Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:40 pm GMT

PDB ID	:	5OFO
EMDB ID	:	EMD-3776
Title	:	Cryo EM structure of the E. coli disaggregase ClpB (BAP form, DWB mutant), in the ATPgammaS state, bound to the model substrate casein
Authors	:	Deville, C.; Carroni, M.; Franke, K.B.; Topf, M.; Bukau, B.; Mogk, A.; Saibil, H.R.
Deposited on	:	2017-07-11
Resolution	:	4.60 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:

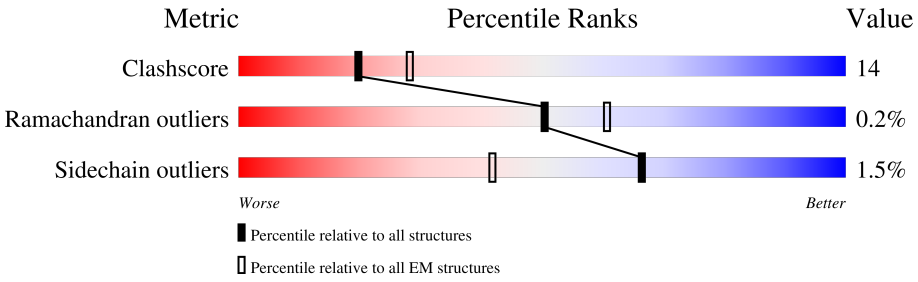
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	871	16% 56% 22% 21%
1	B	871	15% 51% 27% • 21%
1	C	871	17% 52% 26% • 21%
1	D	871	10% 55% 23% • 21%
1	E	871	9% 52% 27% 21%
1	F	871	15% 55% 23% • 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32993 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,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	F	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	E	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	D	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	B	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	A	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	MET	-	initiating methionine	UNP P63284
C	-2	ARG	-	expression tag	UNP P63284
C	-1	GLY	-	expression tag	UNP P63284
C	0	SER	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	745	ILE	ILE	linker	UNP P0ABH9
C	746	LYS	LYS	linker	UNP P0ABH9
C	747	LYS	LYS	linker	UNP P0ABH9
C	748	ILE	ILE	linker	UNP P0ABH9
C	858	GLY	-	expression tag	UNP P63284
C	859	SER	-	expression tag	UNP P63284
C	860	ARG	-	expression tag	UNP P63284
C	861	SER	-	expression tag	UNP P63284
C	862	HIS	-	expression tag	UNP P63284
C	863	HIS	-	expression tag	UNP P63284
C	864	HIS	-	expression tag	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
C	865	HIS	-	expression tag	UNP P63284
C	866	HIS	-	expression tag	UNP P63284
C	867	HIS	-	expression tag	UNP P63284
F	-3	MET	-	initiating methionine	UNP P63284
F	-2	ARG	-	expression tag	UNP P63284
F	-1	GLY	-	expression tag	UNP P63284
F	0	SER	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	745	ILE	ILE	linker	UNP P0ABH9
F	746	LYS	LYS	linker	UNP P0ABH9
F	747	LYS	LYS	linker	UNP P0ABH9
F	748	ILE	ILE	linker	UNP P0ABH9
F	858	GLY	-	expression tag	UNP P63284
F	859	SER	-	expression tag	UNP P63284
F	860	ARG	-	expression tag	UNP P63284
F	861	SER	-	expression tag	UNP P63284
F	862	HIS	-	expression tag	UNP P63284
F	863	HIS	-	expression tag	UNP P63284
F	864	HIS	-	expression tag	UNP P63284
F	865	HIS	-	expression tag	UNP P63284
F	866	HIS	-	expression tag	UNP P63284
F	867	HIS	-	expression tag	UNP P63284
E	-3	MET	-	initiating methionine	UNP P63284
E	-2	ARG	-	expression tag	UNP P63284
E	-1	GLY	-	expression tag	UNP P63284
E	0	SER	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	678	ALA	GLU	engineered mutation	UNP P63284
E	745	ILE	ILE	linker	UNP P0ABH9
E	746	LYS	LYS	linker	UNP P0ABH9
E	747	LYS	LYS	linker	UNP P0ABH9
E	748	ILE	ILE	linker	UNP P0ABH9
E	858	GLY	-	expression tag	UNP P63284
E	859	SER	-	expression tag	UNP P63284
E	860	ARG	-	expression tag	UNP P63284
E	861	SER	-	expression tag	UNP P63284
E	862	HIS	-	expression tag	UNP P63284
E	863	HIS	-	expression tag	UNP P63284
E	864	HIS	-	expression tag	UNP P63284
E	865	HIS	-	expression tag	UNP P63284
E	866	HIS	-	expression tag	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
E	867	HIS	-	expression tag	UNP P63284
D	-3	MET	-	initiating methionine	UNP P63284
D	-2	ARG	-	expression tag	UNP P63284
D	-1	GLY	-	expression tag	UNP P63284
D	0	SER	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	745	ILE	ILE	linker	UNP P0ABH9
D	746	LYS	LYS	linker	UNP P0ABH9
D	747	LYS	LYS	linker	UNP P0ABH9
D	748	ILE	ILE	linker	UNP P0ABH9
D	858	GLY	-	expression tag	UNP P63284
D	859	SER	-	expression tag	UNP P63284
D	860	ARG	-	expression tag	UNP P63284
D	861	SER	-	expression tag	UNP P63284
D	862	HIS	-	expression tag	UNP P63284
D	863	HIS	-	expression tag	UNP P63284
D	864	HIS	-	expression tag	UNP P63284
D	865	HIS	-	expression tag	UNP P63284
D	866	HIS	-	expression tag	UNP P63284
D	867	HIS	-	expression tag	UNP P63284
B	-3	MET	-	initiating methionine	UNP P63284
B	-2	ARG	-	expression tag	UNP P63284
B	-1	GLY	-	expression tag	UNP P63284
B	0	SER	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	745	ILE	ILE	linker	UNP P0ABH9
B	746	LYS	LYS	linker	UNP P0ABH9
B	747	LYS	LYS	linker	UNP P0ABH9
B	748	ILE	ILE	linker	UNP P0ABH9
B	858	GLY	-	expression tag	UNP P63284
B	859	SER	-	expression tag	UNP P63284
B	860	ARG	-	expression tag	UNP P63284
B	861	SER	-	expression tag	UNP P63284
B	862	HIS	-	expression tag	UNP P63284
B	863	HIS	-	expression tag	UNP P63284
B	864	HIS	-	expression tag	UNP P63284
B	865	HIS	-	expression tag	UNP P63284
B	866	HIS	-	expression tag	UNP P63284
B	867	HIS	-	expression tag	UNP P63284
A	-3	MET	-	initiating methionine	UNP P63284

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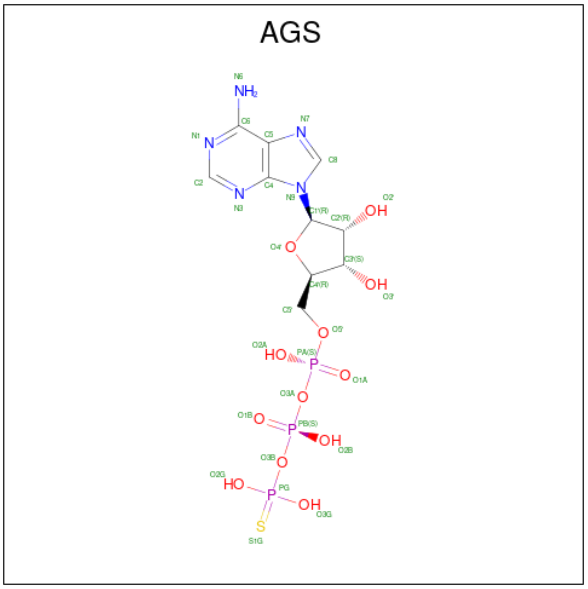
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP P63284
A	-1	GLY	-	expression tag	UNP P63284
A	0	SER	-	expression tag	UNP P63284
A	279	ALA	GLU	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	745	ILE	ILE	linker	UNP P0ABH9
A	746	LYS	LYS	linker	UNP P0ABH9
A	747	LYS	LYS	linker	UNP P0ABH9
A	748	ILE	ILE	linker	UNP P0ABH9
A	858	GLY	-	expression tag	UNP P63284
A	859	SER	-	expression tag	UNP P63284
A	860	ARG	-	expression tag	UNP P63284
A	861	SER	-	expression tag	UNP P63284
A	862	HIS	-	expression tag	UNP P63284
A	863	HIS	-	expression tag	UNP P63284
A	864	HIS	-	expression tag	UNP P63284
A	865	HIS	-	expression tag	UNP P63284
A	866	HIS	-	expression tag	UNP P63284
A	867	HIS	-	expression tag	UNP P63284

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

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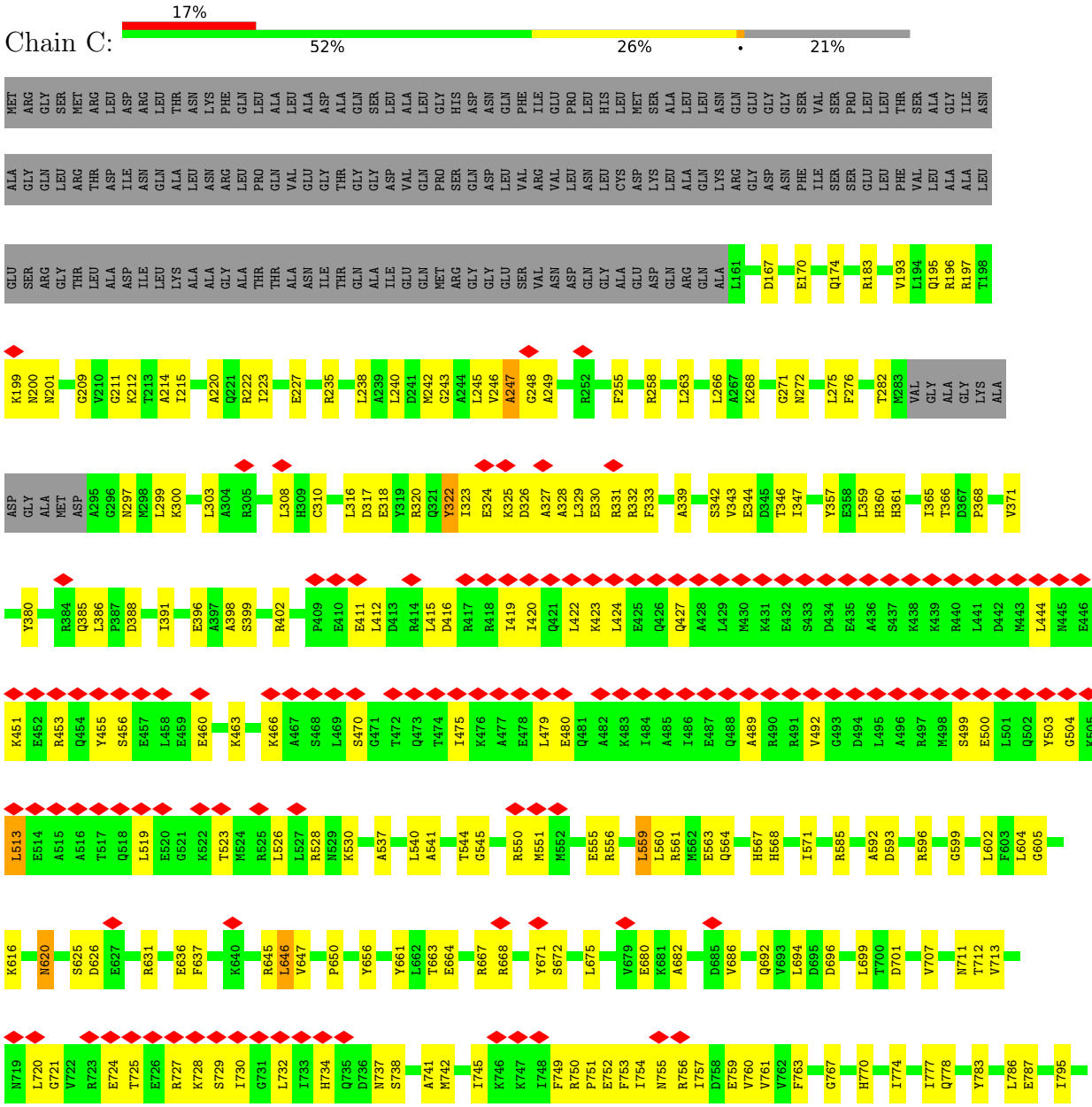
Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

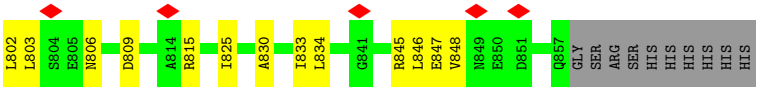
3 Residue-property plots (i)

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,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

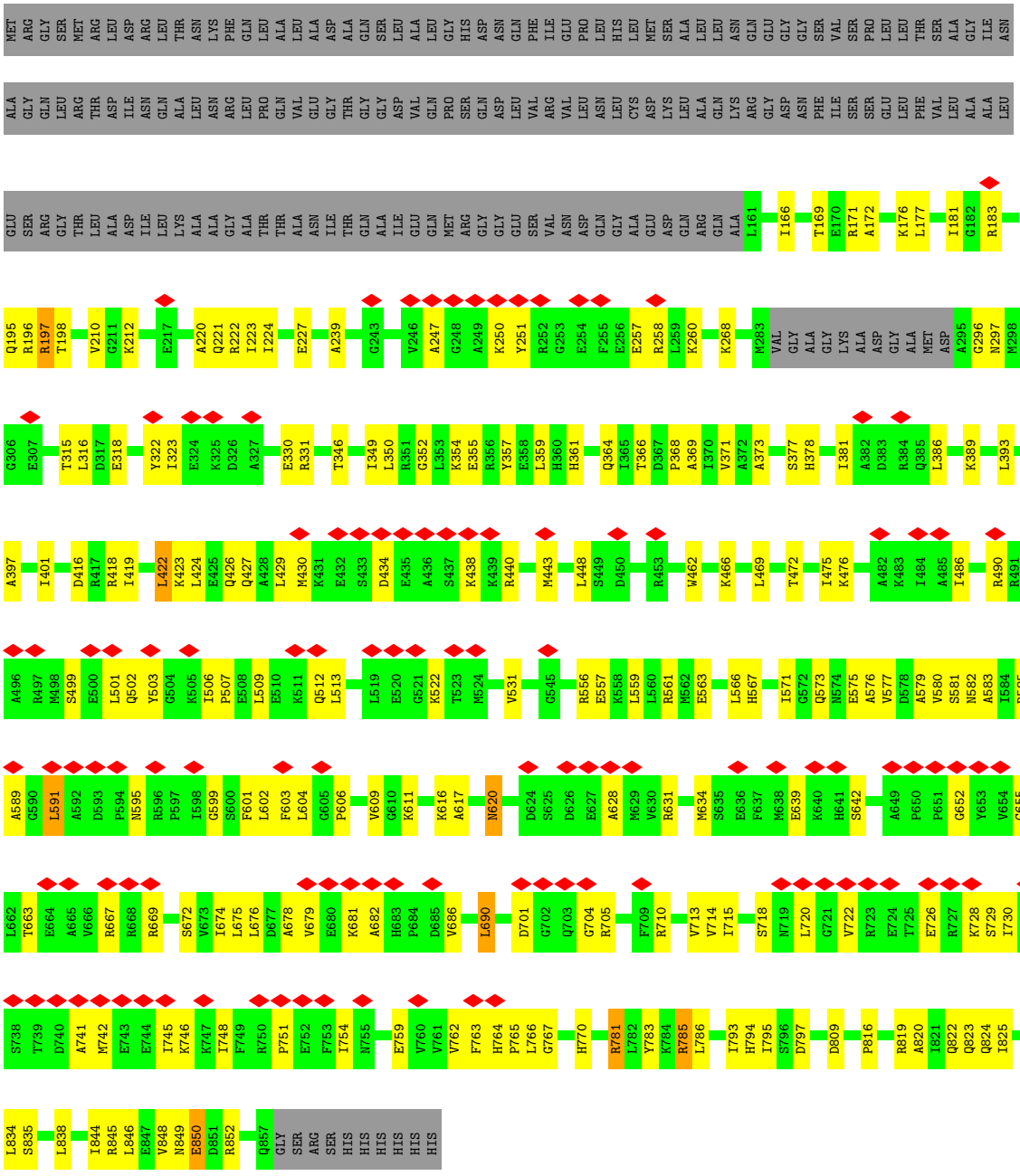
Chain C:





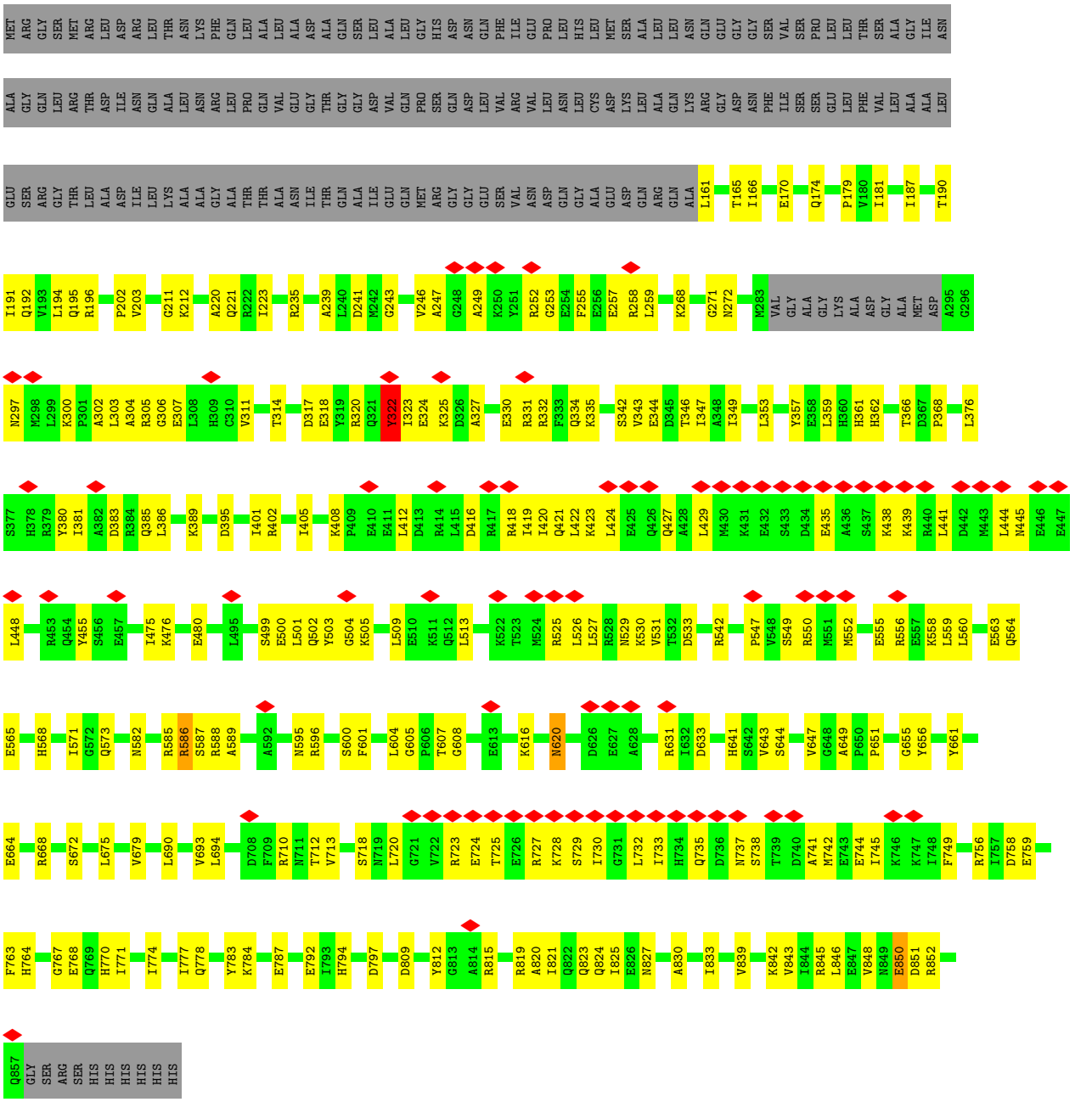
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain F:



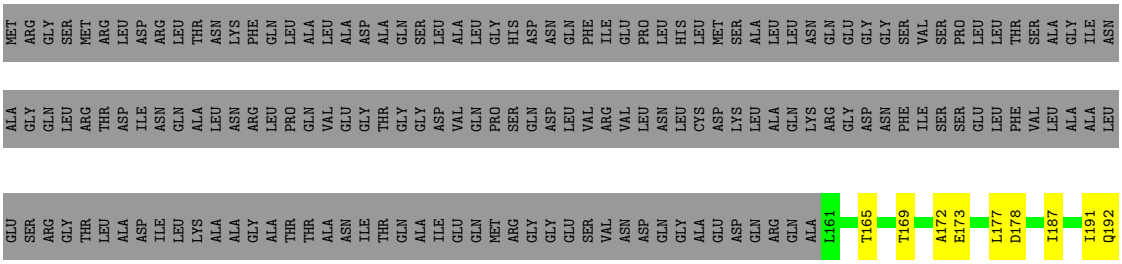
• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

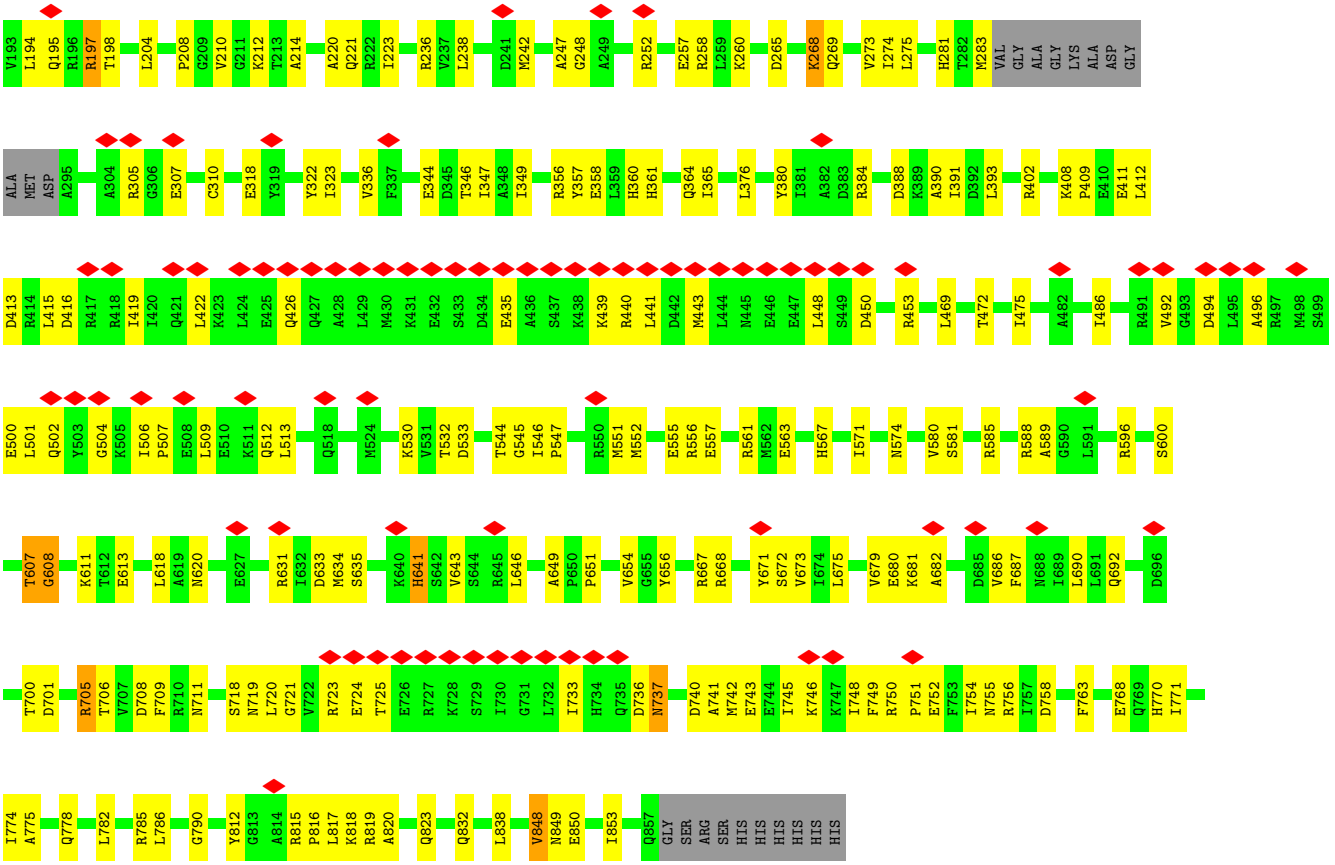
Chain E:



• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

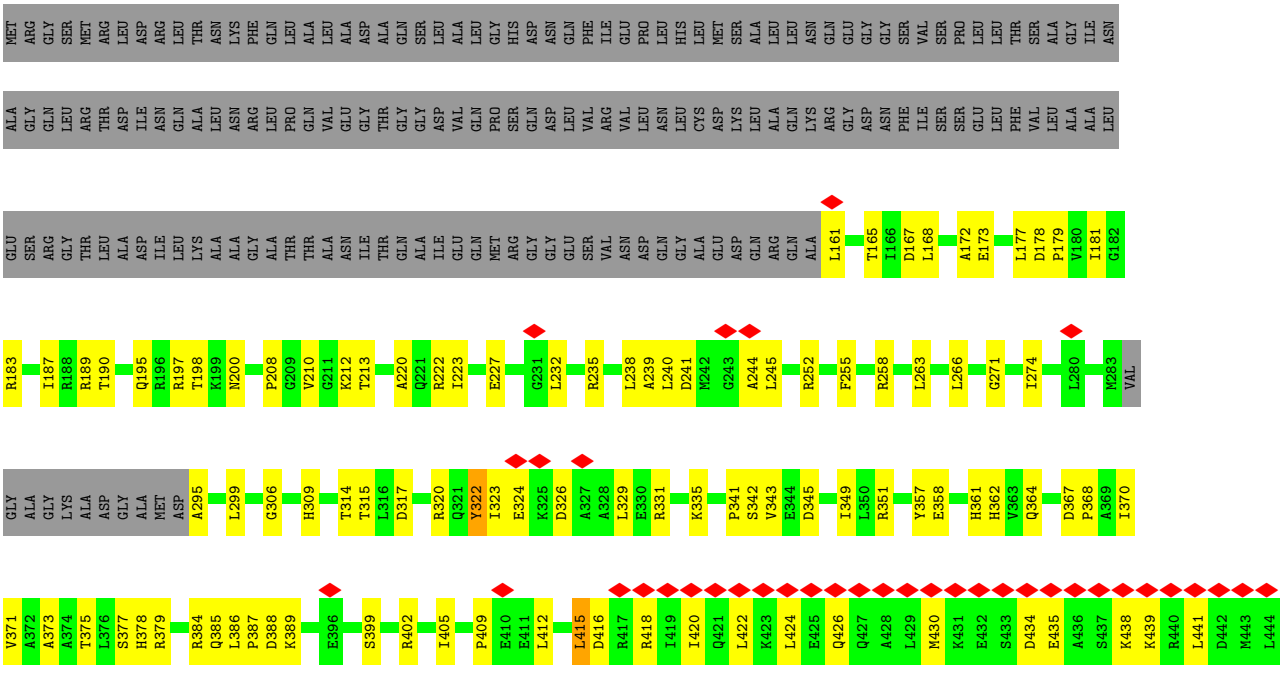
Chain D:

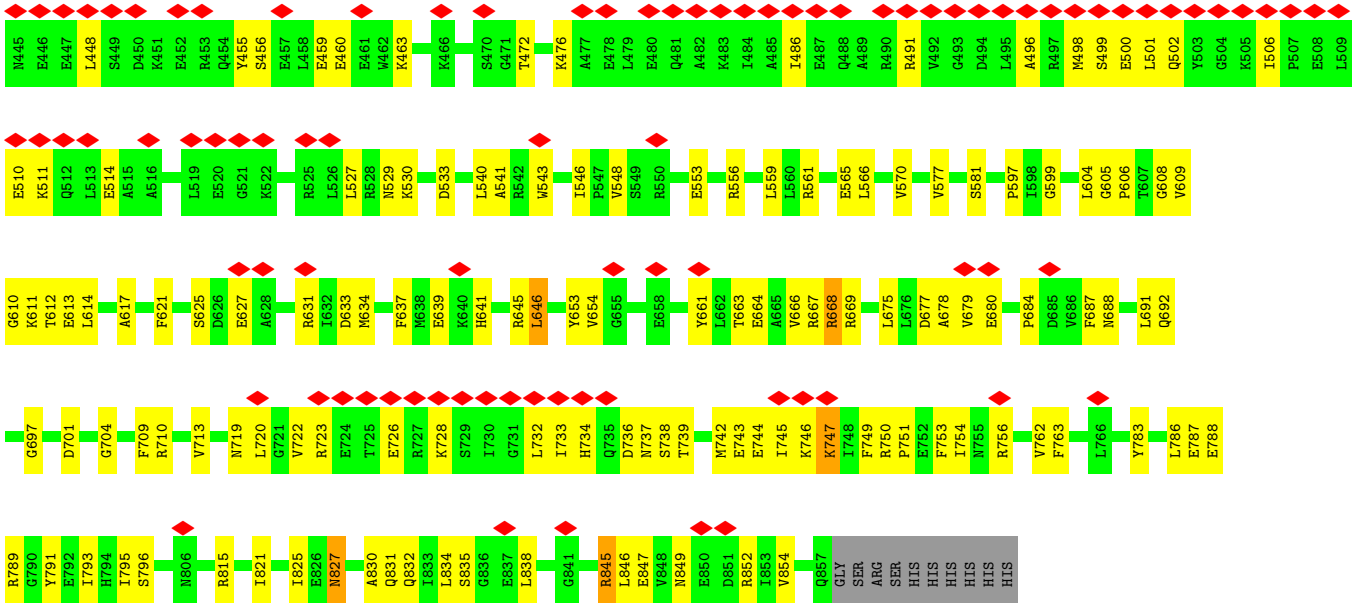




• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

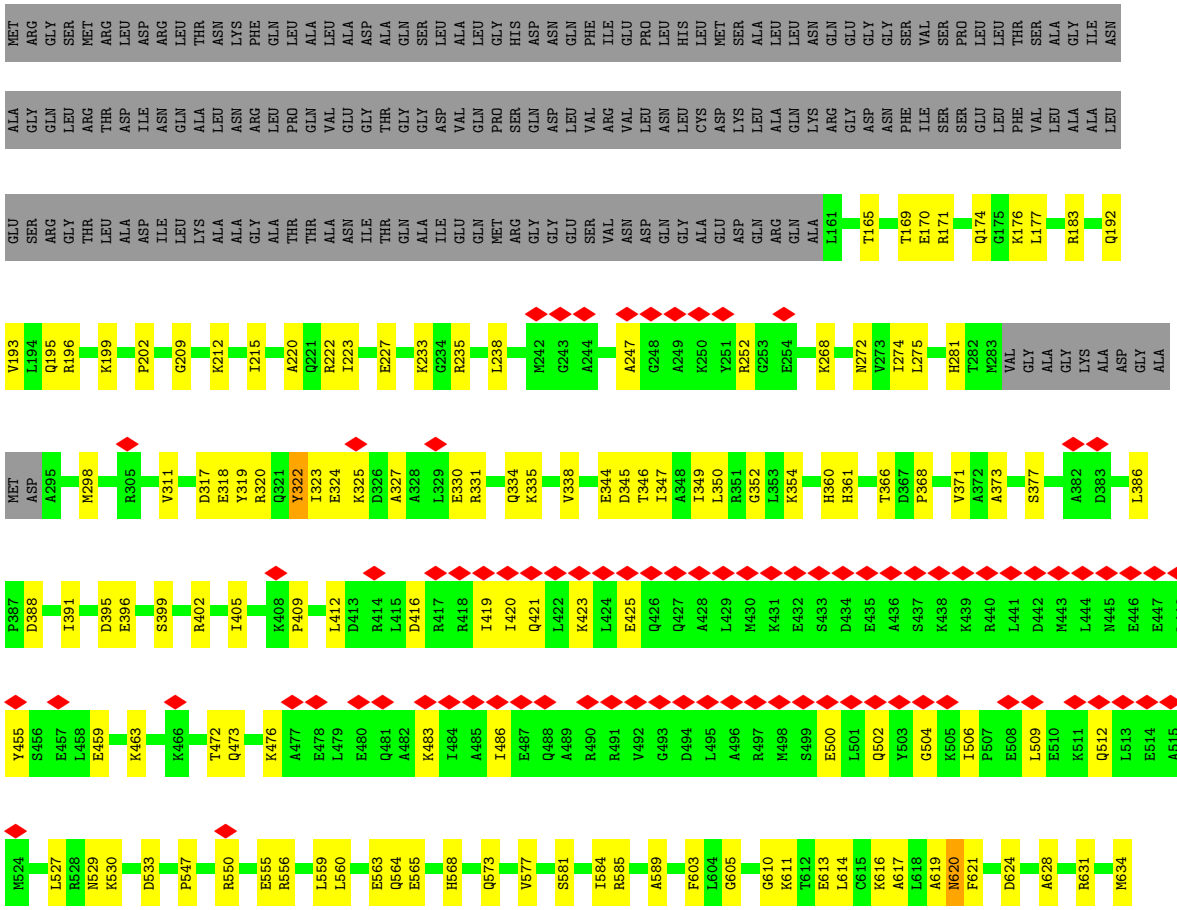
Chain B:

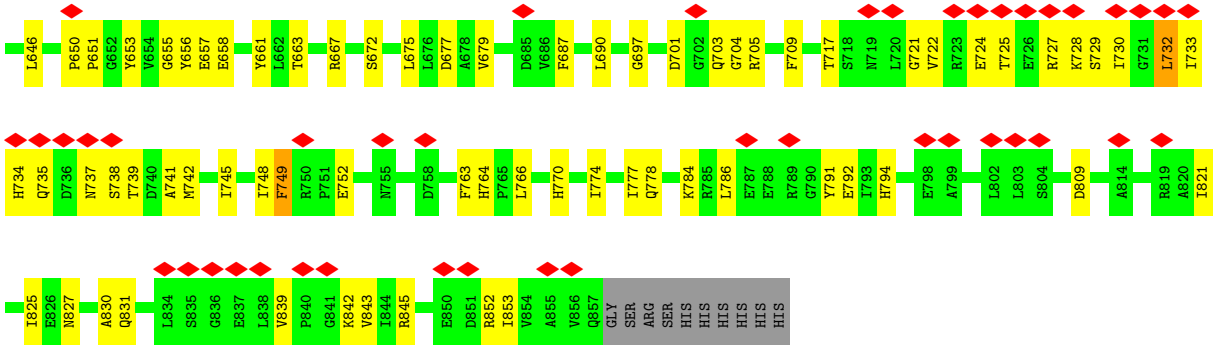




• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain A:




L646
P650
P651
G652
Y653
V654
G655
Y656
E657
E658
Y661
L662
T663
R667
S672
L675
L676
D677
A678
V679
D685
V686
F687
L690
G697
D701
G702
Q703
G704
R705
F709
T717
S718
N719
L720
G721
V722
R723
E724
T725
E726
R727
K728
S729
I730
G731
L732
I733
H734
Q735
D736
N737
S738
T739
D740
A741
M742
I745
I748
F749
R750
P751
E752
N755
D758
F763
H764
P765
L766
H770
I774
I777
Q778
K784
R785
L786
E787
E788
R789
G790
Y791
E792
I793
H794
E798
A799
L802
L803
S804
D809
A814
R819
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I825
E826
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A830
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L834
S835
G836
E837
L838
V839
P840
G841
K842
V843
Y844
R845
E850
D851
R852
I853
V854
A855
V856
Q857
GLY
SER
ARG
SER
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	230000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	350.72, 350.72, 350.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.41	0/5512	0.61	1/7420 (0.0%)
1	B	0.45	1/5512 (0.0%)	0.64	4/7420 (0.1%)
1	C	0.47	0/5512	0.66	1/7420 (0.0%)
1	D	0.45	0/5512	0.65	2/7420 (0.0%)
1	E	0.42	0/5512	0.60	0/7420
1	F	0.38	0/5512	0.61	1/7420 (0.0%)
All	All	0.43	1/33072 (0.0%)	0.63	9/44520 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	3
1	E	0	3
1	F	0	3
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	GLN	C-N	-7.56	1.16	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	413	ASP	CB-CG-OD1	5.88	123.60	118.30
1	B	415	LEU	CB-CG-CD2	-5.79	101.16	111.00
1	A	732	LEU	CA-CB-CG	5.64	128.28	115.30
1	C	513	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	329	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	720	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	548	VAL	C-N-CA	5.13	134.52	121.70
1	B	441	LEU	CA-CB-CG	5.11	127.06	115.30
1	F	690	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	322	TYR	Peptide
1	A	749	PHE	Peptide
1	B	322	TYR	Peptide
1	B	326	ASP	Peptide
1	B	387	PRO	Peptide
1	B	678	ALA	Peptide
1	C	247	ALA	Peptide
1	C	282	THR	Peptide
1	C	322	TYR	Peptide
1	C	324	GLU	Peptide
1	D	608	GLY	Peptide
1	D	848	VAL	Peptide
1	D	849	ASN	Peptide
1	E	322	TYR	Peptide
1	E	324	GLU	Peptide
1	E	850	GLU	Peptide
1	F	848	VAL	Peptide
1	F	849	ASN	Peptide
1	F	850	GLU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5442	0	5553	150	0
1	B	5442	0	5552	169	0
1	C	5442	0	5553	178	0
1	D	5442	0	5553	162	0
1	E	5442	0	5553	166	0
1	F	5442	0	5553	158	0
2	A	31	0	12	3	0
2	B	62	0	24	5	0
2	C	62	0	24	7	0
2	D	62	0	24	10	0
2	E	62	0	24	5	0
2	F	62	0	24	9	0
All	All	32993	0	33449	925	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 14.

