



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:06 PM UTC

PDB ID : 7BQX / pdb_00007bqx
EMDB ID : EMD-30157
Title : Epstein-Barr virus, C5 portal vertex
Authors : Li, Z.; Yu, X.
Deposited on : 2020-03-25
Resolution : 4.20 Å(reported)

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

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

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:

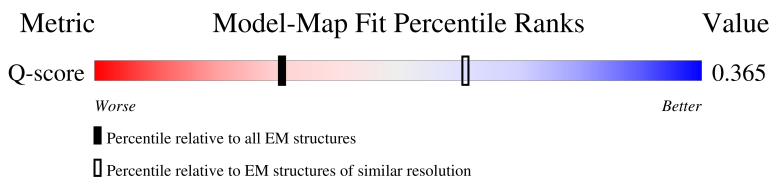
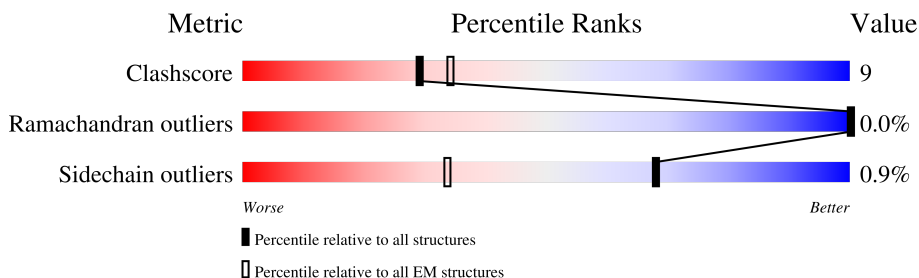
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	5	364	30% 59% 19% 22%
1	e	364	6% 74% 13% 12%
2	6	301	35% 76% 23% .
2	7	301	33% 72% 23% 5%

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Mol	Chain	Length	Quality of chain
2	f	301	
2	g	301	
3	G	570	
3	K	570	
4	C	507	
5	B	3149	
5	O	3149	
6	2	176	
6	Y	176	
6	Z	176	
6	y	176	
7	S	1381	
7	T	1381	
7	W	1381	
7	x	1381	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 61847 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 Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	284	Total	C	N	O	S	0	0
			2199	1421	374	397	7		
1	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		

- Molecule 2 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	297	Total	C	N	O	S	0	0
			2329	1496	385	430	18		
2	7	287	Total	C	N	O	S	0	0
			2262	1452	375	417	18		
2	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
2	g	290	Total	C	N	O	S	0	0
			2272	1464	376	414	18		

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	68	Total	C	N	O	S	0	0
			563	343	113	104	3		
3	G	84	Total	C	N	O	S	0	0
			675	412	135	125	3		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	346	Total	C	N	O	S	0	0
			2705	1733	482	478	12		

- Molecule 5 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	35	Total	C	N	O	0	0
			301	192	61	48		
5	O	29	Total	C	N	O	0	0
			252	163	49	40		

- Molecule 6 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 7 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	1292	Total	C	N	O	S	0	0
			10166	6462	1758	1889	57		
7	T	1305	Total	C	N	O	S	0	0
			10258	6515	1780	1904	59		
7	W	1330	Total	C	N	O	S	0	0
			10456	6648	1808	1941	59		
7	x	1290	Total	C	N	O	S	0	0
			10141	6438	1760	1884	59		

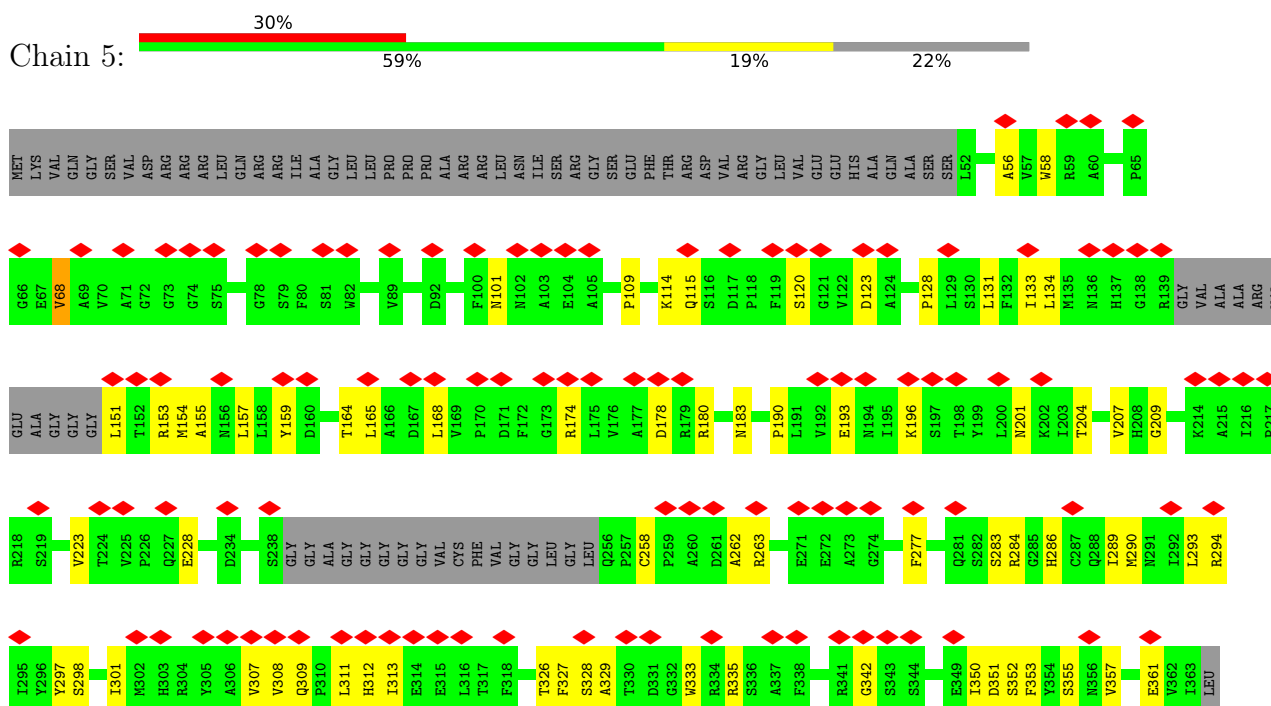
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	89	ILE	THR	conflict	UNP P03226
T	89	ILE	THR	conflict	UNP P03226
W	89	ILE	THR	conflict	UNP P03226
x	89	ILE	THR	conflict	UNP P03226

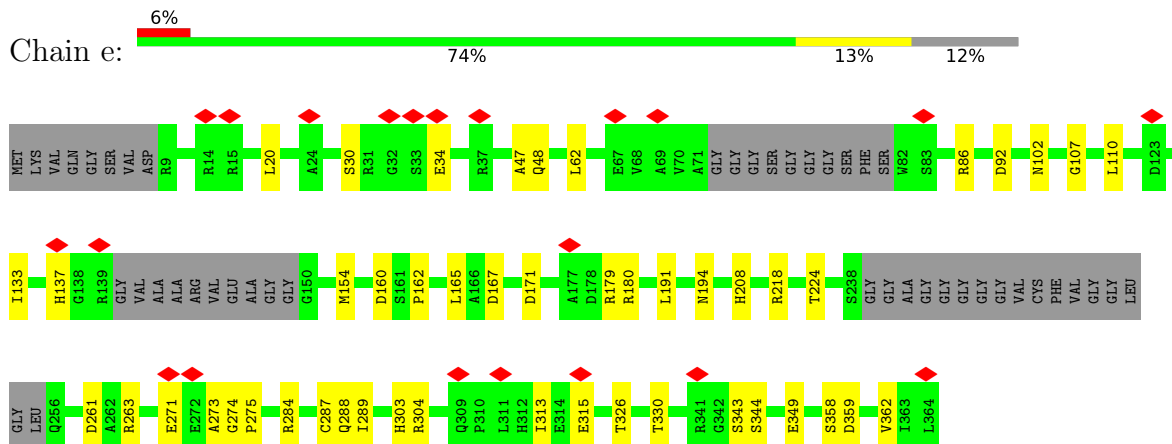
3 Residue-property plots

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.

