



## Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 03:01 AM JST

PDB ID : 6K32  
EMDB ID : EMD-9907  
Title : RdRp complex  
Authors : Li, X.W.  
Deposited on : 2019-05-16  
Resolution : 3.20 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

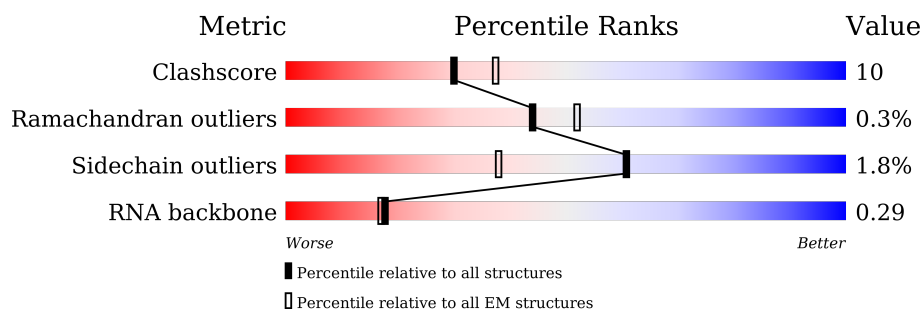
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1208	<div> <div>10%</div> <div>66%</div> <div>28%</div> <div>5%</div> </div>
2	B	559	<div> <div>7%</div> <div>58%</div> <div>26%</div> <div>11%</div> </div>
3	t	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
4	p	3	<div> <div>33%</div> <div>67%</div> </div>
5	C	1220	<div> <div>8%</div> <div>87%</div> <div>12%</div> </div>
6	D	1205	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
6	E	1205	<div> <div>8%</div> <div>89%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	1205	
7	G	1226	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	UTP	A	1306	-	-	X	-
9	MG7	A	1302	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 61364 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1208	Total	C	N	O	S	0	0
			9652	6124	1668	1824	36		

- Molecule 2 is a protein called Viral structural protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	498	Total	C	N	O	S	0	0
			3981	2552	662	749	18		

- Molecule 3 is a RNA chain called RNA (5'-R(P\*UP\*UP\*AP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	t	5	Total	C	N	O	P	0	0
			103	46	14	38	5		

- Molecule 4 is a RNA chain called RNA (5'-D(\*(3PO))-R(\*AP\*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	p	3	Total	C	N	O	P	0	0
			54	20	10	20	4		

- Molecule 5 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	1220	Total	C	N	O	S	0	0
			9622	6072	1676	1836	38		

- Molecule 6 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	1197	Total	C	N	O	S	0	0
			9447	5966	1645	1798	38		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	1191	Total	C	N	O	S	0	0
			9402	5937	1637	1791	37		
6	F	1191	Total	C	N	O	S	0	0
			9402	5937	1637	1791	37		

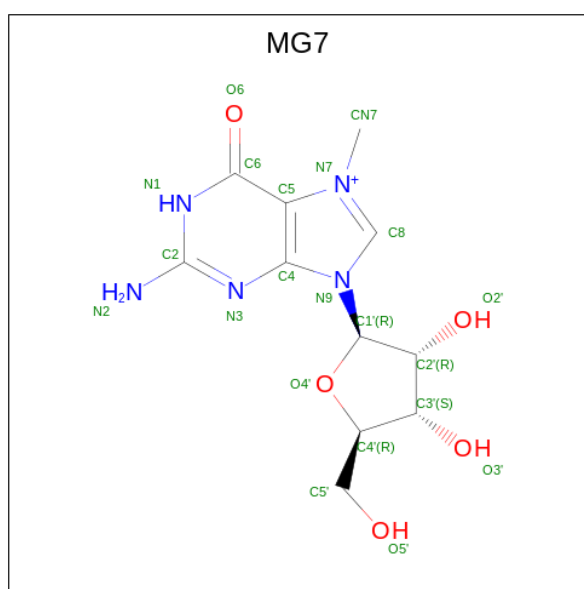
- Molecule 7 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	1218	Total	C	N	O	S	0	0
			9618	6073	1675	1832	38		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

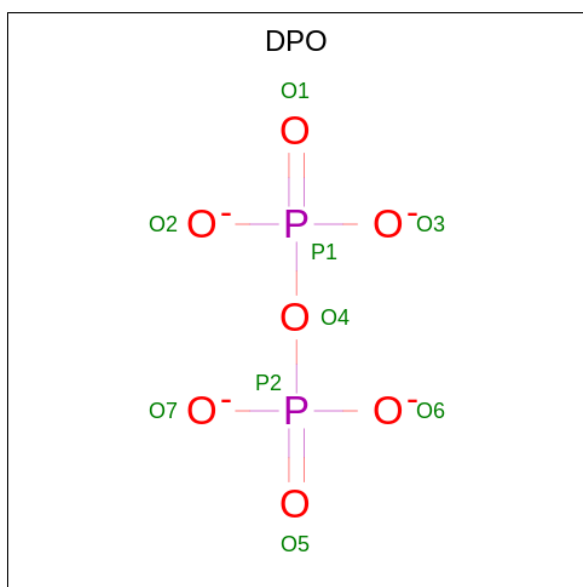
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Mg	0
			2	2	

- Molecule 9 is 7-METHYLGUANOSINE (three-letter code: MG7) (formula: C<sub>11</sub>H<sub>16</sub>N<sub>5</sub>O<sub>5</sub>).



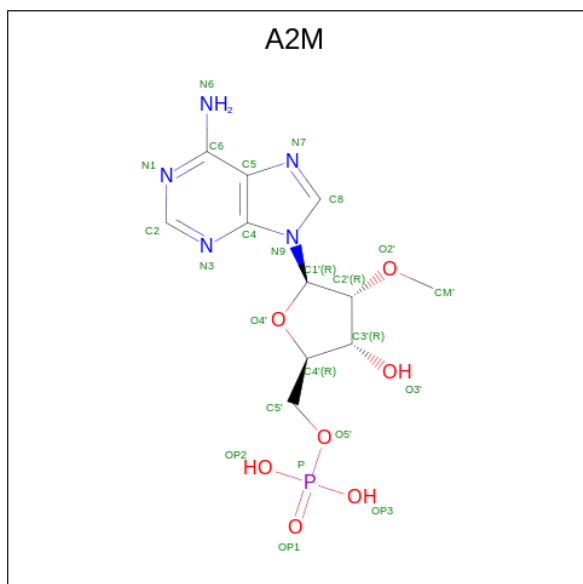
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			21	11	5	5	

- Molecule 10 is DIPHOSPHATE (three-letter code: DPO) (formula: O<sub>7</sub>P<sub>2</sub>).



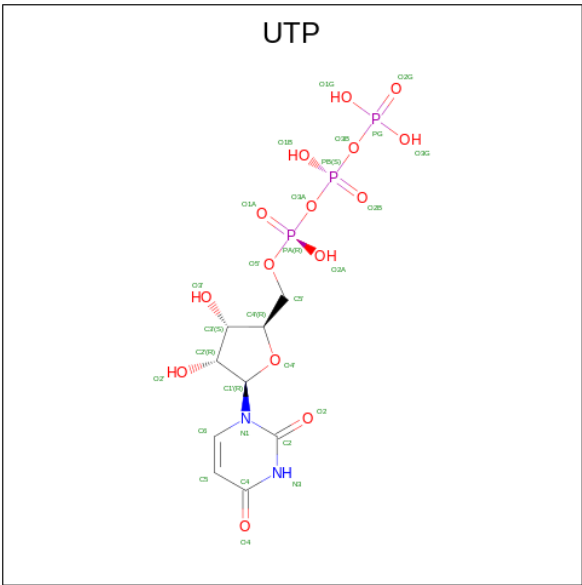
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	O	P	0
			8	6	2	

- Molecule 11 is 2'-O-methyladenosine 5'-(dihydrogen phosphate) (three-letter code: A2M) (formula:  $C_{11}H_{16}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			23	11	5	6	1	

- Molecule 12 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula:  $C_9H_{15}N_2O_{15}P_3$ ).

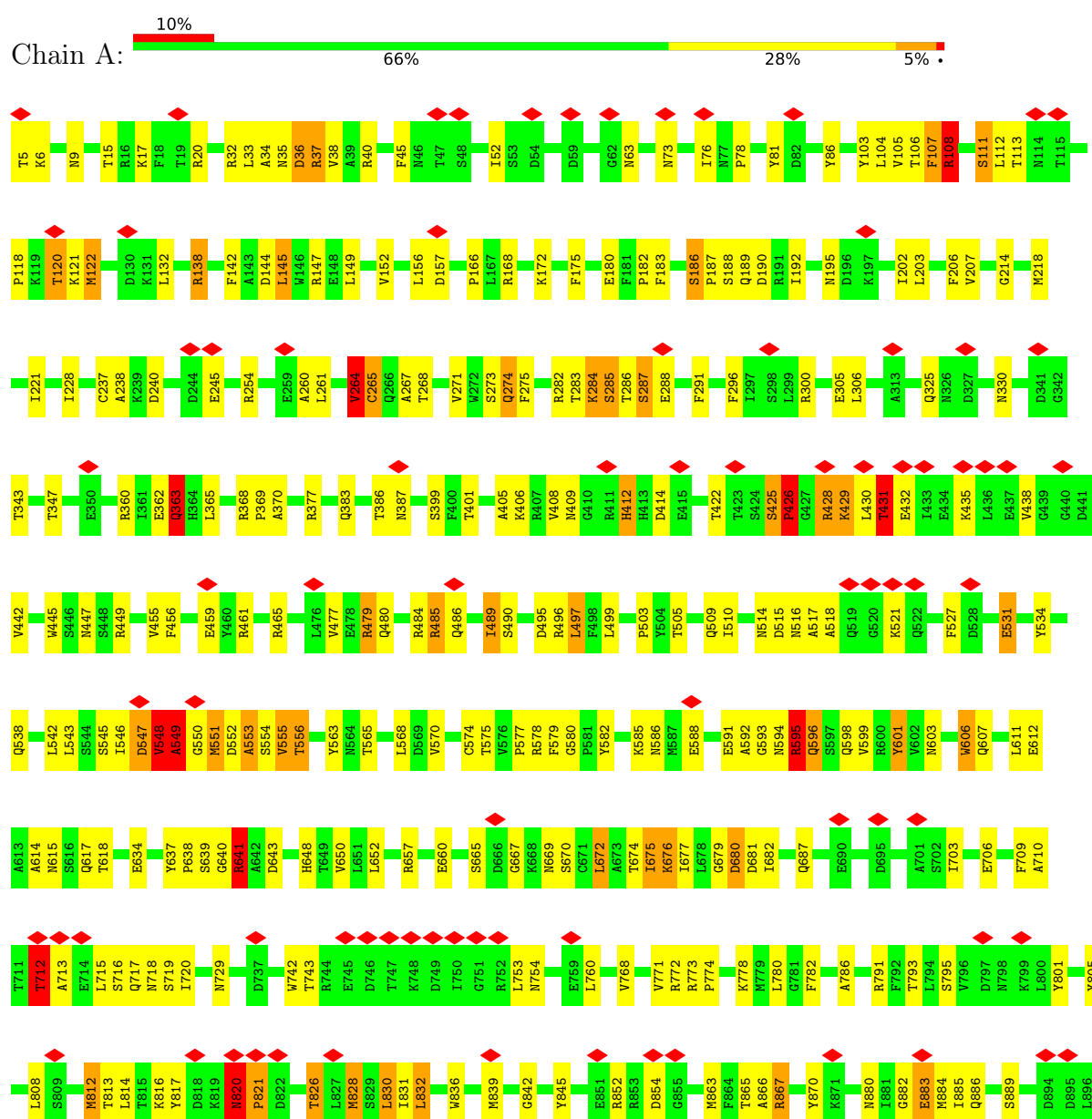


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	29	9	2	15	3	0

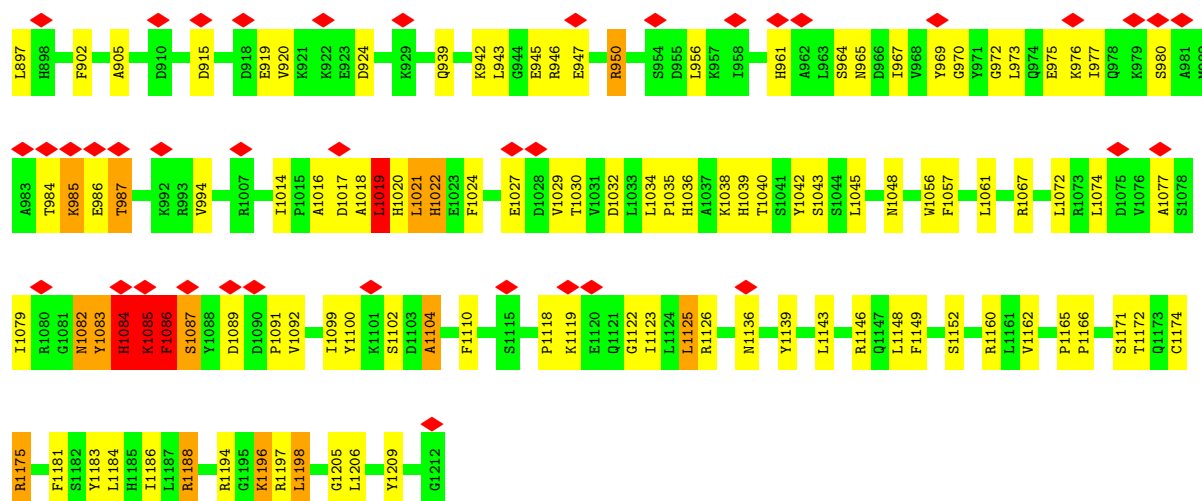
### 3 Residue-property plots

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

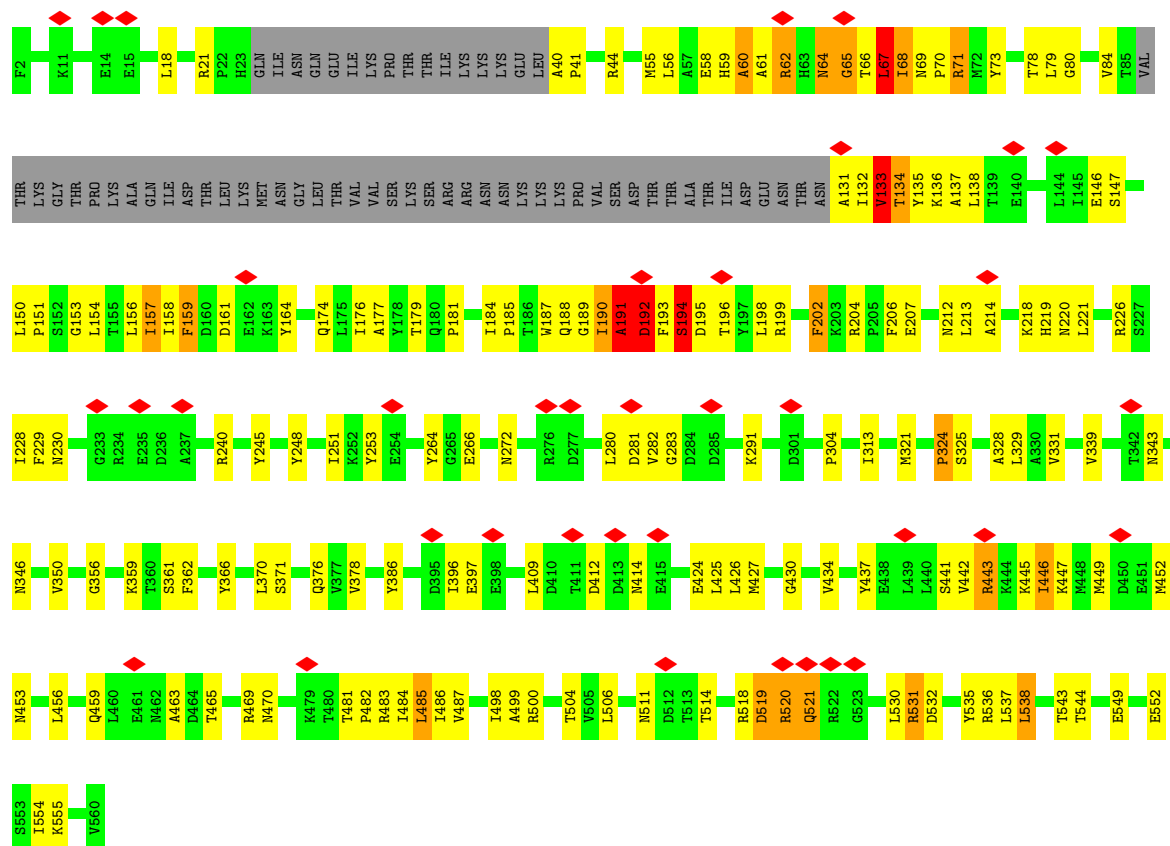
#### • Molecule 1: RNA-dependent RNA polymerase







• Molecule 2: Viral structural protein 4



• Molecule 3: RNA (5'-R(P\*UP\*UP\*AP\*CP\*U)-3')




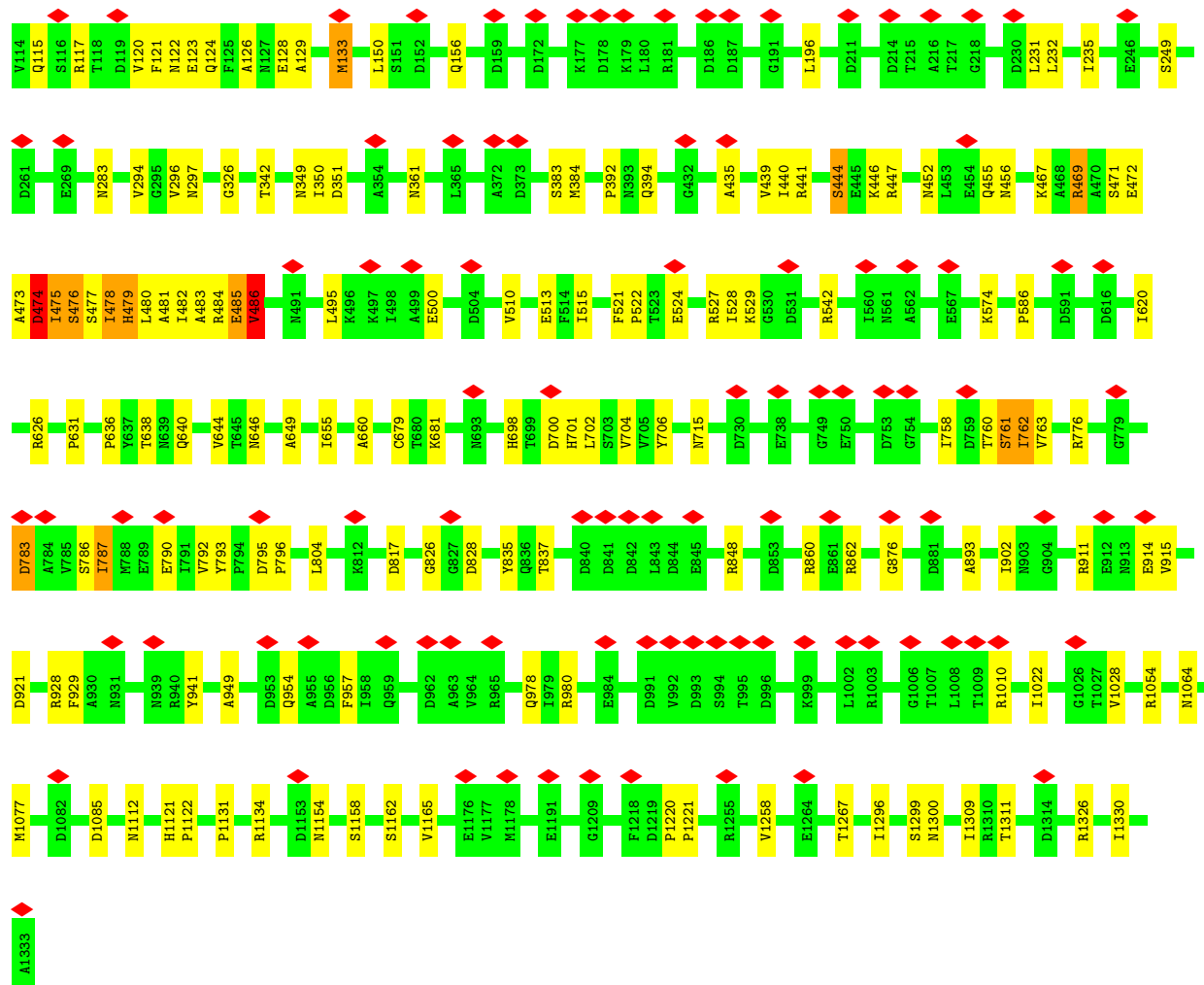
- Molecule 4: RNA (5'-D\*(3PO))-R(\*AP\*G)-3'