All (925) 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:C:500:GLU:O	1:C:504:GLY:HA3	1.48	1.11
1:E:509:LEU:O	1:E:513:LEU:HB2	1.52	1.10
1:C:509:LEU:O	1:C:513:LEU:HB2	1.51	1.09
1:D:751:PRO:O	1:D:755:ASN:HB2	1.58	1.03
1:D:551:MET:O	1:D:555:GLU:HB3	1.62	1.00
1:C:752:GLU:O	1:C:756:ARG:HB2	1.65	0.97
1:E:783:TYR:O	1:E:787:GLU:HB2	1.65	0.96
1:A:412:LEU:O	1:A:416:ASP:HB2	1.65	0.96
1:C:412:LEU:O	1:C:416:ASP:HB2	1.65	0.95
1:C:357:TYR:O	1:C:361:HIS:HB2	1.66	0.95
1:C:499:SER:O	1:C:503:TYR:HB2	1.68	0.92
1:E:412:LEU:O	1:E:416:ASP:HB2	1.68	0.92
1:C:738:SER:O	1:C:742:MET:HB2	1.71	0.91
1:E:499:SER:O	1:E:503:TYR:HB2	1.71	0.90
1:A:555:GLU:O	1:A:559:LEU:HB2	1.71	0.90
1:A:556:ARG:O	1:A:560:LEU:HB2	1.72	0.90
1:B:783:TYR:O	1:B:787:GLU:HB2	1.74	0.87
1:B:830:ALA:O	1:B:834:LEU:HB2	1.75	0.87
1:C:783:TYR:O	1:C:787:GLU:HB2	1.74	0.87
1:E:357:TYR:O	1:E:361:HIS:HB2	1.73	0.87
1:A:616:LYS:O	1:A:620:ASN:HB2	1.73	0.86
1:B:357:TYR:O	1:B:361:HIS:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:MET:O	1:D:556:ARG:HB3	1.79	0.82
1:A:663:THR:O	1:A:667:ARG:HB2	1.80	0.81
1:C:411:GLU:O	1:C:415:LEU:HB2	1.81	0.81
1:E:556:ARG:O	1:E:560:LEU:HB2	1.81	0.80
1:F:357:TYR:O	1:F:361:HIS:HB2	1.83	0.78
1:F:616:LYS:O	1:F:620:ASN:HB2	1.83	0.78
1:D:500:GLU:O	1:D:504:GLY:HA3	1.83	0.78
1:B:553:GLU:HG2	1:B:556:ARG:HE	1.48	0.78
1:F:830:ALA:O	1:F:834:LEU:HB2	1.84	0.77
1:C:728:LYS:HD2	1:C:737:ASN:HD22	1.49	0.76
1:A:821:ILE:O	1:A:825:ILE:HB	1.85	0.76
1:C:318:GLU:O	1:C:322:TYR:HB2	1.86	0.76
1:E:170:GLU:HG2	1:E:174:GLN:HE22	1.50	0.76
1:B:821:ILE:O	1:B:825:ILE:HB	1.87	0.75
1:E:320:ARG:O	1:E:323:ILE:HA	1.86	0.74
1:A:737:ASN:O	1:A:741:ALA:HB3	1.88	0.73
1:C:751:PRO:HB2	1:D:815:ARG:HE	1.54	0.73
1:F:831:GLN:O	1:F:835:SER:HB2	1.88	0.73
1:B:680:GLU:HB2	1:B:720:LEU:HD12	1.70	0.73
1:E:820:ALA:O	1:E:824:GLN:HB2	1.88	0.72
1:B:742:MET:HA	1:B:745:ILE:HG22	1.70	0.72
1:C:323:ILE:HG13	1:C:325:LYS:H	1.53	0.72
1:A:728:LYS:HD2	1:A:737:ASN:HD22	1.55	0.72
1:F:318:GLU:O	1:F:322:TYR:HB2	1.90	0.71
1:B:510:GLU:O	1:B:514:GLU:HB2	1.90	0.71
1:E:737:ASN:O	1:E:741:ALA:HB3	1.91	0.71
1:C:556:ARG:O	1:C:560:LEU:HB2	1.92	0.70
1:F:576:ALA:O	1:F:580:VAL:HB	1.92	0.70
1:E:723:ARG:O	1:E:727:ARG:HB2	1.91	0.70
1:D:435:GLU:O	1:D:439:LYS:HB2	1.92	0.70
1:B:631:ARG:HG3	1:B:675:LEU:HD23	1.74	0.70
1:A:366:THR:HG22	1:A:368:PRO:HD2	1.73	0.69
1:B:786:LEU:HB3	1:B:791:TYR:HB2	1.74	0.69
1:F:423:LYS:O	1:F:427:GLN:HB2	1.92	0.69
1:F:331:ARG:HH21	1:A:209:GLY:H	1.39	0.69
1:D:318:GLU:O	1:D:322:TYR:HB3	1.92	0.69
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.75	0.69
1:C:359:LEU:HD21	1:C:480:GLU:HG2	1.76	0.68
1:C:650:PRO:HG2	1:D:641:HIS:HB3	1.76	0.68
1:F:350:LEU:O	1:F:354:LYS:HB3	1.93	0.68
1:C:571:ILE:HD13	1:C:770:HIS:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:812:TYR:HB3	1:D:755:ASN:HD21	1.59	0.67
1:F:832:GLN:HB3	1:F:838:LEU:HD13	1.73	0.67
1:E:327:ALA:HA	1:E:330:GLU:HG2	1.77	0.67
1:F:509:LEU:O	1:F:513:LEU:HB2	1.95	0.67
1:F:418:ARG:O	1:F:422:LEU:HB2	1.95	0.67
1:D:752:GLU:O	1:D:756:ARG:HB2	1.94	0.67
1:E:424:LEU:HB3	1:D:502:GLN:HE22	1.61	0.66
1:A:631:ARG:HG2	1:A:675:LEU:HD23	1.77	0.66
1:A:327:ALA:O	1:A:331:ARG:HB2	1.95	0.66
1:D:509:LEU:O	1:D:513:LEU:HB2	1.95	0.66
1:C:366:THR:HG22	1:C:368:PRO:HD2	1.77	0.66
1:E:323:ILE:HG13	1:E:325:LYS:H	1.61	0.66
1:C:500:GLU:O	1:C:504:GLY:CA	2.36	0.65
1:C:745:ILE:O	1:C:749:PHE:N	2.23	0.65
1:C:755:ASN:HD21	1:D:812:TYR:HB3	1.61	0.65
1:E:435:GLU:O	1:E:439:LYS:HB2	1.96	0.65
1:B:384:ARG:NH2	1:A:330:GLU:O	2.30	0.65
1:B:384:ARG:HH12	1:A:331:ARG:HA	1.60	0.65
1:F:557:GLU:HG3	1:F:561:ARG:HE	1.61	0.65
1:E:408:LYS:NZ	1:E:455:TYR:OH	2.28	0.64
1:F:195:GLN:O	1:A:402:ARG:NH2	2.31	0.64
1:B:743:GLU:O	1:B:747:LYS:HB2	1.97	0.64
1:F:583:ALA:HA	1:F:586:ARG:HE	1.63	0.64
1:E:679:VAL:HG12	1:E:718:SER:HB3	1.79	0.64
1:F:819:ARG:O	1:F:823:GLN:HB3	1.97	0.64
1:F:296:GLY:HA2	1:F:299:LEU:HD23	1.80	0.64
1:B:739:THR:HA	1:B:742:MET:HB2	1.80	0.63
1:F:820:ALA:O	1:F:824:GLN:HB2	1.99	0.63
1:A:360:HIS:O	1:A:402:ARG:NH1	2.32	0.63
1:C:326:ASP:HB3	1:C:329:LEU:HB2	1.78	0.63
1:F:606:PRO:HB3	1:F:722:VAL:HG23	1.80	0.63
1:E:821:ILE:O	1:E:825:ILE:HB	1.98	0.63
1:D:408:LYS:NZ	1:D:416:ASP:OD2	2.32	0.63
1:F:663:THR:O	1:F:667:ARG:HB2	1.98	0.62
1:B:435:GLU:O	1:B:439:LYS:HB2	1.98	0.62
1:B:617:ALA:O	1:B:621:PHE:HB2	1.98	0.62
1:C:396:GLU:OE2	1:B:189:ARG:NH1	2.31	0.62
1:F:730:ILE:HG12	1:F:767:GLY:HA2	1.79	0.62
2:D:901:AGS:S1G	2:D:901:AGS:O2B	2.57	0.62
1:B:743:GLU:O	1:B:747:LYS:CB	2.48	0.62
2:C:901:AGS:S1G	2:C:901:AGS:O1B	2.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ASP:O	1:D:269:GLN:HB2	2.00	0.62
1:D:236:ARG:HB2	1:D:273:VAL:HG22	1.80	0.62
1:D:571:ILE:HD13	1:D:770:HIS:HB3	1.82	0.62
1:E:555:GLU:O	1:E:559:LEU:HB2	2.00	0.62
1:D:357:TYR:O	1:D:361:HIS:HB2	2.00	0.62
1:C:663:THR:HG23	1:C:707:VAL:HG21	1.82	0.61
1:F:426:GLN:O	1:F:430:MET:N	2.32	0.61
1:B:606:PRO:O	1:B:611:LYS:NZ	2.33	0.61
1:A:419:ILE:HG12	1:A:451:LYS:HB3	1.83	0.61
1:F:196:ARG:HH21	1:A:396:GLU:HB2	1.63	0.61
1:C:318:GLU:O	1:C:322:TYR:CB	2.49	0.61
1:B:745:ILE:HG12	1:B:754:ILE:HG12	1.81	0.61
1:A:212:LYS:NZ	2:A:901:AGS:S1G	2.73	0.61
1:E:728:LYS:HA	1:E:732:LEU:HB3	1.83	0.61
1:D:486:ILE:HD13	1:D:501:LEU:HB2	1.83	0.61
2:E:902:AGS:O1B	2:E:902:AGS:S1G	2.59	0.60
1:E:643:VAL:O	1:E:647:VAL:HB	2.01	0.60
1:B:795:ILE:HG22	1:B:846:LEU:HD12	1.83	0.60
1:A:728:LYS:HA	1:A:732:LEU:HB3	1.83	0.60
1:F:678:ALA:HA	1:F:718:SER:HA	1.83	0.60
1:E:547:PRO:HB2	1:E:550:ARG:HG3	1.83	0.60
1:D:742:MET:O	1:D:746:LYS:CB	2.49	0.60
1:C:199:LYS:NZ	1:C:333:PHE:O	2.33	0.60
1:C:734:HIS:O	1:C:738:SER:HB2	2.02	0.60
1:E:738:SER:O	1:E:742:MET:HB2	2.02	0.60
1:E:812:TYR:O	1:D:755:ASN:ND2	2.35	0.60
1:B:420:ILE:O	1:B:424:LEU:HB2	2.02	0.60
1:A:827:ASN:O	1:A:831:GLN:HB2	2.02	0.59
1:C:631:ARG:NH2	1:B:692:GLN:OE1	2.35	0.59
1:D:194:LEU:HD22	1:D:274:ILE:HD13	1.84	0.59
1:A:655:GLY:HA2	1:A:658:GLU:HB2	1.84	0.59
1:E:401:ILE:HG13	1:E:531:VAL:HG12	1.83	0.59
1:C:721:GLY:O	1:C:725:THR:N	2.34	0.59
1:E:738:SER:O	1:E:742:MET:CB	2.51	0.59
1:D:178:ASP:OD1	1:D:356:ARG:NH1	2.36	0.59
1:A:235:ARG:HG2	1:A:272:ASN:HA	1.84	0.59
1:E:247:ALA:HB3	1:E:258:ARG:HH12	1.68	0.59
1:B:733:ILE:HG13	1:B:736:ASP:H	1.67	0.59
1:E:408:LYS:NZ	1:E:416:ASP:OD2	2.35	0.59
1:B:342:SER:OG	1:B:343:VAL:N	2.34	0.59
2:B:901:AGS:S1G	2:B:901:AGS:O1B	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:MET:O	1:D:746:LYS:HB2	2.02	0.59
1:A:725:THR:HA	1:A:728:LYS:HG2	1.84	0.59
1:C:328:ALA:HA	1:C:331:ARG:HB3	1.85	0.59
1:F:742:MET:O	1:F:746:LYS:CB	2.50	0.59
1:A:361:HIS:HA	1:A:402:ARG:HD3	1.84	0.58
1:E:422:LEU:HD22	1:E:444:LEU:HD11	1.85	0.58
1:E:815:ARG:HD3	1:D:755:ASN:HD22	1.69	0.58
1:D:509:LEU:O	1:D:513:LEU:CB	2.52	0.58
1:C:783:TYR:O	1:C:787:GLU:CB	2.47	0.58
1:F:729:SER:HA	1:F:764:HIS:HB2	1.84	0.58
2:E:901:AGS:S1G	2:E:901:AGS:O2B	2.61	0.58
1:B:426:GLN:O	1:B:430:MET:HB2	2.02	0.58
1:A:564:GLN:O	1:A:568:HIS:ND1	2.35	0.58
1:F:381:ILE:O	1:F:389:LYS:NZ	2.37	0.58
1:F:396:GLU:HB2	1:E:196:ARG:HE	1.68	0.58
1:D:742:MET:HB3	1:D:746:LYS:HB2	1.85	0.58
1:B:743:GLU:OE2	1:B:747:LYS:NZ	2.32	0.58
1:F:663:THR:O	1:F:667:ARG:CB	2.51	0.58
1:B:639:GLU:HG2	1:B:641:HIS:H	1.67	0.58
1:E:395:ASP:OD2	1:D:197:ARG:NH1	2.37	0.58
1:D:581:SER:OG	1:D:585:ARG:NH1	2.36	0.58
1:A:733:ILE:HG22	1:A:735:GLN:H	1.68	0.58
1:A:774:ILE:O	1:A:778:GLN:HB2	2.04	0.58
1:F:795:ILE:HA	1:F:846:LEU:HB2	1.86	0.58
1:E:564:GLN:O	1:E:568:HIS:ND1	2.36	0.58
1:E:582:ASN:HA	1:E:585:ARG:HD2	1.86	0.58
1:E:631:ARG:HG2	1:E:675:LEU:HD23	1.86	0.58
1:D:557:GLU:HG3	1:D:561:ARG:HE	1.68	0.57
1:B:317:ASP:HA	1:B:320:ARG:HB2	1.86	0.57
1:C:316:LEU:HD21	1:C:320:ARG:HE	1.69	0.57
1:C:559:LEU:O	1:C:585:ARG:NH2	2.35	0.57
1:D:450:ASP:HA	1:D:453:ARG:HE	1.69	0.57
1:D:742:MET:HA	1:D:745:ILE:HB	1.86	0.57
1:B:364:GLN:HB2	1:B:530:LYS:HA	1.85	0.57
1:C:170:GLU:HG2	1:C:174:GLN:HE22	1.68	0.57
1:B:181:ILE:HD13	1:B:349:ILE:HA	1.86	0.57
1:B:361:HIS:HA	1:B:402:ARG:HD3	1.85	0.57
1:A:563:GLU:OE2	1:A:585:ARG:NH2	2.37	0.57
1:A:170:GLU:O	1:A:174:GLN:NE2	2.37	0.57
1:F:212:LYS:N	2:F:901:AGS:O3A	2.37	0.57
1:F:686:VAL:O	1:F:690:LEU:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:THR:OG1	2:B:902:AGS:O2G	2.23	0.57
1:E:249:ALA:O	1:D:252:ARG:NH1	2.38	0.57
1:A:520:GLU:OE1	1:A:529:ASN:ND2	2.38	0.57
1:F:819:ARG:O	1:F:823:GLN:CB	2.53	0.57
1:C:537:ALA:O	1:C:541:ALA:HB2	2.05	0.56
1:C:845:ARG:NH1	1:C:847:GLU:OE2	2.33	0.56
1:C:183:ARG:NH2	1:C:339:ALA:O	2.35	0.56
1:F:323:ILE:HD12	1:F:330:GLU:HA	1.86	0.56
1:E:318:GLU:O	1:E:322:TYR:HB2	2.05	0.56
1:D:832:GLN:HB3	1:D:838:LEU:HD13	1.87	0.56
1:B:831:GLN:O	1:B:835:SER:HB2	2.05	0.56
1:A:724:GLU:OE1	1:A:727:ARG:NH2	2.38	0.56
1:E:794:HIS:HB2	1:E:845:ARG:HG2	1.87	0.56
1:D:247:ALA:O	1:D:258:ARG:NH1	2.38	0.56
1:C:756:ARG:NH1	1:D:815:ARG:O	2.38	0.56
1:F:401:ILE:HD13	1:F:531:VAL:HG22	1.88	0.56
2:C:902:AGS:O1B	2:C:902:AGS:S1G	2.63	0.56
1:F:581:SER:OG	1:F:585:ARG:NH1	2.39	0.56
1:F:591:LEU:HD13	1:A:830:ALA:HB3	1.86	0.56
1:D:563:GLU:O	1:D:567:HIS:ND1	2.38	0.56
1:D:611:LYS:NZ	1:D:718:SER:O	2.38	0.56
1:D:700:THR:HA	1:D:706:THR:HA	1.88	0.56
1:C:664:GLU:OE1	1:C:668:ARG:NH2	2.38	0.56
1:F:742:MET:O	1:F:746:LYS:HB2	2.05	0.56
1:D:778:GLN:HE21	1:D:818:LYS:HD3	1.70	0.56
1:B:388:ASP:OD2	1:A:331:ARG:NH1	2.39	0.56
1:A:613:GLU:O	1:A:617:ALA:HB2	2.06	0.56
2:F:901:AGS:S1G	2:F:901:AGS:O2B	2.64	0.56
1:D:388:ASP:HA	1:D:391:ILE:HD12	1.86	0.56
1:C:424:LEU:HA	1:C:427:GLN:HB3	1.87	0.56
1:F:609:VAL:HG11	1:F:765:PRO:HG3	1.86	0.56
1:F:834:LEU:O	1:E:556:ARG:NH1	2.39	0.56
1:E:362:HIS:HA	1:E:476:LYS:HE3	1.86	0.56
1:B:625:SER:OG	1:B:627:GLU:OE1	2.22	0.56
1:E:422:LEU:HB2	1:E:448:LEU:HD13	1.87	0.56
1:B:510:GLU:O	1:B:514:GLU:CB	2.54	0.55
1:F:628:ALA:HB1	1:F:672:SER:HA	1.88	0.55
1:B:646:LEU:HA	1:B:661:TYR:HD2	1.70	0.55
1:B:668:ARG:HD3	1:B:669:ARG:HG3	1.86	0.55
1:E:616:LYS:O	1:E:620:ASN:HB2	2.06	0.55
1:B:728:LYS:HA	1:B:732:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:HA	1:A:347:ILE:HD12	1.89	0.55
1:E:774:ILE:HA	1:E:777:ILE:HG12	1.89	0.55
1:A:183:ARG:HE	1:A:215:ILE:HD11	1.72	0.55
1:C:561:ARG:HB2	1:C:564:GLN:HB3	1.89	0.55
1:F:172:ALA:HB2	1:F:177:LEU:HD12	1.88	0.55
1:B:244:ALA:O	1:B:258:ARG:NH1	2.39	0.55
1:B:744:GLU:HA	1:B:747:LYS:HB3	1.87	0.55
1:E:318:GLU:O	1:E:322:TYR:CB	2.55	0.55
1:A:451:LYS:O	1:A:455:TYR:HB2	2.07	0.55
1:A:605:GLY:H	1:A:722:VAL:HG22	1.72	0.55
1:A:766:LEU:HB3	1:A:770:HIS:HB2	1.89	0.55
1:F:499:SER:O	1:F:503:TYR:HB2	2.07	0.55
1:E:235:ARG:NE	1:E:271:GLY:O	2.39	0.55
1:D:214:ALA:HB2	2:D:901:AGS:H2'	1.88	0.55
1:D:819:ARG:O	1:D:823:GLN:CB	2.55	0.55
1:F:563:GLU:O	1:F:567:HIS:ND1	2.33	0.55
1:A:171:ARG:HE	1:A:176:LYS:HD3	1.70	0.55
1:F:422:LEU:O	1:F:426:GLN:CB	2.55	0.55
1:F:506:ILE:HG13	1:F:507:PRO:HD3	1.88	0.55
1:E:723:ARG:O	1:E:727:ARG:CB	2.55	0.55
1:B:426:GLN:O	1:B:430:MET:CB	2.54	0.55
1:F:559:LEU:O	1:F:585:ARG:NH1	2.38	0.54
1:D:422:LEU:O	1:D:426:GLN:HB2	2.07	0.54
1:D:686:VAL:O	1:D:690:LEU:HB2	2.08	0.54
1:A:774:ILE:HA	1:A:777:ILE:HG12	1.88	0.54
1:B:351:ARG:NH2	1:B:367:ASP:OD2	2.40	0.54
1:B:604:LEU:HB2	1:B:762:VAL:HA	1.87	0.54
1:C:631:ARG:HG2	1:C:675:LEU:HD23	1.89	0.54
1:F:212:LYS:NZ	2:F:901:AGS:O2B	2.40	0.54
1:B:455:TYR:O	1:B:459:GLU:HB3	2.07	0.54
1:C:742:MET:HA	1:C:745:ILE:HB	1.88	0.54
1:F:423:LYS:O	1:F:427:GLN:CB	2.55	0.54
1:F:634:MET:HG3	1:F:679:VAL:HA	1.87	0.54
1:D:567:HIS:NE2	1:D:574:ASN:OD1	2.40	0.54
1:B:375:THR:O	1:B:379:ARG:CB	2.56	0.54
1:F:793:ILE:HA	1:F:844:ILE:HB	1.88	0.54
1:A:687:PHE:HA	1:A:690:LEU:HD12	1.88	0.54
1:C:346:THR:HG21	1:C:386:LEU:HB3	1.88	0.54
1:E:212:LYS:NZ	2:E:901:AGS:S1G	2.81	0.54
1:B:172:ALA:HB2	1:B:177:LEU:HD12	1.90	0.54
1:B:599:GLY:HA3	1:B:713:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:NZ	2:C:901:AGS:O1B	2.39	0.54
1:C:592:ALA:O	1:D:785:ARG:NH1	2.38	0.54
1:E:243:GLY:H	1:E:246:VAL:HG23	1.72	0.54
1:D:546:ILE:HD13	1:D:671:TYR:HD2	1.73	0.54
1:A:502:GLN:HA	1:A:506:ILE:HD13	1.89	0.54
1:F:318:GLU:O	1:F:322:TYR:CB	2.56	0.54
1:E:549:SER:HA	1:E:552:MET:HB3	1.90	0.54
1:E:571:ILE:HD13	1:E:770:HIS:HA	1.89	0.54
1:A:350:LEU:O	1:A:354:LYS:HB3	2.08	0.54
1:E:304:ALA:O	1:E:332:ARG:NH2	2.41	0.54
1:C:667:ARG:NH2	1:B:324:GLU:OE1	2.40	0.53
1:F:197:ARG:NH1	1:F:198:THR:OG1	2.41	0.53
1:F:681:LYS:HE3	1:F:720:LEU:HD21	1.90	0.53
1:B:719:ASN:HA	1:B:722:VAL:HG23	1.90	0.53
1:F:181:ILE:H	2:F:901:AGS:HN62	1.57	0.53
1:F:582:ASN:OD1	1:F:585:ARG:NH2	2.39	0.53
1:D:819:ARG:O	1:D:823:GLN:HB3	2.08	0.53
1:B:405:ILE:HG23	1:B:527:LEU:HD23	1.89	0.53
1:B:745:ILE:HA	1:B:749:PHE:HD2	1.73	0.53
1:A:734:HIS:O	1:A:738:SER:CB	2.56	0.53
1:C:753:PHE:O	1:C:757:ILE:N	2.40	0.53
1:C:774:ILE:O	1:C:778:GLN:HB2	2.08	0.53
1:B:496:ALA:O	1:B:500:GLU:HB2	2.09	0.53
1:B:728:LYS:NZ	1:B:732:LEU:O	2.38	0.53
1:A:193:VAL:HG11	1:A:202:PRO:HB3	1.90	0.53
1:F:509:LEU:O	1:F:513:LEU:CB	2.55	0.53
1:B:435:GLU:O	1:B:439:LYS:CB	2.57	0.53
1:A:199:LYS:HD3	1:A:334:GLN:HB2	1.89	0.53
1:E:661:TYR:OH	1:D:701:ASP:O	2.27	0.53
1:E:737:ASN:O	1:E:741:ALA:CB	2.56	0.53
1:D:737:ASN:O	1:D:741:ALA:HB2	2.09	0.53
1:A:419:ILE:HD13	1:A:455:TYR:HB2	1.89	0.53
1:E:342:SER:OG	1:E:343:VAL:N	2.40	0.53
1:D:585:ARG:O	1:D:589:ALA:HB2	2.08	0.53
1:A:222:ARG:HG3	1:A:227:GLU:HB2	1.90	0.53
1:F:634:MET:HB3	1:F:682:ALA:HB2	1.90	0.53
1:F:686:VAL:O	1:F:690:LEU:HB2	2.09	0.53
1:A:786:LEU:HB3	1:A:791:TYR:HB2	1.90	0.53
1:C:475:ILE:O	1:C:479:LEU:HB2	2.09	0.53
2:F:901:AGS:H5'2	1:E:331:ARG:HH12	1.74	0.53
1:E:586:ARG:HA	1:E:589:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ALA:O	1:C:331:ARG:HB2	2.08	0.52
1:F:734:HIS:NE2	1:F:762:VAL:O	2.39	0.52
1:E:550:ARG:HD3	1:E:588:ARG:HB3	1.91	0.52
1:D:265:ASP:HA	1:D:268:LYS:HG3	1.90	0.52
2:D:901:AGS:O2G	2:D:901:AGS:O2A	2.26	0.52
1:A:405:ILE:HG23	1:A:527:LEU:HD23	1.91	0.52
1:A:839:VAL:HB	1:A:842:LYS:HD3	1.91	0.52
1:C:235:ARG:NH2	1:C:271:GLY:O	2.42	0.52
1:E:220:ALA:HA	1:E:223:ILE:HD12	1.92	0.52
1:A:327:ALA:O	1:A:331:ARG:CB	2.57	0.52
1:C:750:ARG:NH2	2:D:902:AGS:O3B	2.33	0.52
1:F:210:VAL:N	2:F:901:AGS:O1B	2.41	0.52
1:F:434:ASP:HB2	1:F:438:LYS:HG2	1.91	0.52
1:D:634:MET:HB3	1:D:682:ALA:HB2	1.90	0.52
1:A:169:THR:HG22	1:A:220:ALA:HB1	1.92	0.52
1:D:631:ARG:HA	1:D:675:LEU:HB3	1.91	0.52
1:B:208:PRO:HG2	1:A:327:ALA:HB1	1.92	0.52
1:B:358:GLU:O	1:B:362:HIS:N	2.41	0.52
1:B:399:SER:HA	1:B:402:ARG:HE	1.74	0.52
1:C:170:GLU:O	1:C:174:GLN:NE2	2.42	0.52
1:C:456:SER:O	1:C:460:GLU:HB2	2.09	0.52
1:A:165:THR:HB	1:A:238:LEU:HB3	1.90	0.52
1:A:409:PRO:HB2	1:A:412:LEU:HD13	1.92	0.52
1:F:611:LYS:HG2	1:F:763:PHE:HD2	1.74	0.52
1:A:742:MET:HA	1:A:745:ILE:HD12	1.91	0.52
1:C:672:SER:O	1:C:712:THR:OG1	2.22	0.52
1:F:257:GLU:HA	1:F:260:LYS:HE2	1.90	0.52
1:E:191:ILE:HA	1:E:194:LEU:HD12	1.92	0.52
1:E:733:ILE:HG22	1:E:735:GLN:H	1.74	0.52
1:A:577:VAL:O	1:A:581:SER:CB	2.58	0.52
1:D:220:ALA:HA	1:D:223:ILE:HD12	1.90	0.52
1:C:544:THR:OG1	1:C:545:GLY:N	2.41	0.52
1:F:220:ALA:HA	1:F:223:ILE:HD12	1.92	0.52
1:D:532:THR:OG1	1:D:533:ASP:N	2.41	0.52
1:B:235:ARG:NH2	1:B:271:GLY:O	2.43	0.52
1:A:323:ILE:HG13	1:A:325:LYS:H	1.73	0.52
1:A:745:ILE:HA	1:A:748:ILE:HG22	1.91	0.52
1:C:803:LEU:HD11	1:C:825:ILE:HD11	1.91	0.51
1:F:701:ASP:OD1	1:F:704:GLY:N	2.35	0.51
1:E:320:ARG:O	1:E:323:ILE:CA	2.56	0.51
1:E:595:ASN:HA	1:E:710:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:HD21	1:A:589:ALA:HB2	1.92	0.51
1:C:564:GLN:O	1:C:568:HIS:ND1	2.42	0.51
1:C:692:GLN:NE2	1:D:633:ASP:OD2	2.41	0.51
1:E:555:GLU:HA	1:E:558:LYS:HE2	1.92	0.51
1:D:719:ASN:O	1:D:723:ARG:N	2.40	0.51
1:B:195:GLN:HE22	1:B:232:LEU:HD21	1.75	0.51
1:C:245:LEU:HB3	1:C:255:PHE:HE1	1.74	0.51
1:C:774:ILE:HA	1:C:777:ILE:HG12	1.92	0.51
1:F:331:ARG:NH2	2:A:901:AGS:S1G	2.83	0.51
1:F:563:GLU:OE2	1:F:585:ARG:NH2	2.36	0.51
1:B:684:PRO:HA	1:B:687:PHE:HD2	1.74	0.51
1:A:809:ASP:OD1	1:A:809:ASP:N	2.43	0.51
1:C:767:GLY:H	1:C:770:HIS:CD2	2.28	0.51
1:F:652:GLY:HA2	1:A:653:TYR:HB3	1.92	0.51
1:F:835:SER:HA	1:E:556:ARG:HD2	1.92	0.51
1:B:691:LEU:HD11	1:B:753:PHE:HB2	1.93	0.51
1:A:220:ALA:HA	1:A:223:ILE:HD12	1.91	0.51
1:A:738:SER:O	1:A:742:MET:HB3	2.10	0.51
1:F:166:ILE:O	1:F:239:ALA:N	2.41	0.51
1:F:741:ALA:O	1:F:745:ILE:HB	2.11	0.51
1:D:212:LYS:NZ	2:D:901:AGS:O2B	2.31	0.51
1:A:735:GLN:O	1:A:739:THR:OG1	2.26	0.51
1:A:738:SER:O	1:A:742:MET:CB	2.58	0.51
1:C:724:GLU:OE1	1:C:727:ARG:NH2	2.44	0.51
1:F:728:LYS:HG2	1:F:732:LEU:HD23	1.91	0.51
1:B:645:ARG:NH2	1:B:661:TYR:OH	2.43	0.51
1:A:610:GLY:O	1:A:614:LEU:N	2.44	0.51
1:A:619:ALA:HB1	1:A:628:ALA:HB3	1.91	0.51
1:A:724:GLU:O	1:A:728:LYS:HB3	2.11	0.51
1:F:197:ARG:HB3	1:A:360:HIS:CE1	2.45	0.51
1:E:533:ASP:OD1	1:E:533:ASP:N	2.43	0.51
1:D:364:GLN:HB2	1:D:530:LYS:HA	1.92	0.51
1:B:832:GLN:HB3	1:B:838:LEU:HD13	1.93	0.51
1:A:734:HIS:O	1:A:738:SER:HB3	2.11	0.51
1:D:412:LEU:O	1:D:416:ASP:HB2	2.11	0.51
1:B:412:LEU:O	1:B:416:ASP:HB2	2.11	0.51
1:A:547:PRO:HD2	1:A:550:ARG:HD2	1.93	0.51
1:C:759:GLU:OE2	1:D:823:GLN:NE2	2.40	0.50
1:B:222:ARG:HG3	1:B:227:GLU:HB2	1.93	0.50
1:B:751:PRO:HA	1:B:754:ILE:HD12	1.93	0.50
1:F:251:TYR:HA	1:E:252:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:599:GLY:HA3	1:F:713:VAL:HG13	1.93	0.50
1:E:181:ILE:HB	1:E:349:ILE:HD13	1.94	0.50
1:E:314:THR:OG1	1:E:318:GLU:OE1	2.28	0.50
1:D:600:SER:N	1:D:758:ASP:OD2	2.41	0.50
1:D:672:SER:OG	1:D:673:VAL:N	2.45	0.50
1:D:741:ALA:HB1	1:D:745:ILE:HD12	1.92	0.50
1:E:361:HIS:HA	1:E:402:ARG:HD3	1.92	0.50
1:A:663:THR:O	1:A:667:ARG:CB	2.58	0.50
1:C:243:GLY:H	1:C:246:VAL:HG23	1.75	0.50
1:C:361:HIS:HA	1:C:402:ARG:HD3	1.94	0.50
1:C:385:GLN:OE1	1:B:331:ARG:NH2	2.44	0.50
1:C:466:LYS:O	1:C:470:SER:CB	2.59	0.50
2:F:901:AGS:O3G	1:E:330:GLU:OE2	2.29	0.50
1:C:537:ALA:O	1:C:541:ALA:CB	2.59	0.50
1:D:580:VAL:HG11	1:D:618:LEU:HD11	1.94	0.50
1:A:318:GLU:O	1:A:322:TYR:HB3	2.10	0.50
1:A:334:GLN:NE2	1:A:335:LYS:O	2.42	0.50
1:F:422:LEU:HD22	1:F:448:LEU:HD23	1.94	0.50
1:D:733:ILE:HG13	1:D:736:ASP:H	1.77	0.50
1:B:456:SER:O	1:B:460:GLU:HB2	2.10	0.50
1:C:399:SER:HB3	1:B:195:GLN:HB2	1.94	0.50
1:C:402:ARG:NH2	1:B:195:GLN:O	2.45	0.50
1:C:422:LEU:HD22	1:C:444:LEU:HD11	1.93	0.50
1:C:737:ASN:O	1:C:741:ALA:CB	2.59	0.50
1:C:815:ARG:NH1	2:C:902:AGS:O3B	2.33	0.50
1:B:255:PHE:HE2	1:B:295:ALA:HB2	1.76	0.50
1:B:274:ILE:HG12	1:B:309:HIS:HD2	1.76	0.50
1:A:737:ASN:O	1:A:741:ALA:CB	2.58	0.50
1:F:486:ILE:HD13	1:F:501:LEU:HB2	1.94	0.50
1:F:764:HIS:ND1	1:F:765:PRO:O	2.34	0.50
1:E:211:GLY:N	2:E:901:AGS:O1B	2.43	0.50
1:E:694:LEU:HB3	1:E:756:ARG:HB3	1.94	0.50
1:E:819:ARG:NH2	1:D:755:ASN:O	2.44	0.50
1:C:636:GLU:OE1	1:C:645:ARG:NH1	2.44	0.50
1:B:637:PHE:HE1	1:B:645:ARG:HE	1.58	0.50
1:A:533:ASP:N	1:A:533:ASP:OD1	2.40	0.50
1:D:649:ALA:HB3	1:D:656:TYR:HA	1.94	0.49
1:C:327:ALA:O	1:C:331:ARG:CB	2.60	0.49
1:C:734:HIS:O	1:C:738:SER:CB	2.59	0.49
1:F:745:ILE:HA	1:F:748:ILE:HG22	1.93	0.49
1:E:499:SER:HA	1:E:503:TYR:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:SER:HG	1:D:758:ASP:H	1.61	0.49
1:A:170:GLU:HG2	1:A:174:GLN:HE22	1.77	0.49
1:A:196:ARG:HH12	1:A:334:GLN:HG2	1.77	0.49
1:F:396:GLU:OE1	1:E:196:ARG:NH2	2.44	0.49
1:B:533:ASP:N	1:B:533:ASP:OD1	2.44	0.49
1:C:605:GLY:HA3	1:C:763:PHE:HB2	1.94	0.49
1:C:671:TYR:CE1	1:C:711:ASN:HB2	2.47	0.49
1:C:751:PRO:O	1:C:755:ASN:HB2	2.12	0.49
1:F:183:ARG:HE	2:F:901:AGS:HN61	1.60	0.49
1:D:745:ILE:HG23	1:D:749:PHE:HB2	1.94	0.49
1:C:380:TYR:HB2	1:C:540:LEU:HD21	1.94	0.49
1:C:388:ASP:HA	1:C:391:ILE:HD12	1.93	0.49
1:C:663:THR:HG21	1:C:701:ASP:HB3	1.94	0.49
1:E:303:LEU:O	1:E:332:ARG:NE	2.43	0.49
1:E:797:ASP:OD1	1:E:797:ASP:N	2.44	0.49
1:B:540:LEU:HA	1:B:543:TRP:HB2	1.93	0.49
1:A:472:THR:HG22	1:A:476:LYS:HE2	1.94	0.49
1:A:577:VAL:O	1:A:581:SER:HB2	2.13	0.49
1:C:209:GLY:HA2	2:C:901:AGS:H5'1	1.94	0.49
1:C:344:GLU:HA	1:C:347:ILE:HD12	1.94	0.49
1:C:593:ASP:HA	1:D:785:ARG:HH22	1.76	0.49
1:C:599:GLY:HA3	1:C:713:VAL:HG13	1.94	0.49
1:B:663:THR:O	1:B:667:ARG:HB2	2.12	0.49
1:C:475:ILE:HD12	1:C:513:LEU:HG	1.93	0.49
1:C:750:ARG:NH1	2:D:902:AGS:S1G	2.84	0.49
1:E:344:GLU:HA	1:E:347:ILE:HD12	1.94	0.49
1:E:542:ARG:NH1	1:D:192:GLN:OE1	2.46	0.49
1:E:655:GLY:HA3	1:D:651:PRO:HB3	1.94	0.49
1:E:725:THR:HA	1:E:728:LYS:HG2	1.94	0.49
1:B:541:ALA:HA	1:B:546:ILE:H	1.77	0.49
1:C:368:PRO:HA	1:C:371:VAL:HG12	1.93	0.49
1:F:364:GLN:OE1	1:F:476:LYS:NZ	2.44	0.49
1:F:639:GLU:H	1:F:642:SER:HG	1.59	0.49
1:D:197:ARG:HH11	1:D:198:THR:H	1.61	0.49
1:B:499:SER:HA	1:B:502:GLN:HB3	1.94	0.49
1:A:483:LYS:HA	1:A:486:ILE:HG22	1.95	0.49
1:A:628:ALA:HB1	1:A:672:SER:HA	1.94	0.49