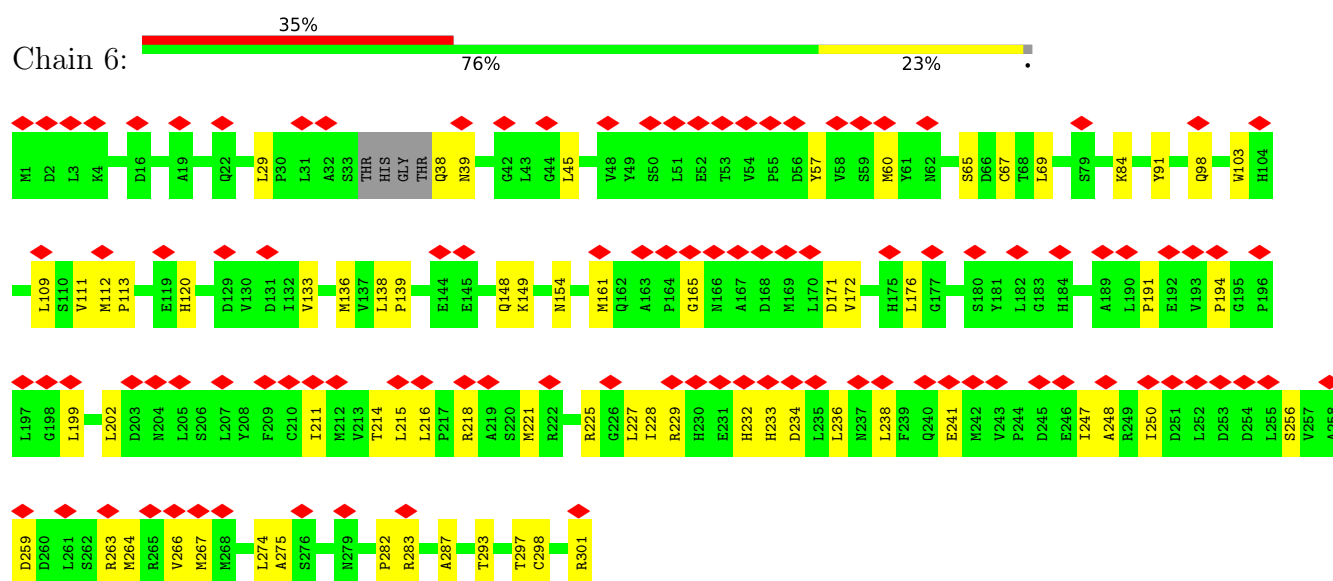
- Molecule 1: Triplex capsid protein 1



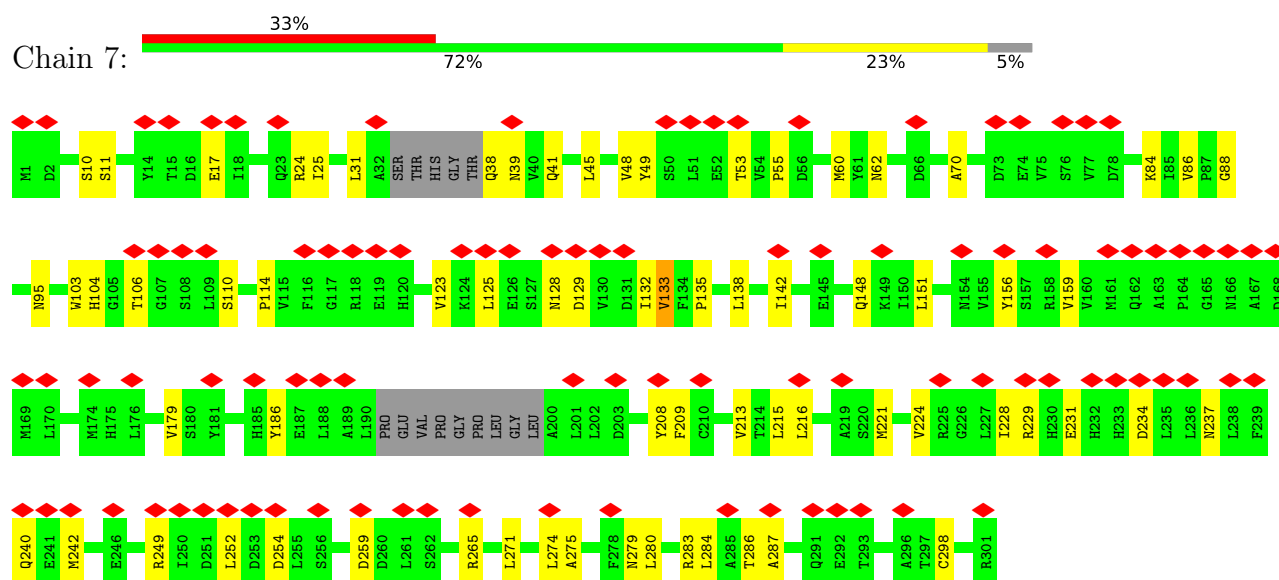
- Molecule 1: Triplex capsid protein 1



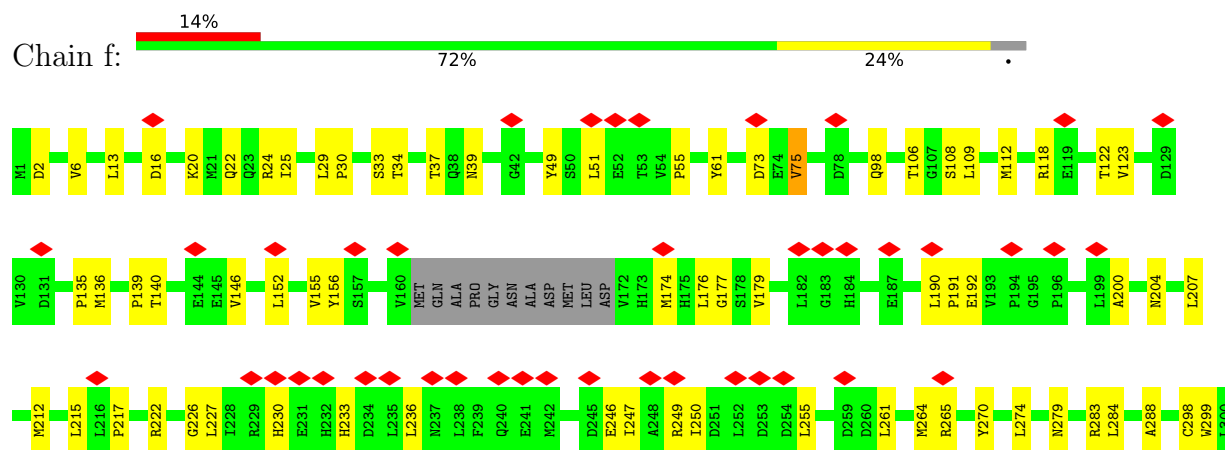
- Molecule 2: Triplex capsid protein 2



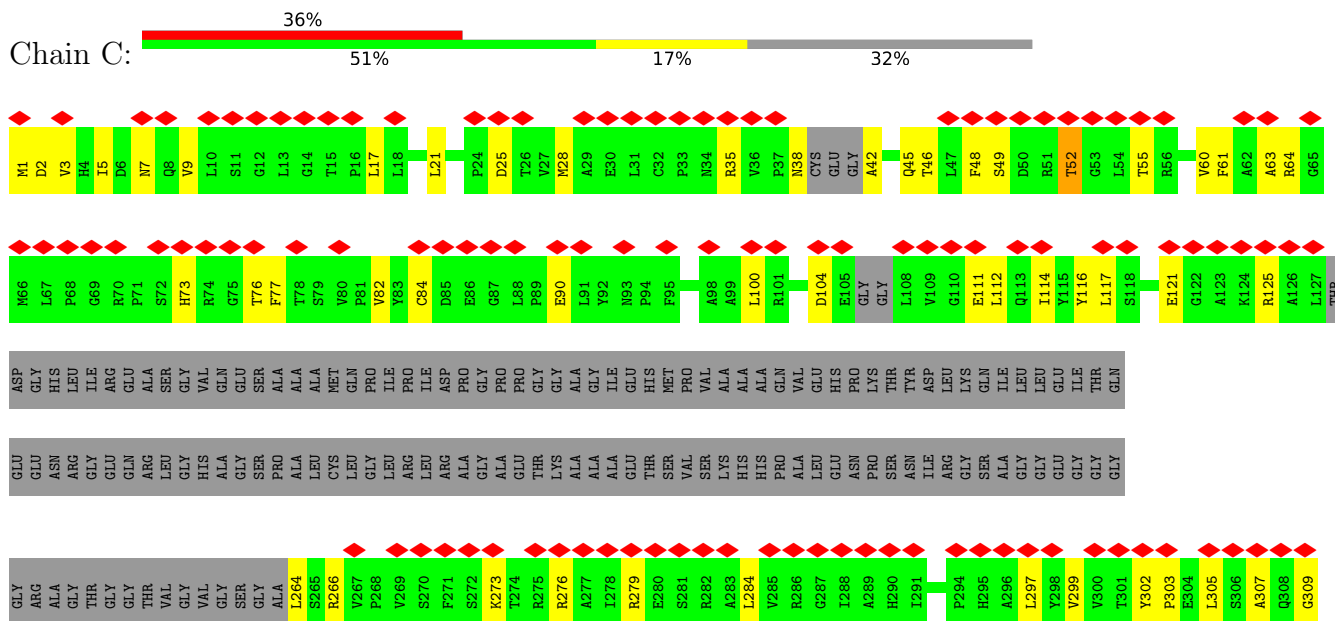
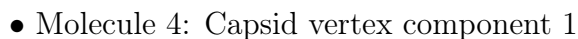
• Molecule 2: Triplex capsid protein 2

