



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:35 PM UTC

PDB ID : 7CYQ / pdb_00007cyq
EMDB ID : EMD-30504
Title : Cryo-EM structure of an extended SARS-CoV-2 replication and transcription complex reveals an intermediate state in cap synthesis
Authors : Yan, L.; Ge, J.; Zheng, L.; Zhang, Y.; Gao, Y.; Wang, T.; Wang, H.; Huang, Y.; Li, M.; Wang, Q.; Rao, Z.; Lou, Z.
Deposited on : 2020-09-04
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

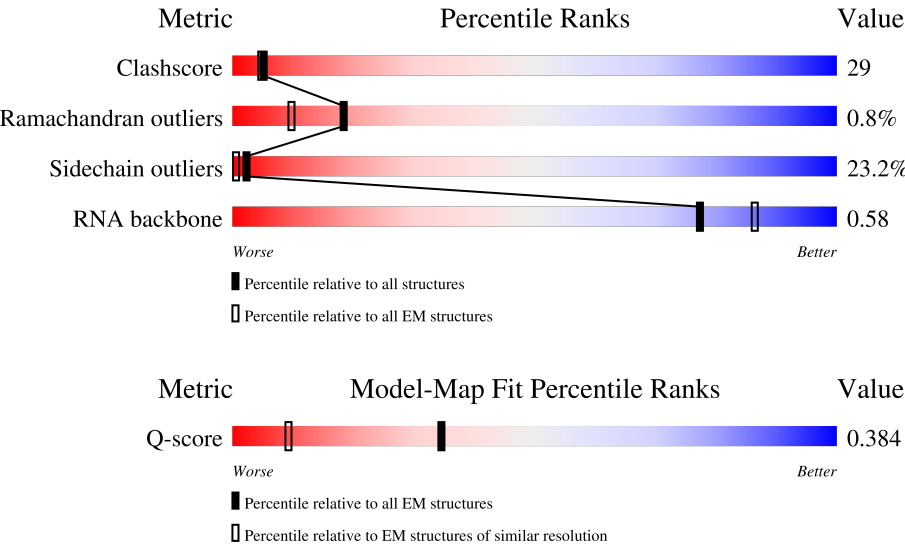
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.83 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.



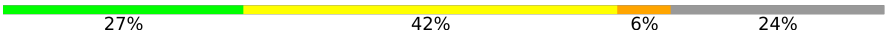
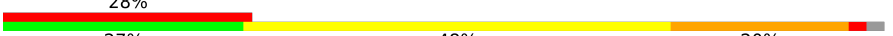
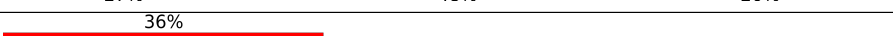
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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

Mol	Chain	Length	Quality of chain
1	A	942	
2	B	198	
2	D	198	

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Mol	Chain	Length	Quality of chain
3	C	83	
4	I	33	
5	J	59	
6	E	601	
6	F	601	
7	G	117	

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
9	GDP	A	1003	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21857 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-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7458	4763	1251	1390	54		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1396	872	240	273	11		
2	D	186	Total	C	N	O	S	0	0
			1414	889	242	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a RNA chain called Primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 5 is a RNA chain called Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	27	Total	C	N	O	P	0	0
			565	253	94	191	27		

- Molecule 6 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	585	Total	C	N	O	S	1	0
			4508	2875	750	848	35		
6	E	586	Total	C	N	O	S	1	0
			4513	2878	751	849	35		

- Molecule 7 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

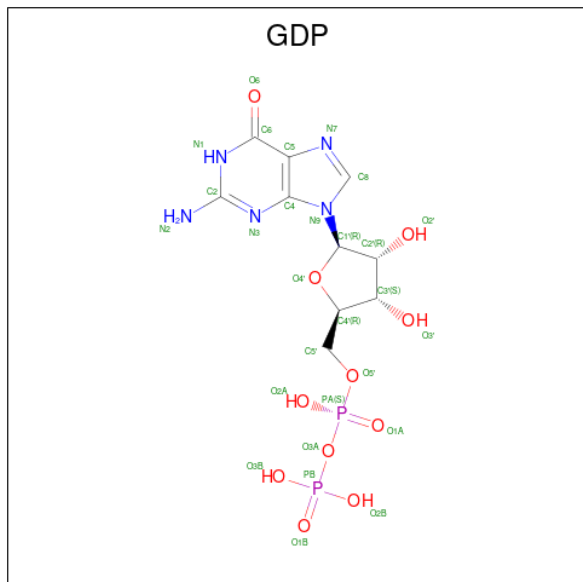
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	SER	-	expression tag	UNP P0DTD1
G	-2	ASN	-	expression tag	UNP P0DTD1
G	-1	ALA	-	expression tag	UNP P0DTD1
G	0	MET	-	expression tag	UNP P0DTD1

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	F	3	Total	Zn	0
			3	3	
8	E	3	Total	Zn	0
			3	3	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

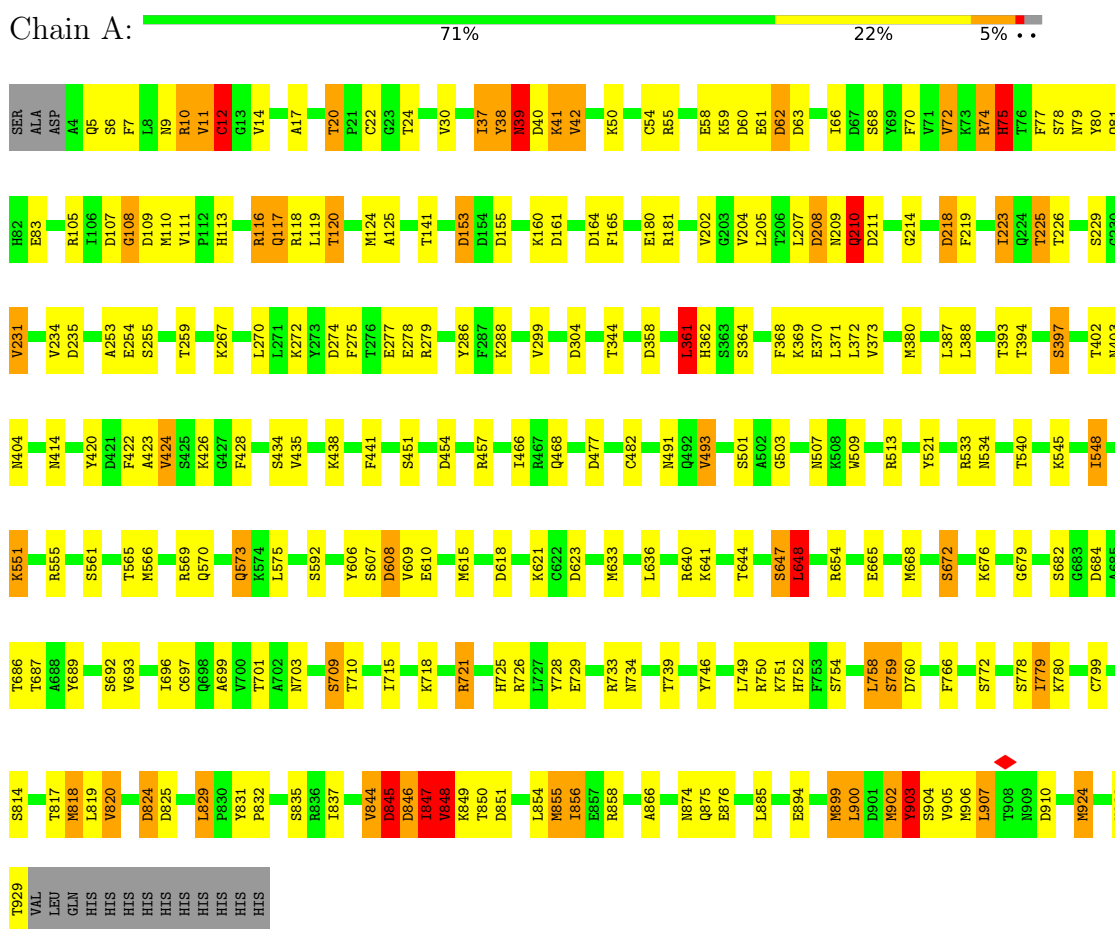
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

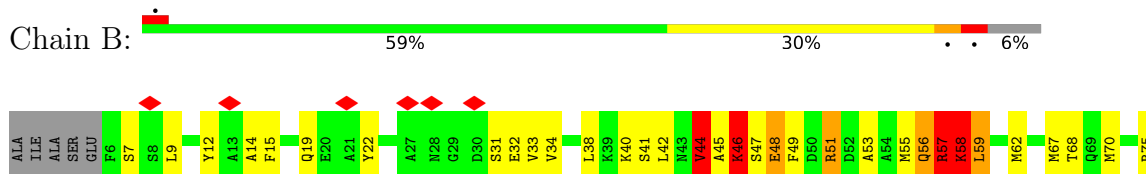
3 Residue-property plots

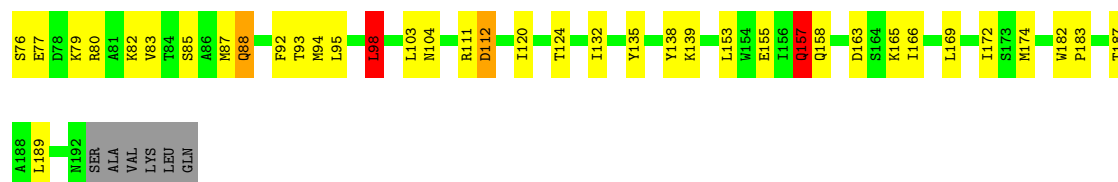
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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-directed RNA polymerase

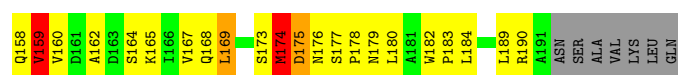
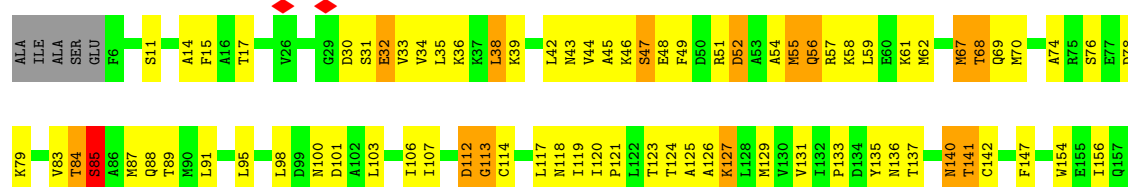


• Molecule 2: Non-structural protein 8





• Molecule 2: Non-structural protein 8



• Molecule 3: Non-structural protein 7



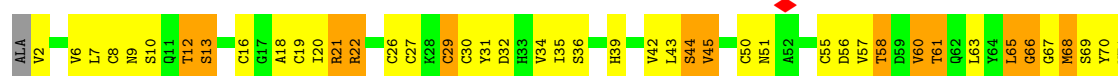
• Molecule 4: Primer

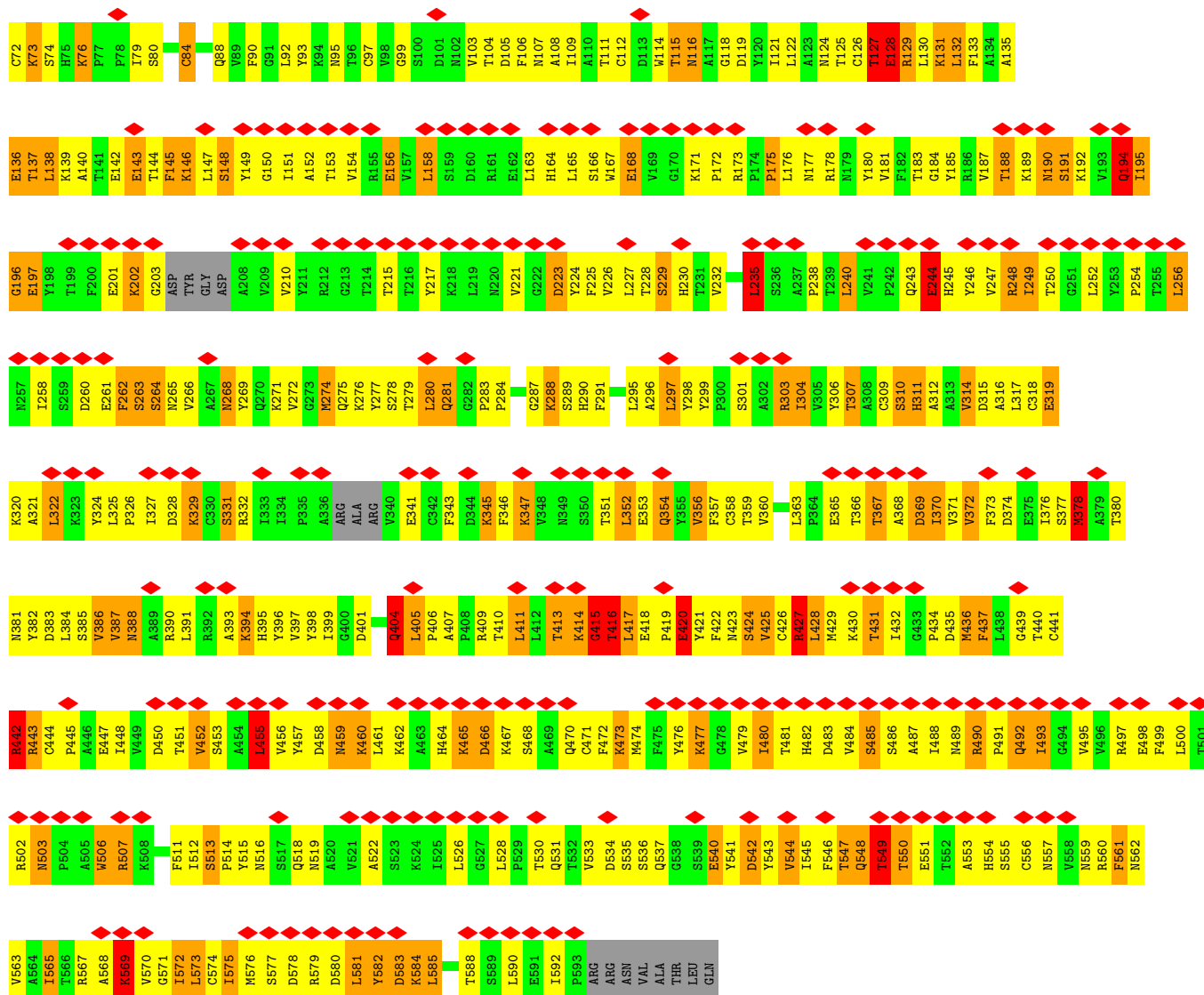


• Molecule 5: Template

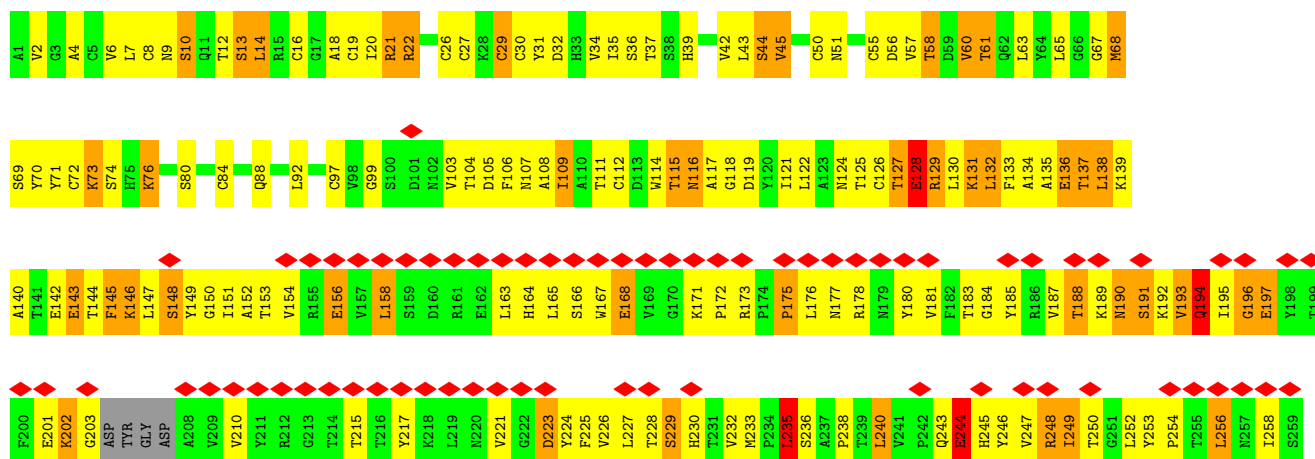


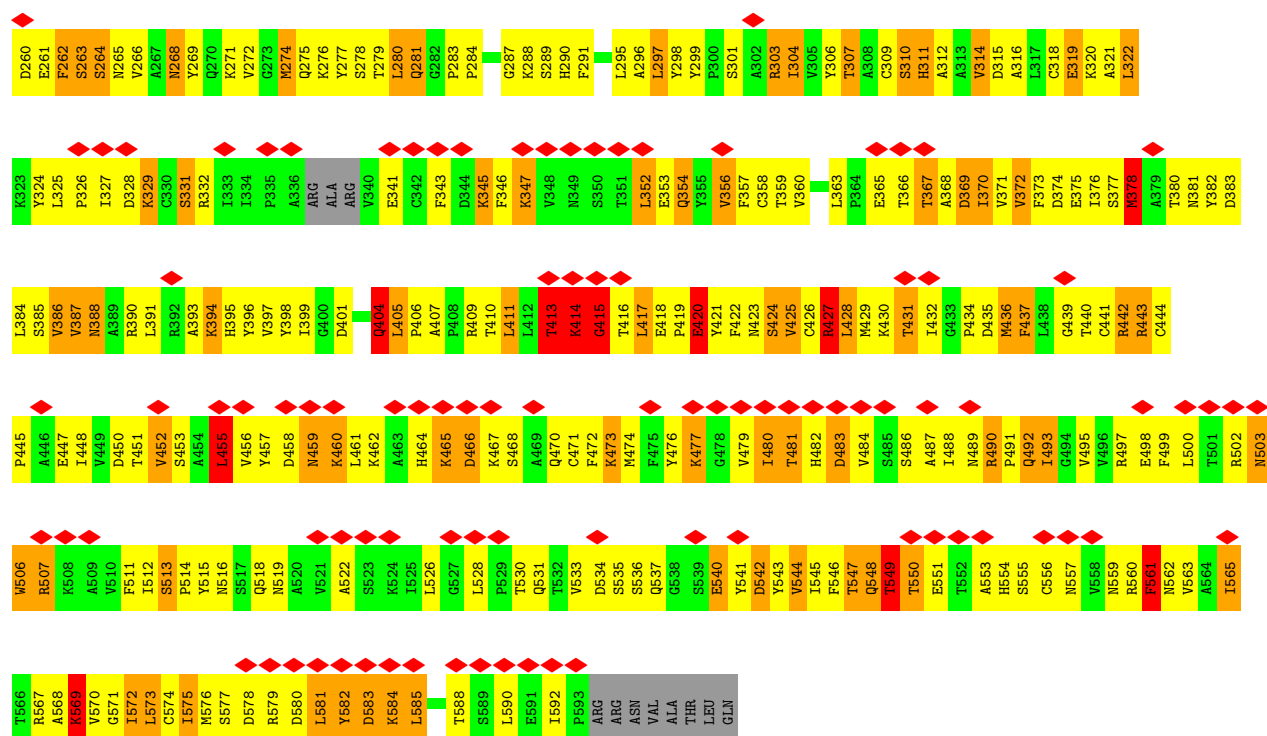
• Molecule 6: Helicase



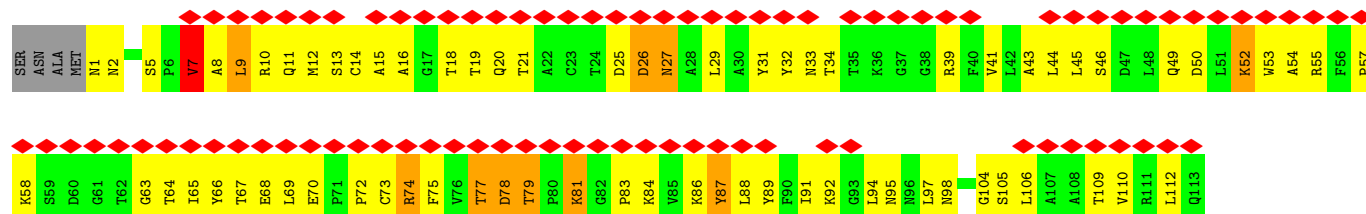
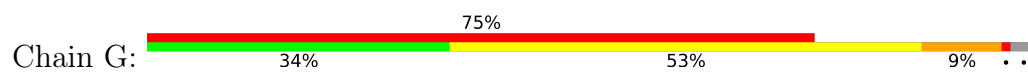


• Molecule 6: Helicase





• Molecule 7: Non-structural protein 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	529558	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.146	Depositor
Minimum map value	-0.897	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GDP

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	0.74	15/7647 (0.2%)	0.96	51/10379 (0.5%)
2	B	0.77	3/1414 (0.2%)	1.00	15/1922 (0.8%)
2	D	0.42	0/1433	0.88	14/1944 (0.7%)
3	C	0.52	0/556	0.53	0/749
4	I	0.42	0/611	0.34	0/953
5	J	0.68	3/628 (0.5%)	0.57	2/974 (0.2%)
6	E	0.30	0/4615	1.17	48/6290 (0.8%)
6	F	0.30	0/4610	1.03	36/6283 (0.6%)
7	G	0.30	0/884	0.90	5/1200 (0.4%)
All	All	0.55	21/22398 (0.1%)	0.99	171/30694 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
2	D	0	1
6	E	0	1
6	F	0	2
7	G	0	1
All	All	0	8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLN	C-O	-8.07	1.14	1.24
1	A	207	LEU	C-O	-7.71	1.14	1.24
1	A	117	GLN	C-O	-7.52	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LEU	CA-C	-7.51	1.42	1.52
1	A	37	ILE	C-O	-7.34	1.16	1.24
1	A	116	ARG	C-O	-7.22	1.15	1.24
1	A	117	GLN	CA-C	-6.83	1.44	1.52
1	A	846	ASP	CA-C	-6.44	1.43	1.52
5	J	26	A	O3'-P	-6.35	1.51	1.61
1	A	116	ARG	CA-C	-6.28	1.45	1.52
5	J	25	G	O3'-P	-6.10	1.51	1.61
1	A	847	ILE	C-O	-5.86	1.17	1.24
1	A	209	ASN	C-O	-5.78	1.15	1.23
1	A	11	VAL	CA-C	-5.72	1.46	1.52
1	A	848	VAL	C-O	-5.61	1.17	1.24
1	A	38	TYR	C-O	-5.58	1.17	1.24
2	B	104	ASN	CA-C	-5.52	1.45	1.52
2	B	75	ARG	CA-C	-5.27	1.46	1.52
5	J	24	U	O3'-P	-5.14	1.53	1.61
1	A	208	ASP	C-O	-5.12	1.17	1.24
2	B	75	ARG	C-O	-5.10	1.18	1.24