1:C:220:ALA:HA	1:C:223:ILE:HD12	1.94	0.49
1:B:641:HIS:HB3	1:A:650:PRO:HB3	1.95	0.49
1:A:346:THR:HG21	1:A:386:LEU:HD22	1.95	0.49
1:A:603:PHE:HB2	1:A:717:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:ASP:HA	1:E:419:ILE:HD12	1.94	0.49
1:E:596:ARG:NH2	1:E:756:ARG:O	2.46	0.49
1:D:305:ARG:NH1	1:D:307:GLU:OE2	2.39	0.49
1:D:585:ARG:O	1:D:589:ALA:CB	2.60	0.49
1:B:472:THR:HG22	1:B:476:LYS:HE2	1.95	0.49
1:C:342:SER:OG	1:C:343:VAL:N	2.46	0.48
1:C:596:ARG:NH2	1:C:756:ARG:O	2.46	0.48
1:C:750:ARG:HG2	1:C:751:PRO:HD2	1.94	0.48
1:F:422:LEU:O	1:F:426:GLN:HB3	2.13	0.48
1:C:211:GLY:O	1:C:215:ILE:N	2.43	0.48
1:C:742:MET:SD	1:D:812:TYR:OH	2.67	0.48
1:D:741:ALA:O	1:D:745:ILE:HB	2.13	0.48
1:B:597:PRO:HA	1:B:710:ARG:HA	1.94	0.48
2:B:902:AGS:O2G	2:B:902:AGS:O1B	2.31	0.48
1:A:318:GLU:O	1:A:322:TYR:CB	2.61	0.48
1:A:745:ILE:O	1:A:749:PHE:N	2.28	0.48
1:A:827:ASN:O	1:A:831:GLN:CB	2.61	0.48
1:C:317:ASP:OD1	1:C:317:ASP:N	2.47	0.48
1:C:750:ARG:HH22	2:D:902:AGS:PB	2.36	0.48
1:F:628:ALA:HB2	1:F:669:ARG:HH11	1.78	0.48
1:A:577:VAL:O	1:A:581:SER:OG	2.31	0.48
1:F:221:GLN:HA	1:F:224:ILE:HG22	1.95	0.48
1:D:346:THR:HA	1:D:349:ILE:HD12	1.95	0.48
1:F:734:HIS:CE1	1:F:764:HIS:HB3	2.48	0.48
1:E:745:ILE:HG23	1:E:749:PHE:HB2	1.95	0.48
1:D:740:ASP:HA	1:D:743:GLU:HG2	1.95	0.48
1:C:263:LEU:HD23	1:C:266:LEU:HD12	1.94	0.48
1:A:319:TYR:O	1:A:323:ILE:C	2.52	0.48
1:A:509:LEU:HA	1:A:512:GLN:HG2	1.96	0.48
1:F:676:LEU:N	1:F:715:ILE:O	2.47	0.48
1:D:643:VAL:HA	1:D:646:LEU:HD23	1.95	0.48
1:D:737:ASN:O	1:D:741:ALA:CB	2.61	0.48
1:B:827:ASN:OD1	1:B:827:ASN:N	2.35	0.48
1:C:195:GLN:O	1:D:402:ARG:NH2	2.46	0.48
1:F:355:GLU:O	1:F:359:LEU:HB2	2.14	0.48
1:F:616:LYS:O	1:F:620:ASN:CB	2.59	0.48
1:D:242:MET:HB2	1:D:283:MET:HE1	1.95	0.48
1:A:275:LEU:O	1:A:311:VAL:N	2.40	0.48
1:A:613:GLU:O	1:A:617:ALA:CB	2.62	0.48
1:A:792:GLU:HB2	1:A:843:VAL:HG23	1.94	0.48
1:C:645:ARG:NH2	1:B:701:ASP:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:378:HIS:HA	1:F:389:LYS:HZ1	1.79	0.48
1:F:783:TYR:HA	1:F:786:LEU:HD12	1.95	0.48
1:A:317:ASP:OD1	1:A:317:ASP:N	2.46	0.48
1:C:238:LEU:O	1:C:276:PHE:N	2.47	0.48
1:F:566:LEU:HD22	1:F:617:ALA:HB1	1.96	0.48
1:E:161:LEU:O	1:E:165:THR:N	2.42	0.48
1:E:402:ARG:NH2	1:D:195:GLN:O	2.39	0.48
1:B:384:ARG:HB2	1:B:389:LYS:HB3	1.96	0.48
1:B:455:TYR:O	1:B:459:GLU:CB	2.62	0.48
1:A:697:GLY:O	1:A:709:PHE:N	2.44	0.48
1:C:214:ALA:N	2:C:901:AGS:O1A	2.46	0.47
1:C:475:ILE:HB	1:C:513:LEU:HD21	1.96	0.47
1:F:825:ILE:HA	1:F:852:ARG:HH22	1.79	0.47
1:E:203:VAL:HB	1:E:335:LYS:HA	1.97	0.47
1:E:441:LEU:HB2	1:E:444:LEU:HB3	1.96	0.47
1:D:344:GLU:HA	1:D:347:ILE:HD12	1.96	0.47
1:B:241:ASP:OD1	1:B:241:ASP:N	2.46	0.47
1:B:456:SER:O	1:B:460:GLU:CB	2.62	0.47
1:A:373:ALA:O	1:A:377:SER:OG	2.26	0.47
1:C:331:ARG:NH2	1:D:208:PRO:O	2.45	0.47
1:C:357:TYR:O	1:C:361:HIS:CB	2.52	0.47
1:C:423:LYS:O	1:C:427:GLN:CB	2.62	0.47
1:B:415:LEU:HA	1:B:418:ARG:HE	1.79	0.47
1:A:646:LEU:HA	1:A:661:TYR:HD2	1.79	0.47
1:B:435:GLU:HB2	1:B:439:LYS:HE3	1.95	0.47
1:F:606:PRO:HG3	1:F:726:GLU:HG2	1.96	0.47
1:D:506:ILE:HG13	1:D:507:PRO:HD3	1.94	0.47
1:B:375:THR:O	1:B:379:ARG:HB2	2.13	0.47
1:C:412:LEU:O	1:C:416:ASP:CB	2.50	0.47
1:F:197:ARG:HG2	1:F:198:THR:HG23	1.96	0.47
1:F:475:ILE:HD11	1:F:512:GLN:HG3	1.95	0.47
1:D:613:GLU:N	2:D:902:AGS:O1A	2.47	0.47
2:B:902:AGS:O3B	2:B:902:AGS:O1A	2.32	0.47
1:B:746:LYS:HE3	1:B:751:PRO:HG3	1.97	0.47
1:C:466:LYS:O	1:C:470:SER:OG	2.29	0.47
1:F:604:LEU:HB2	1:F:762:VAL:HG23	1.97	0.47
1:F:794:HIS:N	1:F:844:ILE:O	2.35	0.47
1:E:435:GLU:O	1:E:439:LYS:CB	2.62	0.47
1:E:582:ASN:OD1	1:E:585:ARG:NH1	2.47	0.47
1:D:492:VAL:HG13	1:D:494:ASP:H	1.80	0.47
1:D:742:MET:O	1:D:746:LYS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG23	1:B:341:PRO:HD3	1.97	0.47
1:B:220:ALA:HA	1:B:223:ILE:HD12	1.97	0.47
1:B:631:ARG:HA	1:B:675:LEU:HB3	1.97	0.47
2:A:901:AGS:O2G	2:A:901:AGS:O2B	2.31	0.47
1:C:303:LEU:HD13	1:C:332:ARG:HG3	1.97	0.47
1:F:197:ARG:NH1	1:A:395:ASP:OD2	2.47	0.47
1:F:297:ASN:ND2	1:A:247:ALA:O	2.43	0.47
1:E:563:GLU:OE2	1:E:585:ARG:NH2	2.47	0.47
1:C:247:ALA:O	1:C:249:ALA:N	2.48	0.47
1:C:499:SER:HA	1:C:503:TYR:HD2	1.80	0.47
1:F:822:GLN:HB2	1:E:586:ARG:HH12	1.79	0.47
1:F:250:LYS:O	1:E:252:ARG:NH1	2.48	0.47
1:F:366:THR:HG23	1:F:369:ALA:H	1.80	0.47
1:F:585:ARG:O	1:F:589:ALA:HB2	2.15	0.47
1:D:816:PRO:O	1:D:820:ALA:CB	2.63	0.47
1:B:263:LEU:HA	1:B:266:LEU:HD12	1.97	0.47
1:B:668:ARG:HH11	1:B:669:ARG:HG3	1.80	0.47
1:F:655:GLY:O	1:F:659:GLY:N	2.48	0.46
1:F:686:VAL:O	1:F:690:LEU:HB3	2.15	0.46
1:E:366:THR:OG1	1:E:531:VAL:O	2.29	0.46
1:B:561:ARG:O	1:B:565:GLU:N	2.41	0.46
1:C:193:VAL:HG13	1:C:196:ARG:HH21	1.79	0.46
1:C:222:ARG:HG3	1:C:227:GLU:HB2	1.97	0.46
1:C:316:LEU:HD22	1:D:668:ARG:NE	2.30	0.46
1:F:674:ILE:O	1:F:715:ILE:N	2.43	0.46
1:E:587:SER:OG	1:E:588:ARG:N	2.48	0.46
1:E:729:SER:HA	1:E:730:ILE:HA	1.66	0.46
1:C:200:ASN:OD1	1:C:200:ASN:N	2.47	0.46
1:C:330:GLU:O	1:D:384:ARG:NH2	2.47	0.46
1:F:222:ARG:O	1:F:227:GLU:N	2.44	0.46
1:E:405:ILE:HD11	1:E:529:ASN:HA	1.98	0.46
1:A:235:ARG:HE	1:A:274:ILE:HD11	1.80	0.46
1:F:247:ALA:O	1:F:258:ARG:NH1	2.48	0.46
1:E:305:ARG:HB3	1:E:307:GLU:HG2	1.96	0.46
1:D:210:VAL:N	2:D:901:AGS:O1B	2.49	0.46
1:D:721:GLY:O	1:D:725:THR:N	2.40	0.46
1:B:367:ASP:HA	1:B:370:ILE:HD12	1.96	0.46
1:E:179:PRO:HA	1:E:221:GLN:HE22	1.81	0.46
1:E:830:ALA:HA	1:E:833:ILE:HG22	1.97	0.46
1:D:611:LYS:HG2	1:D:763:PHE:HE2	1.80	0.46
1:B:666:VAL:HG21	1:B:709:PHE:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:PRO:HG3	1:A:656:TYR:CZ	2.51	0.46
1:C:663:THR:O	1:C:667:ARG:HB2	2.16	0.46
1:F:794:HIS:O	1:F:846:LEU:N	2.42	0.46
1:D:248:GLY:HA3	1:D:258:ARG:HH22	1.80	0.46
1:D:409:PRO:HB2	1:D:412:LEU:HD23	1.98	0.46
1:A:193:VAL:HA	1:A:196:ARG:HD3	1.98	0.46
1:C:419:ILE:HD13	1:C:455:TYR:HB2	1.98	0.46
1:C:656:TYR:HD2	1:D:654:VAL:HG12	1.81	0.46
1:C:756:ARG:HD3	1:D:819:ARG:HG2	1.98	0.46
2:F:902:AGS:O2A	2:F:902:AGS:O1B	2.33	0.46
1:D:633:ASP:OD2	1:D:635:SER:OG	2.33	0.46
1:B:198:THR:HA	1:B:306:GLY:HA3	1.97	0.46
1:B:611:LYS:HG2	1:B:763:PHE:HE2	1.81	0.46
1:B:756:ARG:HD3	1:B:756:ARG:HA	1.78	0.46
1:A:500:GLU:O	1:A:504:GLY:HA3	2.16	0.46
1:C:419:ILE:HG12	1:C:451:LYS:HB3	1.98	0.46
1:F:490:ARG:HH21	1:F:502:GLN:HE21	1.63	0.46
1:B:173:GLU:HG2	1:B:491:ARG:HH12	1.81	0.46
1:B:831:GLN:O	1:B:835:SER:CB	2.63	0.46
1:B:849:ASN:HD22	1:B:852:ARG:HG3	1.80	0.46
1:F:834:LEU:HB3	1:E:556:ARG:CZ	2.46	0.45
1:E:241:ASP:N	1:E:241:ASP:OD1	2.46	0.45
1:E:672:SER:O	1:E:712:THR:OG1	2.26	0.45
1:D:172:ALA:HB2	1:D:177:LEU:HD12	1.97	0.45
1:D:472:THR:HA	1:D:475:ILE:HG22	1.98	0.45
1:F:559:LEU:HD22	1:F:585:ARG:HG2	1.98	0.45
1:E:253:GLY:O	1:E:257:GLU:N	2.48	0.45
1:E:690:LEU:HA	1:E:693:VAL:HG22	1.97	0.45
1:B:317:ASP:N	1:B:317:ASP:OD1	2.49	0.45
1:A:619:ALA:O	1:A:624:ASP:N	2.49	0.45
1:C:167:ASP:HA	1:C:238:LEU:HG	1.97	0.45
1:F:346:THR:HG21	1:F:386:LEU:HD22	1.98	0.45
1:F:742:MET:O	1:F:746:LYS:HB3	2.15	0.45
1:F:766:LEU:HB3	1:F:770:HIS:HB2	1.97	0.45
1:E:565:GLU:HA	1:E:568:HIS:HD1	1.81	0.45
1:D:724:GLU:OE2	1:D:737:ASN:ND2	2.49	0.45
1:B:677:ASP:OD1	1:B:677:ASP:N	2.50	0.45
1:C:450:ASP:OD1	1:C:453:ARG:NH2	2.49	0.45
1:E:608:GLY:H	1:E:815:ARG:HH11	1.64	0.45
1:D:680:GLU:OE2	1:D:718:SER:OG	2.34	0.45
1:D:718:SER:HG	1:D:719:ASN:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:GLU:HB3	1:C:720:LEU:HG	1.99	0.45
1:E:819:ARG:HH22	1:D:756:ARG:HE	1.65	0.45
1:D:197:ARG:HD3	1:D:197:ARG:H	1.81	0.45
1:D:358:GLU:HG3	1:D:365:ILE:HD12	1.98	0.45
1:D:768:GLU:HA	1:D:771:ILE:HD12	1.98	0.45
1:B:168:LEU:HD11	1:B:239:ALA:HB2	1.98	0.45
1:B:323:ILE:HA	1:B:323:ILE:HD13	1.85	0.45
1:B:409:PRO:HD2	1:B:412:LEU:HD12	1.99	0.45
1:B:610:GLY:O	1:B:614:LEU:N	2.48	0.45
1:A:409:PRO:HG3	1:A:527:LEU:HD11	1.98	0.45
1:C:694:LEU:HD23	1:C:757:ILE:HG22	1.99	0.45
1:F:171:ARG:HG2	1:F:176:LYS:HE3	1.99	0.45
1:E:850:GLU:O	1:E:852:ARG:N	2.50	0.45
1:B:245:LEU:O	1:B:258:ARG:NH1	2.50	0.45
1:C:646:LEU:HA	1:C:661:TYR:HD2	1.81	0.45
1:B:167:ASP:HA	1:B:238:LEU:HG	1.97	0.45
1:B:378:HIS:HB2	1:B:386:LEU:HD21	1.98	0.45
1:A:281:HIS:HB2	1:A:322:TYR:CG	2.50	0.45
1:C:466:LYS:O	1:C:470:SER:HB2	2.17	0.45
1:E:768:GLU:HA	1:E:771:ILE:HD12	1.97	0.45
1:D:786:LEU:O	1:D:790:GLY:N	2.50	0.45
1:B:633:ASP:OD1	1:B:634:MET:N	2.50	0.45
1:A:421:GLN:O	1:A:425:GLU:HB2	2.17	0.45
1:E:429:LEU:HD12	1:E:441:LEU:HD13	1.99	0.45
1:E:641:HIS:O	1:E:644:SER:OG	2.26	0.45
1:B:434:ASP:O	1:B:438:LYS:N	2.42	0.45
1:B:815:ARG:HH11	1:A:752:GLU:HB3	1.82	0.45
1:A:192:GLN:O	1:A:195:GLN:NE2	2.50	0.45
1:A:509:LEU:HG	1:A:512:GLN:HE21	1.82	0.45
1:C:489:ALA:HA	1:C:492:VAL:HG12	1.98	0.45
1:C:802:LEU:O	1:C:806:ASN:ND2	2.50	0.45
1:F:797:ASP:N	1:F:797:ASP:OD1	2.48	0.45
1:E:170:GLU:O	1:E:174:GLN:NE2	2.49	0.45
1:E:500:GLU:O	1:E:504:GLY:HA3	2.16	0.45
1:D:544:THR:OG1	1:D:545:GLY:N	2.50	0.45
1:B:653:TYR:HB3	1:B:654:VAL:H	1.62	0.45
1:F:171:ARG:O	1:F:176:LYS:N	2.44	0.44
1:F:462:TRP:CE2	1:F:466:LYS:HD2	2.52	0.44
1:E:187:ILE:O	1:E:190:THR:OG1	2.30	0.44
1:E:441:LEU:O	1:E:445:ASN:N	2.43	0.44
1:E:633:ASP:HB2	1:D:692:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:783:TYR:O	1:E:787:GLU:CB	2.52	0.44
1:D:416:ASP:HA	1:D:419:ILE:HG12	1.99	0.44
1:A:459:GLU:O	1:A:463:LYS:HD2	2.17	0.44
1:A:473:GLN:HA	1:A:476:LYS:HD2	1.98	0.44
1:C:834:LEU:HD22	1:B:559:LEU:HD11	1.98	0.44
1:B:511:LYS:HA	1:B:514:GLU:HB3	1.99	0.44
1:B:566:LEU:HD12	1:B:577:VAL:HG13	1.98	0.44
1:B:734:HIS:O	1:B:738:SER:HB2	2.18	0.44
1:A:323:ILE:HD12	1:A:323:ILE:HA	1.92	0.44
1:A:729:SER:HA	1:A:730:ILE:HA	1.61	0.44
1:F:556:ARG:HA	1:F:559:LEU:HB2	2.00	0.44
1:D:408:LYS:HA	1:D:409:PRO:HD3	1.89	0.44
1:D:596:ARG:HH22	1:D:756:ARG:HD3	1.83	0.44
1:B:847:GLU:N	1:B:854:VAL:O	2.50	0.44
1:C:423:LYS:O	1:C:427:GLN:HB2	2.18	0.44
1:C:519:LEU:O	1:C:523:THR:HB	2.17	0.44
1:E:651:PRO:HA	1:E:656:TYR:CG	2.52	0.44
1:B:200:ASN:OD1	1:B:200:ASN:N	2.50	0.44
1:A:687:PHE:HE2	1:A:748:ILE:HG13	1.83	0.44
1:C:699:LEU:O	1:C:707:VAL:N	2.50	0.44
1:F:604:LEU:HD22	1:F:718:SER:HB3	2.00	0.44
1:C:616:LYS:O	1:C:620:ASN:HB2	2.18	0.44
1:C:646:LEU:HG	1:C:647:VAL:HG23	1.98	0.44
1:C:729:SER:HA	1:C:730:ILE:HA	1.64	0.44
1:D:667:ARG:NH1	1:D:705:ARG:HD3	2.33	0.44
1:B:664:GLU:OE1	1:B:667:ARG:NH2	2.51	0.44
1:A:581:SER:HA	1:A:584:ILE:HD12	2.00	0.44
1:A:784:LYS:HE2	1:A:784:LYS:HB3	1.85	0.44
1:E:420:ILE:HA	1:E:423:LYS:HE2	2.00	0.44
1:E:839:VAL:HB	1:E:842:LYS:HD3	1.98	0.44
1:D:435:GLU:HG3	1:D:439:LYS:HG3	1.98	0.44
1:B:422:LEU:HD13	1:B:448:LEU:HA	1.99	0.44
1:B:498:MET:O	1:B:502:GLN:HB2	2.17	0.44
1:B:697:GLY:O	1:B:709:PHE:N	2.50	0.44
1:A:399:SER:HA	1:A:402:ARG:HE	1.83	0.44
1:C:728:LYS:HA	1:C:732:LEU:HB3	1.99	0.44
1:E:166:ILE:HB	1:E:239:ALA:HB3	1.99	0.44
1:E:846:LEU:HD23	1:E:846:LEU:HA	1.86	0.44
1:D:257:GLU:HA	1:D:260:LYS:HE2	1.99	0.44
1:D:265:ASP:O	1:D:269:GLN:CB	2.66	0.44
1:D:671:TYR:CD1	1:D:711:ASN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:718:SER:OG	1:D:719:ASN:N	2.50	0.44
1:B:796:SER:HB2	1:B:845:ARG:HH21	1.83	0.44
1:A:409:PRO:HD2	1:A:412:LEU:HD22	2.00	0.44
1:A:721:GLY:O	1:A:725:THR:N	2.50	0.44
1:C:550:ARG:HB3	1:C:555:GLU:HB2	2.00	0.43
1:F:373:ALA:O	1:F:377:SER:CB	2.66	0.43
1:F:393:LEU:O	1:F:397:ALA:HB2	2.17	0.43
1:D:322:TYR:HD2	1:D:323:ILE:HG22	1.84	0.43
1:B:608:GLY:HA3	1:B:815:ARG:HE	1.83	0.43
1:A:657:GLU:O	1:A:703:GLN:NE2	2.51	0.43
1:C:551:MET:HA	1:C:556:ARG:NH1	2.33	0.43
1:C:625:SER:OG	1:C:626:ASP:N	2.50	0.43
1:C:664:GLU:HB3	1:C:668:ARG:HH22	1.83	0.43
1:C:245:LEU:O	1:C:258:ARG:NH1	2.51	0.43
1:B:661:TYR:CE1	1:A:704:GLY:HA2	2.53	0.43
1:F:424:LEU:HD13	1:E:502:GLN:HE22	1.83	0.43
1:D:411:GLU:O	1:D:415:LEU:HB2	2.18	0.43
1:C:661:TYR:CE1	1:B:704:GLY:HA2	2.54	0.43
1:E:300:LYS:HA	1:E:303:LEU:HB2	2.00	0.43
1:B:161:LEU:O	1:B:165:THR:N	2.47	0.43
1:B:570:VAL:HG22	1:B:613:GLU:HG3	2.01	0.43
1:F:585:ARG:O	1:F:589:ALA:CB	2.67	0.43
1:E:767:GLY:H	1:E:770:HIS:CD2	2.36	0.43
1:D:169:THR:O	1:D:173:GLU:HB2	2.18	0.43
1:B:274:ILE:HG12	1:B:309:HIS:CD2	2.54	0.43
1:B:606:PRO:HG2	1:B:609:VAL:HG11	2.00	0.43
1:B:723:ARG:HA	1:B:726:GLU:HG2	2.00	0.43
1:B:786:LEU:HD22	1:B:793:ILE:HD11	1.99	0.43
1:C:420:ILE:HA	1:C:423:LYS:HG2	1.99	0.43
1:C:526:LEU:O	1:C:528:ARG:NH1	2.52	0.43
1:C:563:GLU:O	1:C:567:HIS:HB2	2.18	0.43
1:C:682:ALA:HB1	1:C:686:VAL:HG21	2.01	0.43
1:F:416:ASP:HA	1:F:419:ILE:HG12	2.01	0.43
1:E:418:ARG:HA	1:E:421:GLN:HB3	2.00	0.43
1:E:600:SER:N	1:E:758:ASP:OD2	2.51	0.43
1:E:605:GLY:HA3	1:E:763:PHE:HB2	2.01	0.43
1:D:775:ALA:HB2	1:D:817:LEU:HD21	2.01	0.43
1:B:375:THR:O	1:B:379:ARG:HB3	2.18	0.43
1:B:617:ALA:O	1:B:621:PHE:CB	2.65	0.43
1:E:424:LEU:HA	1:E:427:GLN:HB3	2.00	0.43
1:D:187:ILE:O	1:D:191:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:NH1	1:D:198:THR:OG1	2.52	0.43
1:B:688:ASN:OD1	1:B:750:ARG:NH1	2.46	0.43
1:C:756:ARG:CZ	1:D:818:LYS:HB3	2.49	0.43
1:F:393:LEU:O	1:F:397:ALA:CB	2.67	0.43
1:E:383:ASP:O	1:E:385:GLN:NE2	2.52	0.43
1:D:613:GLU:HB2	2:D:902:AGS:H2'	2.00	0.43
1:B:245:LEU:HB3	1:B:255:PHE:HE1	1.84	0.43
1:B:314:THR:OG1	1:B:315:THR:N	2.49	0.43
1:E:429:LEU:HD22	1:E:438:LYS:HG2	2.01	0.42
1:E:501:LEU:HD23	1:E:505:LYS:HD2	1.99	0.42
1:D:816:PRO:O	1:D:820:ALA:HB2	2.18	0.42
1:D:848:VAL:HG12	1:D:853:ILE:HA	2.01	0.42
1:B:646:LEU:HA	1:B:661:TYR:CD2	2.52	0.42
1:C:299:LEU:O	1:C:303:LEU:N	2.44	0.42
1:F:674:ILE:HD12	1:F:714:VAL:HG12	2.01	0.42
1:D:782:LEU:HA	1:D:785:ARG:HD2	2.01	0.42
1:C:637:PHE:HE1	1:C:645:ARG:HD3	1.84	0.42
1:F:373:ALA:O	1:F:377:SER:OG	2.34	0.42
1:F:601:PHE:HB2	1:F:603:PHE:CE2	2.54	0.42
1:F:809:ASP:HB2	1:F:816:PRO:HG2	2.00	0.42
1:E:203:VAL:N	1:E:334:GLN:O	2.51	0.42
1:E:738:SER:O	1:E:742:MET:HB3	2.20	0.42
1:A:388:ASP:HA	1:A:391:ILE:HD12	2.01	0.42
1:F:171:ARG:HB3	1:F:176:LYS:HB2	2.01	0.42
1:F:601:PHE:HD1	1:F:759:GLU:H	1.67	0.42
1:F:631:ARG:HA	1:F:675:LEU:HB3	2.01	0.42
1:E:774:ILE:O	1:E:778:GLN:HB2	2.20	0.42
1:E:809:ASP:N	1:E:809:ASP:OD1	2.50	0.42
1:D:204:LEU:HA	1:D:336:VAL:HB	2.01	0.42
1:D:607:THR:HG22	1:D:608:GLY:H	1.84	0.42
1:B:213:THR:HG22	2:B:901:AGS:PA	2.59	0.42
1:C:300:LYS:HA	1:C:303:LEU:HD12	2.01	0.42
1:B:570:VAL:HG21	1:B:614:LEU:HA	2.01	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.88	0.42
1:A:298:MET:SD	1:A:298:MET:N	2.92	0.42
1:A:701:ASP:OD2	1:A:705:ARG:NH2	2.53	0.42
1:C:240:LEU:HB2	1:C:275:LEU:HD21	2.01	0.42
1:C:326:ASP:OD1	1:C:327:ALA:N	2.52	0.42
1:C:602:LEU:HD23	1:C:760:VAL:HG22	2.01	0.42
1:F:181:ILE:HD11	1:F:352:GLY:HA3	2.01	0.42
1:F:422:LEU:O	1:F:426:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:577:VAL:O	1:F:581:SER:HB2	2.20	0.42
1:F:602:LEU:HD21	1:F:745:ILE:HD13	2.01	0.42
1:D:667:ARG:HH11	1:D:705:ARG:HD3	1.84	0.42
1:B:788:GLU:HG3	1:B:789:ARG:HG3	2.00	0.42
1:A:349:ILE:O	1:A:352:GLY:N	2.52	0.42
1:A:697:GLY:HA2	1:A:709:PHE:HB2	2.02	0.42
1:C:668:ARG:HE	1:B:320:ARG:HH22	1.67	0.42
1:E:720:LEU:HD13	1:E:744:GLU:HG3	2.02	0.42
1:D:390:ALA:HA	1:D:393:LEU:HD12	2.00	0.42
1:A:345:ASP:O	1:A:349:ILE:HG12	2.20	0.42
1:E:346:THR:HG21	1:E:386:LEU:HB3	2.02	0.42
1:D:496:ALA:O	1:D:500:GLU:HB2	2.20	0.42
1:D:750:ARG:O	1:D:754:ILE:N	2.33	0.42
1:B:634:MET:HG3	1:B:679:VAL:HG23	2.01	0.42
1:A:183:ARG:HH22	1:A:338:VAL:HB	1.85	0.42
1:A:565:GLU:HG3	1:A:621:PHE:HE1	1.84	0.42
1:A:794:HIS:H	1:A:845:ARG:HA	1.83	0.42
1:C:604:LEU:N	1:C:761:VAL:O	2.47	0.42
1:C:745:ILE:HG21	1:C:754:ILE:HD11	2.01	0.42
1:E:381:ILE:HB	1:E:389:LYS:HD2	2.01	0.42
1:E:475:ILE:HD12	1:E:513:LEU:HG	2.02	0.42
1:B:240:LEU:HD11	1:B:245:LEU:HD11	2.02	0.42
1:B:605:GLY:HA3	1:B:763:PHE:HB2	2.00	0.42
1:A:320:ARG:HA	1:A:324:GLU:HB2	2.01	0.42
1:C:365:ILE:HD13	1:C:365:ILE:HA	1.93	0.41
1:C:507:PRO:HA	1:C:510:GLU:HB2	2.02	0.41
1:E:376:LEU:O	1:E:380:TYR:HB2	2.20	0.41
1:E:712:THR:OG1	1:E:713:VAL:N	2.53	0.41
1:F:181:ILE:HD13	1:F:349:ILE:HA	2.01	0.41
1:F:315:THR:HG22	1:F:316:LEU:H	1.85	0.41
1:B:178:ASP:HA	1:B:179:PRO:HD3	1.94	0.41
1:B:486:ILE:HD13	1:B:501:LEU:HD12	2.03	0.41
1:A:573:GLN:HE22	1:A:764:HIS:H	1.66	0.41
1:C:696:ASP:OD2	1:D:631:ARG:NH1	2.54	0.41
1:F:429:LEU:HA	1:F:438:LYS:HE2	2.01	0.41
1:E:604:LEU:HD23	1:E:604:LEU:HA	1.87	0.41
1:D:509:LEU:HD23	1:D:512:GLN:HE21	1.84	0.41
1:D:571:ILE:H	1:D:571:ILE:HG13	1.62	0.41
1:A:368:PRO:HA	1:A:371:VAL:HG12	2.02	0.41
1:C:830:ALA:HA	1:C:833:ILE:HG22	2.02	0.41
1:E:525:ARG:HE	1:E:526:LEU:HG	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LEU:HA	1:D:472:THR:HG22	2.01	0.41
1:D:571:ILE:HD11	1:D:774:ILE:HD11	2.03	0.41
1:B:183:ARG:NH2	1:B:341:PRO:HG3	2.35	0.41
1:B:373:ALA:O	1:B:377:SER:CB	2.68	0.41
1:A:611:LYS:HG2	1:A:763:PHE:HE2	1.85	0.41
1:C:343:VAL:O	1:C:346:THR:OG1	2.30	0.41
1:C:530:LYS:HA	1:C:530:LYS:HD3	1.85	0.41
1:D:708:ASP:OD1	1:D:709:PHE:N	2.54	0.41
1:B:299:LEU:HD13	1:B:299:LEU:HA	1.93	0.41
1:A:631:ARG:NH2	1:A:677:ASP:OD2	2.53	0.41
1:C:197:ARG:HG2	1:D:357:TYR:HE1	1.85	0.41
1:C:745:ILE:HG23	1:C:749:PHE:HD2	1.85	0.41
1:F:509:LEU:HD23	1:F:512:GLN:HE21	1.85	0.41
1:E:573:GLN:NE2	1:E:764:HIS:O	2.52	0.41
1:E:607:THR:HG21	1:D:751:PRO:HB2	2.02	0.41
1:E:792:GLU:HB2	1:E:843:VAL:HG23	2.02	0.41
1:B:368:PRO:HA	1:B:371:VAL:HG12	2.02	0.41
1:A:729:SER:HB3	1:A:764:HIS:HB3	2.03	0.41
1:C:242:MET:SD	1:C:242:MET:N	2.91	0.41
1:F:197:ARG:HD3	1:F:197:ARG:H	1.86	0.41
1:F:573:GLN:HE22	1:F:766:LEU:HD22	1.86	0.41
1:F:726:GLU:HA	1:F:765:PRO:HG2	2.01	0.41
1:E:601:PHE:HD1	1:E:759:GLU:HB2	1.85	0.41
1:D:281:HIS:HA	1:D:322:TYR:CZ	2.55	0.41
1:B:187:ILE:O	1:B:190:THR:OG1	2.33	0.41
1:B:208:PRO:HB2	1:A:331:ARG:NE	2.35	0.41
1:B:502:GLN:HA	1:B:506:ILE:HD12	2.03	0.41
1:C:201:ASN:OD1	1:C:310:CYS:N	2.45	0.41
1:F:575:GLU:O	1:F:579:ALA:HB3	2.21	0.41
1:F:751:PRO:HA	1:F:754:ILE:HB	2.02	0.41
1:D:547:PRO:HD2	1:D:588:ARG:HH12	1.85	0.41
1:C:303:LEU:HG	1:C:308:LEU:HD23	2.02	0.41
1:C:360:HIS:CD2	1:B:197:ARG:HB3	2.56	0.41
1:F:169:THR:HG22	1:F:224:ILE:HD13	2.03	0.41
1:F:368:PRO:HA	1:F:371:VAL:HB	2.03	0.41
1:F:751:PRO:HA	1:F:754:ILE:HD12	2.02	0.41
1:E:823:GLN:HA	1:E:827:ASN:ND2	2.36	0.41
1:D:165:THR:HG23	1:D:238:LEU:HD21	2.03	0.41
1:A:821:ILE:HA	1:A:825:ILE:HD12	2.03	0.41
1:C:197:ARG:HD2	1:D:360:HIS:CD2	2.56	0.41
1:E:255:PHE:O	1:E:259:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:564:GLN:HG2	1:E:568:HIS:CE1	2.56	0.41
1:E:724:GLU:OE1	1:E:727:ARG:NH2	2.53	0.41
1:E:784:LYS:HE2	1:E:784:LYS:HB3	1.88	0.41
1:D:634:MET:HG3	1:D:679:VAL:HG23	2.03	0.41
1:B:498:MET:O	1:B:502:GLN:CB	2.69	0.41
1:C:795:ILE:HG12	1:C:846:LEU:HD12	2.03	0.40
1:E:423:LYS:O	1:E:427:GLN:HB2	2.21	0.40
1:D:775:ALA:HA	1:D:817:LEU:HD11	2.03	0.40
1:B:345:ASP:OD1	1:B:345:ASP:N	2.51	0.40
1:A:420:ILE:HA	1:A:423:LYS:HE2	2.03	0.40
1:A:560:LEU:HD13	1:A:560:LEU:HA	1.95	0.40
1:C:212:LYS:N	2:C:901:AGS:O3A	2.54	0.40
1:C:737:ASN:O	1:C:741:ALA:HB3	2.22	0.40
1:F:571:ILE:H	1:F:571:ILE:HG13	1.56	0.40
1:E:192:GLN:HA	1:E:195:GLN:HG2	2.04	0.40
1:E:302:ALA:O	1:E:306:GLY:N	2.53	0.40
1:E:649:ALA:HB3	1:E:656:TYR:N	2.36	0.40
1:E:664:GLU:O	1:E:668:ARG:HG2	2.22	0.40
1:D:275:LEU:HB3	1:D:310:CYS:HA	2.02	0.40
1:B:529:ASN:OD1	1:B:530:LYS:NZ	2.48	0.40
1:A:634:MET:HG3	1:A:679:VAL:HG23	2.03	0.40
1:F:595:ASN:HD22	1:F:710:ARG:HD3	1.86	0.40
1:F:781:ARG:O	1:F:785:ARG:HD3	2.21	0.40
1:E:317:ASP:N	1:E:317:ASP:OD1	2.54	0.40
1:E:353:LEU:HD11	2:E:901:AGS:H2	2.03	0.40
1:E:359:LEU:HD21	1:E:480:GLU:HG2	2.02	0.40
1:E:405:ILE:HG23	1:E:527:LEU:HD23	2.03	0.40
1:D:687:PHE:HD2	1:D:748:ILE:HG12	1.86	0.40
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.86	0.40
1:A:347:ILE:HD11	1:A:371:VAL:HG23	2.02	0.40
1:C:361:HIS:HB3	1:C:398:ALA:HB1	2.03	0.40
1:C:786:LEU:HD23	1:C:786:LEU:HA	1.92	0.40
1:C:809:ASP:N	1:C:809:ASP:OD1	2.54	0.40
1:F:181:ILE:HB	1:F:349:ILE:HG12	2.03	0.40
1:F:469:LEU:HA	1:F:472:THR:HG22	2.03	0.40
1:E:202:PRO:HG2	1:E:311:VAL:HG13	2.03	0.40
1:D:178:ASP:O	1:D:221:GLN:NE2	2.41	0.40
1:D:318:GLU:O	1:D:322:TYR:CB	2.66	0.40
1:D:376:LEU:HD22	1:D:380:TYR:HE2	1.87	0.40
1:D:422:LEU:HD22	1:D:448:LEU:HD23	2.04	0.40
1:A:852:ARG:HB3	1:A:853:ILE:H	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:VAL:O	1:B:581:SER:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	682/871 (78%)	651 (96%)	31 (4%)	0	100	100
1	B	682/871 (78%)	638 (94%)	43 (6%)	1 (0%)	51	85
1	C	682/871 (78%)	636 (93%)	45 (7%)	1 (0%)	51	85
1	D	682/871 (78%)	634 (93%)	46 (7%)	2 (0%)	41	76
1	E	682/871 (78%)	646 (95%)	34 (5%)	2 (0%)	41	76
1	F	682/871 (78%)	658 (96%)	23 (3%)	1 (0%)	51	85
All	All	4092/5226 (78%)	3863 (94%)	222 (5%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	850	GLU
1	D	850	GLU
1	D	441	LEU
1	E	322	TYR
1	E	851	ASP
1	B	322	TYR
1	C	248	GLY

