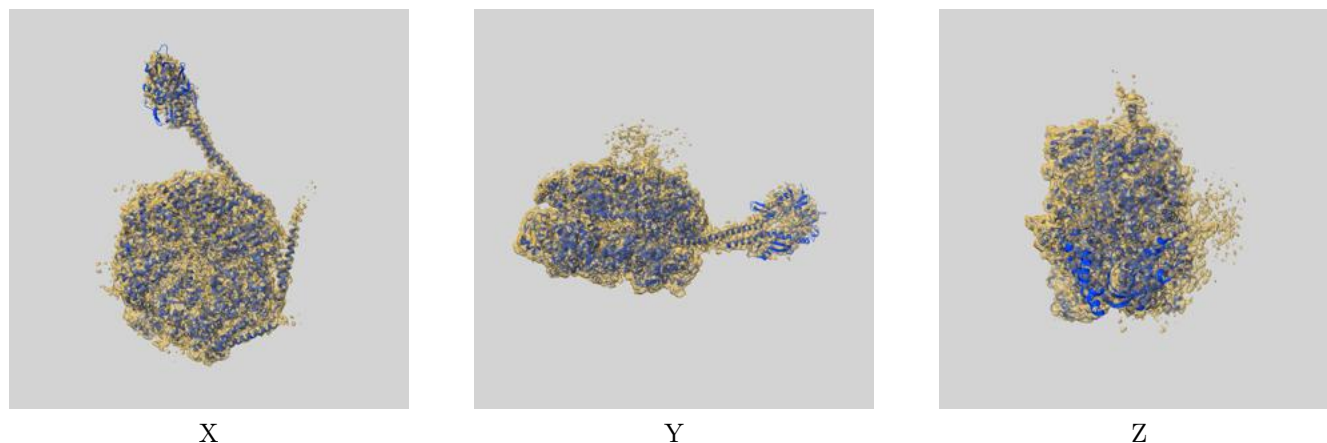
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.28	3.80
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

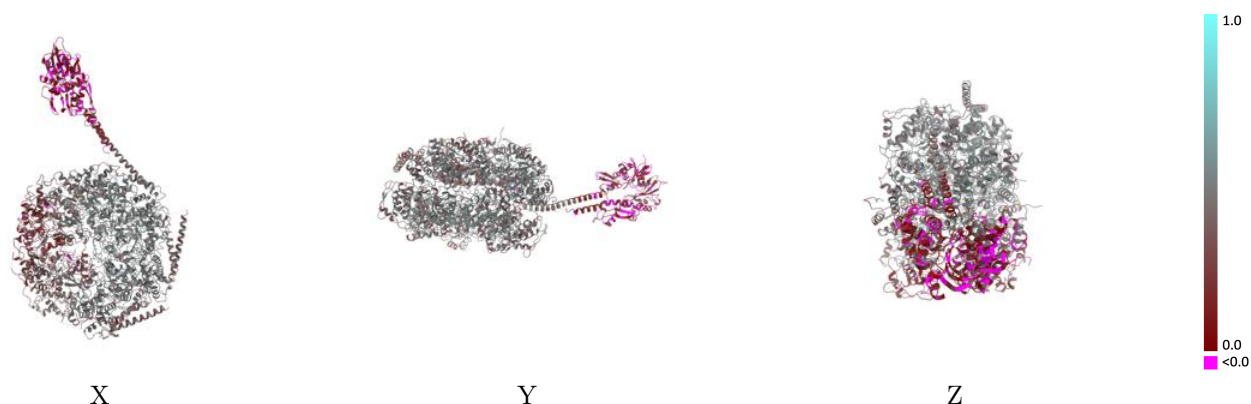
This section contains information regarding the fit between EMDB map EMD-21553 and PDB model 6W6E. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



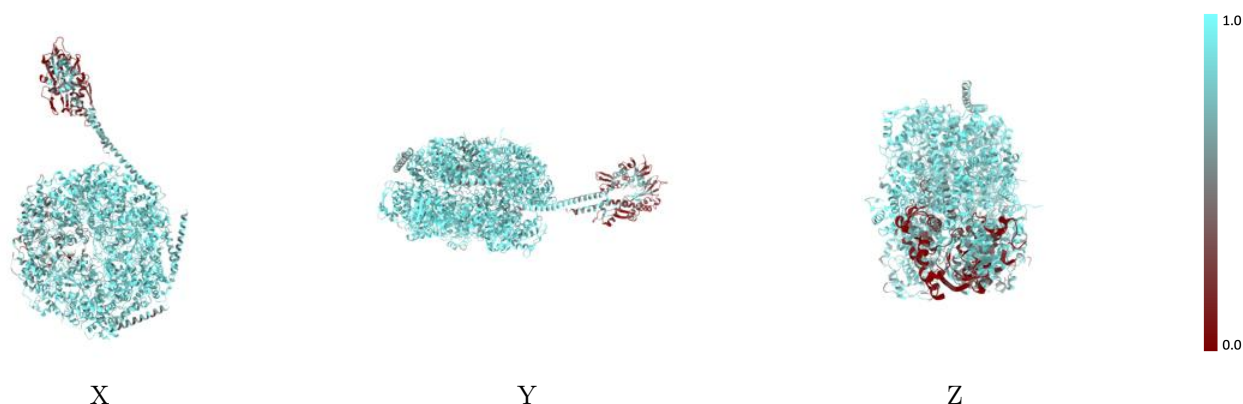
The images above show the 3D surface view of the map at the recommended contour level 0.0126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