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	LEU	N-CA-C	28.12	147.74	111.75
6	F	194	GLN	N-CA-C	25.41	147.09	111.52
1	A	844	VAL	CB-CA-C	-22.32	90.76	111.74
1	A	39	ASN	CB-CA-C	-21.68	75.68	111.24
6	F	194	GLN	CB-CA-C	-20.54	84.33	111.86
6	E	194	GLN	N-CA-C	20.39	140.34	109.96
6	E	405	LEU	N-CA-CB	-20.34	79.32	110.03
1	A	855	MET	CB-CA-C	-19.13	79.87	111.24
1	A	849	LYS	N-CA-C	18.59	138.82	112.04
6	E	405	LEU	N-CA-C	18.41	135.44	109.84
6	E	235	LEU	CB-CA-C	-18.35	79.70	110.16
6	E	404	GLN	CB-CA-C	-15.64	79.33	110.30
6	E	193	VAL	CB-CA-C	15.00	135.89	111.29
1	A	845	ASP	CB-CA-C	14.83	134.01	109.84
6	F	128	GLU	N-CA-CB	-14.04	86.76	110.49
1	A	848	VAL	N-CA-C	-13.94	97.43	110.53
6	E	128	GLU	N-CA-CB	-13.91	89.63	110.07
6	E	194	GLN	N-CA-CB	-13.86	87.62	109.51
1	A	648	LEU	N-CA-C	13.41	125.42	111.07
6	F	66	GLY	N-CA-C	-13.05	87.99	112.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	128	GLU	N-CA-C	12.80	127.75	111.24
1	A	928	HIS	N-CA-C	-12.76	87.39	108.32
6	E	194	GLN	CB-CA-C	-12.57	92.06	110.16
1	A	609	VAL	N-CA-C	-12.46	90.00	108.45
6	F	415	GLY	N-CA-C	12.35	142.45	113.18
1	A	856	ILE	N-CA-CB	-12.07	91.32	111.23
1	A	606	TYR	CB-CA-C	-11.68	96.43	111.50
1	A	850	THR	N-CA-CB	-11.66	92.57	110.06
1	A	39	ASN	N-CA-C	11.51	123.99	110.41
6	F	128	GLU	N-CA-C	11.50	135.29	110.80
7	G	7	VAL	N-CA-C	11.38	133.00	109.34
6	F	189	LYS	N-CA-C	-11.18	100.18	114.04
6	E	14	LEU	N-CA-CB	11.13	129.31	110.49
1	A	608	ASP	N-CA-C	-10.91	87.56	110.80
2	B	158	GLN	N-CA-CB	-10.79	93.31	110.69
6	E	414	LYS	N-CA-C	-10.58	93.29	109.79
7	G	8	ALA	N-CA-C	10.34	123.67	110.33
1	A	855	MET	N-CA-C	10.27	122.53	110.41
6	E	236	SER	N-CA-CB	-10.26	93.15	110.49
6	F	369	ASP	N-CA-C	10.20	126.25	112.68
6	E	369	ASP	N-CA-C	10.19	126.23	112.68
6	E	236	SER	N-CA-C	9.95	131.99	110.80
1	A	845	ASP	N-CA-C	-9.87	94.07	109.76
6	F	127	THR	N-CA-C	-9.79	94.83	109.81
7	G	7	VAL	CB-CA-C	-9.76	95.29	111.29
2	B	104	ASN	N-CA-C	-9.70	101.57	113.50
6	E	483	ASP	N-CA-C	9.51	131.04	110.80
6	E	414	LYS	CB-CA-C	9.40	134.58	113.33
6	F	195	ILE	N-CA-C	9.31	128.71	109.34
6	E	443	ARG	N-CA-CB	-9.12	95.08	110.49
6	F	443	ARG	N-CA-CB	-9.12	95.08	110.49
2	D	175	ASP	N-CA-C	-9.06	102.00	113.23
6	E	550	THR	N-CA-CB	9.04	125.76	110.49
1	A	362	HIS	N-CA-CB	-8.99	97.18	110.84
1	A	850	THR	N-CA-C	8.98	122.19	111.33
6	E	484	VAL	N-CA-CB	8.96	126.01	111.23
2	D	174	MET	N-CA-C	8.94	122.77	111.24
6	E	13	SER	CB-CA-C	-8.86	98.24	111.70
1	A	120	THR	N-CA-CB	-8.79	97.87	111.05
6	E	127	THR	N-CA-C	-8.77	94.88	109.80
1	A	218	ASP	N-CA-C	8.69	123.99	111.56
1	A	12	CYS	N-CA-C	-8.67	96.67	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	ARG	CB-CA-C	-8.62	96.27	109.29
6	E	235	LEU	N-CA-C	8.59	122.41	108.41
1	A	928	HIS	CB-CA-C	8.54	124.32	109.89
1	A	362	HIS	N-CA-C	-8.50	92.89	108.02
2	D	159	VAL	N-CA-C	-8.47	95.81	108.17
6	F	370	ILE	N-CA-CB	8.22	124.80	111.23
6	E	370	ILE	N-CA-CB	8.21	124.77	111.23
1	A	361	LEU	CB-CA-C	-8.17	94.61	110.46
6	F	550	THR	N-CA-CB	8.14	124.18	111.24
1	A	845	ASP	CA-C-N	8.07	134.09	121.26
1	A	845	ASP	C-N-CA	8.07	134.09	121.26
2	D	85	SER	N-CA-CB	-8.07	98.07	110.42
2	D	158	GLN	CB-CA-C	8.04	124.34	109.86
6	E	549	THR	CB-CA-C	-7.71	95.07	110.42
2	B	157	GLN	CB-CA-C	7.49	125.33	110.42
6	F	442	ARG	N-CA-C	7.46	126.68	110.80
6	F	127	THR	CB-CA-C	-7.44	96.25	110.24
2	B	57	ARG	CB-CA-C	7.35	125.04	110.42
1	A	119	LEU	CB-CA-C	-7.31	98.46	112.43
1	A	108	GLY	N-CA-C	-7.29	95.89	113.18
6	F	188	THR	N-CA-C	7.22	120.40	108.48
6	E	569	LYS	CA-CB-CG	7.22	128.54	114.10
6	F	569	LYS	CA-CB-CG	7.21	128.53	114.10
2	B	158	GLN	N-CA-C	-7.20	97.99	109.59
1	A	37	ILE	N-CA-C	7.18	118.16	108.11
1	A	847	ILE	N-CA-CB	7.10	122.94	111.23
1	A	107	ASP	N-CA-C	7.10	125.91	110.80
2	B	44	VAL	N-CA-C	-7.02	105.50	112.17
2	D	84	THR	CB-CA-C	7.02	124.08	110.46
6	F	404	GLN	N-CA-C	6.99	121.88	111.04
1	A	929	THR	N-CA-CB	6.97	123.34	111.50
1	A	849	LYS	CB-CA-C	-6.90	97.93	110.56
6	E	369	ASP	CB-CA-C	-6.86	98.78	110.24
6	F	369	ASP	CB-CA-C	-6.83	98.83	110.24
6	E	172	PRO	CA-C-N	-6.83	106.09	122.74
6	E	172	PRO	C-N-CA	-6.83	106.09	122.74
6	F	172	PRO	CA-C-N	-6.80	106.14	122.74
6	F	172	PRO	C-N-CA	-6.80	106.14	122.74
6	F	549	THR	CB-CA-C	-6.80	96.89	110.42
1	A	37	ILE	N-CA-CB	-6.75	102.09	111.41
2	D	156	ILE	CB-CA-C	-6.63	101.45	111.33
2	B	46	LYS	N-CA-C	-6.62	105.23	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	26	A	C1'-C2'-O2'	-6.55	98.57	108.40
6	F	195	ILE	N-CA-CB	-6.55	100.42	111.23
1	A	368	PHE	N-CA-C	6.55	119.25	111.33
1	A	845	ASP	N-CA-CB	-6.55	99.80	109.95
6	F	196	GLY	N-CA-C	6.42	119.10	110.43
6	E	196	GLY	N-CA-C	6.41	119.08	110.43
6	E	569	LYS	CB-CG-CD	6.39	125.99	111.30
6	F	569	LYS	CB-CG-CD	6.38	125.98	111.30
2	B	56	GLN	N-CA-C	-6.36	104.27	111.14
2	D	169	LEU	N-CA-C	6.32	118.05	111.03
2	B	47	SER	N-CA-C	-6.32	105.72	113.50
6	E	189	LYS	N-CA-C	-6.26	97.46	110.80
1	A	119	LEU	N-CA-C	-6.26	100.07	109.96
2	D	112	ASP	CB-CA-C	6.17	122.70	110.42
6	E	188	THR	N-CA-C	6.16	123.92	110.80
2	B	7	SER	CB-CA-C	6.13	122.62	110.42
2	B	44	VAL	CA-C-N	6.10	132.40	121.66
2	B	44	VAL	C-N-CA	6.10	132.40	121.66
6	F	244	GLU	CA-CB-CG	6.09	126.28	114.10
6	E	244	GLU	CA-CB-CG	6.09	126.28	114.10
6	E	561	PHE	N-CA-C	-6.09	105.61	113.16
1	A	846	ASP	N-CA-C	6.08	119.42	110.30
6	F	415	GLY	CA-C-N	6.07	133.13	121.54
6	F	415	GLY	C-N-CA	6.07	133.13	121.54
6	E	375	GLU	N-CA-C	6.05	119.45	111.28
1	A	647	SER	CB-CA-C	-6.03	100.01	110.45
1	A	846	ASP	CA-C-N	6.02	132.81	121.97
1	A	846	ASP	C-N-CA	6.02	132.81	121.97
2	B	59	LEU	CB-CA-C	-6.00	97.61	109.67
2	D	30	ASP	N-CA-C	5.99	120.33	111.04
6	E	484	VAL	N-CA-C	-5.89	97.09	109.34
6	E	442	ARG	N-CA-C	5.84	120.02	113.01
1	A	107	ASP	CB-CA-C	-5.80	98.88	110.42
7	G	20	GLN	CB-CA-C	-5.75	109.93	116.54
2	D	158	GLN	N-CA-C	-5.74	99.24	108.55
6	E	14	LEU	N-CA-C	-5.63	98.81	110.80
6	F	235	LEU	CB-CA-C	-5.62	100.73	110.45
2	D	126	ALA	N-CA-C	5.60	122.73	110.80
2	B	58	LYS	N-CA-CB	-5.58	101.70	110.46
7	G	8	ALA	N-CA-CB	-5.56	102.72	110.29
2	D	85	SER	N-CA-C	5.53	120.03	113.12
6	E	127	THR	CB-CA-C	-5.45	104.60	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	MET	N-CA-C	5.41	118.68	111.75
6	E	481	THR	N-CA-C	-5.40	101.08	109.24
1	A	609	VAL	N-CA-CB	5.34	120.21	111.45
2	D	159	VAL	N-CA-CB	5.31	120.18	111.58
6	F	455	LEU	CA-CB-CG	5.28	134.77	116.30
6	E	455	LEU	CA-CB-CG	5.26	134.73	116.30
6	E	413	THR	CB-CA-C	-5.26	99.78	109.15
6	E	415	GLY	N-CA-C	5.24	125.60	113.18
6	F	13	SER	N-CA-CB	-5.23	102.59	111.27
6	F	188	THR	CB-CA-C	-5.23	105.06	114.52
6	F	378	MET	CB-CG-SD	5.21	128.33	112.70
6	E	378	MET	CB-CG-SD	5.21	128.33	112.70
1	A	38	TYR	N-CA-CB	-5.20	102.79	110.90
6	F	12	THR	CB-CA-C	-5.17	100.25	111.11
1	A	218	ASP	CB-CA-C	-5.13	105.25	111.82
1	A	117	GLN	N-CA-C	5.11	118.08	109.95
6	F	420	GLU	CA-CB-CG	5.10	124.30	114.10
6	E	420	GLU	CA-CB-CG	5.10	124.29	114.10
5	J	25	G	C1'-C2'-O2'	5.10	119.44	111.80
1	A	209	ASN	N-CA-C	-5.07	104.39	110.88
1	A	75	HIS	N-CA-C	5.04	114.80	108.45
6	F	427	ARG	CG-CD-NE	5.02	123.03	112.00
6	E	427	ARG	CG-CD-NE	5.01	123.02	112.00
6	E	378	MET	CA-CB-CG	5.00	124.11	114.10
1	A	647	SER	N-CA-C	-5.00	103.06	110.46

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ASP	Peptide
1	A	903	TYR	Peptide
2	B	182	TRP	Peptide
2	D	38	LEU	Peptide
6	E	506	TRP	Peptide
6	F	415	GLY	Peptide
6	F	506	TRP	Peptide
7	G	9	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7458	0	7191	186	0
2	B	1396	0	1364	78	0
2	D	1414	0	1416	84	0
3	C	553	0	585	21	0
4	I	545	0	272	23	0
5	J	565	0	291	27	0
6	E	4513	0	4431	390	0
6	F	4508	0	4423	390	0
7	G	868	0	880	62	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
9	A	28	0	12	10	0
10	A	1	0	0	0	0
All	All	21857	0	20865	1225	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 29.