5.3.2 Protein sidechains (i)

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	582/726 (80%)	577 (99%)	5 (1%)	78 87
1	B	582/726 (80%)	573 (98%)	9 (2%)	65 80
1	C	582/726 (80%)	574 (99%)	8 (1%)	67 81
1	D	582/726 (80%)	572 (98%)	10 (2%)	60 78
1	E	582/726 (80%)	575 (99%)	7 (1%)	71 84
1	F	582/726 (80%)	569 (98%)	13 (2%)	52 71
All	All	3492/4356 (80%)	3440 (98%)	52 (2%)	66 80

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	LYS
1	C	272	ASN
1	C	297	ASN
1	C	463	LYS
1	C	559	LEU
1	C	620	ASN
1	C	646	LEU
1	C	848	VAL
1	F	197	ARG
1	F	268	LYS
1	F	422	LEU
1	F	440	ARG
1	F	443	MET
1	F	522	LYS
1	F	591	LEU
1	F	620	ASN
1	F	705	ARG
1	F	737	ASN
1	F	781	ARG
1	F	785	ARG
1	F	845	ARG
1	E	268	LYS

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Mol	Chain	Res	Type
1	E	272	ASN
1	E	297	ASN
1	E	530	LYS
1	E	586	ARG
1	E	620	ASN
1	E	848	VAL
1	D	197	ARG
1	D	268	LYS
1	D	440	ARG
1	D	443	MET
1	D	607	THR
1	D	620	ASN
1	D	641	HIS
1	D	681	LYS
1	D	705	ARG
1	D	737	ASN
1	B	212	LYS
1	B	252	ARG
1	B	335	LYS
1	B	646	LEU
1	B	668	ARG
1	B	737	ASN
1	B	747	LYS
1	B	827	ASN
1	B	845	ARG
1	A	233	LYS
1	A	252	ARG
1	A	268	LYS
1	A	530	LYS
1	A	620	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	C	272	ASN
1	C	297	ASN
1	C	360	HIS
1	C	512	GLN
1	C	582	ASN
1	C	620	ASN
1	C	641	HIS

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Mol	Chain	Res	Type
1	C	711	ASN
1	C	719	ASN
1	C	737	ASN
1	C	755	ASN
1	C	778	GLN
1	C	806	ASN
1	C	824	GLN
1	F	360	HIS
1	F	454	GLN
1	F	502	GLN
1	F	595	ASN
1	F	620	ASN
1	F	703	GLN
1	E	174	GLN
1	E	269	GLN
1	E	272	ASN
1	E	297	ASN
1	E	641	HIS
1	E	755	ASN
1	E	778	GLN
1	E	806	ASN
1	E	822	GLN
1	D	360	HIS
1	D	502	GLN
1	D	512	GLN
1	D	688	ASN
1	D	711	ASN
1	D	719	ASN
1	D	737	ASN
1	D	755	ASN
1	D	806	ASN
1	B	195	GLN
1	B	297	ASN
1	B	806	ASN
1	B	831	GLN
1	B	849	ASN
1	A	174	GLN
1	A	454	GLN
1	A	512	GLN
1	A	719	ASN
1	A	737	ASN
1	A	778	GLN

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Mol	Chain	Res	Type
1	A	806	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	E	901	-	26,33,33	0.75	0	26,52,52	1.25	2 (7%)
2	AGS	F	902	-	26,33,33	0.78	1 (3%)	26,52,52	1.24	2 (7%)
2	AGS	C	901	-	26,33,33	0.80	0	26,52,52	1.05	2 (7%)
2	AGS	B	901	-	26,33,33	0.83	1 (3%)	26,52,52	1.16	2 (7%)
2	AGS	D	902	-	26,33,33	0.78	0	26,52,52	1.36	2 (7%)
2	AGS	C	902	-	26,33,33	0.89	1 (3%)	26,52,52	1.28	3 (11%)
2	AGS	A	901	-	26,33,33	0.81	1 (3%)	26,52,52	1.14	2 (7%)
2	AGS	F	901	-	26,33,33	0.78	1 (3%)	26,52,52	1.05	2 (7%)
2	AGS	B	902	-	26,33,33	0.84	1 (3%)	26,52,52	1.36	2 (7%)
2	AGS	E	902	-	26,33,33	0.84	0	26,52,52	1.30	3 (11%)
2	AGS	D	901	-	26,33,33	0.74	0	26,52,52	1.29	3 (11%)

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
2	AGS	E	901	-	-	4/17/38/38	0/3/3/3
2	AGS	F	902	-	-	4/17/38/38	0/3/3/3
2	AGS	C	901	-	-	6/17/38/38	0/3/3/3
2	AGS	B	901	-	-	5/17/38/38	0/3/3/3
2	AGS	D	902	-	-	5/17/38/38	0/3/3/3
2	AGS	C	902	-	-	4/17/38/38	0/3/3/3
2	AGS	A	901	-	-	6/17/38/38	0/3/3/3
2	AGS	F	901	-	-	6/17/38/38	0/3/3/3
2	AGS	B	902	-	-	4/17/38/38	0/3/3/3
2	AGS	E	902	-	-	4/17/38/38	0/3/3/3
2	AGS	D	901	-	-	6/17/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	AGS	C8-N7	-2.13	1.30	1.34
2	A	901	AGS	PG-S1G	2.05	1.95	1.90
2	B	901	AGS	PG-S1G	2.03	1.95	1.90
2	F	902	AGS	PG-S1G	2.03	1.95	1.90
2	C	902	AGS	C8-N7	-2.01	1.31	1.34
2	F	901	AGS	PG-S1G	2.00	1.95	1.90

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	902	AGS	PA-O3A-PB	-5.69	113.30	132.83
2	D	902	AGS	PA-O3A-PB	-5.58	113.68	132.83
2	F	902	AGS	PA-O3A-PB	-5.09	115.36	132.83
2	E	902	AGS	PA-O3A-PB	-5.02	115.59	132.83
2	D	901	AGS	PA-O3A-PB	-4.58	117.12	132.83
2	E	901	AGS	PA-O3A-PB	-4.41	117.70	132.83
2	C	902	AGS	PA-O3A-PB	-4.38	117.80	132.83
2	A	901	AGS	PA-O3A-PB	-4.38	117.81	132.83
2	F	901	AGS	PA-O3A-PB	-3.77	119.89	132.83
2	B	901	AGS	PA-O3A-PB	-3.75	119.97	132.83
2	C	901	AGS	PA-O3A-PB	-3.54	120.69	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	902	AGS	C1'-N9-C4	2.65	131.30	126.64
2	B	902	AGS	C5-C6-N6	2.58	124.27	120.35
2	E	902	AGS	C5-C6-N6	2.34	123.91	120.35
2	E	901	AGS	C5-C6-N6	2.27	123.81	120.35
2	F	902	AGS	C5-C6-N6	2.27	123.80	120.35
2	D	902	AGS	C5-C6-N6	2.25	123.77	120.35
2	A	901	AGS	C5-C6-N6	2.22	123.73	120.35
2	D	901	AGS	C5-C6-N6	2.20	123.70	120.35
2	B	901	AGS	C5-C6-N6	2.18	123.67	120.35
2	F	901	AGS	C5-C6-N6	2.17	123.66	120.35
2	D	901	AGS	C3'-C2'-C1'	2.17	104.24	100.98
2	E	902	AGS	C1'-N9-C4	2.15	130.41	126.64
2	C	902	AGS	C5-C6-N6	2.07	123.50	120.35
2	C	901	AGS	C5-C6-N6	2.07	123.50	120.35

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	AGS	C5'-O5'-PA-O3A
2	C	902	AGS	C5'-O5'-PA-O1A
2	C	902	AGS	C5'-O5'-PA-O2A
2	C	902	AGS	C5'-O5'-PA-O3A
2	F	901	AGS	C5'-O5'-PA-O1A
2	F	901	AGS	C5'-O5'-PA-O2A
2	F	901	AGS	C5'-O5'-PA-O3A
2	F	902	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	PB-O3A-PA-O5'
2	E	901	AGS	C5'-O5'-PA-O3A
2	E	902	AGS	C5'-O5'-PA-O1A
2	E	902	AGS	C5'-O5'-PA-O2A
2	D	901	AGS	C5'-O5'-PA-O2A
2	D	902	AGS	C5'-O5'-PA-O1A
2	D	902	AGS	C5'-O5'-PA-O2A
2	B	901	AGS	C5'-O5'-PA-O2A
2	B	901	AGS	C5'-O5'-PA-O3A
2	B	902	AGS	C5'-O5'-PA-O1A
2	B	902	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	C5'-O5'-PA-O1A
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	PG-O3B-PB-O1B
2	D	901	AGS	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	901	AGS	PA-O3A-PB-O1B
2	D	902	AGS	O4'-C4'-C5'-O5'
2	C	901	AGS	PG-O3B-PB-O1B
2	D	901	AGS	C4'-C5'-O5'-PA
2	B	901	AGS	C4'-C5'-O5'-PA
2	C	902	AGS	PB-O3A-PA-O5'
2	E	902	AGS	PB-O3A-PA-O5'
2	D	901	AGS	PB-O3A-PA-O5'
2	A	901	AGS	PB-O3A-PA-O5'
2	F	901	AGS	C4'-C5'-O5'-PA
2	F	902	AGS	C5'-O5'-PA-O3A
2	D	901	AGS	C5'-O5'-PA-O3A
2	D	902	AGS	C3'-C4'-C5'-O5'
2	C	901	AGS	PA-O3A-PB-O3B
2	E	901	AGS	C4'-C5'-O5'-PA
2	C	901	AGS	C5'-O5'-PA-O1A
2	F	902	AGS	C5'-O5'-PA-O1A
2	E	901	AGS	C5'-O5'-PA-O1A
2	D	901	AGS	C5'-O5'-PA-O1A
2	F	902	AGS	C4'-C5'-O5'-PA
2	F	901	AGS	PA-O3A-PB-O3B
2	C	901	AGS	C4'-C5'-O5'-PA
2	A	901	AGS	C4'-C5'-O5'-PA
2	F	901	AGS	PG-O3B-PB-O2B
2	B	901	AGS	PB-O3A-PA-O5'
2	B	902	AGS	C4'-C5'-O5'-PA
2	E	902	AGS	C5'-O5'-PA-O3A
2	D	902	AGS	C5'-O5'-PA-O3A
2	B	902	AGS	C5'-O5'-PA-O3A
2	A	901	AGS	C5'-O5'-PA-O3A
2	C	901	AGS	PA-O3A-PB-O2B

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	901	AGS	4	0
2	F	902	AGS	1	0
2	C	901	AGS	5	0
2	B	901	AGS	2	0
2	D	902	AGS	5	0
2	C	902	AGS	2	0