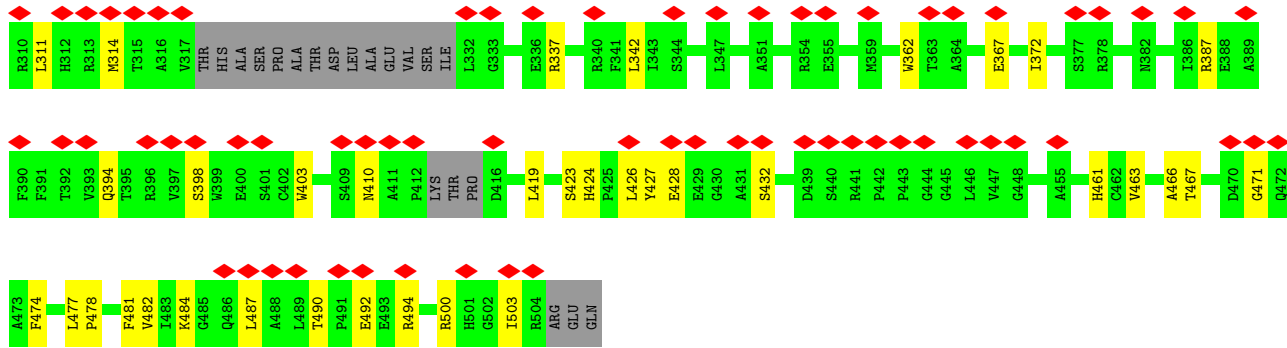


• Molecule 2: Triplex capsid protein 2

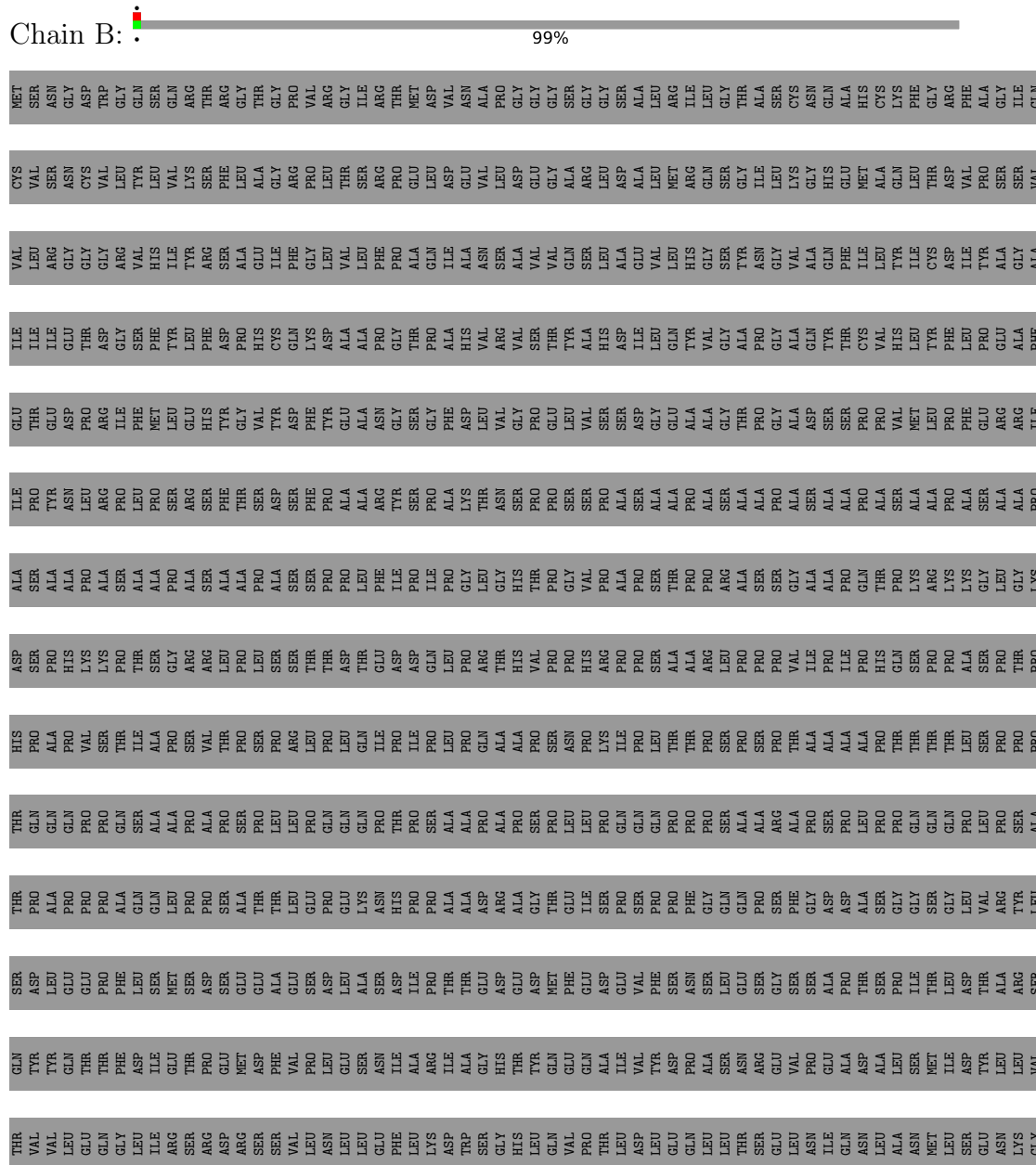


Chain G: 8% 12% . 85%





- Molecule 5: Large tegument protein deneddylase





R3121	PRO	SER	LEU	ALA	ASN	LEU
F3122	VAL	TYR	ALA	ALA	ALA	TYR
V3123	PRO	ILE	ASP	PRO	ASP	ILE
S3124	THR	SER	THR	THR	SER	VAL
Q3125	GLN	ASP	ARG	ARG	ASP	THR
L3126	PHE	LEU	VAL	GLU	HIS	THR
R3127	LEU	ILE	THR	ASP	ASP	ASP
R3128	GLU	ILE	THR	THR	THR	THR
K3129	ASP	LEU	PRO	LEU	PRO	GLU
L3130	ILE	ILE	VAL	ASP	VAL	THR
E3131	ILE	ARG	GLU	GLN	VAL	VAL
R3132	GLU	VAL	GLY	ASN	SER	MET
S3133	VAL	VAL	VAL	GLY	GLY	THR
R3136	THR	THR	THR	ALA	GLY	LEU
L3137	GLY	GLY	GLY	LEU	LEU	LEU
I3138	SER	GLN	GLN	ASN	LEU	ASN
A3139	THR	TYR	GLN	ARG	GLY	PRO
D3140	SER	PRO	SER	GLY	GLY	GLY
L3141	GLY	PRO	PRO	THR	THR	ALA
E3142	ASP	SER	ALA	ASN	THR	PHE
R3143	LEU	GLY	ILE	LEU	LEU	LEU
L3144	VAL	VAL	ALA	ALA	ALA	ALA
K3145	PRO	ARG	ALA	GLY	GLY	PRO
F3146	SER	TYR	ALA	ALA	GLY	GLY
L3147	PRO	ALA	THR	PRO	ARG	ARG
V3148	PRO	PHE	THR	GLY	PRO	PRO
L3149	SER	SER	GLN	GLN	GLN	GLY
A3115	PRO	GLY	GLY	GLY	GLY	GLY
S3116	VAL	VAL	VAL	VAL	VAL	VAL
R3117	THR	THR	THR	THR	THR	THR
V3118	THR	THR	THR	THR	THR	THR
L3119	THR	THR	THR	THR	THR	THR
S3120	THR	THR	THR	THR	THR	THR

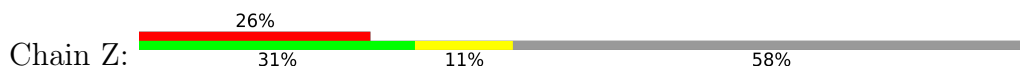
● Molecule 5: Large tegument protein deneddylase

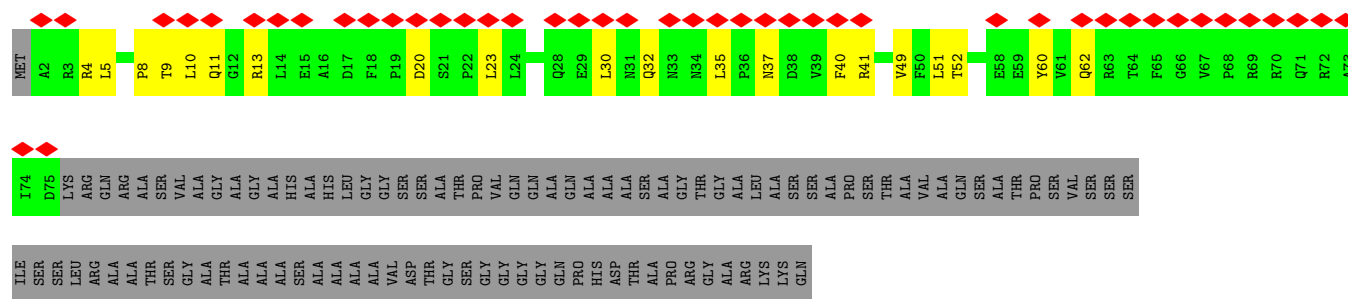
[illegible]