All (1225) 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)
2:D:125:ALA:O	2:D:189:LEU:CD1	1.76	1.33
6:E:194:GLN:O	6:E:194:GLN:CG	1.70	1.33
2:B:41:SER:O	2:B:44:VAL:HG23	1.30	1.30
2:B:42:LEU:O	2:B:45:ALA:HB3	1.39	1.22
6:E:549:THR:CG2	6:E:549:THR:O	1.87	1.21
6:E:185:TYR:HB3	6:E:193:VAL:O	1.38	1.19
6:E:549:THR:O	6:E:549:THR:HG23	1.37	1.17
6:F:369:ASP:O	6:F:394:LYS:HB2	1.45	1.16
6:E:369:ASP:O	6:E:394:LYS:HB2	1.45	1.14
2:B:42:LEU:O	2:B:45:ALA:CB	1.97	1.13
2:D:125:ALA:O	2:D:189:LEU:HD13	1.43	1.12
6:F:549:THR:HG23	6:F:549:THR:O	1.50	1.11
1:A:907:LEU:HG	1:A:910:ASP:OD1	1.36	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:ASP:OD1	1:A:845:ASP:N	1.87	1.08
7:G:15:ALA:HB2	7:G:25:ASP:O	1.57	1.02
1:A:75:HIS:HE1	9:A:1003:GDP:C4	1.77	1.02
6:E:424:SER:O	6:E:427:ARG:NH1	1.93	1.02
6:F:549:THR:O	6:F:549:THR:CG2	2.04	1.01
6:F:424:SER:O	6:F:427:ARG:NH1	1.93	1.00
1:A:607:SER:O	1:A:608:ASP:OD1	1.80	0.99
1:A:75:HIS:CE1	9:A:1003:GDP:C4	2.51	0.99
6:F:404:GLN:O	6:F:405:LEU:HD23	1.63	0.98
2:D:125:ALA:O	2:D:189:LEU:HD12	1.62	0.98
1:A:12:CYS:SG	1:A:17:ALA:HA	2.09	0.93
1:A:907:LEU:CG	1:A:910:ASP:OD1	2.18	0.92
2:B:14:ALA:HB3	2:B:48:GLU:OE2	1.69	0.92
2:B:14:ALA:CB	2:B:48:GLU:OE2	2.15	0.92
6:E:194:GLN:O	6:E:194:GLN:HG2	1.11	0.92
7:G:7:VAL:HG22	7:G:7:VAL:O	1.69	0.91
2:B:42:LEU:HA	2:B:45:ALA:HB2	1.54	0.89
1:A:844:VAL:HG23	1:A:844:VAL:O	1.72	0.89
6:E:57:VAL:HG21	6:E:72:CYS:HB3	1.53	0.89
6:F:57:VAL:HG21	6:F:72:CYS:HB3	1.53	0.88
1:A:39:ASN:O	1:A:40:ASP:OD1	1.92	0.88
6:F:26:CYS:O	6:F:30:CYS:N	2.07	0.88
6:E:553:ALA:O	6:E:557:ASN:ND2	2.07	0.88
4:I:11:G:O6	5:J:49:C:N4	2.08	0.86
6:E:26:CYS:O	6:E:30:CYS:N	2.07	0.86
2:B:42:LEU:O	2:B:45:ALA:N	2.07	0.86
2:B:41:SER:O	2:B:44:VAL:CG2	2.21	0.86
6:F:553:ALA:O	6:F:557:ASN:ND2	2.07	0.86
6:E:490:ARG:HG2	6:E:490:ARG:HH11	1.41	0.86
2:B:46:LYS:O	2:B:46:LYS:NZ	2.07	0.85
6:F:490:ARG:HH11	6:F:490:ARG:HG2	1.41	0.85
6:F:490:ARG:HA	6:F:493:ILE:HB	1.59	0.85
1:A:22:CYS:HB2	1:A:55:ARG:O	1.77	0.85
1:A:75:HIS:HE1	9:A:1003:GDP:N9	1.74	0.85
2:B:15:PHE:CA	2:B:48:GLU:OE1	2.26	0.84
1:A:12:CYS:SG	1:A:17:ALA:CB	2.66	0.84
6:E:490:ARG:HA	6:E:493:ILE:HB	1.59	0.83
2:B:51:ARG:C	2:B:53:ALA:H	1.85	0.83
5:J:25:G:O2'	5:J:26:A:P	2.35	0.83
2:B:15:PHE:HA	2:B:48:GLU:OE1	1.78	0.83
1:A:903:TYR:OH	2:D:67:MET:SD	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:173:SER:OG	2:D:176:ASN:ND2	2.12	0.81
6:E:167:TRP:HB2	6:E:173:ARG:NH1	1.96	0.81
6:F:331:SER:HB2	6:F:353:GLU:HG2	1.63	0.80
6:F:167:TRP:HB2	6:F:173:ARG:NH1	1.96	0.80
6:F:281:GLN:OE1	6:F:429:MET:HE3	1.82	0.80
1:A:116:ARG:HD3	1:A:116:ARG:N	1.96	0.80
2:B:56:GLN:O	2:B:59:LEU:N	2.11	0.79
6:E:248:ARG:HG2	6:E:249:ILE:N	1.97	0.79
6:E:279:THR:HG23	6:E:398:TYR:HB2	1.64	0.79
6:E:281:GLN:OE1	6:E:429:MET:HE3	1.82	0.79
6:E:331:SER:HB2	6:E:353:GLU:HG2	1.63	0.79
6:F:6:VAL:O	6:F:129:ARG:NH2	2.15	0.79
6:E:194:GLN:O	6:E:194:GLN:HG3	1.80	0.79
1:A:12:CYS:SG	1:A:17:ALA:CA	2.71	0.79
6:F:451:THR:O	6:F:584:LYS:NZ	2.16	0.79
6:E:549:THR:O	6:E:550:THR:HG23	1.82	0.79
7:G:81:LYS:HE2	7:G:84:LYS:HE2	1.63	0.79
6:E:6:VAL:O	6:E:129:ARG:NH2	2.15	0.78
2:B:56:GLN:O	2:B:58:LYS:N	2.15	0.78
6:F:284:PRO:HB2	6:F:443:ARG:HH12	1.48	0.78
6:E:451:THR:O	6:E:584:LYS:NZ	2.16	0.78
6:F:248:ARG:HG2	6:F:249:ILE:N	1.97	0.78
2:D:174:MET:O	2:D:177:SER:OG	2.02	0.78
6:E:185:TYR:CB	6:E:193:VAL:O	2.29	0.77
1:A:12:CYS:SG	1:A:17:ALA:HB2	2.24	0.77
2:B:41:SER:C	2:B:44:VAL:HG23	2.08	0.77
6:F:279:THR:HG23	6:F:398:TYR:HB2	1.64	0.77
7:G:29:LEU:HB2	7:G:45:LEU:HB3	1.65	0.77
7:G:73:CYS:HB3	7:G:88:LEU:HB3	1.66	0.77
6:E:26:CYS:HB3	6:E:29:CYS:SG	2.25	0.76
1:A:75:HIS:CE1	9:A:1003:GDP:N9	2.51	0.76
6:E:284:PRO:HB2	6:E:443:ARG:HH12	1.48	0.76
2:B:41:SER:HA	2:B:44:VAL:CG2	2.16	0.76
7:G:58:LYS:HE3	7:G:65:ILE:HG23	1.68	0.76
6:F:26:CYS:HB3	6:F:29:CYS:SG	2.25	0.76
2:D:84:THR:O	2:D:88:GLN:HG3	1.85	0.75
6:E:154:VAL:N	6:E:223:ASP:O	2.19	0.75
6:E:466:ASP:OD1	6:E:466:ASP:N	2.20	0.74
6:E:326:PRO:HD2	6:E:329:LYS:HZ3	1.53	0.74
6:F:36:SER:OG	6:F:107:ASN:ND2	2.21	0.74
6:E:36:SER:OG	6:E:107:ASN:ND2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:73:LYS:HA	6:E:76:LYS:HG2	1.69	0.74
6:E:453:SER:HA	6:E:457:TYR:HB2	1.70	0.74
6:F:154:VAL:N	6:F:223:ASP:O	2.19	0.74
6:E:240:LEU:HD22	6:E:425:VAL:HG23	1.70	0.74
2:B:40:LYS:O	2:B:44:VAL:HG22	1.88	0.73
4:I:22:G:H1	5:J:38:C:H42	1.35	0.73
6:F:240:LEU:HD22	6:F:425:VAL:HG23	1.70	0.73
6:E:445:PRO:HD3	6:E:569:LYS:O	1.88	0.73
6:E:549:THR:O	6:E:549:THR:HG22	1.85	0.73
6:E:388:ASN:OD1	6:E:388:ASN:N	2.22	0.73
6:F:252:LEU:HB3	6:F:299:TYR:HE2	1.53	0.73
6:F:73:LYS:HA	6:F:76:LYS:HG2	1.69	0.73
6:E:252:LEU:HB3	6:E:299:TYR:HE2	1.53	0.72
7:G:70:GLU:HA	7:G:92:LYS:HE3	1.69	0.72
2:B:45:ALA:HA	2:B:48:GLU:HG3	1.71	0.72
6:F:65:LEU:C	6:F:66:GLY:O	2.23	0.72
6:F:453:SER:HA	6:F:457:TYR:HB2	1.70	0.72
2:D:52:ASP:OD1	2:D:52:ASP:N	2.22	0.72
1:A:847:ILE:C	1:A:847:ILE:HD12	2.15	0.72
6:E:365:GLU:HG3	6:E:390:ARG:HA	1.72	0.72
6:F:307:THR:HG21	6:F:387:VAL:HG21	1.71	0.72
7:G:45:LEU:HD13	7:G:88:LEU:HD12	1.72	0.71
6:E:133:PHE:O	6:E:137:THR:OG1	2.08	0.71
2:B:42:LEU:O	2:B:45:ALA:CA	2.38	0.71
6:E:479:VAL:HB	6:E:491:PRO:HG2	1.72	0.71
1:A:414:ASN:HB2	1:A:844:VAL:O	1.90	0.71
4:I:12:G:N1	5:J:48:C:N3	2.32	0.71
6:F:365:GLU:HG3	6:F:390:ARG:HA	1.72	0.71
6:E:542:ASP:OD1	6:E:542:ASP:N	2.21	0.71
2:D:39:LYS:HA	2:D:42:LEU:HB3	1.72	0.71
2:D:112:ASP:OD1	2:D:113:GLY:N	2.24	0.70
6:F:256:LEU:HD23	6:F:256:LEU:H	1.56	0.70
6:F:479:VAL:HB	6:F:491:PRO:HG2	1.72	0.70
2:B:46:LYS:HZ3	2:B:46:LYS:C	1.96	0.70
2:B:51:ARG:HG3	2:B:55:MET:CB	2.21	0.70
6:E:256:LEU:HD23	6:E:256:LEU:H	1.56	0.70
6:E:583:ASP:OD1	6:E:583:ASP:N	2.25	0.70
6:F:133:PHE:O	6:F:137:THR:OG1	2.08	0.70
6:F:427:ARG:HG3	6:F:427:ARG:HH11	1.57	0.70
6:E:307:THR:HG21	6:E:387:VAL:HG21	1.71	0.69
1:A:78:SER:O	1:A:79:ASN:C	2.34	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:12:G:O6	5:J:48:C:N4	2.20	0.69
6:F:443:ARG:NH2	6:F:540:GLU:OE1	2.16	0.69
1:A:358:ASP:H	1:A:534:ASN:HD21	1.38	0.69
5:J:24:U:P	5:J:24:U:H6	2.15	0.69
6:F:542:ASP:N	6:F:542:ASP:OD1	2.21	0.69
6:E:578:ASP:O	6:E:579:ARG:NH1	2.26	0.69
1:A:569:ARG:NH1	5:J:28:U:OP2	2.25	0.69
2:B:95:LEU:O	2:B:98:LEU:HB2	1.93	0.68
6:F:578:ASP:O	6:F:579:ARG:NH1	2.26	0.68
2:D:174:MET:SD	2:D:174:MET:N	2.66	0.68
6:F:284:PRO:HB2	6:F:443:ARG:NH1	2.09	0.68
7:G:7:VAL:O	7:G:7:VAL:HG13	1.93	0.68
6:E:427:ARG:HG3	6:E:427:ARG:HH11	1.56	0.68
1:A:402:THR:HG22	1:A:403:ASN:H	1.57	0.68
6:E:284:PRO:HB2	6:E:443:ARG:NH1	2.09	0.68
6:E:423:ASN:OD1	6:E:426:CYS:N	2.27	0.67
6:F:549:THR:O	6:F:550:THR:HG23	1.94	0.67
2:B:51:ARG:C	2:B:53:ALA:N	2.46	0.67
6:E:190:ASN:OD1	6:E:190:ASN:N	2.27	0.67
2:D:33:VAL:HA	2:D:36:LYS:HB2	1.76	0.67
6:F:466:ASP:OD1	6:F:466:ASP:N	2.20	0.67
6:E:44:SER:OG	6:E:45:VAL:N	2.27	0.67
7:G:45:LEU:HD11	7:G:75:PHE:CZ	2.29	0.67
6:E:443:ARG:O	6:E:569:LYS:HE3	1.95	0.66
6:F:443:ARG:O	6:F:569:LYS:HE3	1.96	0.66
6:F:190:ASN:N	6:F:190:ASN:OD1	2.27	0.66
6:E:441:CYS:O	6:E:464:HIS:CG	2.48	0.66
6:F:287:GLY:O	6:F:291:PHE:N	2.29	0.66
6:E:115:THR:N	6:E:119:ASP:OD2	2.28	0.66
2:B:51:ARG:HG3	2:B:55:MET:HB3	1.77	0.66
6:F:115:THR:N	6:F:119:ASP:OD2	2.28	0.66
6:E:443:ARG:NH2	6:E:540:GLU:OE1	2.16	0.66
2:B:56:GLN:C	2:B:58:LYS:H	2.02	0.66
1:A:116:ARG:NH2	9:A:1003:GDP:O3B	2.19	0.65
2:D:182:TRP:O	2:D:184:LEU:N	2.30	0.65
6:F:116:ASN:N	6:F:119:ASP:OD2	2.28	0.65
6:F:326:PRO:HD2	6:F:329:LYS:NZ	2.11	0.65
6:E:287:GLY:O	6:E:291:PHE:N	2.29	0.65
6:F:139:LYS:O	6:F:143:GLU:HG3	1.96	0.65
6:E:500:LEU:HD12	6:E:506:TRP:HB3	1.79	0.65
1:A:545:LYS:HZ3	1:A:555:ARG:HE	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:116:ASN:N	6:E:119:ASP:OD2	2.28	0.65
6:E:139:LYS:O	6:E:143:GLU:HG3	1.96	0.65
7:G:95:ASN:OD1	7:G:98:ASN:ND2	2.30	0.65
1:A:906:MET:HG3	1:A:907:LEU:H	1.62	0.65
6:E:372:VAL:HB	6:E:399:ILE:HD11	1.79	0.65
2:B:14:ALA:HB1	2:B:48:GLU:OE2	1.96	0.64
2:B:56:GLN:C	2:B:58:LYS:N	2.51	0.64
6:F:275:GLN:O	6:F:395:HIS:ND1	2.30	0.64
6:E:275:GLN:O	6:E:395:HIS:ND1	2.30	0.64
6:F:583:ASP:OD1	6:F:583:ASP:N	2.25	0.64
7:G:11:GLN:HE22	7:G:29:LEU:HA	1.62	0.64
7:G:74:ARG:H	7:G:74:ARG:HD3	1.61	0.64
6:F:500:LEU:HD12	6:F:506:TRP:HB3	1.79	0.64
6:F:306:TYR:HA	6:F:372:VAL:HG23	1.78	0.64
6:E:332:ARG:HH12	6:E:343:PHE:HB2	1.62	0.64
1:A:845:ASP:O	1:A:848:VAL:HB	1.97	0.64
6:F:533:VAL:HG11	6:F:560:ARG:HH21	1.62	0.64
6:E:152:ALA:HB3	6:E:225:PHE:HB2	1.80	0.64
6:E:326:PRO:HD2	6:E:329:LYS:NZ	2.11	0.64
7:G:44:LEU:HD22	7:G:89:TYR:HB2	1.77	0.64
3:C:16:VAL:HG11	2:D:91:LEU:HD22	1.80	0.64
6:F:372:VAL:HB	6:F:399:ILE:HD11	1.80	0.64
6:F:423:ASN:OD1	6:F:426:CYS:N	2.27	0.64
2:B:95:LEU:HA	2:B:98:LEU:HD12	1.78	0.64
6:E:280:LEU:HD11	6:E:399:ILE:HG23	1.80	0.64
6:E:306:TYR:HA	6:E:372:VAL:HG23	1.78	0.64
6:E:243:GLN:HB2	6:E:276:LYS:HB2	1.80	0.64
6:E:154:VAL:HG22	6:E:165:LEU:HD12	1.80	0.63
1:A:210:GLN:NE2	1:A:214:GLY:O	2.31	0.63
6:F:280:LEU:HD11	6:F:399:ILE:HG23	1.80	0.63
6:E:118:GLY:HA2	6:E:121:ILE:HD12	1.80	0.63
6:F:152:ALA:HB3	6:F:225:PHE:HB2	1.80	0.63
6:F:332:ARG:HH12	6:F:343:PHE:HB2	1.62	0.63
6:E:203:GLY:HA2	6:E:210:VAL:HG23	1.81	0.63
6:E:576:MET:HE1	6:E:585:LEU:HB3	1.80	0.63
1:A:75:HIS:HE1	9:A:1003:GDP:C8	2.16	0.63
1:A:38:TYR:HD2	1:A:728:TYR:CD1	2.17	0.63
1:A:824:ASP:OD1	1:A:824:ASP:N	2.30	0.63
6:F:183:THR:HA	6:F:196:GLY:O	1.99	0.63
6:F:415:GLY:O	6:F:416:THR:O	2.16	0.63
6:E:533:VAL:HG11	6:E:560:ARG:HH21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:HD22	1:A:361:LEU:H	1.63	0.62
1:A:758:LEU:O	1:A:760:ASP:N	2.32	0.62
6:E:12:THR:OG1	6:E:13:SER:N	2.28	0.62
6:E:183:THR:HA	6:E:196:GLY:O	1.99	0.62
6:F:326:PRO:HD2	6:F:329:LYS:HZ3	1.63	0.62
2:B:112:ASP:OD1	2:B:112:ASP:N	2.28	0.62
6:F:118:GLY:HA2	6:F:121:ILE:HD12	1.80	0.62
6:F:243:GLN:HB2	6:F:276:LYS:HB2	1.80	0.62
7:G:15:ALA:CB	7:G:25:ASP:O	2.43	0.62
1:A:844:VAL:O	1:A:844:VAL:CG2	2.45	0.62
2:B:12:TYR:HD1	2:B:49:PHE:HE2	1.47	0.62
6:F:154:VAL:HG22	6:F:165:LEU:HD12	1.80	0.62
6:F:480:ILE:HD13	6:F:549:THR:O	1.99	0.62
6:F:576:MET:HE1	6:F:585:LEU:HB3	1.80	0.62
6:E:4:ALA:HA	6:E:10:SER:O	2.00	0.62
6:F:203:GLY:HA2	6:F:210:VAL:HG23	1.81	0.62
6:E:310:SER:O	6:E:314:VAL:N	2.26	0.62
6:F:373:PHE:O	6:F:399:ILE:N	2.33	0.62
6:E:373:PHE:O	6:E:399:ILE:N	2.33	0.62
6:E:13:SER:O	6:E:14:LEU:HG	1.99	0.62
6:F:502:ARG:HG2	6:F:503:ASN:OD1	1.99	0.62
2:D:177:SER:C	2:D:179:ASN:H	2.07	0.62
7:G:45:LEU:HD11	7:G:75:PHE:HZ	1.63	0.62
6:E:7:LEU:HD21	6:E:106:PHE:HB2	1.82	0.61
1:A:38:TYR:CD2	1:A:728:TYR:CD1	2.87	0.61
2:D:74:ALA:HB1	6:F:2:VAL:HG21	1.81	0.61
6:E:502:ARG:HG2	6:E:503:ASN:OD1	1.99	0.61
2:B:12:TYR:CD1	2:B:49:PHE:HE2	2.18	0.61
2:B:103:LEU:O	2:B:103:LEU:HD23	2.01	0.61
1:A:725:HIS:HE1	1:A:729:GLU:OE2	1.84	0.61
6:F:12:THR:OG1	6:F:13:SER:N	2.30	0.61
6:F:249:ILE:HG13	6:F:252:LEU:HD13	1.83	0.61
6:F:310:SER:O	6:F:314:VAL:N	2.26	0.61
1:A:902:MET:HE1	6:F:92:LEU:HD22	1.82	0.61
9:A:1003:GDP:H5'	9:A:1003:GDP:H8	1.65	0.61
6:F:18:ALA:HB3	6:F:39:HIS:HA	1.82	0.61
6:E:18:ALA:HB3	6:E:39:HIS:HA	1.82	0.61
1:A:54:CYS:SG	1:A:74:ARG:NH1	2.74	0.60
1:A:454:ASP:OD2	1:A:457:ARG:NH1	2.34	0.60
1:A:899:MET:HB3	1:A:906:MET:SD	2.41	0.60
1:A:902:MET:HB2	6:F:93:TYR:CE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:SER:N	6:F:95:ASN:OD1	2.25	0.60
6:F:128:GLU:O	6:F:131:LYS:N	2.34	0.60
6:E:473:LYS:HE2	6:E:576:MET:HE3	1.83	0.60
1:A:160:LYS:O	1:A:161:ASP:HB2	2.01	0.60
6:E:128:GLU:O	6:E:131:LYS:N	2.34	0.60
6:E:429:MET:HG2	6:E:434:PRO:HA	1.82	0.60
6:E:548:GLN:HE22	6:E:577:SER:H	1.49	0.60
1:A:414:ASN:ND2	1:A:846:ASP:HB2	2.17	0.60
1:A:503:GLY:O	1:A:507:ASN:ND2	2.34	0.60
6:F:7:LEU:HD21	6:F:106:PHE:HB2	1.82	0.60
6:F:44:SER:OG	6:F:45:VAL:N	2.29	0.60
1:A:358:ASP:OD1	1:A:533:ARG:NH2	2.31	0.60
6:F:243:GLN:HE22	6:F:245:HIS:CE1	2.19	0.60
2:B:55:MET:O	2:B:58:LYS:HB3	2.01	0.60
4:I:22:G:H2'	4:I:23:C:C6	2.37	0.60
6:F:519:ASN:HA	6:F:522:ALA:HB3	1.83	0.60
6:F:429:MET:HG2	6:F:434:PRO:HA	1.83	0.60
6:F:572:ILE:HG12	6:F:573:LEU:H	1.67	0.60
6:E:417:LEU:HD22	6:E:418:GLU:H	1.66	0.60
6:F:465:LYS:HE2	6:F:569:LYS:NZ	2.17	0.60
6:E:185:TYR:HD1	6:E:194:GLN:HA	1.66	0.60
6:F:445:PRO:HD3	6:F:569:LYS:O	2.01	0.60
6:E:519:ASN:HA	6:E:522:ALA:HB3	1.83	0.60
6:F:548:GLN:HE22	6:F:577:SER:H	1.49	0.59
6:F:353:GLU:HB3	6:F:356:VAL:HG13	1.83	0.59
6:F:548:GLN:HE22	6:F:577:SER:N	2.00	0.59
6:E:419:PRO:HA	6:E:422:PHE:CE1	2.37	0.59
6:E:243:GLN:HE22	6:E:245:HIS:CE1	2.19	0.59
6:E:548:GLN:HE22	6:E:577:SER:N	2.00	0.59
6:F:326:PRO:HB2	6:F:329:LYS:HD3	1.84	0.59
6:F:417:LEU:HD22	6:F:418:GLU:H	1.66	0.59
6:E:249:ILE:HG13	6:E:252:LEU:HD13	1.83	0.59
6:E:465:LYS:HE2	6:E:569:LYS:NZ	2.17	0.59
7:G:55:ARG:HG2	7:G:64:THR:HG22	1.84	0.59
1:A:30:VAL:HA	1:A:50:LYS:O	2.02	0.59
6:F:311:HIS:O	6:F:315:ASP:HB2	2.01	0.59
6:E:311:HIS:O	6:E:315:ASP:HB2	2.02	0.59
6:F:419:PRO:HA	6:F:422:PHE:CE1	2.37	0.59
6:E:140:ALA:HA	6:E:143:GLU:OE2	2.02	0.59
6:E:326:PRO:HB2	6:E:329:LYS:HD3	1.84	0.59
1:A:501:SER:OG	5:J:25:G:OP1	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:473:LYS:HE2	6:F:576:MET:HE3	1.83	0.59
6:E:445:PRO:HB3	6:E:465:LYS:HE3	1.85	0.59
5:J:24:U:H2'	5:J:25:G:H5''	1.85	0.59
6:F:445:PRO:HB3	6:F:465:LYS:HE3	1.85	0.59
6:E:368:ALA:N	6:E:391:LEU:HD21	2.17	0.59
5:J:40:U:H2'	5:J:41:G:H8	1.67	0.58
6:F:152:ALA:HB2	6:F:167:TRP:CZ3	2.38	0.58
6:F:417:LEU:HD22	6:F:418:GLU:N	2.18	0.58
6:E:353:GLU:HB3	6:E:356:VAL:HG13	1.83	0.58
6:F:368:ALA:N	6:F:391:LEU:HD21	2.18	0.58
6:E:9:ASN:CG	6:E:129:ARG:HH12	2.11	0.58
6:E:417:LEU:HD22	6:E:418:GLU:N	2.18	0.58
7:G:106:LEU:HD23	7:G:110:VAL:HG21	1.85	0.58
1:A:697:CYS:O	1:A:701:THR:HG22	2.03	0.58
1:A:903:TYR:HB3	1:A:905:VAL:H	1.68	0.58
6:F:388:ASN:OD1	6:F:388:ASN:N	2.22	0.58
6:E:322:LEU:HD22	6:E:327:ILE:HG23	1.85	0.58
6:F:358:CYS:SG	6:F:359:THR:N	2.77	0.58
1:A:718:LYS:HZ2	1:A:721:ARG:HD3	1.67	0.58
6:F:369:ASP:HA	6:F:394:LYS:HE2	1.85	0.58
1:A:41:LYS:NZ	1:A:41:LYS:HB3	2.18	0.58
6:F:140:ALA:HA	6:F:143:GLU:OE2	2.02	0.58
6:F:322:LEU:HD22	6:F:327:ILE:HG23	1.85	0.58
6:F:471:CYS:HB3	6:F:572:ILE:HG22	1.86	0.58
6:E:152:ALA:HB2	6:E:167:TRP:CZ3	2.38	0.58
6:E:358:CYS:SG	6:E:359:THR:N	2.77	0.58
6:E:471:CYS:HB3	6:E:572:ILE:HG22	1.86	0.58
2:D:58:LYS:HA	2:D:61:LYS:NZ	2.18	0.58
6:E:572:ILE:HG12	6:E:573:LEU:H	1.67	0.58
6:F:540:GLU:HB3	6:F:567:ARG:HD3	1.86	0.58
4:I:24:U:H2'	4:I:25:A:H8	1.69	0.57
6:E:131:LYS:HE3	6:E:132:LEU:HD23	1.86	0.57
6:E:548:GLN:OE1	6:E:576:MET:HA	2.04	0.57
1:A:906:MET:HE3	1:A:907:LEU:HD13	1.85	0.57
6:E:369:ASP:HA	6:E:394:LYS:HE2	1.85	0.57
6:F:9:ASN:CG	6:F:129:ARG:HH12	2.11	0.57
6:F:548:GLN:OE1	6:F:576:MET:HA	2.04	0.57
6:E:2:VAL:O	6:E:2:VAL:HG12	2.03	0.57
1:A:39:ASN:OD1	1:A:39:ASN:N	2.37	0.57
6:F:297:LEU:HD21	6:F:324:TYR:HD2	1.70	0.57
6:F:347:LYS:NZ	6:F:353:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:35:ILE:HD12	6:E:36:SER:HB3	1.87	0.57
2:B:22:TYR:HA	2:B:38:LEU:HD13	1.86	0.57
3:C:53:VAL:HG23	2:D:106:ILE:HD13	1.85	0.57
6:F:131:LYS:HE3	6:F:132:LEU:HD23	1.86	0.57
6:F:201:GLU:HG2	6:F:202:LYS:N	2.19	0.57
1:A:7:PHE:O	1:A:11:VAL:HG23	2.03	0.57
5:J:38:C:H2'	5:J:39:A:C8	2.40	0.57
3:C:9:THR:HG21	2:D:98:LEU:HD11	1.87	0.57
2:D:44:VAL:HA	2:D:47:SER:HB2	1.86	0.57
1:A:275:PHE:O	1:A:279:ARG:HG3	2.05	0.57
2:D:15:PHE:CE1	2:D:46:LYS:HB3	2.39	0.57
6:F:65:LEU:HD12	6:F:66:GLY:O	2.05	0.57
6:F:185:TYR:HD1	6:F:194:GLN:HA	1.70	0.57
6:F:563:VAL:O	6:F:567:ARG:NE	2.31	0.57
7:G:16:ALA:HA	7:G:54:ALA:HA	1.86	0.57
6:F:304:ILE:HD12	6:F:370:ILE:HB	1.87	0.56
6:E:147:LEU:HD11	6:E:229:SER:HB3	1.87	0.56
6:E:167:TRP:HB2	6:E:173:ARG:HH12	1.68	0.56
6:E:347:LYS:NZ	6:E:353:GLU:OE1	2.38	0.56
6:E:540:GLU:HB3	6:E:567:ARG:HD3	1.86	0.56
6:F:147:LEU:HD11	6:F:229:SER:HB3	1.87	0.56
1:A:41:LYS:HB3	1:A:41:LYS:HZ3	1.70	0.56
1:A:387:LEU:HD12	1:A:388:LEU:H	1.71	0.56
2:B:15:PHE:N	2:B:48:GLU:OE1	2.39	0.56
6:F:427:ARG:O	6:F:431:THR:OG1	2.22	0.56
6:E:366:THR:HG22	6:E:367:THR:H	1.70	0.56
6:E:499:PHE:HA	6:E:502:ARG:NH1	2.20	0.56
1:A:72:VAL:HG23	1:A:113:HIS:HB3	1.88	0.56
6:F:555:SER:HA	6:F:560:ARG:NH1	2.21	0.56
6:F:35:ILE:HD12	6:F:36:SER:HB3	1.87	0.56
6:E:131:LYS:HG2	6:E:132:LEU:N	2.20	0.56
6:E:297:LEU:HD21	6:E:324:TYR:HD2	1.70	0.56
2:D:67:MET:HG3	6:F:90:PHE:CZ	2.41	0.56
4:I:22:G:H2'	4:I:23:C:H6	1.70	0.56
6:F:366:THR:HG22	6:F:367:THR:H	1.70	0.56
2:D:45:ALA:HA	2:D:48:GLU:OE2	2.06	0.56
6:E:304:ILE:HD12	6:E:370:ILE:HB	1.87	0.56
6:E:427:ARG:O	6:E:431:THR:OG1	2.22	0.56
7:G:9:LEU:HD22	7:G:32:TYR:HE1	1.70	0.56
1:A:814:SER:OG	4:I:33:G:OP1	2.24	0.56
2:D:127:LYS:HZ3	2:D:127:LYS:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HD3	1:A:113:HIS:CD2	2.41	0.56
2:B:132:ILE:HG21	2:B:138:TYR:HB2	1.88	0.56
6:E:332:ARG:NH2	6:E:343:PHE:O	2.39	0.56
1:A:623:ASP:OD1	1:A:623:ASP:N	2.36	0.56
2:B:42:LEU:C	2:B:45:ALA:H	2.11	0.56
6:E:555:SER:HA	6:E:560:ARG:NH1	2.21	0.56
1:A:851:ASP:HB2	2:D:79:LYS:HE2	1.88	0.55
6:F:103:VAL:O	6:F:106:PHE:N	2.38	0.55
6:F:499:PHE:HA	6:F:502:ARG:NH1	2.20	0.55
6:E:103:VAL:O	6:E:106:PHE:N	2.38	0.55
6:F:6:VAL:HG23	6:F:7:LEU:HG	1.89	0.55
6:F:332:ARG:NH2	6:F:343:PHE:O	2.38	0.55
6:E:139:LYS:HD2	6:E:382:TYR:CG	2.41	0.55
6:E:480:ILE:HD13	6:E:549:THR:O	2.06	0.55
7:G:58:LYS:HD2	7:G:63:GLY:HA3	1.89	0.55
6:F:139:LYS:HD2	6:F:382:TYR:CG	2.41	0.55
6:F:185:TYR:HA	6:F:195:ILE:H	1.71	0.55
6:F:167:TRP:HB2	6:F:173:ARG:HH12	1.68	0.55
6:F:386:VAL:HG13	6:F:390:ARG:HD3	1.88	0.55
6:E:572:ILE:HG12	6:E:573:LEU:N	2.22	0.55
1:A:105:ARG:HH12	1:A:108:GLY:HA2	1.69	0.55
1:A:111:VAL:HG13	1:A:113:HIS:CE1	2.42	0.55
2:D:141:THR:OG1	2:D:142:CYS:N	2.38	0.55
6:F:131:LYS:HG2	6:F:132:LEU:N	2.20	0.55
6:E:386:VAL:HG13	6:E:390:ARG:HD3	1.88	0.55
4:I:23:C:H2'	4:I:24:U:C6	2.41	0.55
2:D:168:GLN:H	2:D:168:GLN:CD	2.15	0.55
7:G:31:TYR:HB2	7:G:43:ALA:HB3	1.88	0.55
1:A:10:ARG:O	1:A:10:ARG:NE	2.40	0.55
