Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:36 AM UTC

PDB ID	:	8WW6 / pdb_00008ww6
EMDB ID	:	EMD-37882
Title	:	Structure of ATP-rs-Form AsfvPrimPol Hexamer
Authors	:	Shi, T.H.; Guo, Y.Y.; Yan, R.H.
Deposited on	:	2023-10-25
Resolution	:	3.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

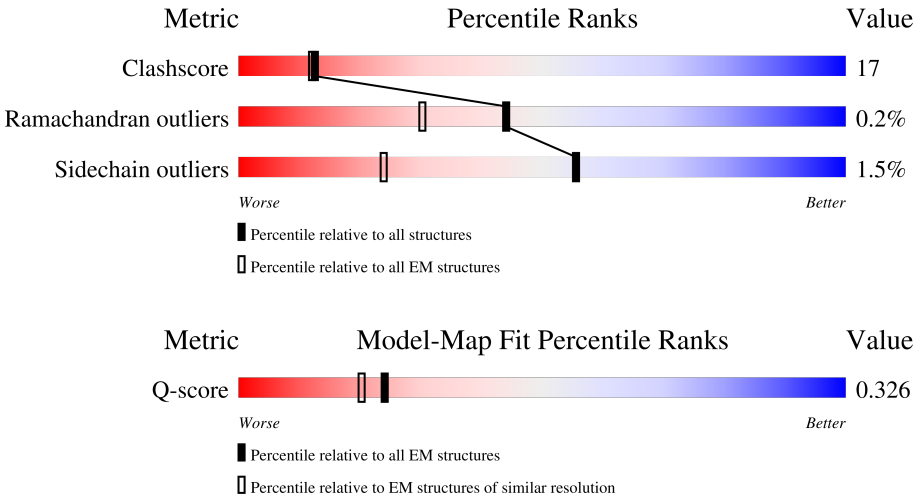
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.73 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10415 (3.23 - 4.23)

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	H	25	44% 56%
2	I	4	50% 50%
3	A	972	8% 45% 22% 34%
3	B	972	43% 22% 34%

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Mol	Chain	Length	Quality of chain
3	C	972	43% 23% 34%
3	D	972	41% 24% 34%
3	E	972	44% 22% 34%
3	F	972	44% 22% 34%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32825 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 DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	25	Total	C	N	O	P	0	0
			500	250	50	175	25		

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

- Molecule 3 is a protein called Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	A	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	C	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		
3	D	644	Total	C	N	O	S	0	0
			5333	3440	907	961	25		
3	E	643	Total	C	N	O	S	0	0
			5328	3436	906	960	26		
3	F	646	Total	C	N	O	S	0	0
			5347	3449	909	963	26		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	963	LEU	-	expression tag	UNP A0A2X0TKI6
B	964	GLU	-	expression tag	UNP A0A2X0TKI6
B	965	ASP	-	expression tag	UNP A0A2X0TKI6
B	966	TYR	-	expression tag	UNP A0A2X0TKI6
B	967	LYS	-	expression tag	UNP A0A2X0TKI6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	968	ASP	-	expression tag	UNP A0A2X0TKI6
B	969	ASP	-	expression tag	UNP A0A2X0TKI6
B	970	ASP	-	expression tag	UNP A0A2X0TKI6
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
A	963	LEU	-	expression tag	UNP A0A2X0TKI6
A	964	GLU	-	expression tag	UNP A0A2X0TKI6
A	965	ASP	-	expression tag	UNP A0A2X0TKI6
A	966	TYR	-	expression tag	UNP A0A2X0TKI6
A	967	LYS	-	expression tag	UNP A0A2X0TKI6
A	968	ASP	-	expression tag	UNP A0A2X0TKI6
A	969	ASP	-	expression tag	UNP A0A2X0TKI6
A	970	ASP	-	expression tag	UNP A0A2X0TKI6
A	971	ASP	-	expression tag	UNP A0A2X0TKI6
A	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
C	966	TYR	-	expression tag	UNP A0A2X0TKI6
C	967	LYS	-	expression tag	UNP A0A2X0TKI6
C	968	ASP	-	expression tag	UNP A0A2X0TKI6
C	969	ASP	-	expression tag	UNP A0A2X0TKI6
C	970	ASP	-	expression tag	UNP A0A2X0TKI6
C	971	ASP	-	expression tag	UNP A0A2X0TKI6
C	972	LYS	-	expression tag	UNP A0A2X0TKI6
D	963	LEU	-	expression tag	UNP A0A2X0TKI6
D	964	GLU	-	expression tag	UNP A0A2X0TKI6
D	965	ASP	-	expression tag	UNP A0A2X0TKI6
D	966	TYR	-	expression tag	UNP A0A2X0TKI6
D	967	LYS	-	expression tag	UNP A0A2X0TKI6
D	968	ASP	-	expression tag	UNP A0A2X0TKI6
D	969	ASP	-	expression tag	UNP A0A2X0TKI6
D	970	ASP	-	expression tag	UNP A0A2X0TKI6
D	971	ASP	-	expression tag	UNP A0A2X0TKI6
D	972	LYS	-	expression tag	UNP A0A2X0TKI6
E	963	LEU	-	expression tag	UNP A0A2X0TKI6
E	964	GLU	-	expression tag	UNP A0A2X0TKI6
E	965	ASP	-	expression tag	UNP A0A2X0TKI6
E	966	TYR	-	expression tag	UNP A0A2X0TKI6
E	967	LYS	-	expression tag	UNP A0A2X0TKI6
E	968	ASP	-	expression tag	UNP A0A2X0TKI6
E	969	ASP	-	expression tag	UNP A0A2X0TKI6

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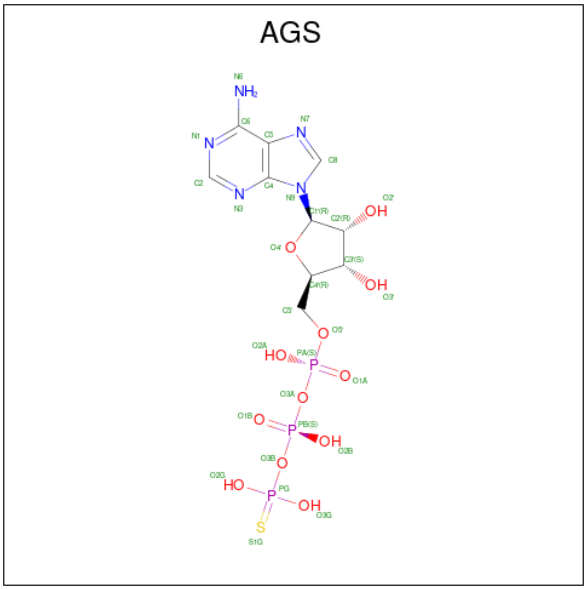
Chain	Residue	Modelled	Actual	Comment	Reference
E	970	ASP	-	expression tag	UNP A0A2X0TKI6
E	971	ASP	-	expression tag	UNP A0A2X0TKI6
E	972	LYS	-	expression tag	UNP A0A2X0TKI6
F	963	LEU	-	expression tag	UNP A0A2X0TKI6
F	964	GLU	-	expression tag	UNP A0A2X0TKI6
F	965	ASP	-	expression tag	UNP A0A2X0TKI6
F	966	TYR	-	expression tag	UNP A0A2X0TKI6
F	967	LYS	-	expression tag	UNP A0A2X0TKI6
F	968	ASP	-	expression tag	UNP A0A2X0TKI6
F	969	ASP	-	expression tag	UNP A0A2X0TKI6
F	970	ASP	-	expression tag	UNP A0A2X0TKI6
F	971	ASP	-	expression tag	UNP A0A2X0TKI6
F	972	LYS	-	expression tag	UNP A0A2X0TKI6

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	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: DNA (25-MER)

Chain H:



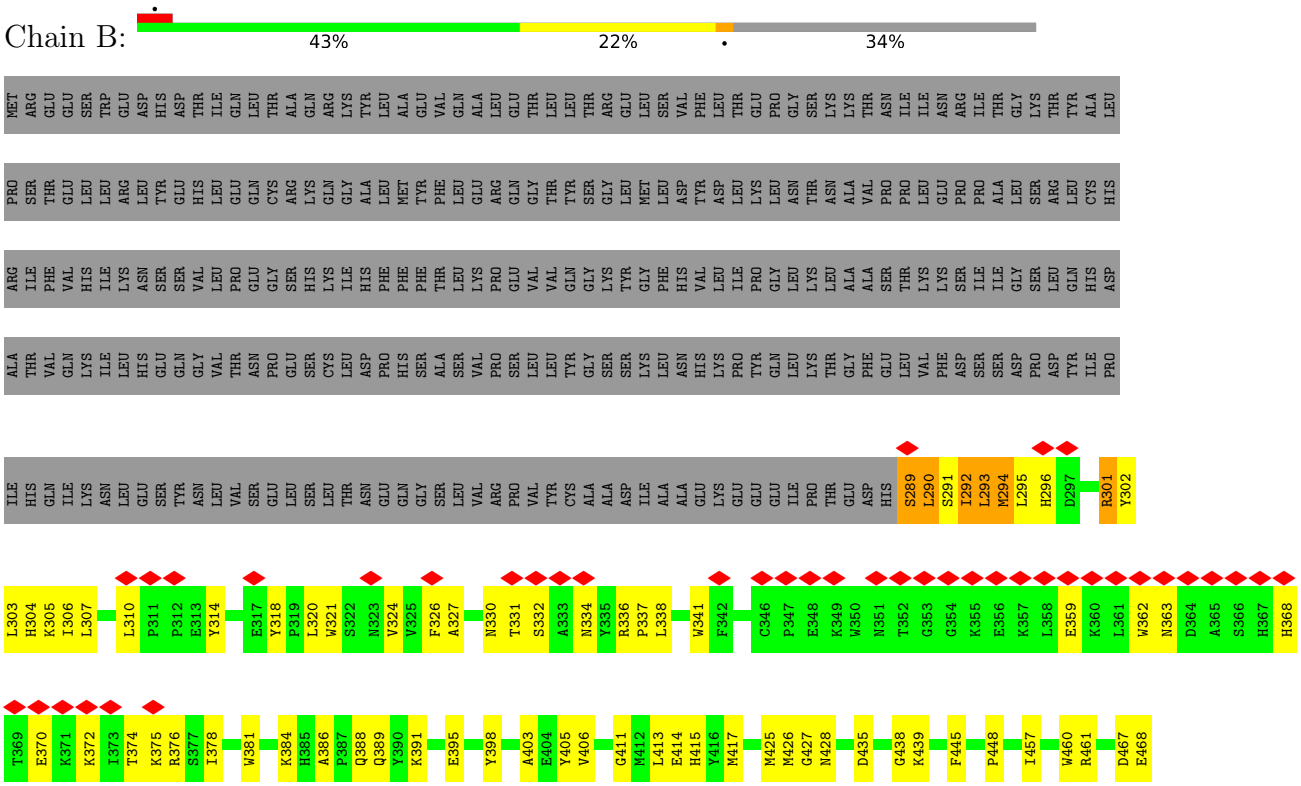
• Molecule 2: DNA (5'-D(P*AP*AP*AP*A)-3')

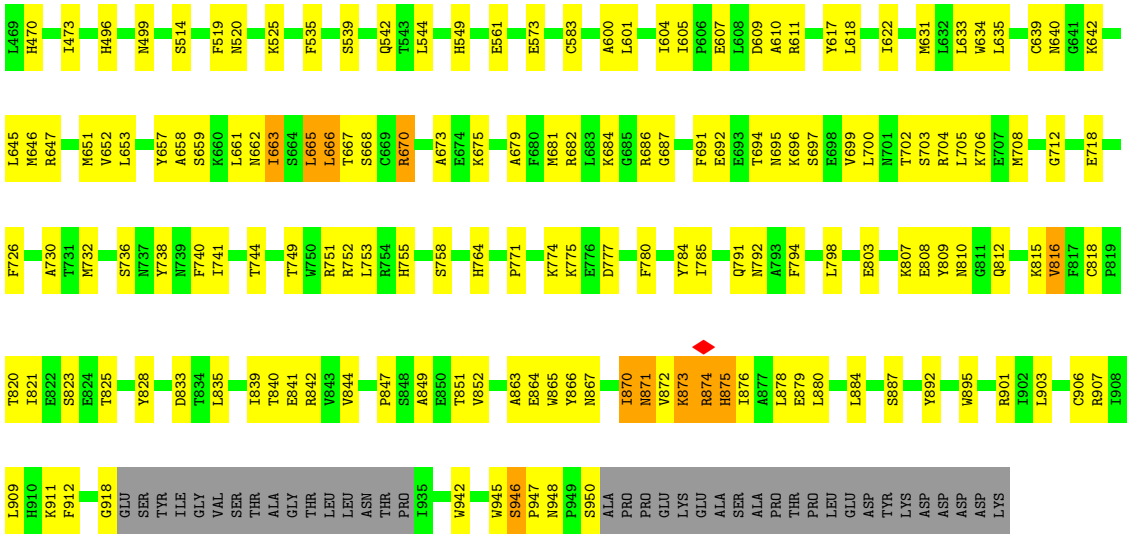
Chain I:



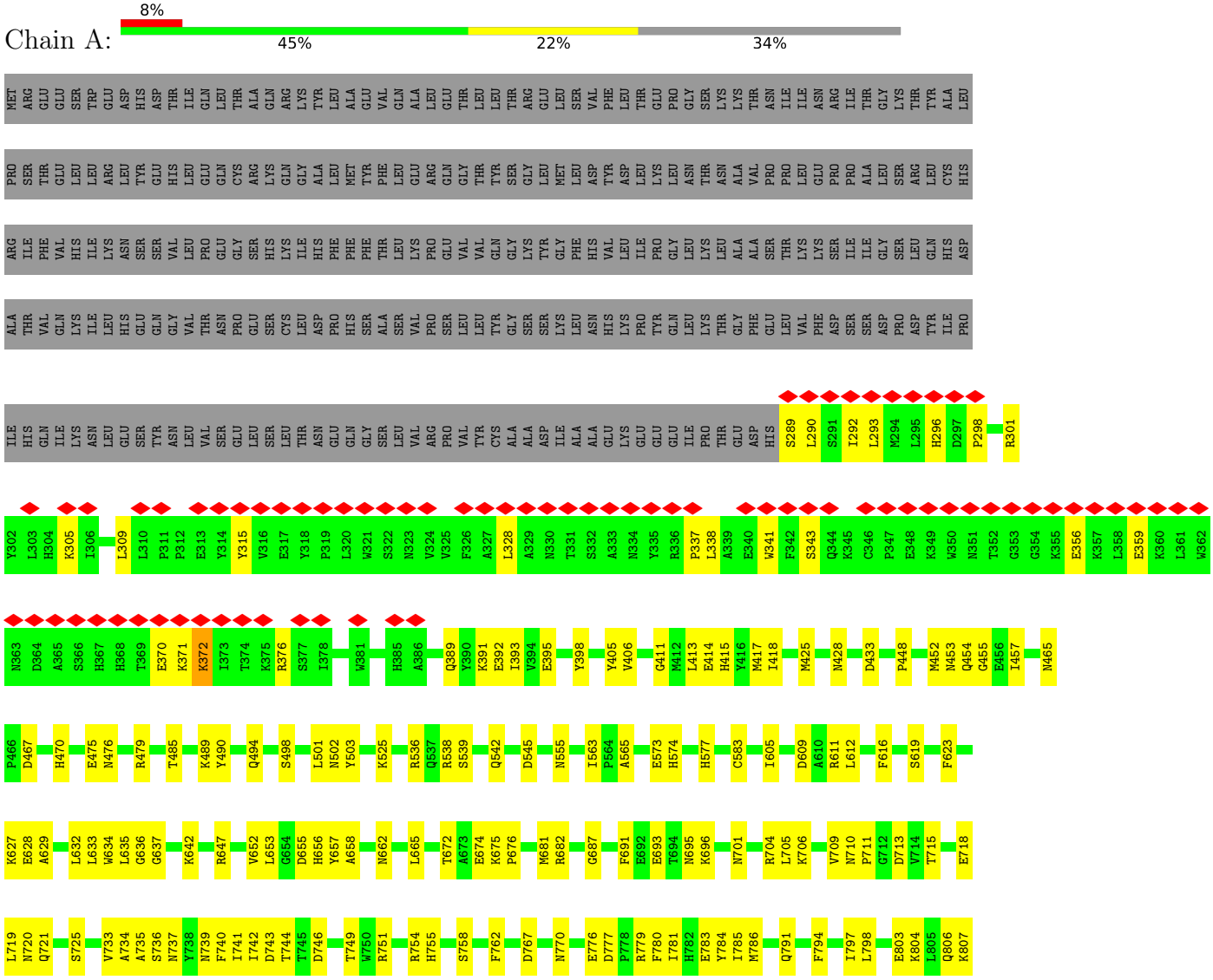
• Molecule 3: Putative primase C962R

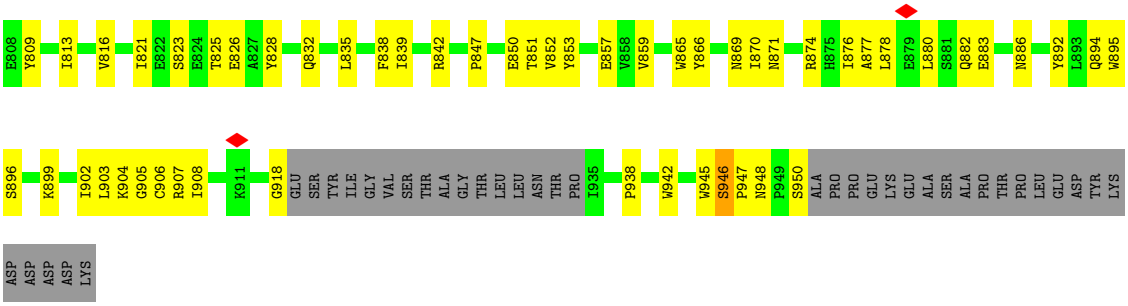
Chain B:





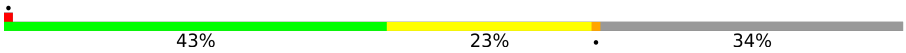
• Molecule 3: Putative primase C962R

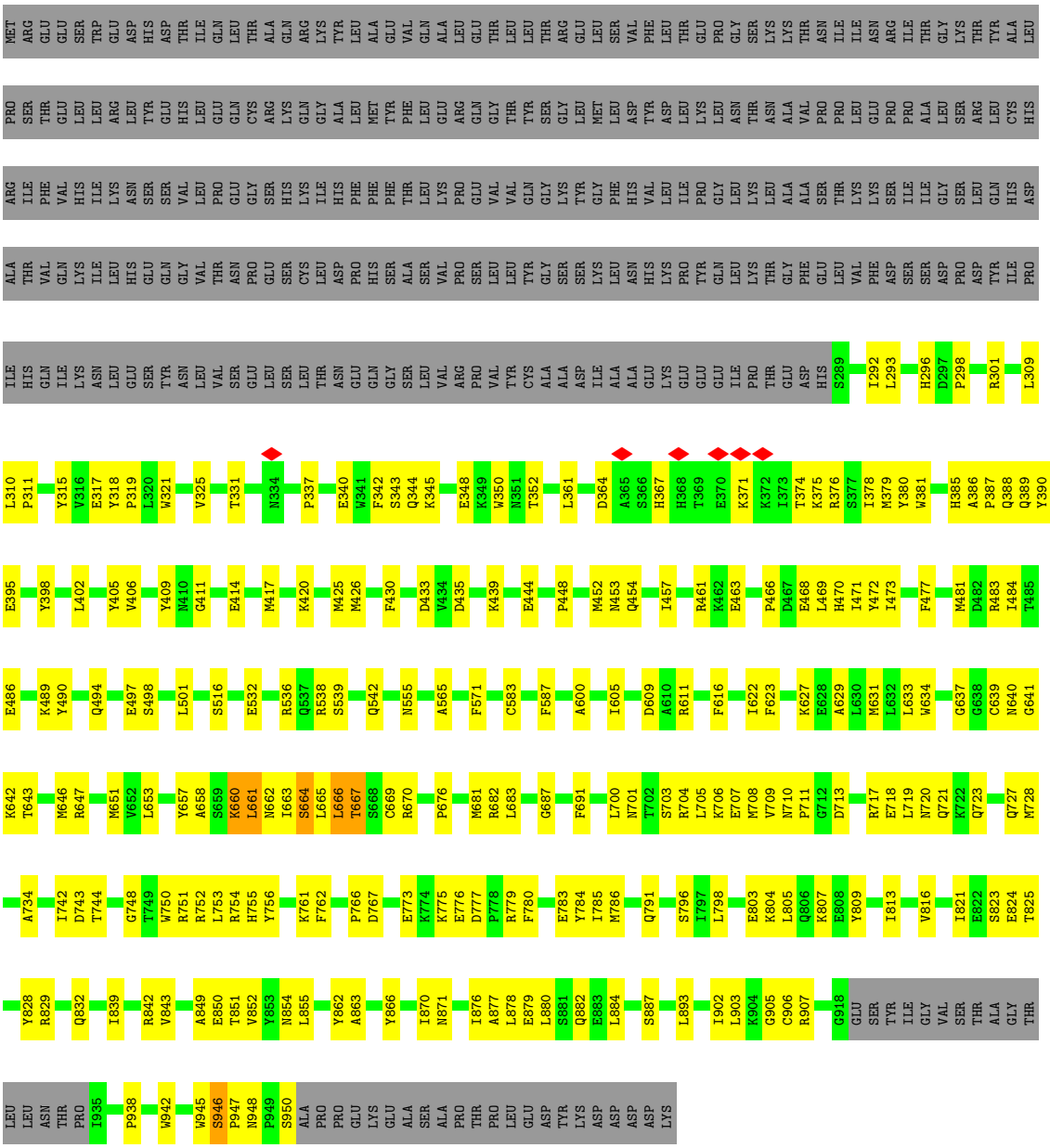




• Molecule 3: Putative primase C962R

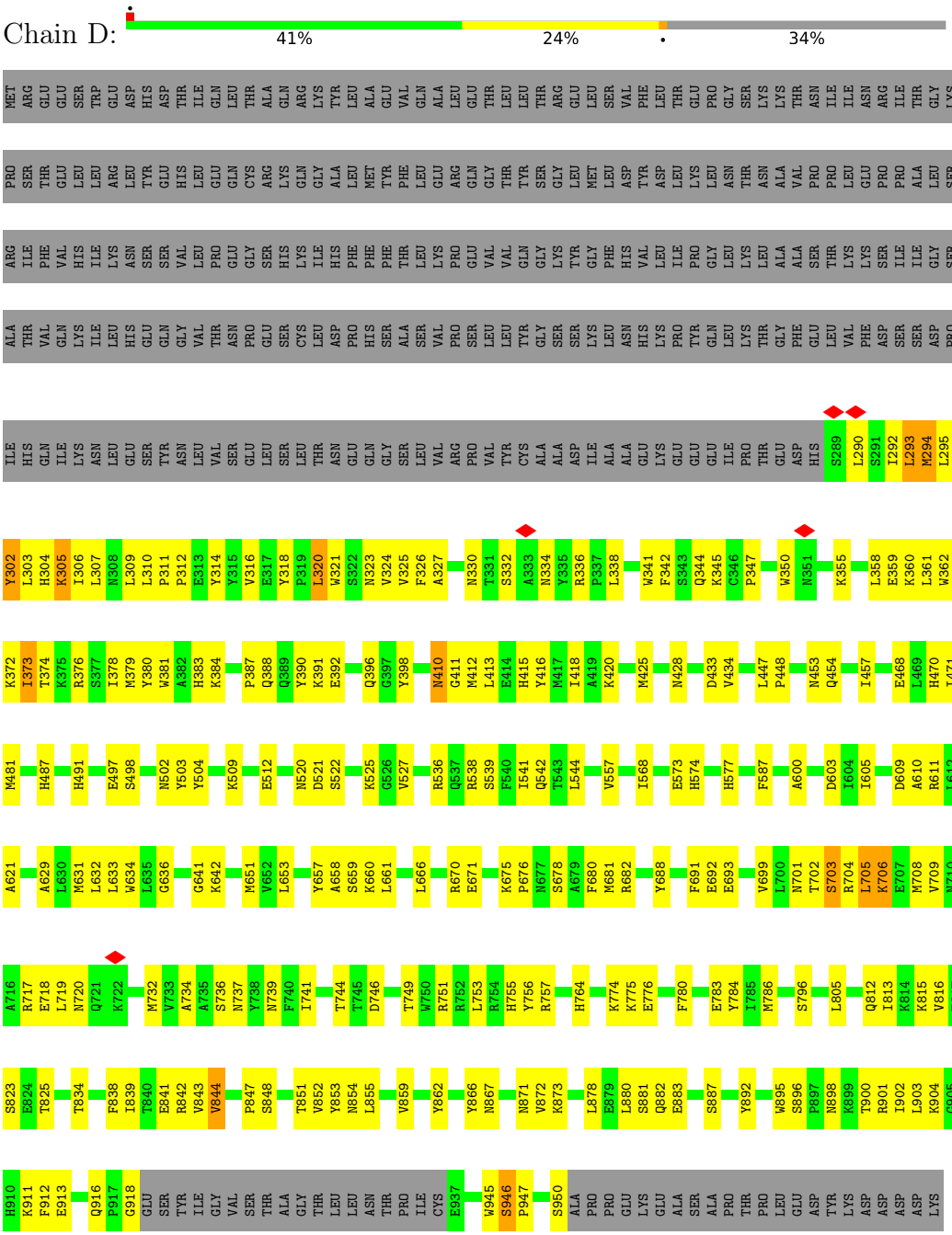
Chain C:





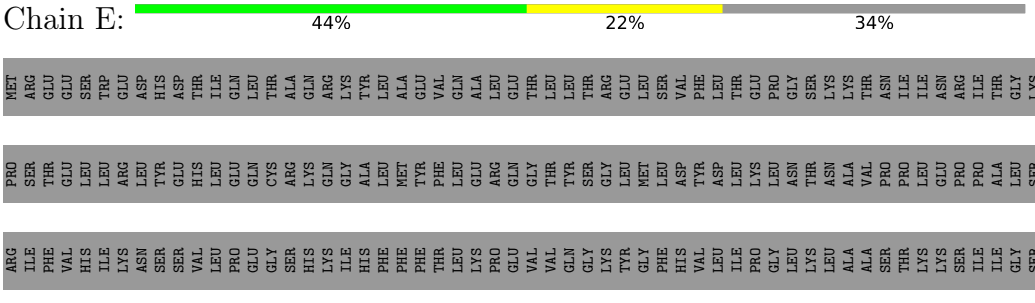
• Molecule 3: Putative primase C962R

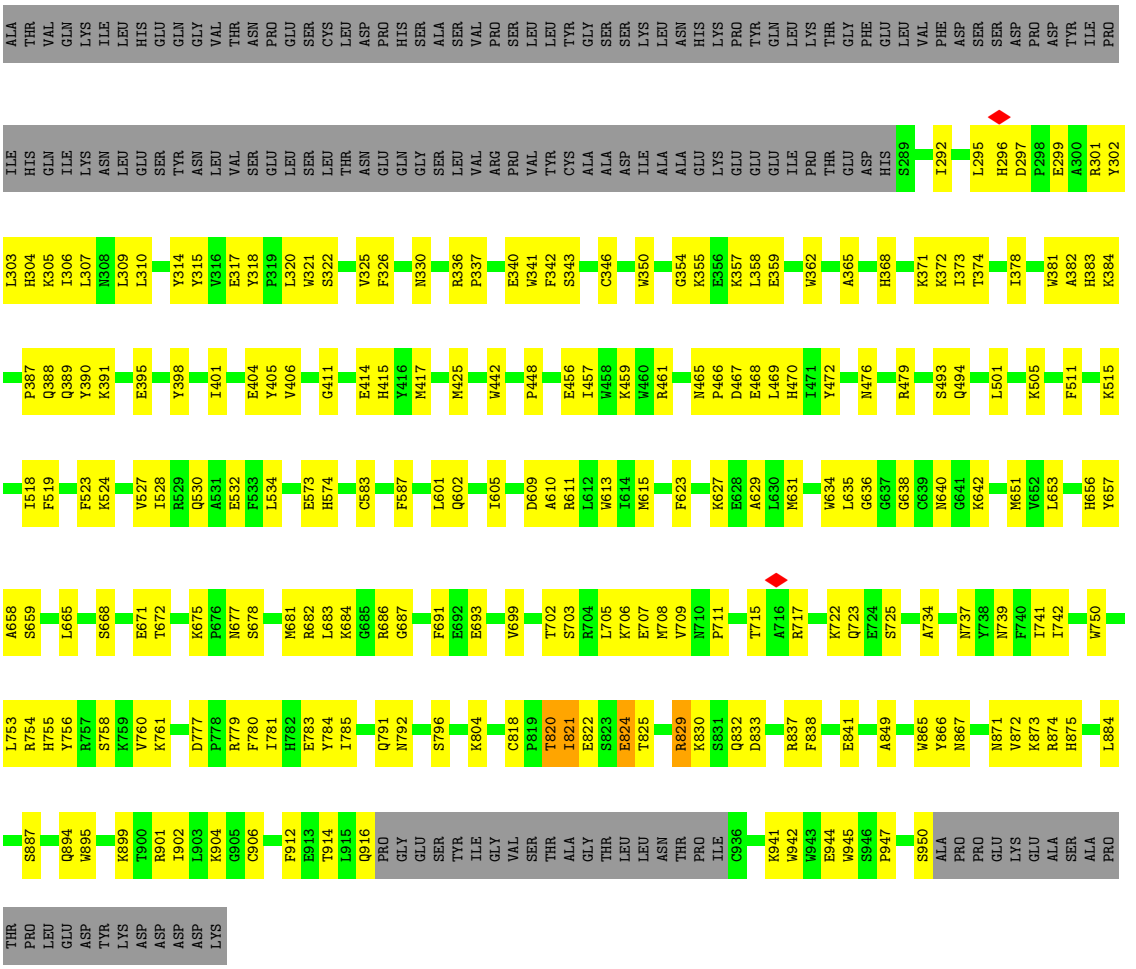
Chain D:



• Molecule 3: Putative primase C962R

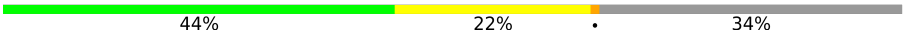
Chain E:

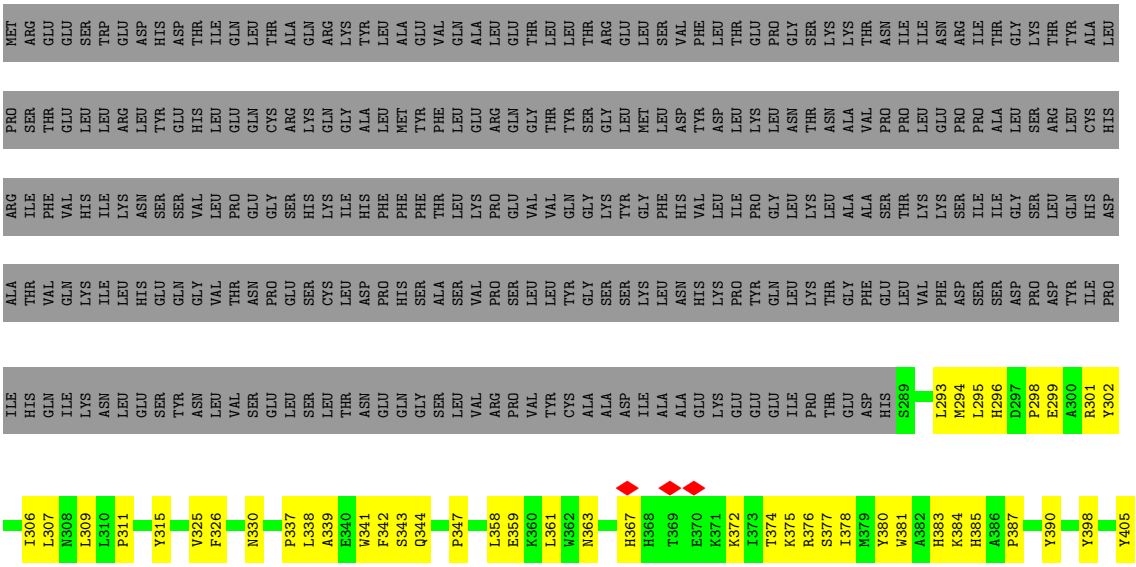


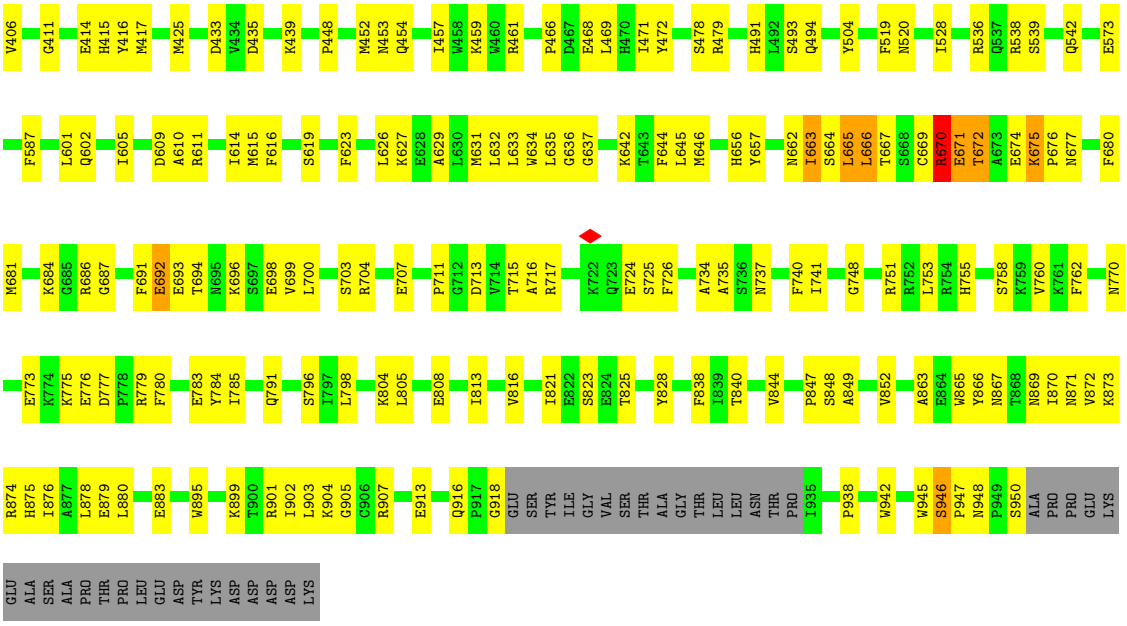


• Molecule 3: Putative primase C962R

Chain F:






V406 G411 E414 H415 Y416 M417 M425 D433 V434 D435 K439 P448 M452 N453 Q454 I457 W458 K459 W460 R461 P466 D467 E468 L469 H470 I471 Y472 S478 R479 H491 L492 S493 Q494 Y504 F519 N520 I528 R536 Q537 R538 S539 Q542 E573
F587 L601 Q602 I605 D609 A610 R611 I614 M615 F616 S619 F623 L626 K627 E628 A629 L630 M631 L632 L633 W634 L635 G636 G637 K642 T643 F644 L645 M646 H656 Y657 N662 I663 S664 L665 L666 T667 S668 C669 R670 E671 T672 A673 E674 K675 P676 N677 F680
M681 K684 G685 R686 G687 F691 E692 E693 T694 N695 K696 S697 E698 V699 L700 S703 R704 E707 P711 G712 D713 V714 T715 A716 R717 K722 Q723 E724 S725 F726 A734 A735 S736 N737 F740 I741 G748 R751 R752 L753 R754 H755 S758 K759 V760 K761 F762 N770
E773 K774 K775 E776 D777 P778 R779 F780 E783 Y784 I785 Q791 S796 I797 L798 K804 L805 E808 I813 V816 I821 E822 S823 E824 T825 Y828 F838 I839 T840 V844 P847 S848 A849 V852 A863 E864 W865 Y866 N867 T868 N869 I870 N871 V872 K873
R874 H875 I876 A877 L878 E879 L880 E883 W895 K899 T900 R901 I902 L903 K904 G905 C906 R907 E913 Q916 P917 G918 GLU SER TYR ILE GLY VAL SER THR ALA GLY THR LEU LEU ASN THR PRO I935 P938 W942 W945 S946 P947 N948 P949 S950 ALA PRO PRO GLU LYS
GLU ALA SER ALA PRO THR PRO LEU GLU ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38908	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.164	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	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, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	H	0.22	0/549	0.55	0/846
2	I	0.13	0/95	0.19	0/144
3	A	0.12	0/5503	0.30	0/7458
3	B	0.16	0/5503	0.39	0/7458
3	C	0.15	0/5503	0.37	0/7458
3	D	0.19	0/5489	0.43	1/7439 (0.0%)
3	E	0.15	0/5483	0.37	0/7430
3	F	0.15	0/5503	0.37	1/7458 (0.0%)
All	All	0.16	0/33628	0.38	2/45691 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	670	ARG	CB-CA-C	-5.29	110.46	116.54
3	D	373	ILE	N-CA-C	-5.25	108.72	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	500	0	301	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	84	0	45	3	0
3	A	5347	0	5216	160	0
3	B	5347	0	5217	210	0
3	C	5347	0	5217	181	0
3	D	5333	0	5202	196	0
3	E	5328	0	5196	172	0
3	F	5347	0	5217	176	0
4	A	31	0	12	7	0
4	B	31	0	12	7	0
4	C	31	0	12	6	0
4	D	31	0	12	5	0
4	E	31	0	12	6	0
4	F	31	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	32825	0	31683	1082	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 17.