WORLDWIDE
PDB
PROTEIN DATA BANK

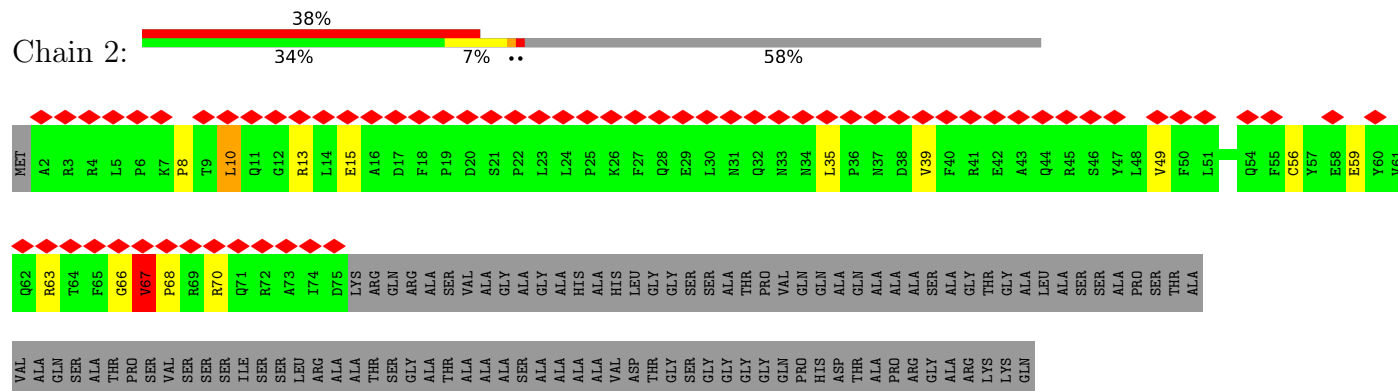
R3121	F3122	V3123	S3124	Q3125	L3126	R3127	R3128	S3129	L3130	E3131	R3132	S3133	T3134	R3135	L3136	L3137	I3138	S3139	D3140	L3141	E3142	R3143	L3144	K3145	F3146	L3147	L3148	L3149
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Chain Y:

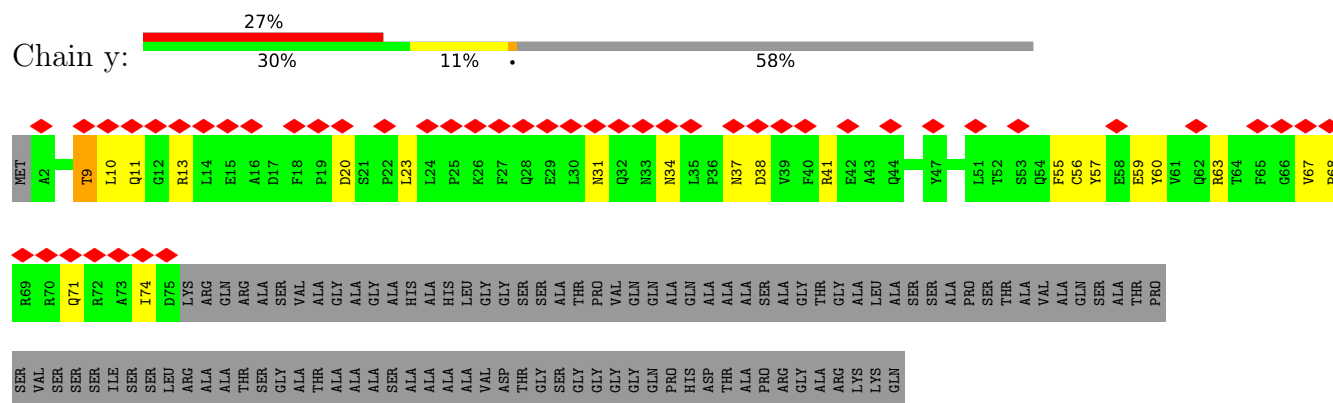




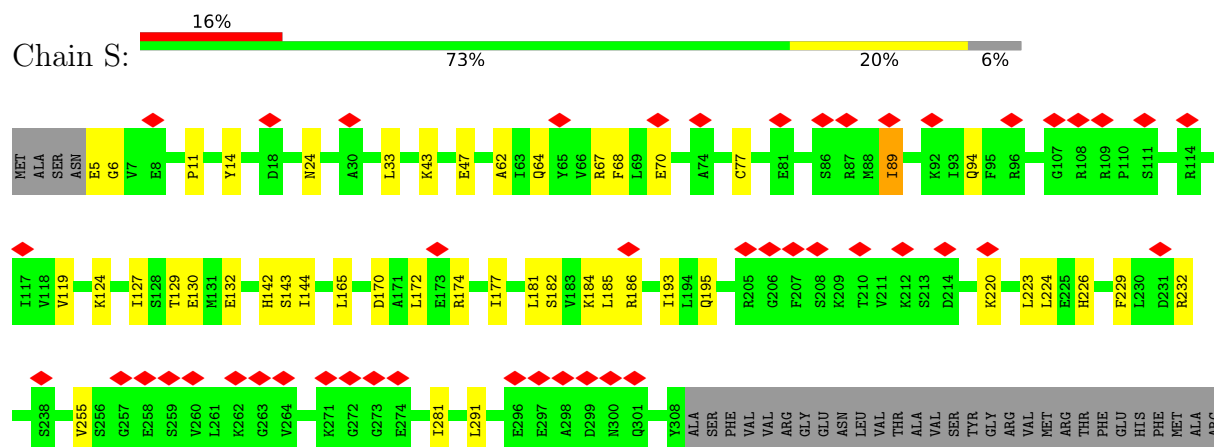
• Molecule 6: Small capsomere-interacting protein