Chain p:  33% 67%




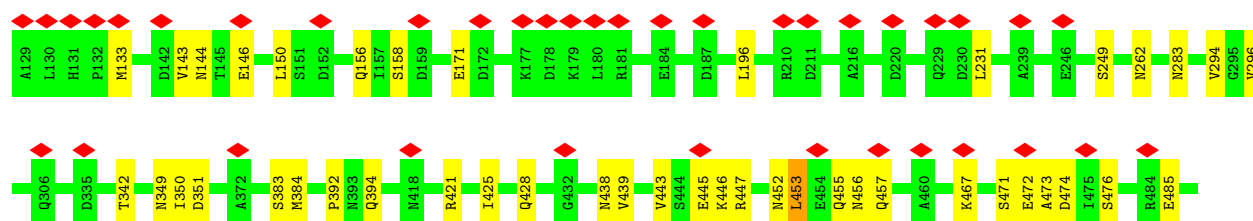
- Molecule 5: VP1

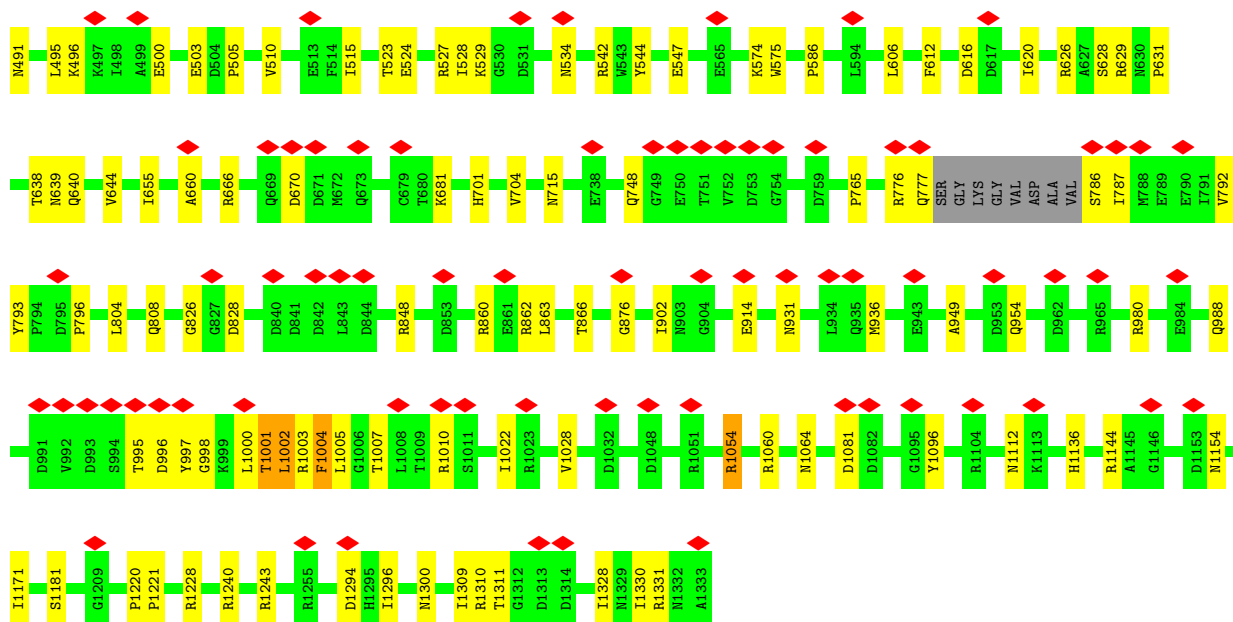
Chain C:  8% 87% 12%



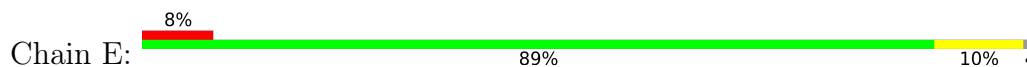
- Molecule 6: VP1

Chain D:  9% 87% 12%





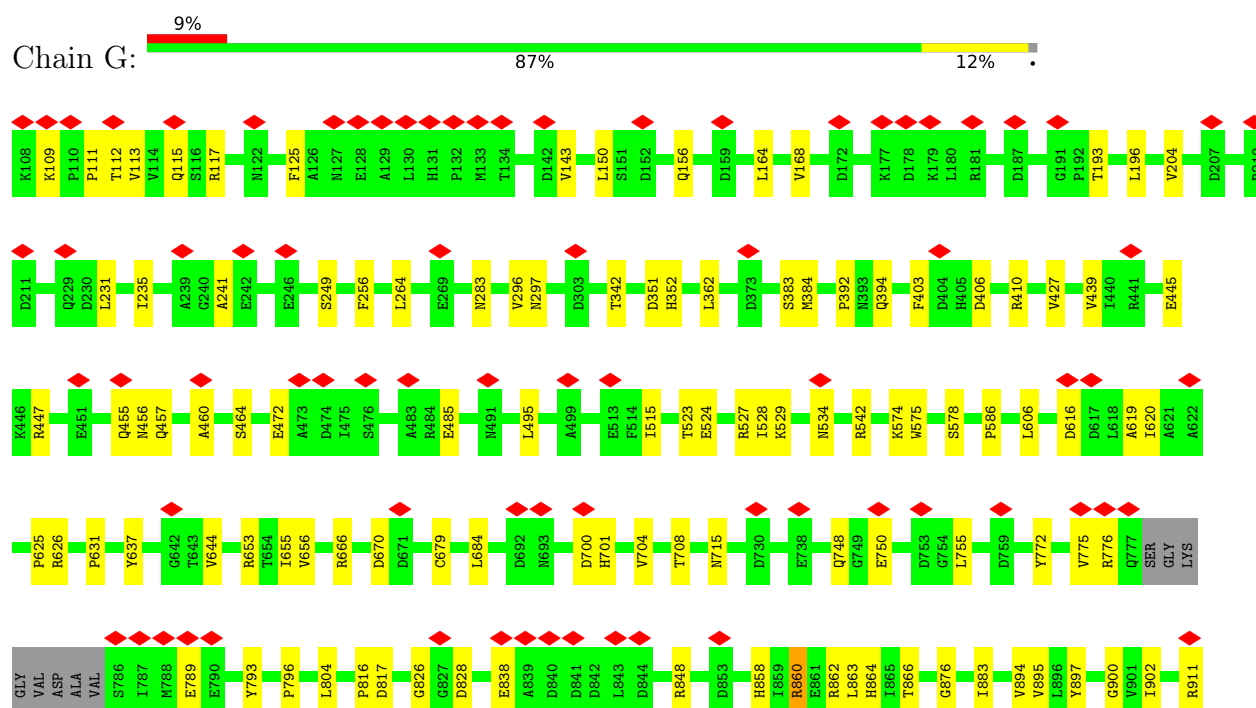
• Molecule 6: VP1

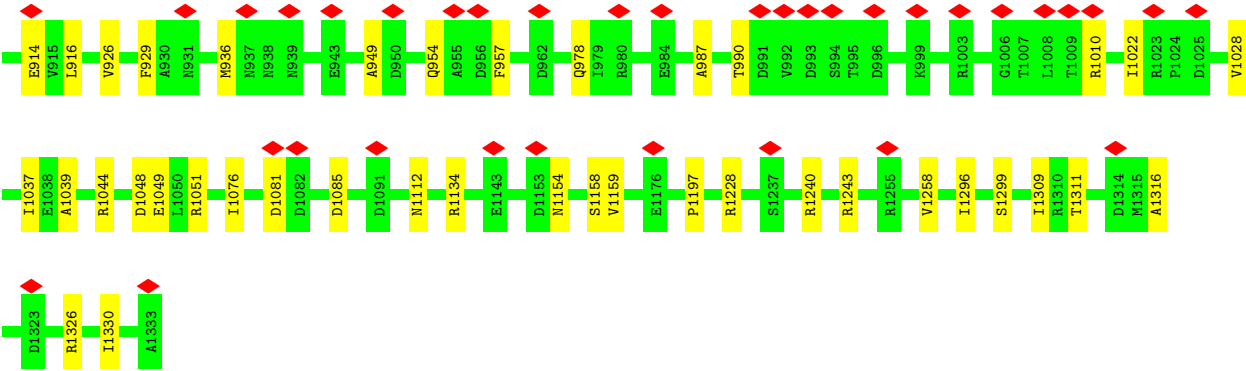


• Molecule 6: VP1



• Molecule 7: VP1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	161.942	Depositor
Minimum map value	-93.427	Depositor
Average map value	2.237	Depositor
Map value standard deviation	16.144	Depositor
Recommended contour level	25.0	Depositor
Map size ( $\text{\AA}$ )	285.75, 285.75, 285.75	wwPDB
Map dimensions	225, 225, 225	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.27, 1.27, 1.27	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PO, A2M, MG7, UTP, MG, DPO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.46	2/9859 (0.0%)	0.76	15/13346 (0.1%)
2	B	0.41	0/4067	0.73	3/5513 (0.1%)
3	t	6.72	26/113 (23.0%)	6.73	40/171 (23.4%)
4	p	2.68	2/46 (4.3%)	2.39	5/71 (7.0%)
5	C	0.35	0/9820	0.57	2/13367 (0.0%)
6	D	0.33	0/9642	0.54	0/13125
6	E	0.33	0/9595	0.54	0/13060
6	F	0.33	0/9595	0.54	0/13060
7	G	0.33	0/9817	0.55	1/13363 (0.0%)
All	All	0.47	30/62554 (0.0%)	0.67	66/85076 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	43
2	B	0	21
5	C	0	7
6	D	0	2
7	G	0	3
All	All	0	76

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	t	1	U	C5'-C4'	-31.53	1.13	1.51
3	t	1	U	C4'-O4'	23.68	1.76	1.45
3	t	1	U	C4'-C3'	-20.28	1.30	1.53
3	t	1	U	C3'-O3'	17.79	1.67	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	p	2	A	C5'-C4'	16.24	1.70	1.51
3	t	2	U	C3'-O3'	16.10	1.64	1.42
3	t	1	U	C3'-C2'	16.08	1.70	1.52
3	t	1	U	C4-O4	14.04	1.34	1.23
3	t	3	A	O3'-P	-13.65	1.44	1.61
3	t	2	U	C5'-C4'	-13.41	1.35	1.51
3	t	2	U	C4'-O4'	13.37	1.62	1.45
3	t	2	U	P-O5'	-12.06	1.47	1.59
3	t	1	U	C4-C5	-11.65	1.33	1.43
3	t	2	U	O4'-C1'	-11.49	1.26	1.41
3	t	2	U	C2'-O2'	11.30	1.56	1.41
3	t	5	U	C3'-O3'	-11.21	1.26	1.42
3	t	2	U	C2'-C1'	-11.01	1.41	1.53
1	A	1083	TYR	C-N	10.95	1.59	1.34
3	t	3	A	O5'-C5'	9.95	1.60	1.44
3	t	3	A	P-O5'	-9.85	1.50	1.59
3	t	2	U	O5'-C5'	-8.46	1.29	1.42
3	t	4	C	O3'-P	-7.94	1.51	1.61
3	t	1	U	O4'-C1'	7.79	1.51	1.41
3	t	1	U	OP3-P	-7.67	1.51	1.61
3	t	3	A	P-OP2	-6.80	1.37	1.49
3	t	2	U	C3'-C2'	-6.71	1.45	1.52
1	A	1082	ASN	C-N	6.36	1.48	1.34
4	p	2	A	C4'-O4'	6.25	1.53	1.45
3	t	1	U	O3'-P	-6.06	1.53	1.61
3	t	1	U	N3-C4	-5.16	1.33	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	t	1	U	O4'-C1'-N1	35.52	136.62	108.20
3	t	1	U	C5'-C4'-C3'	25.64	157.03	116.00
3	t	1	U	C5'-C4'-O4'	-23.09	81.39	109.10
3	t	1	U	N3-C4-C5	21.96	127.78	114.60
3	t	4	C	P-O3'-C3'	-20.39	95.23	119.70
3	t	1	U	C2-N3-C4	-20.29	114.82	127.00
3	t	1	U	C2'-C3'-O3'	-18.73	68.31	109.50
3	t	1	U	C1'-O4'-C4'	-17.81	95.65	109.90
3	t	2	U	P-O3'-C3'	-16.46	99.95	119.70
3	t	1	U	C4'-C3'-O3'	16.21	145.42	113.00
3	t	1	U	C5-C4-O4	-13.39	117.86	125.90
3	t	2	U	C1'-O4'-C4'	-12.93	99.56	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	t	1	U	O5'-C5'-C4'	11.55	133.65	111.70
3	t	2	U	OP1-P-OP2	-11.38	102.54	119.60
3	t	2	U	C1'-C2'-O2'	-11.31	76.66	110.60
3	t	3	A	O5'-C5'-C4'	11.18	132.94	111.70
3	t	3	A	O5'-P-OP1	-10.50	96.25	105.70
3	t	5	U	C4'-C3'-O3'	-10.38	87.61	109.40
2	B	192	ASP	CB-CG-OD1	10.33	127.59	118.30
3	t	1	U	N1-C2-N3	10.19	121.01	114.90
1	A	1086	PHE	CA-C-N	-10.06	95.07	117.20
3	t	1	U	O3'-P-O5'	10.00	123.00	104.00
1	A	497	LEU	CA-CB-CG	9.71	137.64	115.30
3	t	1	U	N3-C4-O4	-9.47	112.77	119.40
4	p	2	A	O4'-C4'-C3'	-8.87	95.13	104.00
3	t	1	U	P-O5'-C5'	-8.86	106.73	120.90
3	t	2	U	O3'-P-O5'	8.86	120.82	104.00
1	A	145	LEU	CA-CB-CG	8.84	135.64	115.30
3	t	3	A	O5'-P-OP2	-8.70	97.87	105.70
3	t	1	U	C3'-C2'-C1'	8.66	108.42	101.50
4	p	2	A	O3'-P-O5'	-8.62	87.61	104.00
3	t	2	U	OP2-P-O3'	8.50	123.91	105.20
3	t	2	U	C5'-C4'-O4'	8.40	119.18	109.10
4	p	2	A	P-O3'-C3'	8.26	129.61	119.70
1	A	1148	LEU	CA-CB-CG	7.93	133.53	115.30
2	B	280	LEU	CA-CB-CG	7.87	133.41	115.30
3	t	2	U	O5'-C5'-C4'	7.69	126.31	111.70
3	t	3	A	C5'-C4'-O4'	-7.49	100.11	109.10
1	A	830	LEU	CA-CB-CG	7.46	132.46	115.30
3	t	1	U	C1'-C2'-O2'	-7.43	88.31	110.60
3	t	1	U	C4-C5-C6	-7.29	115.33	119.70
3	t	2	U	N1-C1'-C2'	7.23	123.39	114.00
3	t	2	U	C2'-C3'-O3'	-7.15	93.77	109.50
3	t	2	U	C3'-C2'-C1'	7.05	107.14	101.50
1	A	854	ASP	C-N-CA	6.78	136.55	122.30
3	t	2	U	C4'-C3'-O3'	6.78	126.56	113.00
3	t	1	U	OP1-P-OP2	-6.69	109.57	119.60
1	A	33	LEU	CA-CB-CG	6.29	129.77	115.30
1	A	542	LEU	CA-CB-CG	6.28	129.74	115.30
3	t	2	U	O4'-C1'-C2'	6.27	113.24	107.60
1	A	1074	LEU	CA-CB-CG	6.15	129.44	115.30
5	C	1258	VAL	C-N-CA	6.13	137.03	121.70
1	A	1045	LEU	CA-CB-CG	6.12	129.38	115.30
4	p	2	A	OP2-P-O3'	6.10	118.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	2	A	C1'-O4'-C4'	-6.03	105.08	109.90
3	t	2	U	O4'-C4'-C3'	-5.93	98.06	104.00
3	t	1	U	C5-C6-N1	-5.88	119.76	122.70
5	C	485	GLU	CB-CA-C	5.60	121.59	110.40
7	G	1258	VAL	C-N-CA	5.41	135.22	121.70
1	A	753	LEU	CA-CB-CG	5.39	127.71	115.30
2	B	538	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	122	MET	CA-CB-CG	5.31	122.32	113.30
3	t	4	C	C4'-C3'-O3'	-5.30	98.27	109.40
1	A	515	ASP	C-N-CA	5.13	134.52	121.70
1	A	832	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	156	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1017	ASP	Peptide
1	A	1018	ALA	Peptide
1	A	1019	LEU	Peptide
1	A	1079	ILE	Peptide
1	A	1084	HIS	Mainchain
1	A	1085	LYS	Peptide
1	A	1086	PHE	Mainchain
1	A	1087	SER	Peptide
1	A	1102	SER	Peptide
1	A	1104	ALA	Peptide
1	A	120	THR	Peptide
1	A	186	SER	Peptide
1	A	264	VAL	Peptide
1	A	285	SER	Peptide
1	A	362	GLU	Peptide
1	A	363	GLN	Peptide
1	A	426	PRO	Peptide
1	A	429	LYS	Peptide
1	A	431	THR	Peptide
1	A	514	ASN	Peptide
1	A	517	ALA	Peptide
1	A	518	ALA	Peptide
1	A	52	ILE	Peptide
1	A	548	VAL	Peptide
1	A	549	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	553	ALA	Peptide
1	A	592	ALA	Peptide
1	A	593	GLY	Peptide
1	A	595	ARG	Peptide
1	A	614	ALA	Peptide
1	A	615	ASN	Peptide
1	A	641	ARG	Peptide
1	A	712	THR	Peptide
1	A	820	ASN	Peptide
1	A	821	PRO	Peptide
1	A	867	ARG	Peptide
1	A	924	ASP	Peptide
1	A	945	GLU	Peptide
1	A	964	SER	Peptide
1	A	972	GLY	Peptide
1	A	984	THR	Peptide
1	A	986	GLU	Peptide
1	A	987	THR	Peptide
2	B	131	ALA	Peptide
2	B	133	VAL	Peptide
2	B	153	GLY	Peptide
2	B	159	PHE	Peptide
2	B	188	GLN	Peptide
2	B	189	GLY	Peptide
2	B	191	ALA	Peptide
2	B	192	ASP	Peptide
2	B	194	SER	Peptide
2	B	202	PHE	Peptide
2	B	324	PRO	Peptide
2	B	441	SER	Peptide
2	B	519	ASP	Peptide
2	B	521	GLN	Peptide
2	B	531	ARG	Sidechain
2	B	60	ALA	Peptide
2	B	64	ASN	Peptide
2	B	65	GLY	Peptide
2	B	67	LEU	Peptide
2	B	68	ILE	Peptide
2	B	80	GLY	Peptide
5	C	472	GLU	Peptide
5	C	474	ASP	Peptide
5	C	475	ILE	Peptide

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Mol	Chain	Res	Type	Group
5	C	476	SER	Peptide
5	C	761	SER	Peptide
5	C	776	ARG	Peptide
5	C	786	SER	Peptide
6	D	452	ASN	Peptide
6	D	456	ASN	Peptide
7	G	109	LYS	Peptide
7	G	111	PRO	Peptide
7	G	578	SER	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9652	0	9538	477	0
2	B	3981	0	3985	264	0
3	t	103	0	52	0	0
4	p	54	0	21	0	0
5	C	9622	0	9521	169	0
6	D	9447	0	9360	164	0
6	E	9402	0	9314	67	0
6	F	9402	0	9314	75	0
7	G	9618	0	9526	100	0
8	A	2	0	0	0	0
9	A	21	0	5	7	0
10	A	8	0	0	1	0
11	A	23	0	10	5	0
12	A	29	0	9	13	0
All	All	61364	0	60655	1114	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 10.