All (1082) 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)
3:B:874:ARG:HH21	3:B:875:HIS:C	1.63	1.06
3:F:667:THR:HA	3:F:700:LEU:HB3	1.48	0.95
3:C:667:THR:HB	3:C:700:LEU:HB3	1.48	0.95
3:D:294:MET:HG3	3:D:301:ARG:HG3	1.51	0.90
3:B:294:MET:HG3	3:B:301:ARG:HG2	1.52	0.88
3:B:681:MET:SD	3:B:684:LYS:NZ	2.48	0.87
3:C:866:TYR:HB2	3:C:870:ILE:HG12	1.59	0.85
3:B:600:ALA:HB1	4:B:1001:AGS:HN62	1.39	0.84
3:B:870:ILE:HA	3:C:877:ALA:HB2	1.59	0.83
3:F:852:VAL:HG21	3:F:903:LEU:HB3	1.63	0.81
3:D:325:VAL:HG21	3:D:358:LEU:HD11	1.60	0.80
3:B:331:THR:HG21	3:B:375:LYS:HB2	1.64	0.80
3:C:854:ASN:H	3:C:902:ILE:HG13	1.48	0.78
3:B:911:LYS:HG3	3:B:912:PHE:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:777:ASP:HB3	3:F:780:PHE:HB2	1.66	0.78
3:A:370:GLU:HG2	3:A:372:LYS:H	1.50	0.77
3:A:777:ASP:HB3	3:A:780:PHE:HB2	1.67	0.76
3:C:498:SER:HA	3:C:501:LEU:HD13	1.68	0.76
3:C:622:ILE:HD11	3:C:798:LEU:HB3	1.66	0.76
3:F:642:LYS:HE2	3:F:735:ALA:HB1	1.66	0.76
3:E:640:ASN:HD21	3:E:758:SER:HB3	1.51	0.75
3:D:415:HIS:HB3	3:D:527:VAL:HA	1.67	0.75
3:B:663:ILE:HA	3:B:691:PHE:CD2	2.22	0.75
3:C:653:LEU:HD23	3:C:658:ALA:HB2	1.68	0.75
3:F:662:ASN:HB3	3:F:665:LEU:HD22	1.66	0.75
3:B:842:ARG:HG3	3:B:909:LEU:HG	1.68	0.74
3:D:344:GLN:HA	3:D:347:PRO:HB3	1.69	0.74
3:C:893:LEU:HA	3:C:903:LEU:HA	1.68	0.74
3:B:386:ALA:HB1	3:B:389:GLN:HE21	1.53	0.74
3:A:850:GLU:HG2	3:A:905:GLY:HA3	1.69	0.73
3:D:303:LEU:HD23	3:D:306:ILE:HD11	1.71	0.73
3:D:296:HIS:CE1	3:D:297:ASP:OD1	2.41	0.73
3:F:298:PRO:HA	3:F:301:ARG:HD3	1.70	0.73
3:B:874:ARG:NH2	3:B:875:HIS:C	2.44	0.73
3:C:331:THR:HG21	3:C:375:LYS:HG2	1.70	0.72
3:E:871:ASN:HB2	3:F:874:ARG:HH22	1.52	0.72
3:F:874:ARG:NH1	3:F:875:HIS:O	2.23	0.72
3:B:293:LEU:HD21	3:B:337:PRO:HB2	1.72	0.72
3:D:294:MET:HA	3:D:301:ARG:HD2	1.71	0.72
3:F:605:ILE:O	3:F:611:ARG:NH1	2.23	0.72
3:A:762:PHE:HB3	3:A:776:GLU:HG3	1.72	0.71
3:E:874:ARG:NH1	3:E:875:HIS:O	2.23	0.71
3:F:635:LEU:HD23	3:F:755:HIS:HE2	1.56	0.71
3:B:741:ILE:HD11	3:C:878:LEU:HD11	1.72	0.71
3:F:748:GLY:HA2	3:F:751:ARG:HD3	1.73	0.71
3:F:406:VAL:HG13	3:F:411:GLY:HA2	1.73	0.70
3:D:600:ALA:HB1	4:D:1001:AGS:HN62	1.57	0.70
3:E:677:ASN:H	3:E:717:ARG:HG2	1.57	0.70
3:B:647:ARG:HH21	3:B:651:MET:HE3	1.56	0.70
3:C:876:ILE:HB	3:C:879:GLU:HG3	1.72	0.70
3:A:718:GLU:OE1	3:A:721:GLN:NE2	2.23	0.70
3:C:767:ASP:H	3:C:773:GLU:HG2	1.57	0.70
3:D:392:GLU:O	3:D:396:GLN:NE2	2.24	0.70
3:A:672:THR:O	3:A:704:ARG:NH1	2.25	0.70
3:C:750:TRP:O	3:C:829:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:425:MET:SD	3:C:472:TYR:OH	2.49	0.69
3:F:306:ILE:HA	3:F:309:LEU:HD12	1.74	0.69
3:B:697:SER:HA	3:B:738:TYR:HB3	1.75	0.69
3:A:413:LEU:HD13	3:A:418:ILE:HD11	1.74	0.69
3:C:468:GLU:HA	3:C:471:ILE:HG12	1.73	0.69
3:C:340:GLU:O	3:C:344:GLN:NE2	2.26	0.69
3:C:785:ILE:O	3:C:791:GLN:NE2	2.22	0.69
3:F:671:GLU:HG3	3:F:675:LYS:HE2	1.74	0.69
3:F:699:VAL:HB	3:F:741:ILE:HB	1.74	0.69
3:E:315:TYR:O	3:E:321:TRP:NE1	2.20	0.68
3:A:498:SER:HA	3:A:501:LEU:HD13	1.75	0.68
3:D:371:LYS:NZ	3:D:573:GLU:OE2	2.26	0.68
3:C:661:LEU:HB3	3:C:691:PHE:CE1	2.28	0.68
3:C:605:ILE:O	3:C:611:ARG:NH1	2.27	0.68
3:E:330:ASN:ND2	3:E:373:ILE:O	2.27	0.67
3:E:310:LEU:HD21	3:E:382:ALA:HA	1.76	0.67
3:E:315:TYR:HE2	3:E:346:CYS:H	1.42	0.67
3:C:293:LEU:HD21	3:C:337:PRO:HB2	1.75	0.67
3:B:895:TRP:HA	3:B:901:ARG:HA	1.74	0.67
3:A:642:LYS:HD3	3:A:735:ALA:HB1	1.76	0.67
3:B:863:ALA:HA	3:B:866:TYR:CZ	2.30	0.67
3:A:785:ILE:O	3:A:791:GLN:NE2	2.25	0.67
3:A:636:GLY:HA3	3:A:758:SER:HB3	1.76	0.67
3:E:387:PRO:HA	3:E:390:TYR:HE1	1.58	0.67
3:E:629:ALA:HB2	3:E:711:PRO:HD3	1.77	0.67
3:C:433:ASP:OD1	3:C:536:ARG:NH1	2.28	0.66
3:E:448:PRO:HG3	3:E:457:ILE:HD11	1.77	0.66
3:B:703:SER:HB3	3:A:695:ASN:HB3	1.77	0.66
3:B:871:ASN:HD22	3:C:876:ILE:HA	1.59	0.66
3:A:448:PRO:HG3	3:A:457:ILE:HD11	1.76	0.66
3:E:785:ILE:O	3:E:791:GLN:NE2	2.23	0.66
3:A:433:ASP:OD1	3:A:536:ARG:NH1	2.29	0.66
3:A:681:MET:HG3	3:A:718:GLU:HB2	1.77	0.66
3:F:691:PHE:HB2	3:F:734:ALA:HA	1.76	0.66
3:F:375:LYS:O	3:F:376:ARG:HG2	1.95	0.66
3:D:379:MET:O	3:D:383:HIS:ND1	2.29	0.66
3:A:635:LEU:HD23	3:A:755:HIS:HE2	1.60	0.65
3:E:301:ARG:O	3:E:304:HIS:ND1	2.28	0.65
3:B:600:ALA:HB1	4:B:1001:AGS:N6	2.09	0.65
3:B:751:ARG:NH2	4:A:1001:AGS:S1G	2.69	0.65
3:E:902:ILE:O	3:E:904:LYS:NZ	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:667:THR:HA	3:F:700:LEU:CB	2.25	0.65
3:A:376:ARG:HD2	3:A:428:ASN:HB2	1.78	0.65
3:F:326:PHE:O	3:F:330:ASN:ND2	2.30	0.65
3:D:521:ASP:OD2	3:E:530:GLN:NE2	2.30	0.65
3:F:448:PRO:HG3	3:F:457:ILE:HD11	1.79	0.65
3:A:874:ARG:HH22	3:F:872:VAL:H	1.45	0.65
3:D:415:HIS:HA	3:D:527:VAL:HG22	1.77	0.65
3:D:603:ASP:HB3	3:D:774:LYS:HE3	1.77	0.65
3:E:365:ALA:O	3:E:368:HIS:ND1	2.29	0.65
3:D:776:GLU:HA	4:D:1001:AGS:H1'	1.79	0.65
3:F:913:GLU:HG3	3:F:916:GLN:HE22	1.61	0.65
3:D:314:TYR:HH	3:D:381:TRP:CD1	2.15	0.65
3:B:301:ARG:HH11	3:B:301:ARG:HA	1.62	0.64
3:C:727:GLN:NE2	3:C:728:MET:O	2.30	0.64
3:B:849:ALA:HB1	3:B:907:ARG:HH21	1.63	0.64
3:F:669:CYS:HB2	3:F:704:ARG:HG2	1.79	0.64
3:A:490:TYR:O	3:A:494:GLN:NE2	2.30	0.64
3:A:605:ILE:O	3:A:611:ARG:NH1	2.31	0.64
3:D:312:PRO:HA	3:D:345:LYS:NZ	2.13	0.64
3:B:668:SER:HB3	3:B:705:LEU:HD21	1.78	0.64
3:C:639:CYS:SG	3:D:751:ARG:NH2	2.70	0.64
3:D:678:SER:HB3	3:D:719:LEU:HB2	1.78	0.64
3:C:555:ASN:ND2	3:C:583:CYS:SG	2.70	0.64
3:B:368:HIS:NE2	3:B:370:GLU:OE2	2.26	0.63
3:A:779:ARG:NH1	3:A:784:TYR:OH	2.30	0.63
3:D:851:THR:OG1	3:D:907:ARG:NH1	2.32	0.63
3:E:605:ILE:O	3:E:611:ARG:NH1	2.31	0.63
3:C:466:PRO:HB2	3:C:469:LEU:HB3	1.80	0.63
3:C:375:LYS:O	3:C:376:ARG:HG2	1.98	0.63
3:C:681:MET:HE3	3:C:718:GLU:HG3	1.81	0.63
3:E:442:TRP:NE1	3:E:532:GLU:OE2	2.30	0.63
3:C:701:ASN:ND2	3:C:743:ASP:O	2.31	0.63
3:D:293:LEU:HA	3:D:296:HIS:ND1	2.14	0.63
1:H:6:DT:H5"	3:A:719:LEU:HD11	1.79	0.63
3:B:668:SER:HA	3:B:670:ARG:HH21	1.63	0.63
3:A:853:TYR:HB2	3:A:857:GLU:HG2	1.81	0.63
3:A:675:LYS:HB2	3:A:676:PRO:HD3	1.80	0.62
3:C:600:ALA:HB1	4:C:1001:AGS:HN62	1.62	0.62
3:E:425:MET:HE1	3:E:472:TYR:HE1	1.64	0.62
3:B:605:ILE:O	3:B:611:ARG:NH1	2.32	0.62
3:B:687:GLY:HA2	3:B:730:ALA:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1001:AGS:H8	4:B:1001:AGS:H5'2	1.81	0.62
3:F:674:GLU:O	3:F:717:ARG:HG2	1.99	0.62
3:A:637:GLY:O	3:A:737:ASN:ND2	2.33	0.62
3:B:874:ARG:NH2	3:B:875:HIS:O	2.29	0.62
1:H:23:DT:O4	2:I:2:DA:N6	2.33	0.62
3:B:370:GLU:HB2	3:B:372:LYS:HD3	1.81	0.62
3:A:706:LYS:O	3:A:710:ASN:ND2	2.33	0.62
3:F:785:ILE:O	3:F:791:GLN:NE2	2.23	0.62
3:C:850:GLU:HA	3:C:905:GLY:HA2	1.82	0.62
3:D:302:TYR:HA	3:D:305:LYS:HD2	1.80	0.62
3:D:670:ARG:HA	3:D:704:ARG:HH22	1.64	0.62
3:E:777:ASP:HB3	3:E:780:PHE:HB2	1.81	0.61
3:B:376:ARG:NH2	3:B:428:ASN:O	2.27	0.61
3:A:293:LEU:HD21	3:A:337:PRO:HB2	1.82	0.61
3:C:435:ASP:OD1	3:C:439:LYS:N	2.29	0.61
3:D:290:LEU:HA	3:D:293:LEU:HD12	1.81	0.61
3:D:839:ILE:O	3:D:843:VAL:N	2.24	0.61
3:B:359:GLU:OE1	3:B:363:ASN:ND2	2.34	0.61
3:D:481:MET:N	3:D:481:MET:HE2	2.14	0.61
3:F:539:SER:HB2	3:F:542:GLN:HE22	1.65	0.61
3:F:672:THR:HG23	3:F:675:LYS:H	1.64	0.61
3:B:665:LEU:HD12	3:B:670:ARG:HH12	1.64	0.61
3:D:854:ASN:HD22	3:D:900:THR:HG22	1.65	0.61
3:E:467:ASP:OD1	3:E:468:GLU:N	2.33	0.61
3:C:706:LYS:O	3:C:710:ASN:ND2	2.33	0.61
3:D:867:ASN:HB3	3:D:872:VAL:HG12	1.82	0.61
3:B:293:LEU:HB2	3:B:301:ARG:HH22	1.64	0.61
3:D:307:LEU:HD21	3:D:342:PHE:HD1	1.66	0.61
3:E:750:TRP:CD2	3:E:829:ARG:HD2	2.36	0.61
3:F:662:ASN:O	3:F:665:LEU:HB2	2.00	0.61
3:F:779:ARG:NH1	3:F:784:TYR:OH	2.34	0.61
3:B:496:HIS:CE1	3:B:499:ASN:HD21	2.19	0.61
3:B:871:ASN:HB2	3:B:873:LYS:HZ3	1.66	0.61
3:D:290:LEU:HD13	3:D:341:TRP:CD2	2.35	0.61
3:B:699:VAL:HA	3:B:741:ILE:HB	1.81	0.61
3:E:691:PHE:HB2	3:E:734:ALA:HA	1.83	0.60
3:F:775:LYS:NZ	3:F:776:GLU:O	2.33	0.60
3:E:395:GLU:HA	3:E:398:TYR:CZ	2.36	0.60
3:C:720:ASN:O	3:C:721:GLN:NE2	2.34	0.60
3:E:777:ASP:O	4:E:1001:AGS:O2'	2.20	0.60
3:E:610:ALA:HB2	3:E:820:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:539:SER:HB2	3:A:542:GLN:HE22	1.67	0.60
3:B:289:SER:HB3	3:B:292:ILE:HB	1.82	0.60
3:C:661:LEU:HB3	3:C:691:PHE:HE1	1.67	0.60
3:B:863:ALA:HA	3:B:866:TYR:CE2	2.36	0.59
3:C:666:LEU:HD12	3:C:700:LEU:HD13	1.83	0.59
3:C:777:ASP:HB3	3:C:780:PHE:HB2	1.84	0.59
3:F:762:PHE:HB3	3:F:776:GLU:HG3	1.84	0.59
3:B:290:LEU:HD12	3:B:341:TRP:HB2	1.85	0.59
3:C:946:SER:HB2	3:C:950:SER:HA	1.84	0.59
3:E:405:TYR:CD2	3:E:417:MET:HB2	2.38	0.59
3:B:467:ASP:OD1	3:B:468:GLU:N	2.35	0.59
3:D:302:TYR:CE1	3:D:306:ILE:HD13	2.37	0.59
3:D:898:ASN:O	3:D:900:THR:OG1	2.20	0.59
3:C:539:SER:HB2	3:C:542:GLN:HE22	1.68	0.59
3:D:783:GLU:HA	3:D:786:MET:HE1	1.85	0.59
3:F:684:LYS:HD3	3:F:726:PHE:HB2	1.85	0.59
3:B:302:TYR:HA	3:B:305:LYS:HE2	1.83	0.59
3:B:700:LEU:HB3	3:B:705:LEU:HD11	1.85	0.59
3:A:877:ALA:HB2	3:F:870:ILE:HA	1.85	0.59
3:A:892:TYR:HD2	3:A:904:LYS:HB2	1.68	0.59
3:E:583:CYS:O	3:E:792:ASN:ND2	2.36	0.59
4:F:1001:AGS:O2B	4:F:1001:AGS:O1A	2.20	0.59
3:E:755:HIS:HB3	3:E:825:THR:HA	1.85	0.58
3:A:293:LEU:O	3:A:296:HIS:NE2	2.36	0.58
3:F:338:LEU:HA	3:F:341:TRP:HD1	1.68	0.58
3:F:387:PRO:HA	3:F:390:TYR:HE1	1.69	0.58
3:B:818:CYS:SG	3:B:820:THR:OG1	2.61	0.58
3:A:642:LYS:NZ	3:A:736:SER:O	2.37	0.58
3:C:629:ALA:HB2	3:C:711:PRO:HD3	1.86	0.58
3:D:848:SER:OG	3:D:907:ARG:NH1	2.37	0.58
3:D:852:VAL:HG11	3:D:903:LEU:HB3	1.84	0.58
3:E:350:TRP:O	3:E:355:LYS:N	2.29	0.58
3:A:405:TYR:CD2	3:A:417:MET:HB2	2.38	0.58
3:D:491:HIS:HB3	3:D:504:TYR:HE2	1.67	0.58
3:D:605:ILE:O	3:D:611:ARG:NH1	2.37	0.58
3:C:849:ALA:HB1	3:C:907:ARG:HB2	1.85	0.58
3:D:371:LYS:HZ1	3:D:574:HIS:HA	1.68	0.58
3:B:840:THR:HA	3:B:844:VAL:HB	1.86	0.57
3:D:487:HIS:CE1	3:D:491:HIS:CE1	2.92	0.57
3:C:863:ALA:HA	3:C:866:TYR:CE2	2.39	0.57
3:D:659:SER:HB2	3:D:682:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1001:AGS:H8	4:F:1001:AGS:H5'2	1.85	0.57
3:E:303:LEU:HA	3:E:306:ILE:HG12	1.86	0.57
3:E:895:TRP:HB2	3:E:899:LYS:HA	1.87	0.57
3:F:777:ASP:O	4:F:1001:AGS:O2'	2.23	0.57
3:E:659:SER:HB2	3:E:682:ARG:HH21	1.68	0.57
3:A:657:TYR:O	3:A:687:GLY:N	2.38	0.57
3:C:870:ILE:HG13	3:C:871:ASN:N	2.18	0.57
3:D:892:TYR:HB2	3:D:904:LYS:HB2	1.86	0.57
3:C:292:ILE:O	3:C:296:HIS:ND1	2.31	0.57
3:C:395:GLU:HA	3:C:398:TYR:CZ	2.39	0.57
1:H:3:DT:H2"	1:H:4:DT:C6	2.40	0.57
3:B:946:SER:HB3	3:B:947:PRO:HD2	1.85	0.57
3:F:636:GLY:HA2	3:F:758:SER:HB3	1.87	0.57
3:F:946:SER:HB2	3:F:950:SER:HA	1.86	0.57
1:H:14:DT:H2"	1:H:15:DT:C6	2.40	0.56
3:B:851:THR:N	3:B:906:CYS:O	2.36	0.56
3:D:878:LEU:O	3:D:882:GLN:NE2	2.36	0.56
3:E:470:HIS:HE1	3:E:528:ILE:HD13	1.71	0.56
3:B:395:GLU:HA	3:B:398:TYR:CZ	2.40	0.56
3:A:475:GLU:O	3:A:479:ARG:NH1	2.38	0.56
3:F:433:ASP:OD1	3:F:536:ARG:NH1	2.37	0.56
3:F:675:LYS:HD2	3:F:676:PRO:HD2	1.87	0.56
3:B:634:TRP:HZ3	3:B:758:SER:HB2	1.70	0.56
3:B:852:VAL:HG11	3:B:903:LEU:HB3	1.86	0.56
3:C:348:GLU:O	3:C:352:THR:N	2.37	0.56
3:D:653:LEU:HD23	3:D:658:ALA:HB2	1.87	0.56
3:A:414:GLU:OE2	3:F:520:ASN:HA	2.05	0.56
3:D:290:LEU:HD13	3:D:341:TRP:CG	2.40	0.56
3:F:325:VAL:HG21	3:F:358:LEU:HD21	1.88	0.56
3:B:290:LEU:HA	3:B:293:LEU:HD12	1.87	0.56
3:A:298:PRO:O	3:A:301:ARG:NH1	2.39	0.56
3:A:720:ASN:ND2	3:A:721:GLN:OE1	2.39	0.56
3:D:521:ASP:OD1	3:D:525:LYS:NZ	2.34	0.56
3:D:872:VAL:O	3:E:874:ARG:NH2	2.39	0.56
3:B:878:LEU:HD11	3:A:870:ILE:HG23	1.88	0.56
3:E:425:MET:HE1	3:E:472:TYR:CE1	2.40	0.56
4:E:1001:AGS:H8	4:E:1001:AGS:H5'2	1.88	0.56
3:D:834:THR:OG1	3:D:862:TYR:OH	2.20	0.55
3:E:325:VAL:HG13	3:E:362:TRP:HE3	1.70	0.55
3:E:699:VAL:HA	3:E:741:ILE:HB	1.87	0.55
3:E:912:PHE:HE1	3:F:902:ILE:HD13	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:902:ILE:O	3:F:904:LYS:NZ	2.39	0.55
3:A:305:LYS:HD2	3:A:393:ILE:HG23	1.88	0.55
3:E:365:ALA:HA	3:E:368:HIS:HB3	1.88	0.55
3:B:652:VAL:HG21	3:B:794:PHE:HD2	1.70	0.55
3:B:777:ASP:HB3	3:B:780:PHE:HB2	1.89	0.55
3:B:874:ARG:NH2	3:B:876:ILE:HA	2.21	0.55
3:E:657:TYR:O	3:E:687:GLY:N	2.36	0.55
3:B:635:LEU:HD23	3:B:755:HIS:NE2	2.22	0.55
3:C:402:LEU:HD22	3:C:484:ILE:HG13	1.89	0.55
3:C:448:PRO:HG3	3:C:457:ILE:HD11	1.88	0.55
3:F:493:SER:OG	3:F:494:GLN:NE2	2.40	0.55
3:C:842:ARG:NH2	3:D:853:TYR:OH	2.39	0.55
3:D:680:PHE:HZ	3:D:704:ARG:HG2	1.71	0.55
3:B:809:TYR:CE1	3:B:815:LYS:HB2	2.41	0.55
3:A:616:PHE:O	3:A:619:SER:OG	2.22	0.55
3:A:675:LYS:HE2	3:F:676:PRO:O	2.06	0.55
3:E:336:ARG:HE	3:E:362:TRP:CD1	2.25	0.55
3:A:545:ASP:OD1	3:A:577:HIS:N	2.32	0.55
3:D:378:ILE:HA	3:D:381:TRP:HE3	1.71	0.55
3:D:388:GLN:OE1	3:D:391:LYS:NZ	2.39	0.55
3:B:617:TYR:HD2	3:B:618:LEU:HD22	1.71	0.55
3:F:663:ILE:HA	3:F:691:PHE:CG	2.42	0.55
3:A:563:ILE:HD11	3:A:806:GLN:HB3	1.89	0.55
4:A:1001:AGS:O2B	4:A:1001:AGS:O1A	2.25	0.55
3:C:852:VAL:HG11	3:C:903:LEU:HB3	1.89	0.55
3:B:301:ARG:HH11	3:B:304:HIS:HB2	1.72	0.54
3:D:859:VAL:HG13	3:D:880:LEU:HD12	1.88	0.54
3:F:657:TYR:O	3:F:687:GLY:N	2.32	0.54
3:B:604:ILE:HD13	3:B:645:LEU:HD21	1.90	0.54
3:C:876:ILE:HG22	3:C:878:LEU:H	1.71	0.54
3:D:298:PRO:HA	3:D:301:ARG:NE	2.22	0.54
3:C:600:ALA:HB1	4:C:1001:AGS:N6	2.22	0.54
3:C:828:TYR:OH	3:C:832:GLN:NE2	2.39	0.54
3:D:301:ARG:H	3:D:301:ARG:HD3	1.73	0.54
3:E:388:GLN:HA	3:E:391:LYS:NZ	2.22	0.54
3:E:668:SER:H	3:E:703:SER:HB2	1.71	0.54
3:B:682:ARG:NH2	3:C:723:GLN:O	2.41	0.54
3:B:712:GLY:HA2	3:A:647:ARG:HH12	1.72	0.54
3:F:848:SER:HB3	3:F:918:GLY:HA2	1.88	0.54
3:B:670:ARG:H	3:B:670:ARG:HE	1.55	0.54
3:B:874:ARG:HH22	3:B:876:ILE:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:326:PHE:HE1	3:D:361:LEU:HB3	1.73	0.54
3:E:636:GLY:HA3	3:E:640:ASN:ND2	2.22	0.54
3:E:945:TRP:HZ3	3:E:947:PRO:HA	1.73	0.54
3:C:641:GLY:H	4:C:1001:AGS:PB	2.30	0.54
3:C:804:LYS:HA	3:C:807:LYS:HE2	1.90	0.54
3:E:388:GLN:HA	3:E:391:LYS:HZ2	1.73	0.54
3:F:669:CYS:HB3	3:F:703:SER:HB2	1.89	0.54
3:F:453:ASN:OD1	3:F:454:GLN:N	2.39	0.54
3:C:643:THR:HA	3:C:646:MET:HE2	1.89	0.54
3:E:895:TRP:HB3	3:E:901:ARG:HA	1.90	0.54
3:F:387:PRO:HA	3:F:390:TYR:CE1	2.43	0.54
3:F:715:THR:HA	3:F:725:SER:HA	1.90	0.54
3:D:636:GLY:HA3	3:D:757:ARG:HG3	1.90	0.53
3:D:706:LYS:HD2	3:D:706:LYS:N	2.22	0.53
3:E:309:LEU:HD22	3:E:389:GLN:HG3	1.89	0.53
3:E:665:LEU:HD21	3:E:708:MET:HE2	1.90	0.53
3:F:363:ASN:O	3:F:367:HIS:ND1	2.32	0.53
3:A:783:GLU:HA	3:A:786:MET:HE1	1.90	0.53
3:D:296:HIS:CE1	3:D:297:ASP:CG	2.86	0.53
3:A:804:LYS:HZ1	3:A:945:TRP:CG	2.26	0.53
3:E:613:TRP:CD1	3:E:818:CYS:HB3	2.42	0.53
3:B:673:ALA:H	3:B:675:LYS:HE3	1.72	0.53
3:D:434:VAL:H	3:D:536:ARG:HH12	1.54	0.53
3:F:740:PHE:O	3:F:828:TYR:OH	2.26	0.53
3:B:326:PHE:HB3	3:B:372:LYS:HD2	1.90	0.53
3:A:629:ALA:HB2	3:A:711:PRO:HD3	1.90	0.53
3:A:767:ASP:OD1	3:A:770:ASN:ND2	2.38	0.53
3:D:866:TYR:HE2	3:D:873:LYS:HG2	1.73	0.53
3:C:463:GLU:OE2	3:D:538:ARG:NH2	2.41	0.53
3:D:839:ILE:HG23	3:D:843:VAL:HB	1.91	0.53
3:E:894:GLN:H	3:E:904:LYS:HG2	1.73	0.53
3:F:849:ALA:HB1	3:F:907:ARG:HH21	1.74	0.53
1:H:13:DT:H1'	1:H:14:DT:H5'	1.91	0.53
3:B:810:ASN:O	3:B:812:GLN:NE2	2.41	0.53
4:A:1001:AGS:O1A	4:A:1001:AGS:O2G	2.26	0.53
3:C:637:GLY:H	3:C:640:ASN:HB2	1.74	0.53
3:D:453:ASN:OD1	3:D:454:GLN:N	2.37	0.53
3:D:642:LYS:HG2	4:D:1001:AGS:O1B	2.08	0.53
3:E:299:GLU:O	3:E:303:LEU:HG	2.09	0.53
3:B:406:VAL:HG23	3:B:411:GLY:HA2	1.91	0.53
3:B:634:TRP:CZ3	3:B:642:LYS:HE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:290:LEU:HD11	3:D:304:HIS:HD2	1.73	0.53
3:B:583:CYS:O	3:B:792:ASN:ND2	2.42	0.53
3:C:616:PHE:HA	3:C:805:LEU:HD11	1.91	0.53
3:E:297:ASP:HB3	3:E:299:GLU:HG3	1.90	0.53
3:E:781:ILE:HD12	4:E:1001:AGS:H3'	1.91	0.53
3:B:653:LEU:HD23	3:B:658:ALA:HB2	1.90	0.52
3:C:634:TRP:HB3	3:C:756:TYR:HB3	1.92	0.52
3:F:663:ILE:O	3:F:667:THR:HG23	2.10	0.52
3:D:290:LEU:HA	3:D:293:LEU:CD1	2.39	0.52
3:F:425:MET:HE2	3:F:472:TYR:CE2	2.44	0.52
1:H:22:DT:O4	2:I:3:DA:N6	2.43	0.52
3:B:663:ILE:HA	3:B:691:PHE:CE2	2.43	0.52
3:A:652:VAL:HG21	3:A:794:PHE:HD2	1.74	0.52
3:C:371:LYS:H	3:C:371:LYS:HD2	1.74	0.52
3:C:490:TYR:O	3:C:494:GLN:NE2	2.42	0.52
3:A:376:ARG:HH21	3:A:573:GLU:HG3	1.74	0.52
3:C:701:ASN:HD21	3:C:744:THR:HB	1.75	0.52
3:E:493:SER:OG	3:E:494:GLN:NE2	2.43	0.52
3:B:867:ASN:OD1	3:B:872:VAL:HA	2.08	0.52
3:A:701:ASN:HA	3:A:705:LEU:HD22	1.90	0.52