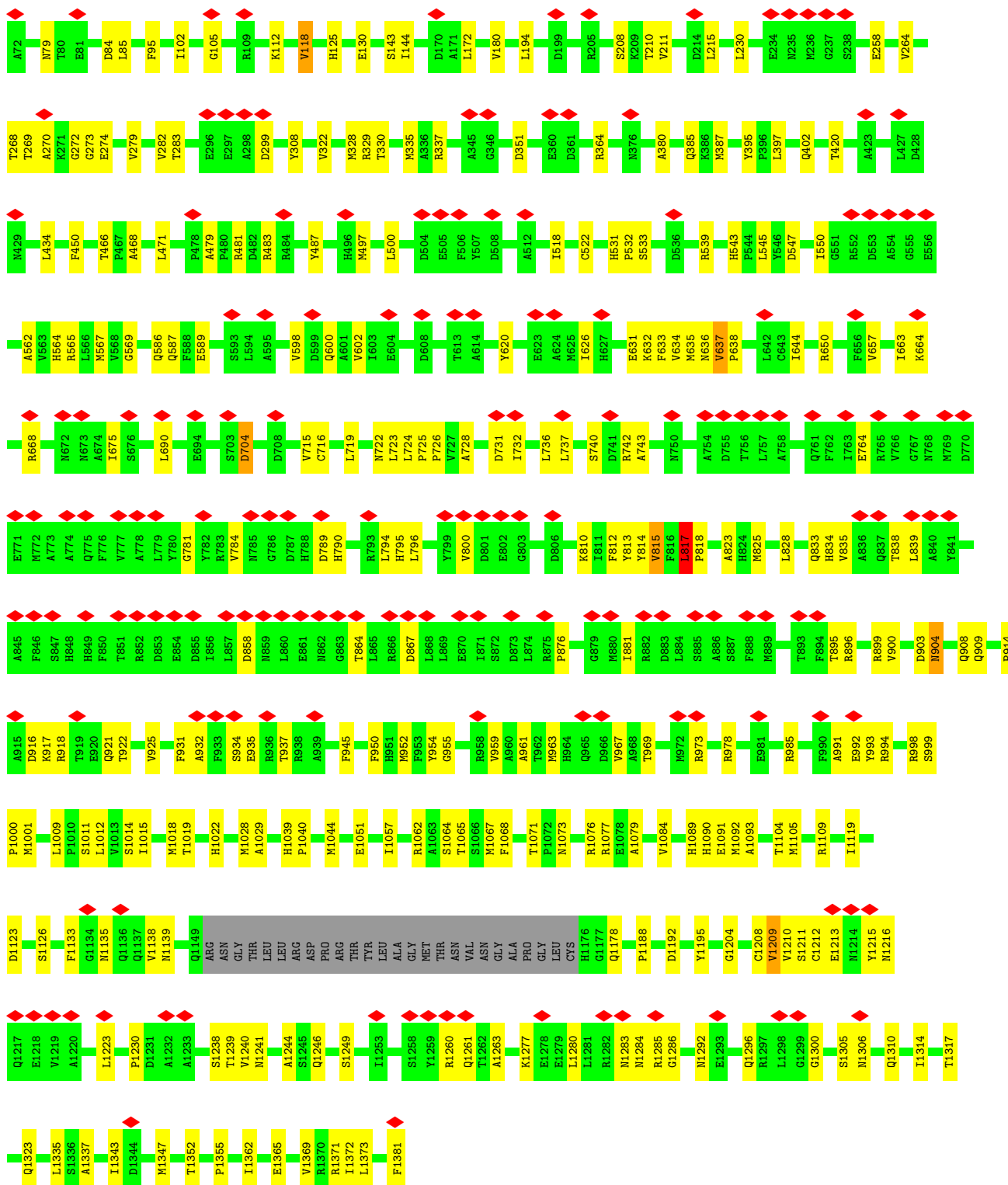


• Molecule 6: Small capsomere-interacting protein

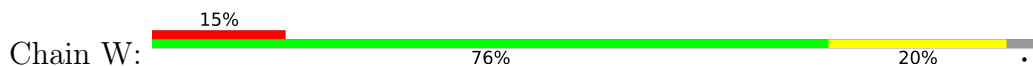


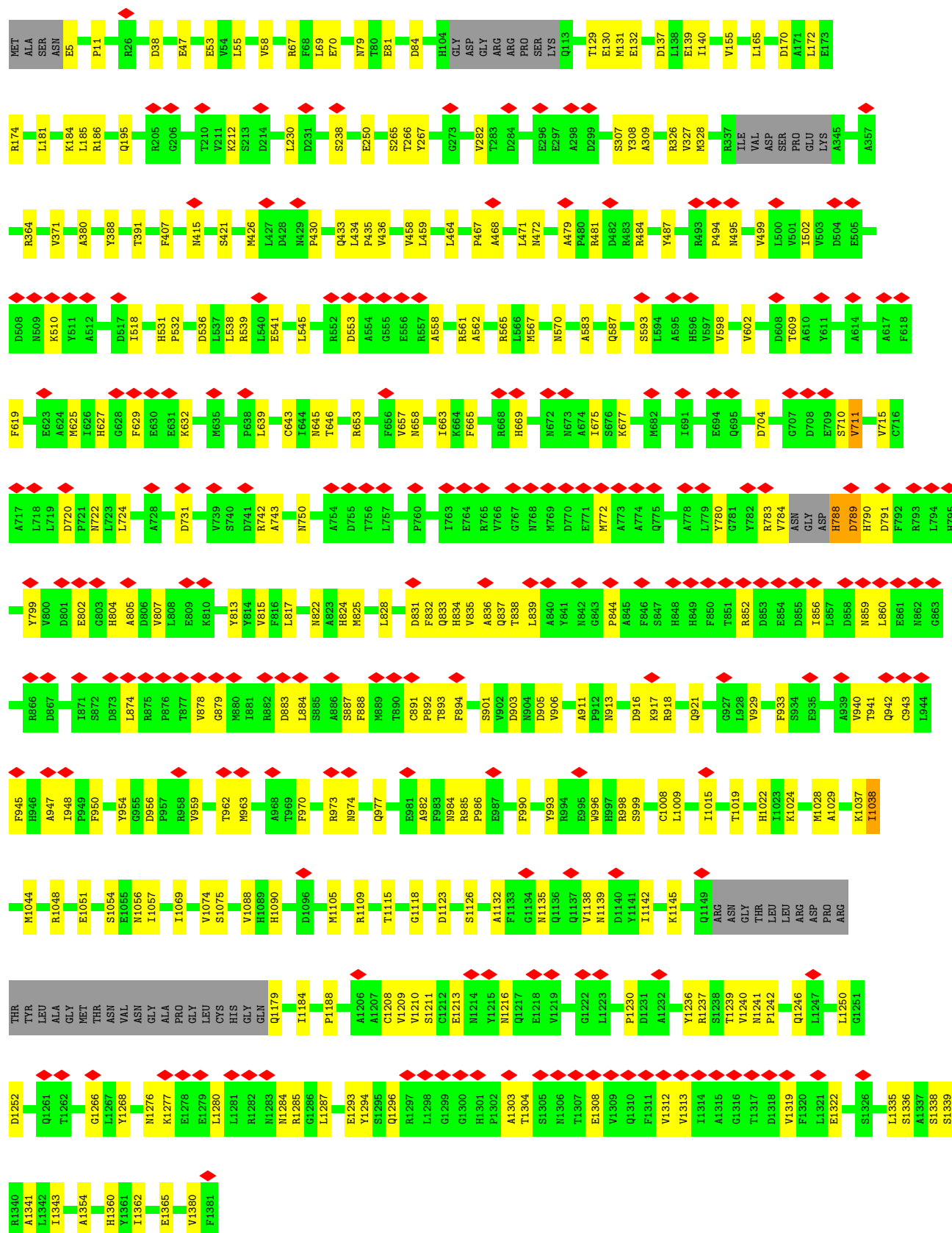
• Molecule 7: Major capsid protein





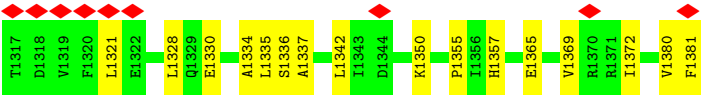
• Molecule 7: Major capsid protein





• Molecule 7: Major capsid protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	28639	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 ($e^-/\text{\AA}^2$)	48	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	0.063	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	5	0.27	0/2263	0.61	0/3088
1	e	0.36	0/2572	0.59	0/3503
2	6	0.29	0/2377	0.61	0/3236
2	7	0.32	0/2306	0.66	0/3135
2	f	0.30	0/2327	0.55	2/3169 (0.1%)
2	g	0.34	0/2319	0.59	0/3155
3	G	0.31	0/684	0.72	1/924 (0.1%)
3	K	0.26	0/570	0.59	0/765
4	C	0.30	0/2770	0.65	2/3763 (0.1%)
5	B	0.24	0/304	0.55	0/404
5	O	0.28	0/255	0.64	0/339
6	2	0.28	0/636	0.68	1/861 (0.1%)
6	Y	0.31	0/636	0.59	0/861
6	Z	0.27	0/636	0.58	0/861
6	y	0.27	0/636	0.60	0/861
7	S	0.38	0/10405	0.61	3/14142 (0.0%)
7	T	0.38	0/10500	0.62	5/14271 (0.0%)
7	W	0.36	0/10699	0.59	4/14539 (0.0%)
7	x	0.41	2/10380 (0.0%)	0.64	2/14109 (0.0%)
All	All	0.36	2/63275 (0.0%)	0.62	20/85986 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	0	1
1	e	0	1
2	g	0	1
6	2	0	1
7	T	0	1
7	x	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	x	362	GLN	C-N	14.74	1.51	1.33
7	x	392	GLN	C-N	-5.56	1.24	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	x	362	GLN	CA-C-N	13.07	133.94	119.83
7	x	362	GLN	C-N-CA	13.07	133.94	119.83
7	S	890	THR	CA-C-N	7.83	131.29	120.65
7	S	890	THR	C-N-CA	7.83	131.29	120.65
7	W	436	VAL	N-CA-C	-6.90	107.15	113.71
7	T	1263	ALA	CA-C-N	6.29	124.20	120.24
7	T	1263	ALA	C-N-CA	6.29	124.20	120.24
7	W	711	VAL	N-CA-C	-6.12	106.77	112.83
7	S	89	ILE	N-CA-C	-6.07	105.91	111.67
2	f	139	PRO	CA-C-N	5.54	127.02	120.09
2	f	139	PRO	C-N-CA	5.54	127.02	120.09
7	T	800	VAL	CA-C-N	5.43	130.53	122.82
7	T	800	VAL	C-N-CA	5.43	130.53	122.82
3	G	14	LEU	N-CA-C	5.33	114.98	108.11
4	C	52	THR	CA-C-N	5.18	131.55	121.41
4	C	52	THR	C-N-CA	5.18	131.55	121.41
6	2	67	VAL	N-CA-C	5.16	120.03	108.88
7	W	1038	ILE	CA-C-N	5.09	127.47	120.39
7	W	1038	ILE	C-N-CA	5.09	127.47	120.39
7	T	817	LEU	CA-CB-CG	5.05	133.97	116.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	2	66	GLY	Peptide
1	5	312	HIS	Peptide
7	T	817	LEU	Peptide
1	e	20	LEU	Peptide
2	g	232	HIS	Peptide

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Mol	Chain	Res	Type	Group
7	x	1211	SER	Peptide
7	x	361	ASP	Mainchain
7	x	669	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	2199	0	2144	40	0
1	e	2505	0	2480	34	0
2	6	2329	0	2363	54	0
2	7	2262	0	2293	53	0
2	f	2279	0	2316	51	0
2	g	2272	0	2308	43	0
3	G	675	0	678	15	0
3	K	563	0	566	12	0
4	C	2705	0	2712	70	0
5	B	301	0	328	4	0
5	O	252	0	269	7	0
6	2	621	0	611	10	0
6	Y	621	0	611	11	0
6	Z	621	0	611	14	0
6	y	621	0	611	15	0
7	S	10166	0	9995	193	0
7	T	10258	0	10093	211	0
7	W	10456	0	10286	192	0
7	x	10141	0	9977	218	0
All	All	61847	0	61252	1150	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 9.