All (1114) 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)
5:C:473:ALA:HB2	5:C:761:SER:CB	1.42	1.49
1:A:1077:ALA:HB2	1:A:1086:PHE:CE2	1.55	1.39
2:B:185:PRO:HG3	6:D:1000:LEU:CD2	1.51	1.36
5:C:473:ALA:CB	5:C:761:SER:HB2	1.59	1.31
2:B:185:PRO:CG	6:D:1000:LEU:HD22	1.61	1.29
1:A:489:ILE:HD13	1:A:490:SER:N	1.46	1.28
1:A:274:GLN:HE21	1:A:274:GLN:N	1.34	1.24
1:A:1082:ASN:O	1:A:1083:TYR:CD1	1.90	1.24
2:B:60:ALA:HB1	2:B:65:GLY:O	1.34	1.23
1:A:594:ASN:OD1	6:D:1007:THR:HG21	1.36	1.20
2:B:190:ILE:CD1	2:B:191:ALA:H	1.54	1.18
1:A:479:ARG:HG2	1:A:479:ARG:HH11	1.07	1.15
1:A:81:TYR:CE1	1:A:112:LEU:HD11	1.83	1.14
2:B:190:ILE:HD11	2:B:192:ASP:CG	1.65	1.14
2:B:194:SER:CB	6:D:995:THR:HB	1.78	1.13
5:C:440:ILE:HG21	5:C:478:ILE:HD11	1.23	1.13
2:B:194:SER:HB2	6:D:995:THR:HB	1.26	1.12
1:A:808:LEU:CB	1:A:814:LEU:HD11	1.78	1.11
1:A:550:GLY:HA2	12:A:1306:UTP:O1B	1.48	1.11
1:A:286:THR:HG22	1:A:718:ASN:ND2	1.66	1.11
1:A:1022:HIS:HD2	1:A:1181:PHE:CD2	1.69	1.10
1:A:1022:HIS:HD2	1:A:1181:PHE:CE2	1.70	1.10
1:A:1022:HIS:CD2	1:A:1181:PHE:CD2	2.39	1.09
2:B:443:ARG:HB3	5:C:133:MET:CE	1.82	1.09
6:D:425:ILE:HD11	6:D:1004:PHE:HD2	1.19	1.08
1:A:1172:THR:HG22	6:F:455:GLN:O	1.52	1.07
2:B:190:ILE:CD1	2:B:191:ALA:N	2.17	1.06
1:A:1194:ARG:NE	7:G:113:VAL:HG12	1.69	1.06
1:A:1166:PRO:HB2	6:F:451:GLU:OE1	1.54	1.06
2:B:190:ILE:HD12	2:B:191:ALA:N	1.68	1.05
5:C:440:ILE:CG2	5:C:478:ILE:HD11	1.85	1.05
1:A:274:GLN:H	1:A:274:GLN:NE2	1.53	1.05
1:A:795:SER:HB2	11:A:1304:A2M:HM'1	1.33	1.05
1:A:808:LEU:HB2	1:A:814:LEU:HD11	1.09	1.05
1:A:1077:ALA:CB	1:A:1086:PHE:CE2	2.39	1.05
1:A:1077:ALA:HB2	1:A:1086:PHE:CZ	1.90	1.04
2:B:41:PRO:HG2	6:D:146:GLU:HG3	1.38	1.04
2:B:41:PRO:HD2	6:D:146:GLU:OE2	1.56	1.03
2:B:59:HIS:ND1	2:B:137:ALA:HB1	1.73	1.03
2:B:443:ARG:HB3	5:C:133:MET:HE3	1.33	1.03
2:B:190:ILE:HD12	2:B:191:ALA:H	0.89	1.02
2:B:514:THR:HG21	5:C:120:VAL:HG13	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG22	1:A:718:ASN:HD21	1.15	1.01
1:A:428:ARG:HE	1:A:429:LYS:HA	1.20	1.01
1:A:551:MET:HB2	12:A:1306:UTP:O2A	1.58	1.01
2:B:378:VAL:CG1	2:B:484:ILE:HD11	1.90	1.01
5:C:485:GLU:OE2	5:C:522:PRO:HD2	1.59	1.01
1:A:188:SER:HB2	9:A:1302:MG7:O6	1.60	1.01
1:A:105:VAL:HG13	1:A:240:ASP:O	1.59	1.01
2:B:190:ILE:HD11	2:B:192:ASP:OD1	1.58	1.00
1:A:399:SER:OG	5:C:787:ILE:HG22	1.61	1.00
1:A:428:ARG:HD3	1:A:429:LYS:N	1.77	0.99
1:A:1022:HIS:CD2	1:A:1181:PHE:CE2	2.50	0.99
1:A:428:ARG:NE	1:A:429:LYS:HA	1.78	0.98
2:B:443:ARG:CB	5:C:133:MET:HE3	1.94	0.98
1:A:449:ARG:HH12	1:A:497:LEU:HG	1.28	0.98
6:D:473:ALA:HB2	6:D:765:PRO:HB3	1.44	0.98
1:A:81:TYR:CE1	1:A:112:LEU:CD1	2.46	0.98
1:A:1022:HIS:NE2	1:A:1181:PHE:CD1	2.32	0.97
1:A:186:SER:OG	9:A:1302:MG7:CN7	2.11	0.97
1:A:1057:PHE:CG	7:G:117:ARG:HD3	1.99	0.97
2:B:67:LEU:HB2	2:B:73:TYR:HE2	1.26	0.97
2:B:146:GLU:O	6:D:133:MET:HE2	1.65	0.97
2:B:147:SER:HA	6:D:133:MET:CG	1.95	0.96
1:A:489:ILE:HD13	1:A:490:SER:H	1.21	0.96
1:A:425:SER:HB3	1:A:426:PRO:CD	1.94	0.96
1:A:1162:VAL:HG22	1:A:1198:LEU:CD1	1.95	0.96
5:C:485:GLU:O	5:C:486:VAL:HG13	1.67	0.95
2:B:59:HIS:CE1	2:B:137:ALA:HB1	2.02	0.94
1:A:81:TYR:CD1	1:A:112:LEU:CD1	2.50	0.94
1:A:81:TYR:CD1	1:A:112:LEU:HD12	2.02	0.94
1:A:1166:PRO:HB2	6:F:451:GLU:CD	1.88	0.94
1:A:549:ALA:HA	12:A:1306:UTP:O1B	1.70	0.92
2:B:156:LEU:O	2:B:157:ILE:HG13	1.69	0.92
1:A:479:ARG:HH11	1:A:479:ARG:CG	1.81	0.92
2:B:378:VAL:HG12	2:B:484:ILE:HD11	1.50	0.91
2:B:41:PRO:HG2	6:D:146:GLU:CG	2.01	0.90
1:A:1057:PHE:HB2	7:G:117:ARG:HD3	1.53	0.90
1:A:1038:LYS:HB2	7:G:125:PHE:CE2	2.06	0.90
2:B:67:LEU:HB2	2:B:73:TYR:CE2	2.06	0.90
1:A:81:TYR:HE1	1:A:112:LEU:HD11	1.31	0.90
1:A:1162:VAL:HG22	1:A:1198:LEU:HD12	1.53	0.90
6:D:425:ILE:HD11	6:D:1004:PHE:CD2	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:VAL:HG11	1:A:709:PHE:HB3	1.53	0.89
2:B:443:ARG:CB	5:C:133:MET:CE	2.50	0.89
1:A:674:THR:HB	5:C:444:SER:HB2	1.55	0.89
1:A:795:SER:CB	11:A:1304:A2M:HM'1	2.03	0.88
1:A:674:THR:CB	5:C:444:SER:HB2	2.03	0.88
1:A:596:GLN:HA	1:A:596:GLN:NE2	1.88	0.88
2:B:442:VAL:HG21	5:C:128:GLU:HG3	1.54	0.88
1:A:144:ASP:OD2	10:A:1303:DPO:O3	1.92	0.87
2:B:190:ILE:HD13	2:B:192:ASP:N	1.89	0.87
1:A:81:TYR:HB2	1:A:111:SER:OG	1.75	0.87
1:A:104:LEU:HB2	1:A:132:LEU:HD21	1.56	0.87
2:B:60:ALA:CB	2:B:65:GLY:O	2.22	0.87
2:B:378:VAL:HG12	2:B:484:ILE:CD1	2.05	0.86
1:A:521:LYS:HD3	1:A:1084:HIS:HD1	1.40	0.86
2:B:514:THR:HB	2:B:531:ARG:HH11	1.41	0.85
2:B:264:TYR:HE1	5:C:115:GLN:O	1.59	0.85
2:B:452:MET:HE2	2:B:530:LEU:CD2	2.05	0.85
2:B:264:TYR:CG	5:C:117:ARG:HG2	2.11	0.85
2:B:147:SER:HA	6:D:133:MET:CE	2.07	0.85
1:A:104:LEU:HB2	1:A:132:LEU:CD2	2.07	0.85
1:A:274:GLN:N	1:A:274:GLN:NE2	2.20	0.84
1:A:449:ARG:NH1	1:A:497:LEU:HG	1.93	0.84
1:A:596:GLN:HA	1:A:596:GLN:HE21	1.42	0.84
1:A:1057:PHE:CB	7:G:117:ARG:HD3	2.07	0.84
1:A:386:THR:HG22	5:C:129:ALA:HB2	1.60	0.84
1:A:551:MET:CB	12:A:1306:UTP:O2A	2.25	0.84
2:B:185:PRO:HG3	6:D:1000:LEU:HD22	0.85	0.83
1:A:428:ARG:HD3	1:A:429:LYS:CA	2.08	0.83
2:B:483:ARG:HG2	2:B:484:ILE:HG23	1.60	0.83
2:B:518:ARG:NH1	5:C:115:GLN:NE2	2.26	0.83
1:A:595:ARG:HG2	1:A:595:ARG:HH11	1.43	0.82
1:A:795:SER:HB2	11:A:1304:A2M:CM'	2.09	0.82
1:A:1022:HIS:CD2	1:A:1181:PHE:CG	2.66	0.82
1:A:274:GLN:HB3	5:C:446:LYS:HE2	1.60	0.82
2:B:156:LEU:O	2:B:157:ILE:CG1	2.27	0.82
1:A:399:SER:CB	5:C:787:ILE:HG22	2.10	0.82
1:A:550:GLY:CA	12:A:1306:UTP:O1B	2.26	0.81
2:B:452:MET:HE2	2:B:530:LEU:HD21	1.62	0.81
1:A:286:THR:CG2	1:A:718:ASN:HD21	1.93	0.81
2:B:378:VAL:HG12	2:B:484:ILE:CG1	2.09	0.81
1:A:665:SER:HA	5:C:790:GLU:HG2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:PRO:HD2	5:C:123:GLU:HG2	1.62	0.81
1:A:606:TRP:HA	1:A:606:TRP:HE3	1.42	0.81
1:A:672:LEU:HD23	1:A:672:LEU:O	1.81	0.81
1:A:801:TYR:OH	1:A:816:LYS:HG3	1.81	0.81
1:A:1194:ARG:HE	7:G:113:VAL:CG1	1.94	0.80
1:A:606:TRP:HA	1:A:606:TRP:CE3	2.13	0.80
1:A:1057:PHE:CD1	7:G:117:ARG:HD3	2.16	0.80
1:A:1082:ASN:O	1:A:1083:TYR:CG	2.34	0.80
1:A:489:ILE:CD1	1:A:490:SER:N	2.40	0.80
6:D:998:GLY:O	6:D:1001:THR:HG22	1.80	0.80
1:A:265:CYS:SG	1:A:285:SER:OG	2.38	0.80
2:B:190:ILE:CD1	2:B:192:ASP:OD1	2.29	0.80
2:B:339:VAL:HG23	2:B:484:ILE:HD13	1.64	0.80
1:A:105:VAL:CG1	1:A:240:ASP:O	2.29	0.80
1:A:1077:ALA:HB2	1:A:1086:PHE:HE2	1.41	0.80
1:A:808:LEU:HB2	1:A:814:LEU:CD1	2.04	0.80
1:A:531:GLU:OE2	1:A:674:THR:HG21	1.81	0.80
2:B:442:VAL:HG22	5:C:124:GLN:NE2	1.97	0.80
2:B:147:SER:HA	6:D:133:MET:HG2	1.63	0.79
2:B:190:ILE:HD13	2:B:192:ASP:H	1.47	0.79
1:A:549:ALA:CA	12:A:1306:UTP:O1B	2.29	0.79
2:B:190:ILE:HD13	2:B:191:ALA:N	1.95	0.79
1:A:1162:VAL:CG2	1:A:1198:LEU:CD1	2.60	0.79
1:A:489:ILE:CG1	1:A:639:SER:O	2.30	0.79
1:A:37:ARG:HB2	1:A:37:ARG:CZ	2.13	0.78
1:A:428:ARG:CD	1:A:429:LYS:HA	2.14	0.78
1:A:430:LEU:HD11	1:A:435:LYS:NZ	1.97	0.78
1:A:1194:ARG:HE	7:G:113:VAL:HG12	1.44	0.78
1:A:793:THR:HG21	11:A:1304:A2M:OP1	1.83	0.78
6:F:452:ASN:ND2	7:G:460:ALA:HB1	1.99	0.78
1:A:479:ARG:HG2	1:A:479:ARG:NH1	1.89	0.78
5:C:473:ALA:CB	5:C:761:SER:CB	2.38	0.78
1:A:1194:ARG:NE	7:G:113:VAL:CG1	2.48	0.77
1:A:577:PRO:HG3	6:D:476:SER:OG	1.86	0.76
2:B:221:LEU:HD22	2:B:226:ARG:HD3	1.67	0.76
2:B:78:THR:HA	2:B:154:LEU:O	1.86	0.76
2:B:150:LEU:HD11	2:B:154:LEU:HD21	1.67	0.76
2:B:187:TRP:HB2	2:B:192:ASP:OD2	1.86	0.76
2:B:147:SER:CB	6:D:133:MET:HG3	2.17	0.75
2:B:378:VAL:HG11	2:B:484:ILE:HD11	1.66	0.75
2:B:339:VAL:CG2	2:B:484:ILE:HD13	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:MET:CE	2:B:530:LEU:HD21	2.16	0.75
2:B:514:THR:HG21	5:C:120:VAL:CG1	2.17	0.75
1:A:37:ARG:HA	1:A:40:ARG:NH2	2.02	0.74
1:A:370:ALA:HB1	5:C:126:ALA:HA	1.67	0.74
2:B:518:ARG:HH11	5:C:115:GLN:NE2	1.85	0.74
2:B:442:VAL:CG2	5:C:124:GLN:HE21	1.99	0.74
1:A:284:LYS:NZ	1:A:718:ASN:HD22	1.85	0.74
2:B:190:ILE:CD1	2:B:192:ASP:CG	2.52	0.74
6:F:452:ASN:HD21	7:G:460:ALA:HB1	1.53	0.74
1:A:1022:HIS:NE2	1:A:1181:PHE:CG	2.55	0.74
1:A:108:ARG:HG3	1:A:108:ARG:O	1.88	0.74
2:B:67:LEU:N	2:B:67:LEU:HD12	2.02	0.74
1:A:406:LYS:HE3	6:D:496:LYS:HE3	1.68	0.74
6:D:473:ALA:CB	6:D:765:PRO:HB3	2.17	0.74
1:A:591:GLU:O	1:A:594:ASN:N	2.21	0.73
2:B:156:LEU:C	2:B:157:ILE:HG13	2.09	0.73
5:C:435:ALA:HA	5:C:479:HIS:CE1	2.23	0.73
1:A:594:ASN:OD1	6:D:1007:THR:CG2	2.29	0.73
2:B:147:SER:HB2	6:D:133:MET:HG3	1.70	0.73
2:B:147:SER:CA	6:D:133:MET:CG	2.66	0.73
1:A:531:GLU:OE2	1:A:674:THR:CG2	2.37	0.73
2:B:251:ILE:HD12	2:B:251:ILE:O	1.88	0.73
1:A:363:GLN:N	1:A:363:GLN:OE1	2.22	0.73
1:A:555:VAL:O	1:A:556:THR:O	2.07	0.73
2:B:151:PRO:HG3	6:D:144:ASN:ND2	2.04	0.73
5:C:474:ASP:OD1	5:C:474:ASP:N	2.15	0.73
2:B:156:LEU:CD1	2:B:179:THR:HG21	2.20	0.72
2:B:185:PRO:CB	6:D:1000:LEU:HD22	2.18	0.72
1:A:425:SER:HB3	1:A:426:PRO:HD3	1.72	0.72
1:A:882:GLY:O	1:A:885:ILE:HG13	1.89	0.72
2:B:425:LEU:O	2:B:425:LEU:HD12	1.89	0.72
1:A:430:LEU:HD11	1:A:435:LYS:HZ3	1.54	0.72
1:A:808:LEU:HD23	1:A:814:LEU:HD21	1.72	0.72
1:A:186:SER:OG	9:A:1302:MG7:H71	1.90	0.71
1:A:665:SER:HA	5:C:790:GLU:CG	2.20	0.71
2:B:147:SER:CA	6:D:133:MET:HG2	2.20	0.71
2:B:190:ILE:O	2:B:191:ALA:HB3	1.88	0.71
2:B:304:PRO:CD	5:C:123:GLU:HG2	2.19	0.71
6:D:421:ARG:NH2	6:D:1004:PHE:HE1	1.87	0.71
2:B:220:ASN:HD21	6:D:1310:ARG:NH1	1.88	0.71
2:B:485:LEU:HD23	2:B:485:LEU:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:ARG:HB3	5:C:133:MET:HE1	1.71	0.71
1:A:667:GLY:HA2	5:C:792:VAL:HG13	1.73	0.71
1:A:449:ARG:HH12	1:A:497:LEU:CG	2.02	0.70
1:A:274:GLN:HE21	1:A:274:GLN:H	0.73	0.70
1:A:489:ILE:HD13	1:A:489:ILE:C	2.12	0.70
1:A:405:ALA:O	1:A:409:ASN:HB2	1.91	0.70
1:A:425:SER:HB3	1:A:426:PRO:HD2	1.73	0.70
2:B:442:VAL:HG21	5:C:128:GLU:CG	2.22	0.70
5:C:473:ALA:HB2	5:C:761:SER:HB3	1.63	0.70
5:C:1064:ASN:HD21	5:C:1296:ILE:HD11	1.56	0.70
1:A:271:VAL:HG11	1:A:282:ARG:HD3	1.73	0.70
5:C:480:LEU:O	5:C:480:LEU:HD12	1.92	0.70
2:B:229:PHE:HA	2:B:251:ILE:HD11	1.74	0.70
1:A:406:LYS:HE3	6:D:496:LYS:CE	2.22	0.69
2:B:56:LEU:CD2	2:B:67:LEU:HD23	2.21	0.69
1:A:574:CYS:HG	1:A:575:THR:H	1.38	0.69
2:B:185:PRO:HG3	6:D:1000:LEU:CG	2.21	0.69
1:A:554:SER:O	1:A:556:THR:N	2.25	0.69
5:C:513:GLU:CG	5:C:760:THR:O	2.41	0.69
6:D:425:ILE:CD1	6:D:1004:PHE:HD2	2.02	0.69
6:F:452:ASN:ND2	7:G:460:ALA:CB	2.55	0.69
2:B:190:ILE:O	2:B:191:ALA:CB	2.40	0.69
1:A:36:ASP:O	1:A:40:ARG:CZ	2.41	0.69
2:B:18:LEU:HB3	2:B:202:PHE:HE2	1.58	0.69
2:B:67:LEU:HD22	2:B:73:TYR:CD2	2.27	0.69
5:C:435:ALA:HA	5:C:479:HIS:HE1	1.56	0.69
1:A:808:LEU:CD2	1:A:814:LEU:HD21	2.23	0.69
2:B:41:PRO:CD	6:D:146:GLU:OE2	2.38	0.69
2:B:146:GLU:O	6:D:133:MET:CE	2.41	0.69
1:A:1022:HIS:NE2	1:A:1181:PHE:CE1	2.55	0.68
1:A:425:SER:CB	1:A:426:PRO:CD	2.69	0.68
1:A:1057:PHE:CG	7:G:117:ARG:CD	2.74	0.68
1:A:406:LYS:CE	6:D:496:LYS:HE3	2.23	0.68
1:A:485:ARG:CD	1:A:485:ARG:H	2.07	0.68
1:A:428:ARG:HD3	1:A:429:LYS:HA	1.76	0.68
1:A:426:PRO:HA	1:A:447:ASN:O	1.94	0.67
1:A:568:LEU:HD22	1:A:606:TRP:CZ3	2.30	0.67
1:A:268:THR:HG22	1:A:283:THR:HB	1.76	0.67
1:A:598:GLN:HG3	1:A:598:GLN:O	1.94	0.67
1:A:1036:HIS:HA	1:A:1039:HIS:HD2	1.60	0.67
1:A:37:ARG:HG3	1:A:40:ARG:NH2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:ILE:HG22	1:A:1016:ALA:H	1.59	0.67
1:A:1082:ASN:O	1:A:1083:TYR:CE1	2.48	0.67
1:A:1027:GLU:OE1	1:A:1197:ARG:NH1	2.27	0.66
1:A:386:THR:CG2	5:C:129:ALA:HB2	2.26	0.66
1:A:284:LYS:NZ	1:A:729:ASN:HD22	1.93	0.66
1:A:430:LEU:CD1	1:A:435:LYS:NZ	2.58	0.66
1:A:521:LYS:HE2	1:A:1084:HIS:CE1	2.30	0.66
2:B:62:ARG:NH1	2:B:62:ARG:HG2	2.10	0.66
5:C:383:SER:HB3	5:C:796:PRO:HG3	1.77	0.66
6:D:453:LEU:C	6:D:453:LEU:HD23	2.16	0.66
1:A:218:MET:HG2	1:A:780:LEU:HB2	1.78	0.66
1:A:36:ASP:N	1:A:36:ASP:OD1	2.29	0.66
1:A:78:PRO:HB2	1:A:108:ARG:HB3	1.77	0.66
2:B:378:VAL:HG12	2:B:484:ILE:HG13	1.78	0.65
1:A:36:ASP:O	1:A:40:ARG:NH1	2.30	0.65
2:B:264:TYR:CE1	5:C:115:GLN:O	2.45	0.65
2:B:531:ARG:HH22	5:C:122:ASN:ND2	1.94	0.65
1:A:985:LYS:HD2	1:A:987:THR:HG23	1.79	0.65
2:B:147:SER:HA	6:D:133:MET:HG3	1.79	0.65
1:A:399:SER:OG	5:C:787:ILE:CG2	2.41	0.65
2:B:147:SER:HA	6:D:133:MET:HE2	1.78	0.65
5:C:481:ALA:O	5:C:484:ARG:N	2.29	0.65
1:A:1022:HIS:CD2	1:A:1181:PHE:CZ	2.85	0.65
5:C:485:GLU:OE2	5:C:636:PRO:HB3	1.97	0.65
1:A:479:ARG:CG	1:A:479:ARG:NH1	2.51	0.64
1:A:595:ARG:HH11	1:A:595:ARG:CG	2.10	0.64
6:D:1001:THR:HG22	6:D:1002:LEU:N	2.12	0.64
6:D:425:ILE:CD1	6:D:1004:PHE:CD2	2.80	0.64
2:B:442:VAL:CG2	5:C:128:GLU:HG3	2.26	0.64
6:D:457:GLN:HA	6:D:457:GLN:OE1	1.98	0.64
6:D:383:SER:HB3	6:D:796:PRO:HG3	1.79	0.64
5:C:485:GLU:OE1	5:C:521:PHE:HA	1.98	0.64
1:A:37:ARG:HD3	9:A:1302:MG7:O3'	1.98	0.63
6:D:998:GLY:O	6:D:1002:LEU:N	2.27	0.63
1:A:489:ILE:CD1	1:A:490:SER:H	2.06	0.63
1:A:618:THR:HB	1:A:634:GLU:HB2	1.79	0.63
2:B:67:LEU:HD12	2:B:67:LEU:H	1.61	0.63
2:B:378:VAL:CG1	2:B:484:ILE:CD1	2.70	0.63
1:A:547:ASP:O	1:A:712:THR:HG22	1.98	0.63
2:B:185:PRO:CG	6:D:1000:LEU:HB2	2.28	0.63
6:D:1064:ASN:HD21	6:D:1296:ILE:HD11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:529:LYS:HG3	6:F:586:PRO:HG2	1.80	0.63
1:A:545:SER:C	1:A:546:ILE:HD12	2.19	0.63
1:A:261:LEU:O	1:A:264:VAL:HG22	1.99	0.63
5:C:473:ALA:HB2	5:C:761:SER:HB2	0.66	0.63
2:B:442:VAL:CG2	5:C:124:GLN:NE2	2.61	0.62
1:A:618:THR:HG23	1:A:638:PRO:HD3	1.80	0.62
1:A:675:ILE:HD11	1:A:677:ILE:HD11	1.81	0.62
2:B:59:HIS:CE1	2:B:137:ALA:CB	2.80	0.62
1:A:499:LEU:HB3	1:A:612:GLU:HB2	1.81	0.62
6:D:1001:THR:CG2	6:D:1002:LEU:N	2.62	0.62
6:F:231:LEU:HB3	6:F:249:SER:HB2	1.79	0.62
6:F:704:VAL:HG12	6:F:1330:ILE:HD11	1.81	0.62
6:F:452:ASN:HD22	7:G:460:ALA:HB3	1.64	0.62
1:A:386:THR:HG22	5:C:129:ALA:CB	2.30	0.62
2:B:185:PRO:HG2	6:D:1000:LEU:HB2	1.82	0.62
5:C:440:ILE:HD12	5:C:482:ILE:HD11	1.82	0.62
1:A:175:PHE:HB2	1:A:182:PRO:HG2	1.82	0.61
1:A:582:TYR:OH	1:A:611:LEU:HD13	2.00	0.61
1:A:599:VAL:HG23	1:A:599:VAL:O	1.99	0.61
6:E:848:ARG:HH11	6:E:914:GLU:HB3	1.65	0.61
1:A:1162:VAL:HG22	1:A:1198:LEU:HD13	1.81	0.61
2:B:531:ARG:HH22	5:C:122:ASN:CG	2.03	0.61
1:A:1196:LYS:N	1:A:1196:LYS:HD2	2.10	0.61
1:A:967:ILE:HD11	1:A:1091:PRO:HB2	1.81	0.61
5:C:297:ASN:HD21	5:C:1299:SER:HB2	1.66	0.61
1:A:870:TYR:OH	1:A:1188:ARG:NH1	2.34	0.61
2:B:195:ASP:O	2:B:198:LEU:N	2.34	0.61
5:C:440:ILE:HG22	5:C:478:ILE:HD11	1.81	0.61
1:A:429:LYS:NZ	1:A:456:PHE:HE2	1.99	0.61
2:B:331:VAL:HG21	2:B:543:THR:HG21	1.83	0.61
1:A:284:LYS:CE	1:A:718:ASN:HD22	2.14	0.60
1:A:1118:PRO:HD3	6:D:446:LYS:HE3	1.82	0.60
6:E:231:LEU:HB3	6:E:249:SER:HB2	1.82	0.60
2:B:324:PRO:HG3	2:B:552:GLU:HG2	1.82	0.60
1:A:37:ARG:HD3	9:A:1302:MG7:C3'	2.32	0.60
1:A:363:GLN:H	1:A:363:GLN:CD	2.05	0.60
2:B:229:PHE:HE1	2:B:253:TYR:CD2	2.19	0.60
6:D:848:ARG:HH11	6:D:914:GLU:HB3	1.66	0.60
1:A:1072:LEU:HD11	5:C:455:GLN:HE21	1.67	0.60
2:B:187:TRP:CB	2:B:192:ASP:OD2	2.48	0.60
1:A:549:ALA:HB3	1:A:710:ALA:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:THR:OG1	5:C:444:SER:HB2	2.00	0.60
1:A:812:MET:HG2	1:A:812:MET:O	2.00	0.60
2:B:66:THR:HG23	2:B:66:THR:O	2.01	0.60
2:B:304:PRO:HD2	5:C:123:GLU:CG	2.30	0.60
6:F:297:ASN:HD21	6:F:1299:SER:HB2	1.67	0.60
6:F:626:ARG:NH1	6:F:715:ASN:O	2.35	0.60
7:G:620:ILE:HD11	7:G:631:PRO:HG2	1.82	0.60
1:A:578:ARG:HG2	2:B:177:ALA:HA	1.82	0.60
2:B:147:SER:CA	6:D:133:MET:HG3	2.32	0.60
5:C:828:ASP:OD2	5:C:862:ARG:NH2	2.35	0.60
6:D:828:ASP:OD2	6:D:862:ARG:NH2	2.35	0.60
2:B:443:ARG:HB2	5:C:133:MET:HE3	1.83	0.60
2:B:531:ARG:HH22	5:C:122:ASN:HD21	1.48	0.60
1:A:611:LEU:C	1:A:611:LEU:HD23	2.22	0.59
7:G:626:ARG:NH1	7:G:715:ASN:O	2.35	0.59
1:A:489:ILE:HG12	1:A:639:SER:O	2.03	0.59
1:A:284:LYS:NZ	1:A:729:ASN:ND2	2.50	0.59
1:A:555:VAL:O	1:A:555:VAL:HG12	2.02	0.59
2:B:264:TYR:CD2	5:C:117:ARG:HG2	2.37	0.59
6:E:1044:ARG:NH1	6:E:1049:GLU:OE1	2.34	0.59
6:F:515:ILE:HG21	6:F:655:ILE:HG21	1.85	0.59
1:A:1040:THR:HG23	1:A:1056:TRP:HE1	1.68	0.59
2:B:156:LEU:HD12	2:B:181:PRO:HB3	1.84	0.59
2:B:481:THR:OG1	2:B:482:PRO:HD2	2.02	0.59
2:B:56:LEU:HD23	2:B:67:LEU:HD23	1.85	0.59
6:F:196:LEU:HD23	6:F:296:VAL:HG11	1.85	0.59
7:G:666:ARG:NH1	7:G:670:ASP:OD2	2.34	0.59
1:A:377:ARG:NH1	2:B:325:SER:OG	2.36	0.59
6:F:452:ASN:HD22	7:G:460:ALA:CB	2.15	0.59
1:A:956:LEU:HD22	1:A:1110:PHE:HB3	1.84	0.59
6:D:997:TYR:O	6:D:1001:THR:HB	2.03	0.59
1:A:588:GLU:HG2	6:D:1003:ARG:NH2	2.17	0.58
1:A:703:ILE:HA	1:A:706:GLU:HG2	1.85	0.58
6:E:666:ARG:NH1	6:E:670:ASP:OD2	2.30	0.58
5:C:469:ARG:HG2	5:C:469:ARG:HH21	1.69	0.58
6:E:196:LEU:HD23	6:E:296:VAL:HG11	1.84	0.58
6:D:231:LEU:HB3	6:D:249:SER:HB2	1.85	0.58
6:D:666:ARG:NH1	6:D:670:ASP:OD2	2.35	0.58
1:A:521:LYS:HD3	1:A:1084:HIS:ND1	2.12	0.58
6:F:383:SER:HB3	6:F:796:PRO:HG3	1.85	0.58
7:G:168:VAL:HG22	7:G:204:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASN:HA	1:A:76:ILE:HG22	1.84	0.58
1:A:791:ARG:NH2	1:A:817:TYR:OH	2.36	0.58
6:D:626:ARG:NH1	6:D:715:ASN:O	2.37	0.58