6:E:353:GLU:OE2	6:E:354:GLN:N	2.39	0.55
6:F:332:ARG:HG3	6:F:357:PHE:O	2.07	0.54
2:D:54:ALA:HA	2:D:57:ARG:NH1	2.22	0.54
6:F:269:TYR:CE1	6:F:295:LEU:HB2	2.42	0.54
6:E:145:PHE:CD1	6:E:145:PHE:C	2.86	0.54
6:E:465:LYS:HE2	6:E:569:LYS:HZ3	1.71	0.54
4:I:25:A:H2'	4:I:26:G:C8	2.42	0.54
6:F:368:ALA:H	6:F:391:LEU:HD21	1.72	0.54
6:F:548:GLN:NE2	6:F:575:ILE:O	2.41	0.54
6:E:548:GLN:NE2	6:E:575:ILE:O	2.41	0.54
1:A:699:ALA:O	1:A:703:ASN:ND2	2.39	0.54
1:A:851:ASP:HB3	1:A:854:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:353:GLU:OE2	6:F:354:GLN:N	2.39	0.54
6:F:572:ILE:HG12	6:F:573:LEU:N	2.22	0.54
6:E:573:LEU:HD22	6:E:574:CYS:N	2.23	0.54
6:F:145:PHE:C	6:F:145:PHE:HD1	2.16	0.54
6:F:492:GLN:HE22	6:F:549:THR:H	1.54	0.54
6:F:515:TYR:O	6:F:518:GLN:N	2.29	0.54
6:E:184:GLY:O	6:E:195:ILE:HB	2.08	0.54
6:E:252:LEU:HB3	6:E:299:TYR:CE2	2.39	0.54
6:E:378:MET:O	6:E:407:ALA:HB2	2.08	0.54
6:E:6:VAL:HG23	6:E:7:LEU:HG	1.89	0.54
6:E:145:PHE:C	6:E:145:PHE:HD1	2.16	0.54
6:E:269:TYR:CE1	6:E:295:LEU:HB2	2.42	0.54
2:B:42:LEU:C	2:B:45:ALA:CB	2.79	0.54
2:B:42:LEU:CA	2:B:45:ALA:HB2	2.33	0.54
3:C:45:THR:O	3:C:45:THR:OG1	2.26	0.54
6:F:573:LEU:HD22	6:F:574:CYS:N	2.23	0.54
6:E:332:ARG:HG3	6:E:357:PHE:O	2.07	0.54
6:E:492:GLN:HE22	6:E:549:THR:H	1.54	0.54
6:E:563:VAL:O	6:E:567:ARG:NE	2.31	0.54
1:A:725:HIS:CE1	1:A:729:GLU:OE2	2.61	0.53
6:F:401:ASP:O	6:F:404:GLN:HG2	2.08	0.53
6:E:243:GLN:HG2	6:E:277:TYR:CE2	2.43	0.53
6:E:248:ARG:HH11	6:E:250:THR:HA	1.73	0.53
6:E:277:TYR:HA	6:E:396:TYR:O	2.09	0.53
7:G:68:GLU:OE2	7:G:92:LYS:HD2	2.07	0.53
1:A:75:HIS:HE1	9:A:1003:GDP:C5	2.26	0.53
6:F:145:PHE:O	6:F:148:SER:OG	2.26	0.53
6:F:116:ASN:N	6:F:116:ASN:OD1	2.42	0.53
6:F:145:PHE:C	6:F:145:PHE:CD1	2.86	0.53
6:F:378:MET:O	6:F:407:ALA:HB2	2.08	0.53
6:E:145:PHE:O	6:E:148:SER:OG	2.26	0.53
1:A:78:SER:O	1:A:80:TYR:N	2.41	0.53
5:J:24:U:H6	5:J:24:U:O5'	1.91	0.53
6:E:142:GLU:O	6:E:145:PHE:HB3	2.08	0.53
2:B:41:SER:CA	2:B:44:VAL:CG2	2.87	0.53
6:F:490:ARG:HG2	6:F:490:ARG:NH1	2.13	0.53
6:E:492:GLN:NE2	6:E:547:THR:HG22	2.23	0.53
1:A:155:ASP:OD1	1:A:155:ASP:N	2.35	0.53
2:D:61:LYS:H	2:D:61:LYS:HD3	1.73	0.53
6:F:473:LYS:HZ2	6:F:474[B]:MET:C	2.15	0.53
6:E:368:ALA:H	6:E:391:LEU:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:THR:O	7:G:83:PRO:HA	2.08	0.53
6:F:142:GLU:O	6:F:145:PHE:HB3	2.08	0.53
6:F:184:GLY:O	6:F:195:ILE:HB	2.08	0.53
6:F:248:ARG:HH11	6:F:250:THR:HA	1.73	0.53
1:A:55:ARG:NH1	1:A:55:ARG:HB2	2.24	0.53
2:D:173:SER:OG	2:D:174:MET:N	2.41	0.53
6:F:442:ARG:HA	6:F:464:HIS:CE1	2.44	0.53
7:G:9:LEU:HD13	7:G:34:THR:H	1.73	0.53
6:E:116:ASN:N	6:E:116:ASN:OD1	2.42	0.53
6:E:401:ASP:O	6:E:404:GLN:HG2	2.08	0.53
6:E:50:CYS:HA	6:E:70:TYR:O	2.08	0.53
6:E:107:ASN:O	6:E:111:THR:OG1	2.24	0.53
6:E:262:PHE:O	6:E:265:ASN:HB2	2.09	0.53
1:A:61:GLU:C	1:A:63:ASP:H	2.17	0.52
1:A:569:ARG:O	1:A:573:GLN:HB2	2.09	0.52
2:B:157:GLN:HG2	2:B:189:LEU:HD12	1.91	0.52
6:F:243:GLN:HG2	6:F:277:TYR:CE2	2.44	0.52
6:F:476:TYR:CD2	6:F:492:GLN:HG3	2.44	0.52
6:F:492:GLN:NE2	6:F:547:THR:HG22	2.23	0.52
1:A:78:SER:C	1:A:80:TYR:N	2.64	0.52
1:A:105:ARG:HB3	1:A:110:MET:SD	2.49	0.52
2:B:55:MET:SD	2:B:55:MET:C	2.92	0.52
6:E:114:TRP:CE3	6:E:119:ASP:HB3	2.45	0.52
4:I:24:U:H2'	4:I:25:A:C8	2.44	0.52
6:E:476:TYR:CD2	6:E:492:GLN:HG3	2.44	0.52
1:A:899:MET:HE1	2:D:68:THR:HA	1.91	0.52
6:F:50:CYS:HA	6:F:70:TYR:O	2.08	0.52
6:F:277:TYR:HA	6:F:396:TYR:O	2.09	0.52
1:A:746:TYR:CZ	1:A:750:ARG:HD2	2.45	0.52
6:F:472:PHE:CE2	6:F:506:TRP:HH2	2.28	0.52
6:E:20:ILE:HD12	6:E:20:ILE:H	1.75	0.52
1:A:41:LYS:NZ	1:A:41:LYS:CB	2.72	0.52
1:A:358:ASP:H	1:A:534:ASN:ND2	2.07	0.52
2:B:42:LEU:C	2:B:45:ALA:HB3	2.28	0.52
6:F:262:PHE:N	6:F:262:PHE:CD1	2.78	0.52
6:F:548:GLN:NE2	6:F:577:SER:H	2.08	0.52
6:E:21:ARG:HG3	6:E:136:GLU:HG2	1.91	0.52
6:E:115:THR:OG1	6:E:116:ASN:OD1	2.15	0.52
6:E:417:LEU:HD11	6:E:421:TYR:O	2.10	0.52
6:E:473:LYS:HD3	6:E:473:LYS:C	2.35	0.52
3:C:58:VAL:HG22	2:D:119:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:PHE:HE1	2:D:46:LYS:HB3	1.74	0.52
2:D:101:ASP:OD1	2:D:101:ASP:N	2.43	0.52
2:D:117:LEU:HD11	2:D:131:VAL:HG23	1.91	0.52
6:F:437:PHE:HB2	6:F:460:LYS:NZ	2.25	0.52
6:E:548:GLN:NE2	6:E:577:SER:H	2.08	0.52
2:B:12:TYR:HD1	2:B:49:PHE:CE2	2.28	0.52
2:D:147:PHE:HB3	2:D:154:TRP:HB2	1.91	0.52
6:F:455:LEU:HB2	6:F:584:LYS:HZ2	1.75	0.52
6:E:201:GLU:HG2	6:E:202:LYS:N	2.24	0.52
7:G:50:ASP:HA	7:G:89:TYR:OH	2.10	0.52
6:F:417:LEU:HD11	6:F:421:TYR:O	2.10	0.52
1:A:38:TYR:CD1	1:A:38:TYR:C	2.88	0.51
6:F:21:ARG:HG3	6:F:136:GLU:HG2	1.91	0.51
6:F:262:PHE:O	6:F:265:ASN:HB2	2.09	0.51
6:F:495:VAL:HA	6:F:498:GLU:HB3	1.92	0.51
6:E:435:ASP:O	6:E:436:MET:HE2	2.10	0.51
2:B:19:GLN:CD	2:B:42:LEU:HD12	2.35	0.51
6:F:435:ASP:O	6:F:436:MET:HE2	2.10	0.51
6:E:476:TYR:HD2	6:E:492:GLN:HG3	1.75	0.51
1:A:847:ILE:HG22	2:D:79:LYS:HD3	1.93	0.51
4:I:21:U:C2	4:I:22:G:C8	2.98	0.51
6:F:252:LEU:HB3	6:F:299:TYR:CE2	2.39	0.51
6:E:439:GLY:HA2	6:E:461:LEU:HD23	1.93	0.51
6:E:512:ILE:HA	6:E:531:GLN:HB3	1.92	0.51
2:D:159:VAL:HG13	2:D:167:VAL:O	2.11	0.51
6:F:20:ILE:HD12	6:F:20:ILE:H	1.75	0.51
6:F:322:LEU:HD22	6:F:327:ILE:HA	1.92	0.51
6:F:548:GLN:O	6:F:550:THR:N	2.44	0.51
6:F:474[A]:MET:HB3	6:F:575:ILE:HA	1.92	0.51
6:E:271:LYS:HZ3	6:E:274:MET:HE2	1.75	0.51
6:F:271:LYS:HZ3	6:F:274:MET:HE2	1.75	0.51
6:E:472:PHE:CE2	6:E:506:TRP:HH2	2.28	0.51
6:F:114:TRP:CE3	6:F:119:ASP:HB3	2.45	0.51
6:F:476:TYR:HD2	6:F:492:GLN:HG3	1.75	0.51
6:E:262:PHE:N	6:E:262:PHE:CD1	2.78	0.51
6:E:490:ARG:HH11	6:E:490:ARG:CG	2.20	0.51
6:E:495:VAL:HA	6:E:498:GLU:HB3	1.92	0.51
1:A:858:ARG:HG2	4:I:30:G:H5'	1.93	0.51
6:E:126:CYS:HB2	6:E:130:LEU:HD23	1.93	0.51
6:E:154:VAL:HG13	6:E:163:LEU:HB3	1.93	0.51
6:F:152:ALA:HB2	6:F:167:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:154:VAL:HG13	6:F:163:LEU:HB3	1.93	0.51
6:E:512:ILE:HD11	6:E:544:VAL:HB	1.93	0.51
7:G:32:TYR:HA	7:G:41:VAL:HA	1.92	0.51
2:D:103:LEU:O	2:D:107:ILE:HG13	2.11	0.51
2:D:127:LYS:CB	2:D:127:LYS:NZ	2.73	0.51
6:E:437:PHE:HB2	6:E:460:LYS:NZ	2.25	0.51
6:F:114:TRP:O	6:F:411:LEU:HB3	2.11	0.50
6:F:277:TYR:CB	6:F:396:TYR:HB2	2.42	0.50
6:F:473:LYS:HD3	6:F:473:LYS:C	2.35	0.50
6:E:322:LEU:HD22	6:E:327:ILE:HA	1.92	0.50
7:G:53:TRP:HD1	7:G:66:TYR:HD2	1.59	0.50
2:D:135:TYR:HB2	2:D:182:TRP:CZ2	2.46	0.50
6:F:115:THR:O	6:F:413:THR:N	2.30	0.50
6:F:512:ILE:HA	6:F:531:GLN:HB3	1.92	0.50
6:E:455:LEU:HB2	6:E:584:LYS:HZ2	1.76	0.50
6:E:561:PHE:O	6:E:565:ILE:HG12	2.11	0.50
1:A:6:SER:HA	1:A:9:ASN:HD22	1.77	0.50
6:F:561:PHE:O	6:F:565:ILE:HG12	2.11	0.50
6:E:152:ALA:HB2	6:E:167:TRP:CH2	2.46	0.50
6:E:277:TYR:CB	6:E:396:TYR:HB2	2.42	0.50
7:G:73:CYS:N	7:G:88:LEU:O	2.44	0.50
6:F:439:GLY:HA2	6:F:461:LEU:HD23	1.92	0.50
6:E:114:TRP:O	6:E:411:LEU:HB3	2.11	0.50
1:A:20:THR:HG22	1:A:59:LYS:HE3	1.93	0.50
1:A:120:THR:HB	1:A:211:ASP:HB2	1.93	0.50
1:A:818:MET:HE2	1:A:831:TYR:CD1	2.47	0.50
2:B:51:ARG:CG	2:B:55:MET:HB3	2.41	0.50
5:J:39:A:H2'	5:J:40:U:O4'	2.11	0.50
6:F:476:TYR:CG	6:F:477:LYS:N	2.79	0.50
6:F:512:ILE:HD11	6:F:544:VAL:HB	1.94	0.50
6:E:21:ARG:NH1	6:E:232:VAL:O	2.40	0.50
6:E:122:LEU:O	6:E:126:CYS:HB3	2.11	0.50
6:E:275:GLN:OE1	6:E:278:SER:OG	2.26	0.50
1:A:78:SER:OG	1:A:79:ASN:N	2.44	0.50
6:F:107:ASN:O	6:F:111:THR:OG1	2.24	0.50
6:E:268:ASN:OD1	6:E:268:ASN:N	2.45	0.50
6:E:490:ARG:HG2	6:E:490:ARG:NH1	2.13	0.50
6:F:68:MET:N	6:F:68:MET:HE2	2.27	0.50
6:F:122:LEU:O	6:F:126:CYS:HB3	2.11	0.50
6:F:360:VAL:HG11	6:F:383:ASP:HB3	1.94	0.50
6:E:55:CYS:SG	6:E:56:ASP:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:55:CYS:SG	6:F:56:ASP:N	2.84	0.50
6:F:473:LYS:HZ2	6:F:474[A]:MET:C	2.17	0.50
6:F:581:LEU:HG	6:F:581:LEU:O	2.12	0.50
3:C:23:GLU:HA	3:C:29:TRP:HB2	1.94	0.49
3:C:71:LEU:HD11	2:D:107:ILE:HG22	1.94	0.49
5:J:47:A:H2'	5:J:48:C:C6	2.47	0.49
6:F:311:HIS:CE1	6:F:359:THR:HG1	2.29	0.49
6:F:457:TYR:O	6:F:459:ASN:N	2.45	0.49
6:E:447:GLU:HA	6:E:467:LYS:HG3	1.94	0.49
6:E:548:GLN:CD	6:E:576:MET:HA	2.37	0.49
6:F:548:GLN:CD	6:F:576:MET:HA	2.38	0.49
6:E:176:LEU:HG	6:E:177:ASN:OD1	2.12	0.49
6:E:360:VAL:HG11	6:E:383:ASP:HB3	1.94	0.49
6:E:581:LEU:O	6:E:581:LEU:HG	2.12	0.49
1:A:62:ASP:OD1	1:A:62:ASP:N	2.43	0.49
6:F:126:CYS:HB2	6:F:130:LEU:HD23	1.93	0.49
6:F:131:LYS:NZ	6:F:238:PRO:HA	2.27	0.49
6:E:68:MET:N	6:E:68:MET:HE2	2.27	0.49
6:E:265:ASN:HB3	6:E:269:TYR:CZ	2.47	0.49
7:G:10:ARG:HB2	7:G:32:TYR:CZ	2.47	0.49
7:G:49:GLN:HA	7:G:87:TYR:CD2	2.47	0.49
6:F:176:LEU:HG	6:F:177:ASN:OD1	2.12	0.49
6:F:465:LYS:HE2	6:F:569:LYS:HZ1	1.76	0.49
6:F:490:ARG:HH11	6:F:490:ARG:CG	2.20	0.49
6:F:533:VAL:HG11	6:F:560:ARG:NH2	2.28	0.49
6:F:573:LEU:HD22	6:F:574:CYS:H	1.77	0.49
4:I:25:A:H2'	4:I:26:G:H8	1.77	0.49
6:F:493:ILE:HD11	6:F:522:ALA:HB2	1.94	0.49
6:E:256:LEU:H	6:E:256:LEU:CD2	2.24	0.49
2:D:31:SER:OG	2:D:32:GLU:N	2.43	0.49
2:D:123:THR:C	2:D:125:ALA:H	2.20	0.49
6:F:447:GLU:HA	6:F:467:LYS:HG3	1.94	0.49
6:E:131:LYS:NZ	6:E:238:PRO:HA	2.27	0.49
6:E:245:HIS:HA	6:E:275:GLN:HA	1.95	0.49
6:E:457:TYR:O	6:E:459:ASN:N	2.45	0.49
1:A:647:SER:OG	1:A:648:LEU:N	2.42	0.49
2:D:168:GLN:H	2:D:168:GLN:NE2	2.10	0.49
6:F:135:ALA:HA	6:F:138:LEU:HG	1.95	0.49
6:F:265:ASN:HB3	6:F:269:TYR:CZ	2.47	0.49
6:F:265:ASN:HB3	6:F:269:TYR:CE2	2.48	0.49
6:F:268:ASN:N	6:F:268:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:275:GLN:OE1	6:F:278:SER:OG	2.26	0.49
6:E:265:ASN:HB3	6:E:269:TYR:CE2	2.48	0.49
7:G:12:MET:SD	7:G:14:CYS:HB2	2.53	0.49
6:F:158:LEU:CD2	6:F:164:HIS:HB2	2.43	0.49
7:G:31:TYR:HE2	7:G:45:LEU:HB2	1.77	0.49
6:F:271:LYS:HA	6:F:274:MET:HB2	1.94	0.48
6:F:276:LYS:O	6:F:396:TYR:N	2.38	0.48
6:F:540:GLU:HB2	6:F:567:ARG:O	2.13	0.48
6:E:108:ALA:O	6:E:112:CYS:HB2	2.12	0.48
6:E:271:LYS:HA	6:E:274:MET:HB2	1.94	0.48
6:E:319:GLU:OE1	6:E:319:GLU:HA	2.13	0.48
6:E:427:ARG:HH11	6:E:427:ARG:CG	2.25	0.48
6:E:473:LYS:HZ2	6:E:474[A]:MET:C	2.21	0.48
6:F:369:ASP:O	6:F:394:LYS:CB	2.38	0.48
6:F:470:GLN:C	6:F:571:GLY:HA2	2.39	0.48
6:E:16:CYS:SG	6:E:39:HIS:HB3	2.53	0.48
6:E:310:SER:HB3	6:E:312:ALA:H	1.78	0.48
6:E:573:LEU:HD22	6:E:574:CYS:H	1.78	0.48
2:B:82:LYS:HB2	2:B:82:LYS:NZ	2.28	0.48
2:D:182:TRP:O	2:D:182:TRP:HE3	1.96	0.48
6:F:115:THR:OG1	6:F:116:ASN:OD1	2.15	0.48
1:A:116:ARG:HD3	1:A:116:ARG:H	1.74	0.48
2:B:42:LEU:HA	2:B:45:ALA:CB	2.36	0.48
2:D:42:LEU:O	2:D:45:ALA:N	2.43	0.48
2:D:127:LYS:HB2	2:D:127:LYS:NZ	2.28	0.48
6:F:108:ALA:O	6:F:112:CYS:HB2	2.12	0.48
6:F:406:PRO:HB3	6:F:422:PHE:CE1	2.48	0.48
6:E:34:VAL:HG21	6:E:60:VAL:HG11	1.95	0.48
6:E:406:PRO:HB3	6:E:422:PHE:CE1	2.48	0.48
6:E:540:GLU:HB2	6:E:567:ARG:O	2.13	0.48
1:A:615:MET:HB2	1:A:766:PHE:HE1	1.78	0.48
6:F:569:LYS:HE2	6:F:569:LYS:CA	2.43	0.48
6:E:142:GLU:O	6:E:146:LYS:HG2	2.14	0.48
6:E:470:GLN:C	6:E:571:GLY:HA2	2.39	0.48
6:E:487:ALA:HB3	6:E:515:TYR:CD2	2.49	0.48
6:E:493:ILE:HD11	6:E:522:ALA:HB2	1.94	0.48
6:E:537:GLN:HA	6:E:567:ARG:NH1	2.29	0.48
1:A:5:GLN:OE1	1:A:9:ASN:ND2	2.43	0.48
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.72	0.48
6:E:283:PRO:HG2	6:E:461:LEU:HD21	1.96	0.48
6:E:378:MET:SD	6:E:378:MET:C	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:22:G:HO2'	4:I:23:C:P	2.36	0.48
6:F:256:LEU:H	6:F:256:LEU:CD2	2.24	0.48
6:E:135:ALA:HA	6:E:138:LEU:HG	1.95	0.48
1:A:778:SER:OG	1:A:779:ILE:N	2.43	0.48
2:B:12:TYR:CB	2:B:49:PHE:CE2	2.91	0.48
2:B:31:SER:OG	2:B:32:GLU:N	2.47	0.48
3:C:65:ALA:HB1	3:C:70:LYS:NZ	2.28	0.48
2:D:165:LYS:NZ	2:D:165:LYS:HB3	2.28	0.48
6:F:6:VAL:HG23	6:F:7:LEU:H	1.79	0.48
6:F:16:CYS:SG	6:F:39:HIS:HB3	2.53	0.48
6:F:126:CYS:HB2	6:F:130:LEU:CD2	2.44	0.48
6:E:118:GLY:O	6:E:122:LEU:HG	2.14	0.48
6:E:150:GLY:HA3	6:E:167:TRP:HB3	1.96	0.48
6:E:158:LEU:CD2	6:E:164:HIS:HB2	2.43	0.48
6:E:569:LYS:CA	6:E:569:LYS:HE2	2.43	0.48
1:A:211:ASP:OD1	1:A:211:ASP:N	2.41	0.48
6:F:21:ARG:NH1	6:F:232:VAL:O	2.40	0.48
6:F:34:VAL:HG21	6:F:60:VAL:HG11	1.95	0.48
6:F:150:GLY:HA3	6:F:167:TRP:HB3	1.96	0.48
6:F:310:SER:HB3	6:F:312:ALA:H	1.78	0.48
6:F:544:VAL:HG23	6:F:572:ILE:HG13	1.96	0.48
6:E:369:ASP:O	6:E:394:LYS:CB	2.38	0.48
1:A:10:ARG:HD2	1:A:10:ARG:HA	1.47	0.48
6:F:245:HIS:HA	6:F:275:GLN:HA	1.95	0.48
6:F:262:PHE:HB3	6:F:265:ASN:CG	2.39	0.48
6:F:319:GLU:OE1	6:F:319:GLU:HA	2.13	0.48
6:E:414:LYS:HB3	6:E:414:LYS:HE3	1.47	0.48
1:A:848:VAL:HA	1:A:855:MET:HE3	1.96	0.47
6:F:283:PRO:HG2	6:F:461:LEU:HD21	1.96	0.47
6:F:318:CYS:HA	6:F:321:ALA:HB2	1.96	0.47
6:E:126:CYS:HB2	6:E:130:LEU:CD2	2.44	0.47
7:G:18:THR:O	7:G:52:LYS:HB2	2.14	0.47
1:A:226:THR:O	1:A:229:SER:OG	2.32	0.47
1:A:592:SER:HB2	5:J:30:C:H4'	1.96	0.47
1:A:607:SER:OG	1:A:608:ASP:N	2.47	0.47
1:A:820:VAL:HG21	1:A:829:LEU:HD22	1.96	0.47
2:D:121:PRO:O	2:D:190:ARG:NH1	2.47	0.47
6:F:142:GLU:O	6:F:146:LYS:HG2	2.14	0.47
6:F:153:THR:HA	6:F:224:TYR:HA	1.96	0.47
6:F:378:MET:SD	6:F:378:MET:C	2.97	0.47
6:E:9:ASN:HB2	6:E:129:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:544:VAL:HG23	6:E:572:ILE:HG13	1.96	0.47
1:A:125:ALA:HB2	1:A:208:ASP:HB3	1.96	0.47
1:A:493:VAL:HG11	1:A:570:GLN:HG2	1.95	0.47
5:J:24:U:P	5:J:24:U:C6	3.04	0.47
6:F:118:GLY:O	6:F:122:LEU:HG	2.14	0.47
6:F:487:ALA:HB3	6:F:515:TYR:CD2	2.49	0.47
6:E:515:TYR:O	6:E:518:GLN:N	2.29	0.47
6:E:153:THR:HA	6:E:224:TYR:HA	1.96	0.47
6:E:298:TYR:CZ	6:E:299:TYR:HE1	2.33	0.47
1:A:758:LEU:HD23	1:A:759:SER:H	1.79	0.47
6:F:470:GLN:HB2	6:F:570:VAL:O	2.14	0.47
6:E:276:LYS:O	6:E:396:TYR:N	2.38	0.47
6:E:476:TYR:CG	6:E:477:LYS:N	2.79	0.47
6:E:512:ILE:N	6:E:545:ILE:O	2.28	0.47
7:G:75:PHE:CZ	7:G:86:LYS:HB2	2.49	0.47
7:G:75:PHE:CE2	7:G:86:LYS:HB2	2.49	0.47
6:F:128:GLU:HG2	6:F:129:ARG:N	2.30	0.47
6:F:298:TYR:CZ	6:F:299:TYR:HE1	2.33	0.47
6:F:427:ARG:HH11	6:F:427:ARG:CG	2.25	0.47
6:F:474[B]:MET:HB3	6:F:575:ILE:HA	1.96	0.47
6:E:180:TYR:OH	6:E:410:THR:HG22	2.15	0.47
6:E:185:TYR:CD1	6:E:194:GLN:HA	2.49	0.47
6:E:441:CYS:O	6:E:464:HIS:ND1	2.47	0.47
6:E:470:GLN:HB2	6:E:570:VAL:O	2.14	0.47
6:E:473:LYS:HZ2	6:E:474[B]:MET:C	2.22	0.47
7:G:95:ASN:OD1	7:G:95:ASN:N	2.48	0.47
1:A:551:LYS:HE2	1:A:551:LYS:HB3	1.58	0.47
1:A:844:VAL:C	1:A:845:ASP:OD1	2.54	0.47
2:B:51:ARG:O	2:B:53:ALA:N	2.47	0.47
4:I:13:U:H2'	4:I:14:A:O4'	2.14	0.47
6:F:6:VAL:HG23	6:F:7:LEU:N	2.29	0.47
6:F:473:LYS:HE3	6:F:582:TYR:HD1	1.79	0.47
6:E:128:GLU:HG2	6:E:129:ARG:N	2.30	0.47
6:E:311:HIS:CE1	6:E:359:THR:HG1	2.32	0.47
6:E:452:VAL:O	6:E:455:LEU:HB3	2.15	0.47
1:A:733:ARG:NH2	7:G:2:ASN:OD1	2.45	0.47
1:A:902:MET:HE3	1:A:903:TYR:CZ	2.50	0.47
6:F:371:VAL:O	6:F:397:VAL:N	2.48	0.47
6:E:262:PHE:HB3	6:E:265:ASN:CG	2.39	0.47
6:E:473:LYS:HE3	6:E:582:TYR:HD1	1.79	0.47
7:G:12:MET:HG3	7:G:39:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:105:SER:O	7:G:109:THR:HG22	2.14	0.47
1:A:37:ILE:O	1:A:37:ILE:HG23	2.15	0.47
1:A:38:TYR:CD2	1:A:728:TYR:CE1	3.03	0.47
1:A:686:THR:O	1:A:686:THR:OG1	2.30	0.47
1:A:709:SER:O	1:A:709:SER:OG	2.26	0.47
2:B:45:ALA:HA	2:B:48:GLU:HB2	1.96	0.47
6:E:178:ARG:O	6:E:181:VAL:HG23	2.15	0.47
6:E:318:CYS:HA	6:E:321:ALA:HB2	1.96	0.47
1:A:218:ASP:OD1	1:A:218:ASP:C	2.58	0.47
6:E:6:VAL:HG23	6:E:7:LEU:N	2.29	0.47
6:E:548:GLN:O	6:E:550:THR:N	2.47	0.47
2:B:79:LYS:HB2	2:B:79:LYS:HE3	1.83	0.46
6:F:34:VAL:HG23	6:F:39:HIS:O	2.16	0.46
6:F:51:ASN:OD1	6:F:69:SER:HB3	2.15	0.46
6:F:477:LYS:HZ2	6:F:579:ARG:HE	1.63	0.46
6:F:537:GLN:HA	6:F:567:ARG:NH1	2.29	0.46
6:E:117:ALA:HB2	6:E:415:GLY:O	2.15	0.46
7:G:94:LEU:HG	7:G:98:ASN:HB2	1.97	0.46
1:A:61:GLU:C	1:A:63:ASP:N	2.73	0.46
1:A:277:GLU:H	1:A:277:GLU:CD	2.23	0.46
1:A:900:LEU:HD23	1:A:900:LEU:HA	1.71	0.46
6:F:8:CYS:SG	6:F:99:GLY:N	2.86	0.46
6:F:178:ARG:O	6:F:181:VAL:HG23	2.15	0.46
6:F:180:TYR:OH	6:F:410:THR:HG22	2.15	0.46
6:E:274:MET:HE2	6:E:274:MET:HB3	1.77	0.46
6:E:371:VAL:O	6:E:397:VAL:N	2.48	0.46
7:G:10:ARG:HB3	7:G:11:GLN:H	1.51	0.46
2:B:41:SER:CA	2:B:44:VAL:HG23	2.46	0.46
6:F:452:VAL:O	6:F:455:LEU:HB3	2.15	0.46
6:E:34:VAL:HG23	6:E:39:HIS:O	2.15	0.46
6:E:370:ILE:HA	6:E:395:HIS:O	2.15	0.46
1:A:77:PHE:O	1:A:77:PHE:CG	2.68	0.46
1:A:218:ASP:OD1	1:A:218:ASP:O	2.33	0.46
2:B:135:TYR:OH	2:B:139:LYS:HE3	2.16	0.46
5:J:43:U:H2'	5:J:44:A:H8	1.81	0.46
6:E:51:ASN:OD1	6:E:69:SER:HB3	2.15	0.46
1:A:38:TYR:CD1	1:A:38:TYR:O	2.69	0.46
1:A:692:SER:O	1:A:696:ILE:HG13	2.16	0.46
6:F:185:TYR:CD1	6:F:194:GLN:HA	2.49	0.46
6:E:6:VAL:HG23	6:E:7:LEU:H	1.79	0.46
6:E:406:PRO:HB3	6:E:422:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:503:ASN:OD1	6:E:503:ASN:N	2.49	0.46
3:C:27:LYS:HB3	3:C:27:LYS:HE2	1.70	0.46
6:F:67:GLY:C	6:F:68:MET:HE2	2.41	0.46
6:F:280:LEU:HD21	6:F:399:ILE:HG13	1.98	0.46
6:F:503:ASN:OD1	6:F:503:ASN:N	2.49	0.46
6:E:21:ARG:HD3	6:E:136:GLU:HG3	1.96	0.46
2:B:165:LYS:HB3	2:B:165:LYS:HE2	1.71	0.46
2:D:51:ARG:HB3	2:D:51:ARG:CZ	2.46	0.46
6:F:158:LEU:HD21	6:F:164:HIS:HB2	1.98	0.46
2:D:55:MET:O	2:D:59:LEU:HG	2.16	0.46
6:F:21:ARG:HD3	6:F:136:GLU:HG3	1.96	0.46
6:F:511:PHE:CB	6:F:519:ASN:HD21	2.28	0.46
6:F:542:ASP:HA	6:F:569:LYS:H	1.81	0.46
1:A:369:LYS:O	1:A:373:VAL:HG13	2.16	0.46
2:B:31:SER:OG	2:B:33:VAL:N	2.46	0.46
2:B:174:MET:HE3	2:B:174:MET:O	2.16	0.46
2:D:100:ASN:HB3	2:D:103:LEU:HD12	1.97	0.46
6:F:9:ASN:HB2	6:F:129:ARG:HH12	1.79	0.46
6:F:104:THR:O	6:F:108:ALA:HB2	2.16	0.46
6:F:245:HIS:CE1	6:F:275:GLN:HE21	2.34	0.46
6:F:473:LYS:HD3	6:F:474[A]:MET:N	2.30	0.46
6:E:55:CYS:SG	6:E:57:VAL:HG22	2.56	0.46
6:E:248:ARG:NH1	6:E:250:THR:HA	2.31	0.46
7:G:74:ARG:H	7:G:74:ARG:CD	2.23	0.46
1:A:254:GLU:OE1	1:A:286:TYR:OH	2.15	0.46
2:D:14:ALA:O	2:D:17:THR:OG1	2.29	0.46
6:F:370:ILE:HA	6:F:395:HIS:O	2.15	0.46
6:F:381:ASN:OD1	6:F:424:SER:OG	2.32	0.46
6:F:476:TYR:O	6:F:579:ARG:NH2	2.49	0.46
6:E:104:THR:O	6:E:108:ALA:HB2	2.16	0.46
6:E:476:TYR:O	6:E:579:ARG:NH2	2.49	0.46
2:D:154:TRP:HA	2:D:189:LEU:O	2.16	0.45