All (1150) 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)
7:x:395:TYR:CE1	7:x:397:LEU:HB2	1.14	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:395:TYR:HE1	7:S:397:LEU:CB	1.13	1.55
7:x:395:TYR:HE1	7:x:397:LEU:CB	1.21	1.50
7:S:395:TYR:CE1	7:S:397:LEU:CB	2.01	1.44
7:S:395:TYR:CE1	7:S:397:LEU:HB2	1.53	1.41
7:S:395:TYR:CE1	7:S:397:LEU:CG	1.97	1.40
7:S:395:TYR:HE1	7:S:397:LEU:CG	1.26	1.29
7:T:1133:PHE:HB2	7:T:1139:ASN:OD1	1.21	1.27
7:T:518:ILE:HD12	7:T:992:GLU:OE2	1.37	1.19
7:x:1133:PHE:CB	7:x:1139:ASN:OD1	1.93	1.17
7:x:1133:PHE:HB2	7:x:1139:ASN:OD1	1.01	1.16
7:W:518:ILE:HD12	7:W:993:TYR:CE1	1.83	1.13
7:x:1133:PHE:HB2	7:x:1139:ASN:CG	1.72	1.13
7:x:1133:PHE:N	7:x:1139:ASN:HD21	1.50	1.09
7:W:780:TYR:O	7:W:784:VAL:HG22	1.51	1.09
7:x:395:TYR:CE1	7:x:397:LEU:CB	2.07	1.06
7:T:518:ILE:HD12	7:T:992:GLU:CD	1.79	1.05
7:x:395:TYR:CZ	7:x:397:LEU:HB2	1.92	1.05
7:S:395:TYR:CE1	7:S:397:LEU:HG	1.55	1.03
7:W:1132:ALA:HB1	7:W:1139:ASN:ND2	1.72	1.02
7:W:518:ILE:HD12	7:W:993:TYR:CD1	1.94	1.00
7:T:79:ASN:HB3	7:T:308:TYR:HD1	1.26	0.98
7:W:518:ILE:HG22	7:W:999:SER:OG	1.65	0.96
2:6:264:MET:HE1	2:7:209:PHE:CZ	2.00	0.96
7:x:1133:PHE:H	7:x:1139:ASN:ND2	1.64	0.95
7:T:1372:ILE:CD1	7:T:1381:PHE:HD1	1.83	0.90
7:W:518:ILE:CD1	7:W:993:TYR:CE1	2.54	0.90
7:W:788:HIS:O	7:W:791:ASP:N	2.06	0.89
7:x:1133:PHE:H	7:x:1139:ASN:HD21	1.19	0.87
7:S:395:TYR:CD1	7:S:397:LEU:HB2	2.10	0.86
7:W:518:ILE:HD12	7:W:993:TYR:HE1	1.37	0.86
7:W:518:ILE:CD1	7:W:993:TYR:HE1	1.88	0.86
7:W:1132:ALA:HB1	7:W:1139:ASN:HD21	1.35	0.86
7:T:1133:PHE:CB	7:T:1139:ASN:OD1	2.17	0.85
2:7:224:VAL:O	2:7:228:ILE:HB	1.76	0.84
7:T:79:ASN:HB3	7:T:308:TYR:CD1	2.11	0.84
7:T:395:TYR:HD1	7:T:397:LEU:H	1.25	0.84
7:x:1133:PHE:CA	7:x:1139:ASN:HD21	1.90	0.83
7:T:1372:ILE:HD11	7:T:1381:PHE:CD1	2.14	0.82
7:W:79:ASN:ND2	7:W:308:TYR:CE1	2.47	0.81
7:x:68:PHE:CD1	7:x:176:LEU:CD2	2.65	0.80
7:T:518:ILE:CD1	7:T:992:GLU:OE2	2.27	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:788:HIS:O	7:W:790:HIS:N	2.15	0.79
7:x:1133:PHE:N	7:x:1139:ASN:ND2	2.23	0.78
7:x:68:PHE:CD1	7:x:176:LEU:HD23	2.19	0.77
7:T:1133:PHE:HB2	7:T:1139:ASN:CG	2.10	0.77
7:T:1372:ILE:CD1	7:T:1381:PHE:CD1	2.68	0.77
7:T:1372:ILE:HD13	7:T:1381:PHE:HD1	1.50	0.76
1:5:164:THR:O	1:5:168:LEU:HB2	1.83	0.76
7:x:395:TYR:CD1	7:x:398:ASN:OD1	2.39	0.76
7:T:395:TYR:HE1	7:T:397:LEU:CG	1.99	0.75
7:x:395:TYR:HE1	7:x:397:LEU:CA	1.98	0.75
7:T:518:ILE:HD12	7:T:992:GLU:OE1	1.86	0.75
7:T:1372:ILE:HD11	7:T:1381:PHE:HD1	1.51	0.75
4:C:45:GLN:OE1	4:C:55:THR:OG1	2.06	0.72
7:S:518:ILE:HG22	7:S:999:SER:OG	1.88	0.72
7:W:79:ASN:HD22	7:W:308:TYR:HE1	1.35	0.71
7:T:644:ILE:HD11	7:T:675:ILE:HG12	1.72	0.71
7:x:395:TYR:CE1	7:x:397:LEU:CA	2.71	0.71
7:T:395:TYR:CE1	7:T:397:LEU:HB2	2.26	0.71
2:6:264:MET:CE	2:7:209:PHE:CZ	2.74	0.70
2:f:246:GLU:O	2:f:250:ILE:HB	1.93	0.69
7:x:899:ARG:HE	7:x:920:GLU:HB3	1.58	0.68
7:W:645:ASN:HD21	7:W:675:ILE:HA	1.59	0.68
7:W:1132:ALA:CB	7:W:1139:ASN:HD21	2.06	0.68
2:6:264:MET:HE1	2:7:209:PHE:CE1	2.29	0.68
7:S:395:TYR:CD1	7:S:397:LEU:N	2.60	0.68
7:W:609:THR:HA	7:W:653:ARG:HD3	1.76	0.67
7:W:499:VAL:HA	7:W:502:ILE:HD12	1.77	0.67
2:7:17:GLU:HG2	2:7:125:LEU:HD22	1.77	0.66
7:T:1292:ASN:O	7:T:1296:GLN:HB2	1.96	0.66
7:x:68:PHE:CE1	7:x:180:VAL:HG21	2.31	0.66
1:e:110:LEU:HD11	1:e:191:LEU:HD12	1.79	0.65
7:W:567:MET:SD	7:W:1022:HIS:ND1	2.68	0.65
7:W:839:LEU:HD21	7:W:884:LEU:HG	1.78	0.65
7:x:395:TYR:CE1	7:x:397:LEU:N	2.65	0.65
2:f:55:PRO:HD2	2:f:191:PRO:HB3	1.79	0.65
7:W:5:GLU:N	7:W:38:ASP:OD2	2.30	0.64
3:G:61:LEU:HA	3:G:64:ARG:HE	1.63	0.64
7:T:335:MET:HG2	7:x:319:VAL:HG21	1.79	0.64
2:6:165:GLY:HA3	4:C:503:ILE:H	1.63	0.64
7:W:518:ILE:CG1	7:W:993:TYR:HE1	2.10	0.64
2:7:114:PRO:HD3	2:7:135:PRO:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:810:LYS:O	7:T:814:TYR:HB2	1.98	0.64
1:e:224:THR:HG22	1:e:349:GLU:HG2	1.80	0.64
3:G:24:TRP:HB2	1:e:303:HIS:HD2	1.63	0.63
7:W:1209:VAL:HG23	7:W:1210:VAL:HG13	1.79	0.63
1:5:180:ARG:HD2	1:5:183:ASN:HD21	1.64	0.63
7:W:805:ALA:HB2	7:x:972:MET:HG3	1.81	0.63
5:O:3135:HIS:HD2	5:O:3138:ILE:HD11	1.63	0.63
7:T:1261:GLN:HE21	7:T:1314:ILE:HA	1.64	0.63
7:T:1135:ASN:HB3	7:T:1138:VAL:HG12	1.80	0.63
2:7:231:GLU:HG2	2:7:234:ASP:HB2	1.80	0.63
7:W:518:ILE:HD12	7:W:993:TYR:HD1	1.61	0.63
4:C:305:LEU:HD12	4:C:307:ALA:H	1.63	0.63
7:S:1117:MET:SD	7:S:1371:ARG:NH1	2.72	0.63
2:6:259:ASP:OD1	4:C:264:LEU:N	2.30	0.62
7:x:191:MET:HB2	7:x:1106:THR:HG22	1.79	0.62
2:7:151:LEU:HD21	2:7:209:PHE:CD2	2.34	0.62
7:S:1355:PRO:HA	7:S:1362:ILE:HG22	1.81	0.62
7:W:69:LEU:HD21	7:W:79:ASN:HD21	1.63	0.62
7:W:308:TYR:CE1	7:W:1069:ILE:HG13	2.35	0.62
2:f:246:GLU:HA	2:f:249:ARG:HG2	1.81	0.62
4:C:426:LEU:HD22	4:C:461:HIS:HB2	1.81	0.62
7:T:724:LEU:O	7:T:921:GLN:NE2	2.33	0.62
7:x:176:LEU:HD11	7:x:1069:ILE:HD12	1.81	0.62
3:K:34:VAL:HG13	4:C:362:TRP:HB2	1.81	0.61
7:S:11:PRO:HB3	7:S:47:GLU:HB3	1.82	0.61