3:E:683:LEU:HA	3:E:686:ARG:HB2	1.90	0.52
3:A:634:TRP:HZ3	3:A:758:SER:HB2	1.73	0.52
3:C:315:TYR:HA	3:C:321:TRP:HB2	1.91	0.52
3:E:292:ILE:HA	3:E:295:LEU:HB2	1.92	0.52
3:C:663:ILE:HB	3:C:691:PHE:HB3	1.90	0.52
3:D:448:PRO:HG3	3:D:457:ILE:HD11	1.91	0.52
3:D:732:MET:HE3	3:D:732:MET:HA	1.92	0.52
3:A:315:TYR:OH	3:A:343:SER:O	2.27	0.52
3:F:326:PHE:HZ	3:F:361:LEU:HD12	1.75	0.52
3:B:318:TYR:HA	3:B:321:TRP:NE1	2.23	0.52
3:B:876:ILE:HG13	3:A:871:ASN:HB3	1.91	0.52
3:A:555:ASN:ND2	3:A:583:CYS:SG	2.82	0.52
3:C:707:GLU:OE1	3:C:707:GLU:N	2.31	0.52
3:F:378:ILE:HA	3:F:381:TRP:HD1	1.75	0.52
3:F:716:ALA:HB2	3:F:726:PHE:HD1	1.75	0.52
3:B:290:LEU:H	3:B:290:LEU:HD22	1.75	0.51
3:B:290:LEU:HB3	3:B:341:TRP:CE3	2.45	0.51
3:B:666:LEU:HD21	3:B:732:MET:HE2	1.91	0.51
3:E:866:TYR:HH	3:E:875:HIS:CD2	2.25	0.51
3:F:677:ASN:OD1	3:F:680:PHE:N	2.43	0.51
4:A:1001:AGS:O2B	4:A:1001:AGS:O2G	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:LEU:HD12	3:D:734:ALA:HB3	1.92	0.51
3:B:668:SER:HB2	3:B:704:ARG:HB2	1.90	0.51
3:E:387:PRO:HA	3:E:390:TYR:CE1	2.42	0.51
3:E:702:THR:HA	3:E:705:LEU:HB3	1.92	0.51
3:B:398:TYR:CE2	3:B:425:MET:HG3	2.45	0.51
3:A:398:TYR:CD2	3:A:425:MET:HG3	2.45	0.51
3:D:376:ARG:NH2	3:D:428:ASN:O	2.43	0.51
3:D:621:ALA:HB1	3:D:688:TYR:HB2	1.93	0.51
3:E:615:MET:HE3	3:E:615:MET:HA	1.92	0.51
3:B:622:ILE:HD11	3:B:798:LEU:HB3	1.93	0.51
3:B:755:HIS:HB3	3:B:825:THR:HA	1.92	0.51
3:A:865:TRP:NE1	3:A:869:ASN:HD22	2.08	0.51
3:D:318:TYR:HA	3:D:321:TRP:HB3	1.93	0.51
3:D:946:SER:HB3	3:D:947:PRO:HD2	1.92	0.51
3:B:291:SER:HA	3:B:294:MET:HE3	1.93	0.51
3:A:945:TRP:O	3:A:950:SER:OG	2.27	0.51
3:C:657:TYR:O	3:C:687:GLY:N	2.34	0.51
3:D:290:LEU:HD22	3:D:341:TRP:NE1	2.26	0.51
3:D:312:PRO:HA	3:D:345:LYS:HZ2	1.75	0.51
3:D:323:ASN:OD1	3:D:324:VAL:N	2.43	0.51
3:D:410:ASN:N	3:D:410:ASN:OD1	2.40	0.51
3:E:750:TRP:CE3	3:E:829:ARG:HD2	2.46	0.51
3:F:398:TYR:CE1	3:F:425:MET:HA	2.45	0.51
3:B:808:GLU:O	3:B:810:ASN:N	2.43	0.51
3:A:395:GLU:HA	3:A:398:TYR:CZ	2.46	0.51
3:A:691:PHE:HB2	3:A:734:ALA:HA	1.92	0.51
3:F:339:ALA:O	3:F:343:SER:N	2.36	0.51
3:F:852:VAL:HG11	3:F:903:LEU:H	1.75	0.51
3:A:415:HIS:CD2	3:A:415:HIS:H	2.28	0.51
3:C:676:PRO:HD3	3:C:717:ARG:HH12	1.75	0.51
3:C:713:ASP:OD1	3:C:713:ASP:N	2.43	0.51
3:C:748:GLY:HA2	3:C:751:ARG:HG2	1.93	0.51
3:E:315:TYR:C	3:E:321:TRP:HE1	2.15	0.51
3:F:616:PHE:HB3	3:F:805:LEU:HD12	1.93	0.51
3:B:697:SER:HB2	3:C:878:LEU:HD13	1.93	0.50
3:C:609:ASP:OD1	3:C:609:ASP:N	2.41	0.50
3:D:947:PRO:O	3:D:950:SER:OG	2.27	0.50
3:A:619:SER:HA	3:A:798:LEU:HD11	1.93	0.50
3:A:635:LEU:HD23	3:A:755:HIS:NE2	2.26	0.50
3:F:663:ILE:HA	3:F:691:PHE:CD1	2.47	0.50
3:A:632:LEU:HB3	3:A:733:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:386:ALA:HB1	3:C:389:GLN:HE21	1.75	0.50
3:C:780:PHE:HA	3:C:784:TYR:HD2	1.77	0.50
3:E:636:GLY:HA3	3:E:640:ASN:HD22	1.74	0.50
1:H:16:DT:H2'	1:H:17:DT:O4'	2.11	0.50
3:F:637:GLY:O	3:F:737:ASN:ND2	2.44	0.50
3:B:405:TYR:CD2	3:B:417:MET:HB2	2.47	0.50
3:C:425:MET:HG3	3:C:426:MET:HG2	1.94	0.50
3:C:662:ASN:HD22	3:C:665:LEU:HG	1.75	0.50
3:D:634:TRP:HB3	3:D:756:TYR:HB3	1.92	0.50
3:D:854:ASN:HA	3:D:903:LEU:H	1.76	0.50
1:H:9:DT:H2'	1:H:10:DT:C6	2.46	0.50
3:B:708:MET:HE2	3:B:708:MET:HA	1.93	0.50
3:C:343:SER:HB3	3:C:350:TRP:HD1	1.76	0.50
3:C:664:SER:HA	3:C:667:THR:HG23	1.94	0.50
3:D:822:GLU:HA	3:D:825:THR:HB	1.93	0.50
3:E:602:GLN:HB2	3:E:942:TRP:CZ2	2.47	0.50
3:B:414:GLU:HG3	3:B:415:HIS:H	1.77	0.50
3:A:838:PHE:HE1	3:A:842:ARG:HD2	1.76	0.50
3:C:640:ASN:HB3	4:C:1001:AGS:O1B	2.12	0.50
3:D:539:SER:HB2	3:D:542:GLN:HE22	1.77	0.50
3:E:304:HIS:HB2	3:E:341:TRP:CZ3	2.46	0.50
3:F:359:GLU:O	3:F:363:ASN:ND2	2.43	0.50
3:B:290:LEU:HD13	3:B:290:LEU:N	2.26	0.50
3:B:381:TRP:HA	3:B:384:LYS:HG2	1.94	0.50
3:E:305:LYS:O	3:E:309:LEU:HG	2.12	0.50
3:E:640:ASN:ND2	3:E:758:SER:HB3	2.23	0.50
3:B:448:PRO:HG3	3:B:457:ILE:HD11	1.93	0.50
3:C:946:SER:HB3	3:C:947:PRO:HD2	1.94	0.50
3:B:684:LYS:HE3	3:B:726:PHE:CG	2.47	0.49
3:B:946:SER:HB2	3:B:950:SER:HA	1.94	0.49
3:A:628:GLU:OE2	3:A:813:ILE:N	2.45	0.49
3:A:674:GLU:OE1	3:A:676:PRO:HD2	2.11	0.49
3:C:387:PRO:HA	3:C:390:TYR:HE1	1.76	0.49
3:C:750:TRP:HE3	3:C:829:ARG:HH11	1.60	0.49
3:C:766:PRO:HG3	3:C:775:LYS:HB2	1.92	0.49
3:D:764:HIS:HA	3:D:775:LYS:HD2	1.94	0.49
3:E:330:ASN:HB3	3:E:374:THR:HG22	1.92	0.49
3:B:438:GLY:O	3:B:439:LYS:HD3	2.11	0.49
3:C:643:THR:HB	3:C:647:ARG:HH22	1.76	0.49
3:C:755:HIS:HD1	3:C:828:TYR:HB2	1.78	0.49
3:F:813:ILE:O	3:F:816:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:840:THR:HG22	3:F:844:VAL:HG11	1.94	0.49
3:F:895:TRP:CD1	3:F:899:LYS:HD3	2.46	0.49
3:A:662:ASN:HB3	3:A:665:LEU:HD23	1.95	0.49
3:A:751:ARG:O	3:A:754:ARG:NH1	2.44	0.49
3:C:477:PHE:O	3:C:481:MET:HG2	2.12	0.49
3:D:838:PHE:O	3:D:841:GLU:HG3	2.12	0.49
3:B:525:LYS:HD3	3:B:525:LYS:C	2.37	0.49
3:B:635:LEU:HD13	3:B:736:SER:O	2.12	0.49
3:D:312:PRO:O	3:D:316:VAL:HG23	2.12	0.49
3:D:843:VAL:HG12	3:D:844:VAL:HG23	1.92	0.49
3:E:755:HIS:O	3:E:824:GLU:HB3	2.13	0.49
3:E:838:PHE:HB2	3:E:865:TRP:CZ3	2.47	0.49
3:A:609:ASP:N	3:A:609:ASP:OD1	2.43	0.49
3:A:616:PHE:HZ	3:A:804:LYS:HE3	1.76	0.49
3:D:641:GLY:HA2	4:D:1001:AGS:O1A	2.12	0.49
3:D:895:TRP:HB3	3:D:901:ARG:HA	1.94	0.49
3:E:292:ILE:HB	3:E:296:HIS:CE1	2.48	0.49
3:E:707:GLU:OE1	3:E:707:GLU:N	2.38	0.49
3:F:457:ILE:O	3:F:459:LYS:NZ	2.43	0.49
3:F:663:ILE:HG12	3:F:694:THR:HG22	1.94	0.49
3:C:342:PHE:O	3:C:345:LYS:HG2	2.12	0.49
3:D:755:HIS:HB3	3:D:825:THR:HA	1.95	0.49
3:E:656:HIS:O	3:E:686:ARG:NH1	2.45	0.49
3:F:293:LEU:HD11	3:F:337:PRO:HB2	1.94	0.49
3:B:519:PHE:HE2	3:C:409:TYR:CZ	2.31	0.49
3:B:665:LEU:HD21	3:B:679:ALA:HB1	1.94	0.49
3:A:755:HIS:HB3	3:A:825:THR:HA	1.94	0.49
3:D:398:TYR:CE2	3:D:425:MET:HG3	2.48	0.49
3:D:609:ASP:OD1	3:D:610:ALA:N	2.44	0.49
3:F:938:PRO:HG3	3:F:942:TRP:HB3	1.94	0.49
3:B:634:TRP:CH2	3:B:642:LYS:HG2	2.48	0.49
3:D:666:LEU:HD12	3:D:705:LEU:HB2	1.95	0.49
3:D:702:THR:HA	3:D:705:LEU:HD23	1.94	0.49
3:E:623:PHE:HB3	3:E:627:LYS:HE2	1.94	0.49
4:E:1001:AGS:O3A	4:E:1001:AGS:O2G	2.30	0.49
3:A:852:VAL:HG22	3:A:908:ILE:HD11	1.95	0.49
3:C:623:PHE:HB3	3:C:627:LYS:HE2	1.94	0.49
3:D:344:GLN:HB2	3:D:347:PRO:HG3	1.95	0.49
3:B:604:ILE:HD11	4:B:1001:AGS:HN61	1.77	0.48
3:D:911:LYS:HD2	3:D:912:PHE:N	2.28	0.48
3:E:470:HIS:CE1	3:E:528:ILE:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:638:GLY:O	4:E:1001:AGS:O2G	2.30	0.48
3:E:947:PRO:O	3:E:950:SER:OG	2.23	0.48
3:F:681:MET:HE1	3:F:716:ALA:HB1	1.95	0.48
3:B:332:SER:OG	3:B:334:ASN:OD1	2.31	0.48
3:B:667:THR:HA	3:B:700:LEU:HG	1.95	0.48
3:B:764:HIS:O	3:B:775:LYS:NZ	2.46	0.48
3:B:871:ASN:HB2	3:B:873:LYS:NZ	2.29	0.48
3:B:874:ARG:HE	3:B:875:HIS:N	2.11	0.48
3:F:669:CYS:H	3:F:703:SER:HB2	1.78	0.48
3:D:350:TRP:HZ3	3:D:355:LYS:HD3	1.78	0.48
3:D:544:LEU:HD21	3:D:577:HIS:HB3	1.94	0.48
3:E:635:LEU:HD21	3:E:739:ASN:HA	1.95	0.48
3:F:642:LYS:O	3:F:646:MET:HG2	2.13	0.48
3:B:292:ILE:HG23	3:B:296:HIS:CE1	2.49	0.48
3:B:336:ARG:HD2	3:B:362:TRP:CD1	2.48	0.48
3:A:946:SER:HB3	3:A:947:PRO:HD2	1.96	0.48
3:D:703:SER:O	3:D:704:ARG:HB2	2.12	0.48
3:E:322:SER:O	3:E:326:PHE:HD1	1.97	0.48
3:E:371:LYS:HE2	3:E:574:HIS:HA	1.96	0.48
3:E:865:TRP:CE3	3:E:866:TYR:HB3	2.49	0.48
3:E:867:ASN:HB3	3:E:872:VAL:HG12	1.96	0.48
3:F:295:LEU:N	3:F:301:ARG:HH21	2.12	0.48
3:F:383:HIS:HA	3:F:390:TYR:CZ	2.48	0.48
3:F:452:MET:HE1	3:F:457:ILE:HB	1.95	0.48
3:B:609:ASP:OD1	3:B:609:ASP:N	2.44	0.48
3:B:841:GLU:CD	3:B:865:TRP:HE1	2.22	0.48
3:A:847:PRO:HD2	3:A:918:GLY:HA3	1.95	0.48
3:C:395:GLU:OE2	3:C:483:ARG:NH1	2.38	0.48
3:D:629:ALA:HB2	3:D:711:PRO:HD3	1.96	0.48
3:B:670:ARG:H	3:B:670:ARG:NE	2.12	0.48
3:C:762:PHE:HB3	3:C:776:GLU:HG3	1.96	0.48
3:E:383:HIS:HA	3:E:390:TYR:CE1	2.48	0.48
3:E:401:ILE:O	3:E:404:GLU:HG2	2.13	0.48
3:B:808:GLU:HG3	3:B:809:TYR:CD2	2.48	0.48
3:E:395:GLU:HA	3:E:398:TYR:CE1	2.49	0.48
3:F:293:LEU:O	3:F:294:MET:HE2	2.13	0.48
3:B:290:LEU:HA	3:B:293:LEU:CD1	2.44	0.48
3:A:895:TRP:HB2	3:A:899:LYS:HA	1.96	0.48
3:F:867:ASN:HA	3:F:871:ASN:O	2.12	0.48
3:D:321:TRP:CZ2	3:D:358:LEU:HD22	2.49	0.48
3:D:744:THR:OG1	3:D:746:ASP:OD1	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:315:TYR:CE1	3:E:343:SER:HA	2.49	0.48
3:F:296:HIS:O	3:F:301:ARG:NH1	2.47	0.48
1:H:4:DT:H4'	1:H:5:DT:H5'	1.96	0.47
3:D:913:GLU:HB3	3:D:916:GLN:OE1	2.12	0.47
3:E:944:GLU:HG3	3:E:945:TRP:N	2.29	0.47
3:F:663:ILE:HA	3:F:691:PHE:CD2	2.49	0.47
3:B:866:TYR:CE1	3:B:873:LYS:HG2	2.49	0.47
3:C:660:LYS:NZ	3:D:715:THR:H	2.12	0.47
3:D:320:LEU:O	3:D:324:VAL:HG22	2.13	0.47
3:F:849:ALA:O	3:F:905:GLY:HA2	2.14	0.47
3:B:755:HIS:HD1	3:B:828:TYR:HB2	1.78	0.47
3:A:371:LYS:HE3	3:A:574:HIS:CD2	2.48	0.47
3:A:850:GLU:HA	3:A:905:GLY:HA3	1.95	0.47
3:D:359:GLU:OE1	3:D:360:LYS:NZ	2.40	0.47
3:E:466:PRO:HB2	3:E:469:LEU:HB3	1.95	0.47
3:E:914:THR:H	3:E:916:GLN:HE22	1.62	0.47
3:B:307:LEU:HA	3:B:310:LEU:HD23	1.96	0.47
3:A:538:ARG:HH12	3:F:461:ARG:HH22	1.62	0.47
3:A:746:ASP:OD2	3:A:749:THR:OG1	2.28	0.47
3:C:298:PRO:O	3:C:301:ARG:HG2	2.14	0.47
3:D:321:TRP:CH2	3:D:358:LEU:HB2	2.49	0.47
3:F:299:GLU:HA	3:F:302:TYR:CE2	2.48	0.47
3:B:395:GLU:OE1	3:B:398:TYR:OH	2.20	0.47
3:B:780:PHE:HA	3:B:784:TYR:HD2	1.79	0.47
3:C:783:GLU:HA	3:C:786:MET:HE1	1.95	0.47
3:F:821:ILE:C	3:F:823:SER:H	2.22	0.47
3:B:835:LEU:O	3:B:839:ILE:HG12	2.15	0.47
3:A:406:VAL:HG13	3:A:411:GLY:HA2	1.97	0.47
3:C:444:GLU:OE1	3:C:461:ARG:NH2	2.41	0.47
3:B:293:LEU:HB2	3:B:301:ARG:NH2	2.29	0.47
3:B:427:GLY:HA2	3:B:535:PHE:CE2	2.50	0.47
3:B:712:GLY:HA2	3:A:647:ARG:NH1	2.29	0.47
3:B:911:LYS:HG3	3:B:912:PHE:N	2.22	0.47
3:A:309:LEU:HB3	3:A:389:GLN:NE2	2.29	0.47
3:A:938:PRO:HG3	3:A:942:TRP:HB3	1.97	0.47
3:C:378:ILE:HA	3:C:381:TRP:HE3	1.79	0.47
3:D:711:PRO:O	3:D:712:GLY:C	2.57	0.47
3:E:292:ILE:HD11	3:E:337:PRO:HG2	1.95	0.47
3:E:321:TRP:O	3:E:325:VAL:HG23	2.14	0.47
3:E:684:LYS:NZ	3:E:725:SER:O	2.39	0.47
3:F:435:ASP:OD1	3:F:439:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:321:TRP:HA	3:B:324:VAL:HG12	1.96	0.47
3:C:821:ILE:C	3:C:823:SER:H	2.23	0.47
3:E:318:TYR:O	3:E:321:TRP:HB2	2.15	0.47
3:A:681:MET:HE3	3:A:718:GLU:HB2	1.95	0.47
3:A:715:THR:HA	3:A:725:SER:HA	1.97	0.47
3:A:883:GLU:HA	3:A:886:ASN:HB2	1.96	0.47
3:C:298:PRO:HA	3:C:301:ARG:HG2	1.97	0.47
3:C:779:ARG:NH1	3:C:784:TYR:OH	2.48	0.47
3:D:661:LEU:HB2	3:D:691:PHE:HE1	1.79	0.47
3:D:671:GLU:HB3	3:D:675:LYS:HE3	1.97	0.47
3:D:821:ILE:C	3:D:823:SER:H	2.23	0.47
3:E:336:ARG:O	3:E:340:GLU:HG2	2.15	0.47
3:E:706:LYS:HA	3:E:709:VAL:HB	1.97	0.47
3:B:771:PRO:O	3:B:774:LYS:NZ	2.38	0.47
3:B:884:LEU:O	3:B:887:SER:OG	2.27	0.47
3:F:466:PRO:HB2	3:F:469:LEU:HB3	1.95	0.47
3:F:670:ARG:HH22	3:F:671:GLU:HG2	1.80	0.47
3:B:639:CYS:HA	4:B:1001:AGS:O3A	2.15	0.46
3:B:873:LYS:HB3	3:B:873:LYS:HE3	1.30	0.46
3:A:835:LEU:O	3:A:839:ILE:HG12	2.15	0.46
3:C:379:MET:HE1	3:C:390:TYR:CD2	2.50	0.46
3:D:416:TYR:HE2	3:D:420:LYS:HZ3	1.59	0.46
3:D:676:PRO:HB2	3:D:720:ASN:H	1.80	0.46
3:E:821:ILE:HD12	3:E:822:GLU:H	1.79	0.46
3:B:539:SER:HA	3:B:542:GLN:HE22	1.80	0.46
3:B:631:MET:HB3	3:B:753:LEU:HD23	1.97	0.46
3:A:392:GLU:HA	3:A:395:GLU:HB3	1.97	0.46
3:D:290:LEU:HD22	3:D:341:TRP:CD1	2.51	0.46
3:E:461:ARG:NH2	3:F:538:ARG:HH12	2.14	0.46
3:F:619:SER:HA	3:F:798:LEU:HD12	1.95	0.46
3:C:631:MET:O	3:C:754:ARG:N	2.44	0.46
3:C:641:GLY:HA2	4:C:1001:AGS:O1A	2.15	0.46
3:C:742:ILE:H	3:C:832:GLN:CD	2.24	0.46
3:D:502:ASN:OD1	3:D:503:TYR:N	2.48	0.46
3:E:671:GLU:HB2	3:E:675:LYS:HB2	1.97	0.46
3:E:884:LEU:O	3:E:887:SER:OG	2.32	0.46
3:A:563:ILE:HD13	3:A:807:LYS:HG2	1.98	0.46
3:E:631:MET:HB3	3:E:753:LEU:HD23	1.97	0.46
3:A:414:GLU:CD	3:A:415:HIS:N	2.74	0.46
3:A:693:GLU:CD	3:A:737:ASN:H	2.24	0.46
3:A:777:ASP:H	4:A:1001:AGS:H1'	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:293:LEU:HA	3:C:296:HIS:HE1	1.80	0.46
3:C:681:MET:HG2	3:C:718:GLU:HG3	1.98	0.46
3:C:839:ILE:HA	3:C:843:VAL:HG22	1.97	0.46
3:C:854:ASN:OD1	3:C:855:LEU:N	2.48	0.46
3:D:370:GLU:CD	3:D:372:LYS:H	2.23	0.46
3:E:354:GLY:HA2	3:E:357:LYS:HG2	1.98	0.46
3:F:631:MET:HB3	3:F:753:LEU:HD23	1.96	0.46
3:F:633:LEU:HD21	3:F:740:PHE:HD2	1.81	0.46
3:B:303:LEU:HA	3:B:306:ILE:HG12	1.97	0.46
3:C:532:GLU:N	3:C:532:GLU:OE1	2.49	0.46
3:F:377:SER:OG	3:F:573:GLU:OE2	2.31	0.46
3:F:380:TYR:HD1	3:F:384:LYS:HZ2	1.62	0.46
3:B:294:MET:HE2	3:B:294:MET:HB2	1.71	0.46
3:C:380:TYR:CE2	3:C:571:PHE:HB3	2.51	0.46
3:D:327:ALA:HB2	3:D:373:ILE:HD11	1.98	0.46
3:D:660:LYS:NZ	3:D:692:GLU:OE2	2.33	0.46
3:E:829:ARG:HH11	3:E:829:ARG:HA	1.81	0.46
3:F:777:ASP:H	4:F:1001:AGS:H1'	1.81	0.46
3:B:388:GLN:O	3:B:391:LYS:HG2	2.15	0.46
3:A:635:LEU:HD13	3:A:736:SER:O	2.16	0.46
3:C:704:ARG:HB3	3:C:708:MET:HE1	1.98	0.46
3:D:433:ASP:HB3	3:D:541:ILE:HG13	1.98	0.46
3:E:354:GLY:O	3:E:358:LEU:HB3	2.16	0.46
3:A:894:GLN:HG3	3:A:895:TRP:H	1.81	0.46
3:D:676:PRO:HA	3:D:717:ARG:HB3	1.96	0.46
3:F:946:SER:HB3	3:F:947:PRO:HD2	1.97	0.46
3:B:601:LEU:HD22	3:B:942:TRP:HH2	1.80	0.46
3:B:640:ASN:HB3	3:B:642:LYS:HG3	1.97	0.46
3:B:695:ASN:OD1	3:B:696:LYS:N	2.48	0.46
3:D:303:LEU:HA	3:D:306:ILE:HG12	1.98	0.46
3:D:693:GLU:HG2	4:D:1001:AGS:S1G	2.56	0.46
3:E:693:GLU:OE1	3:E:737:ASN:N	2.45	0.46
3:F:344:GLN:HA	3:F:347:PRO:HB3	1.97	0.46
3:F:398:TYR:CZ	3:F:425:MET:HA	2.50	0.46
3:F:468:GLU:HA	3:F:471:ILE:HG12	1.96	0.46
3:B:301:ARG:HA	3:B:301:ARG:HD3	1.30	0.45
3:B:301:ARG:NH1	3:B:304:HIS:HB2	2.31	0.45
3:A:616:PHE:CZ	3:A:804:LYS:HE3	2.50	0.45
3:D:812:GLN:HB2	3:D:815:LYS:HE2	1.97	0.45
3:D:883:GLU:O	3:D:887:SER:N	2.49	0.45
3:B:691:PHE:CE1	3:B:732:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:LEU:HD11	3:A:338:LEU:HD22	1.99	0.45
3:A:847:PRO:HA	3:A:906:CYS:HB2	1.97	0.45
3:D:294:MET:HE2	3:D:301:ARG:HA	1.98	0.45
3:E:678:SER:O	3:E:681:MET:HG3	2.16	0.45
3:A:876:ILE:HG23	3:A:878:LEU:HG	1.99	0.45
3:C:945:TRP:O	3:C:950:SER:OG	2.31	0.45
3:F:675:LYS:O	3:F:676:PRO:C	2.58	0.45
3:B:425:MET:HE2	3:B:425:MET:HB3	1.87	0.45
3:B:661:LEU:HB2	3:B:691:PHE:HE1	1.82	0.45
3:C:783:GLU:O	3:C:784:TYR:HB2	2.16	0.45
3:D:330:ASN:HB3	3:D:374:THR:HG22	1.98	0.45
3:E:753:LEU:O	3:E:754:ARG:NH1	2.37	0.45
1:H:5:DT:OP1	3:C:717:ARG:NH2	2.49	0.45
3:B:663:ILE:HG22	3:B:692:GLU:H	1.82	0.45
3:A:470:HIS:HE1	3:A:525:LYS:NZ	2.14	0.45
3:C:405:TYR:OH	3:C:420:LYS:HD2	2.17	0.45
3:C:682:ARG:O	3:C:683:LEU:HB2	2.17	0.45
3:E:634:TRP:CH2	3:E:642:LYS:HB3	2.52	0.45
3:F:675:LYS:HE3	3:F:675:LYS:HB3	1.40	0.45
3:F:755:HIS:H	3:F:825:THR:HG1	1.64	0.45
3:B:607:GLU:HB2	3:B:610:ALA:HB3	1.99	0.45
3:B:702:THR:O	3:B:706:LYS:HG2	2.17	0.45
3:A:838:PHE:HB2	3:A:865:TRP:CZ3	2.52	0.45
3:C:293:LEU:HA	3:C:296:HIS:CE1	2.52	0.45
3:C:587:PHE:HA	3:C:796:SER:HB3	1.97	0.45
3:D:332:SER:OG	3:D:334:ASN:OD1	2.23	0.45
3:D:848:SER:HB3	3:D:906:CYS:HA	1.98	0.45
3:D:945:TRP:O	3:D:950:SER:OG	2.34	0.45
3:E:849:ALA:O	3:E:906:CYS:N	2.49	0.45
3:E:610:ALA:HB2	3:E:820:THR:CG2	2.47	0.45
3:E:671:GLU:C	3:E:672:THR:HG1	2.24	0.45
3:F:587:PHE:HA	3:F:796:SER:HB3	1.98	0.45
3:F:693:GLU:CD	3:F:737:ASN:H	2.24	0.45
3:B:849:ALA:HB3	3:B:907:ARG:HB2	1.98	0.45
3:A:713:ASP:OD1	3:A:725:SER:OG	2.34	0.45
3:A:821:ILE:C	3:A:823:SER:H	2.24	0.45
4:A:1001:AGS:H8	4:A:1001:AGS:H5'2	1.98	0.45
3:C:642:LYS:HG2	4:C:1001:AGS:O1B	2.17	0.45
3:D:557:VAL:HG13	3:D:568:ILE:HB	1.99	0.45
3:E:587:PHE:HA	3:E:796:SER:HB3	1.98	0.45
3:B:633:LEU:HD13	3:B:740:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:633:LEU:O	3:D:755:HIS:HA	2.17	0.45
3:D:780:PHE:HA	3:D:784:TYR:CD2	2.52	0.45
3:F:666:LEU:HD22	3:F:666:LEU:HA	1.79	0.45
3:B:876:ILE:O	3:B:878:LEU:N	2.49	0.45
3:A:882:GLN:N	3:A:882:GLN:OE1	2.50	0.45
3:C:321:TRP:O	3:C:325:VAL:HG23	2.17	0.45
3:C:780:PHE:HA	3:C:784:TYR:CD2	2.52	0.45
3:C:850:GLU:HG2	3:C:905:GLY:HA2	1.99	0.45
3:D:842:ARG:HG3	3:D:843:VAL:HG23	1.99	0.45
3:E:374:THR:OG1	3:E:573:GLU:OE1	2.32	0.45
3:E:742:ILE:O	3:E:832:GLN:HG3	2.17	0.45
3:B:438:GLY:C	3:B:439:LYS:HD3	2.41	0.44
3:B:945:TRP:CH2	3:B:948:ASN:HA	2.51	0.44
3:C:809:TYR:CZ	3:C:816:VAL:HG23	2.52	0.44
3:D:682:ARG:HH21	3:E:722:LYS:NZ	2.15	0.44
3:E:307:LEU:HD13	3:E:342:PHE:HD1	1.82	0.44
3:F:866:TYR:HA	3:F:869:ASN:HB3	1.98	0.44