6:F:500:GLU:HG3	6:F:510:VAL:HG21	1.84	0.58
6:F:644:VAL:HG22	7:G:574:LYS:HG3	1.86	0.58
2:B:442:VAL:HG12	2:B:446:ILE:HD12	1.85	0.58
1:A:485:ARG:H	1:A:485:ARG:HD2	1.69	0.58
1:A:1057:PHE:CD1	7:G:117:ARG:CD	2.85	0.58
2:B:134:THR:OG1	2:B:135:TYR:N	2.37	0.58
1:A:429:LYS:HZ1	1:A:456:PHE:HE2	1.47	0.58
1:A:1082:ASN:C	1:A:1083:TYR:CG	2.77	0.58
2:B:531:ARG:NH2	5:C:122:ASN:OD1	2.37	0.58
6:D:515:ILE:HG21	6:D:655:ILE:HG21	1.86	0.58
6:E:704:VAL:HG12	6:E:1330:ILE:HD11	1.85	0.58
7:G:156:GLN:NE2	7:G:1311:THR:O	2.37	0.58
2:B:481:THR:OG1	2:B:482:PRO:CD	2.52	0.58
5:C:761:SER:O	5:C:763:VAL:N	2.37	0.58
6:D:196:LEU:HD23	6:D:296:VAL:HG11	1.85	0.58
1:A:45:PHE:HE1	1:A:172:LYS:HA	1.69	0.57
1:A:383:GLN:HG3	1:A:565:THR:HG22	1.85	0.57
2:B:133:VAL:HA	2:B:136:LYS:HB2	1.84	0.57
2:B:206:PHE:CG	2:B:221:LEU:HD11	2.39	0.57
6:F:264:LEU:HD11	6:F:362:LEU:HD23	1.85	0.57
2:B:350:VAL:HG21	2:B:498:ILE:HD13	1.85	0.57
5:C:513:GLU:HG3	5:C:760:THR:O	2.04	0.57
1:A:1061:LEU:O	1:A:1160:ARG:NH2	2.38	0.57
2:B:147:SER:O	6:D:133:MET:HG2	2.04	0.57
5:C:761:SER:C	5:C:763:VAL:H	2.08	0.57
6:D:453:LEU:HD23	6:D:453:LEU:O	2.04	0.57
6:F:1134:ARG:NH1	6:F:1158:SER:OG	2.37	0.57
2:B:41:PRO:CG	6:D:146:GLU:HG3	2.24	0.57
6:E:626:ARG:NH1	6:E:715:ASN:O	2.38	0.57
7:G:231:LEU:HB3	7:G:249:SER:HB2	1.86	0.57
5:C:529:LYS:HG3	5:C:586:PRO:HG2	1.86	0.57
1:A:672:LEU:HD23	1:A:672:LEU:C	2.24	0.57
2:B:68:ILE:HG23	2:B:68:ILE:O	2.04	0.57
5:C:620:ILE:HD11	5:C:631:PRO:HG2	1.87	0.57
1:A:813:THR:O	1:A:831:ILE:CG2	2.53	0.57
2:B:62:ARG:HG2	2:B:62:ARG:HH11	1.69	0.57
7:G:817:ASP:OD1	7:G:1010:ARG:NH2	2.38	0.57
7:G:848:ARG:HH11	7:G:914:GLU:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:CE	6:D:496:LYS:CE	2.83	0.56
9:A:1302:MG7:O6	9:A:1302:MG7:H71	2.05	0.56
2:B:465:THR:HA	2:B:470:ASN:HD22	1.70	0.56
1:A:261:LEU:O	1:A:264:VAL:CG2	2.53	0.56
2:B:191:ALA:O	6:D:996:ASP:OD2	2.24	0.56
1:A:343:THR:HA	1:A:743:THR:HG21	1.87	0.56
1:A:505:THR:O	1:A:509:GLN:NE2	2.38	0.56
5:C:474:ASP:OD2	5:C:477:SER:HB2	2.06	0.56
6:D:980:ARG:HG3	6:D:1010:ARG:HD3	1.86	0.56
7:G:826:GLY:HA3	7:G:949:ALA:HB2	1.87	0.56
1:A:428:ARG:CD	1:A:429:LYS:CA	2.76	0.56
1:A:808:LEU:HB3	1:A:814:LEU:HD11	1.79	0.56
1:A:1171:SER:HB2	1:A:1174:CYS:HB2	1.88	0.56
2:B:371:SER:HB3	2:B:378:VAL:HG22	1.87	0.56
1:A:265:CYS:O	1:A:286:THR:OG1	2.21	0.56
1:A:430:LEU:CD1	1:A:435:LYS:HZ3	2.15	0.56
2:B:535:TYR:CZ	5:C:122:ASN:ND2	2.73	0.56
2:B:64:ASN:O	2:B:64:ASN:ND2	2.39	0.56
2:B:506:LEU:HD12	2:B:544:THR:HG22	1.88	0.56
5:C:235:ILE:HG23	5:C:978:GLN:HE21	1.71	0.56
6:E:524:GLU:OE2	6:E:527:ARG:NH1	2.39	0.56
6:D:660:ALA:HB1	6:D:681:LYS:HE3	1.87	0.56
1:A:104:LEU:HG	1:A:104:LEU:O	2.05	0.56
1:A:813:THR:O	1:A:831:ILE:HG22	2.05	0.56
2:B:437:TYR:OH	2:B:445:LYS:HD3	2.05	0.56
6:F:235:ILE:HG23	6:F:978:GLN:HE21	1.71	0.56
1:A:429:LYS:NZ	1:A:456:PHE:CE2	2.74	0.56
1:A:716:SER:HB3	1:A:719:SER:HB2	1.88	0.56
1:A:950:ARG:HD2	1:A:970:GLY:HA3	1.87	0.56
2:B:194:SER:HB2	6:D:996:ASP:H	1.71	0.56
5:C:485:GLU:CD	5:C:522:PRO:HD2	2.23	0.56
1:A:428:ARG:CD	1:A:429:LYS:N	2.61	0.55
1:A:489:ILE:HG13	1:A:639:SER:O	2.06	0.55
1:A:106:THR:O	1:A:106:THR:OG1	2.22	0.55
1:A:568:LEU:CD2	1:A:606:TRP:CZ3	2.89	0.55
2:B:283:GLY:H	2:B:313:ILE:HB	1.72	0.55
2:B:206:PHE:CD2	2:B:221:LEU:HD11	2.41	0.55
6:F:828:ASP:OD2	6:F:862:ARG:NH2	2.40	0.55
7:G:704:VAL:HG12	7:G:1330:ILE:HD11	1.89	0.55
1:A:296:PHE:HB3	1:A:300:ARG:HH21	1.71	0.55
2:B:55:MET:O	2:B:59:HIS:CD2	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG23	5:C:124:GLN:HE21	1.69	0.55
1:A:1030:THR:HG22	1:A:1196:LYS:HE2	1.86	0.55
2:B:427:MET:O	2:B:430:GLY:HA2	2.06	0.55
5:C:485:GLU:O	5:C:486:VAL:CG1	2.50	0.55
6:E:644:VAL:HG22	6:F:574:LYS:HG3	1.86	0.55
6:E:817:ASP:OD1	6:E:1010:ARG:NH2	2.39	0.55
1:A:107:PHE:O	1:A:108:ARG:CB	2.55	0.55
6:E:485:GLU:HG3	6:E:523:THR:HB	1.88	0.55
7:G:196:LEU:HD23	7:G:296:VAL:HG11	1.88	0.55
1:A:275:PHE:CD2	5:C:467:LYS:HG2	2.42	0.55
2:B:62:ARG:HH11	2:B:62:ARG:CG	2.18	0.55
5:C:817:ASP:OD1	5:C:1010:ARG:NH2	2.40	0.55
6:F:451:GLU:OE2	7:G:464:SER:CB	2.54	0.55
7:G:1134:ARG:NH1	7:G:1158:SER:OG	2.39	0.55
6:D:620:ILE:HD11	6:D:631:PRO:HG2	1.89	0.55
6:E:828:ASP:OD2	6:E:862:ARG:NH2	2.40	0.55
2:B:156:LEU:HD12	2:B:179:THR:HG21	1.87	0.55
2:B:194:SER:OG	6:D:995:THR:HB	2.06	0.55
5:C:626:ARG:NH1	5:C:715:ASN:O	2.40	0.55
6:D:384:MET:HG3	6:D:793:TYR:HD1	1.72	0.55
7:G:515:ILE:HG21	7:G:655:ILE:HG21	1.88	0.55
1:A:37:ARG:HG3	1:A:40:ARG:HH22	1.72	0.54
5:C:456:ASN:ND2	5:C:679:CYS:SG	2.80	0.54
5:C:1134:ARG:NH1	5:C:1158:SER:OG	2.40	0.54
1:A:422:THR:HB	1:A:976:LYS:HE2	1.89	0.54
2:B:132:ILE:O	2:B:135:TYR:N	2.40	0.54
2:B:409:LEU:O	2:B:414:ASN:ND2	2.36	0.54
1:A:180:GLU:OE1	1:A:195:ASN:ND2	2.41	0.54
1:A:268:THR:HG22	1:A:283:THR:CB	2.36	0.54
1:A:489:ILE:HD11	1:A:640:GLY:HA3	1.89	0.54
1:A:939:GLN:HE22	2:B:69:ASN:H	1.54	0.54
6:E:515:ILE:HG21	6:E:655:ILE:HG21	1.90	0.54
6:F:620:ILE:HD11	6:F:631:PRO:HG2	1.88	0.54
6:D:421:ARG:NH2	6:D:1004:PHE:CE1	2.74	0.54
1:A:947:GLU:HA	1:A:950:ARG:HE	1.73	0.54
2:B:194:SER:CB	6:D:995:THR:CB	2.70	0.54
2:B:194:SER:HB2	6:D:996:ASP:N	2.23	0.54
6:D:606:LEU:HD22	6:D:655:ILE:HG12	1.89	0.54
6:F:392:PRO:HG2	6:F:394:GLN:HG3	1.89	0.54
7:G:235:ILE:HG23	7:G:978:GLN:HE21	1.73	0.54
2:B:531:ARG:NH1	5:C:122:ASN:OD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:980:ARG:HG3	6:E:1010:ARG:HD3	1.90	0.54
1:A:489:ILE:HD11	1:A:639:SER:O	2.08	0.54
1:A:531:GLU:OE2	1:A:676:LYS:HD3	2.07	0.54
1:A:555:VAL:O	1:A:556:THR:C	2.46	0.54
6:F:342:THR:HB	6:F:1309:ILE:HD11	1.90	0.54
1:A:284:LYS:HZ3	1:A:729:ASN:ND2	2.06	0.53
1:A:465:ARG:NH1	1:A:495:ASP:OD1	2.41	0.53
1:A:550:GLY:HA2	12:A:1306:UTP:PB	2.47	0.53
6:F:666:ARG:NH1	6:F:670:ASP:OD2	2.41	0.53
7:G:383:SER:HB3	7:G:796:PRO:HG3	1.90	0.53
1:A:915:ASP:O	1:A:919:GLU:N	2.40	0.53
2:B:41:PRO:CG	6:D:146:GLU:CG	2.83	0.53
6:D:1060:ARG:NH2	6:D:1294:ASP:OD1	2.40	0.53
1:A:260:ALA:O	1:A:264:VAL:HG13	2.08	0.53
5:C:156:GLN:NE2	5:C:1311:THR:O	2.42	0.53
6:F:653:ARG:HH12	7:G:542:ARG:HG2	1.74	0.53
7:G:524:GLU:OE2	7:G:527:ARG:NH1	2.41	0.53
1:A:138:ARG:HB3	1:A:192:ILE:HD11	1.91	0.53
2:B:412:ASP:OD2	2:B:520:ARG:NH2	2.42	0.53
1:A:652:LEU:HD22	1:A:682:ILE:HD11	1.91	0.53
1:A:778:LYS:O	1:A:845:TYR:OH	2.26	0.53
2:B:41:PRO:HB3	6:D:143:VAL:HG12	1.91	0.53
2:B:442:VAL:CB	5:C:128:GLU:HG3	2.39	0.53
5:C:481:ALA:O	5:C:482:ILE:C	2.44	0.53
6:E:500:GLU:HG3	6:E:510:VAL:HG21	1.91	0.53
6:F:1060:ARG:NH2	6:F:1294:ASP:OD1	2.41	0.53
1:A:37:ARG:CZ	1:A:37:ARG:CB	2.86	0.53
1:A:138:ARG:NH2	1:A:190:ASP:OD1	2.42	0.53
2:B:154:LEU:N	2:B:154:LEU:HD23	2.23	0.53
5:C:384:MET:HG3	5:C:793:TYR:HD1	1.74	0.53
6:E:826:GLY:HA3	6:E:949:ALA:HB2	1.91	0.53
6:F:350:ILE:O	6:F:1300:ASN:ND2	2.42	0.53
7:G:485:GLU:HG3	7:G:523:THR:HB	1.90	0.53
5:C:469:ARG:HG2	5:C:469:ARG:NH2	2.24	0.53
1:A:479:ARG:NH1	1:A:480:GLN:O	2.42	0.52
1:A:1162:VAL:CG2	1:A:1198:LEU:HD13	2.37	0.52
2:B:41:PRO:HG3	6:D:143:VAL:CG1	2.39	0.52
2:B:199:ARG:O	2:B:199:ARG:HG2	2.08	0.52
2:B:264:TYR:CD1	5:C:117:ARG:HG2	2.44	0.52
5:C:644:VAL:HG22	6:D:574:LYS:HG3	1.90	0.52
6:E:328:GLY:H	6:E:347:ALA:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:HIS:O	1:A:1022:HIS:ND1	2.42	0.52
7:G:384:MET:HG3	7:G:793:TYR:HD1	1.73	0.52
1:A:489:ILE:HD11	1:A:640:GLY:CA	2.39	0.52
1:A:543:LEU:HD22	1:A:720:ILE:HD12	1.92	0.52
5:C:638:THR:OG1	5:C:640:GLN:NE2	2.43	0.52
6:D:156:GLN:NE2	6:D:1311:THR:O	2.42	0.52
6:E:392:PRO:HG2	6:E:394:GLN:HG3	1.91	0.52
6:E:858:HIS:O	6:E:862:ARG:NH1	2.41	0.52
7:G:954:GLN:HB2	7:G:957:PHE:HB3	1.90	0.52
1:A:406:LYS:HE3	6:D:496:LYS:CD	2.39	0.52
5:C:574:LYS:HG3	7:G:644:VAL:HG22	1.90	0.52
6:E:445:GLU:O	6:E:447:ARG:NH1	2.42	0.52
6:E:495:LEU:HD13	6:E:528:ILE:HD12	1.90	0.52
1:A:283:THR:O	1:A:283:THR:OG1	2.22	0.52
1:A:442:VAL:HA	1:A:445:TRP:HD1	1.75	0.52
1:A:546:ILE:HD12	1:A:546:ILE:N	2.24	0.52
2:B:453:ASN:O	2:B:456:LEU:HB2	2.10	0.52
5:C:361:ASN:OD1	5:C:1054:ARG:NH1	2.43	0.52
6:E:700:ASP:HB3	6:E:1326:ARG:HG2	1.91	0.52
1:A:1122:GLY:HA3	6:D:467:LYS:NZ	2.24	0.52
2:B:185:PRO:CG	6:D:1000:LEU:CB	2.88	0.52
1:A:1125:LEU:HD21	6:D:455:GLN:CB	2.40	0.52
2:B:84:VAL:HG11	2:B:138:LEU:HB3	1.91	0.52
5:C:848:ARG:HH11	5:C:914:GLU:HB3	1.75	0.52
5:C:980:ARG:HG3	5:C:1010:ARG:HD3	1.91	0.52
1:A:377:ARG:NH2	2:B:544:THR:O	2.43	0.52
2:B:356:GLY:O	2:B:511:ASN:ND2	2.42	0.52
1:A:801:TYR:CE1	1:A:826:THR:OG1	2.60	0.52
2:B:442:VAL:HG11	5:C:128:GLU:HG3	1.91	0.52
6:D:826:GLY:HA3	6:D:949:ALA:HB2	1.92	0.52
6:E:529:LYS:HG3	6:E:586:PRO:HG2	1.92	0.52
1:A:271:VAL:CG1	1:A:282:ARG:HD3	2.39	0.51
1:A:574:CYS:SG	1:A:575:THR:N	2.83	0.51
1:A:816:LYS:O	1:A:817:TYR:HD1	1.93	0.51
1:A:1029:VAL:HB	7:G:472:GLU:OE1	2.10	0.51
2:B:185:PRO:HG3	6:D:1000:LEU:CB	2.39	0.51
7:G:392:PRO:HG2	7:G:394:GLN:HG3	1.91	0.51
1:A:430:LEU:CD1	1:A:435:LYS:HZ1	2.23	0.51
1:A:814:LEU:HD23	1:A:830:LEU:CB	2.41	0.51
2:B:56:LEU:CD2	2:B:67:LEU:CD2	2.88	0.51
2:B:452:MET:CE	2:B:530:LEU:CD2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:485:GLU:HG3	6:D:523:THR:HB	1.92	0.51
1:A:546:ILE:N	1:A:546:ILE:CD1	2.72	0.51
1:A:1125:LEU:HD21	6:D:455:GLN:HB3	1.92	0.51
1:A:801:TYR:HE1	1:A:828:MET:HB3	1.76	0.51
1:A:774:PRO:HB2	1:A:863:MET:HG3	1.93	0.51
1:A:942:LYS:HB3	1:A:943:LEU:O	2.10	0.51
1:A:330:ASN:OD1	1:A:772:ARG:NH1	2.43	0.51
1:A:805:TYR:CD1	1:A:816:LYS:HE3	2.46	0.51
1:A:1019:LEU:HD23	1:A:1206:LEU:CD1	2.40	0.51
6:D:350:ILE:O	6:D:1300:ASN:ND2	2.44	0.51
6:D:1022:ILE:HG22	6:D:1028:VAL:HA	1.93	0.51
1:A:386:THR:O	1:A:386:THR:OG1	2.25	0.51
1:A:603:ASN:OD1	1:A:606:TRP:HB2	2.10	0.51
2:B:62:ARG:NH1	2:B:62:ARG:CG	2.73	0.51
6:D:491:ASN:HD21	6:D:748:GLN:HE21	1.58	0.51
1:A:412:HIS:NE2	1:A:414:ASP:HB2	2.25	0.51
1:A:1072:LEU:CD1	5:C:455:GLN:HE21	2.24	0.51
2:B:229:PHE:HD1	2:B:251:ILE:HD11	1.76	0.51
2:B:443:ARG:HB2	5:C:133:MET:CE	2.39	0.51
6:E:616:ASP:HB2	6:E:631:PRO:HB2	1.93	0.51
7:G:529:LYS:HG3	7:G:586:PRO:HG2	1.93	0.51
1:A:81:TYR:CE1	1:A:112:LEU:HD12	2.31	0.51
1:A:771:VAL:HG22	1:A:773:ARG:H	1.76	0.51
1:A:1032:ASP:OD1	1:A:1160:ARG:NH1	2.44	0.51
5:C:704:VAL:HG12	5:C:1330:ILE:HD11	1.92	0.51
6:D:529:LYS:HG3	6:D:586:PRO:HG2	1.93	0.51
6:F:554:ARG:HD2	6:F:594:LEU:HD13	1.92	0.51
1:A:431:THR:HB	1:A:435:LYS:HB2	1.94	0.50
1:A:648:HIS:CD2	12:A:1306:UTP:O3'	2.63	0.50
5:C:231:LEU:HB3	5:C:249:SER:HB2	1.92	0.50
5:C:783:ASP:OD1	5:C:783:ASP:N	2.33	0.50
1:A:865:THR:O	1:A:867:ARG:NH1	2.44	0.50
1:A:1194:ARG:HE	7:G:113:VAL:HG11	1.75	0.50
1:A:1196:LYS:N	1:A:1196:LYS:CD	2.73	0.50
6:D:524:GLU:OE2	6:D:527:ARG:NH1	2.44	0.50
1:A:107:PHE:O	1:A:108:ARG:HB3	2.11	0.50
1:A:175:PHE:HB3	1:A:203:LEU:HD21	1.93	0.50
1:A:489:ILE:CD1	1:A:489:ILE:C	2.77	0.50
1:A:555:VAL:C	1:A:556:THR:O	2.48	0.50
5:C:515:ILE:HG21	5:C:655:ILE:HG21	1.93	0.50
5:C:876:GLY:HA2	5:C:902:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:524:GLU:OE2	6:F:527:ARG:NH1	2.44	0.50
1:A:284:LYS:HD2	1:A:284:LYS:O	2.11	0.50
1:A:284:LYS:HE2	1:A:718:ASN:HD22	1.75	0.50
7:G:1048:ASP:HB2	7:G:1051:ARG:HG2	1.93	0.50
7:G:1240:ARG:HD2	7:G:1243:ARG:HB2	1.94	0.50
1:A:1024:PHE:HD2	1:A:1198:LEU:HD22	1.76	0.50
2:B:40:ALA:O	2:B:44:ARG:NH1	2.43	0.50
2:B:79:LEU:HD13	6:D:438:ASN:HD22	1.76	0.50
1:A:1100:TYR:HA	1:A:1104:ALA:HB2	1.94	0.50
1:A:1126:ARG:CD	5:C:452:ASN:HD21	2.24	0.50
6:D:644:VAL:HG22	6:E:574:LYS:HG3	1.93	0.50
6:F:876:GLY:HA2	6:F:902:ILE:HA	1.91	0.50
1:A:78:PRO:HB2	1:A:108:ARG:CB	2.42	0.50
1:A:586:ASN:HD21	6:D:428:GLN:HE22	1.59	0.50
6:D:495:LEU:HD13	6:D:528:ILE:HD12	1.93	0.50
2:B:190:ILE:HD12	2:B:190:ILE:N	2.27	0.50
2:B:61:ALA:O	2:B:62:ARG:C	2.50	0.50
2:B:272:ASN:HB2	2:B:321:MET:HG3	1.93	0.50
6:D:392:PRO:HG2	6:D:394:GLN:HG3	1.94	0.50
6:D:1081:ASP:HB2	6:D:1228:ARG:HB2	1.93	0.50
6:E:384:MET:HG3	6:E:793:TYR:HD1	1.77	0.50
1:A:142:PHE:HE2	1:A:760:LEU:HD13	1.76	0.49
1:A:574:CYS:HG	1:A:575:THR:N	2.09	0.49
1:A:1057:PHE:HB2	7:G:117:ARG:CD	2.36	0.49
6:F:529:LYS:HE2	6:F:586:PRO:HD2	1.93	0.49
1:A:527:PHE:HZ	1:A:1067:ARG:HA	1.77	0.49
2:B:221:LEU:N	2:B:221:LEU:HD23	2.27	0.49
5:C:196:LEU:HD23	5:C:296:VAL:HG11	1.93	0.49
5:C:954:GLN:HB2	5:C:957:PHE:HB3	1.94	0.49
6:F:326:GLY:H	6:F:1267:THR:HG21	1.76	0.49
6:F:1064:ASN:HD21	6:F:1296:ILE:HD11	1.77	0.49
1:A:37:ARG:CA	1:A:40:ARG:NH2	2.75	0.49
1:A:459:GLU:HG2	1:A:465:ARG:HB2	1.94	0.49
1:A:516:ASN:HD22	1:A:657:ARG:HE	1.60	0.49
2:B:150:LEU:CD1	2:B:154:LEU:HD21	2.38	0.49
6:E:350:ILE:O	6:E:1300:ASN:ND2	2.45	0.49
2:B:21:ARG:HB2	2:B:202:PHE:HA	1.95	0.49
6:E:156:GLN:NE2	6:E:1311:THR:O	2.44	0.49
1:A:489:ILE:CD1	1:A:639:SER:O	2.60	0.49
1:A:883:GLU:O	1:A:886:GLN:HB3	2.12	0.49
1:A:35:ASN:HA	1:A:147:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:LYS:O	1:A:817:TYR:CD1	2.66	0.49
1:A:1126:ARG:CD	5:C:452:ASN:ND2	2.75	0.49
2:B:67:LEU:HD22	2:B:73:TYR:HD2	1.74	0.49
2:B:531:ARG:NH2	5:C:122:ASN:HD21	2.10	0.49
1:A:578:ARG:O	1:A:580:GLY:N	2.46	0.49
2:B:147:SER:CB	6:D:133:MET:CG	2.90	0.49
7:G:1022:ILE:HG22	7:G:1028:VAL:HA	1.94	0.49
1:A:305:GLU:HG3	1:A:306:LEU:HD12	1.95	0.49
6:F:858:HIS:O	6:F:862:ARG:NH1	2.46	0.49
1:A:839:MET:HE3	1:A:905:ALA:HB3	1.95	0.49
2:B:207:GLU:O	2:B:212:ASN:ND2	2.45	0.49
2:B:376:GLN:HE22	2:B:483:ARG:NH1	2.11	0.49
1:A:399:SER:HG	5:C:787:ILE:HG22	1.75	0.48
1:A:585:LYS:HE2	1:A:607:GLN:HE22	1.78	0.48
2:B:425:LEU:HD12	2:B:425:LEU:C	2.32	0.48
5:C:837:THR:OG1	5:C:911:ARG:NH1	2.46	0.48
1:A:866:ALA:HB2	1:A:1143:LEU:HD23	1.95	0.48
1:A:1024:PHE:HB3	1:A:1198:LEU:HB2	1.96	0.48
2:B:44:ARG:NH2	6:D:143:VAL:O	2.46	0.48
2:B:59:HIS:HA	2:B:62:ARG:HG3	1.94	0.48
2:B:486:ILE:HG22	2:B:486:ILE:O	2.12	0.48
5:C:524:GLU:OE2	5:C:527:ARG:NH1	2.46	0.48
2:B:55:MET:O	2:B:59:HIS:HD2	1.95	0.48
6:F:384:MET:HG3	6:F:793:TYR:HD1	1.78	0.48
7:G:1081:ASP:HB2	7:G:1228:ARG:HB2	1.95	0.48
1:A:606:TRP:CE3	1:A:606:TRP:CA	2.92	0.48
1:A:884:MET:HE3	1:A:884:MET:HB3	1.64	0.48
2:B:158:ILE:HA	2:B:164:TYR:HE2	1.78	0.48
1:A:34:ALA:O	1:A:40:ARG:NH1	2.46	0.48
1:A:551:MET:N	12:A:1306:UTP:O2A	2.46	0.48
1:A:1021:LEU:N	1:A:1021:LEU:HD12	2.29	0.48
6:D:1004:PHE:HD1	6:D:1004:PHE:O	1.96	0.48
7:G:858:HIS:O	7:G:862:ARG:NH1	2.47	0.48
1:A:261:LEU:C	1:A:264:VAL:HG22	2.34	0.48
1:A:883:GLU:OE1	1:A:883:GLU:HA	2.13	0.48
1:A:920:VAL:HG11	1:A:994:VAL:HG22	1.96	0.48
5:C:469:ARG:HD2	5:C:510:VAL:HG22	1.96	0.48
7:G:193:THR:HA	7:G:296:VAL:HG13	1.95	0.48
7:G:616:ASP:HB3	7:G:619:ALA:HB3	1.96	0.48
2:B:397:GLU:HA	2:B:397:GLU:OE1	2.14	0.47
6:D:500:GLU:HG3	6:D:510:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:495:LEU:HD13	7:G:528:ILE:HD12	1.95	0.47
1:A:106:THR:CG2	1:A:202:ILE:HG21	2.44	0.47
1:A:268:THR:HG22	1:A:283:THR:CG2	2.43	0.47
1:A:1087:SER:O	1:A:1089:ASP:N	2.47	0.47
2:B:147:SER:HB2	6:D:133:MET:CG	2.41	0.47
2:B:484:ILE:HG13	2:B:484:ILE:O	2.15	0.47
5:C:700:ASP:HB3	5:C:1326:ARG:HG2	1.96	0.47
6:F:252:LEU:O	6:F:256:PHE:N	2.47	0.47
1:A:20:ARG:NH2	1:A:852:ARG:O	2.47	0.47
2:B:41:PRO:HG3	6:D:143:VAL:HG12	1.96	0.47
1:A:601:TYR:C	1:A:601:TYR:CD1	2.88	0.47
2:B:147:SER:C	6:D:133:MET:HG2	2.35	0.47
2:B:264:TYR:HB3	5:C:117:ARG:HD3	1.97	0.47
6:D:777:GLN:HB2	6:D:786:SER:HA	1.95	0.47
1:A:286:THR:O	1:A:287:SER:C	2.52	0.47
1:A:412:HIS:C	1:A:412:HIS:CD2	2.85	0.47
2:B:446:ILE:HG12	2:B:536:ARG:NH1	2.30	0.47
6:D:534:ASN:ND2	6:D:575:TRP:O	2.42	0.47
6:D:804:LEU:O	6:D:808:GLN:N	2.48	0.47
6:F:656:VAL:O	6:F:660:ALA:N	2.45	0.47
1:A:521:LYS:CE	1:A:1084:HIS:CE1	2.98	0.47
1:A:591:GLU:O	1:A:594:ASN:HB2	2.15	0.47
5:C:826:GLY:HA3	5:C:949:ALA:HB2	1.97	0.47
5:C:1022:ILE:HG22	5:C:1028:VAL:HA	1.96	0.47
6:E:860:ARG:HE	6:E:864:HIS:HE2	1.61	0.47
7:G:828:ASP:OD2	7:G:862:ARG:NH2	2.47	0.47
1:A:499:LEU:HD22	1:A:611:LEU:HD22	1.96	0.47
1:A:814:LEU:CD2	1:A:830:LEU:HB3	2.44	0.47
2:B:156:LEU:HD13	2:B:176:ILE:CD1	2.45	0.47
5:C:529:LYS:HE2	5:C:586:PRO:HD2	1.96	0.47
6:D:638:THR:HB	6:D:640:GLN:HE21	1.79	0.47
6:E:473:ALA:HB2	6:E:769:GLN:HG3	1.96	0.47
7:G:164:LEU:N	7:G:351:ASP:OD2	2.42	0.47
1:A:575:THR:HA	1:A:603:ASN:HD22	1.80	0.47
2:B:71:ARG:HH11	2:B:71:ARG:HB2	1.79	0.47
2:B:339:VAL:HG21	2:B:484:ILE:HD13	1.91	0.47
6:D:704:VAL:HG12	6:D:1330:ILE:HD11	1.96	0.47
2:B:532:ASP:OD1	5:C:121:PHE:CD2	2.68	0.47
1:A:1166:PRO:CB	6:F:451:GLU:CD	2.73	0.47
2:B:376:GLN:HE22	2:B:483:ARG:HH12	1.62	0.47
6:D:1096:TYR:CD1	6:D:1136:HIS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:256:PHE:HE2	7:G:990:THR:HG21	1.79	0.47
7:G:776:ARG:NH2	7:G:789:GLU:OE1	2.47	0.47
7:G:860:ARG:HE	7:G:864:HIS:HE2	1.62	0.47
6:E:164:LEU:N	6:E:351:ASP:OD2	2.46	0.46
6:E:351:ASP:OD1	6:E:351:ASP:N	2.48	0.46
7:G:150:LEU:HA	7:G:804:LEU:HD21	1.97	0.46
1:A:267:ALA:HB1	1:A:325:GLN:HB2	1.98	0.46
1:A:274:GLN:HB3	5:C:446:LYS:CE	2.39	0.46
7:G:383:SER:O	7:G:708:THR:OG1	2.27	0.46
1:A:63:ASN:N	1:A:63:ASN:OD1	2.49	0.46
1:A:961:HIS:NE2	1:A:1099:ILE:HG12	2.30	0.46