6:F:248:ARG:NH1	6:F:250:THR:HA	2.31	0.45
6:F:405:LEU:HD22	6:F:405:LEU:HA	1.80	0.45
6:F:477:LYS:NZ	6:F:579:ARG:HE	2.14	0.45
6:E:381:ASN:OD1	6:E:424:SER:OG	2.32	0.45
6:E:437:PHE:CD1	6:E:437:PHE:C	2.94	0.45
6:E:533:VAL:HG11	6:E:560:ARG:NH2	2.27	0.45
7:G:18:THR:O	7:G:19:THR:HB	2.16	0.45
1:A:272:LYS:NZ	1:A:278:GLU:OE2	2.49	0.45
7:G:5:SER:O	7:G:5:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:LYS:HZ2	7:G:64:THR:N	2.14	0.45
1:A:109:ASP:N	1:A:109:ASP:OD1	2.48	0.45
2:B:70:MET:HE3	6:E:92:LEU:HG	1.98	0.45
6:F:304:ILE:HG23	6:F:306:TYR:HE1	1.81	0.45
6:E:67:GLY:C	6:E:68:MET:HE2	2.41	0.45
1:A:218:ASP:O	1:A:218:ASP:CG	2.56	0.45
1:A:438:LYS:HB2	1:A:438:LYS:HE2	1.54	0.45
1:A:513:ARG:HG3	1:A:513:ARG:HH11	1.82	0.45
6:F:58:THR:O	6:F:58:THR:OG1	2.34	0.45
6:E:245:HIS:CE1	6:E:275:GLN:HE21	2.34	0.45
6:E:304:ILE:HG23	6:E:306:TYR:HE1	1.81	0.45
6:E:369:ASP:O	6:E:370:ILE:HG12	2.16	0.45
6:E:477:LYS:NZ	6:E:579:ARG:HE	2.14	0.45
1:A:153:ASP:OD1	1:A:153:ASP:N	2.49	0.45
2:B:155:GLU:O	2:B:155:GLU:HG3	2.17	0.45
6:F:264:SER:C	6:F:265:ASN:HD22	2.24	0.45
6:F:406:PRO:HB3	6:F:422:PHE:CZ	2.51	0.45
6:F:452:VAL:HA	6:F:455:LEU:HD12	1.99	0.45
1:A:759:SER:O	1:A:759:SER:OG	2.15	0.45
6:F:19:CYS:HA	6:F:39:HIS:CE1	2.52	0.45
1:A:77:PHE:O	1:A:77:PHE:CD2	2.69	0.45
1:A:358:ASP:CG	1:A:533:ARG:HH21	2.19	0.45
1:A:676:LYS:NZ	1:A:679:GLY:O	2.46	0.45
6:F:55:CYS:SG	6:F:57:VAL:HG22	2.56	0.45
6:E:31:TYR:HD2	6:E:88:GLN:N	2.15	0.45
1:A:899:MET:HA	1:A:902:MET:HG2	1.98	0.45
6:F:296:ALA:HB1	6:F:325:LEU:HD11	1.98	0.45
6:F:388:ASN:HA	6:F:391:LEU:O	2.17	0.45
6:F:425:VAL:O	6:F:428:LEU:HB3	2.16	0.45
6:F:473:LYS:HD3	6:F:474[B]:MET:N	2.30	0.45
6:F:489:ASN:HD21	6:F:492:GLN:HB2	1.82	0.45
6:E:284:PRO:HB3	6:E:537:GLN:OE1	2.16	0.45
6:E:388:ASN:HA	6:E:391:LEU:O	2.17	0.45
6:E:425:VAL:O	6:E:428:LEU:HB3	2.16	0.45
6:E:473:LYS:HD3	6:E:474[A]:MET:N	2.32	0.45
6:E:511:PHE:CB	6:E:519:ASN:HD21	2.29	0.45
1:A:61:GLU:O	1:A:63:ASP:N	2.50	0.45
2:B:15:PHE:CB	2:B:48:GLU:OE1	2.65	0.45
2:B:166:ILE:HD12	2:B:166:ILE:H	1.82	0.45
2:D:85:SER:O	2:D:89:THR:HG23	2.17	0.45
2:D:113:GLY:HA3	2:D:133:PRO:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ASN:OD1	2:D:140:ASN:N	2.50	0.45
6:F:31:TYR:HD2	6:F:88:GLN:N	2.15	0.45
6:F:152:ALA:N	6:F:225:PHE:O	2.43	0.45
6:F:492:GLN:OE1	6:F:577:SER:OG	2.34	0.45
6:E:373:PHE:HB3	6:E:398:TYR:HD1	1.82	0.45
6:E:495:VAL:O	6:E:499:PHE:N	2.36	0.45
1:A:760:ASP:C	1:A:760:ASP:OD1	2.59	0.45
2:D:100:ASN:HD22	2:D:103:LEU:HD12	1.82	0.45
6:F:31:TYR:HA	6:F:34:VAL:HG12	1.99	0.45
6:F:452:VAL:HG23	6:F:457:TYR:HD2	1.82	0.45
6:E:19:CYS:HA	6:E:39:HIS:CE1	2.52	0.45
6:E:58:THR:O	6:E:58:THR:OG1	2.34	0.45
6:E:158:LEU:HD21	6:E:164:HIS:HB2	1.98	0.45
6:E:265:ASN:OD1	6:E:291:PHE:HA	2.16	0.45
6:E:578:ASP:OD1	6:E:580:ASP:N	2.50	0.45
2:D:127:LYS:HZ3	2:D:127:LYS:CB	2.31	0.44
6:F:156:GLU:CD	6:F:156:GLU:N	2.76	0.44
6:F:437:PHE:CD1	6:F:437:PHE:C	2.94	0.44
6:F:445:PRO:HA	6:F:464:HIS:HB3	1.99	0.44
6:E:264:SER:C	6:E:265:ASN:HD22	2.24	0.44
6:E:473:LYS:HD3	6:E:474[B]:MET:N	2.32	0.44
7:G:57:PRO:HA	7:G:64:THR:HG23	1.99	0.44
1:A:274:ASP:HB2	2:B:111:ARG:HH12	1.81	0.44
1:A:420:TYR:O	1:A:424:VAL:HG13	2.17	0.44
6:E:452:VAL:HG23	6:E:457:TYR:HD2	1.82	0.44
1:A:205:LEU:HD22	1:A:234:VAL:HG12	1.99	0.44
1:A:607:SER:O	1:A:608:ASP:CG	2.57	0.44
2:B:31:SER:HB3	2:B:34:VAL:HG23	1.99	0.44
3:C:54:SER:O	3:C:57:SER:OG	2.35	0.44
2:D:31:SER:HB3	2:D:34:VAL:HB	1.99	0.44
5:J:25:G:HO2'	5:J:26:A:P	2.25	0.44
5:J:39:A:C6	5:J:40:U:C4	3.06	0.44
6:F:265:ASN:OD1	6:F:291:PHE:HA	2.16	0.44
6:F:369:ASP:O	6:F:370:ILE:HG12	2.16	0.44
6:F:373:PHE:HB3	6:F:398:TYR:HD1	1.82	0.44
6:F:578:ASP:OD1	6:F:580:ASP:N	2.50	0.44
6:E:296:ALA:HB1	6:E:325:LEU:HD11	1.98	0.44
6:E:483:ASP:OD1	6:E:483:ASP:N	2.50	0.44
6:E:542:ASP:HA	6:E:569:LYS:H	1.81	0.44
7:G:7:VAL:O	7:G:7:VAL:CG2	2.38	0.44
2:B:45:ALA:HA	2:B:48:GLU:CG	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:SER:HB3	2:D:49:PHE:HB2	1.99	0.44
6:F:31:TYR:O	6:F:34:VAL:HG12	2.18	0.44
6:F:235:LEU:HD12	6:F:385:SER:OG	2.17	0.44
6:F:249:ILE:HG12	6:F:252:LEU:HB2	2.00	0.44
6:F:351:THR:O	6:F:353:GLU:N	2.51	0.44
6:E:8:CYS:SG	6:E:99:GLY:N	2.86	0.44
6:E:280:LEU:HD21	6:E:399:ILE:HG13	1.98	0.44
1:A:58:GLU:O	1:A:66:ILE:HG22	2.17	0.44
3:C:28:LEU:HD12	3:C:28:LEU:HA	1.75	0.44
6:E:249:ILE:HG12	6:E:252:LEU:HB2	2.00	0.44
7:G:7:VAL:O	7:G:7:VAL:CG1	2.54	0.44
1:A:223:ILE:HD12	7:G:104:GLY:HA2	2.00	0.44
2:B:15:PHE:HB2	2:B:48:GLU:OE1	2.18	0.44
3:C:47:GLU:HA	3:C:50:GLU:HG2	1.99	0.44
2:D:177:SER:HB2	2:D:182:TRP:HZ2	1.81	0.44
6:F:316:ALA:HA	6:F:319:GLU:HG2	1.99	0.44
6:E:235:LEU:HD12	6:E:385:SER:OG	2.18	0.44
6:E:316:ALA:HA	6:E:319:GLU:HG2	1.98	0.44
1:A:125:ALA:CB	1:A:208:ASP:HB3	2.47	0.44
1:A:566:MET:HE3	1:A:566:MET:HB2	1.78	0.44
2:B:12:TYR:HB2	2:B:49:PHE:CE2	2.52	0.44
6:F:9:ASN:CB	6:F:129:ARG:HH12	2.31	0.44
6:F:284:PRO:HB3	6:F:537:GLN:OE1	2.17	0.44
6:F:387:VAL:HA	6:F:390:ARG:HB2	1.99	0.44
6:F:399:ILE:HD12	6:F:399:ILE:H	1.82	0.44
6:F:414:LYS:HE3	6:F:414:LYS:HB3	1.46	0.44
6:E:489:ASN:HD21	6:E:492:GLN:HB2	1.82	0.44
6:E:545:ILE:HA	6:E:573:LEU:HB3	1.99	0.44
1:A:75:HIS:CE1	9:A:1003:GDP:C8	3.02	0.44
1:A:388:LEU:HD22	1:A:672:SER:HB3	1.98	0.44
5:J:24:U:O5'	5:J:24:U:C6	2.70	0.44
5:J:40:U:C2	5:J:41:G:C8	3.06	0.44
6:E:445:PRO:HA	6:E:464:HIS:HB3	1.99	0.44
7:G:78:ASP:O	7:G:79:THR:HG23	2.17	0.44
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.77	0.44
1:A:906:MET:HE3	1:A:907:LEU:CD1	2.48	0.44
6:F:346:PHE:CD1	6:F:346:PHE:N	2.86	0.44
6:E:31:TYR:O	6:E:34:VAL:HG12	2.18	0.44
6:E:156:GLU:N	6:E:156:GLU:CD	2.76	0.44
6:E:377:SER:CB	6:E:404:GLN:O	2.66	0.44
2:B:41:SER:HA	2:B:44:VAL:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:GLY:C	6:F:195:ILE:HB	2.43	0.43
6:F:244:GLU:CD	6:F:244:GLU:C	2.86	0.43
6:F:441:CYS:O	6:F:464:HIS:ND1	2.51	0.43
2:D:58:LYS:HD2	6:F:79:ILE:HG21	1.99	0.43
5:J:40:U:H2'	5:J:41:G:C8	2.51	0.43
5:J:48:C:H2'	5:J:49:C:C6	2.53	0.43
6:F:395:HIS:C	6:F:396:TYR:CD1	2.96	0.43
6:E:9:ASN:CB	6:E:129:ARG:HH12	2.31	0.43
6:E:549:THR:O	6:E:550:THR:CG2	2.59	0.43
6:F:127:THR:O	6:F:130:LEU:HB2	2.18	0.43
6:F:507:ARG:HH12	6:F:526:LEU:HB3	1.83	0.43
6:F:545:ILE:HA	6:F:573:LEU:HB3	1.99	0.43
6:E:31:TYR:HA	6:E:34:VAL:HG12	1.99	0.43
6:E:32:ASP:O	6:E:35:ILE:HG13	2.19	0.43
6:E:72:CYS:O	6:E:76:LYS:N	2.52	0.43
7:G:54:ALA:HB3	7:G:67:THR:OG1	2.19	0.43
1:A:575:LEU:HD22	1:A:641:LYS:HG3	2.01	0.43
2:B:57:ARG:O	2:B:57:ARG:HG2	2.16	0.43
2:B:62:MET:HE2	2:B:62:MET:HB3	1.72	0.43
3:C:57:SER:CB	2:D:120:ILE:HG13	2.49	0.43
2:D:114:CYS:HA	2:D:131:VAL:O	2.17	0.43
4:I:17:A:H2'	4:I:18:G:H8	1.82	0.43
6:F:288:LYS:HB2	6:F:288:LYS:HE2	1.44	0.43
6:F:483:ASP:OD1	6:F:483:ASP:N	2.50	0.43
6:E:473:LYS:HZ3	6:E:576:MET:HG3	1.83	0.43
1:A:422:PHE:CZ	1:A:426:LYS:HE2	2.53	0.43
1:A:441:PHE:CE1	1:A:548:ILE:HG13	2.53	0.43
3:C:56:LEU:HD23	2:D:106:ILE:HD11	2.01	0.43
6:F:419:PRO:HA	6:F:422:PHE:CZ	2.54	0.43
6:F:561:PHE:CD1	6:F:561:PHE:C	2.96	0.43
6:E:346:PHE:CD1	6:E:346:PHE:N	2.86	0.43
7:G:72:PRO:HB3	7:G:89:TYR:CZ	2.54	0.43
2:B:88:GLN:O	2:B:92:PHE:HD1	2.00	0.43
6:F:72:CYS:O	6:F:76:LYS:N	2.52	0.43
6:E:244:GLU:C	6:E:244:GLU:CD	2.86	0.43
6:E:395:HIS:C	6:E:396:TYR:CD1	2.97	0.43
6:E:452:VAL:HA	6:E:455:LEU:HD12	1.99	0.43
7:G:78:ASP:OD1	7:G:78:ASP:N	2.50	0.43
1:A:689:TYR:O	1:A:693:VAL:HG23	2.18	0.43
6:F:32:ASP:O	6:F:35:ILE:HG13	2.18	0.43
6:E:514:PRO:HB3	6:E:560:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:561:PHE:CD1	6:E:561:PHE:C	2.96	0.43
1:A:751:LYS:HB3	1:A:752:HIS:CD2	2.53	0.43
6:F:60:VAL:HG13	6:F:61:THR:H	1.83	0.43
6:F:150:GLY:HA2	6:F:168:GLU:HB2	2.01	0.43
6:F:514:PRO:HB3	6:F:560:ARG:NH2	2.34	0.43
6:E:175:PRO:HG2	6:E:180:TYR:HE2	1.83	0.43
6:E:192:LYS:HG3	6:E:224:TYR:OH	2.18	0.43
6:E:569:LYS:HE2	6:E:569:LYS:HA	2.01	0.43
1:A:304:ASP:HB2	1:A:636:LEU:HD13	2.01	0.43
6:F:9:ASN:HB2	6:F:129:ARG:HH22	1.84	0.43
6:F:418:GLU:HB3	6:F:420:GLU:H	1.83	0.43
6:F:513:SER:HB3	6:F:519:ASN:OD1	2.18	0.43
6:E:150:GLY:HA2	6:E:168:GLU:HB2	2.01	0.43
6:E:197:GLU:H	6:E:197:GLU:HG2	1.47	0.43
6:E:477:LYS:HZ2	6:E:579:ARG:HE	1.65	0.43
1:A:12:CYS:SG	1:A:12:CYS:O	2.77	0.43
1:A:899:MET:O	1:A:903:TYR:HB2	2.18	0.43
4:I:21:U:N3	4:I:22:G:N7	2.66	0.43
6:F:303:ARG:HA	6:F:354:GLN:O	2.19	0.43
6:E:542:ASP:HB3	6:E:569:LYS:HB3	2.00	0.43
6:F:44:SER:O	6:F:45:VAL:C	2.61	0.42
6:F:201:GLU:HG2	6:F:202:LYS:H	1.83	0.42
6:F:437:PHE:C	6:F:437:PHE:HD1	2.27	0.42
6:E:9:ASN:HB2	6:E:129:ARG:HH22	1.84	0.42
6:E:184:GLY:C	6:E:195:ILE:HB	2.43	0.42
6:E:418:GLU:HB3	6:E:420:GLU:H	1.84	0.42
6:E:465:LYS:HG3	6:E:466:ASP:H	1.83	0.42
2:D:175:ASP:O	2:D:178:PRO:HD2	2.18	0.42
6:F:465:LYS:HG3	6:F:466:ASP:H	1.83	0.42
6:E:387:VAL:HA	6:E:390:ARG:HB2	1.99	0.42
6:E:437:PHE:C	6:E:437:PHE:HD1	2.27	0.42
6:E:442:ARG:HA	6:E:464:HIS:CE1	2.54	0.42
6:E:492:GLN:OE1	6:E:577:SER:OG	2.34	0.42
6:E:513:SER:HB3	6:E:519:ASN:OD1	2.18	0.42
3:C:5:ASP:O	3:C:9:THR:HG22	2.20	0.42
6:F:152:ALA:O	6:F:224:TYR:HA	2.19	0.42
6:F:175:PRO:HG2	6:F:180:TYR:HE2	1.84	0.42
6:F:311:HIS:CE1	6:F:359:THR:HB	2.54	0.42
6:F:391:LEU:HD22	6:F:393:ALA:HB2	2.02	0.42
6:F:485:SER:O	6:F:485:SER:OG	2.33	0.42
6:E:60:VAL:HG13	6:E:61:THR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:399:ILE:HD12	6:E:399:ILE:H	1.82	0.42
6:E:507:ARG:HH12	6:E:526:LEU:HB3	1.83	0.42
1:A:164:ASP:OD1	1:A:165:PHE:N	2.52	0.42
2:D:173:SER:N	2:D:176:ASN:OD1	2.53	0.42
5:J:38:C:H2'	5:J:39:A:O4'	2.19	0.42
6:F:192:LYS:HG3	6:F:224:TYR:OH	2.18	0.42
6:F:548:GLN:H	6:F:548:GLN:HG3	1.46	0.42
6:E:177:ASN:HB3	6:E:178:ARG:H	1.73	0.42
6:E:419:PRO:HA	6:E:422:PHE:CZ	2.54	0.42
1:A:513:ARG:HG3	1:A:513:ARG:NH1	2.34	0.42
2:D:55:MET:HG3	2:D:56:GLN:N	2.35	0.42
6:F:7:LEU:HD11	6:F:106:PHE:CG	2.55	0.42
6:E:548:GLN:H	6:E:548:GLN:HG3	1.46	0.42
1:A:225:THR:HG22	1:A:226:THR:H	1.85	0.42
1:A:503:GLY:HA3	1:A:561:SER:HA	2.01	0.42
2:B:42:LEU:HG	2:B:45:ALA:HB3	2.02	0.42
2:D:35:LEU:O	2:D:39:LYS:NZ	2.44	0.42
6:F:295:LEU:HA	6:F:298:TYR:HB3	2.02	0.42
6:E:152:ALA:O	6:E:224:TYR:HA	2.19	0.42
7:G:91:ILE:H	7:G:91:ILE:HG13	1.54	0.42
1:A:304:ASP:OD1	1:A:304:ASP:N	2.50	0.42
2:D:55:MET:HE3	2:D:55:MET:HB2	1.74	0.42
2:D:147:PHE:O	2:D:154:TRP:HD1	2.02	0.42
6:F:346:PHE:N	6:F:346:PHE:HD1	2.18	0.42
6:F:542:ASP:HB3	6:F:569:LYS:HB3	2.00	0.42
6:F:579:ARG:HA	6:F:579:ARG:HD3	1.83	0.42
6:E:22:ARG:HH11	6:E:22:ARG:CG	2.33	0.42
6:E:303:ARG:HA	6:E:354:GLN:O	2.19	0.42
6:E:307:THR:HA	6:E:358:CYS:O	2.20	0.42
7:G:45:LEU:HD12	7:G:87:TYR:O	2.20	0.42
1:A:70:PHE:CE2	1:A:117:GLN:HG2	2.55	0.42
2:D:177:SER:HB2	2:D:182:TRP:CZ2	2.55	0.42
6:F:252:LEU:O	6:F:254:PRO:HD3	2.20	0.42
6:F:322:LEU:HD11	6:F:345:LYS:HB2	2.02	0.42
6:F:445:PRO:HG2	6:F:447:GLU:HG3	2.02	0.42
6:E:152:ALA:N	6:E:225:PHE:O	2.43	0.42
6:E:304:ILE:HD11	6:E:372:VAL:HG13	2.01	0.42
1:A:825:ASP:OD1	1:A:825:ASP:N	2.51	0.42
6:F:307:THR:HA	6:F:358:CYS:O	2.20	0.42
6:F:406:PRO:HB2	6:F:409:ARG:HH12	1.84	0.42
6:E:21:ARG:HB2	6:E:133:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:124:ASN:C	6:E:126:CYS:H	2.28	0.42
6:E:149:TYR:HA	6:E:171:LYS:HB3	2.02	0.42
6:E:311:HIS:CE1	6:E:359:THR:HB	2.54	0.42
6:E:322:LEU:HD11	6:E:345:LYS:HB2	2.02	0.42
1:A:654:ARG:HE	1:A:654:ARG:HB3	1.66	0.42
1:A:924:MET:HB3	1:A:924:MET:HE2	1.77	0.42
2:B:51:ARG:HG3	2:B:55:MET:HB2	1.98	0.42
6:F:366:THR:O	6:F:391:LEU:HA	2.20	0.42
6:E:109:ILE:HD13	6:E:134:ALA:HB2	2.02	0.42
6:E:187:VAL:HA	6:E:191:SER:O	2.20	0.42
6:E:366:THR:O	6:E:391:LEU:HA	2.20	0.42
6:E:114:TRP:HE3	6:E:119:ASP:HB3	1.85	0.41
6:E:233:MET:HE2	6:E:233:MET:HB2	1.90	0.41
6:E:391:LEU:HD22	6:E:393:ALA:HB2	2.02	0.41
6:E:511:PHE:HB3	6:E:519:ASN:HD21	1.85	0.41
4:I:20:A:C6	5:J:41:G:C6	3.08	0.41
6:F:422:PHE:HB2	6:F:426:CYS:SG	2.60	0.41
6:E:252:LEU:O	6:E:254:PRO:HD3	2.20	0.41
6:E:428:LEU:O	6:E:432:ILE:N	2.42	0.41
7:G:26:ASP:O	7:G:27:ASN:HB3	2.20	0.41
1:A:509:TRP:CZ3	2:B:87:MET:HG2	2.56	0.41
6:F:151:ILE:O	6:F:167:TRP:HA	2.20	0.41
6:F:187:VAL:HA	6:F:191:SER:O	2.20	0.41
6:E:295:LEU:HA	6:E:298:TYR:HB3	2.02	0.41
6:E:422:PHE:HB2	6:E:426:CYS:SG	2.60	0.41
2:B:19:GLN:OE1	2:B:19:GLN:HA	2.20	0.41
3:C:12:VAL:O	3:C:16:VAL:HG12	2.20	0.41
6:F:149:TYR:HA	6:F:171:LYS:HB3	2.02	0.41
6:F:541:TYR:HD2	6:F:543:TYR:H	1.68	0.41
1:A:540:THR:OG1	1:A:665:GLU:OE1	2.21	0.41
1:A:856:ILE:H	1:A:856:ILE:HG13	1.42	0.41
2:B:169:LEU:HA	2:B:172:ILE:HD12	2.02	0.41
3:C:70:LYS:HB2	3:C:70:LYS:HE2	1.67	0.41
6:F:61:THR:HA	6:F:84:CYS:HB3	2.02	0.41
6:F:304:ILE:HD11	6:F:372:VAL:HG13	2.01	0.41
6:F:565:ILE:HG12	6:F:565:ILE:H	1.37	0.41
6:E:346:PHE:N	6:E:346:PHE:HD1	2.18	0.41
6:E:445:PRO:HG2	6:E:447:GLU:HG3	2.02	0.41
6:E:579:ARG:HA	6:E:579:ARG:HD3	1.83	0.41
3:C:39:ILE:HD13	3:C:52:MET:HG2	2.03	0.41
4:I:20:A:C2	4:I:21:U:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:ARG:HB2	6:F:133:PHE:CE1	2.55	0.41
6:E:115:THR:O	6:E:413:THR:N	2.30	0.41
6:E:329:LYS:HB2	6:E:329:LYS:HE2	1.76	0.41
1:A:253:ALA:O	1:A:259:THR:HA	2.19	0.41
1:A:615:MET:HB2	1:A:766:PHE:CE1	2.55	0.41
1:A:874:ASN:OD1	1:A:875:GLN:N	2.54	0.41
3:C:51:LYS:HB2	3:C:51:LYS:HE2	1.83	0.41
2:D:182:TRP:CE3	2:D:184:LEU:HG	2.55	0.41
6:F:22:ARG:CG	6:F:22:ARG:HH11	2.33	0.41
6:F:124:ASN:C	6:F:126:CYS:H	2.28	0.41
6:F:246:TYR:N	6:F:274:MET:O	2.54	0.41
6:F:377:SER:HB3	6:F:401:ASP:O	2.21	0.41
6:F:455:LEU:HB2	6:F:584:LYS:NZ	2.35	0.41
6:F:511:PHE:HB3	6:F:519:ASN:HD21	1.85	0.41
6:E:21:ARG:HG3	6:E:136:GLU:CG	2.51	0.41
6:E:406:PRO:HB2	6:E:409:ARG:HH12	1.84	0.41
6:E:565:ILE:HG12	6:E:565:ILE:H	1.37	0.41
1:A:38:TYR:O	1:A:38:TYR:HD1	2.02	0.41
1:A:370:GLU:HA	1:A:373:VAL:HG22	2.03	0.41
6:F:21:ARG:HG3	6:F:136:GLU:CG	2.51	0.41
6:F:195:ILE:HG22	6:F:196:GLY:N	2.36	0.41
6:E:151:ILE:O	6:E:167:TRP:HA	2.20	0.41
6:E:512:ILE:HB	6:E:546:PHE:CG	2.56	0.41
6:E:514:PRO:O	6:E:516:ASN:ND2	2.54	0.41
1:A:466:ILE:HD12	1:A:466:ILE:HA	1.87	0.41
1:A:633:MET:HE2	1:A:633:MET:HB3	1.90	0.41
3:C:57:SER:HB3	2:D:120:ILE:HG13	2.02	0.41
2:D:62:MET:HE2	2:D:62:MET:HB3	1.90	0.41
2:D:95:LEU:HD23	2:D:95:LEU:HA	1.96	0.41
2:D:117:LEU:HD12	2:D:129:MET:O	2.21	0.41
6:F:151:ILE:H	6:F:168:GLU:HB2	1.86	0.41
6:F:156:GLU:HB2	6:F:164:HIS:HB3	2.03	0.41
6:F:480:ILE:CD1	6:F:549:THR:O	2.67	0.41
6:F:514:PRO:O	6:F:516:ASN:ND2	2.54	0.41
6:E:7:LEU:HD11	6:E:106:PHE:CG	2.55	0.41
6:E:13:SER:O	6:E:13:SER:OG	2.21	0.41
6:E:156:GLU:HB2	6:E:164:HIS:HB3	2.03	0.41
6:E:246:TYR:N	6:E:274:MET:O	2.54	0.41
6:E:445:PRO:HB3	6:E:465:LYS:HG2	2.03	0.41
6:E:455:LEU:HD11	6:E:562:ASN:ND2	2.36	0.41
6:E:541:TYR:HD2	6:E:543:TYR:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:556:CYS:SG	6:E:578:ASP:HB3	2.61	0.41
6:E:568:ALA:HB2	6:E:572:ILE:HB	2.02	0.41
7:G:9:LEU:HB3	7:G:32:TYR:O	2.21	0.41
7:G:9:LEU:HD23	7:G:9:LEU:HA	1.87	0.41
7:G:19:THR:HA	7:G:53:TRP:CG	2.54	0.41
7:G:45:LEU:HD12	7:G:45:LEU:HA	1.68	0.41
1:A:491:ASN:HB3	1:A:521:TYR:CD2	2.56	0.41
2:D:70:MET:HG3	6:F:92:LEU:HD21	2.03	0.41
2:D:162:ALA:HB2	2:D:183:PRO:HG2	2.03	0.41
6:F:63:LEU:HD23	6:F:71:TYR:C	2.46	0.41
6:F:114:TRP:HE3	6:F:119:ASP:HB3	1.85	0.41
6:F:156:GLU:CD	6:E:253:TYR:OH	2.64	0.41
6:F:512:ILE:HB	6:F:546:PHE:CG	2.56	0.41
6:F:561:PHE:C	6:F:561:PHE:HD1	2.29	0.41
6:E:290:HIS:NE2	6:E:320:LYS:HE3	2.37	0.41
6:E:559:ASN:HA	6:E:562:ASN:HB2	2.03	0.41
1:A:715:ILE:HB	1:A:721:ARG:HG2	2.03	0.40
2:B:46:LYS:O	2:B:46:LYS:CD	2.69	0.40
4:I:11:G:N1	5:J:49:C:N3	2.54	0.40
4:I:12:G:N2	5:J:48:C:O2	2.34	0.40
4:I:20:A:H2'	4:I:21:U:C6	2.57	0.40
6:E:35:ILE:HG13	6:E:35:ILE:H	1.79	0.40
6:E:359:THR:HG22	6:E:360:VAL:N	2.36	0.40
7:G:21:THR:O	7:G:21:THR:OG1	2.34	0.40
1:A:78:SER:O	1:A:81:GLN:N	2.55	0.40
1:A:83:GLU:HG3	1:A:219:PHE:HB2	2.03	0.40
3:C:14:LEU:HD22	3:C:36:HIS:CG	2.56	0.40
6:F:119:ASP:O	6:F:122:LEU:HB2	2.21	0.40
6:F:428:LEU:O	6:F:432:ILE:N	2.42	0.40
6:E:195:ILE:HG22	6:E:196:GLY:N	2.36	0.40
6:E:435:ASP:C	6:E:436:MET:HE2	2.47	0.40
1:A:75:HIS:CE1	9:A:1003:GDP:C1'	3.04	0.40
1:A:388:LEU:HD23	1:A:397:SER:OG	2.22	0.40
1:A:423:ALA:O	1:A:428:PHE:HB2	2.22	0.40
2:D:182:TRP:N	2:D:183:PRO:HD2	2.36	0.40
6:F:156:GLU:HB2	6:F:164:HIS:CB	2.51	0.40
6:F:195:ILE:HD13	6:F:195:ILE:HG21	1.84	0.40
6:F:197:GLU:H	6:F:197:GLU:HG2	1.47	0.40
6:F:260:ASP:O	6:F:263:SER:OG	2.39	0.40
6:F:290:HIS:NE2	6:F:320:LYS:HE3	2.36	0.40
6:F:465:LYS:HG3	6:F:466:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:568:ALA:HB2	6:F:572:ILE:HB	2.02	0.40
6:E:37:THR:OG1	6:E:39:HIS:HB2	2.22	0.40
6:E:129:ARG:HA	6:E:132:LEU:HD21	2.04	0.40
6:E:156:GLU:HB2	6:E:164:HIS:CB	2.51	0.40
6:E:195:ILE:HD13	6:E:195:ILE:HG21	1.84	0.40
1:A:202:VAL:HG13	1:A:231:VAL:HG13	2.03	0.40
1:A:718:LYS:HZ2	1:A:721:ARG:CD	2.32	0.40
1:A:837:ILE:HG21	1:A:866:ALA:HB2	2.04	0.40
2:D:118:ASN:OD1	2:D:118:ASN:N	2.54	0.40
2:D:177:SER:O	2:D:179:ASN:N	2.49	0.40
6:F:514:PRO:HB3	6:F:560:ARG:HH22	1.86	0.40
6:F:559:ASN:HA	6:F:562:ASN:HB2	2.02	0.40
6:E:473:LYS:HB3	6:E:588:THR:O	2.22	0.40
2:B:46:LYS:O	2:B:46:LYS:CE	2.70	0.40
6:F:143:GLU:HG3	6:F:143:GLU:H	1.74	0.40
6:F:306:TYR:HB3	6:F:317:LEU:HD13	2.04	0.40
6:F:359:THR:HG22	6:F:360:VAL:N	2.36	0.40
6:F:473:LYS:HB3	6:F:588:THR:O	2.22	0.40
6:F:556:CYS:SG	6:F:578:ASP:HB3	2.61	0.40
6:E:21:ARG:C	6:E:22:ARG:HG3	2.45	0.40
6:E:63:LEU:HD23	6:E:71:TYR:C	2.46	0.40
6:E:260:ASP:O	6:E:263:SER:OG	2.39	0.40
6:E:377:SER:HB3	6:E:401:ASP:O	2.21	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	924/942 (98%)	853 (92%)	67 (7%)	4 (0%)	30	48
2	B	185/198 (93%)	163 (88%)	19 (10%)	3 (2%)	7	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	184/198 (93%)	159 (86%)	24 (13%)	1 (0%)	24	43
3	C	70/83 (84%)	69 (99%)	1 (1%)	0	100	100
6	E	581/601 (97%)	485 (84%)	91 (16%)	5 (1%)	14	27
6	F	580/601 (96%)	486 (84%)	87 (15%)	7 (1%)	10	22
7	G	111/117 (95%)	96 (86%)	13 (12%)	2 (2%)	6	14
All	All	2635/2740 (96%)	2311 (88%)	302 (12%)	22 (1%)	18	31