3:B:293:LEU:HD13	3:B:338:LEU:HB2	1.98	0.44
3:A:693:GLU:OE1	3:A:737:ASN:N	2.50	0.44
3:D:311:PRO:HG2	3:D:314:TYR:CZ	2.53	0.44
3:D:681:MET:HG3	3:D:718:GLU:HA	1.98	0.44
3:E:301:ARG:HA	3:E:304:HIS:ND1	2.32	0.44
3:E:511:PHE:O	3:E:515:LYS:HG3	2.18	0.44
3:B:519:PHE:CD2	3:C:417:MET:HE3	2.51	0.44
3:A:859:VAL:HA	3:A:880:LEU:HD12	2.00	0.44
3:E:702:THR:HB	3:E:706:LYS:HZ2	1.83	0.44
3:B:327:ALA:HB1	3:B:378:ILE:HD11	2.00	0.44
3:B:435:ASP:OD1	3:B:435:ASP:N	2.50	0.44
3:B:780:PHE:HA	3:B:784:TYR:CD2	2.52	0.44
3:A:635:LEU:O	3:A:758:SER:N	2.35	0.44
3:A:655:ASP:OD1	3:A:656:HIS:N	2.51	0.44
3:C:662:ASN:ND2	3:C:665:LEU:HG	2.32	0.44
3:D:412:MET:HE2	3:D:412:MET:HB3	1.74	0.44
3:D:680:PHE:CZ	3:D:704:ARG:HG2	2.51	0.44
3:F:644:PHE:HD2	3:F:645:LEU:HD22	1.83	0.44
3:F:694:THR:HG21	3:F:740:PHE:CE1	2.53	0.44
3:F:713:ASP:OD2	3:F:725:SER:OG	2.35	0.44
3:F:863:ALA:HA	3:F:866:TYR:CE1	2.53	0.44
3:B:681:MET:HE3	3:B:718:GLU:OE1	2.17	0.44
3:B:847:PRO:HD2	3:B:918:GLY:HA2	1.98	0.44
3:A:309:LEU:HD13	3:A:389:GLN:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:660:LYS:HZ1	3:D:715:THR:H	1.65	0.44
3:C:709:VAL:HG11	3:C:752:ARG:HB3	1.99	0.44
3:D:347:PRO:HB2	3:D:350:TRP:NE1	2.33	0.44
3:D:425:MET:HE2	3:D:425:MET:HB3	1.70	0.44
3:D:509:LYS:O	3:D:512:GLU:HG3	2.17	0.44
3:E:383:HIS:HA	3:E:390:TYR:CZ	2.52	0.44
3:F:663:ILE:HD12	3:F:691:PHE:CD2	2.53	0.44
3:F:838:PHE:HB2	3:F:865:TRP:CZ3	2.53	0.44
3:F:840:THR:HA	3:F:844:VAL:HB	1.99	0.44
3:B:375:LYS:O	3:B:376:ARG:HG2	2.17	0.44
3:A:623:PHE:HB3	3:A:627:LYS:HE2	1.98	0.44
3:D:320:LEU:HA	3:D:323:ASN:ND2	2.32	0.44
3:E:653:LEU:HD23	3:E:658:ALA:HB2	2.00	0.44
3:F:601:LEU:HD22	3:F:942:TRP:HH2	1.82	0.44
3:F:609:ASP:OD1	3:F:610:ALA:N	2.49	0.44
3:F:629:ALA:HB2	3:F:711:PRO:HD3	2.00	0.44
1:H:17:DT:H2'	1:H:18:DT:O4'	2.18	0.44
3:A:398:TYR:CE2	3:A:425:MET:HG3	2.53	0.44
3:C:653:LEU:HG	3:C:657:TYR:HB2	2.00	0.44
3:D:616:PHE:CD1	3:D:805:LEU:HD12	2.53	0.44
3:E:381:TRP:HD1	3:E:384:LYS:HE2	1.81	0.44
3:E:465:ASN:O	3:E:467:ASP:N	2.50	0.44
3:E:837:ARG:O	3:E:841:GLU:CB	2.66	0.44
3:F:694:THR:HG21	3:F:740:PHE:CZ	2.53	0.44
3:B:445:PHE:HB2	3:B:460:TRP:CZ3	2.52	0.44
3:B:866:TYR:O	3:B:871:ASN:N	2.51	0.44
3:A:475:GLU:CD	3:A:479:ARG:HH12	2.26	0.44
3:A:740:PHE:O	3:A:828:TYR:OH	2.35	0.44
3:C:426:MET:HE3	3:C:426:MET:HB3	1.84	0.44
3:C:691:PHE:HD2	3:C:734:ALA:HB2	1.83	0.44
3:C:851:THR:N	3:C:906:CYS:O	2.48	0.44
3:E:518:ILE:O	3:E:524:LYS:NZ	2.41	0.44
3:E:779:ARG:HB2	3:E:783:GLU:HG3	2.00	0.44
3:F:671:GLU:HG3	3:F:675:LYS:CE	2.46	0.44
3:B:330:ASN:HD22	3:B:374:THR:HG22	1.83	0.44
3:B:659:SER:HB3	3:B:686:ARG:NH1	2.33	0.44
3:D:909:LEU:HB2	3:D:913:GLU:HB2	1.99	0.44
3:F:326:PHE:CZ	3:F:361:LEU:HD12	2.53	0.44
3:F:375:LYS:HG3	3:F:376:ARG:H	1.83	0.44
3:F:665:LEU:HD12	3:F:665:LEU:HA	1.81	0.44
3:B:294:MET:HE2	3:B:301:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:301:ARG:HA	3:B:301:ARG:NH1	2.31	0.43
3:B:653:LEU:HG	3:B:657:TYR:HB2	2.00	0.43
3:B:809:TYR:CE2	3:B:816:VAL:HG23	2.52	0.43
3:A:485:THR:HG22	3:A:489:LYS:NZ	2.33	0.43
3:A:742:ILE:H	3:A:832:GLN:CD	2.26	0.43
3:C:660:LYS:HB3	3:C:660:LYS:HE2	1.33	0.43
3:C:704:ARG:HA	3:C:707:GLU:CD	2.43	0.43
3:B:661:LEU:HB2	3:B:691:PHE:CE1	2.53	0.43
3:A:290:LEU:HD13	3:A:341:TRP:CD2	2.53	0.43
3:A:794:PHE:HA	3:A:797:ILE:HD12	1.99	0.43
3:C:470:HIS:O	3:C:473:ILE:HG22	2.18	0.43
3:D:314:TYR:CD1	3:D:320:LEU:HD13	2.53	0.43
3:E:830:LYS:HA	3:E:830:LYS:HD3	1.68	0.43
3:E:867:ASN:HA	3:E:871:ASN:O	2.19	0.43
3:F:670:ARG:HB3	3:F:671:GLU:H	1.52	0.43
1:H:4:DT:H1'	1:H:5:DT:C6	2.53	0.43
3:B:301:ARG:CZ	3:B:341:TRP:HZ3	2.32	0.43
3:B:304:HIS:HA	3:B:307:LEU:CD2	2.48	0.43
3:B:604:ILE:CD1	4:B:1001:AGS:HN61	2.31	0.43
3:A:414:GLU:OE1	3:F:519:PHE:HB3	2.18	0.43
3:D:813:ILE:O	3:D:816:VAL:HG12	2.17	0.43
3:E:317:GLU:HB2	3:E:320:LEU:HD12	2.00	0.43
3:E:406:VAL:HG13	3:E:411:GLY:HA2	2.00	0.43
3:E:651:MET:HE2	3:E:651:MET:HA	1.99	0.43
3:F:372:LYS:O	3:F:374:THR:HG23	2.18	0.43
3:B:847:PRO:HB2	3:B:892:TYR:CE1	2.53	0.43
3:A:356:GLU:HG2	3:A:359:GLU:HB3	2.00	0.43
3:C:705:LEU:O	3:C:709:VAL:HG23	2.18	0.43
3:D:470:HIS:O	3:D:473:ILE:HG22	2.19	0.43
3:D:520:ASN:OD1	3:D:522:SER:N	2.51	0.43
3:F:616:PHE:HD1	3:F:805:LEU:HB2	1.82	0.43
3:F:674:GLU:O	3:F:717:ARG:NH1	2.52	0.43
3:A:414:GLU:CD	3:A:415:HIS:H	2.27	0.43
3:D:380:TYR:CZ	3:D:384:LYS:HD3	2.53	0.43
3:E:336:ARG:HB3	3:E:337:PRO:HD3	1.99	0.43
3:B:413:LEU:HA	3:B:417:MET:SD	2.59	0.43
3:B:833:ASP:OD1	3:B:833:ASP:N	2.51	0.43
3:B:874:ARG:NH2	3:B:876:ILE:N	2.67	0.43
3:A:476:ASN:HA	3:A:479:ARG:NH2	2.33	0.43
3:D:302:TYR:CZ	3:D:306:ILE:HD13	2.54	0.43
3:D:387:PRO:HA	3:D:390:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:447:LEU:HD23	3:D:447:LEU:HA	1.85	0.43
3:B:336:ARG:HD2	3:B:362:TRP:HD1	1.83	0.43
3:E:372:LYS:O	3:E:374:THR:HG23	2.19	0.43
3:E:609:ASP:OD1	3:E:609:ASP:N	2.51	0.43
3:F:414:GLU:HG3	3:F:415:HIS:H	1.84	0.43
3:F:667:THR:CA	3:F:700:LEU:HB3	2.34	0.43
3:F:699:VAL:CB	3:F:741:ILE:HB	2.44	0.43
3:F:876:ILE:O	3:F:879:GLU:HG2	2.18	0.43
3:B:633:LEU:HD13	3:B:740:PHE:HD2	1.83	0.43
3:C:651:MET:HE2	3:C:651:MET:HA	1.99	0.43
3:C:676:PRO:HB3	3:C:717:ARG:HB3	2.01	0.43
3:C:681:MET:HG2	3:C:718:GLU:CD	2.43	0.43
3:D:746:ASP:OD1	3:D:746:ASP:N	2.49	0.43
3:D:818:CYS:HB3	3:D:821:ILE:HG22	2.01	0.43
3:E:601:LEU:HD11	3:E:615:MET:SD	2.59	0.43
3:F:847:PRO:HD2	3:F:918:GLY:HA3	2.01	0.43
3:B:301:ARG:NH2	3:B:341:TRP:HZ3	2.17	0.43
3:A:454:GLN:OE1	3:A:455:GLY:N	2.51	0.43
3:A:865:TRP:CE3	3:A:866:TYR:HB3	2.53	0.43
3:D:855:LEU:O	3:D:859:VAL:HG23	2.19	0.43
3:E:378:ILE:HD12	3:E:378:ILE:H	1.84	0.43
3:F:663:ILE:HG22	3:F:692:GLU:HG2	1.99	0.43
3:F:681:MET:HE3	3:F:717:ARG:O	2.18	0.43
3:B:668:SER:HB3	3:B:705:LEU:CD2	2.48	0.43
3:B:785:ILE:O	3:B:791:GLN:NE2	2.28	0.43
3:B:821:ILE:C	3:B:823:SER:H	2.26	0.43
3:A:715:THR:HB	3:A:725:SER:HB2	2.01	0.43
3:D:303:LEU:CD2	3:D:306:ILE:HD11	2.45	0.43
3:D:703:SER:C	3:D:705:LEU:H	2.27	0.43
3:E:634:TRP:HB3	3:E:756:TYR:HB3	2.00	0.43
3:B:803:GLU:HB3	3:B:807:LYS:NZ	2.34	0.42
3:B:874:ARG:NH2	3:B:876:ILE:CA	2.82	0.42
3:A:502:ASN:OD1	3:A:503:TYR:N	2.51	0.42
3:A:870:ILE:HG22	3:A:871:ASN:ND2	2.34	0.42
3:C:430:PHE:CE2	3:C:469:LEU:HD13	2.54	0.42
3:D:867:ASN:HA	3:D:871:ASN:O	2.19	0.42
3:E:702:THR:HB	3:E:706:LYS:NZ	2.34	0.42
3:F:528:ILE:HD13	3:F:528:ILE:HA	1.87	0.42
3:F:602:GLN:O	3:F:611:ARG:NH1	2.51	0.42
3:F:633:LEU:HD21	3:F:740:PHE:CD2	2.54	0.42
3:C:486:GLU:HA	3:C:489:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:945:TRP:CH2	3:C:948:ASN:HA	2.55	0.42
3:D:314:TYR:CD1	3:D:314:TYR:N	2.87	0.42
3:E:528:ILE:O	3:E:532:GLU:HG2	2.18	0.42
3:F:634:TRP:CH2	3:F:642:LYS:HG2	2.53	0.42
3:B:842:ARG:NH1	3:B:864:GLU:OE2	2.53	0.42
3:A:695:ASN:OD1	3:A:696:LYS:N	2.52	0.42
3:C:779:ARG:HB2	3:C:783:GLU:HG3	2.00	0.42
3:D:699:VAL:HG23	3:D:741:ILE:HB	2.02	0.42
3:D:706:LYS:NZ	3:D:749:THR:HA	2.34	0.42
3:F:294:MET:HA	3:F:301:ARG:HE	1.85	0.42
3:F:315:TYR:CE1	3:F:343:SER:HA	2.54	0.42
3:B:413:LEU:HG	3:B:514:SER:HB3	2.01	0.42
3:A:414:GLU:N	3:A:417:MET:SD	2.92	0.42
3:A:851:THR:HG21	3:A:907:ARG:HH12	1.83	0.42
3:D:292:ILE:O	3:D:295:LEU:HG	2.18	0.42
3:D:293:LEU:H	3:D:293:LEU:HG	1.53	0.42
3:D:360:LYS:HA	3:D:360:LYS:HD3	1.85	0.42
3:E:523:PHE:O	3:E:527:VAL:HG23	2.19	0.42
3:B:314:TYR:O	3:B:320:LEU:HD22	2.19	0.42
3:B:700:LEU:HD13	3:B:740:PHE:HB3	2.02	0.42
3:A:682:ARG:HA	3:A:682:ARG:HD3	1.89	0.42
3:E:760:VAL:C	3:E:761:LYS:HD3	2.44	0.42
3:F:405:TYR:CD1	3:F:417:MET:HG2	2.55	0.42
3:F:601:LEU:HD11	3:F:615:MET:HE3	2.01	0.42
3:F:616:PHE:CD1	3:F:805:LEU:HB2	2.54	0.42
3:F:783:GLU:O	3:F:784:TYR:HB2	2.20	0.42
3:B:662:ASN:HB3	3:B:665:LEU:HD13	2.01	0.42
3:A:633:LEU:O	3:A:755:HIS:HA	2.19	0.42
3:C:309:LEU:HD22	3:C:389:GLN:HG3	2.02	0.42
3:C:364:ASP:HA	3:C:367:HIS:NE2	2.34	0.42
3:C:761:LYS:HE2	3:C:761:LYS:HB2	1.91	0.42
3:E:821:ILE:HD13	3:E:821:ILE:HA	1.81	0.42
3:F:760:VAL:HG13	3:F:773:GLU:HA	2.01	0.42
3:F:873:LYS:HA	3:F:873:LYS:HD2	1.84	0.42
3:B:470:HIS:O	3:B:473:ILE:HG22	2.19	0.42
3:B:818:CYS:HB3	3:B:821:ILE:HG22	2.01	0.42
3:A:945:TRP:CH2	3:A:948:ASN:HA	2.54	0.42
3:C:854:ASN:N	3:C:902:ILE:HG13	2.26	0.42
3:D:631:MET:HB3	3:D:753:LEU:HD13	2.02	0.42
3:E:783:GLU:O	3:E:784:TYR:HB2	2.20	0.42
3:F:478:SER:OG	3:F:479:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:880:LEU:HD13	3:F:883:GLU:HB3	2.01	0.42
3:A:701:ASN:ND2	3:A:743:ASP:O	2.50	0.42
3:A:783:GLU:O	3:A:784:TYR:HB2	2.20	0.42
3:D:701:ASN:OD1	3:D:744:THR:HB	2.20	0.42
3:E:519:PHE:HD1	3:F:416:TYR:HB3	1.84	0.42
3:E:671:GLU:HG2	3:E:672:THR:N	2.35	0.42
3:F:707:GLU:OE1	3:F:707:GLU:N	2.37	0.42
3:B:744:THR:HG21	3:B:749:THR:HG21	2.01	0.42
3:A:371:LYS:HE3	3:A:574:HIS:CG	2.55	0.42
3:A:701:ASN:ND2	3:A:744:THR:HB	2.35	0.42
3:E:304:HIS:HA	3:E:307:LEU:HG	2.02	0.42
3:E:691:PHE:HD2	3:E:734:ALA:HB2	1.85	0.42
3:F:294:MET:C	3:F:301:ARG:HH21	2.28	0.42
3:F:804:LYS:O	3:F:808:GLU:HG2	2.20	0.42
3:A:465:ASN:O	3:A:467:ASP:N	2.53	0.42
3:A:894:GLN:HB2	3:A:904:LYS:NZ	2.35	0.42
3:D:330:ASN:HB2	3:D:374:THR:HA	2.01	0.42
3:D:359:GLU:HB3	3:D:360:LYS:NZ	2.34	0.42
3:D:896:SER:HB3	3:D:902:ILE:HD12	2.02	0.42
3:F:770:ASN:HB3	3:F:773:GLU:HG3	2.00	0.42
1:H:3:DT:H1'	1:H:4:DT:O5'	2.19	0.41
3:A:653:LEU:HD22	3:A:658:ALA:HB2	2.02	0.41
3:C:565:ALA:N	3:C:803:GLU:OE2	2.53	0.41
3:C:669:CYS:SG	3:C:670:ARG:N	2.93	0.41
3:E:336:ARG:HH22	3:E:359:GLU:CD	2.29	0.41
3:E:476:ASN:HA	3:E:479:ARG:HE	1.85	0.41
3:F:311:PRO:HG3	3:F:385:HIS:NE2	2.35	0.41
3:F:904:LYS:HD3	3:F:904:LYS:HA	1.69	0.41
3:B:293:LEU:H	3:B:293:LEU:HG	1.56	0.41
3:A:896:SER:HB3	3:A:902:ILE:HD12	2.02	0.41
3:C:367:HIS:O	3:C:367:HIS:ND1	2.52	0.41
3:D:587:PHE:HA	3:D:796:SER:HB3	2.01	0.41
3:D:717:ARG:HA	3:D:717:ARG:HD2	1.80	0.41
3:E:307:LEU:HD13	3:E:342:PHE:CD1	2.54	0.41
3:E:350:TRP:CZ2	3:E:355:LYS:HD3	2.55	0.41
3:E:355:LYS:HD2	3:E:355:LYS:HA	1.83	0.41
3:F:876:ILE:HG22	3:F:878:LEU:H	1.85	0.41
3:F:945:TRP:CH2	3:F:948:ASN:HA	2.55	0.41
1:H:4:DT:H1'	1:H:5:DT:N1	2.35	0.41
3:A:706:LYS:HA	3:A:709:VAL:HG12	2.02	0.41
3:A:779:ARG:HB2	3:A:783:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:631:MET:HB2	3:D:709:VAL:HG22	2.02	0.41
3:D:736:SER:OG	3:D:737:ASN:N	2.54	0.41
3:D:909:LEU:HD23	3:D:909:LEU:H	1.85	0.41
3:E:899:LYS:C	3:E:901:ARG:H	2.28	0.41
3:F:358:LEU:HA	3:F:361:LEU:HB2	2.01	0.41
3:F:656:HIS:O	3:F:686:ARG:NH1	2.53	0.41
3:B:290:LEU:HD12	3:B:341:TRP:CG	2.55	0.41
3:A:781:ILE:HD12	4:A:1001:AGS:H3'	2.02	0.41
3:C:481:MET:HE3	3:C:481:MET:HA	2.01	0.41
3:C:516:SER:HB3	3:D:412:MET:SD	2.60	0.41
3:D:653:LEU:HG	3:D:657:TYR:HB2	2.01	0.41
3:D:882:GLN:H	3:D:882:GLN:HG2	1.70	0.41
3:E:833:ASP:OD1	3:E:833:ASP:N	2.51	0.41
3:E:873:LYS:HD2	3:E:873:LYS:HA	1.90	0.41
2:I:2:DA:H2"	2:I:3:DA:C8	2.56	0.41
3:B:544:LEU:HD23	3:B:544:LEU:HA	1.91	0.41
3:C:406:VAL:HG13	3:C:411:GLY:HA2	2.03	0.41
3:C:884:LEU:O	3:C:887:SER:OG	2.28	0.41
3:D:387:PRO:HA	3:D:390:TYR:HE1	1.84	0.41
3:D:497:GLU:OE1	3:D:498:SER:N	2.53	0.41
3:E:457:ILE:O	3:E:459:LYS:NZ	2.51	0.41
3:E:715:THR:OG1	3:E:723:GLN:HB2	2.20	0.41
3:F:605:ILE:HD13	3:F:611:ARG:HA	2.03	0.41
3:B:289:SER:O	3:B:293:LEU:HG	2.21	0.41
3:B:697:SER:CB	3:C:878:LEU:HD13	2.50	0.41
3:A:634:TRP:CZ3	3:A:758:SER:HB2	2.55	0.41
3:A:780:PHE:HA	3:A:784:TYR:HD2	1.85	0.41
3:C:701:ASN:C	3:C:703:SER:H	2.28	0.41
3:D:307:LEU:HD22	3:D:341:TRP:CZ3	2.56	0.41
3:D:853:TYR:O	3:D:853:TYR:CG	2.73	0.41
3:E:414:GLU:N	3:E:417:MET:SD	2.92	0.41
3:E:501:LEU:O	3:E:505:LYS:HD2	2.20	0.41
3:F:615:MET:HE2	3:F:615:MET:HA	2.02	0.41
1:H:3:DT:H4'	1:H:4:DT:OP1	2.18	0.41
3:C:633:LEU:HD21	3:C:753:LEU:HD12	2.01	0.41
3:D:293:LEU:HD13	3:D:338:LEU:HD13	2.03	0.41
3:D:411:GLY:O	3:D:413:LEU:HG	2.20	0.41
3:D:468:GLU:HA	3:D:471:ILE:HG22	2.01	0.41
3:D:739:ASN:N	3:D:739:ASN:OD1	2.52	0.41
3:E:302:TYR:O	3:E:306:ILE:HG23	2.21	0.41
3:E:414:GLU:HG3	3:E:415:HIS:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:403:ALA:HA	3:B:406:VAL:HG12	2.01	0.41
3:C:361:LEU:HA	3:C:364:ASP:OD2	2.21	0.41
3:C:452:MET:HG2	3:C:453:ASN:O	2.21	0.41
3:C:755:HIS:ND1	3:C:824:GLU:OE1	2.54	0.41
3:C:755:HIS:HB3	3:C:825:THR:HA	2.02	0.41
3:D:651:MET:HE2	3:D:651:MET:HB2	1.84	0.41
3:D:783:GLU:O	3:D:784:TYR:HB2	2.21	0.41
3:F:666:LEU:HB2	3:F:691:PHE:CE2	2.56	0.41
3:F:716:ALA:N	3:F:724:GLU:O	2.53	0.41
3:B:374:THR:OG1	3:B:573:GLU:OE1	2.30	0.41
3:B:549:HIS:ND1	3:B:561:GLU:HA	2.35	0.41
3:B:694:THR:OG1	3:B:696:LYS:O	2.38	0.41
3:B:879:GLU:HG2	3:B:880:LEU:N	2.36	0.41
3:A:804:LYS:HE2	3:A:945:TRP:HB2	2.03	0.41
3:A:823:SER:O	3:A:826:GLU:HG3	2.21	0.41
3:C:310:LEU:HD23	3:C:310:LEU:HA	1.93	0.41
3:C:311:PRO:HG3	3:C:385:HIS:CD2	2.56	0.41
3:C:317:GLU:O	3:C:321:TRP:HB3	2.21	0.41
3:C:345:LYS:O	3:C:345:LYS:HG3	2.21	0.41
3:C:386:ALA:HB1	3:C:389:GLN:NE2	2.36	0.41
3:C:453:ASN:OD1	3:C:454:GLN:N	2.51	0.41
3:C:461:ARG:CZ	3:D:538:ARG:HH12	2.33	0.41
3:C:676:PRO:HB2	3:C:719:LEU:H	1.85	0.41
3:C:753:LEU:O	3:C:754:ARG:NE	2.54	0.41
3:C:938:PRO:HG3	3:C:942:TRP:HB3	2.02	0.41
3:D:301:ARG:O	3:D:304:HIS:HB3	2.20	0.41
3:D:613:TRP:HZ3	3:D:632:LEU:HD12	1.85	0.41
3:E:314:TYR:HA	3:E:320:LEU:HD13	2.02	0.41
3:E:343:SER:HB3	3:E:350:TRP:CD1	2.56	0.41
3:E:804:LYS:HE3	3:E:804:LYS:HB3	1.82	0.41
3:F:491:HIS:HB3	3:F:504:TYR:CE2	2.56	0.41
3:F:666:LEU:HB2	3:F:691:PHE:HE2	1.85	0.41
3:B:646:MET:N	3:B:646:MET:HE2	2.36	0.41
3:A:565:ALA:N	3:A:803:GLU:OE2	2.36	0.41
3:D:336:ARG:HD2	3:D:362:TRP:CD1	2.56	0.41
3:E:779:ARG:O	3:E:783:GLU:HG3	2.20	0.41
3:E:818:CYS:O	3:E:821:ILE:HG22	2.21	0.41
3:E:941:LYS:O	3:E:944:GLU:HG2	2.20	0.41
3:F:299:GLU:HA	3:F:302:TYR:CD2	2.56	0.41
3:B:304:HIS:O	3:B:307:LEU:HG	2.21	0.40
3:B:337:PRO:O	3:B:341:TRP:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:600:ALA:CB	4:B:1001:AGS:HN62	2.22	0.40
3:B:706:LYS:HA	3:B:752:ARG:HH22	1.86	0.40
3:B:878:LEU:HD22	3:A:741:ILE:HD12	2.03	0.40
3:A:739:ASN:OD1	3:A:739:ASN:N	2.52	0.40
3:A:809:TYR:CZ	3:A:816:VAL:HG23	2.56	0.40
3:C:374:THR:OG1	3:C:375:LYS:N	2.55	0.40
3:C:878:LEU:HA	3:C:882:GLN:OE1	2.22	0.40
3:D:855:LEU:HD23	3:D:881:SER:HA	2.03	0.40
3:E:456:GLU:HA	3:E:459:LYS:HE2	2.03	0.40
3:E:534:LEU:HD23	3:E:534:LEU:HA	1.85	0.40
3:F:307:LEU:HB3	3:F:342:PHE:HE1	1.87	0.40
3:F:614:ILE:HD12	3:F:632:LEU:HD11	2.03	0.40
3:F:623:PHE:HB3	3:F:627:LYS:HE2	2.03	0.40
3:F:899:LYS:C	3:F:901:ARG:H	2.28	0.40
3:B:290:LEU:HD12	3:B:341:TRP:CB	2.51	0.40
3:B:945:TRP:O	3:B:950:SER:OG	2.37	0.40
3:A:391:LYS:HE3	3:A:391:LYS:HB3	1.96	0.40
3:A:612:LEU:HD22	3:A:945:TRP:HD1	1.85	0.40
3:C:862:TYR:CG	3:C:880:LEU:HD21	2.56	0.40
3:D:296:HIS:CG	3:D:297:ASP:N	2.89	0.40
3:D:847:PRO:HD2	3:D:918:GLY:HA2	2.03	0.40
3:E:476:ASN:HA	3:E:479:ARG:HH21	1.87	0.40
3:B:376:ARG:HE	3:B:428:ASN:HA	1.87	0.40
3:B:426:MET:HG2	3:B:426:MET:O	2.21	0.40
3:A:289:SER:HA	3:A:292:ILE:HD12	2.04	0.40
3:A:452:MET:HG2	3:A:453:ASN:O	2.21	0.40
3:D:756:TYR:CG	3:D:757:ARG:N	2.90	0.40
3:E:780:PHE:HB3	4:E:1001:AGS:O2'	2.22	0.40
3:B:461:ARG:CZ	3:C:538:ARG:HH12	2.34	0.40
3:B:520:ASN:ND2	3:C:414:GLU:OE2	2.54	0.40
3:A:672:THR:HA	3:A:704:ARG:HH12	1.86	0.40
3:A:672:THR:C	3:A:704:ARG:HH12	2.28	0.40
3:A:780:PHE:HA	3:A:784:TYR:CD2	2.57	0.40
3:C:497:GLU:OE1	3:C:498:SER:N	2.54	0.40
3:C:804:LYS:HE3	3:C:804:LYS:HB3	1.78	0.40
3:C:813:ILE:O	3:C:816:VAL:HG12	2.22	0.40
3:D:480:VAL:C	3:D:481:MET:HE2	2.46	0.40
3:A:852:VAL:HG21	3:A:903:LEU:HD23	2.04	0.40
3:C:318:TYR:N	3:C:319:PRO:HD2	2.37	0.40
3:C:676:PRO:HD3	3:C:717:ARG:NH1	2.36	0.40
3:C:707:GLU:HA	3:C:710:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:626:LEU:HD11	3:F:711:PRO:HB2	2.03	0.40
3:F:636:GLY:HA3	3:F:642:LYS:HD2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	642/972 (66%)	590 (92%)	50 (8%)	2 (0%)	36	65
3	B	642/972 (66%)	585 (91%)	55 (9%)	2 (0%)	36	65
3	C	642/972 (66%)	590 (92%)	50 (8%)	2 (0%)	36	65
3	D	640/972 (66%)	578 (90%)	60 (9%)	2 (0%)	36	65
3	E	639/972 (66%)	565 (88%)	74 (12%)	0	100	100
3	F	642/972 (66%)	574 (89%)	67 (10%)	1 (0%)	43	71
All	All	3847/5832 (66%)	3482 (90%)	356 (9%)	9 (0%)	44	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	844	VAL
3	B	946	SER
3	A	372	LYS
3	C	388	GLN
3	C	946	SER
3	D	946	SER
3	F	946	SER
3	B	816	VAL
3	A	946	SER