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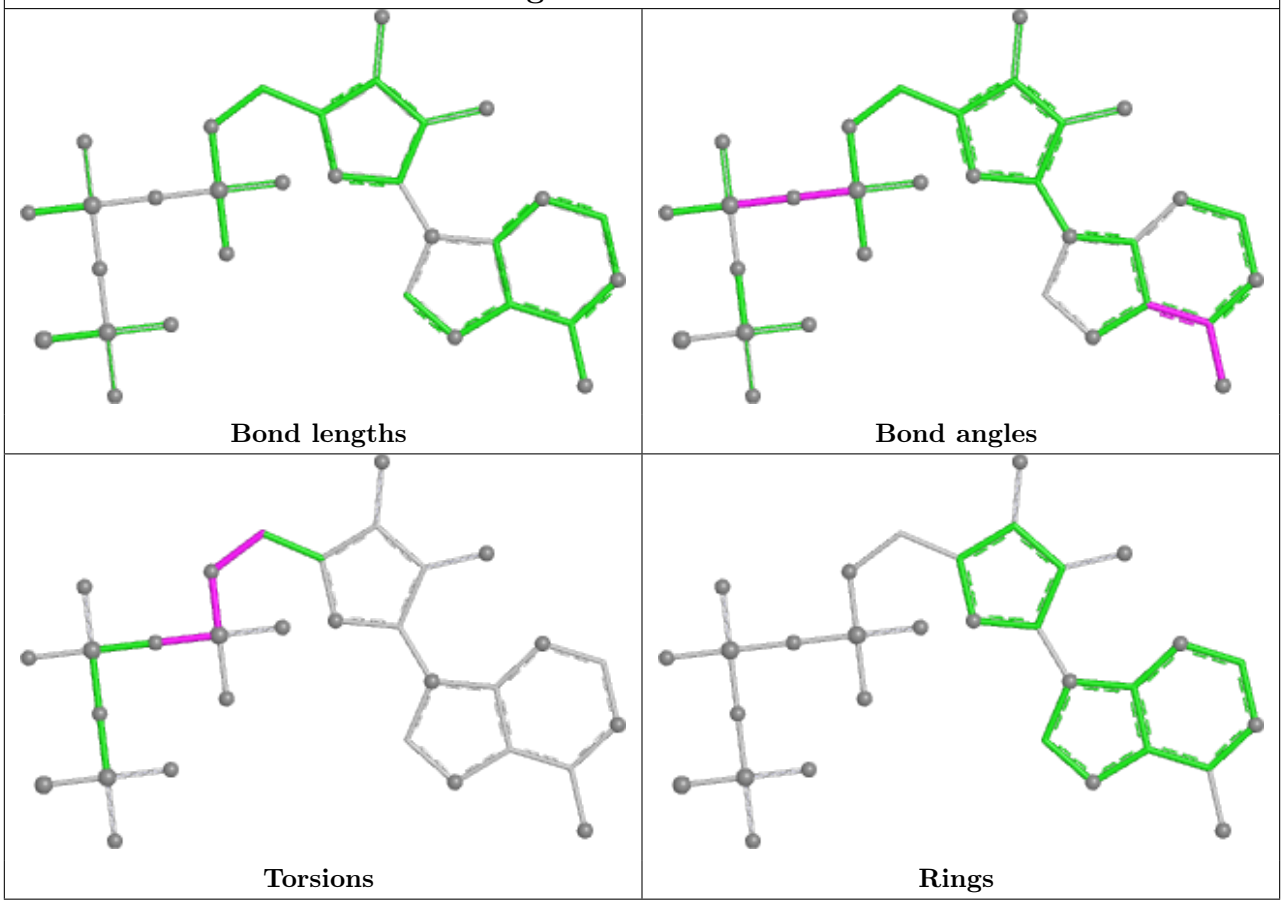
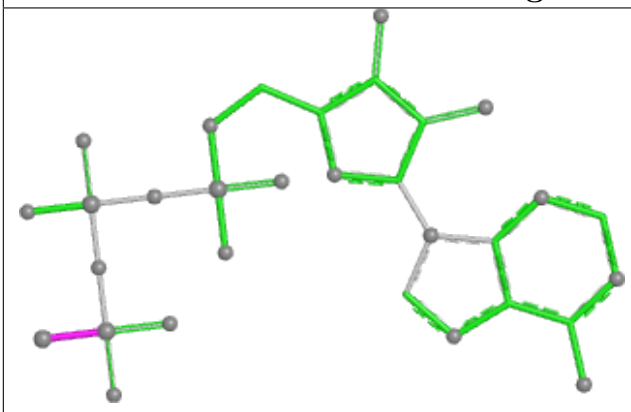
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	3	0
2	F	901	AGS	8	0
2	B	902	AGS	3	0
2	E	902	AGS	1	0
2	D	901	AGS	5	0

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 then 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 E 901



Ligand AGS F 902



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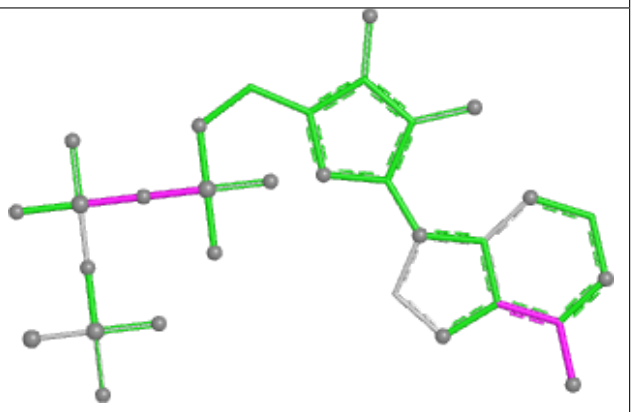
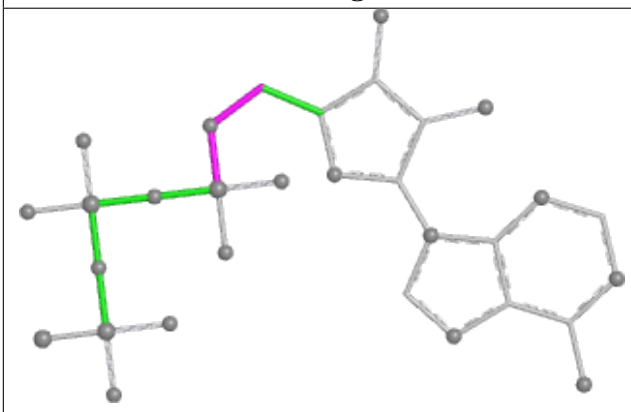


Bond angles



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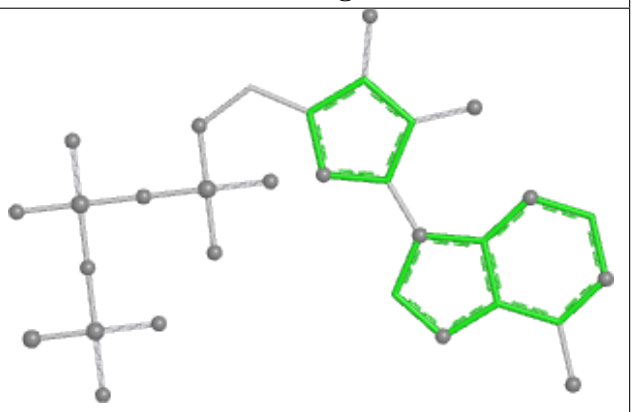
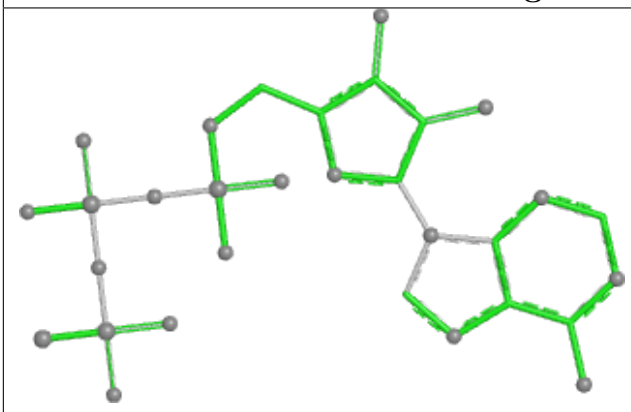


Rings

Ligand AGS C 901



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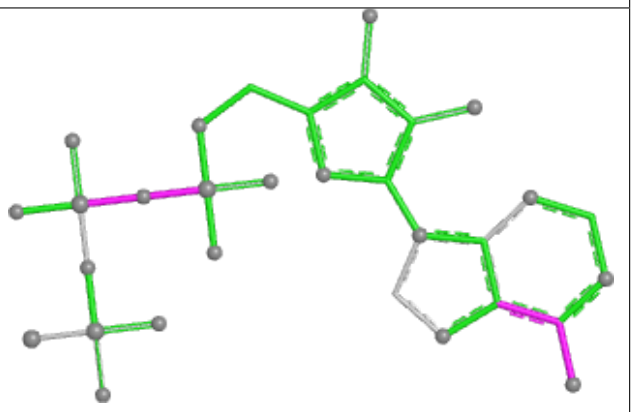

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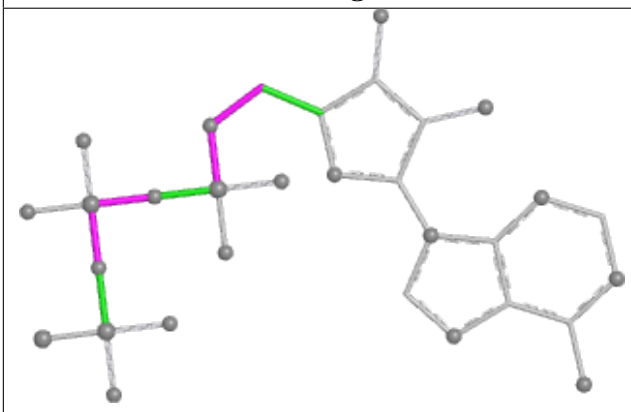

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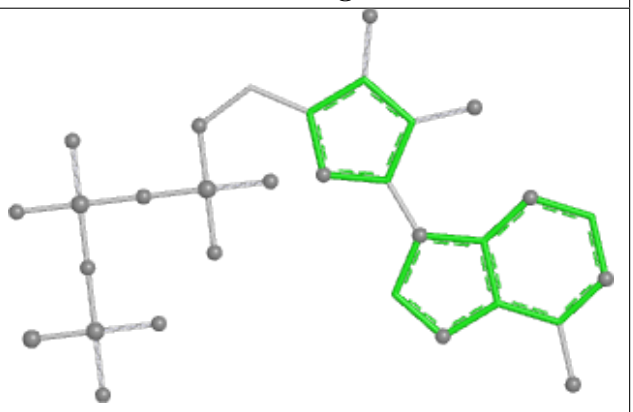

Rings

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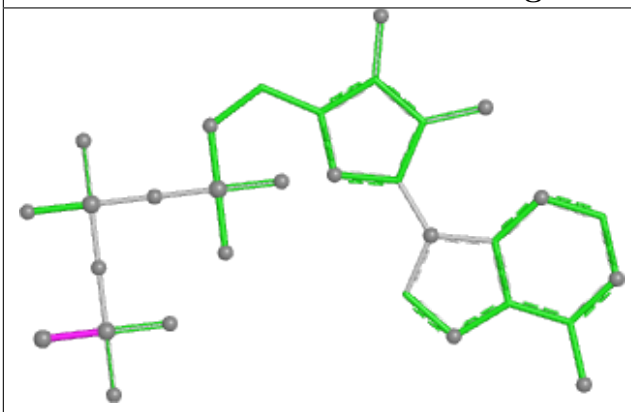

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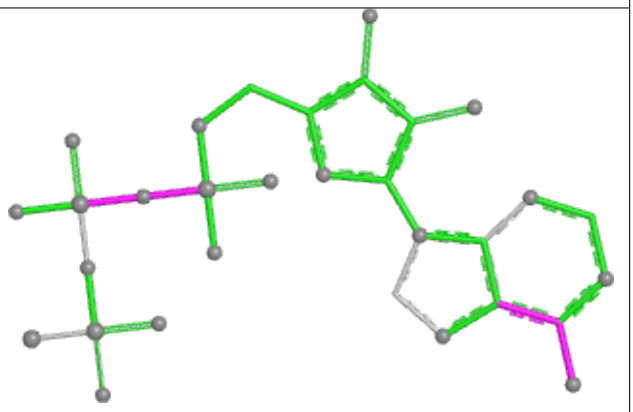

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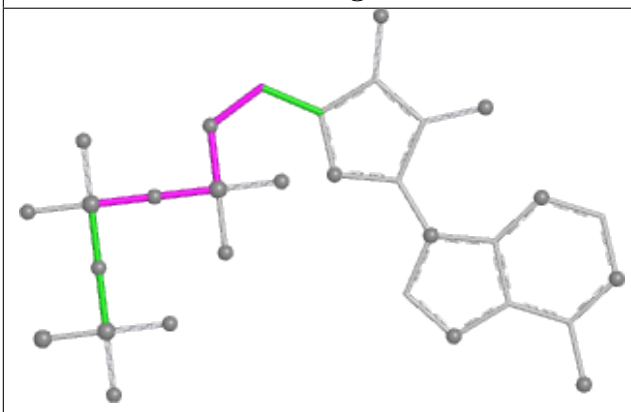

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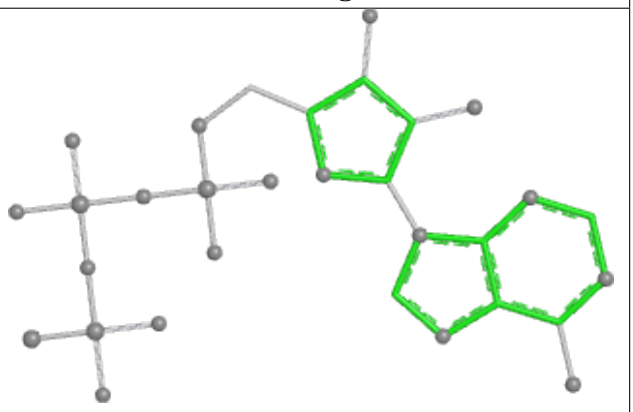

Rings

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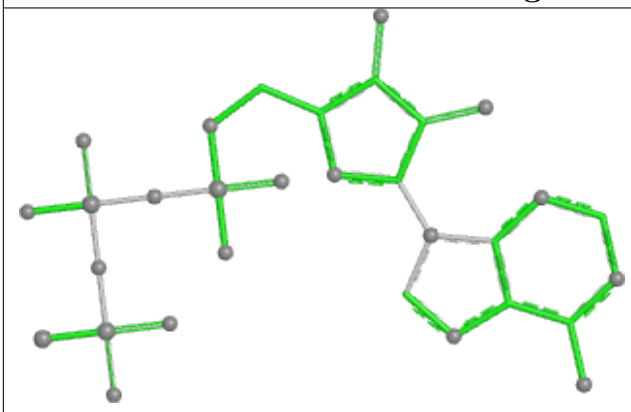

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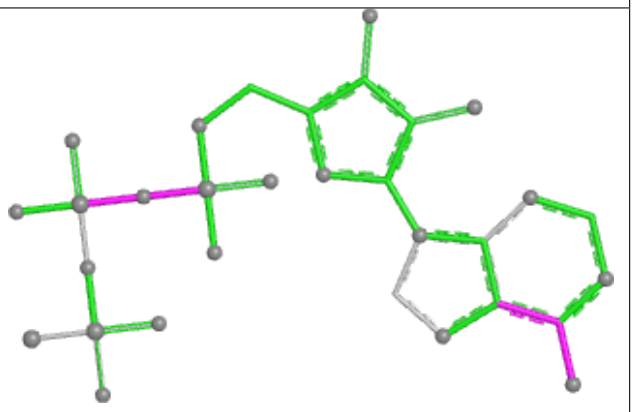

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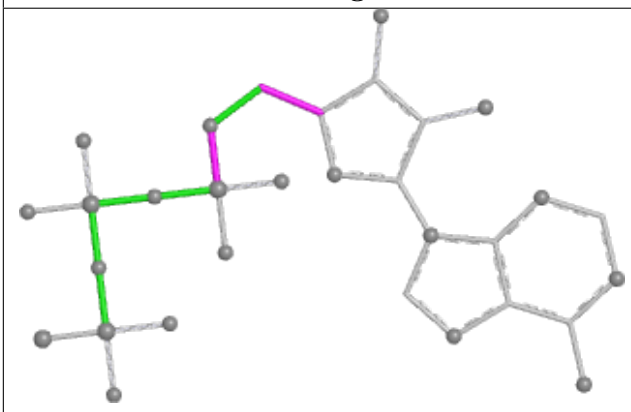

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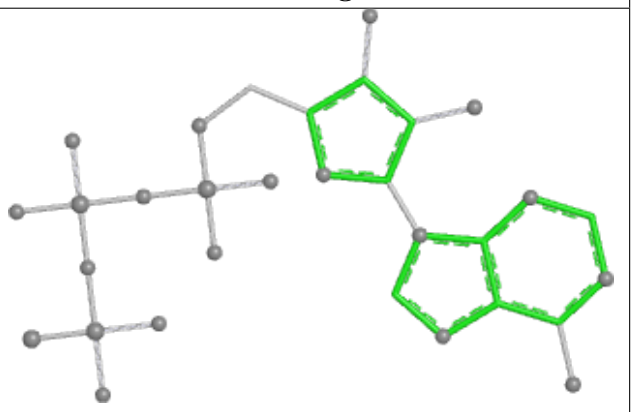
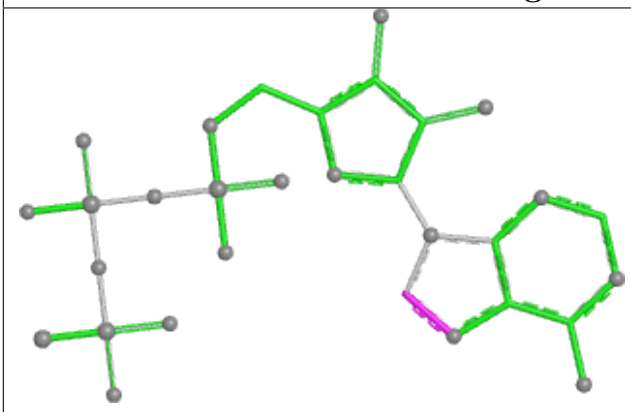


Rings

Ligand AGS C 902



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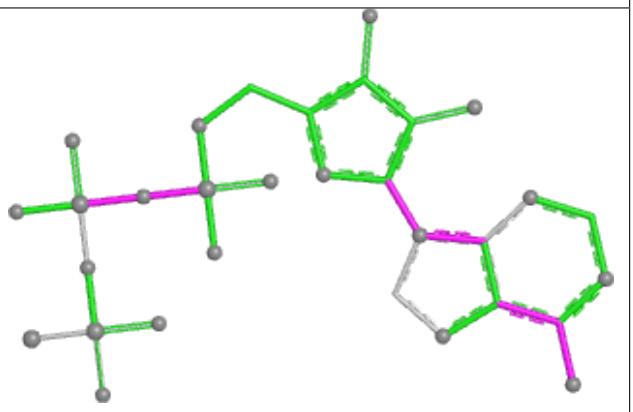

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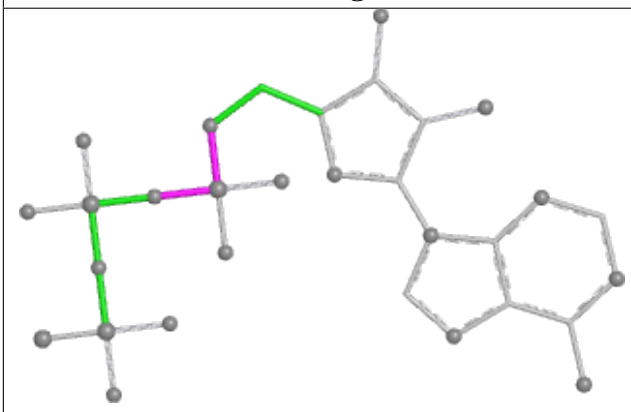

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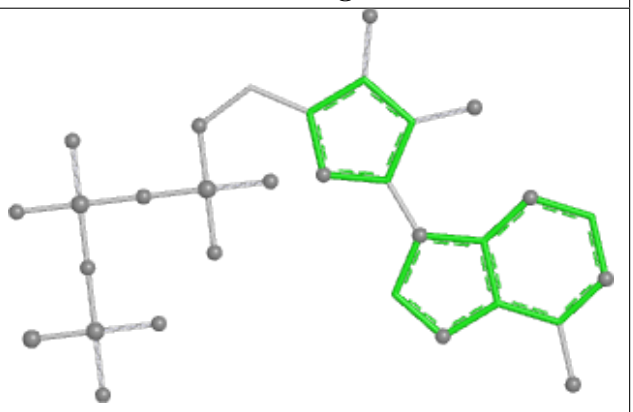
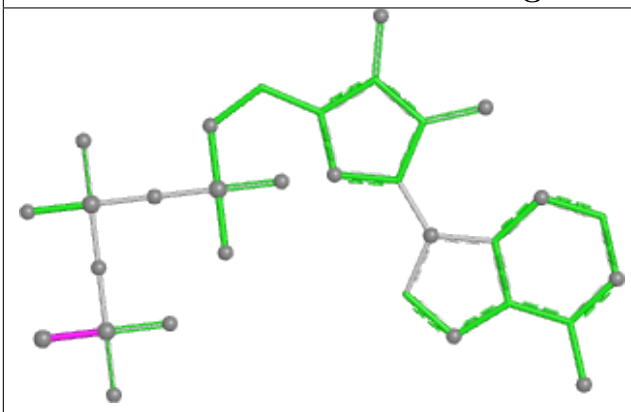
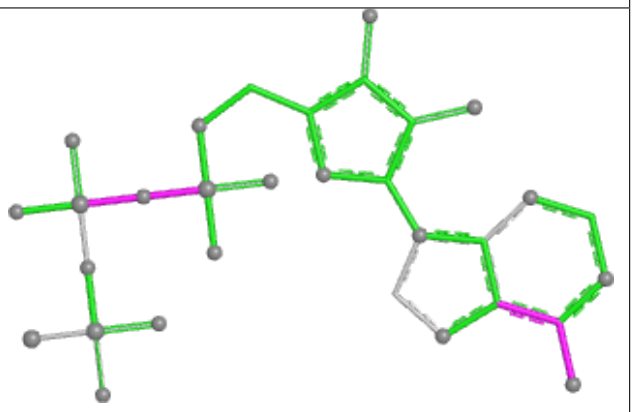
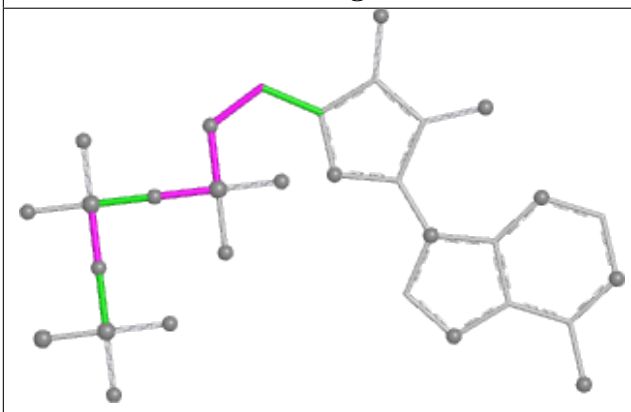
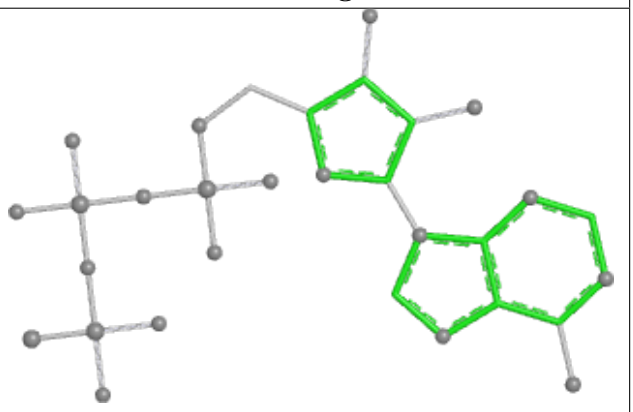
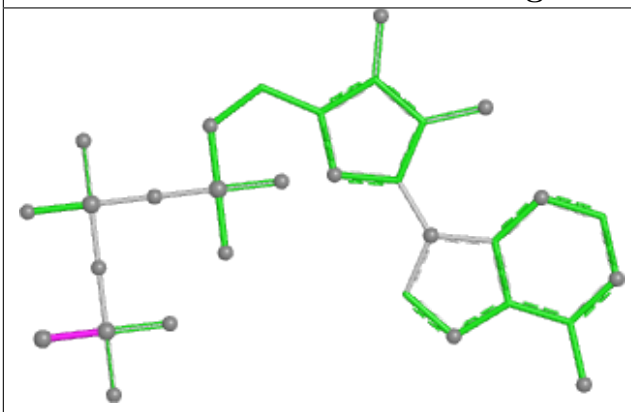