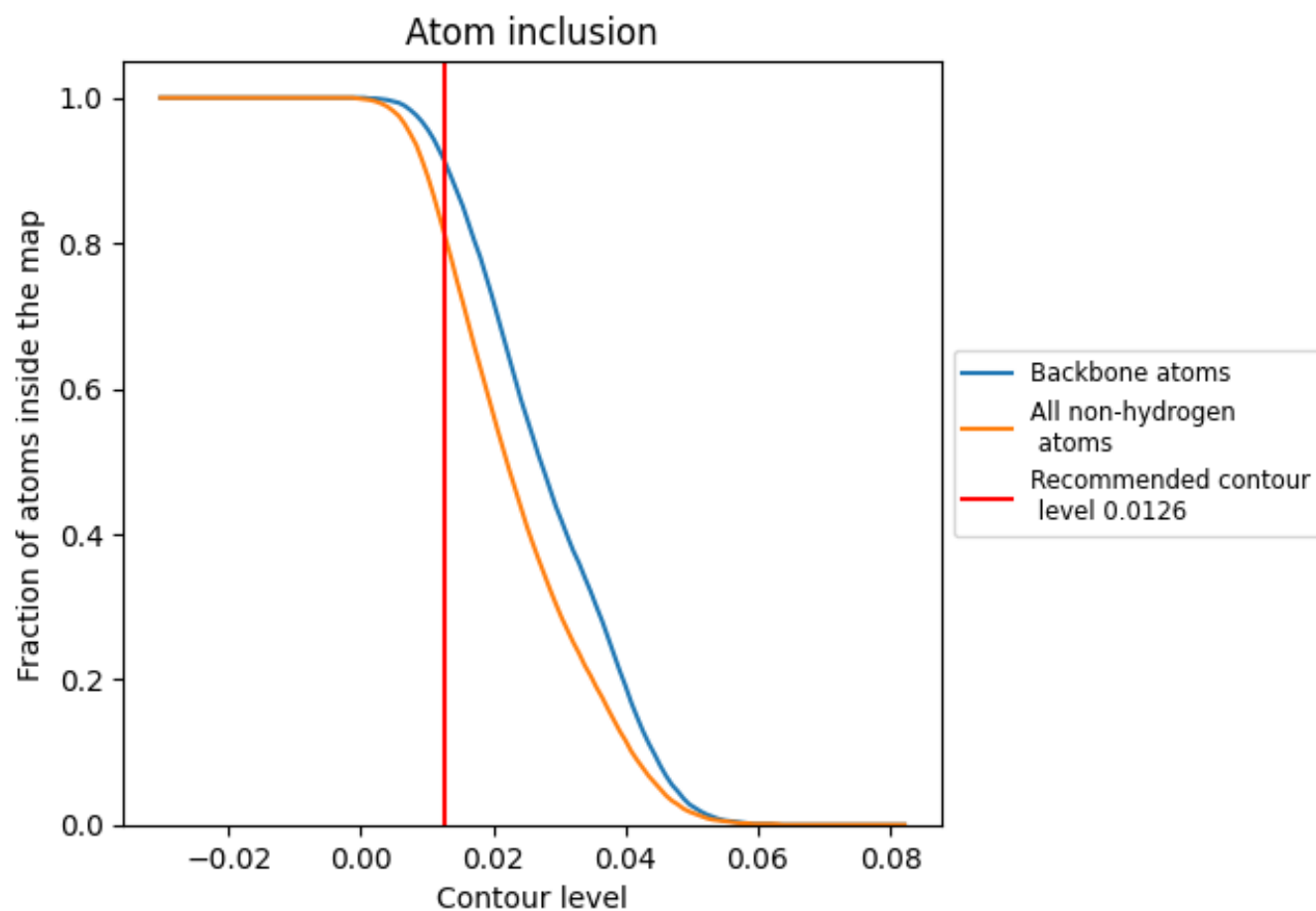
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.3930
A	0.8770	0.4410
B	0.9060	0.4790
C	0.8960	0.4740
D	0.8980	0.4550
E	0.8140	0.3490
F	0.7430	0.3330
I	0.3440	0.0540
N	0.9620	0.4860

1.0

0.0

<0.0