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	
3	A	581/879 (66%)	581 (100%)	0	100	100
3	B	581/879 (66%)	565 (97%)	16 (3%)	38	58
3	C	581/879 (66%)	576 (99%)	5 (1%)	70	74
3	D	579/879 (66%)	564 (97%)	15 (3%)	40	60
3	E	579/879 (66%)	575 (99%)	4 (1%)	76	77
3	F	581/879 (66%)	570 (98%)	11 (2%)	50	65
All	All	3482/5274 (66%)	3431 (98%)	51 (2%)	55	68

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	289	SER
3	B	290	LEU
3	B	292	ILE
3	B	293	LEU
3	B	294	MET
3	B	295	LEU
3	B	301	ARG
3	B	663	ILE
3	B	665	LEU
3	B	666	LEU
3	B	670	ARG
3	B	870	ILE
3	B	871	ASN
3	B	873	LYS
3	B	874	ARG
3	B	875	HIS
3	C	660	LYS
3	C	661	LEU
3	C	664	SER
3	C	666	LEU
3	C	667	THR
3	D	293	LEU

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Mol	Chain	Res	Type
3	D	294	MET
3	D	296	HIS
3	D	301	ARG
3	D	302	TYR
3	D	305	LYS
3	D	309	LEU
3	D	310	LEU
3	D	320	LEU
3	D	410	ASN
3	D	418	ILE
3	D	703	SER
3	D	705	LEU
3	D	706	LYS
3	D	708	MET
3	E	820	THR
3	E	821	ILE
3	E	824	GLU
3	E	829	ARG
3	F	663	ILE
3	F	664	SER
3	F	665	LEU
3	F	666	LEU
3	F	670	ARG
3	F	671	GLU
3	F	672	THR
3	F	675	LYS
3	F	692	GLU
3	F	696	LYS
3	F	698	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	308	ASN
3	B	330	ASN
3	B	383	HIS
3	B	389	GLN
3	B	496	HIS
3	B	764	HIS
3	B	765	ASN
3	B	871	ASN
3	B	882	GLN

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Mol	Chain	Res	Type
3	B	916	GLN
3	A	323	ASN
3	A	389	GLN
3	A	470	HIS
3	A	555	ASN
3	A	599	ASN
3	A	710	ASN
3	A	869	ASN
3	A	871	ASN
3	A	875	HIS
3	A	894	GLN
3	C	344	GLN
3	C	491	HIS
3	C	555	ASN
3	C	695	ASN
3	C	701	ASN
3	C	710	ASN
3	C	721	GLN
3	C	723	GLN
3	C	747	HIS
3	C	836	HIS
3	C	894	GLN
3	D	363	ASN
3	D	396	GLN
3	D	450	GLN
3	D	487	HIS
3	D	491	HIS
3	D	656	HIS
3	D	764	HIS
3	D	765	ASN
3	D	792	ASN
3	E	323	ASN
3	E	640	ASN
3	E	720	ASN
3	E	810	ASN
3	E	869	ASN
3	F	388	GLN
3	F	494	GLN
3	F	765	ASN
3	F	782	HIS
3	F	810	ASN
3	F	836	HIS

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Mol	Chain	Res	Type
3	F	875	HIS
3	F	882	GLN
3	F	916	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AGS	D	1001	5	32,33,33	2.03	7 (21%)	45,52,52	1.87	10 (22%)
4	AGS	E	1001	5	32,33,33	0.53	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	C	1001	5	32,33,33	2.04	9 (28%)	45,52,52	1.87	10 (22%)
4	AGS	A	1001	5	32,33,33	0.50	1 (3%)	45,52,52	0.68	1 (2%)
4	AGS	B	1001	5	32,33,33	2.03	7 (21%)	45,52,52	1.85	11 (24%)
4	AGS	F	1001	5	32,33,33	0.50	1 (3%)	45,52,52	0.67	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	D	1001	5	-	8/21/38/38	0/3/3/3
4	AGS	E	1001	5	-	9/21/38/38	0/3/3/3
4	AGS	C	1001	5	-	7/21/38/38	0/3/3/3
4	AGS	A	1001	5	-	11/21/38/38	0/3/3/3
4	AGS	B	1001	5	-	9/21/38/38	0/3/3/3
4	AGS	F	1001	5	-	7/21/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	AGS	PG-S1G	7.92	2.07	1.90
4	C	1001	AGS	PG-S1G	7.92	2.07	1.90
4	D	1001	AGS	PG-S1G	7.91	2.07	1.90
4	C	1001	AGS	C5-C4	4.65	1.47	1.39
4	D	1001	AGS	C5-C4	4.63	1.47	1.39
4	B	1001	AGS	C5-C4	4.59	1.47	1.39
4	D	1001	AGS	C5-C6	2.69	1.48	1.41
4	B	1001	AGS	C5-C6	2.60	1.48	1.41
4	C	1001	AGS	C5-C6	2.59	1.48	1.41
4	B	1001	AGS	C8-N7	2.34	1.36	1.31
4	C	1001	AGS	C5-N7	-2.29	1.34	1.39
4	D	1001	AGS	C5-N7	-2.28	1.34	1.39
4	B	1001	AGS	C5-N7	-2.28	1.34	1.39
4	D	1001	AGS	C8-N7	2.25	1.36	1.31
4	C	1001	AGS	C8-N7	2.24	1.36	1.31
4	F	1001	AGS	PG-S1G	2.13	1.95	1.90
4	A	1001	AGS	PG-S1G	2.12	1.95	1.90
4	C	1001	AGS	PA-O3A	2.11	1.61	1.59
4	B	1001	AGS	PG-O2G	2.10	1.61	1.54
4	B	1001	AGS	PA-O3A	2.10	1.61	1.59
4	E	1001	AGS	PG-S1G	2.09	1.95	1.90
4	C	1001	AGS	PB-O3A	2.05	1.61	1.59
4	C	1001	AGS	PG-O2G	2.05	1.61	1.54
4	D	1001	AGS	PG-O2G	2.04	1.61	1.54
4	D	1001	AGS	PB-O3A	2.04	1.61	1.59
4	C	1001	AGS	C4-N9	-2.00	1.33	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1001	AGS	C5-C4-N3	-5.70	118.87	126.72
4	D	1001	AGS	C5-C4-N3	-5.66	118.93	126.72
4	B	1001	AGS	C5-C4-N3	-5.60	119.01	126.72
4	C	1001	AGS	N3-C4-N9	4.66	135.09	127.17
4	D	1001	AGS	N3-C4-N9	4.61	135.01	127.17
4	B	1001	AGS	N3-C4-N9	4.55	134.90	127.17
4	F	1001	AGS	PB-O3B-PG	-3.75	119.46	133.17
4	A	1001	AGS	PB-O3B-PG	-3.71	119.61	133.17
4	E	1001	AGS	PB-O3B-PG	-3.69	119.66	133.17
4	B	1001	AGS	C2-N3-C4	3.61	120.64	111.83
4	C	1001	AGS	C2-N3-C4	3.60	120.61	111.83
4	D	1001	AGS	C2-N3-C4	3.58	120.58	111.83
4	D	1001	AGS	PB-O3B-PG	-3.52	120.29	133.17
4	D	1001	AGS	C4-C5-N7	-3.31	106.79	110.58
4	C	1001	AGS	C4-C5-N7	-3.30	106.81	110.58
4	B	1001	AGS	C4-C5-N7	-3.26	106.85	110.58
4	B	1001	AGS	N3-C2-N1	-3.23	123.69	128.58
4	B	1001	AGS	PB-O3B-PG	-3.17	121.56	133.17
4	C	1001	AGS	N3-C2-N1	-3.16	123.80	128.58
4	D	1001	AGS	N3-C2-N1	-3.15	123.81	128.58
4	C	1001	AGS	PB-O3B-PG	-3.03	122.08	133.17
4	C	1001	AGS	C4-N9-C8	2.92	108.81	105.74
4	B	1001	AGS	C4-N9-C8	2.91	108.79	105.74
4	D	1001	AGS	C4-N9-C8	2.88	108.77	105.74
4	D	1001	AGS	C5-N7-C8	2.48	107.34	103.45
4	C	1001	AGS	C5-N7-C8	2.46	107.31	103.45
4	B	1001	AGS	C5-N7-C8	2.42	107.26	103.45
4	C	1001	AGS	C3'-C2'-C1'	2.39	105.99	101.46
4	D	1001	AGS	C3'-C2'-C1'	2.36	105.92	101.46
4	B	1001	AGS	C3'-C2'-C1'	2.29	105.79	101.46
4	B	1001	AGS	N9-C8-N7	-2.06	111.01	113.94
4	B	1001	AGS	C6-C5-N7	2.06	136.06	132.09
4	C	1001	AGS	N9-C8-N7	-2.05	111.03	113.94
4	D	1001	AGS	N9-C8-N7	-2.04	111.04	113.94

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	AGS	C5'-O5'-PA-O2A
4	B	1001	AGS	C5'-O5'-PA-O3A
4	A	1001	AGS	C5'-O5'-PA-O1A
4	A	1001	AGS	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	1001	AGS	C5'-O5'-PA-O3A
4	A	1001	AGS	O4'-C4'-C5'-O5'
4	C	1001	AGS	C5'-O5'-PA-O1A
4	C	1001	AGS	C5'-O5'-PA-O3A
4	D	1001	AGS	C5'-O5'-PA-O2A
4	D	1001	AGS	C5'-O5'-PA-O3A
4	E	1001	AGS	C3'-C4'-C5'-O5'
4	F	1001	AGS	C5'-O5'-PA-O1A
4	F	1001	AGS	C5'-O5'-PA-O2A
4	F	1001	AGS	C5'-O5'-PA-O3A
4	F	1001	AGS	O4'-C4'-C5'-O5'
4	F	1001	AGS	C3'-C4'-C5'-O5'
4	B	1001	AGS	C3'-C4'-C5'-O5'
4	A	1001	AGS	C3'-C4'-C5'-O5'
4	D	1001	AGS	O4'-C4'-C5'-O5'
4	E	1001	AGS	O4'-C4'-C5'-O5'
4	C	1001	AGS	C3'-C4'-C5'-O5'
4	D	1001	AGS	C3'-C4'-C5'-O5'
4	A	1001	AGS	C4'-C5'-O5'-PA
4	C	1001	AGS	O4'-C4'-C5'-O5'
4	B	1001	AGS	O4'-C4'-C5'-O5'
4	F	1001	AGS	C4'-C5'-O5'-PA
4	B	1001	AGS	PB-O3A-PA-O1A
4	A	1001	AGS	PB-O3A-PA-O1A
4	E	1001	AGS	PB-O3A-PA-O1A
4	B	1001	AGS	PG-O3B-PB-O3A
4	D	1001	AGS	C4'-C5'-O5'-PA
4	E	1001	AGS	PG-O3B-PB-O3A
4	C	1001	AGS	C5'-O5'-PA-O2A
4	E	1001	AGS	C4'-C5'-O5'-PA
4	E	1001	AGS	PA-O3A-PB-O2B
4	A	1001	AGS	PG-O3B-PB-O1B
4	D	1001	AGS	PB-O3A-PA-O1A
4	F	1001	AGS	PA-O3A-PB-O1B
4	A	1001	AGS	PB-O3B-PG-O2G
4	C	1001	AGS	PB-O3B-PG-O3G
4	B	1001	AGS	C4'-C5'-O5'-PA
4	C	1001	AGS	C4'-C5'-O5'-PA
4	B	1001	AGS	PG-O3B-PB-O2B
4	E	1001	AGS	PG-O3B-PB-O2B
4	B	1001	AGS	PB-O3A-PA-O2A
4	A	1001	AGS	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	1001	AGS	PB-O3A-PA-O2A
4	D	1001	AGS	PG-O3B-PB-O3A
4	A	1001	AGS	PB-O3A-PA-O2A
4	E	1001	AGS	PA-O3A-PB-O1B
4	E	1001	AGS	PB-O3A-PA-O2A

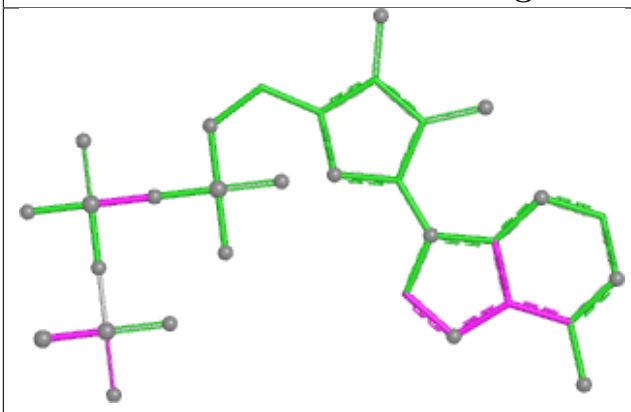
There are no ring outliers.

6 monomers are involved in 35 short contacts:

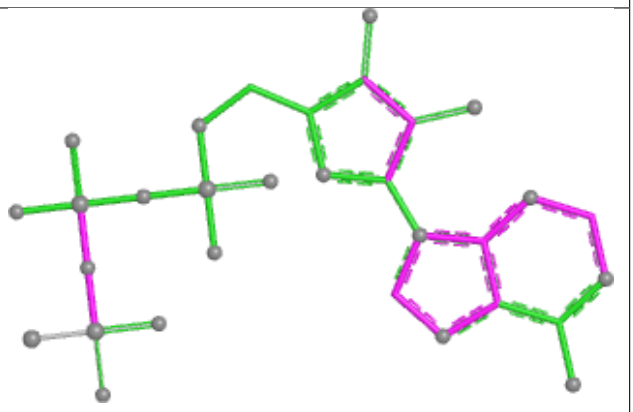
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1001	AGS	5	0
4	E	1001	AGS	6	0
4	C	1001	AGS	6	0
4	A	1001	AGS	7	0
4	B	1001	AGS	7	0
4	F	1001	AGS	4	0