1:A:1019:LEU:HD23	1:A:1206:LEU:HD13	1.98	0.46
1:A:1022:HIS:CD2	1:A:1181:PHE:CD1	2.97	0.46
5:C:474:ASP:OD2	5:C:477:SER:CB	2.64	0.46
6:D:776:ARG:HD2	6:D:787:ILE:HD11	1.96	0.46
7:G:883:ILE:HG23	7:G:895:VAL:HG11	1.97	0.46
1:A:516:ASN:ND2	1:A:657:ARG:HE	2.13	0.46
1:A:531:GLU:OE2	1:A:674:THR:HG23	2.15	0.46
2:B:220:ASN:HD21	6:D:1310:ARG:HH12	1.62	0.46
5:C:761:SER:C	5:C:763:VAL:N	2.68	0.46
6:E:439:VAL:HG23	6:E:701:HIS:CD2	2.51	0.46
7:G:863:LEU:HA	7:G:866:THR:HG22	1.97	0.46
1:A:106:THR:HG22	1:A:202:ILE:CB	2.45	0.46
1:A:274:GLN:CB	5:C:446:LYS:HE2	2.38	0.46
1:A:1194:ARG:CD	7:G:113:VAL:HG12	2.43	0.46
2:B:194:SER:OG	6:D:995:THR:CB	2.63	0.46
2:B:220:ASN:ND2	6:D:1310:ARG:HH12	2.14	0.46
1:A:1186:ILE:HD11	1:A:1198:LEU:HD11	1.97	0.46
2:B:346:ASN:HA	2:B:483:ARG:O	2.16	0.46
5:C:392:PRO:HG2	5:C:394:GLN:HG3	1.97	0.46
7:G:902:ILE:HD12	7:G:929:PHE:HE1	1.81	0.46
1:A:510:ILE:HG21	1:A:650:VAL:HG22	1.98	0.46
6:D:471:SER:O	6:D:765:PRO:HG3	2.16	0.46
1:A:406:LYS:CD	6:D:496:LYS:HE3	2.46	0.46
1:A:499:LEU:HB3	1:A:612:GLU:CB	2.45	0.46
1:A:551:MET:HB3	12:A:1306:UTP:H5'1	1.98	0.46
1:A:667:GLY:CA	5:C:792:VAL:HG13	2.45	0.46
1:A:669:ASN:ND2	5:C:435:ALA:O	2.30	0.46
6:E:875:THR:HG22	6:E:898:GLN:HB3	1.97	0.46
2:B:535:TYR:CE1	5:C:122:ASN:ND2	2.84	0.46
6:E:171:GLU:OE2	6:E:1181:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:1022:ILE:HG22	6:E:1028:VAL:HA	1.98	0.46
7:G:772:TYR:HB2	7:G:775:VAL:HG23	1.97	0.46
1:A:409:ASN:OD1	1:A:575:THR:O	2.35	0.45
2:B:453:ASN:O	2:B:456:LEU:N	2.49	0.45
6:E:529:LYS:HE2	6:E:586:PRO:HD2	1.98	0.45
6:E:902:ILE:HD12	6:E:929:PHE:HE1	1.81	0.45
7:G:816:PRO:HG3	7:G:987:ALA:HB2	1.97	0.45
1:A:166:PRO:HB2	1:A:228:ILE:HD11	1.96	0.45
2:B:204:ARG:HE	2:B:226:ARG:NH1	2.15	0.45
6:E:1064:ASN:HD21	6:E:1296:ILE:HD11	1.80	0.45
7:G:427:VAL:HG11	7:G:755:LEU:HD21	1.98	0.45
1:A:939:GLN:NE2	2:B:69:ASN:H	2.15	0.45
2:B:79:LEU:HD13	6:D:438:ASN:HB2	1.98	0.45
6:D:150:LEU:HA	6:D:804:LEU:HD21	1.98	0.45
6:D:639:ASN:ND2	6:D:1328:ILE:O	2.50	0.45
7:G:700:ASP:HB3	7:G:1326:ARG:HG2	1.98	0.45
1:A:1020:HIS:CD2	1:A:1139:TYR:HE1	2.35	0.45
1:A:1042:TYR:HA	1:A:1043:SER:HA	1.65	0.45
2:B:463:ALA:HB2	2:B:469:ARG:HD3	1.99	0.45
6:D:439:VAL:HG23	6:D:701:HIS:CD2	2.52	0.45
6:D:1002:LEU:O	6:D:1002:LEU:HD23	2.15	0.45
1:A:1175:ARG:NH2	7:G:457:GLN:OE1	2.48	0.45
6:E:427:VAL:HG11	6:E:755:LEU:HD21	1.98	0.45
6:E:653:ARG:HH12	6:F:542:ARG:HG2	1.80	0.45
6:F:495:LEU:HD13	6:F:528:ILE:HD12	1.98	0.45
6:F:902:ILE:HD12	6:F:929:PHE:HE1	1.82	0.45
7:G:1076:ILE:HG22	7:G:1159:VAL:HG11	1.99	0.45
1:A:942:LYS:HB3	1:A:943:LEU:C	2.37	0.45
2:B:240:ARG:HA	2:B:245:TYR:HB2	1.97	0.45
2:B:339:VAL:HG23	2:B:484:ILE:HG21	1.99	0.45
5:C:542:ARG:HG2	7:G:653:ARG:HH12	1.82	0.45
5:C:698:HIS:HA	5:C:702:LEU:HB2	1.98	0.45
5:C:795:ASP:OD1	5:C:795:ASP:N	2.50	0.45
1:A:428:ARG:CD	1:A:428:ARG:C	2.85	0.45
1:A:461:ARG:HG3	2:B:174:GLN:HA	1.99	0.45
1:A:549:ALA:C	12:A:1306:UTP:O1B	2.54	0.45
1:A:1197:ARG:HD2	1:A:1197:ARG:O	2.16	0.45
6:E:168:VAL:HG22	6:E:204:VAL:HG22	1.98	0.45
7:G:897:TYR:OH	7:G:900:GLY:O	2.27	0.45
1:A:534:TYR:CE1	1:A:538:GLN:OE1	2.70	0.45
1:A:884:MET:HE3	1:A:889:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:PHE:O	1:A:1086:PHE:CD1	2.70	0.45
2:B:519:ASP:O	2:B:521:GLN:N	2.50	0.45
1:A:37:ARG:CG	1:A:40:ARG:NH2	2.80	0.45
1:A:660:GLU:OE1	1:A:672:LEU:HD22	2.17	0.45
1:A:106:THR:HG22	1:A:202:ILE:HB	1.99	0.44
1:A:768:VAL:O	1:A:1048:ASN:ND2	2.51	0.44
5:C:150:LEU:HA	5:C:804:LEU:HD21	1.98	0.44
5:C:482:ILE:HG23	5:C:706:TYR:OH	2.17	0.44
6:D:342:THR:HB	6:D:1309:ILE:HD11	1.99	0.44
6:E:326:GLY:H	6:E:1267:THR:HG21	1.81	0.44
7:G:838:GLU:HG2	7:G:911:ARG:HH12	1.81	0.44
1:A:601:TYR:CD1	1:A:601:TYR:O	2.70	0.44
2:B:41:PRO:HG2	6:D:146:GLU:CD	2.36	0.44
5:C:231:LEU:HD13	5:C:232:LEU:HG	1.99	0.44
6:D:998:GLY:O	6:D:1002:LEU:HB2	2.17	0.44
6:F:387:THR:OG1	6:F:1320:VAL:O	2.30	0.44
1:A:360:ARG:H	1:A:553:ALA:HB1	1.83	0.44
2:B:442:VAL:HG22	5:C:124:GLN:HG2	2.00	0.44
6:D:1004:PHE:O	6:D:1004:PHE:CD1	2.70	0.44
6:F:626:ARG:NH2	6:F:710:SER:O	2.46	0.44
7:G:456:ASN:ND2	7:G:679:CYS:SG	2.90	0.44
1:A:284:LYS:C	1:A:284:LYS:CD	2.85	0.44
1:A:965:ASN:ND2	1:A:975:GLU:OE2	2.51	0.44
6:E:748:GLN:NE2	6:E:750:GLU:OE1	2.51	0.44
6:F:863:LEU:HA	6:F:866:THR:HG22	2.00	0.44
7:G:656:VAL:HG13	7:G:684:LEU:HD12	1.99	0.44
1:A:86:TYR:OH	1:A:104:LEU:HA	2.17	0.44
1:A:406:LYS:HD2	6:D:496:LYS:HE3	1.99	0.44
1:A:637:TYR:OH	1:A:643:ASP:OD1	2.35	0.44
1:A:1146:ARG:HD3	1:A:1149:PHE:CE1	2.53	0.44
5:C:440:ILE:CG2	5:C:478:ILE:CD1	2.75	0.44
6:F:256:PHE:HE2	6:F:990:THR:HG21	1.81	0.44
6:F:923:TYR:O	6:F:928:ARG:NH1	2.50	0.44
6:F:967:LEU:HD11	6:F:1062:ILE:HG21	2.00	0.44
1:A:499:LEU:HB3	1:A:612:GLU:CG	2.48	0.44
1:A:687:GLN:NE2	5:C:476:SER:H	2.14	0.44
6:D:503:GLU:HA	6:D:542:ARG:HH21	1.81	0.44
6:F:1167:ASP:OD1	6:F:1167:ASP:N	2.50	0.44
7:G:403:PHE:HE2	7:G:625:PRO:HD3	1.81	0.44
1:A:275:PHE:CE2	5:C:467:LYS:HG2	2.53	0.44
1:A:1057:PHE:CE1	7:G:117:ARG:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:PHE:O	1:A:1086:PHE:CG	2.70	0.44
1:A:1205:GLY:O	1:A:1209:TYR:N	2.49	0.44
2:B:147:SER:HA	6:D:133:MET:HE3	1.94	0.44
5:C:762:ILE:O	5:C:762:ILE:HG23	2.17	0.44
6:D:171:GLU:OE2	6:D:1181:SER:OG	2.31	0.44
2:B:156:LEU:O	2:B:157:ILE:HG12	2.13	0.44
6:D:931:ASN:ND2	6:D:936:MET:O	2.50	0.44
6:D:1220:PRO:HA	6:D:1221:PRO:HD3	1.85	0.44
6:F:171:GLU:OE2	6:F:1181:SER:OG	2.33	0.44
7:G:1037:ILE:HG23	7:G:1039:ALA:H	1.81	0.44
1:A:555:VAL:HG21	1:A:648:HIS:HE1	1.82	0.44
1:A:1022:HIS:CD2	1:A:1181:PHE:CE1	3.06	0.44
5:C:294:VAL:O	5:C:349:ASN:ND2	2.43	0.44
1:A:549:ALA:N	12:A:1306:UTP:O1B	2.51	0.43
1:A:568:LEU:HA	1:A:606:TRP:HZ3	1.83	0.43
1:A:1057:PHE:CD1	7:G:117:ARG:CG	3.01	0.43
1:A:1126:ARG:HD2	5:C:452:ASN:ND2	2.33	0.43
2:B:79:LEU:HD22	6:D:792:VAL:HG11	2.00	0.43
2:B:194:SER:CA	6:D:995:THR:HB	2.43	0.43
1:A:286:THR:O	1:A:288:GLU:N	2.51	0.43
1:A:286:THR:CB	1:A:718:ASN:HD21	2.31	0.43
1:A:445:TRP:HE3	1:A:980:SER:HB3	1.83	0.43
1:A:612:GLU:OE2	1:A:641:ARG:NH1	2.37	0.43
1:A:973:LEU:O	1:A:977:ILE:HD12	2.19	0.43
2:B:79:LEU:HD13	6:D:438:ASN:ND2	2.33	0.43
2:B:485:LEU:HD12	2:B:487:VAL:HG13	2.01	0.43
5:C:351:ASP:OD1	5:C:351:ASP:N	2.50	0.43
6:E:1086:PRO:HB2	6:E:1236:ILE:HB	1.99	0.43
7:G:748:GLN:NE2	7:G:750:GLU:OE1	2.52	0.43
7:G:876:GLY:HA2	7:G:902:ILE:HA	2.00	0.43
1:A:496:ARG:HH22	1:A:617:GLN:HB3	1.83	0.43
2:B:370:LEU:HD22	2:B:378:VAL:HG11	1.99	0.43
5:C:495:LEU:HD13	5:C:528:ILE:HD12	1.99	0.43
6:E:392:PRO:HD3	6:E:1317:VAL:HG12	1.99	0.43
1:A:120:THR:O	1:A:122:MET:N	2.51	0.43
2:B:159:PHE:HB3	2:B:184:ILE:HB	2.00	0.43
2:B:185:PRO:HB3	6:D:1000:LEU:HD22	1.99	0.43
2:B:229:PHE:HD1	2:B:251:ILE:CD1	2.31	0.43
2:B:229:PHE:CD1	2:B:251:ILE:HD11	2.53	0.43
1:A:438:VAL:HG21	1:A:455:VAL:HG13	1.99	0.43
1:A:591:GLU:OE1	1:A:598:GLN:CD	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:HE22	5:C:476:SER:H	1.66	0.43
1:A:1021:LEU:N	1:A:1021:LEU:CD1	2.82	0.43
5:C:326:GLY:H	5:C:1267:THR:HG21	1.83	0.43
5:C:439:VAL:HG23	5:C:701:HIS:CD2	2.53	0.43
6:E:433:TYR:HD1	6:E:799:THR:HG21	1.82	0.43
7:G:112:THR:O	7:G:115:GLN:N	2.47	0.43
1:A:412:HIS:O	1:A:412:HIS:CG	2.70	0.43
2:B:350:VAL:HB	2:B:504:THR:HG22	1.99	0.43
2:B:426:LEU:HA	2:B:426:LEU:HD23	1.69	0.43
6:E:852:TYR:HB2	6:E:920:PRO:HA	2.01	0.43
7:G:606:LEU:HD22	7:G:655:ILE:HG12	2.00	0.43
1:A:106:THR:HG22	1:A:202:ILE:HG21	2.01	0.43
1:A:291:PHE:CE2	1:A:715:LEU:HD11	2.53	0.43
1:A:1146:ARG:HD3	1:A:1149:PHE:HE1	1.84	0.43
1:A:1184:LEU:HD22	1:A:1184:LEU:HA	1.80	0.43
2:B:228:ILE:HD13	2:B:248:TYR:HB3	1.99	0.43
6:E:594:LEU:HD23	6:E:597:ALA:HB3	2.00	0.43
6:F:164:LEU:N	6:F:351:ASP:OD2	2.52	0.43
6:F:376:ILE:HG23	6:F:389:PHE:HB2	2.00	0.43
6:F:795:ASP:N	6:F:795:ASP:OD1	2.52	0.43
5:C:500:GLU:HG3	5:C:510:VAL:HG21	2.00	0.43
6:D:351:ASP:N	6:D:351:ASP:OD1	2.52	0.43
1:A:503:PRO:O	1:A:563:TYR:OH	2.30	0.43
1:A:1119:LYS:O	1:A:1123:ILE:HD12	2.19	0.43
1:A:1165:PRO:HA	1:A:1166:PRO:HD3	1.77	0.43
2:B:304:PRO:HB3	5:C:120:VAL:HG11	2.00	0.43
6:D:1144:ARG:HH12	6:D:1171:ILE:HD11	1.84	0.43
2:B:64:ASN:ND2	2:B:64:ASN:C	2.72	0.43
2:B:386:TYR:OH	2:B:459:GLN:OE1	2.37	0.43
2:B:481:THR:HA	2:B:482:PRO:HD3	1.81	0.43
5:C:484:ARG:CZ	5:C:758:ILE:HD12	2.49	0.43
7:G:534:ASN:ND2	7:G:575:TRP:O	2.44	0.43
1:A:795:SER:CB	11:A:1304:A2M:CM'	2.81	0.42
2:B:67:LEU:N	2:B:67:LEU:CD1	2.73	0.42
5:C:660:ALA:HB1	5:C:681:LYS:HE3	2.00	0.42
6:D:262:ASN:HA	6:D:1054:ARG:HH12	1.84	0.42
6:D:863:LEU:HA	6:D:866:THR:HG22	2.01	0.42
6:E:954:GLN:HB3	6:E:957:PHE:HB3	2.00	0.42
6:E:1081:ASP:HB2	6:E:1228:ARG:HB2	2.01	0.42
7:G:926:VAL:HG22	7:G:936:MET:HG2	1.99	0.42
1:A:369:PRO:HB2	1:A:383:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:HA	2:B:214:ALA:HA	1.85	0.42
6:E:639:ASN:ND2	6:E:1328:ILE:O	2.52	0.42
1:A:273:SER:HB2	5:C:471:SER:HB2	2.01	0.42
1:A:284:LYS:HE2	1:A:717:GLN:OE1	2.19	0.42
1:A:942:LYS:HD2	1:A:942:LYS:HA	1.70	0.42
6:E:1134:ARG:NH1	6:E:1158:SER:OG	2.53	0.42
1:A:206:PHE:HZ	1:A:238:ALA:HB2	1.84	0.42
1:A:546:ILE:HB	1:A:682:ILE:HB	2.01	0.42
1:A:594:ASN:CG	6:D:1007:THR:HG21	2.25	0.42
1:A:601:TYR:O	1:A:601:TYR:HD1	2.01	0.42
1:A:820:ASN:HA	1:A:821:PRO:HD2	1.86	0.42
2:B:147:SER:HA	6:D:133:MET:SD	2.60	0.42
5:C:350:ILE:O	5:C:1300:ASN:ND2	2.52	0.42
6:F:156:GLN:NE2	6:F:1311:THR:O	2.48	0.42
6:F:241:ALA:HB2	6:F:1197:PRO:HB2	2.02	0.42
6:F:681:LYS:HG2	6:F:685:ARG:HH12	1.83	0.42
7:G:342:THR:HB	7:G:1309:ILE:HD11	2.01	0.42
1:A:104:LEU:HD12	1:A:104:LEU:C	2.40	0.42
6:E:505:PRO:HG3	6:E:666:ARG:HG3	2.00	0.42
1:A:599:VAL:CG1	6:D:1003:ARG:NH2	2.82	0.42
1:A:897:LEU:HB3	1:A:902:PHE:HB2	2.01	0.42
2:B:437:TYR:CZ	2:B:445:LYS:HD3	2.54	0.42
5:C:1131:PRO:O	5:C:1162:SER:OG	2.31	0.42
6:E:307:VAL:HG21	6:E:1245:ILE:HG22	2.02	0.42
6:F:772:TYR:HB2	6:F:775:VAL:HG23	2.02	0.42
7:G:1085:ASP:OD1	7:G:1085:ASP:N	2.51	0.42
1:A:107:PHE:HD1	1:A:107:PHE:C	2.22	0.42
1:A:203:LEU:HD12	1:A:206:PHE:HB2	2.01	0.42
1:A:268:THR:HA	1:A:283:THR:HA	2.02	0.42
1:A:548:VAL:CG1	1:A:709:PHE:HB3	2.36	0.42
2:B:220:ASN:ND2	6:D:1310:ARG:NH1	2.62	0.42
2:B:281:ASP:HA	2:B:282:VAL:HA	1.80	0.42
6:D:1240:ARG:HD2	6:D:1243:ARG:HB2	2.01	0.42
6:E:235:ILE:HG23	6:E:978:GLN:HE21	1.85	0.42
6:F:307:VAL:HG21	6:F:1245:ILE:HG22	2.02	0.42
6:F:427:VAL:HG11	6:F:755:LEU:HD21	2.02	0.42
1:A:15:THR:HB	1:A:17:LYS:HG2	2.01	0.42
1:A:149:LEU:HB2	1:A:207:VAL:HG13	2.02	0.42
1:A:221:ILE:HA	1:A:772:ARG:HD3	2.02	0.42
1:A:477:VAL:HB	1:A:489:ILE:O	2.20	0.42
1:A:638:PRO:HG2	1:A:641:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:342:THR:HB	5:C:1309:ILE:HD11	2.02	0.42
6:F:439:VAL:HG23	6:F:701:HIS:CD2	2.55	0.42
1:A:365:LEU:HB3	2:B:537:LEU:HD11	2.01	0.42
1:A:568:LEU:HB3	1:A:606:TRP:HH2	1.85	0.42
1:A:1085:LYS:HG2	1:A:1146:ARG:NH1	2.34	0.42
2:B:156:LEU:HG	2:B:179:THR:HG21	2.02	0.42
6:D:996:ASP:O	6:D:996:ASP:OD1	2.38	0.42
6:F:455:GLN:HE21	6:F:455:GLN:HB2	1.60	0.42
1:A:186:SER:HG	9:A:1302:MG7:CN7	2.26	0.42
1:A:284:LYS:HD2	1:A:284:LYS:C	2.40	0.42
1:A:832:LEU:HD23	1:A:836:TRP:CZ3	2.55	0.42
1:A:939:GLN:NE2	2:B:70:PRO:HD3	2.34	0.42
1:A:1032:ASP:HB3	7:G:445:GLU:HA	2.02	0.42
1:A:1175:ARG:HH11	7:G:455:GLN:NE2	2.18	0.42
2:B:161:ASP:HB3	2:B:164:TYR:HB3	2.01	0.42
2:B:212:ASN:HB2	2:B:219:HIS:NE2	2.35	0.42
2:B:324:PRO:HB3	2:B:549:GLU:HG2	2.00	0.42
2:B:499:ALA:HA	2:B:500:ARG:HA	1.77	0.42
6:D:544:TYR:HB3	6:D:547:GLU:HB2	2.00	0.42
6:F:612:PHE:CG	6:F:1331:ARG:HD3	2.55	0.42
1:A:107:PHE:C	1:A:107:PHE:CD1	2.93	0.41
1:A:152:VAL:HG23	1:A:742:TRP:CH2	2.55	0.41
1:A:531:GLU:CD	1:A:676:LYS:CE	2.88	0.41
1:A:754:ASN:ND2	1:A:842:GLY:HA2	2.35	0.41
2:B:442:VAL:HG22	5:C:124:GLN:CD	2.40	0.41
5:C:893:ALA:HB1	5:C:915:VAL:HG22	2.02	0.41
6:D:616:ASP:HB2	6:D:631:PRO:HB2	2.01	0.41
6:F:1076:ILE:HG22	6:F:1159:VAL:HG11	2.02	0.41
7:G:1044:ARG:NH1	7:G:1049:GLU:OE1	2.53	0.41
1:A:679:GLY:HA2	1:A:680:ASP:HA	1.76	0.41
1:A:967:ILE:HG23	1:A:1092:VAL:HG22	2.02	0.41
1:A:1077:ALA:CB	1:A:1086:PHE:HE2	2.10	0.41
6:E:383:SER:HB3	6:E:796:PRO:HG3	2.00	0.41
6:E:835:TYR:CD1	6:E:941:TYR:HB3	2.55	0.41
6:F:451:GLU:OE2	7:G:464:SER:HB3	2.20	0.41
7:G:894:VAL:HG22	7:G:916:LEU:HB3	2.01	0.41
1:A:489:ILE:HG12	1:A:639:SER:OG	2.20	0.41
1:A:670:SER:OG	5:C:441:ARG:HD3	2.20	0.41
5:C:646:ASN:HB3	5:C:649:ALA:HB3	2.02	0.41
5:C:835:TYR:CD1	5:C:941:TYR:HB3	2.55	0.41
6:F:150:LEU:HA	6:F:804:LEU:HD21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HA	1:A:570:VAL:HG22	2.02	0.41
1:A:599:VAL:HG21	6:D:1000:LEU:HD12	2.02	0.41
2:B:218:LYS:HA	6:D:158:SER:HB2	2.02	0.41
1:A:406:LYS:HE3	6:D:496:LYS:HD3	2.02	0.41
1:A:1196:LYS:HD2	1:A:1196:LYS:HA	1.71	0.41
2:B:434:VAL:HG11	2:B:518:ARG:HG2	2.02	0.41
6:D:474:ASP:OD1	6:D:474:ASP:N	2.54	0.41
7:G:297:ASN:ND2	7:G:1299:SER:HB2	2.35	0.41
1:A:157:ASP:OD2	1:A:168:ARG:NH2	2.52	0.41
1:A:808:LEU:HD22	1:A:814:LEU:HD21	2.00	0.41
1:A:814:LEU:HD23	1:A:830:LEU:HB2	2.02	0.41
6:D:876:GLY:HA2	6:D:902:ILE:HA	2.01	0.41
6:F:403:PHE:HE2	6:F:625:PRO:HD3	1.84	0.41
1:A:5:THR:HA	1:A:6:LYS:HA	1.66	0.41
1:A:32:ARG:O	1:A:36:ASP:OD1	2.39	0.41
1:A:152:VAL:HG11	1:A:214:GLY:HA3	2.03	0.41
6:D:294:VAL:O	6:D:349:ASN:ND2	2.39	0.41
6:E:733:VAL:HG12	6:E:743:PRO:HA	2.03	0.41
1:A:145:LEU:HD21	1:A:183:PHE:HE2	1.85	0.41
1:A:363:GLN:OE1	1:A:363:GLN:CA	2.69	0.41
1:A:484:ARG:NH1	12:A:1306:UTP:O3A	2.54	0.41
1:A:665:SER:CA	5:C:790:GLU:HG2	2.41	0.41
2:B:291:LYS:NZ	2:B:361:SER:OG	2.54	0.41
2:B:325:SER:O	2:B:329:LEU:N	2.53	0.41
5:C:1077:MET:HG3	5:C:1165:VAL:HG22	2.03	0.41
6:D:505:PRO:HG3	6:D:666:ARG:HG3	2.02	0.41
6:E:342:THR:HB	6:E:1309:ILE:HD11	2.02	0.41
7:G:352:HIS:HE1	7:G:1296:ILE:HA	1.85	0.41
7:G:439:VAL:HG23	7:G:701:HIS:CD2	2.56	0.41
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.94	0.41
1:A:595:ARG:CG	1:A:595:ARG:NH1	2.72	0.41
1:A:1152:SER:O	1:A:1183:TYR:OH	2.30	0.41
2:B:146:GLU:C	6:D:133:MET:HE2	2.38	0.41
2:B:366:TYR:CE1	2:B:554:ILE:HD11	2.56	0.41
5:C:484:ARG:CB	5:C:484:ARG:HH11	2.34	0.41
6:D:453:LEU:O	6:D:453:LEU:CG	2.69	0.41
6:D:612:PHE:CG	6:D:1331:ARG:HD3	2.55	0.41
6:E:795:ASP:OD1	6:E:795:ASP:N	2.53	0.41
6:E:894:VAL:HG22	6:E:916:LEU:HB3	2.02	0.41
7:G:264:LEU:HD11	7:G:362:LEU:HD23	2.03	0.41
1:A:1019:LEU:O	1:A:1019:LEU:CD2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:SER:HB3	2:B:328:ALA:HB3	2.04	0.41
5:C:481:ALA:O	5:C:483:ALA:N	2.53	0.41
6:D:628:SER:OG	6:D:629:ARG:N	2.54	0.41
6:E:294:VAL:O	6:E:349:ASN:ND2	2.42	0.41
6:F:954:GLN:HB2	6:F:957:PHE:HB3	2.02	0.41
7:G:143:VAL:HG11	7:G:1316:ALA:HB1	2.03	0.41
1:A:5:THR:HB	1:A:6:LYS:HD2	2.02	0.40
2:B:147:SER:CA	6:D:133:MET:CE	2.91	0.40
2:B:266:GLU:CD	6:D:988:GLN:NE2	2.74	0.40
2:B:506:LEU:HD21	2:B:538:LEU:HD11	2.02	0.40
6:E:660:ALA:HB1	6:E:681:LYS:HE3	2.03	0.40
6:E:876:GLY:HA2	6:E:902:ILE:HA	2.03	0.40
6:E:1174:THR:HG23	6:E:1201:LEU:HD11	2.02	0.40
6:F:485:GLU:HG3	6:F:523:THR:HB	2.02	0.40
1:A:237:CYS:HA	1:A:245:GLU:HG2	2.02	0.40
1:A:284:LYS:HE2	1:A:718:ASN:ND2	2.36	0.40
1:A:363:GLN:CG	1:A:363:GLN:O	2.68	0.40
1:A:946:ARG:HD2	1:A:969:TYR:CE2	2.56	0.40
2:B:193:PHE:N	6:D:996:ASP:HB2	2.36	0.40
2:B:442:VAL:CG1	5:C:128:GLU:HG3	2.51	0.40
5:C:440:ILE:HG22	5:C:478:ILE:CD1	2.50	0.40
5:C:902:ILE:HD12	5:C:929:PHE:HE1	1.86	0.40
5:C:1085:ASP:OD1	5:C:1085:ASP:N	2.54	0.40
6:E:231:LEU:HD13	6:E:232:LEU:HG	2.04	0.40
7:G:351:ASP:OD1	7:G:351:ASP:N	2.54	0.40
1:A:438:VAL:HG13	1:A:442:VAL:HG23	2.04	0.40
6:D:529:LYS:HE2	6:D:586:PRO:HD2	2.02	0.40
6:F:1096:TYR:CD1	6:F:1136:HIS:HB3	2.56	0.40
1:A:103:TYR:HA	1:A:347:THR:HG21	2.03	0.40
1:A:485:ARG:CD	1:A:485:ARG:N	2.80	0.40
1:A:782:PHE:O	1:A:786:ALA:N	2.54	0.40
2:B:156:LEU:CG	2:B:179:THR:HG21	2.51	0.40
2:B:190:ILE:CG1	2:B:192:ASP:OD1	2.69	0.40
5:C:921:ASP:OD1	5:C:928:ARG:NH2	2.54	0.40
5:C:1121:HIS:HA	5:C:1122:PRO:HD3	1.93	0.40
6:D:443:VAL:HG13	6:D:445:GLU:H	1.86	0.40
6:F:352:HIS:HE1	6:F:1296:ILE:HA	1.85	0.40
6:F:534:ASN:ND2	6:F:575:TRP:O	2.46	0.40
6:F:656:VAL:HG13	6:F:684:LEU:HD12	2.02	0.40
7:G:406:ASP:HB3	7:G:410:ARG:HH22	1.87	0.40
1:A:203:LEU:HA	1:A:206:PHE:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:O	1:A:284:LYS:CG	2.70	0.40
2:B:359:LYS:HA	2:B:362:PHE:HB3	2.04	0.40
2:B:532:ASP:OD1	5:C:121:PHE:CE2	2.74	0.40
5:C:1220:PRO:HA	5:C:1221:PRO:HD3	1.87	0.40
7:G:241:ALA:HB2	7:G:1197:PRO:HB2	2.02	0.40
7:G:529:LYS:HE2	7:G:586:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1206/1208 (100%)	1091 (90%)	96 (8%)	19 (2%)	9	43
2	B	492/559 (88%)	437 (89%)	50 (10%)	5 (1%)	15	54
5	C	1218/1220 (100%)	1152 (95%)	64 (5%)	2 (0%)	47	79
6	D	1193/1205 (99%)	1127 (94%)	66 (6%)	0	100	100
6	E	1187/1205 (98%)	1120 (94%)	67 (6%)	0	100	100
6	F	1187/1205 (98%)	1124 (95%)	63 (5%)	0	100	100
7	G	1214/1226 (99%)	1133 (93%)	81 (7%)	0	100	100
All	All	7697/7828 (98%)	7184 (93%)	487 (6%)	26 (0%)	44	74