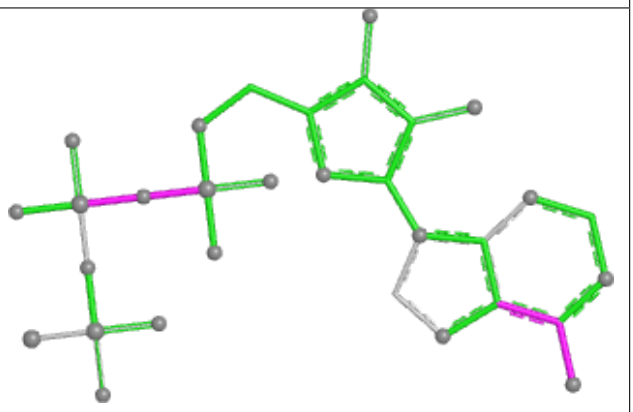
Rings

Ligand AGS A 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

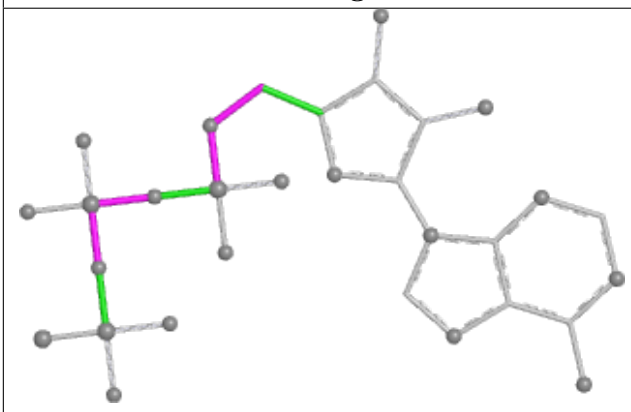
Ligand AGS F 901



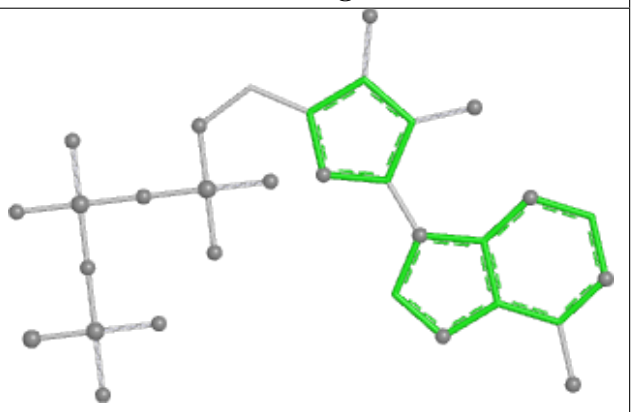
Bond lengths



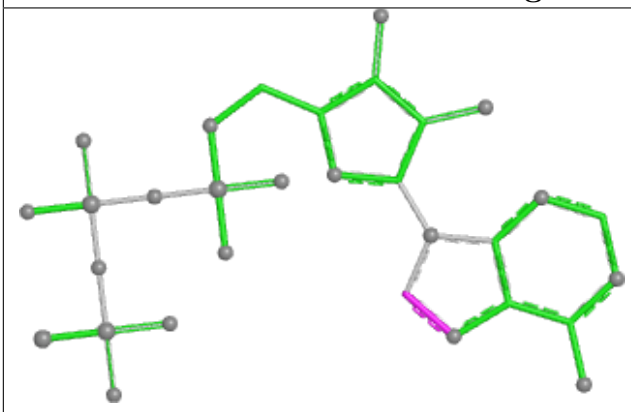
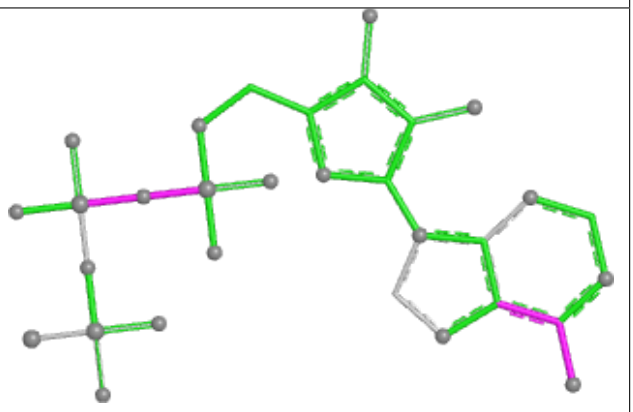
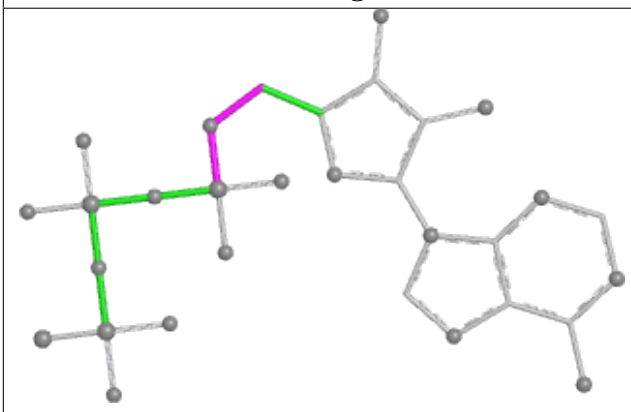
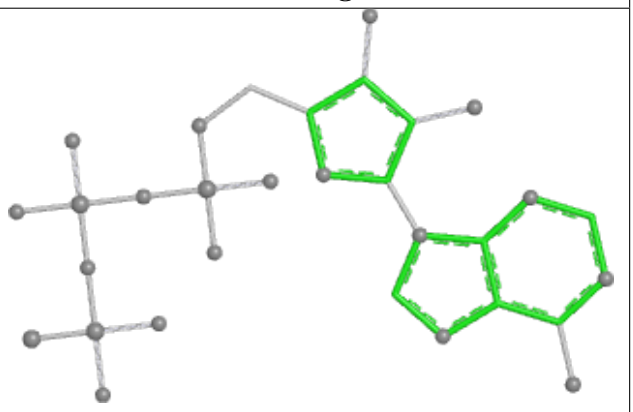
Bond angles



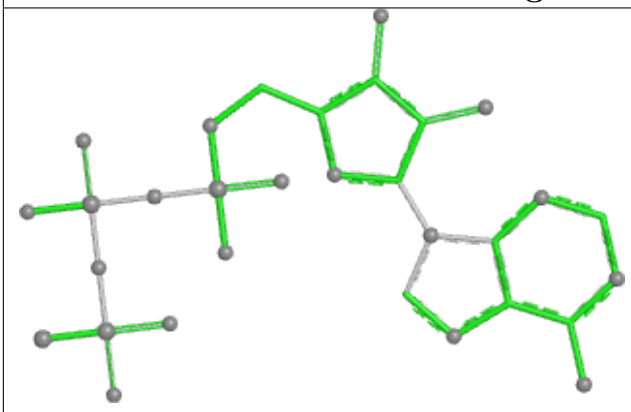
Torsions



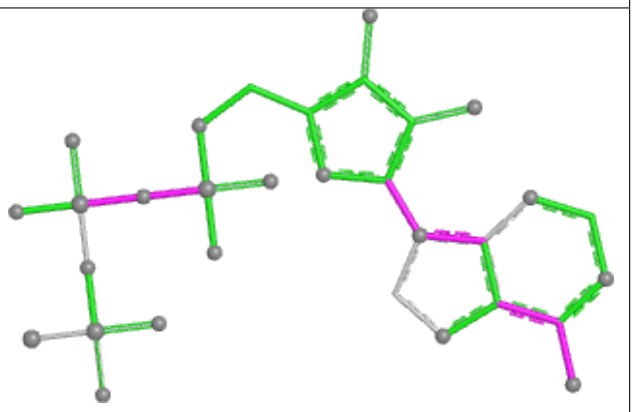
Rings

Ligand AGS B 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

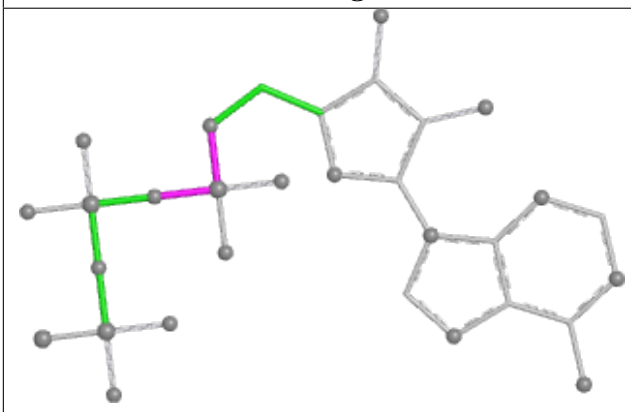
Ligand AGS E 902



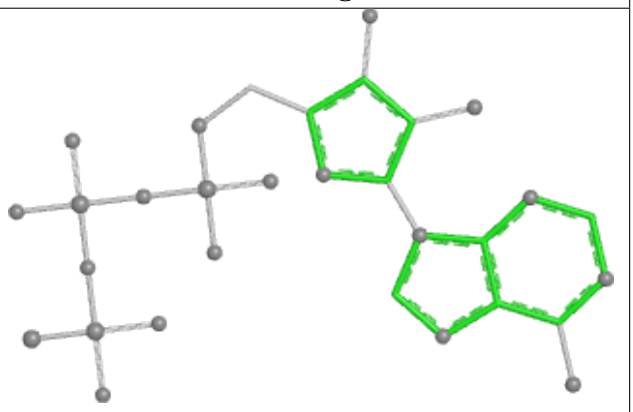
Bond lengths



Bond angles

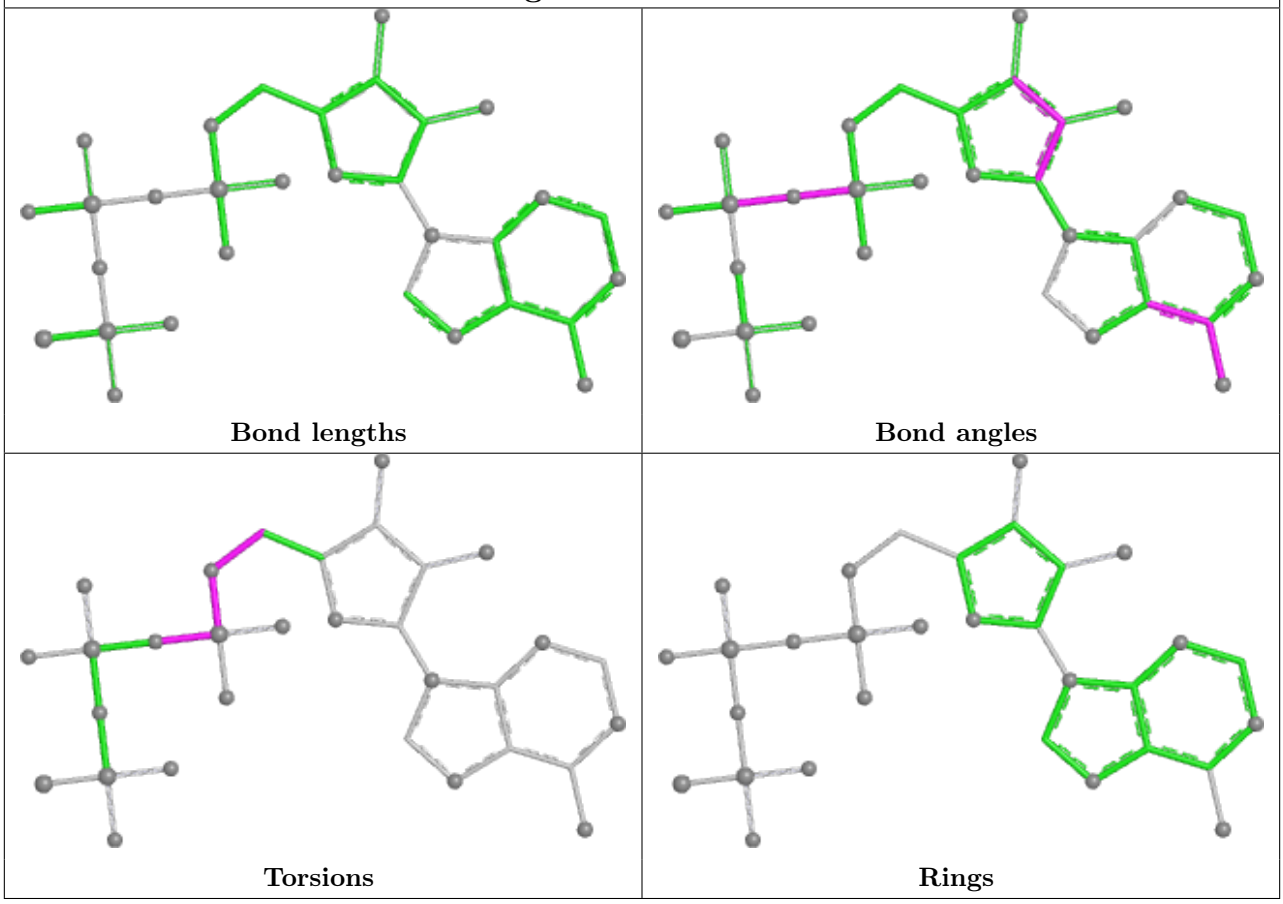


Torsions



Rings

Ligand AGS D 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	385:GLN	C	386:LEU	N	1.16

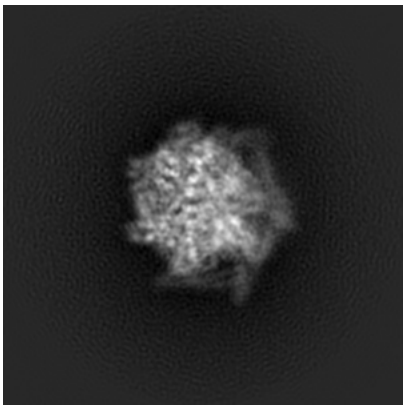
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3776. These allow visual inspection of the internal detail of the map and identification of artifacts.

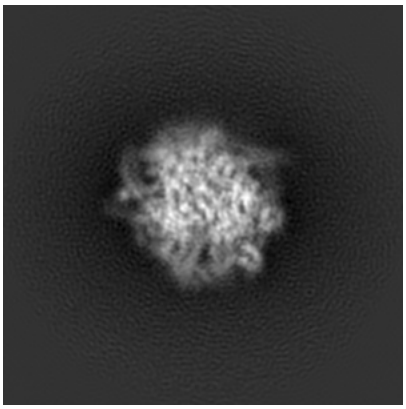
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

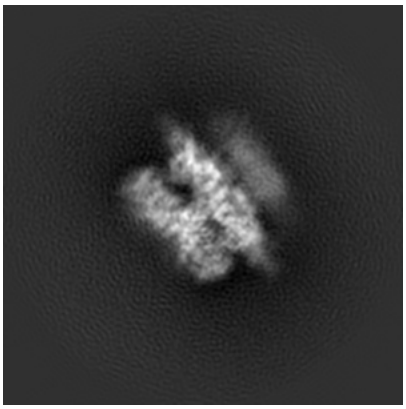
6.1.1 Primary map



X

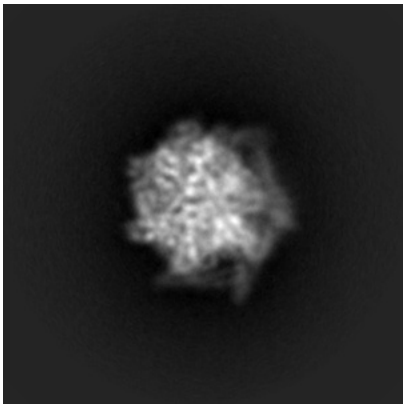


Y

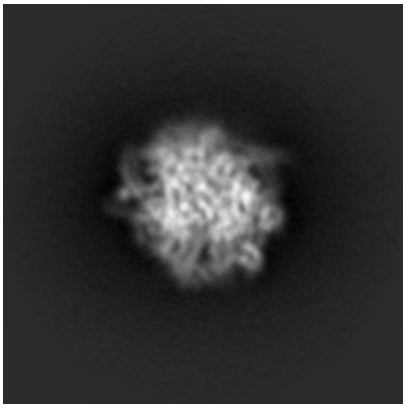


Z

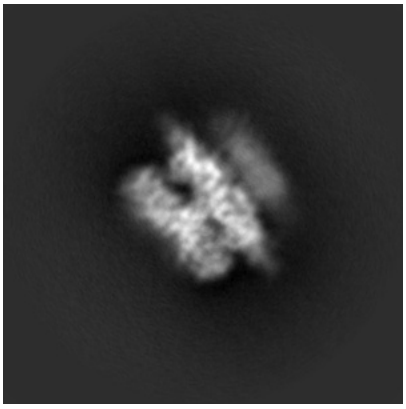
6.1.2 Raw map



X



Y

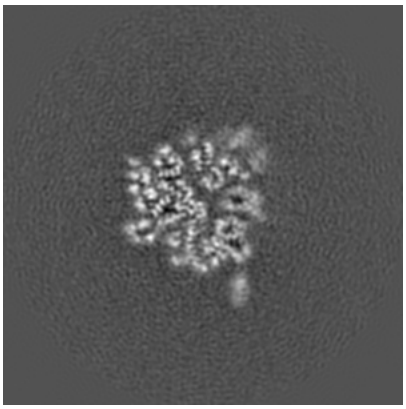


Z

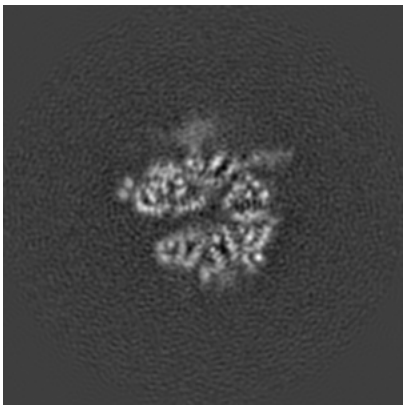
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

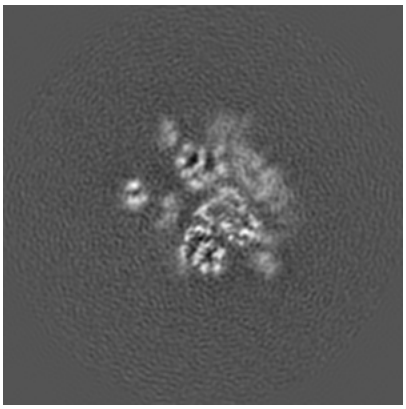
6.2.1 Primary map



X Index: 128

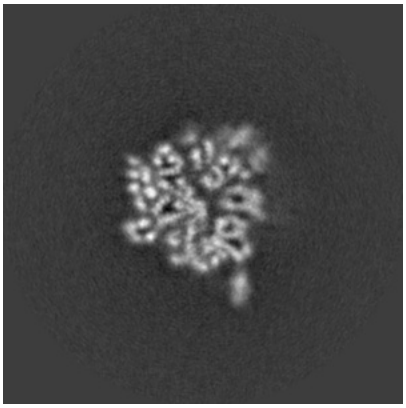


Y Index: 128

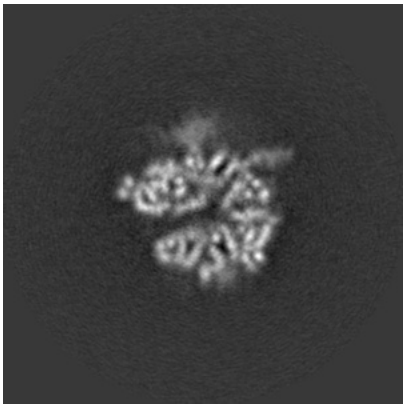


Z Index: 128

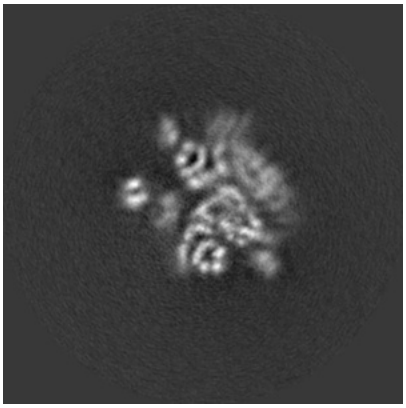
6.2.2 Raw map



X Index: 128



Y Index: 128

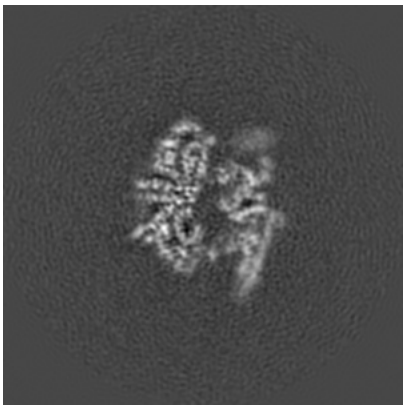


Z Index: 128

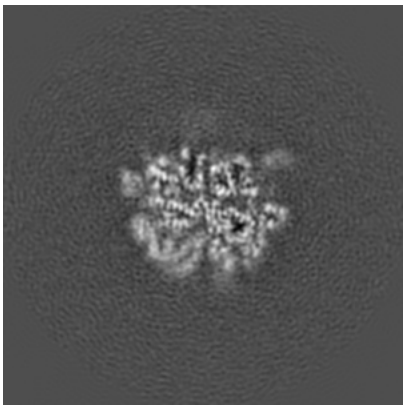
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

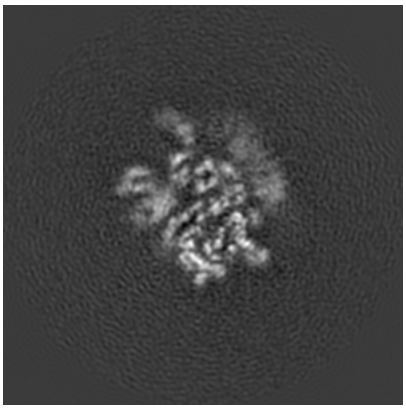
6.3.1 Primary map



X Index: 120

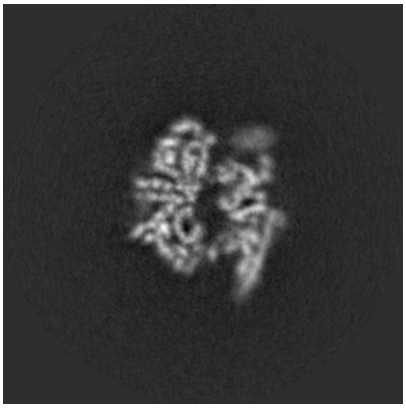


Y Index: 120

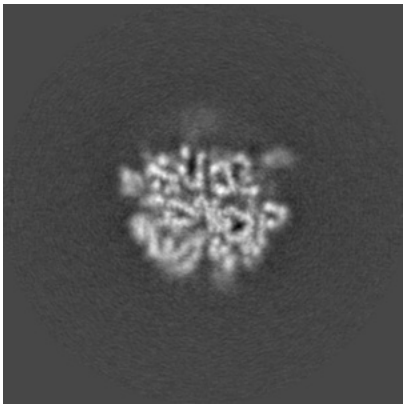


Z Index: 114

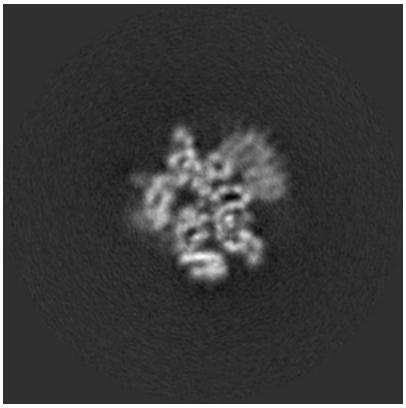
6.3.2 Raw map



X Index: 120



Y Index: 120

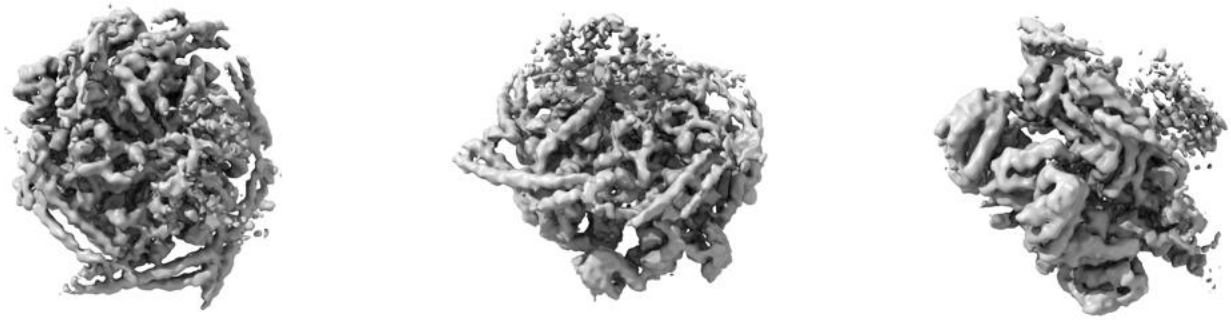


Z Index: 106

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

6.4 Orthogonal surface views (i)

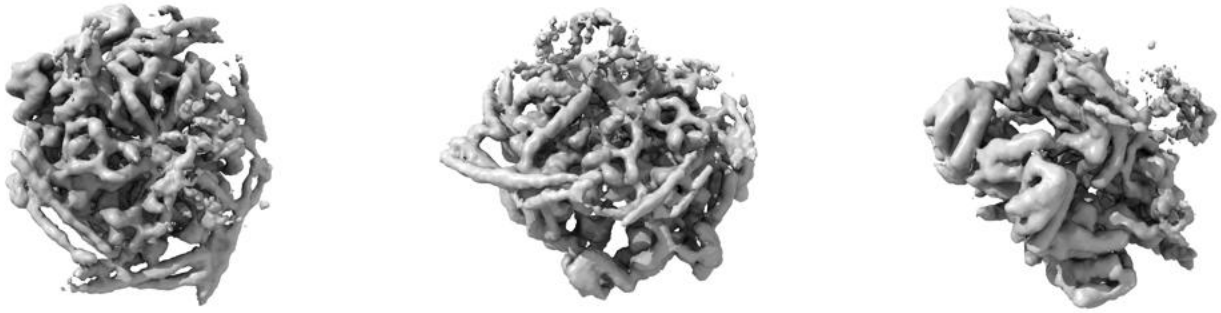
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

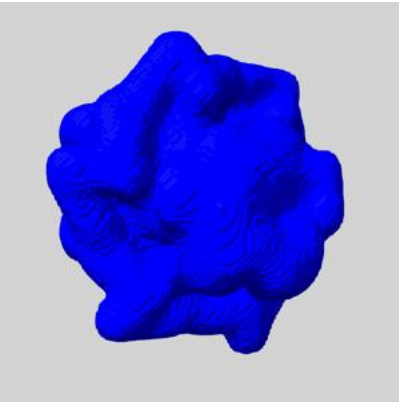
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