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

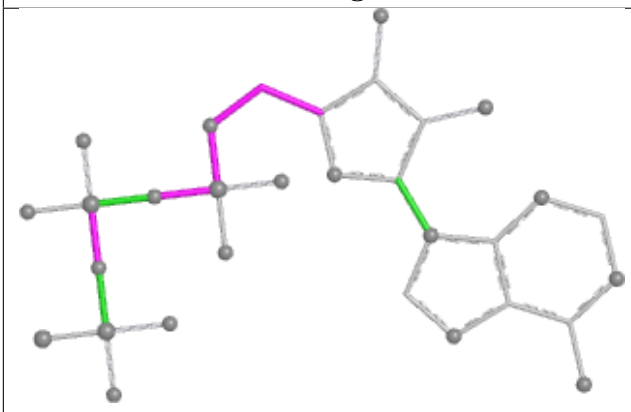
Ligand AGS D 1001



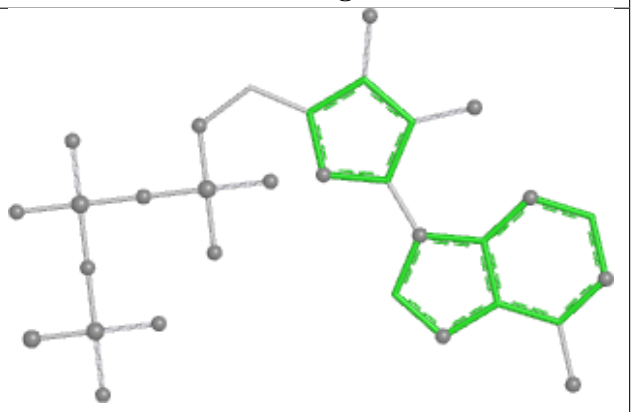
Bond lengths



Bond angles

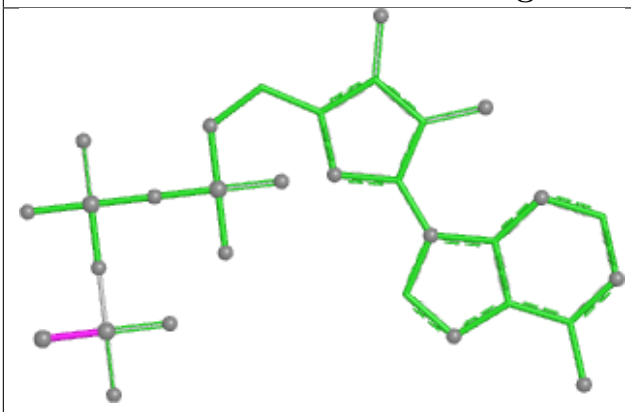


Torsions

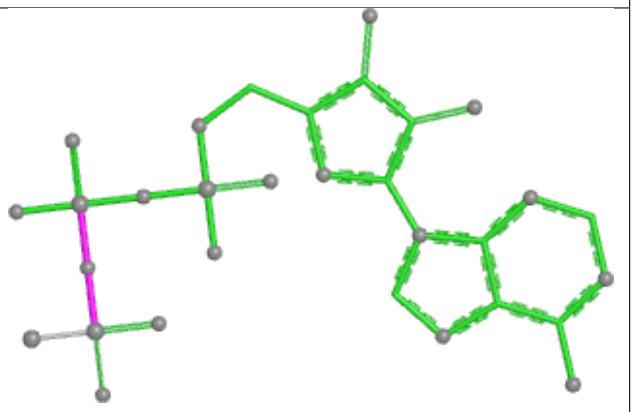


Rings

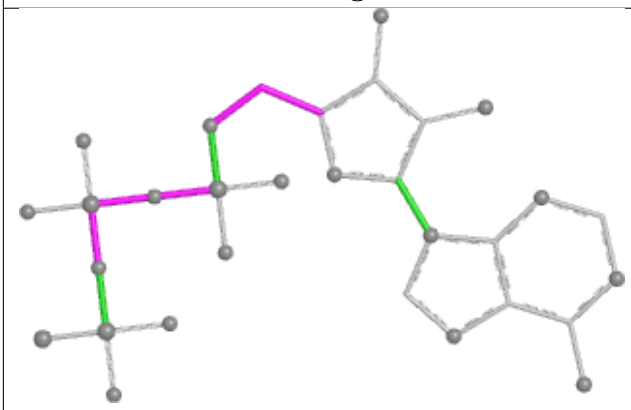
Ligand AGS E 1001



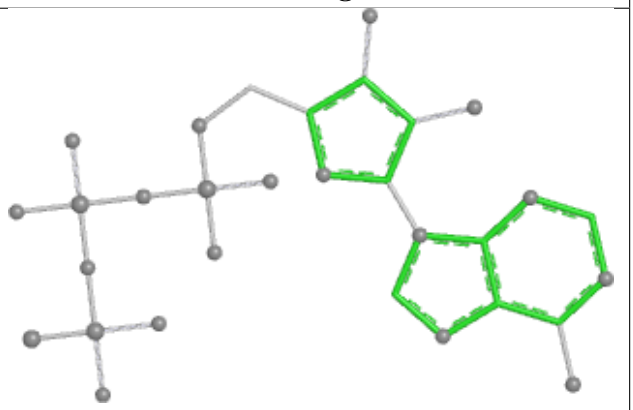
Bond lengths



Bond angles

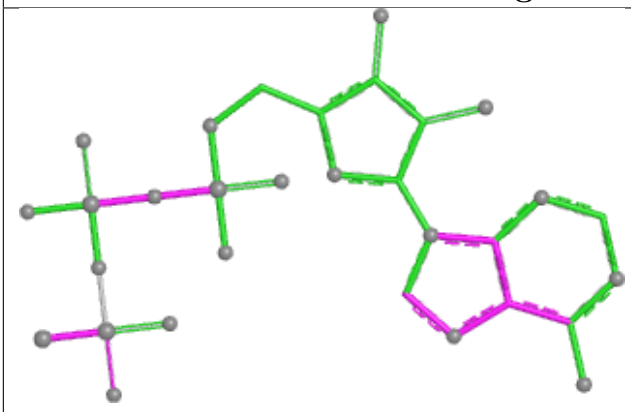


Torsions

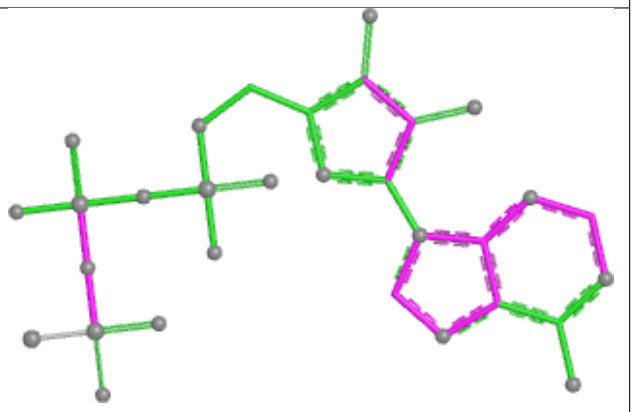


Rings

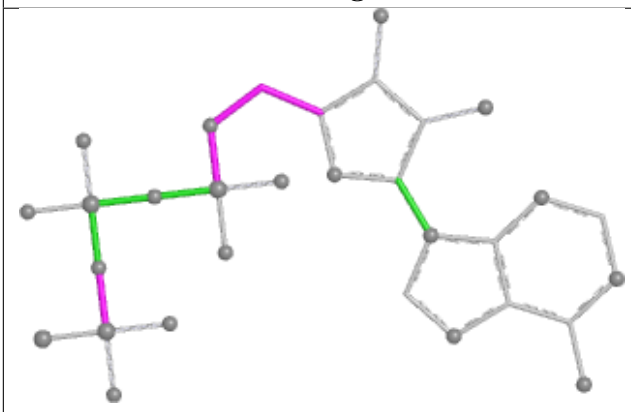
Ligand AGS C 1001



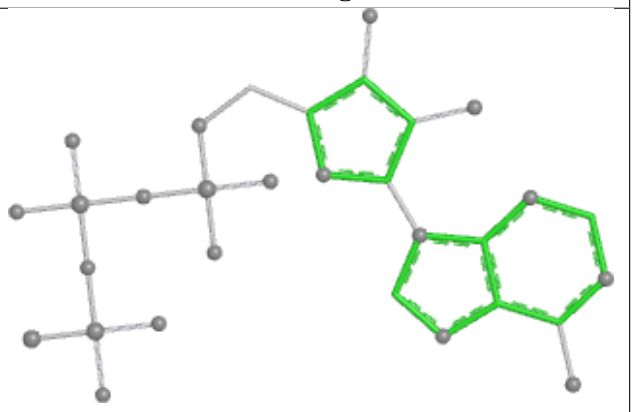
Bond lengths



Bond angles

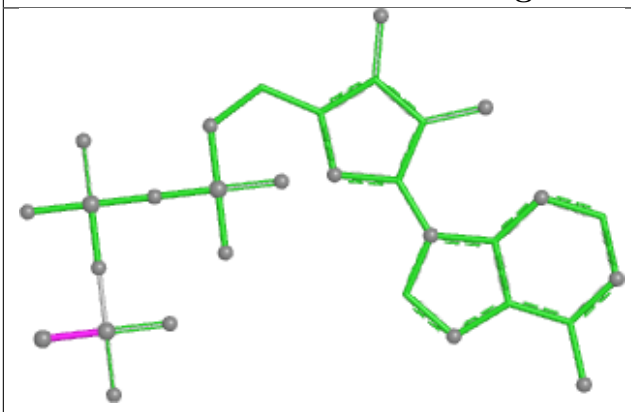


Torsions

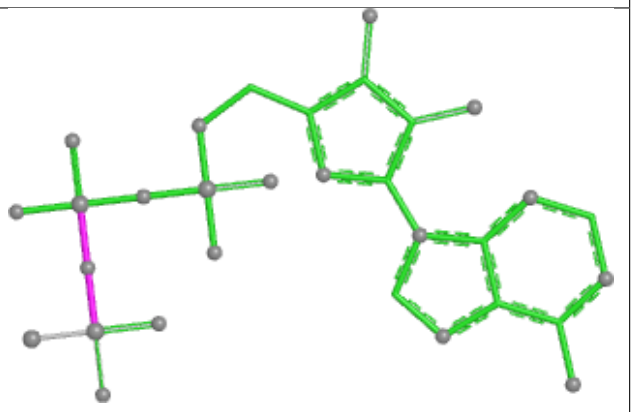


Rings

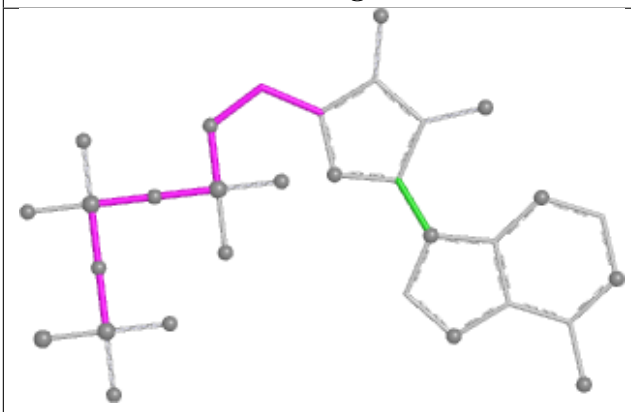
Ligand AGS A 1001



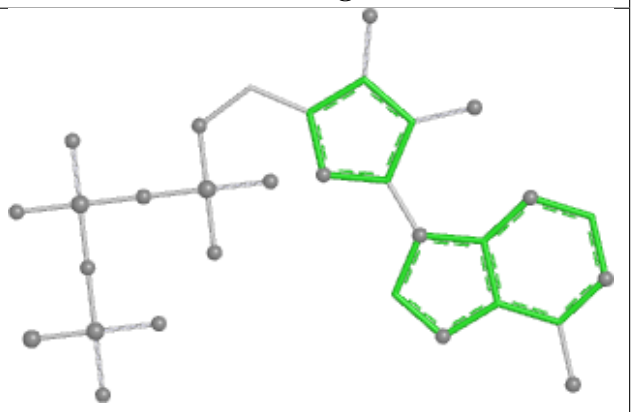
Bond lengths



Bond angles

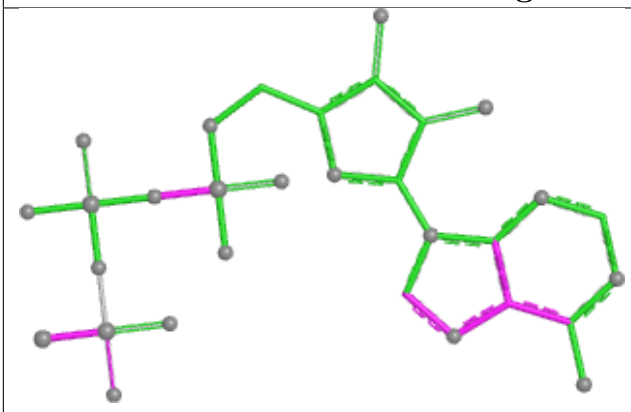


Torsions

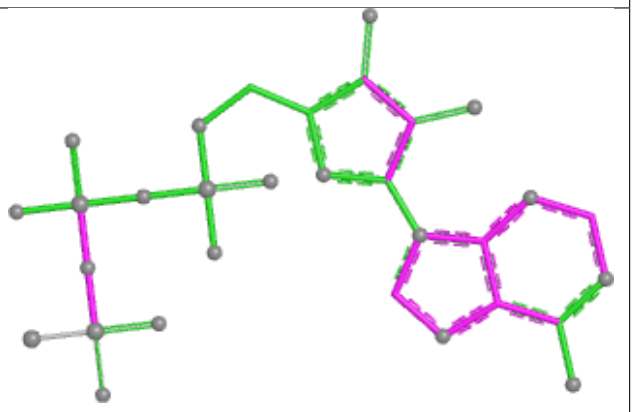


Rings

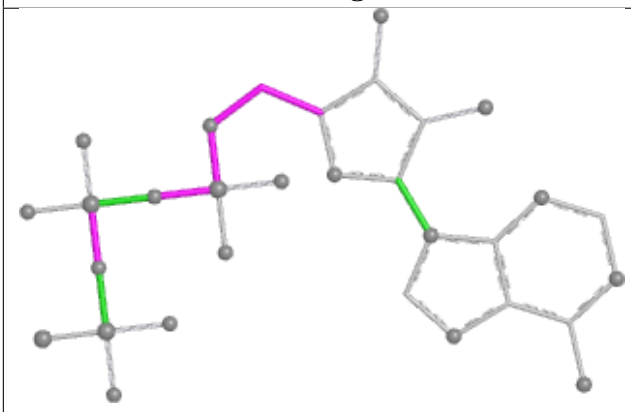
Ligand AGS B 1001



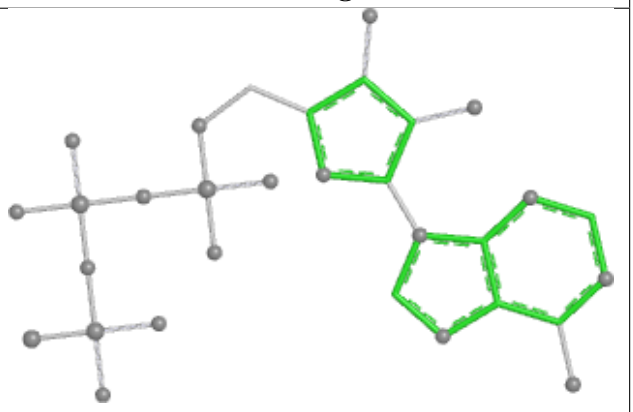
Bond lengths



Bond angles

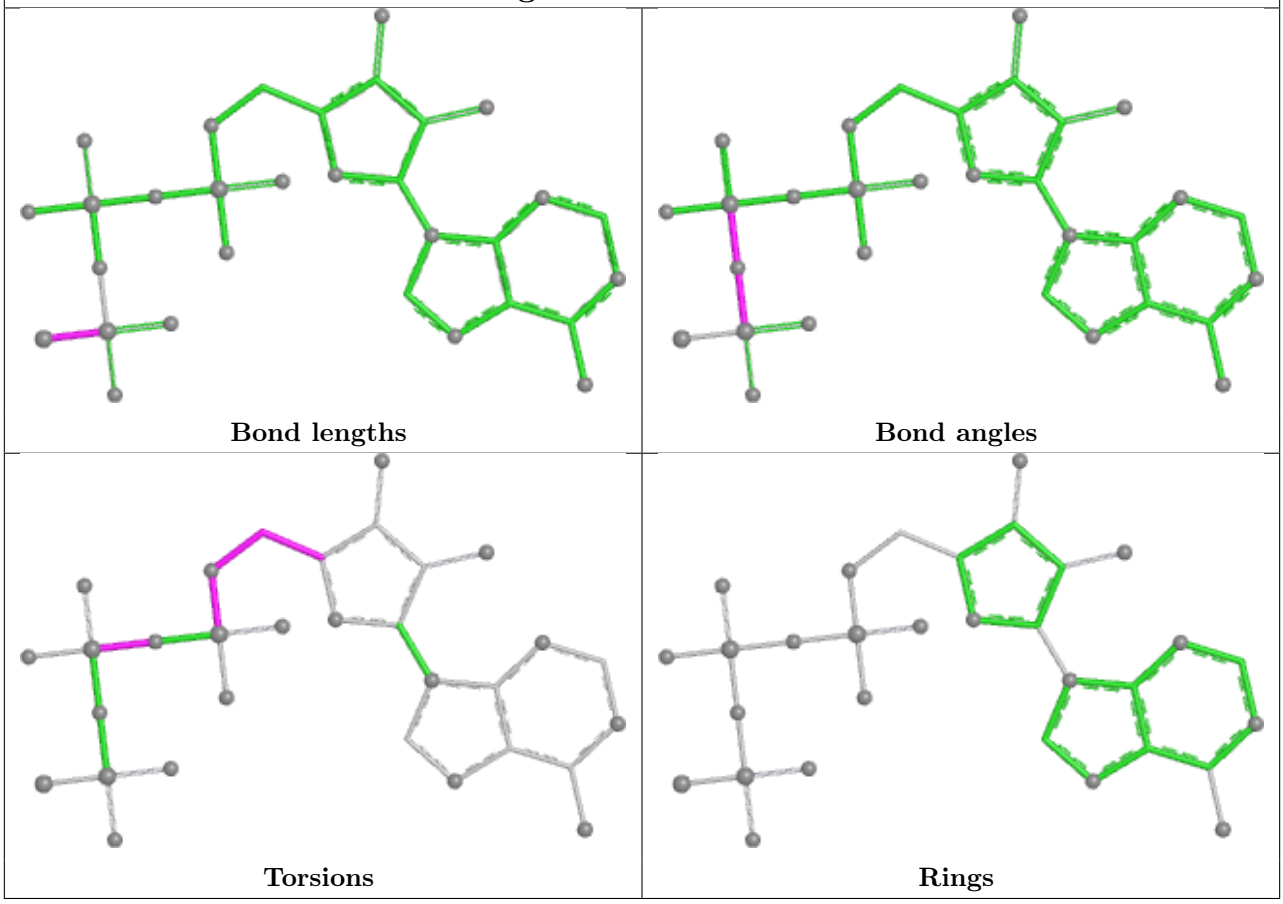


Torsions



Rings

Ligand AGS F 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

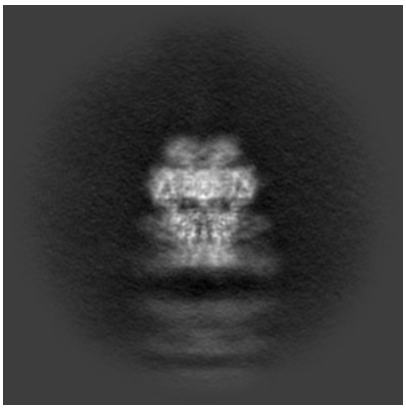
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37882. These allow visual inspection of the internal detail of the map and identification of artifacts.

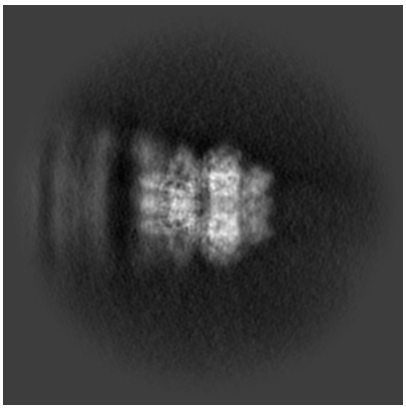
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

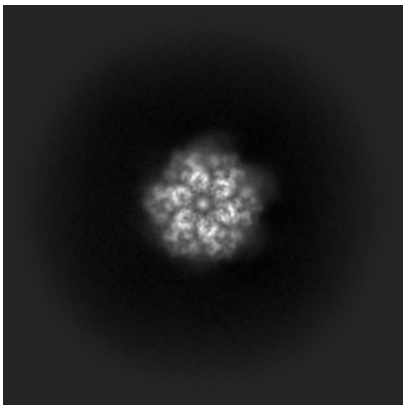
6.1.1 Primary map



X

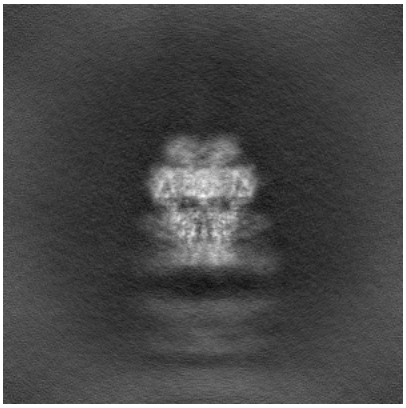


Y

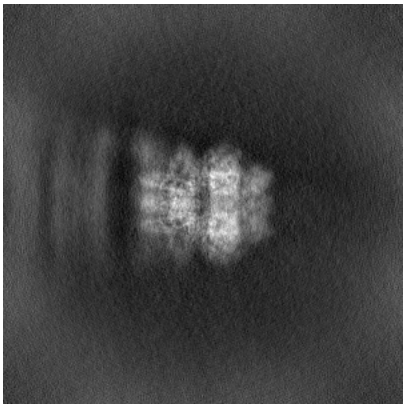


Z

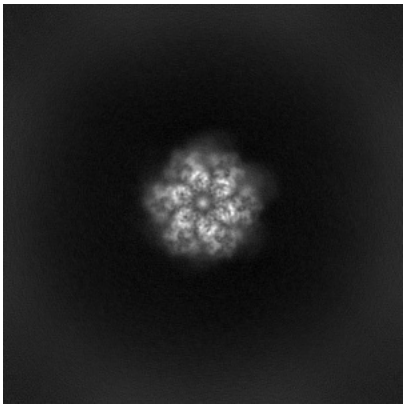
6.1.2 Raw map



X



Y

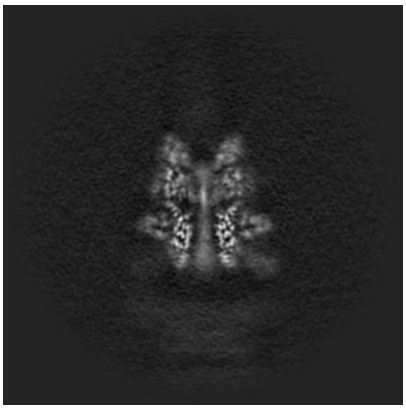


Z

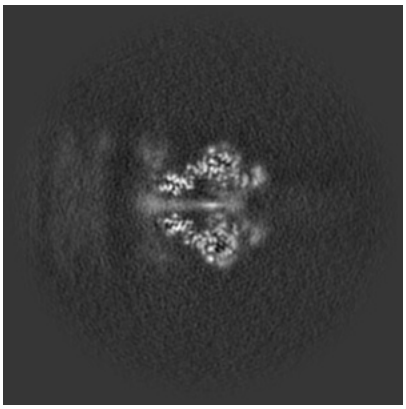
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

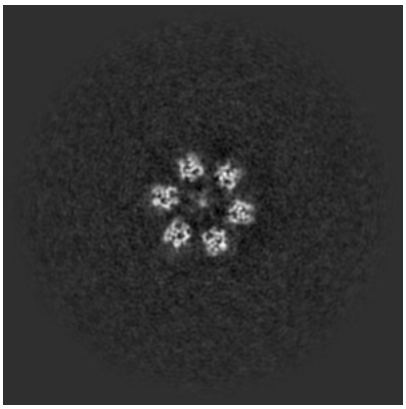
6.2.1 Primary map



X Index: 192



Y Index: 192

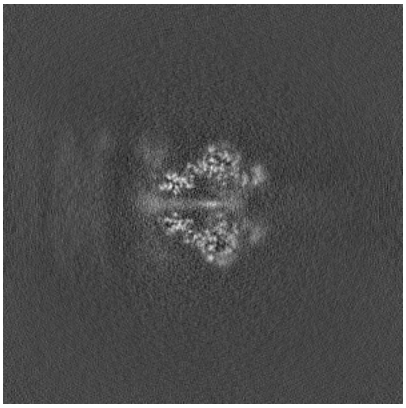


Z Index: 192

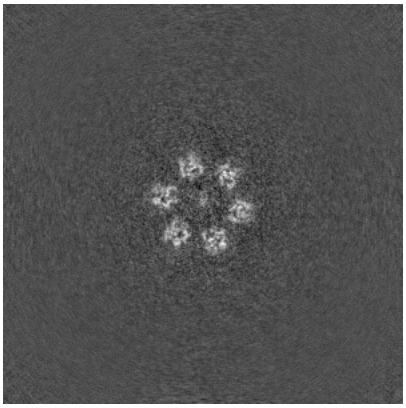
6.2.2 Raw map



X Index: 192



Y Index: 192

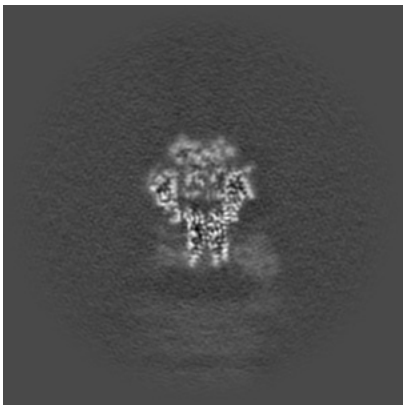


Z Index: 192

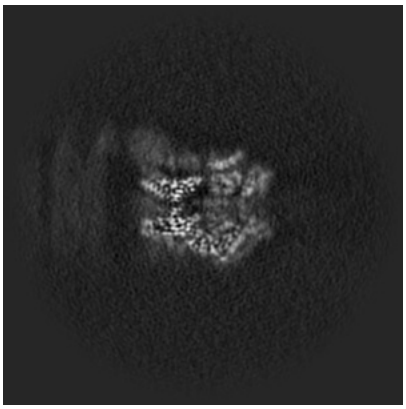
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

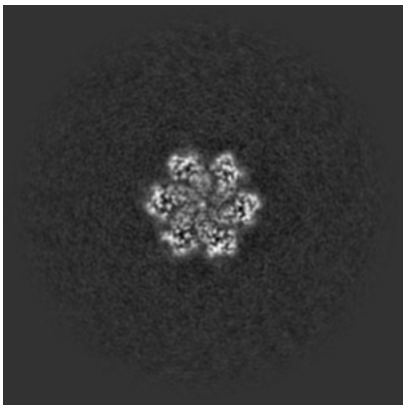
6.3.1 Primary map



X Index: 211

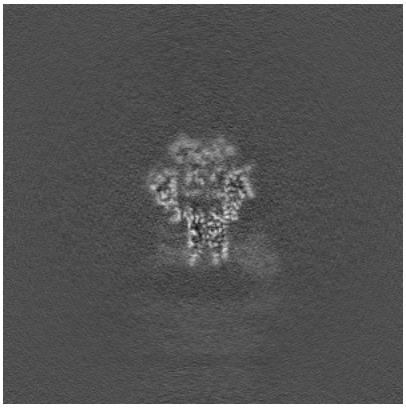


Y Index: 203

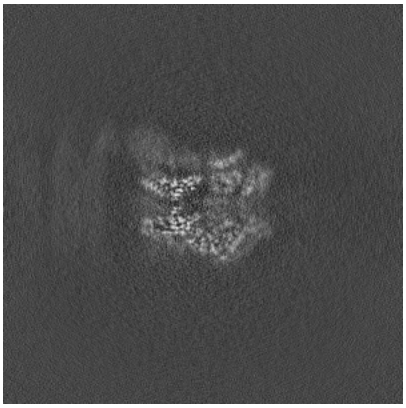


Z Index: 201

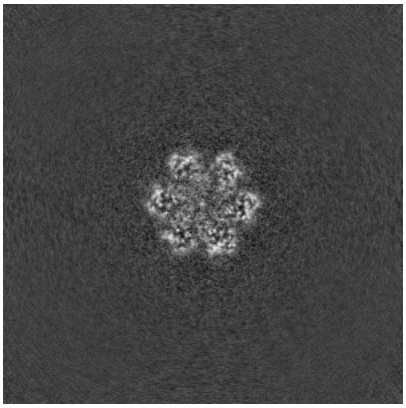
6.3.2 Raw map



X Index: 211



Y Index: 203

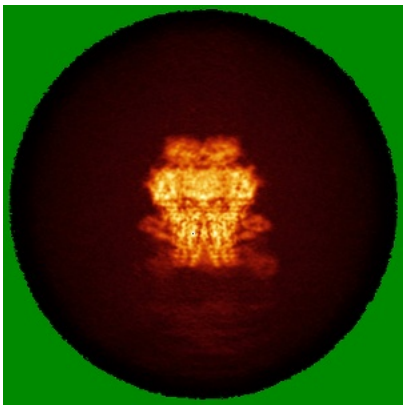


Z Index: 201

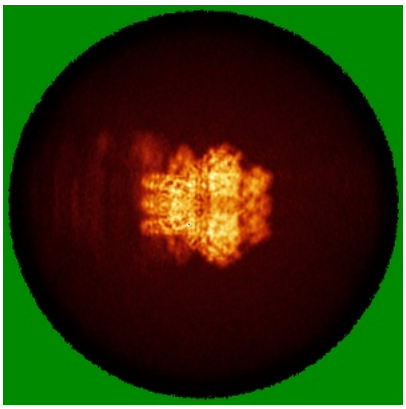
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

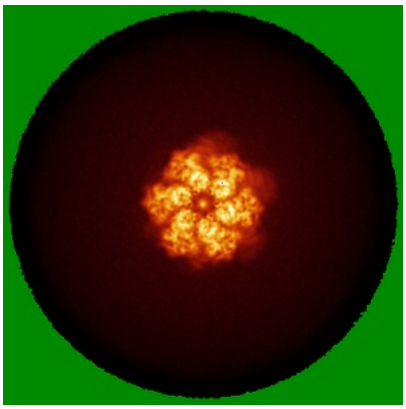
6.4.1 Primary map



X

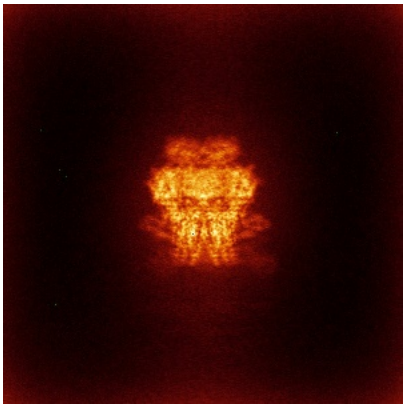


Y

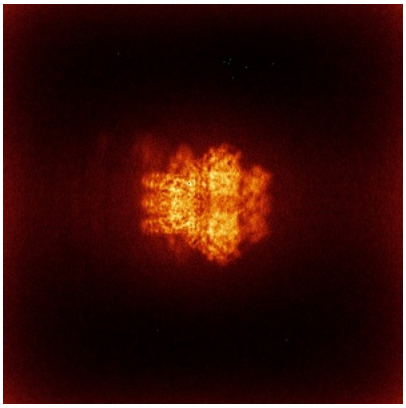


Z

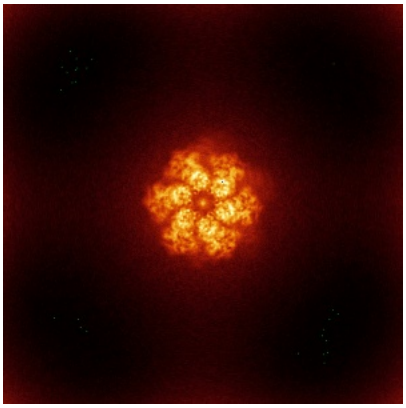
6.4.2 Raw map



X



Y

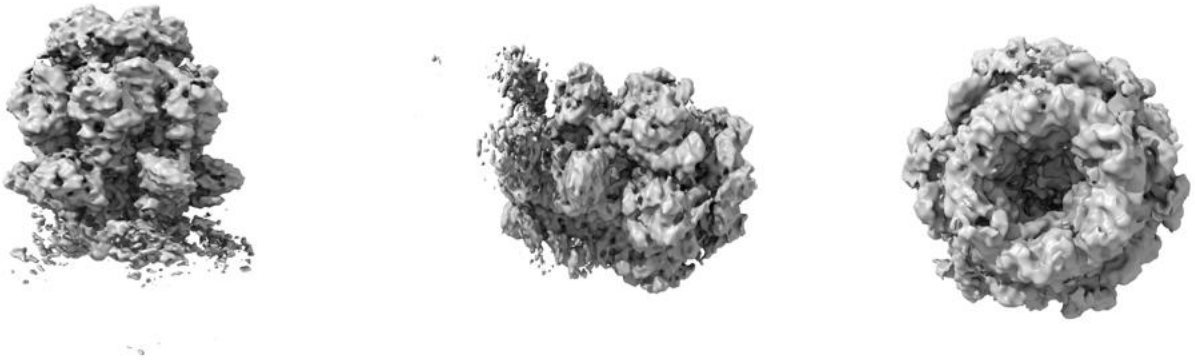


Z

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

6.5 Orthogonal surface views (i)

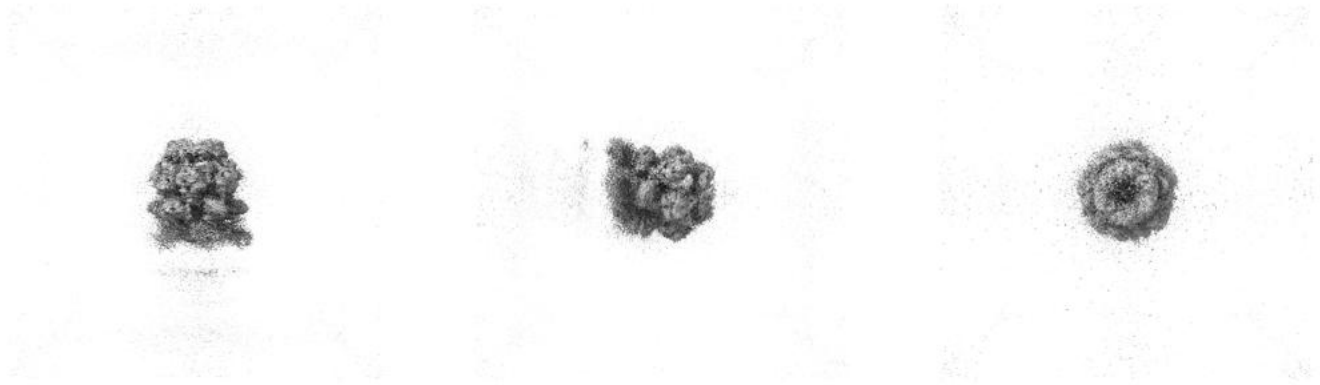
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