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	PRO
1	A	425	SER
1	A	432	GLU
1	A	549	ALA
1	A	555	VAL

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Mol	Chain	Res	Type
1	A	556	THR
1	A	985	LYS
5	C	486	VAL
1	A	121	LYS
1	A	431	THR
1	A	579	PHE
2	B	157	ILE
2	B	191	ALA
2	B	196	THR
1	A	108	ARG
1	A	426	PRO
1	A	287	SER
2	B	192	ASP
1	A	712	THR
1	A	713	ALA
1	A	118	PRO
1	A	641	ARG
2	B	134	THR
5	C	787	ILE
1	A	1034	LEU
1	A	1035	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1049/1049 (100%)	992 (95%)	57 (5%)	22	58
2	B	435/492 (88%)	417 (96%)	18 (4%)	30	66
5	C	1063/1063 (100%)	1048 (99%)	15 (1%)	67	86
6	D	1044/1049 (100%)	1031 (99%)	13 (1%)	71	88
6	E	1039/1049 (99%)	1033 (99%)	6 (1%)	86	94
6	F	1039/1049 (99%)	1033 (99%)	6 (1%)	86	94
7	G	1064/1069 (100%)	1058 (99%)	6 (1%)	86	94
All	All	6733/6820 (99%)	6612 (98%)	121 (2%)	61	82