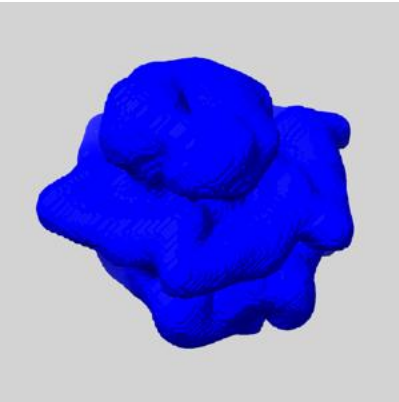
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

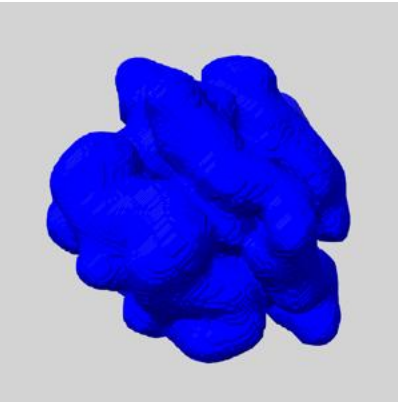
6.5.1 emd_3776_msk_1.map (i)



X



Y

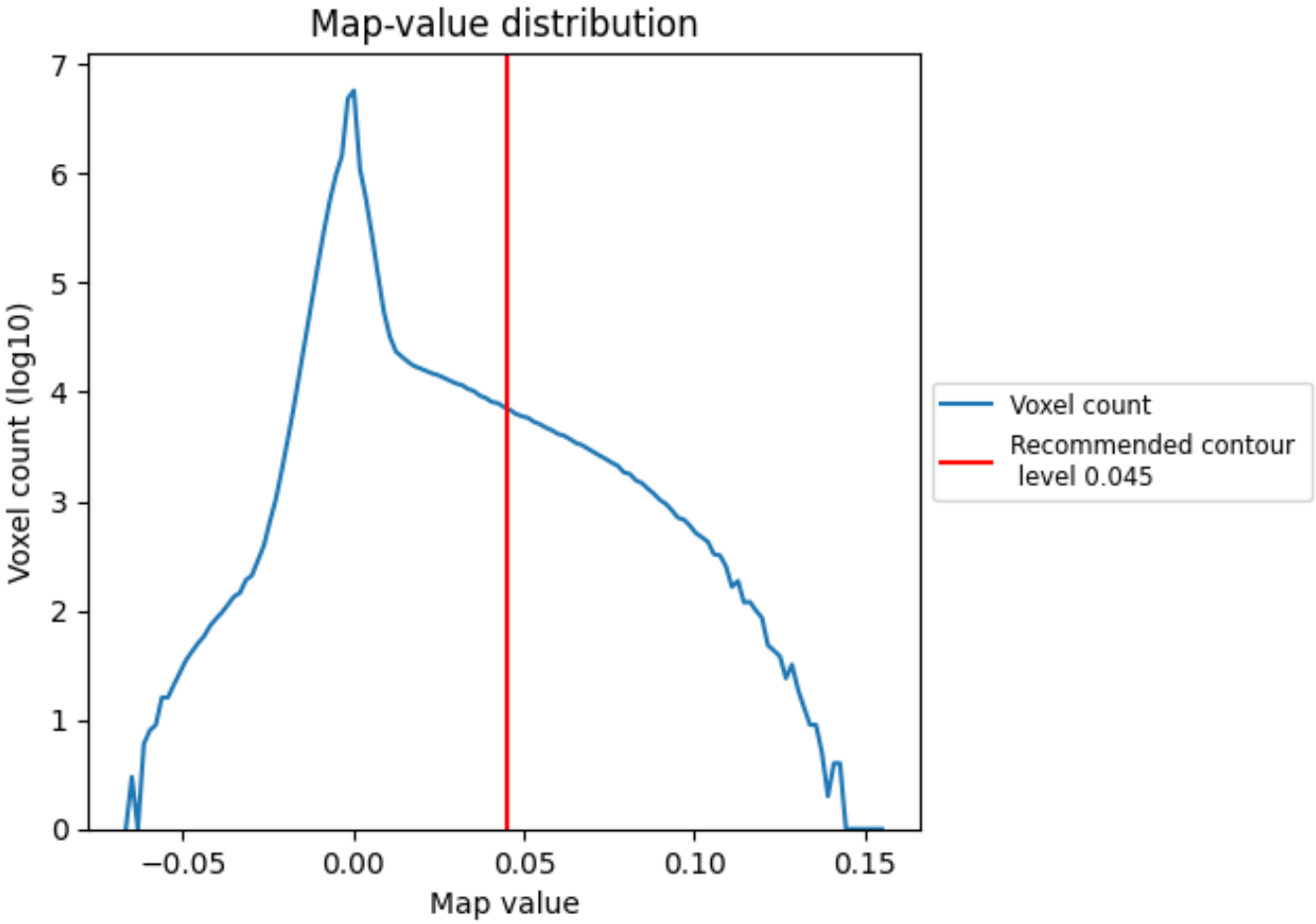


Z

7 Map analysis

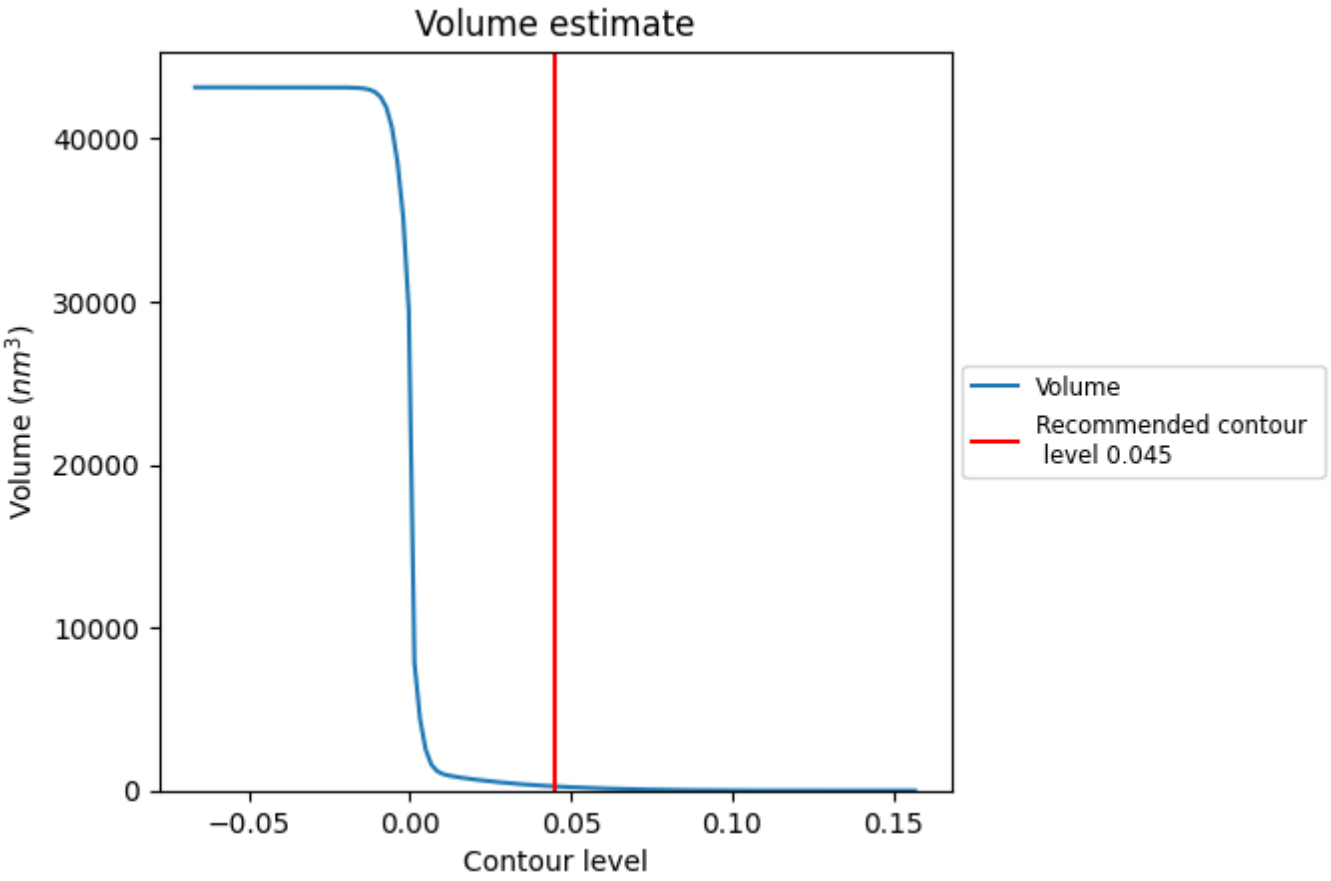
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

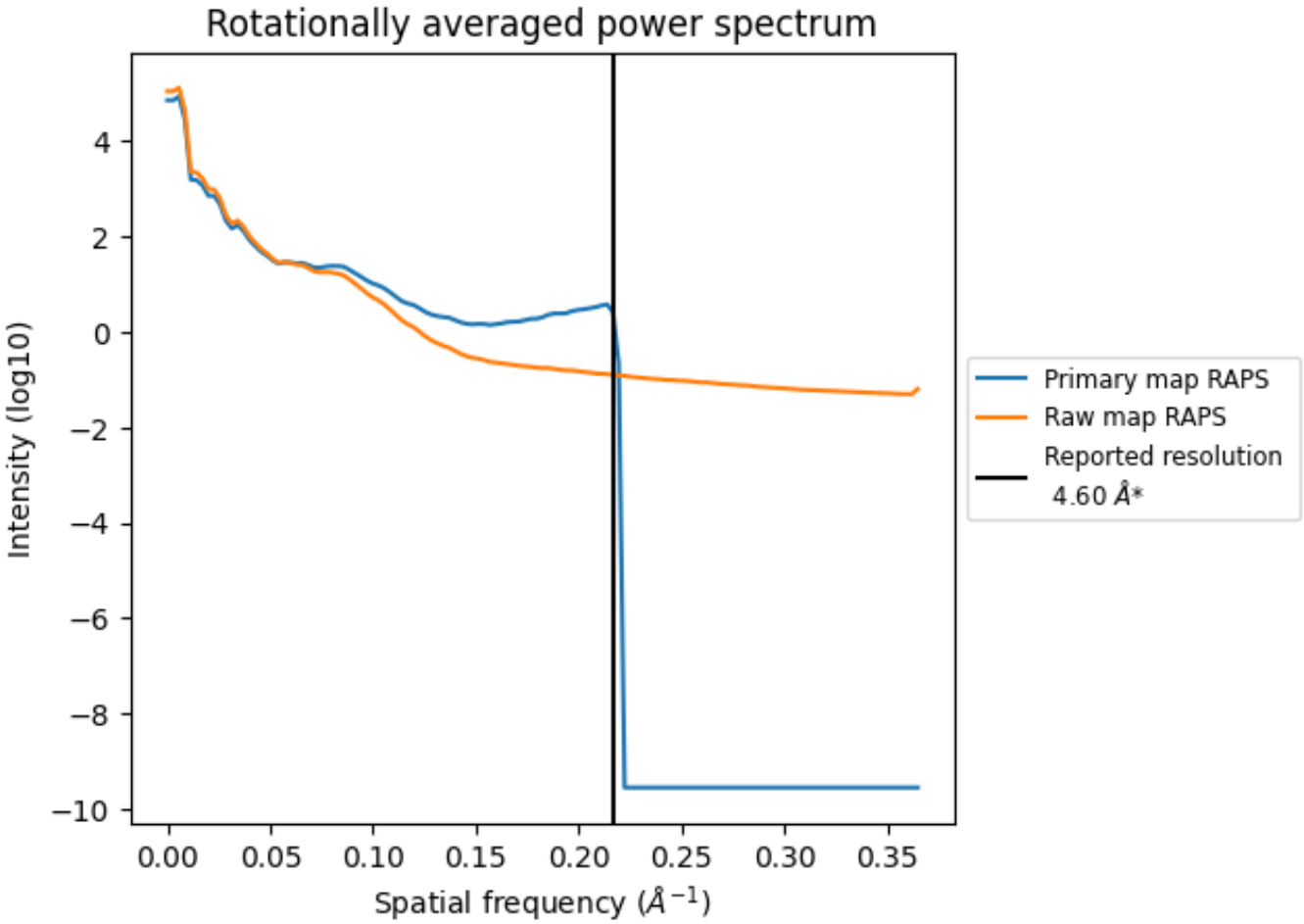
7.2 Volume estimate



The volume at the recommended contour level is 257 nm^3; this corresponds to an approximate mass of 232 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 (i)

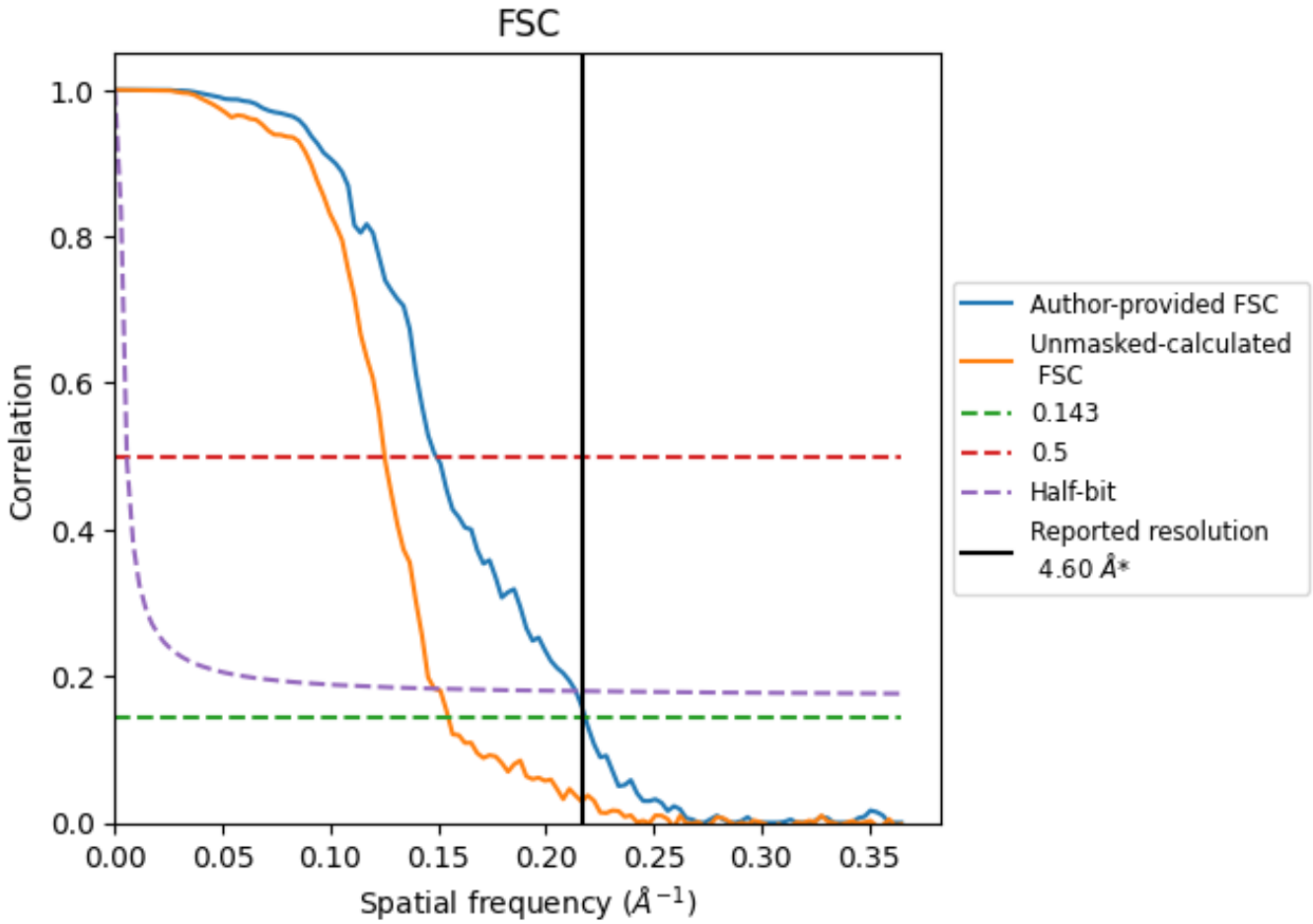


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

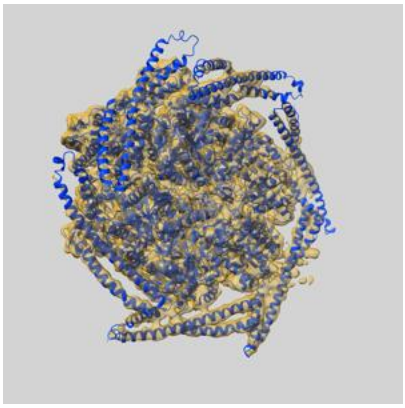
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.58	6.71	4.67
Unmasked-calculated*	6.46	7.99	6.75

*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 6.46 differs from the reported value 4.6 by more than 10 %

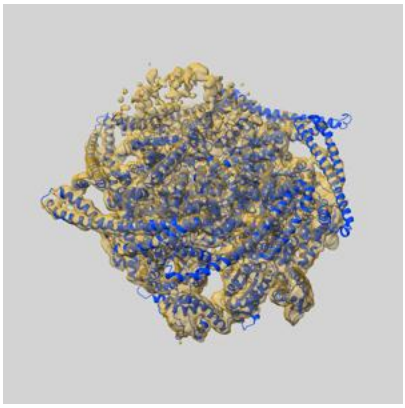
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3776 and PDB model 5OFO. Per-residue inclusion information can be found in section 3 on page 8.

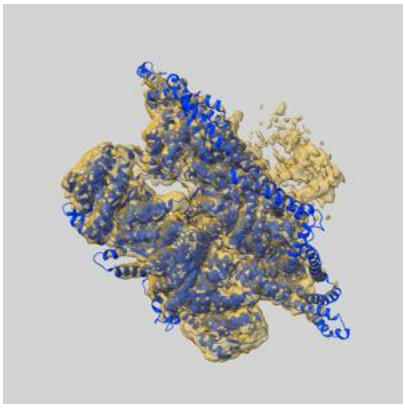
9.1 Map-model overlay



X



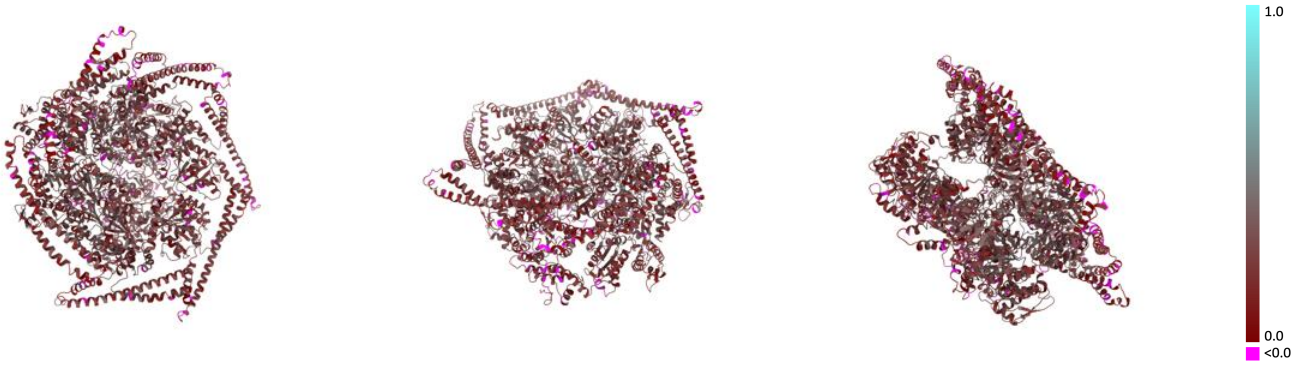
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

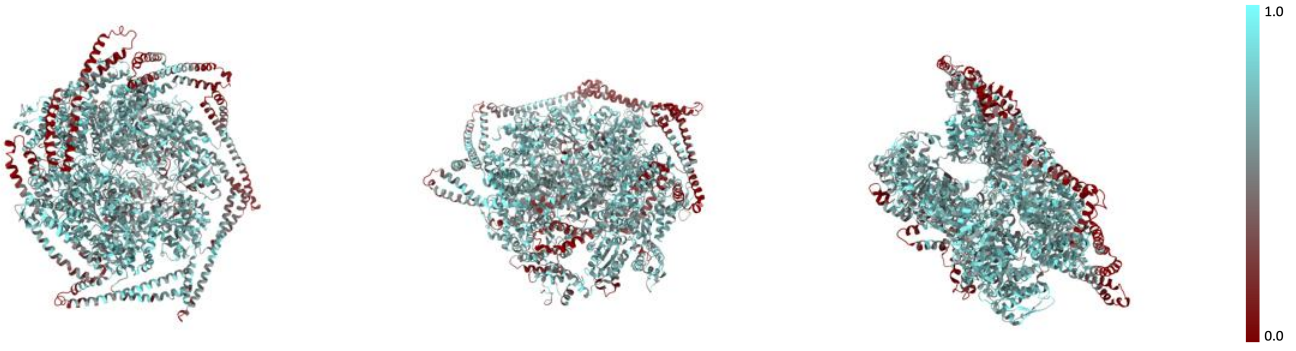
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

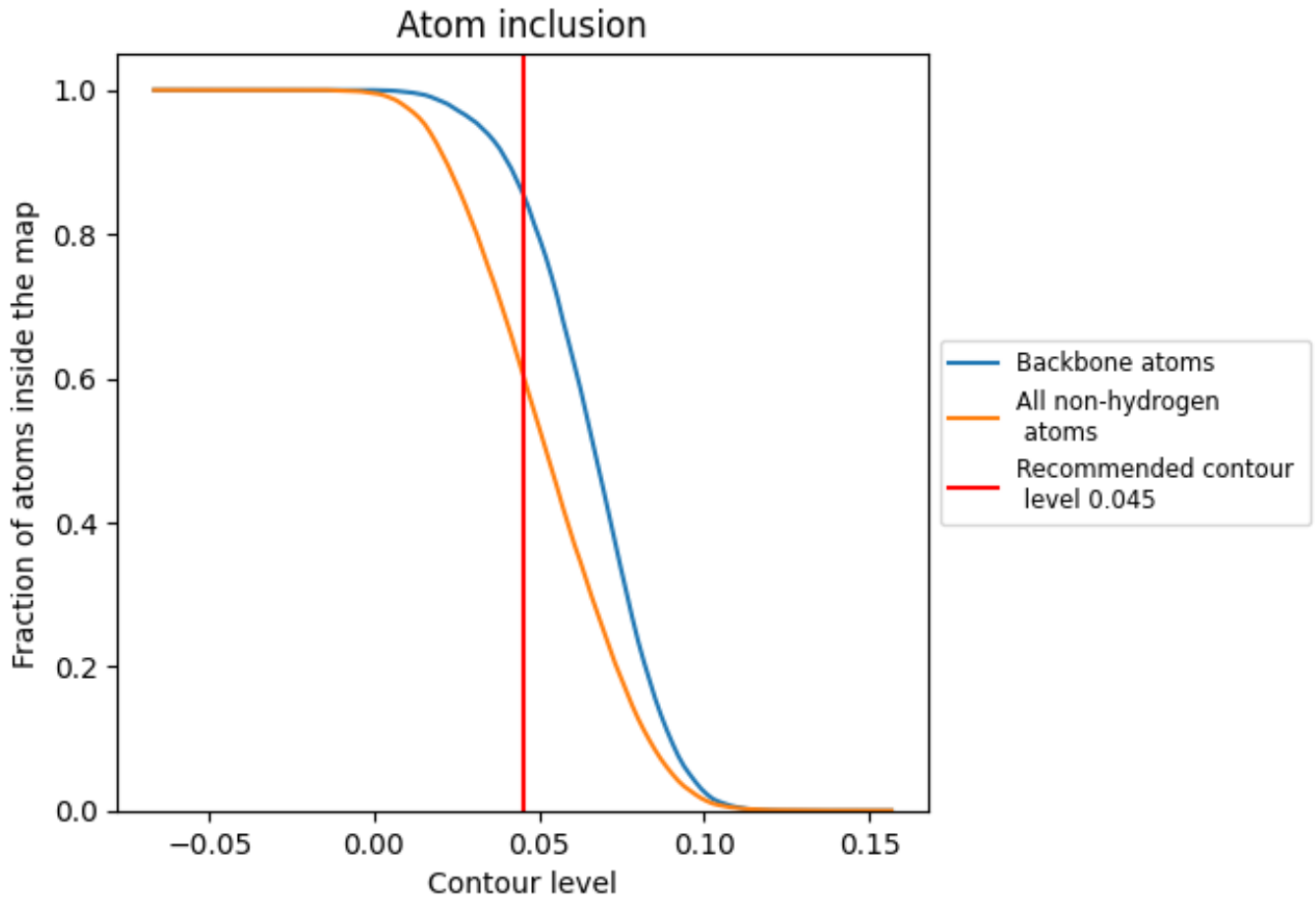
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 61% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6078	0.2350
A	0.5861	0.2190
B	0.6035	0.2390
C	0.5912	0.2470
D	0.6400	0.2560
E	0.6367	0.2490
F	0.5890	0.2030