7:T:1188:PRO:HD2	7:T:1241:ASN:HB2	1.81	0.61
7:W:1048:ARG:NH1	7:W:1118:GLY:O	2.33	0.61
7:x:395:TYR:HD1	7:x:398:ASN:OD1	1.82	0.61
7:x:1133:PHE:CG	7:x:1139:ASN:OD1	2.53	0.61
2:6:264:MET:HE1	2:7:209:PHE:HZ	1.61	0.61
7:S:1064:SER:HB3	7:S:1102:SER:HB2	1.81	0.61
7:x:1069:ILE:HD13	7:x:1092:MET:SD	2.40	0.61
2:g:236:LEU:HA	2:g:239:PHE:HB3	1.83	0.61
7:x:940:VAL:HG23	7:x:941:THR:HG23	1.83	0.61
1:5:193:GLU:HB2	1:5:204:THR:HB	1.83	0.61
7:T:481:ARG:HG2	7:T:483:ARG:H	1.65	0.61
7:W:1132:ALA:HB1	7:W:1139:ASN:HD22	1.65	0.61
7:W:1135:ASN:HB3	7:W:1138:VAL:HG12	1.83	0.61
4:C:7:ASN:ND2	4:C:61:PHE:H	1.99	0.61
6:Z:8:PRO:HD3	7:T:834:HIS:HD2	1.65	0.61
6:2:67:VAL:HG23	6:2:68:PRO:HD3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:395:TYR:CD1	7:x:397:LEU:N	2.69	0.60
2:7:95:ASN:HB2	2:7:103:TRP:HE1	1.66	0.60
7:S:608:ASP:HB3	7:S:653:ARG:HE	1.66	0.60
7:W:942:GLN:NE2	7:W:943:CYS:SG	2.75	0.60
7:x:1069:ILE:CD1	7:x:1092:MET:SD	2.88	0.60
7:x:84:ASP:OD1	7:x:84:ASP:N	2.32	0.60
7:S:543:HIS:HD2	7:S:545:LEU:H	1.48	0.60
7:x:68:PHE:HD1	7:x:177:ILE:HG12	1.65	0.60
7:x:522:CYS:O	7:x:1003:LYS:NZ	2.34	0.60
7:S:541:GLU:OE1	7:S:565:ARG:NH2	2.35	0.60
2:g:279:ASN:OD1	2:g:283:ARG:NH1	2.35	0.60
4:C:7:ASN:HD21	4:C:61:PHE:N	2.00	0.59
7:W:715:VAL:HG23	7:W:1029:ALA:HA	1.82	0.59
7:x:955:GLY:HA3	7:x:985:ARG:HE	1.67	0.59
7:T:959:VAL:HG12	7:T:963:MET:HE2	1.85	0.59
7:T:1076:ARG:NH2	1:e:62:LEU:O	2.36	0.59
7:W:435:PRO:HB3	7:W:1338:SER:HB3	1.84	0.59
7:W:479:ALA:O	7:W:539:ARG:NH2	2.36	0.59
7:S:810:LYS:O	7:S:814:TYR:HB2	2.03	0.59
7:x:828:LEU:HD22	7:x:930:ALA:HB2	1.84	0.59
7:S:1264:VAL:HG12	7:S:1266:GLY:H	1.68	0.59
7:W:844:PRO:HG3	7:W:859:ASN:HD22	1.65	0.59
3:G:70:LEU:HD11	5:O:3145:LYS:HD3	1.84	0.59
7:x:541:GLU:OE1	7:x:565:ARG:NH2	2.34	0.59
7:x:1133:PHE:HB2	7:x:1139:ASN:ND2	2.14	0.59
6:y:67:VAL:HG23	6:y:68:PRO:HD3	1.85	0.59
7:T:329:ARG:HG2	7:T:330:THR:HG23	1.85	0.59
7:x:783:ARG:NH2	7:x:888:PHE:O	2.36	0.59
7:T:1208:CYS:HB2	7:T:1211:SER:HB3	1.84	0.58
7:x:1192:ASP:OD2	7:x:1237:ARG:NH1	2.36	0.58
2:f:298:CYS:SG	2:f:299:TRP:N	2.76	0.58
7:T:518:ILE:HG22	7:T:1000:PRO:HD3	1.84	0.58
6:2:13:ARG:HD3	6:2:15:GLU:H	1.69	0.58
7:S:600:GLN:HE22	7:S:1011:SER:HA	1.68	0.58
7:W:788:HIS:C	7:W:790:HIS:N	2.61	0.58
7:x:1124:PHE:HA	7:x:1127:VAL:HG12	1.85	0.58
2:g:221:MET:SD	2:g:249:ARG:NH2	2.76	0.58
7:S:658:ASN:OD1	7:S:658:ASN:N	2.35	0.58
7:T:518:ILE:CD1	7:T:992:GLU:OE1	2.51	0.58
7:W:265:SER:O	7:W:364:ARG:NH1	2.36	0.58
4:C:387:ARG:O	4:C:387:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:77:CYS:SG	7:x:184:LYS:NZ	2.77	0.58
7:x:1335:LEU:HB2	7:x:1365:GLU:HB2	1.84	0.58
7:x:399:ARG:NH1	7:x:1321:LEU:O	2.36	0.58
1:5:56:ALA:HB1	7:S:144:ILE:HD11	1.85	0.58
7:W:430:PRO:HA	7:W:433:GLN:HE21	1.69	0.58
2:7:208:TYR:HB3	2:7:274:LEU:HD11	1.86	0.58
7:S:874:LEU:HG	7:S:876:PRO:HD3	1.84	0.58
6:Y:32:GLN:NE2	6:Y:35:LEU:O	2.37	0.57
6:Y:37:ASN:OD1	6:Y:41:ARG:NH2	2.37	0.57
7:x:177:ILE:HD12	7:x:387:MET:HE1	1.86	0.57
7:T:664:LYS:HG2	7:T:668:ARG:HH12	1.69	0.57
7:S:904:ASN:ND2	7:S:917:LYS:O	2.36	0.57
7:x:837:GLN:HB3	6:y:10:LEU:HD11	1.86	0.57
4:C:466:ALA:HB3	4:C:474:PHE:HB2	1.87	0.57
7:S:456:LEU:HD21	7:S:1031:ILE:HA	1.85	0.57
7:T:704:ASP:N	7:T:704:ASP:OD1	2.37	0.57
7:W:940:VAL:HG13	7:W:941:THR:HG23	1.86	0.57
7:x:903:ASP:N	7:x:903:ASP:OD1	2.37	0.57
4:C:403:TRP:HA	4:C:467:THR:HG21	1.87	0.57
7:W:561:ARG:NH2	7:W:916:ASP:OD1	2.37	0.57
7:W:1213:GLU:HB3	7:W:1216:ASN:HD21	1.69	0.57
7:x:564:HIS:O	7:x:998:ARG:NH2	2.37	0.57
7:S:955:GLY:HA3	7:S:985:ARG:HE	1.70	0.57
7:T:395:TYR:HE1	7:T:397:LEU:HB2	1.69	0.57
7:T:817:LEU:HD13	7:T:825:MET:HE1	1.86	0.57
7:x:995:GLU:HG3	7:x:997:HIS:H	1.68	0.57
4:C:7:ASN:HD21	4:C:61:PHE:H	1.53	0.57
7:S:1213:GLU:O	7:S:1284:ASN:ND2	2.38	0.57
7:T:337:ARG:NH1	7:T:351:ASP:OD1	2.34	0.57
7:x:68:PHE:CD1	7:x:177:ILE:HG12	2.40	0.57
3:K:24:TRP:HB2	4:C:372:ILE:HG13	1.86	0.56
7:S:224:LEU:O	7:S:232:ARG:NH2	2.38	0.56
7:W:1051:GLU:H	7:W:1115:THR:HB	1.69	0.56
6:Z:37:ASN:HB3	6:Z:41:ARG:HH21	1.70	0.56
7:S:916:ASP:HB3	7:S:994:ARG:HH21	1.70	0.56
7:S:395:TYR:HD1	7:S:397:LEU:H	1.47	0.56
7:S:492:ARG:HB3	7:S:988:GLN:HG3	1.86	0.56
7:S:903:ASP:OD2	7:S:918:ARG:NE	2.37	0.56
7:T:420:THR:HG21	7:T:1355:PRO:HD2	1.86	0.56
3:K:47:GLU:OE2	3:K:50:ARG:NH2	2.36	0.56
7:S:564:HIS:O	7:S:998:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:1195:TYR:O	7:x:1200:ASN:ND2	2.38	0.56
4:C:394:GLN:NE2	4:C:428:GLU:OE1	2.39	0.56
7:S:129:THR:OG1	7:S:130:GLU:N	2.36	0.56
7:T:632:LYS:O	7:T:636:ASN:ND2	2.37	0.56
7:W:1074:VAL:HG12	7:W:1088:VAL:HG12	1.88	0.56
7:x:1208:CYS:HB2	7:x:1211:SER:HB3	1.88	0.56
1:e:263:ARG:HG2	1:e:326:THR:HG22	1.87	0.56
2:7:45:LEU:HB2	2:7:133:VAL:HG13	1.87	0.56
7:T:724:LEU:HD22	7:T:732:ILE:HD12	1.86	0.56
1:5:262:ALA:HB2	1:5:329:ALA:HB2	1.87	0.56
7:S:402:GLN:HE22	7:S:1303:ALA:HB3	1.71	0.56
7:T:395:TYR:HE1	7:T:397:LEU:CB	2.18	0.56