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	36	ASP
1	A	37	ARG
1	A	38	VAL
1	A	107	PHE
1	A	108	ARG
1	A	111	SER
1	A	113	THR
1	A	138	ARG
1	A	189	GLN
1	A	254	ARG
1	A	264	VAL
1	A	265	CYS
1	A	274	GLN
1	A	284	LYS
1	A	363	GLN
1	A	368	ARG
1	A	387	ASN
1	A	408	VAL
1	A	412	HIS
1	A	428	ARG
1	A	479	ARG
1	A	485	ARG
1	A	486	GLN
1	A	489	ILE
1	A	531	GLU
1	A	547	ASP
1	A	548	VAL
1	A	551	MET
1	A	552	ASP
1	A	595	ARG
1	A	596	GLN
1	A	601	TYR
1	A	606	TRP
1	A	672	LEU
1	A	675	ILE
1	A	676	LYS
1	A	680	ASP
1	A	681	ASP
1	A	812	MET
1	A	820	ASN
1	A	826	THR

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Mol	Chain	Res	Type
1	A	828	MET
1	A	880	ASN
1	A	883	GLU
1	A	950	ARG
1	A	1019	LEU
1	A	1021	LEU
1	A	1022	HIS
1	A	1084	HIS
1	A	1085	LYS
1	A	1125	LEU
1	A	1136	ASN
1	A	1175	ARG
1	A	1188	ARG
1	A	1196	LYS
1	A	1198	LEU
2	B	58	GLU
2	B	62	ARG
2	B	67	LEU
2	B	71	ARG
2	B	133	VAL
2	B	190	ILE
2	B	194	SER
2	B	230	ASN
2	B	343	ASN
2	B	396	ILE
2	B	424	GLU
2	B	443	ARG
2	B	446	ILE
2	B	447	LYS
2	B	449	MET
2	B	485	LEU
2	B	520	ARG
2	B	555	LYS
5	C	133	MET
5	C	283	ASN
5	C	444	SER
5	C	447	ARG
5	C	469	ARG
5	C	474	ASP
5	C	475	ILE
5	C	478	ILE
5	C	479	HIS

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Mol	Chain	Res	Type
5	C	486	VAL
5	C	762	ILE
5	C	783	ASP
5	C	860	ARG
5	C	1112	ASN
5	C	1154	ASN
6	D	283	ASN
6	D	447	ARG
6	D	453	LEU
6	D	472	GLU
6	D	860	ARG
6	D	954	GLN
6	D	1001	THR
6	D	1002	LEU
6	D	1004	PHE
6	D	1005	LEU
6	D	1054	ARG
6	D	1112	ASN
6	D	1154	ASN
6	E	283	ASN
6	E	447	ARG
6	E	637	TYR
6	E	860	ARG
6	E	1112	ASN
6	E	1154	ASN
6	F	283	ASN
6	F	447	ARG
6	F	455	GLN
6	F	860	ARG
6	F	1112	ASN
6	F	1154	ASN
7	G	283	ASN
7	G	447	ARG
7	G	637	TYR
7	G	860	ARG
7	G	1112	ASN
7	G	1154	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	126	HIS
1	A	263	ASN
1	A	274	GLN
1	A	387	ASN
1	A	514	ASN
1	A	538	GLN
1	A	586	ASN
1	A	596	GLN
1	A	607	GLN
1	A	648	HIS
1	A	687	GLN
1	A	700	ASN
1	A	718	ASN
1	A	729	ASN
1	A	754	ASN
1	A	807	ASN
1	A	880	ASN
1	A	939	GLN
1	A	1020	HIS
1	A	1039	HIS
1	A	1136	ASN
2	B	59	HIS
2	B	63	HIS
2	B	64	ASN
2	B	188	GLN
2	B	220	ASN
2	B	230	ASN
2	B	319	HIS
2	B	343	ASN
2	B	346	ASN
2	B	376	GLN
2	B	470	ASN
2	B	527	GLN
5	C	115	GLN
5	C	124	GLN
5	C	148	GLN
5	C	452	ASN
5	C	456	ASN
5	C	479	HIS
5	C	640	GLN
5	C	698	HIS
5	C	748	GLN

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Mol	Chain	Res	Type
5	C	821	ASN
5	C	942	HIS
5	C	978	GLN
5	C	1112	ASN
6	D	346	HIS
6	D	438	ASN
6	D	491	ASN
6	D	640	GLN
6	D	698	HIS
6	D	711	ASN
6	D	821	ASN
6	D	954	GLN
6	D	988	GLN
6	D	1112	ASN
6	E	148	GLN
6	E	283	ASN
6	E	346	HIS
6	E	698	HIS
6	E	724	HIS
6	E	821	ASN
6	E	1112	ASN
6	E	1142	ASN
6	F	284	ASN
6	F	346	HIS
6	F	452	ASN
6	F	491	ASN
6	F	748	GLN
6	F	978	GLN
6	F	1112	ASN
6	F	1332	ASN
7	G	148	GLN
7	G	455	GLN
7	G	577	GLN
7	G	748	GLN
7	G	821	ASN
7	G	942	HIS
7	G	978	GLN
7	G	1112	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	t	4/5 (80%)	3 (75%)	0
4	p	1/3 (33%)	1 (100%)	0
All	All	5/8 (62%)	4 (80%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	t	2	U
3	t	3	A
3	t	4	C
4	p	3	G

There are no RNA pucker outliers to report.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
11	A2M	A	1304	10	18,25,26	4.17	9 (50%)	18,36,39	4.11	10 (55%)
9	MG7	A	1302	10	20,23,23	8.75	10 (50%)	17,35,35	4.56	6 (35%)
10	DPO	A	1303	9,11	3,7,8	1.10	0	6,10,13	1.75	1 (16%)
12	UTP	A	1306	8	22,30,30	2.31	4 (18%)	27,47,47	1.77	5 (18%)

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
11	A2M	A	1304	10	-	3/5/27/28	0/3/3/3
9	MG7	A	1302	10	-	2/2/22/22	0/3/3/3
10	DPO	A	1303	9,11	-	0/2/5/6	-
12	UTP	A	1306	8	-	5/20/38/38	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1302	MG7	O3'-C3'	-19.58	0.96	1.43
9	A	1302	MG7	C2'-C1'	-18.31	1.26	1.53
9	A	1302	MG7	O2'-C2'	-13.92	1.10	1.43
9	A	1302	MG7	CN7-N7	-12.66	1.18	1.47
9	A	1302	MG7	C3'-C2'	-11.50	1.21	1.53
9	A	1302	MG7	O4'-C1'	-11.31	1.25	1.41
9	A	1302	MG7	C3'-C4'	-9.68	1.28	1.53
11	A	1304	A2M	O4'-C1'	-9.53	1.27	1.41
12	A	1306	UTP	O2'-C2'	-9.29	1.21	1.43
9	A	1302	MG7	C5'-C4'	-8.07	1.24	1.51
11	A	1304	A2M	C3'-C2'	-6.38	1.38	1.52
11	A	1304	A2M	O3'-C3'	-6.15	1.28	1.43
11	A	1304	A2M	C3'-C4'	-6.14	1.37	1.53
11	A	1304	A2M	O2'-CM'	5.63	1.62	1.42
11	A	1304	A2M	C5'-C4'	5.40	1.68	1.51
9	A	1302	MG7	O4'-C4'	-4.60	1.34	1.45
11	A	1304	A2M	O5'-C5'	-4.58	1.33	1.44
11	A	1304	A2M	O2'-C2'	-3.09	1.34	1.42
12	A	1306	UTP	PB-O1B	3.00	1.69	1.55
12	A	1306	UTP	C2-N3	-2.62	1.33	1.38
12	A	1306	UTP	O5'-C5'	-2.53	1.35	1.44
11	A	1304	A2M	C8-N7	-2.19	1.30	1.34
9	A	1302	MG7	C8-N9	2.06	1.36	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1302	MG7	O4'-C4'-C5'	-11.62	84.10	109.21
11	A	1304	A2M	C1'-N9-C4	11.54	146.91	126.64
9	A	1302	MG7	C5'-C4'-C3'	9.30	137.51	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1302	MG7	C3'-C2'-C1'	8.86	114.31	100.98
11	A	1304	A2M	O2'-C2'-C1'	5.57	120.13	109.09
11	A	1304	A2M	O4'-C4'-C5'	5.55	127.64	109.37
9	A	1302	MG7	O3'-C3'-C4'	5.36	126.55	111.05
11	A	1304	A2M	CM'-O2'-C2'	5.36	128.59	114.52
12	A	1306	UTP	O2'-C2'-C1'	5.26	130.26	110.85
12	A	1306	UTP	PB-O3A-PA	-4.68	116.75	132.83
11	A	1304	A2M	O5'-C5'-C4'	4.25	123.45	108.99
11	A	1304	A2M	N3-C2-N1	-3.93	122.53	128.68
11	A	1304	A2M	O4'-C1'-C2'	3.86	113.27	106.59
11	A	1304	A2M	C2'-C3'-C4'	3.83	110.31	101.99
10	A	1303	DPO	O7-P2-O4	3.59	116.61	104.64
12	A	1306	UTP	PB-O3B-PG	-3.52	120.75	132.83
9	A	1302	MG7	C2-N1-C6	-2.51	120.47	125.10
9	A	1302	MG7	O2'-C2'-C1'	2.35	119.52	110.85
11	A	1304	A2M	C4-C5-N7	-2.31	106.99	109.40
12	A	1306	UTP	C3'-C2'-C1'	2.23	104.34	100.98
12	A	1306	UTP	C5-C4-N3	-2.18	118.50	123.31
11	A	1304	A2M	O3'-C3'-C4'	2.11	117.16	111.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1304	A2M	C3'-C4'-C5'-O5'
12	A	1306	UTP	C5'-O5'-PA-O1A
12	A	1306	UTP	C5'-O5'-PA-O3A
12	A	1306	UTP	O4'-C1'-N1-C6
12	A	1306	UTP	C2'-C1'-N1-C6
9	A	1302	MG7	C3'-C4'-C5'-O5'
9	A	1302	MG7	O4'-C4'-C5'-O5'
11	A	1304	A2M	O4'-C4'-C5'-O5'
12	A	1306	UTP	C4'-C5'-O5'-PA
11	A	1304	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

4 monomers are involved in 26 short contacts:

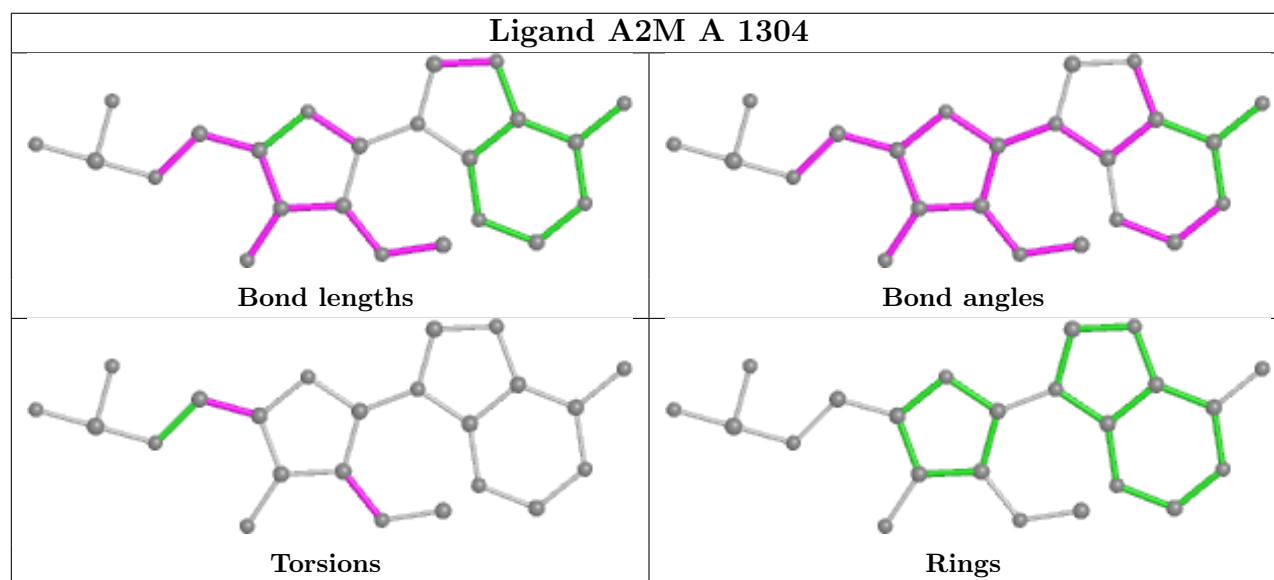
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1304	A2M	5	0
9	A	1302	MG7	7	0

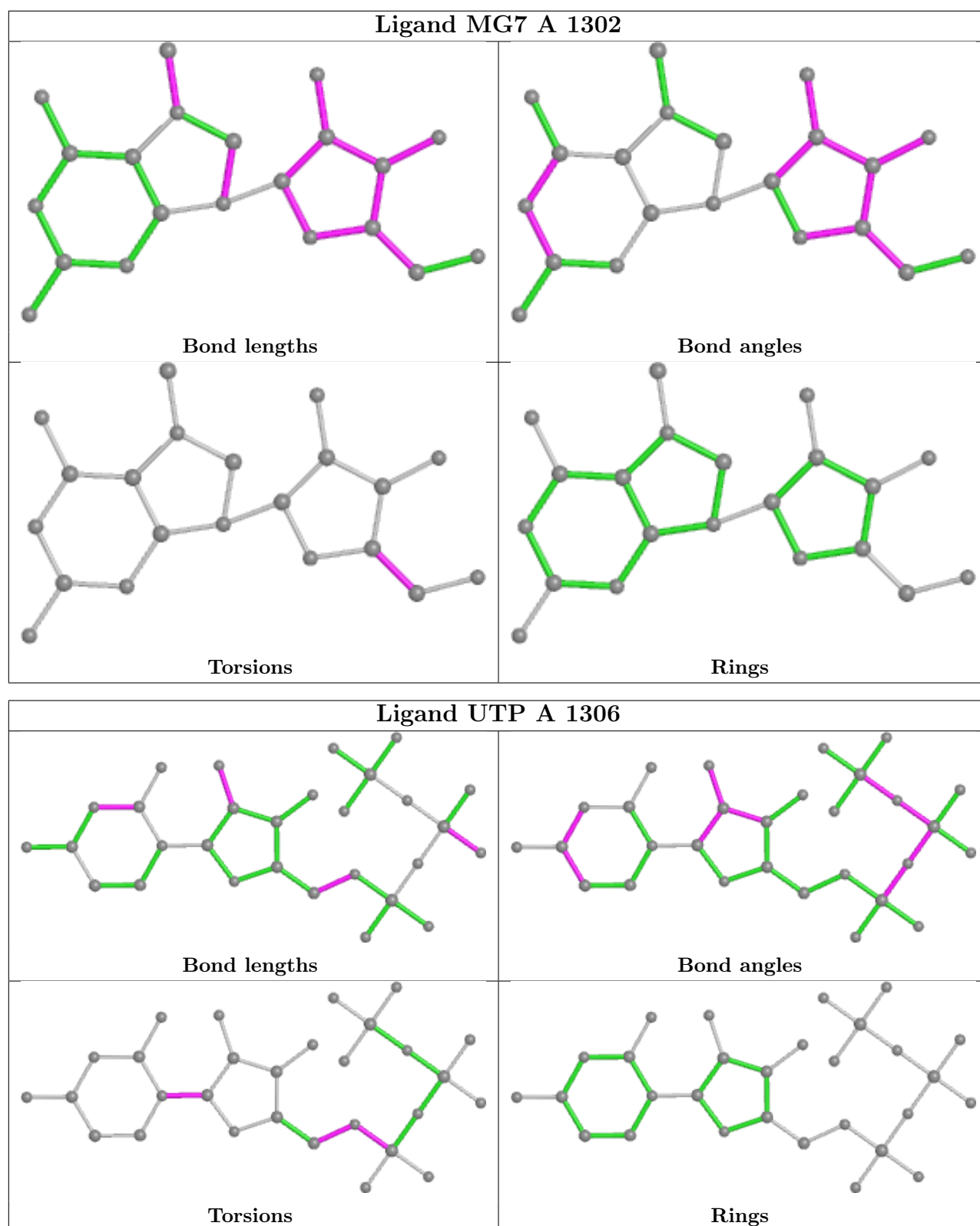
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1303	DPO	1	0
12	A	1306	UTP	13	0

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





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

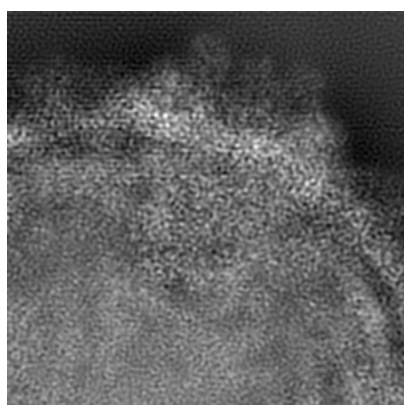
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9907. These allow visual inspection of the internal detail of the map and identification of artifacts.

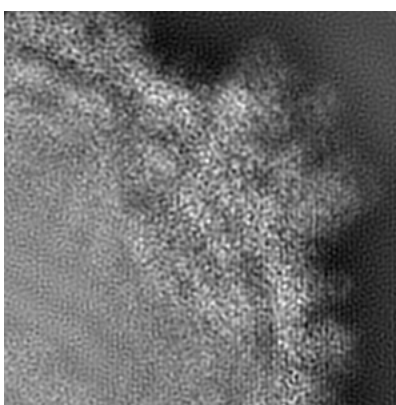
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

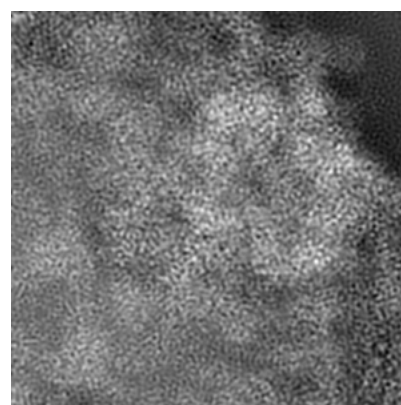
#### 6.1.1 Primary map



X



Y

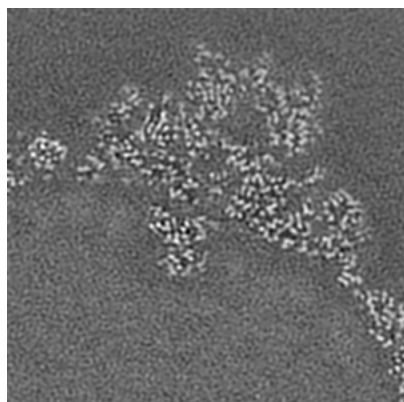


Z

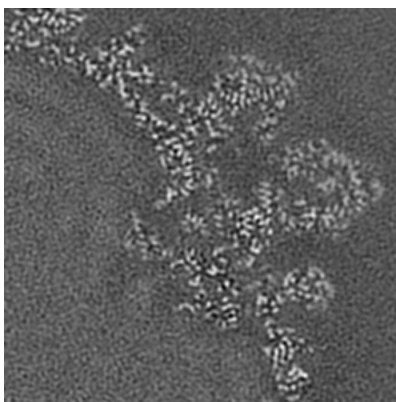
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

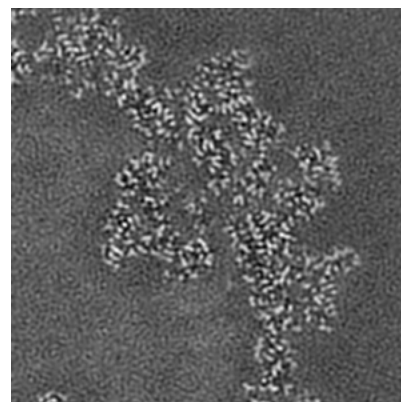
#### 6.2.1 Primary map



X Index: 112



Y Index: 112

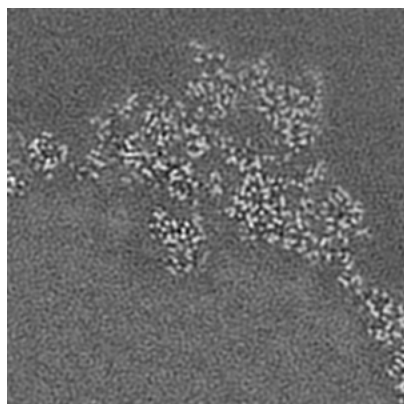


Z Index: 112

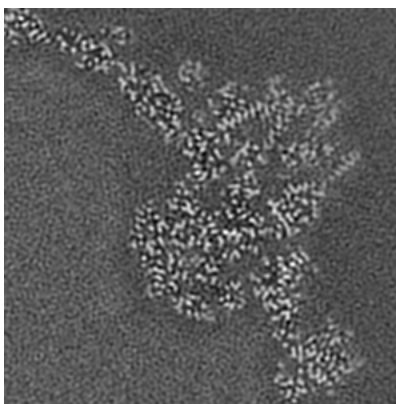
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