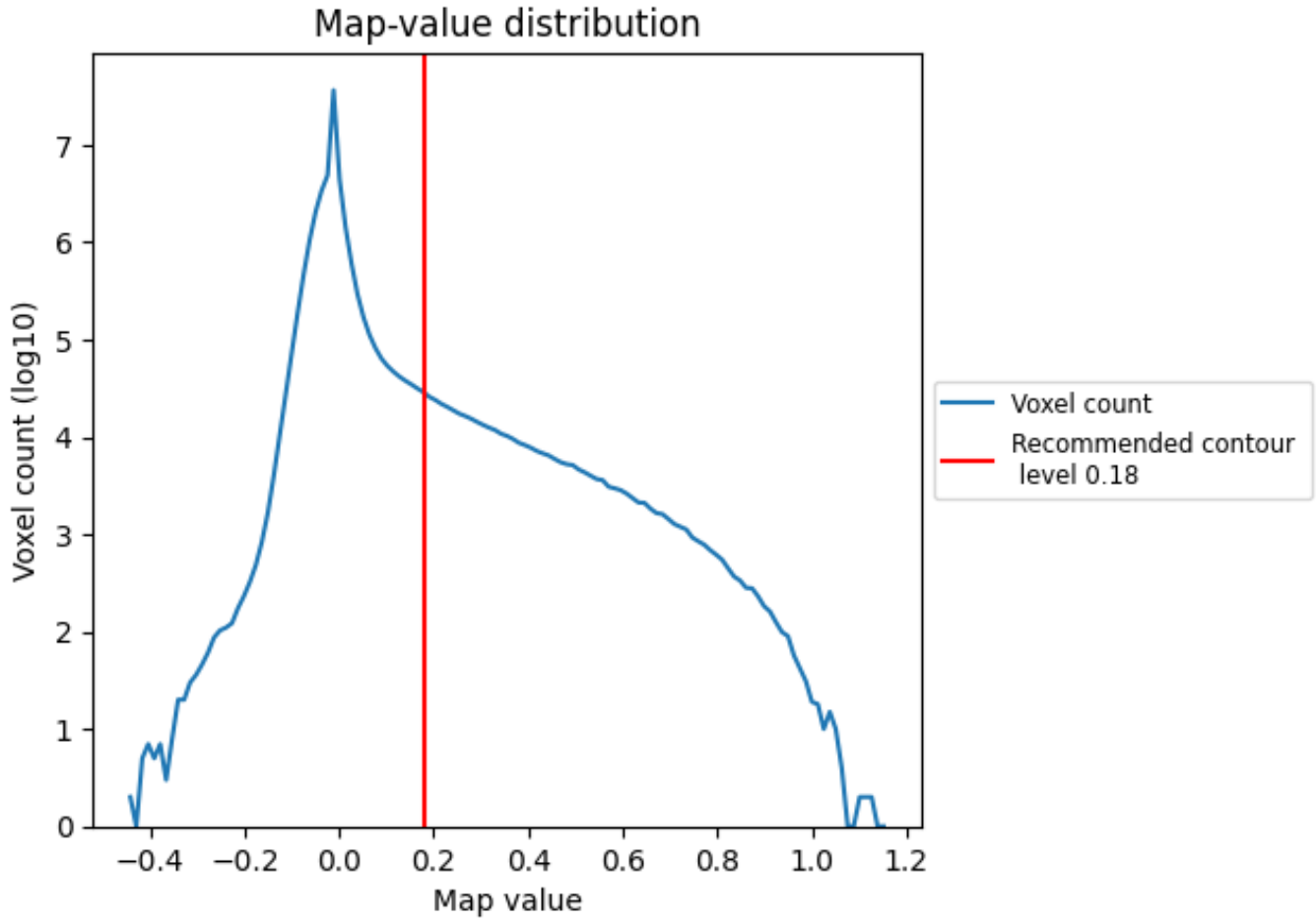
6.6 Mask visualisation (i)

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

7 Map analysis

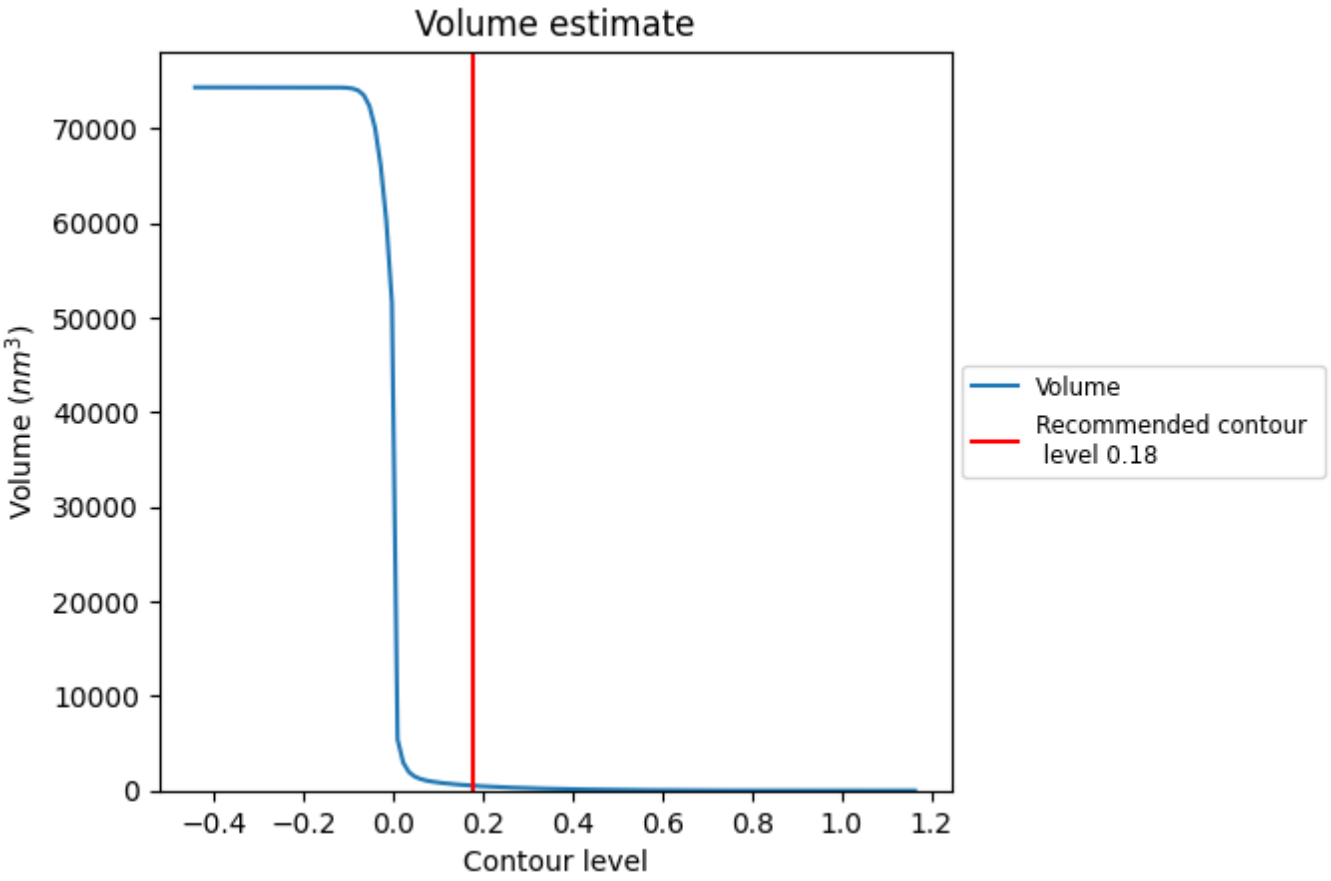
This section contains the results of statistical analysis of the map.

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.

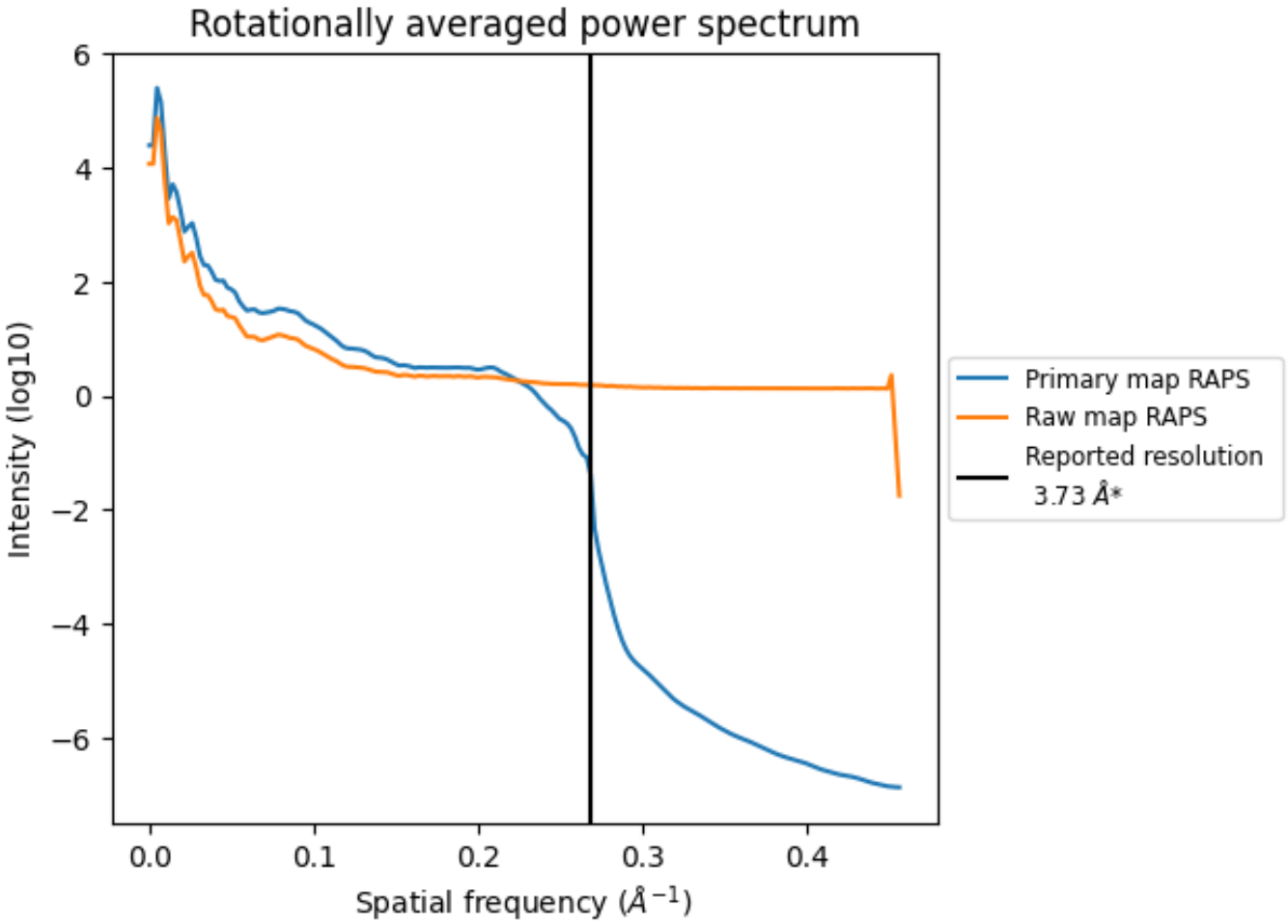
7.2 Volume estimate



The volume at the recommended contour level is 512 nm^3; this corresponds to an approximate mass of 463 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)

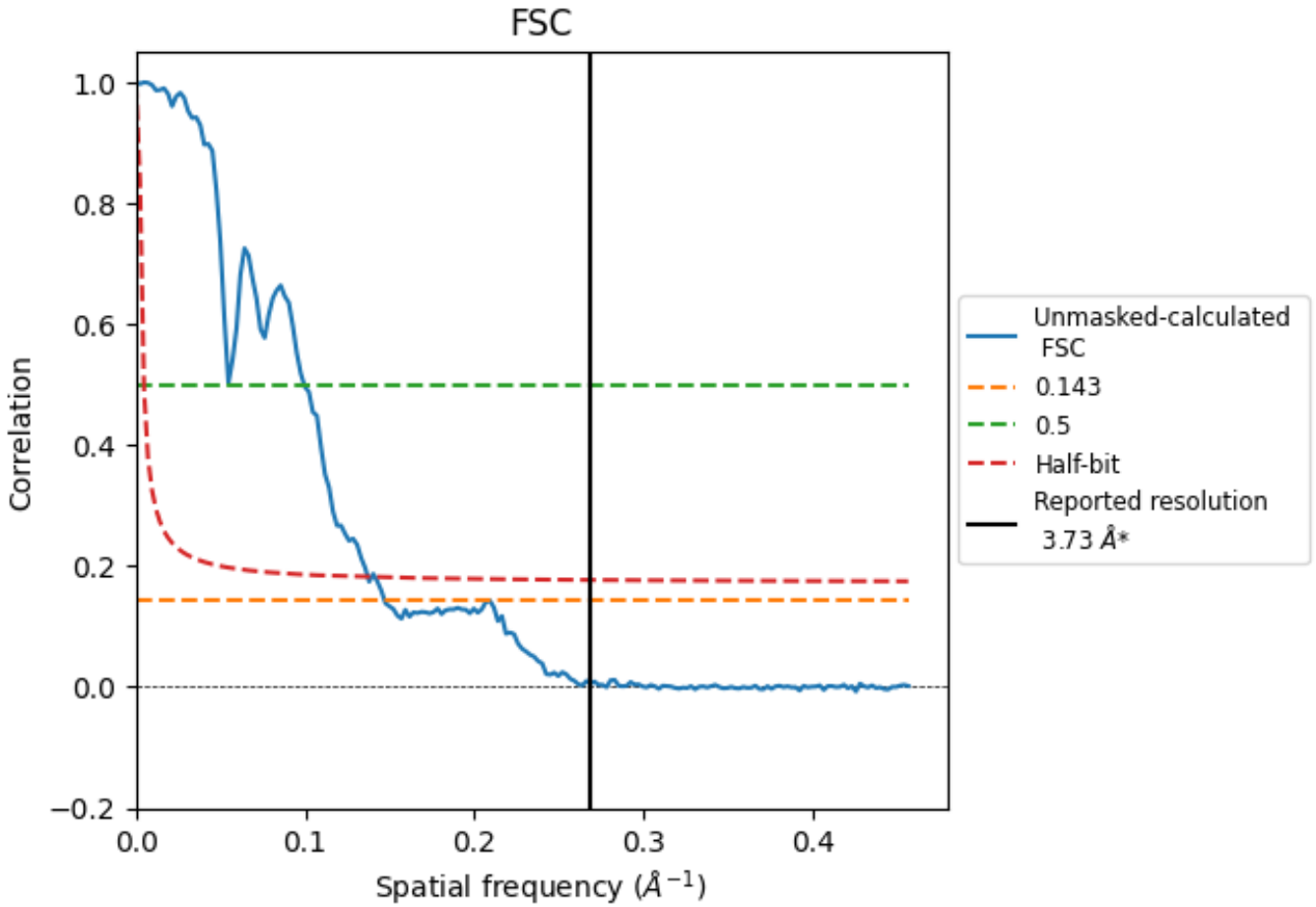


*Reported resolution corresponds to spatial frequency of 0.268 Å^{-1}

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 0.268 Å^{-1}

8.2 Resolution estimates (i)

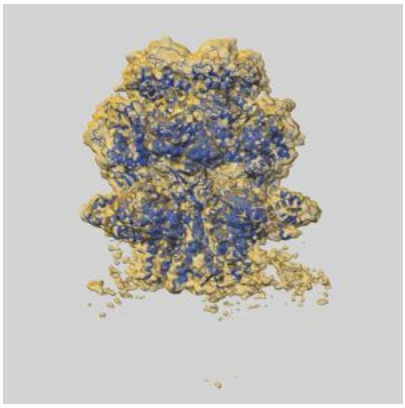
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.81	10.05	7.29

*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 6.81 differs from the reported value 3.73 by more than 10 %

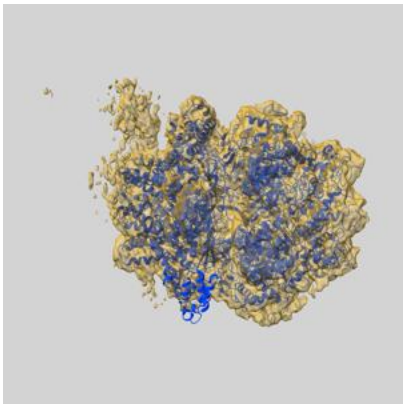
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37882 and PDB model 8WW6. Per-residue inclusion information can be found in section 3 on page 8.

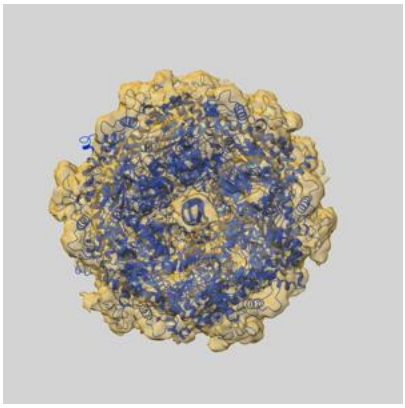
9.1 Map-model overlay



X



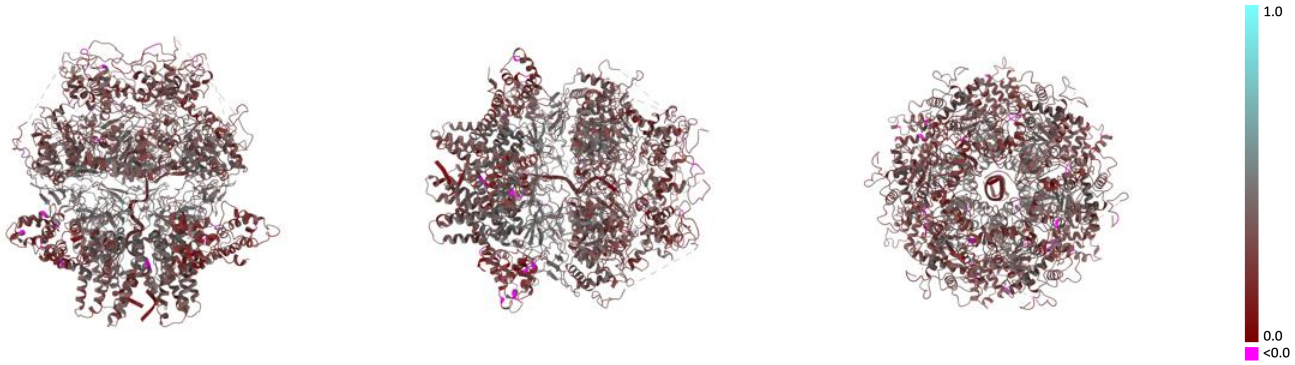
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

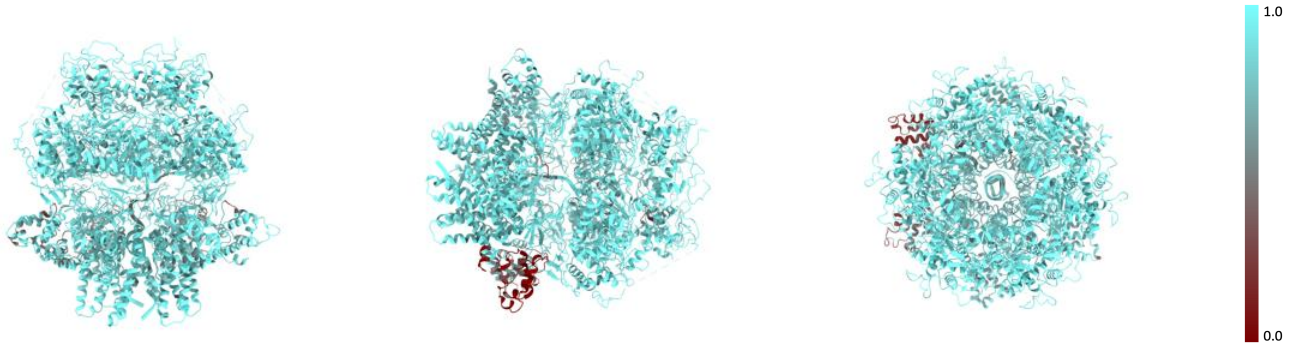
9.2 Q-score mapped to coordinate model (i)



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.

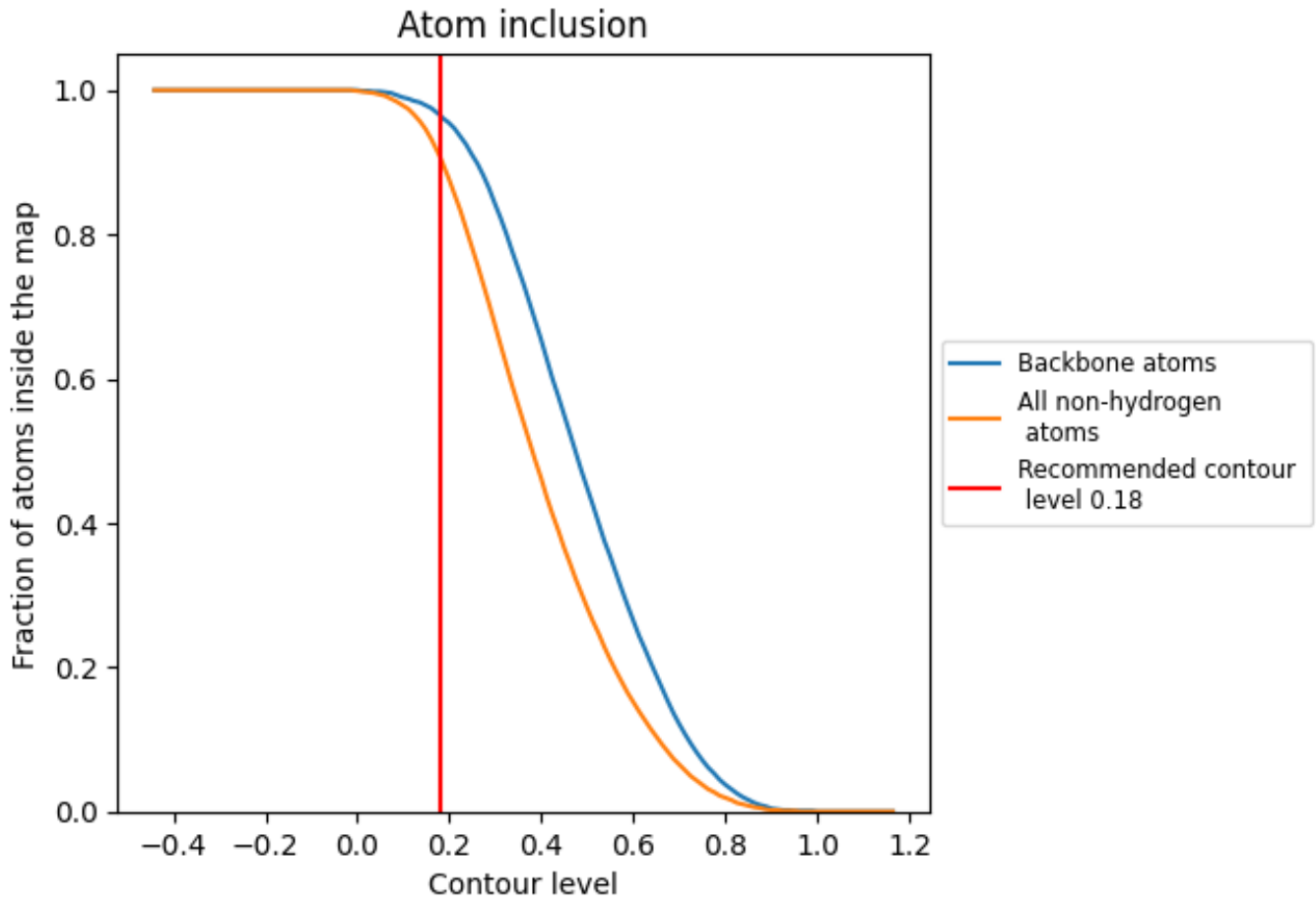
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.18).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.3260
A	0.8340	0.3170
B	0.8770	0.3250
C	0.9350	0.3340
D	0.9310	0.3390
E	0.9300	0.3360
F	0.9430	0.3270
H	0.8280	0.1500
I	0.9880	0.1090