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	847	ILE
2	B	183	PRO
2	B	57	ARG
2	B	98	LEU
6	F	352	LEU
6	F	416	THR
6	F	442	ARG
6	F	484	VAL
6	F	549	THR
7	G	27	ASN
1	A	907	LEU
6	E	549	THR
6	E	352	LEU
1	A	832	PRO
6	E	415	GLY
2	D	113	GLY
7	G	7	VAL
1	A	42	VAL
6	F	175	PRO
6	F	249	ILE
6	E	175	PRO
6	E	249	ILE

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	817/833 (98%)	725 (89%)	92 (11%)	5	12
2	B	144/167 (86%)	120 (83%)	24 (17%)	2	3
2	D	149/167 (89%)	122 (82%)	27 (18%)	2	2
3	C	67/77 (87%)	58 (87%)	9 (13%)	4	8
6	E	498/523 (95%)	320 (64%)	178 (36%)	0	0
6	F	498/523 (95%)	318 (64%)	180 (36%)	0	0
7	G	94/97 (97%)	79 (84%)	15 (16%)	2	4
All	All	2267/2387 (95%)	1742 (77%)	525 (23%)	2	0

All (525) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	12	CYS
1	A	14	VAL
1	A	20	THR
1	A	24	THR
1	A	39	ASN
1	A	41	LYS
1	A	42	VAL
1	A	62	ASP
1	A	68	SER
1	A	72	VAL
1	A	74	ARG
1	A	75	HIS
1	A	118	ARG
1	A	141	THR
1	A	153	ASP
1	A	180	GLU
1	A	181	ARG
1	A	204	VAL
1	A	210	GLN
1	A	223	ILE
1	A	225	THR
1	A	231	VAL
1	A	235	ASP
1	A	255	SER
1	A	267	LYS
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	288	LYS
1	A	299	VAL
1	A	344	THR
1	A	361	LEU
1	A	364	SER
1	A	372	LEU
1	A	380	MET
1	A	393	THR
1	A	394	THR
1	A	397	SER
1	A	404	ASN
1	A	424	VAL
1	A	434	SER
1	A	435	VAL
1	A	451	SER
1	A	468	GLN
1	A	477	ASP
1	A	482	CYS
1	A	493	VAL
1	A	548	ILE
1	A	551	LYS
1	A	565	THR
1	A	573	GLN
1	A	610	GLU
1	A	618	ASP
1	A	621	LYS
1	A	640	ARG
1	A	644	THR
1	A	648	LEU
1	A	668	MET
1	A	672	SER
1	A	682	SER
1	A	684	ASP
1	A	687	THR
1	A	709	SER
1	A	710	THR
1	A	721	ARG
1	A	726	ARG
1	A	734	ASN
1	A	739	THR
1	A	754	SER
1	A	758	LEU