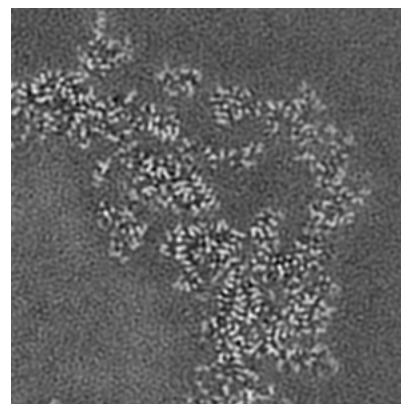
### 6.3.1 Primary map



X Index: 113



Y Index: 90

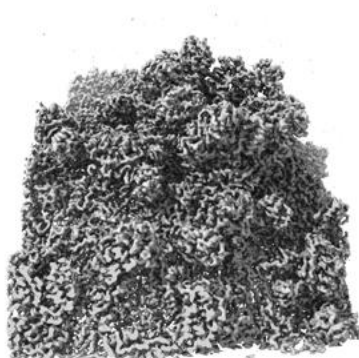


Z Index: 131

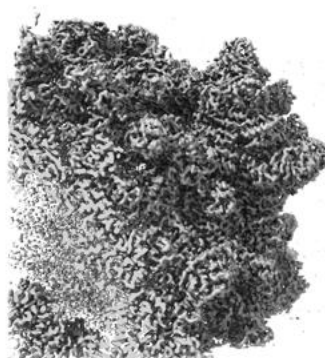
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

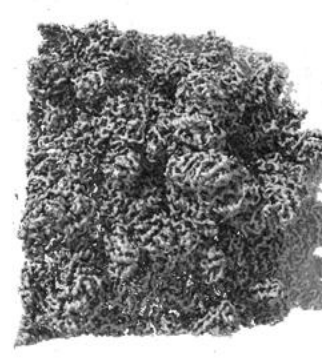
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

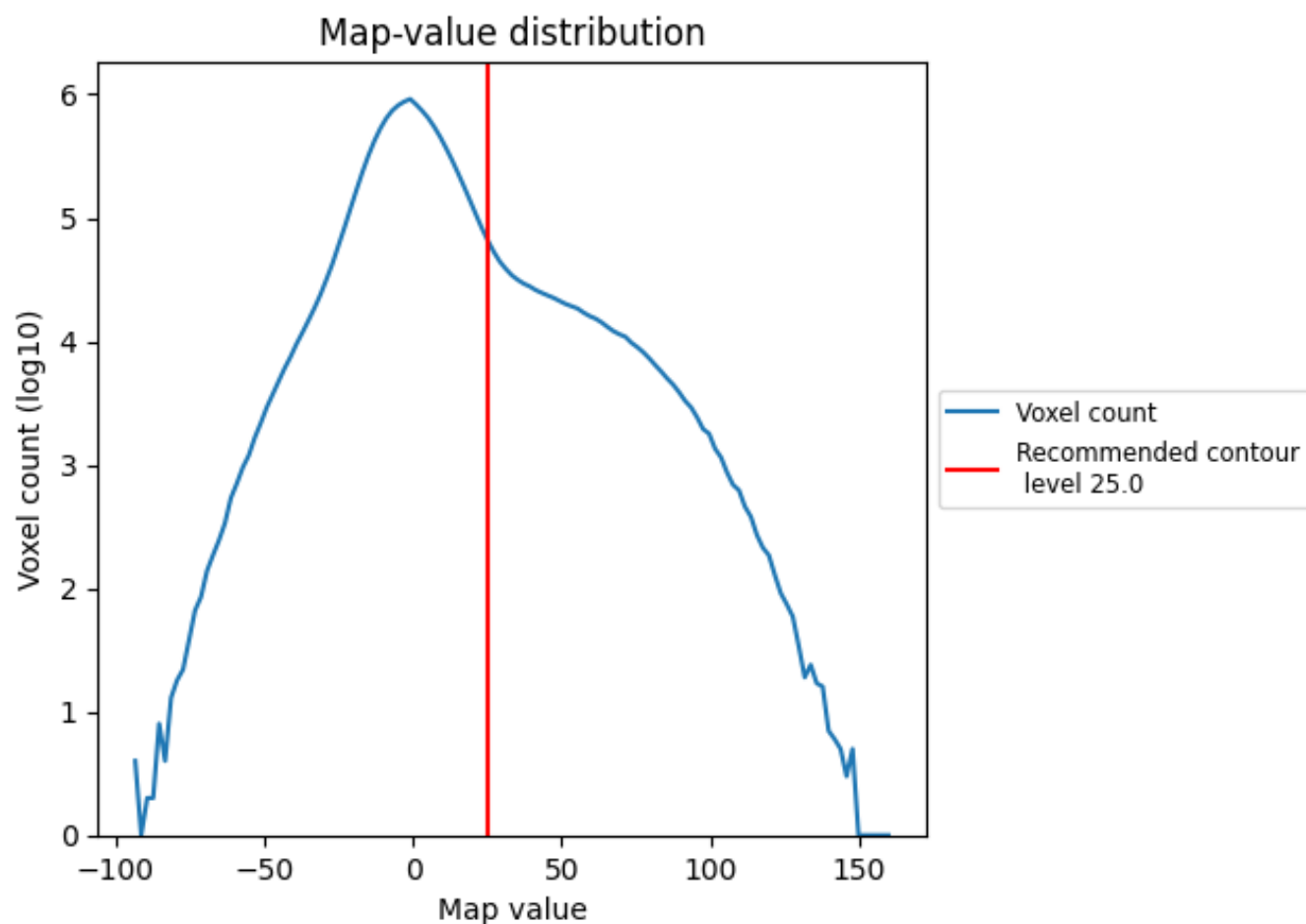
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

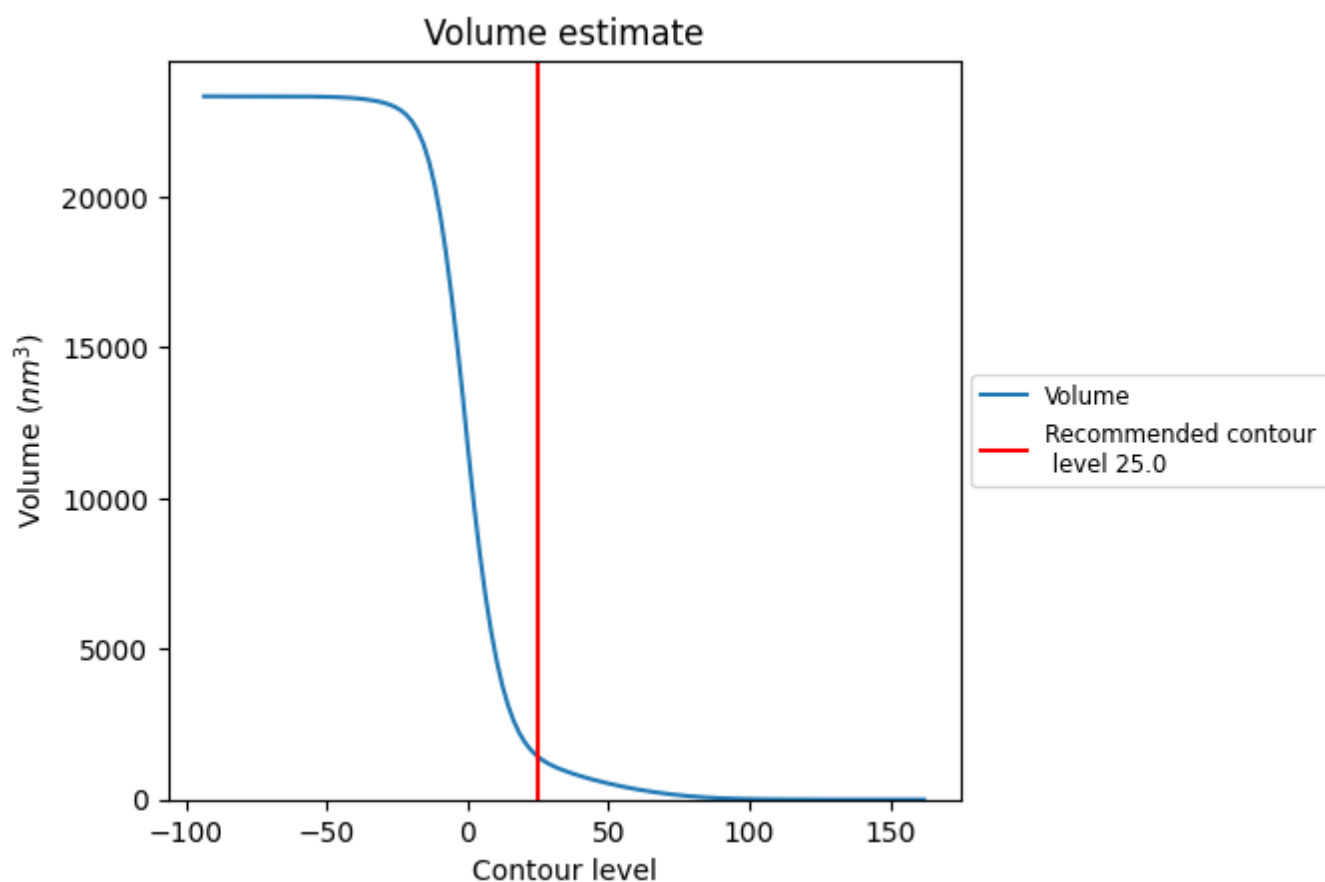
### 7.1 Map-value distribution [i](#)



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



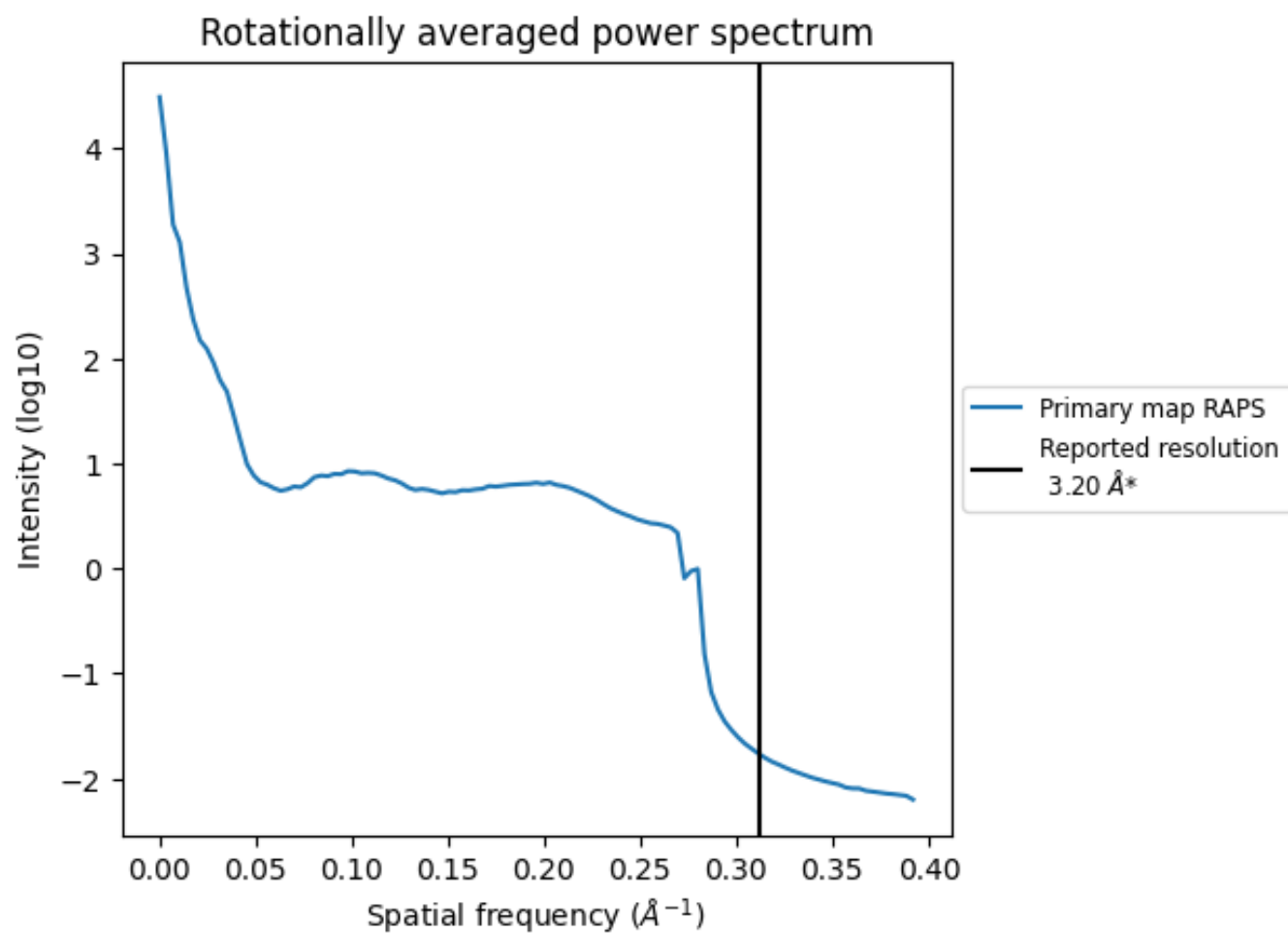
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1428 nm<sup>3</sup>; this corresponds to an approximate mass of 1290 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 0.312 Å<sup>-1</sup>

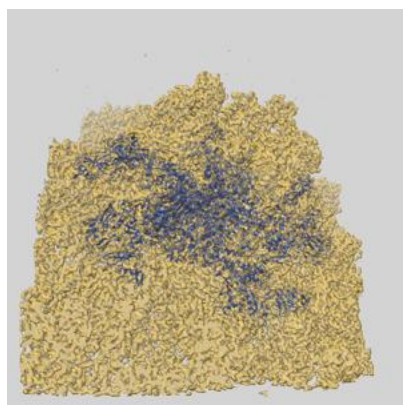
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

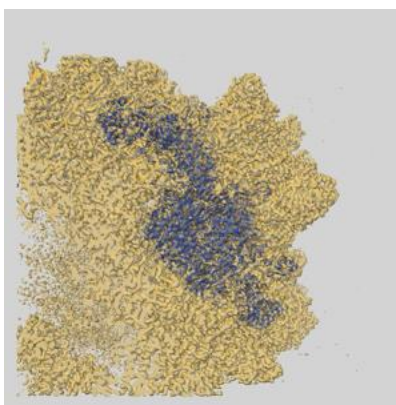
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9907 and PDB model 6K32. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

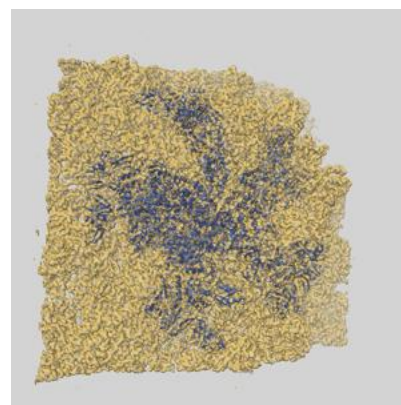
### 9.1 Map-model overlay [i](#)



X



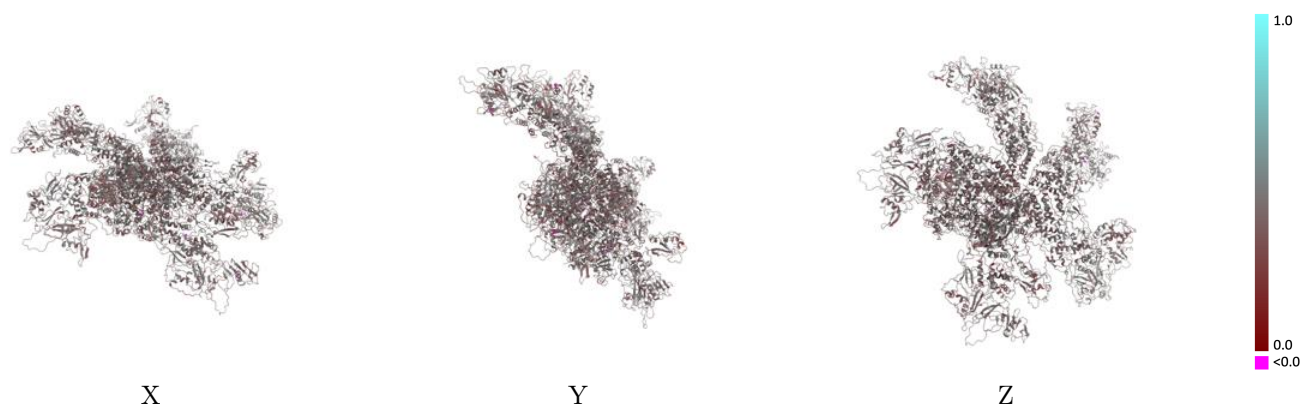
Y



Z

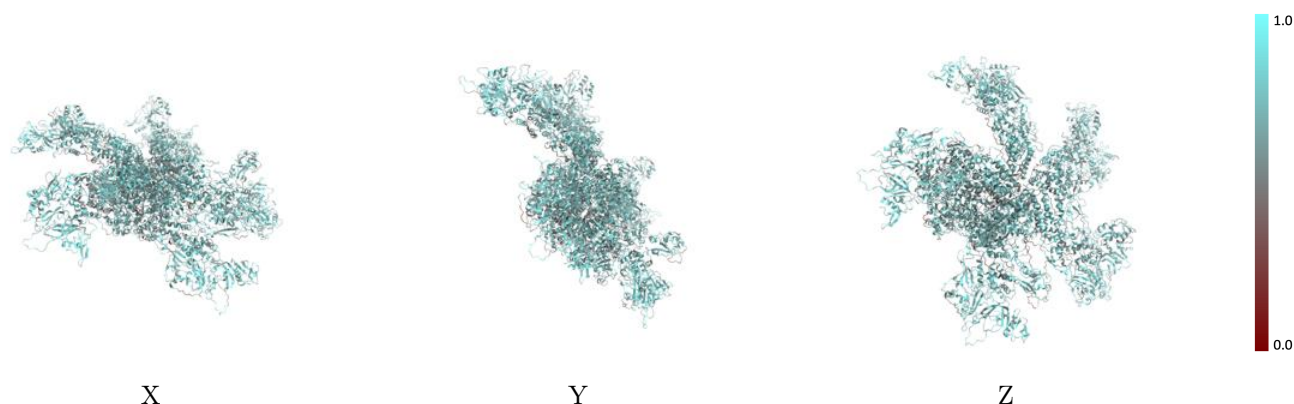
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



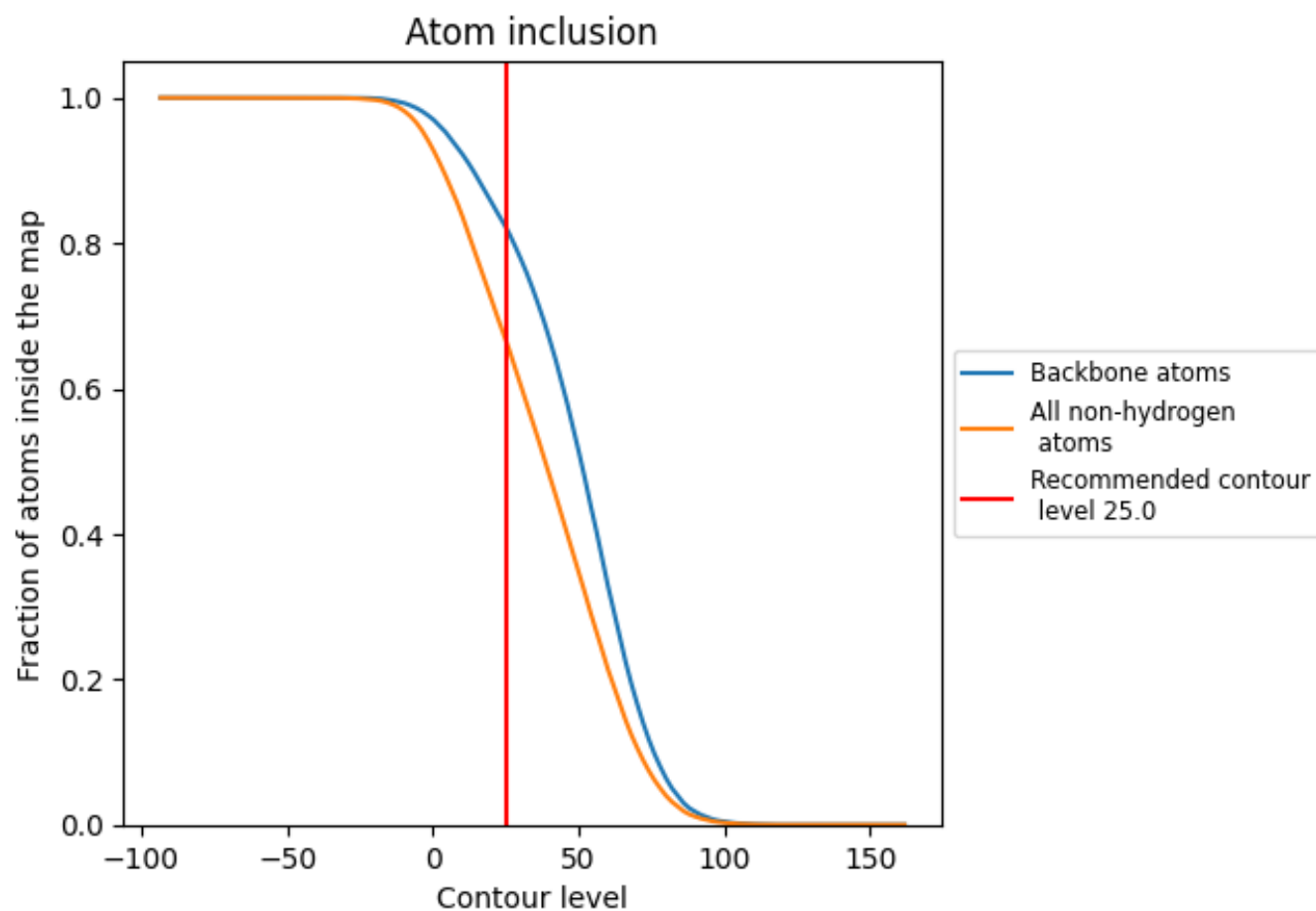
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (25.0).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 67% 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 (25.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6676</div>	<div><div></div>0.3950</div>
A	<div><div></div>0.6484</div>	<div><div></div>0.3890</div>
B	<div><div></div>0.6694</div>	<div><div></div>0.4030</div>
C	<div><div></div>0.6750</div>	<div><div></div>0.3950</div>
D	<div><div></div>0.6643</div>	<div><div></div>0.3900</div>
E	<div><div></div>0.6756</div>	<div><div></div>0.4010</div>
F	<div><div></div>0.6757</div>	<div><div></div>0.3940</div>
G	<div><div></div>0.6683</div>	<div><div></div>0.3980</div>
p	<div><div></div>0.5556</div>	<div><div></div>0.3690</div>
t	<div><div></div>0.5437</div>	<div><div></div>0.3410</div>

1.0

0.0

<0.0