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Mol	Chain	Res	Type
1	A	759	SER
1	A	772	SER
1	A	779	ILE
1	A	780	LYS
1	A	799	CYS
1	A	817	THR
1	A	818	MET
1	A	819	LEU
1	A	820	VAL
1	A	824	ASP
1	A	829	LEU
1	A	835	SER
1	A	845	ASP
1	A	847	ILE
1	A	848	VAL
1	A	876	GLU
1	A	885	LEU
1	A	894	GLU
1	A	899	MET
1	A	900	LEU
1	A	902	MET
1	A	903	TYR
1	A	924	MET
2	B	9	LEU
2	B	44	VAL
2	B	46	LYS
2	B	48	GLU
2	B	57	ARG
2	B	58	LYS
2	B	67	MET
2	B	68	THR
2	B	76	SER
2	B	77	GLU
2	B	80	ARG
2	B	83	VAL
2	B	85	SER
2	B	88	GLN
2	B	93	THR
2	B	94	MET
2	B	98	LEU
2	B	112	ASP
2	B	120	ILE

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Mol	Chain	Res	Type
2	B	124	THR
2	B	153	LEU
2	B	157	GLN
2	B	163	ASP
2	B	187	THR
3	C	2	LYS
3	C	10	SER
3	C	18	GLN
3	C	27	LYS
3	C	45	THR
3	C	52	MET
3	C	53	VAL
3	C	66	VAL
3	C	70	LYS
2	D	32	GLU
2	D	38	LEU
2	D	43	ASN
2	D	47	SER
2	D	52	ASP
2	D	55	MET
2	D	56	GLN
2	D	67	MET
2	D	68	THR
2	D	69	GLN
2	D	76	SER
2	D	78	ASP
2	D	83	VAL
2	D	85	SER
2	D	87	MET
2	D	124	THR
2	D	127	LYS
2	D	136	ASN
2	D	137	THR
2	D	140	ASN
2	D	141	THR
2	D	159	VAL
2	D	160	VAL
2	D	164	SER
2	D	169	LEU
2	D	174	MET
2	D	180	LEU
6	F	10	SER

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Mol	Chain	Res	Type
6	F	21	ARG
6	F	22	ARG
6	F	27	CYS
6	F	29	CYS
6	F	42	VAL
6	F	43	LEU
6	F	44	SER
6	F	45	VAL
6	F	58	THR
6	F	60	VAL
6	F	61	THR
6	F	65	LEU
6	F	68	MET
6	F	73	LYS
6	F	74	SER
6	F	76	LYS
6	F	80	SER
6	F	84	CYS
6	F	97	CYS
6	F	105	ASP
6	F	109	ILE
6	F	115	THR
6	F	116	ASN
6	F	125	THR
6	F	127	THR
6	F	128	GLU
6	F	129	ARG
6	F	131	LYS
6	F	132	LEU
6	F	136	GLU
6	F	137	THR
6	F	138	LEU
6	F	143	GLU
6	F	144	THR
6	F	145	PHE
6	F	146	LYS
6	F	148	SER
6	F	156	GLU
6	F	158	LEU
6	F	166	SER
6	F	168	GLU
6	F	188	THR

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Mol	Chain	Res	Type
6	F	190	ASN
6	F	191	SER
6	F	194	GLN
6	F	197	GLU
6	F	202	LYS
6	F	215	THR
6	F	217	TYR
6	F	221	VAL
6	F	223	ASP
6	F	226	VAL
6	F	227	LEU
6	F	228	THR
6	F	229	SER
6	F	230	HIS
6	F	235	LEU
6	F	240	LEU
6	F	244	GLU
6	F	247	VAL
6	F	248	ARG
6	F	256	LEU
6	F	258	ILE
6	F	261	GLU
6	F	262	PHE
6	F	263	SER
6	F	264	SER
6	F	266	VAL
6	F	268	ASN
6	F	272	VAL
6	F	274	MET
6	F	280	LEU
6	F	281	GLN
6	F	288	LYS
6	F	289	SER
6	F	297	LEU
6	F	301	SER
6	F	303	ARG
6	F	304	ILE
6	F	307	THR
6	F	309	CYS
6	F	310	SER
6	F	311	HIS
6	F	314	VAL

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Mol	Chain	Res	Type
6	F	319	GLU
6	F	322	LEU
6	F	328	ASP
6	F	329	LYS
6	F	331	SER
6	F	341	GLU
6	F	345	LYS
6	F	347	LYS
6	F	352	LEU
6	F	354	GLN
6	F	356	VAL
6	F	363	LEU
6	F	367	THR
6	F	372	VAL
6	F	374	ASP
6	F	376	ILE
6	F	378	MET
6	F	380	THR
6	F	384	LEU
6	F	386	VAL
6	F	387	VAL
6	F	388	ASN
6	F	394	LYS
6	F	404	GLN
6	F	405	LEU
6	F	411	LEU
6	F	413	THR
6	F	414	LYS
6	F	416	THR
6	F	417	LEU
6	F	420	GLU
6	F	424	SER
6	F	425	VAL
6	F	427	ARG
6	F	428	LEU
6	F	430	LYS
6	F	431	THR
6	F	436	MET
6	F	437	PHE
6	F	440	THR
6	F	442	ARG
6	F	444	CYS

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Mol	Chain	Res	Type
6	F	448	ILE
6	F	450	ASP
6	F	452	VAL
6	F	455	LEU
6	F	456	VAL
6	F	458	ASP
6	F	459	ASN
6	F	460	LYS
6	F	462	LYS
6	F	465	LYS
6	F	466	ASP
6	F	468	SER
6	F	473	LYS
6	F	477	LYS
6	F	480	ILE
6	F	481	THR
6	F	482	HIS
6	F	485	SER
6	F	486	SER
6	F	488	ILE
6	F	490	ARG
6	F	492	GLN
6	F	493	ILE
6	F	497	ARG
6	F	503	ASN
6	F	507	ARG
6	F	513	SER
6	F	528	LEU
6	F	530	THR
6	F	534	ASP
6	F	535	SER
6	F	536	SER
6	F	540	GLU
6	F	542	ASP
6	F	544	VAL
6	F	547	THR
6	F	548	GLN
6	F	549	THR
6	F	551	GLU
6	F	554	HIS
6	F	561	PHE
6	F	565	ILE

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Mol	Chain	Res	Type
6	F	569	LYS
6	F	572	ILE
6	F	573	LEU
6	F	575	ILE
6	F	581	LEU
6	F	582	TYR
6	F	583	ASP
6	F	584	LYS
6	F	585	LEU
6	F	590	LEU
6	F	592	ILE
6	E	10	SER
6	E	21	ARG
6	E	22	ARG
6	E	27	CYS
6	E	29	CYS
6	E	42	VAL
6	E	43	LEU
6	E	44	SER
6	E	45	VAL
6	E	58	THR
6	E	60	VAL
6	E	61	THR
6	E	65	LEU
6	E	68	MET
6	E	73	LYS
6	E	74	SER
6	E	76	LYS
6	E	80	SER
6	E	84	CYS
6	E	97	CYS
6	E	105	ASP
6	E	109	ILE
6	E	115	THR
6	E	116	ASN
6	E	125	THR
6	E	127	THR
6	E	128	GLU
6	E	129	ARG
6	E	131	LYS
6	E	132	LEU
6	E	136	GLU

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Mol	Chain	Res	Type
6	E	137	THR
6	E	138	LEU
6	E	143	GLU
6	E	144	THR
6	E	145	PHE
6	E	146	LYS
6	E	148	SER
6	E	156	GLU
6	E	158	LEU
6	E	166	SER
6	E	168	GLU
6	E	188	THR
6	E	190	ASN
6	E	191	SER
6	E	194	GLN
6	E	197	GLU
6	E	202	LYS
6	E	215	THR
6	E	217	TYR
6	E	221	VAL
6	E	223	ASP
6	E	226	VAL
6	E	227	LEU
6	E	228	THR
6	E	229	SER
6	E	230	HIS
6	E	235	LEU
6	E	240	LEU
6	E	244	GLU
6	E	247	VAL
6	E	248	ARG
6	E	256	LEU
6	E	258	ILE
6	E	261	GLU
6	E	262	PHE
6	E	263	SER
6	E	264	SER
6	E	266	VAL
6	E	268	ASN
6	E	272	VAL
6	E	274	MET
6	E	280	LEU

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Mol	Chain	Res	Type
6	E	281	GLN
6	E	288	LYS
6	E	289	SER
6	E	297	LEU
6	E	301	SER
6	E	303	ARG
6	E	304	ILE
6	E	307	THR
6	E	309	CYS
6	E	310	SER
6	E	311	HIS
6	E	314	VAL
6	E	319	GLU
6	E	322	LEU
6	E	328	ASP
6	E	329	LYS
6	E	331	SER
6	E	341	GLU
6	E	345	LYS
6	E	347	LYS
6	E	352	LEU
6	E	354	GLN
6	E	356	VAL
6	E	363	LEU
6	E	367	THR
6	E	372	VAL
6	E	374	ASP
6	E	376	ILE
6	E	378	MET
6	E	380	THR
6	E	384	LEU
6	E	386	VAL
6	E	387	VAL
6	E	388	ASN
6	E	394	LYS
6	E	404	GLN
6	E	405	LEU
6	E	411	LEU
6	E	413	THR
6	E	414	LYS
6	E	416	THR
6	E	417	LEU

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Mol	Chain	Res	Type
6	E	420	GLU
6	E	424	SER
6	E	425	VAL
6	E	427	ARG
6	E	428	LEU
6	E	430	LYS
6	E	431	THR
6	E	436	MET
6	E	437	PHE
6	E	440	THR
6	E	444	CYS
6	E	448	ILE
6	E	450	ASP
6	E	452	VAL
6	E	455	LEU
6	E	456	VAL
6	E	458	ASP
6	E	459	ASN
6	E	460	LYS
6	E	462	LYS
6	E	465	LYS
6	E	466	ASP
6	E	468	SER
6	E	473	LYS
6	E	477	LYS
6	E	480	ILE
6	E	481	THR
6	E	482	HIS
6	E	486	SER
6	E	488	ILE
6	E	490	ARG
6	E	492	GLN
6	E	493	ILE
6	E	497	ARG
6	E	503	ASN
6	E	507	ARG
6	E	513	SER
6	E	528	LEU
6	E	530	THR
6	E	534	ASP
6	E	535	SER
6	E	536	SER

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Mol	Chain	Res	Type
6	E	540	GLU
6	E	542	ASP
6	E	544	VAL
6	E	547	THR
6	E	548	GLN
6	E	549	THR
6	E	551	GLU
6	E	554	HIS
6	E	561	PHE
6	E	565	ILE
6	E	569	LYS
6	E	572	ILE
6	E	573	LEU
6	E	575	ILE
6	E	581	LEU
6	E	582	TYR
6	E	583	ASP
6	E	584	LYS
6	E	585	LEU
6	E	590	LEU
6	E	592	ILE
7	G	1	ASN
7	G	13	SER
7	G	26	ASP
7	G	33	ASN
7	G	46	SER
7	G	52	LYS
7	G	69	LEU
7	G	74	ARG
7	G	77	THR
7	G	78	ASP
7	G	79	THR
7	G	81	LYS
7	G	87	TYR
7	G	97	LEU
7	G	112	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	75	HIS

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Mol	Chain	Res	Type
1	A	113	HIS
1	A	357	GLN
1	A	362	HIS
1	A	492	GLN
1	A	534	ASN
1	A	713	ASN
1	A	725	HIS
1	A	734	ASN
1	A	789	GLN
1	A	790	ASN
1	A	822	GLN
1	A	928	HIS
3	C	34	GLN
2	D	168	GLN
6	F	107	ASN
6	F	179	ASN
6	F	194	GLN
6	F	245	HIS
6	F	265	ASN
6	F	464	HIS
6	F	482	HIS
6	F	516	ASN
6	F	548	GLN
6	F	554	HIS
6	F	562	ASN
6	E	107	ASN
6	E	194	GLN
6	E	245	HIS
6	E	265	ASN
6	E	464	HIS
6	E	482	HIS
6	E	516	ASN
6	E	548	GLN
6	E	562	ASN
7	G	11	GLN
7	G	98	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/33 (72%)	2 (8%)	1 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	J	26/59 (44%)	2 (7%)	1 (3%)
All	All	50/92 (54%)	4 (8%)	2 (4%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	15	G
4	I	23	C
5	J	25	G
5	J	26	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	22	G
5	J	25	G

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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
9	GDP	A	1003	10	29,30,30	1.19	3 (10%)	45,47,47	1.77	8 (17%)

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
9	GDP	A	1003	10	-	1/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GDP	C5-C4	3.01	1.47	1.38
9	A	1003	GDP	C6-N1	-2.72	1.33	1.38
9	A	1003	GDP	C5-N7	-2.37	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	GDP	C5-C4-N3	-6.21	118.51	128.39
9	A	1003	GDP	C2-N3-C4	4.93	120.80	112.30
9	A	1003	GDP	N9-C4-N3	4.64	135.22	125.95
9	A	1003	GDP	C6-C5-N7	2.89	135.54	130.29
9	A	1003	GDP	C4-C5-N7	-2.42	106.84	110.67
9	A	1003	GDP	C3'-C2'-C1'	2.32	105.84	101.46
9	A	1003	GDP	O6-C6-C5	-2.12	120.94	126.53
9	A	1003	GDP	C2'-C1'-N9	-2.08	107.47	113.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1003	GDP	O4'-C4'-C5'-O5'

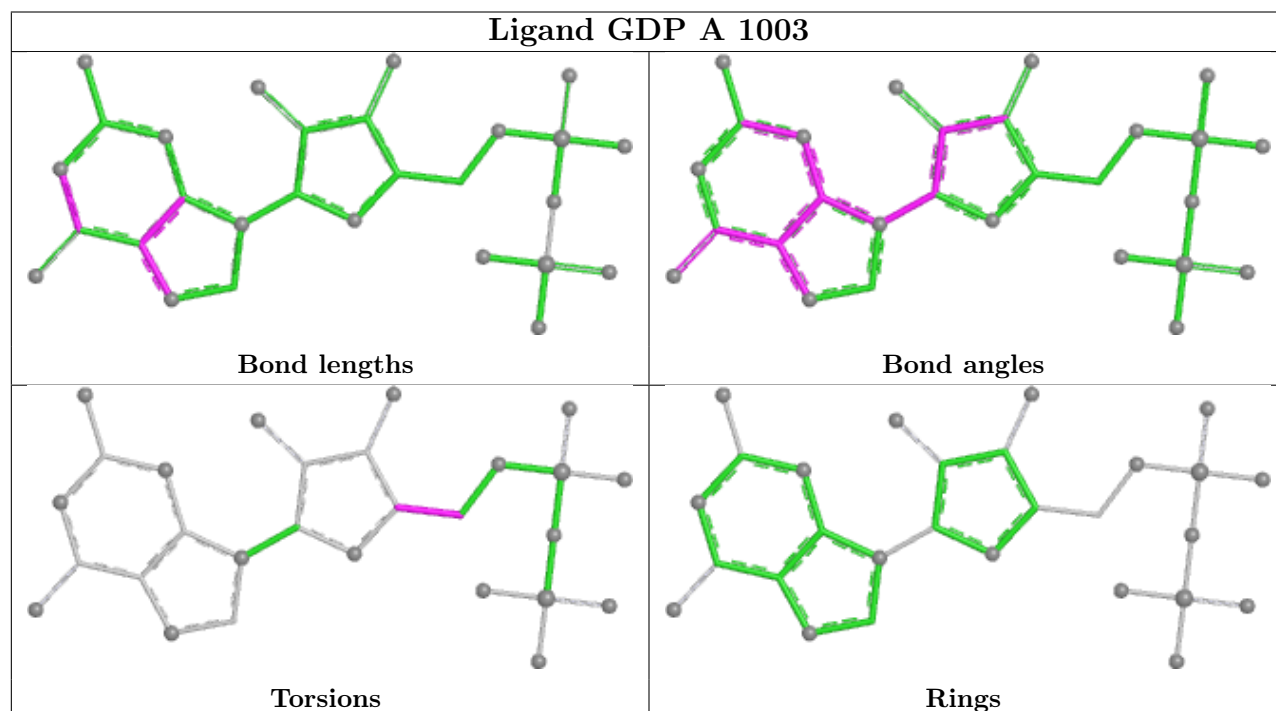
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1003	GDP	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

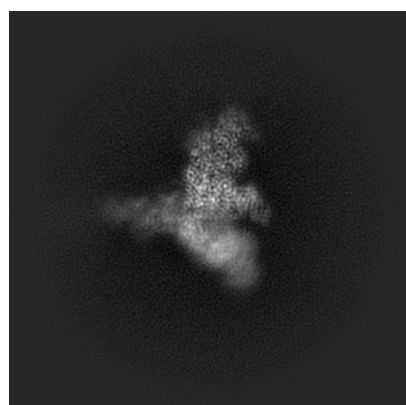
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30504. These allow visual inspection of the internal detail of the map and identification of artifacts.

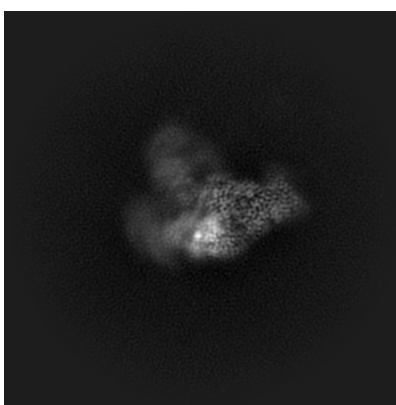
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

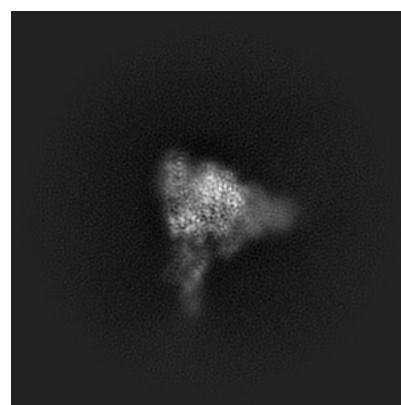
6.1.1 Primary map



X



Y

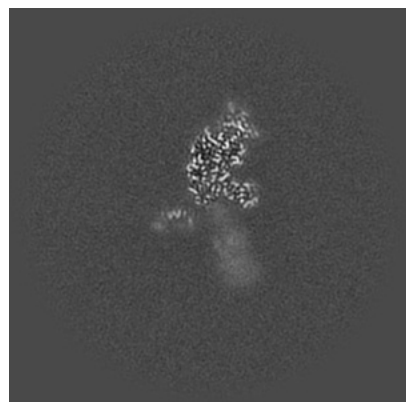


Z

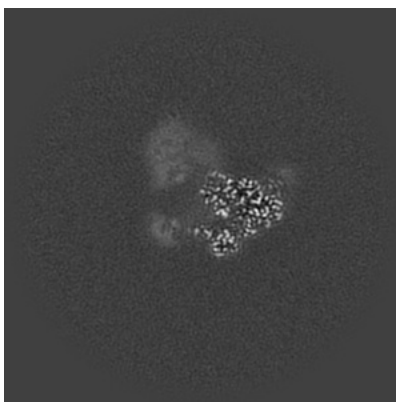
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

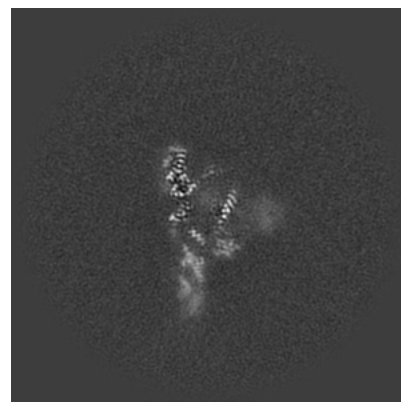
6.2.1 Primary map



X Index: 224



Y Index: 224

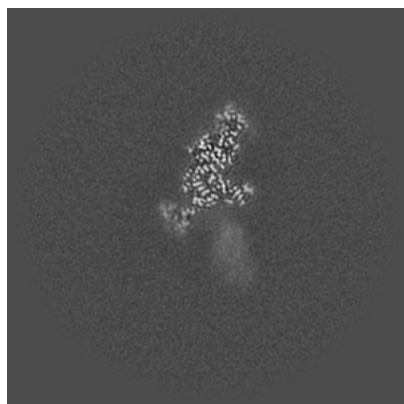


Z Index: 224

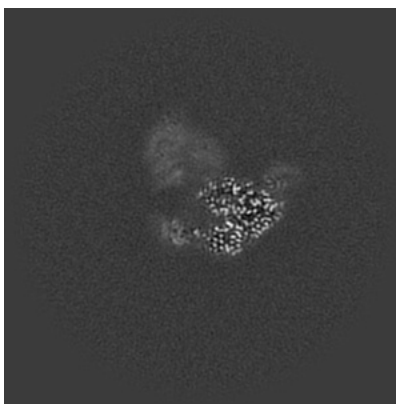
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

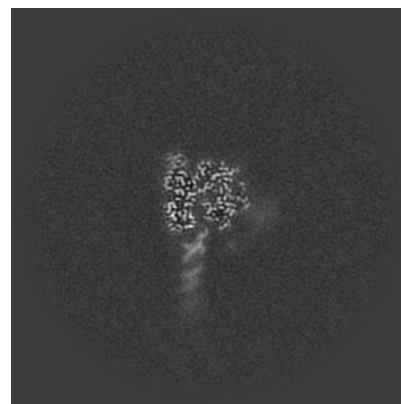
6.3.1 Primary map



X Index: 232



Y Index: 218

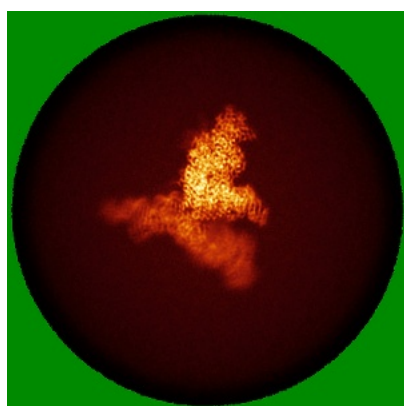


Z Index: 236

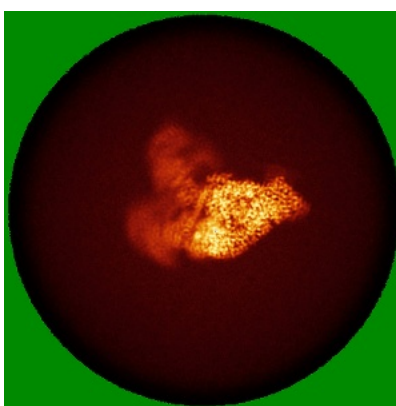
The images above show the largest variance slices of the map in three orthogonal directions.

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

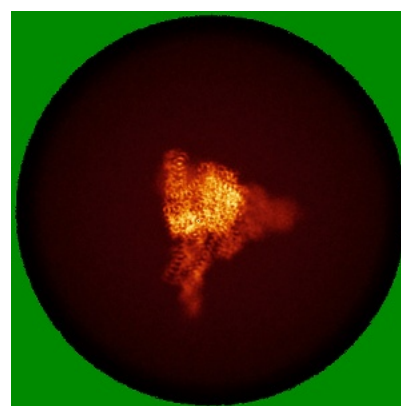
6.4.1 Primary map



X



Y

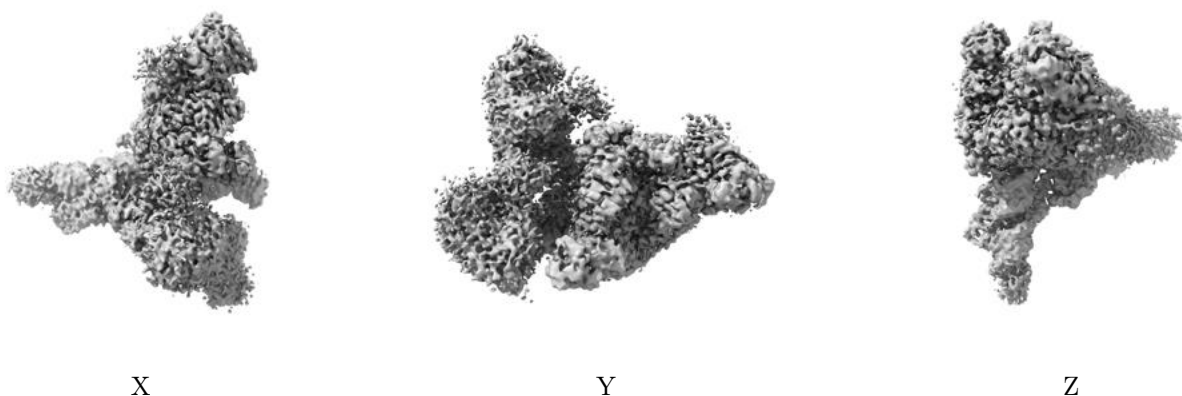


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

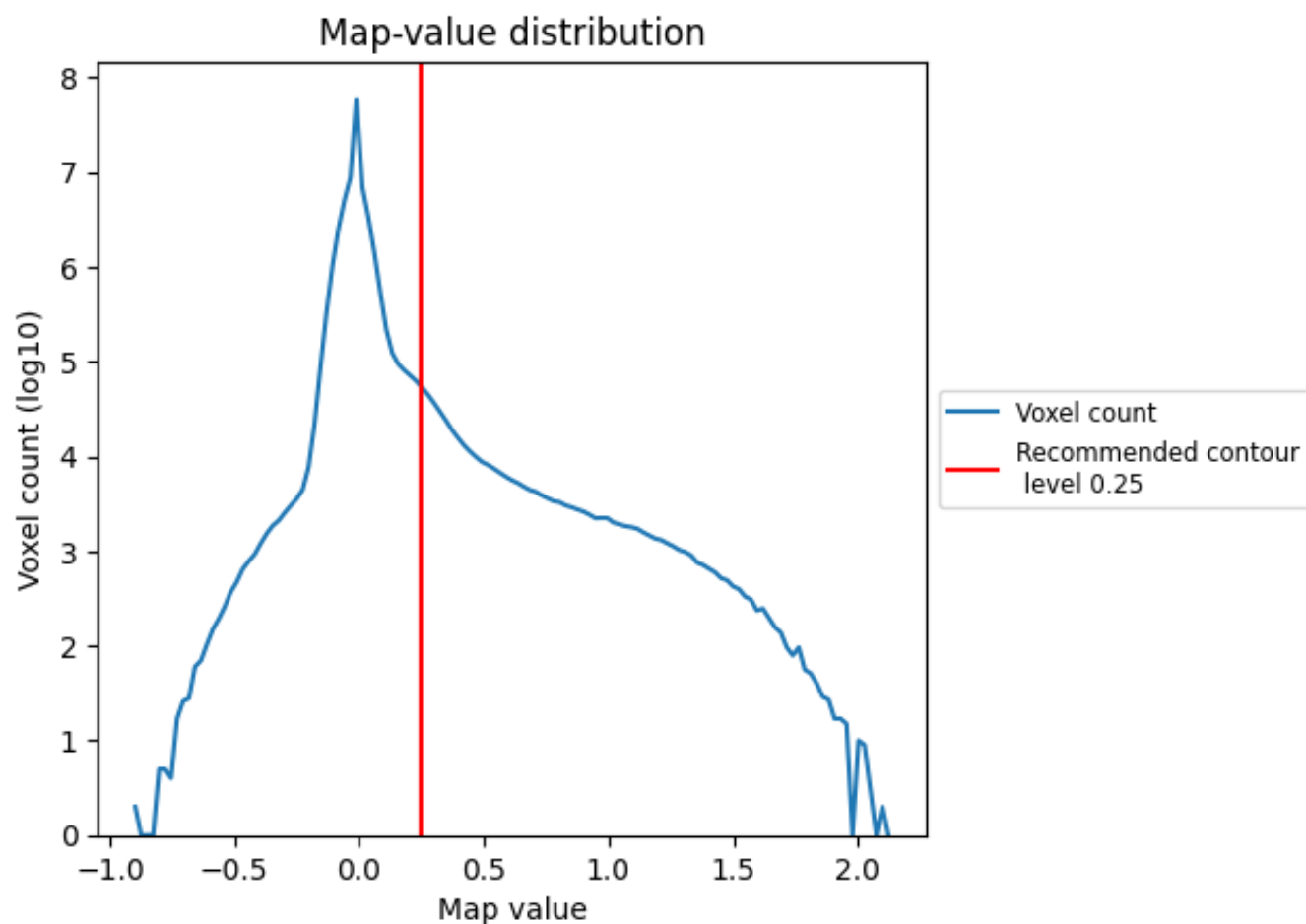
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

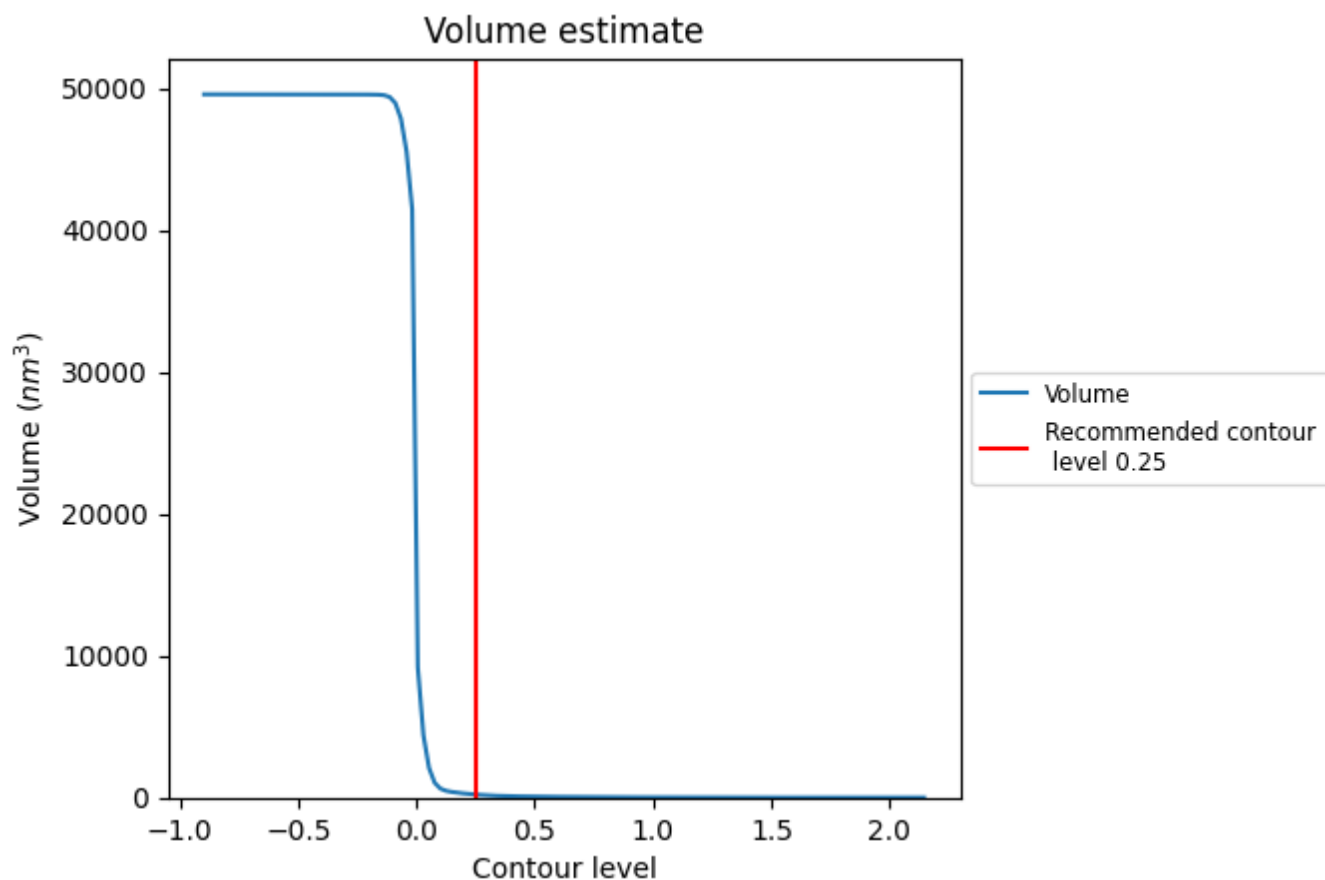
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

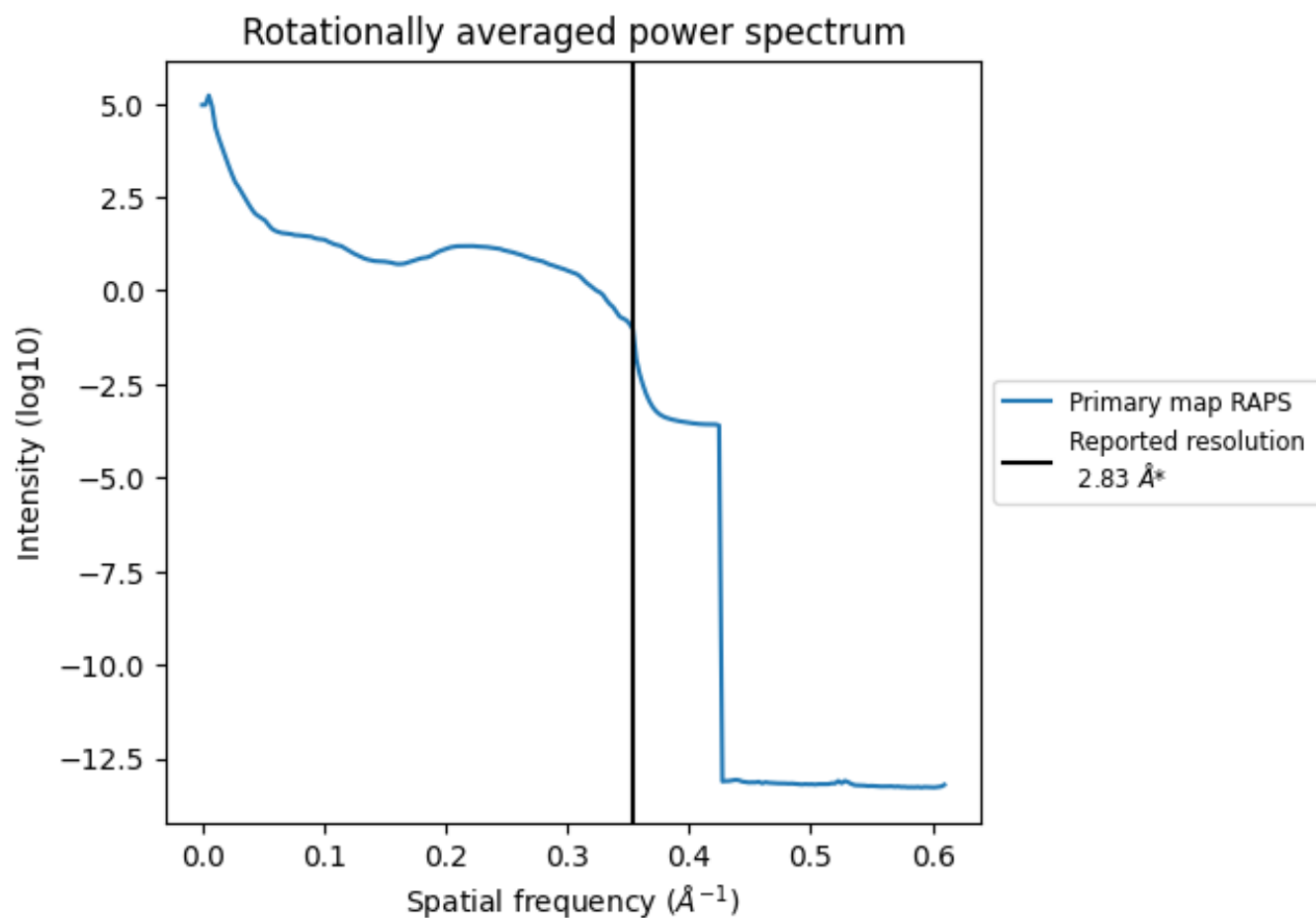
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm^3 ; this corresponds to an approximate mass of 192 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

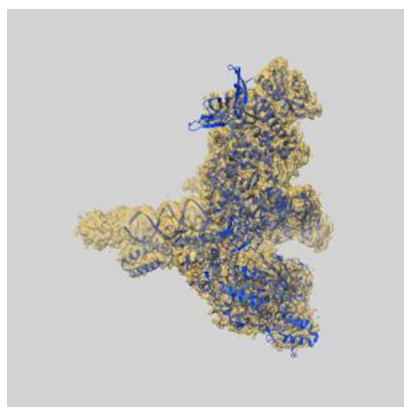
8 Fourier-Shell correlation ⓘ

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

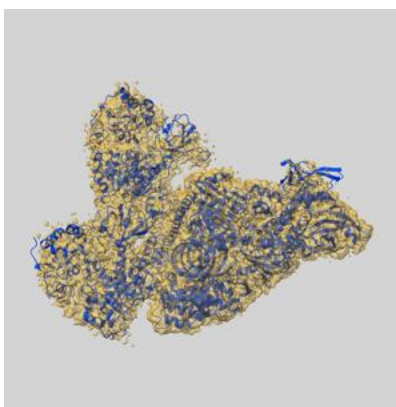
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30504 and PDB model 7CYQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

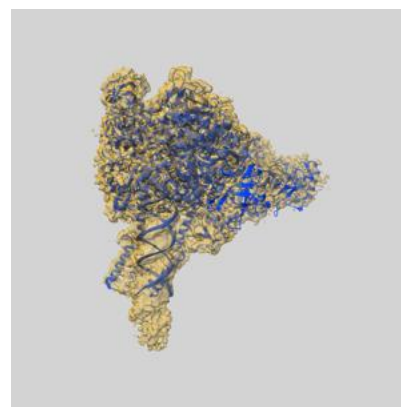
9.1 Map-model overlay [i](#)



X



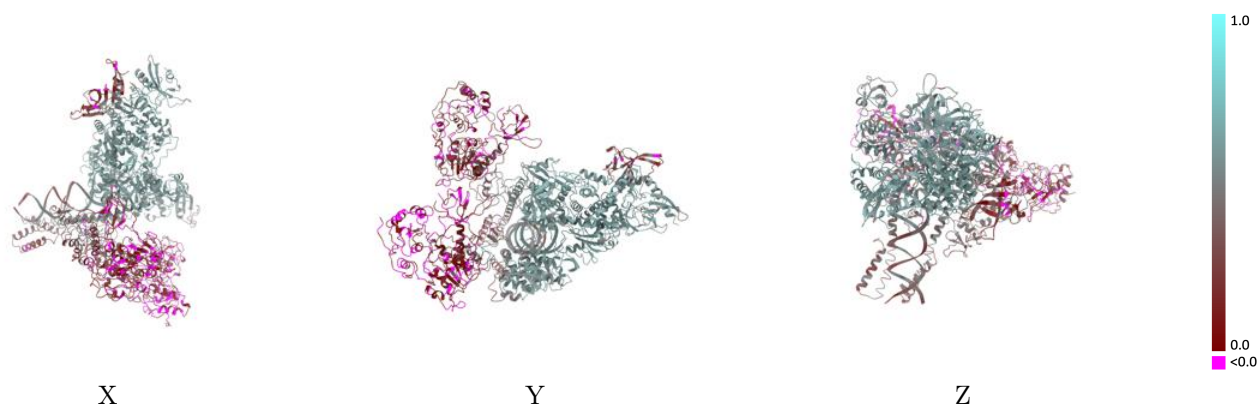
Y



Z

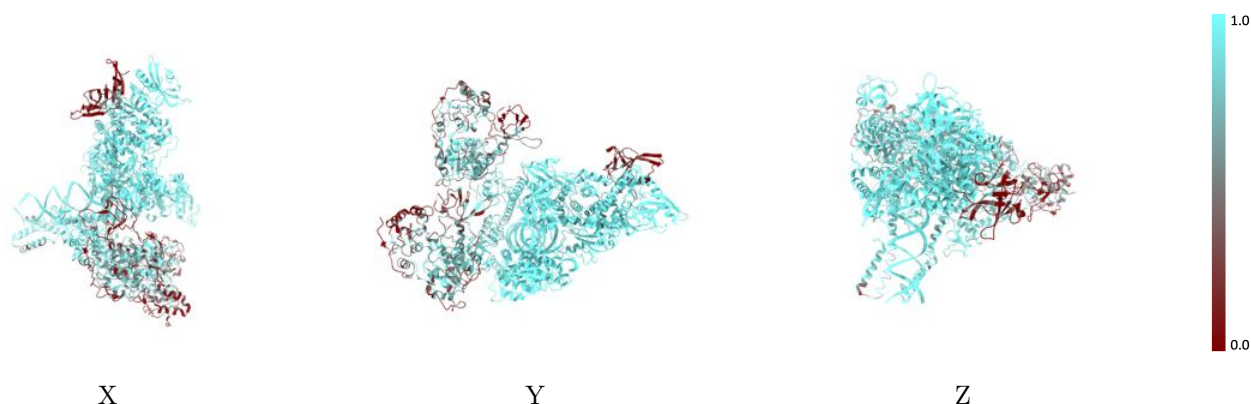
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



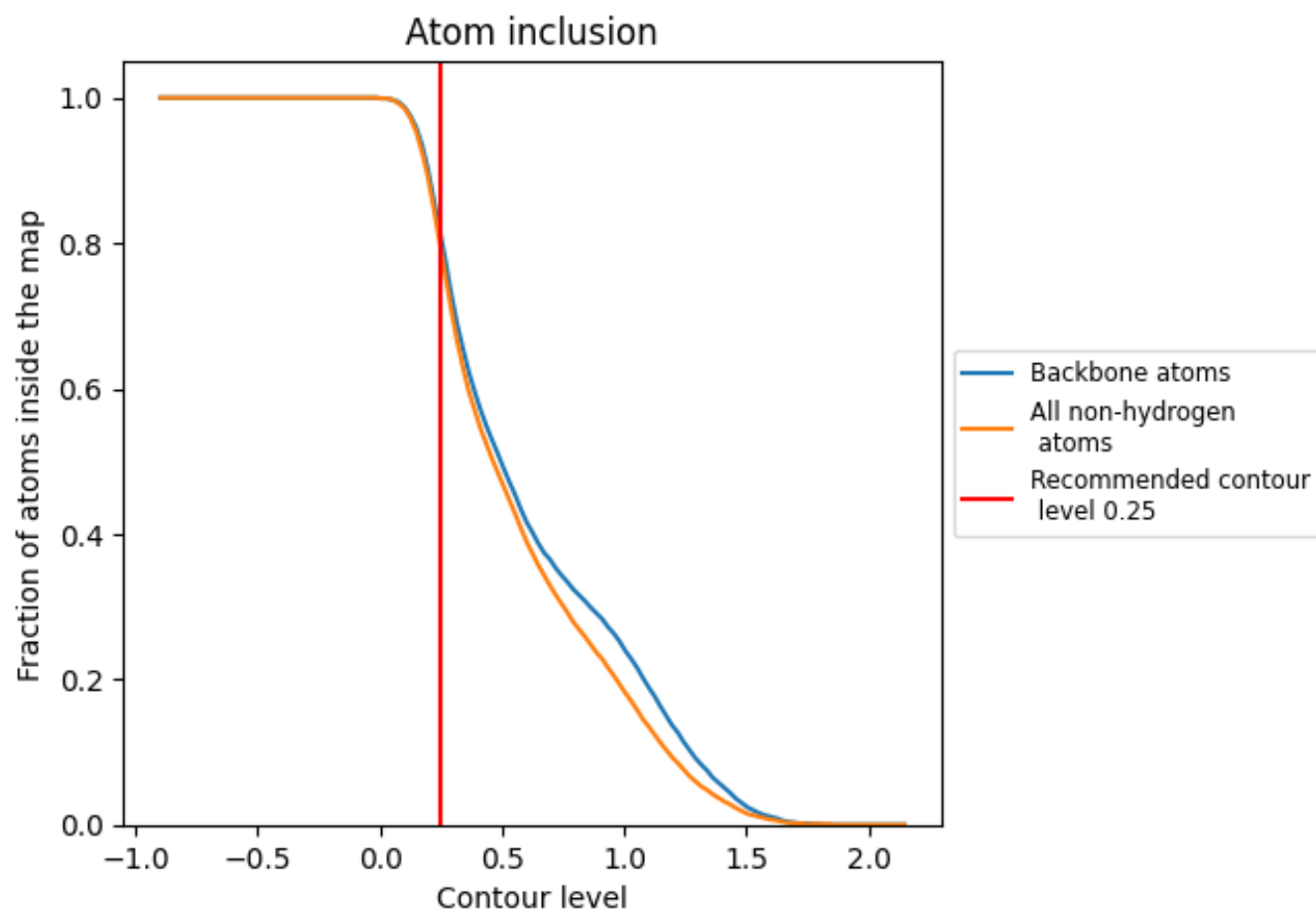
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.3840
A	0.9860	0.5900
B	0.9390	0.5000
C	0.9780	0.5660
D	0.9420	0.4740
E	0.6220	0.2140
F	0.5620	0.1140
G	0.2540	0.3280
I	0.9980	0.4550
J	0.9820	0.4770

1.0

0.0

<0.0