7:T:731:ASP:HA	7:T:796:LEU:HD13	1.88	0.56
7:x:864:THR:HG23	6:y:9:THR:HG22	1.87	0.56
2:g:13:LEU:N	2:g:77:VAL:O	2.38	0.56
7:S:671:GLY:O	7:T:650:ARG:NH1	2.39	0.56
7:T:1068:PHE:HB2	7:T:1093:ALA:HB3	1.87	0.56
7:W:704:ASP:OD2	7:W:1145:LYS:NZ	2.37	0.56
7:x:1133:PHE:CD2	7:x:1139:ASN:OD1	2.58	0.56
6:y:23:LEU:HD21	6:y:55:PHE:HB2	1.87	0.56
7:W:1285:ARG:NH2	7:W:1293:GLU:OE1	2.39	0.55
7:x:844:PRO:HG3	7:x:859:ASN:HD22	1.71	0.55
7:x:1304:THR:HG22	7:x:1311:PHE:H	1.70	0.55
1:e:171:ASP:OD1	1:e:171:ASP:N	2.37	0.55
7:S:693:LEU:HD22	7:S:1019:THR:HG21	1.88	0.55
7:S:860:LEU:HD13	7:S:866:ARG:HG3	1.88	0.55
7:T:466:THR:HG22	7:T:468:ALA:H	1.71	0.55
7:T:867:ASP:N	7:T:867:ASP:OD1	2.39	0.55
2:f:176:LEU:HD22	2:g:261:LEU:HD21	1.87	0.55
4:C:7:ASN:OD1	4:C:61:PHE:HB2	2.06	0.55
7:S:395:TYR:CE1	7:S:397:LEU:N	2.74	0.55
7:T:1216:ASN:O	7:T:1284:ASN:ND2	2.38	0.55
7:W:172:LEU:HD21	7:W:1090:HIS:HB2	1.87	0.55
7:x:1074:VAL:HG23	7:x:1088:VAL:HG22	1.88	0.55
7:x:720:ASP:O	7:x:810:LYS:NZ	2.40	0.55
7:x:905:ASP:OD2	7:x:1024:LYS:NZ	2.40	0.55
2:f:255:LEU:HD22	2:g:166:ASN:HB3	1.89	0.55
4:C:7:ASN:CG	4:C:61:PHE:H	2.15	0.55
7:S:518:ILE:HG22	7:S:999:SER:HG	1.69	0.55
7:W:518:ILE:CD1	7:W:993:TYR:CD1	2.80	0.55
4:C:5:ILE:HG12	4:C:273:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:539:ARG:HA	7:W:1246:GLN:HE22	1.70	0.55
7:x:269:THR:HA	7:x:302:ILE:HG22	1.89	0.55
7:S:170:ASP:OD1	7:S:174:ARG:NH1	2.40	0.55
7:T:743:ALA:O	7:T:918:ARG:NH2	2.40	0.55
7:W:817:LEU:HB3	7:W:825:MET:HE1	1.88	0.55
7:S:828:LEU:HB2	7:S:930:ALA:HB2	1.88	0.55
7:T:279:VAL:HG12	7:T:380:ALA:HB3	1.88	0.55
2:6:57:TYR:H	2:6:60:MET:HE3	1.71	0.55
7:T:395:TYR:HE1	7:T:397:LEU:HG	1.70	0.55
7:T:395:TYR:CE1	7:T:397:LEU:HG	2.42	0.54
7:T:497:MET:HG2	7:T:896:ARG:HG2	1.89	0.54
7:T:815:VAL:HG23	7:T:1018:MET:HB3	1.88	0.54
1:5:307:VAL:HG23	1:5:308:VAL:HG13	1.89	0.54
2:6:234:ASP:OD2	2:6:234:ASP:N	2.37	0.54
4:C:48:PHE:HE2	4:C:55:THR:CG2	2.20	0.54
7:x:395:TYR:CZ	7:x:397:LEU:HD23	2.43	0.54
2:g:33:SER:O	2:g:38:GLN:NE2	2.41	0.54
3:G:39:LEU:HB2	4:C:426:LEU:HD11	1.90	0.54
4:C:21:LEU:HD21	4:C:297:LEU:HD21	1.89	0.54
5:O:3147:LEU:HA	7:x:793:ARG:HH12	1.73	0.54
7:S:474:LEU:HD11	7:S:542:LEU:HD21	1.90	0.54
7:T:273:GLY:O	7:T:274:GLU:HG3	2.07	0.54
7:T:1209:VAL:HG23	7:T:1283:ASN:HD22	1.72	0.54
7:x:1350:LYS:HD2	7:x:1380:VAL:HB	1.89	0.54
6:Y:70:ARG:NH1	6:Z:11:GLN:O	2.40	0.54
7:S:486:THR:OG1	7:S:552:ARG:NH2	2.34	0.54
7:T:531:HIS:HD2	7:T:533:SER:H	1.53	0.54
7:T:916:ASP:OD1	7:T:994:ARG:NH2	2.40	0.54
7:W:1266:GLY:HA2	7:W:1312:VAL:HG22	1.89	0.54
7:x:919:THR:OG1	7:x:996:TRP:NE1	2.40	0.54
1:5:258:CYS:HB2	2:6:67:CYS:HA	1.89	0.54
2:6:111:VAL:H	2:6:283:ARG:HH21	1.55	0.54
6:Z:9:THR:OG1	6:Z:10:LEU:N	2.40	0.54
7:x:1068:PHE:HB2	7:x:1093:ALA:HB3	1.88	0.54
7:S:433:GLN:OE1	7:S:1360:HIS:NE2	2.39	0.54
7:S:609:THR:HG22	7:S:653:ARG:HB3	1.90	0.54
7:S:1048:ARG:NH1	7:S:1117:MET:O	2.41	0.54
7:T:814:TYR:HB3	7:T:1022:HIS:HE1	1.72	0.54
7:S:400:ARG:NH1	7:S:1051:GLU:OE2	2.38	0.54
7:T:1178:GLN:HE21	7:T:1310:GLN:HG2	1.73	0.54
4:C:42:ALA:N	4:C:60:VAL:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:76:THR:OG1	4:C:77:PHE:N	2.38	0.54
7:T:814:TYR:OH	7:T:921:GLN:NE2	2.41	0.54
7:W:959:VAL:HA	7:W:962:THR:HG22	1.90	0.54
7:x:1283:ASN:HB3	7:x:1290:MET:HG3	1.90	0.54
4:C:423:SER:O	4:C:432:SER:OG	2.24	0.54
7:T:1365:GLU:OE1	7:T:1371:ARG:NH1	2.39	0.54
7:W:903:ASP:HA	7:W:918:ARG:HA	1.90	0.54
7:x:1342:LEU:HD11	7:x:1357:HIS:HB2	1.89	0.54
2:f:118:ARG:O	2:f:122:THR:OG1	2.24	0.54
2:f:200:ALA:O	2:f:204:ASN:ND2	2.40	0.54
2:7:279:ASN:OD1	2:7:283:ARG:NH1	2.38	0.53
7:W:5:GLU:HG2	7:W:38:ASP:OD1	2.08	0.53
7:x:609:THR:HA	7:x:653:ARG:HD3	1.89	0.53
7:T:934:SER:OG	7:T:935:GLU:N	2.41	0.53
5:B:3129:LYS:HA	5:B:3132:ARG:HE	1.72	0.53
7:T:724:LEU:HD21	7:T:736:LEU:HD11	1.90	0.53
7:T:282:VAL:HG12	7:T:1057:ILE:HG23	1.91	0.53
7:W:856:ILE:HG13	7:W:878:VAL:HG22	1.91	0.53
7:x:68:PHE:HA	7:x:177:ILE:HD11	1.90	0.53
4:C:17:LEU:HB3	4:C:82:VAL:HG23	1.89	0.53
7:x:209:LYS:NZ	7:x:1211:SER:OG	2.41	0.53
7:W:1028:MET:HG3	7:W:1142:ILE:HD11	1.90	0.53
7:x:764:GLU:OE2	7:x:795:HIS:ND1	2.41	0.53
7:W:467:PRO:HB2	7:W:471:LEU:HD23	1.90	0.53
2:6:172:VAL:O	2:6:176:LEU:HB3	2.09	0.53
7:T:434:LEU:O	7:T:587:GLN:NE2	2.41	0.53
7:x:482:ASP:N	7:x:482:ASP:OD1	2.42	0.53
7:x:934:SER:HB3	7:x:937:THR:HG23	1.91	0.53
6:Z:20:ASP:OD1	6:Z:20:ASP:N	2.34	0.53
7:W:665:PHE:O	7:W:669:HIS:N	2.37	0.53
7:W:1236:TYR:OH	7:W:1237:ARG:NH1	2.42	0.53
1:5:133:ILE:HB	1:5:155:ALA:HB1	1.91	0.53
7:S:520:LEU:HG	7:S:537:LEU:HD11	1.90	0.53
7:W:84:ASP:OD1	7:W:84:ASP:N	2.40	0.53
2:f:174:MET:SD	2:f:174:MET:N	2.81	0.53
3:G:70:LEU:HA	3:G:73:ILE:HG12	1.91	0.52
7:S:655:ALA:O	7:S:683:TYR:OH	2.26	0.52
2:6:171:ASP:OD2	2:6:171:ASP:N	2.41	0.52
2:7:86:VAL:HG13	2:7:88:GLY:H	1.73	0.52
7:S:1048:ARG:HG2	7:S:1182:CYS:HB3	1.91	0.52
7:T:586:GLN:NE2	7:T:589:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:230:LEU:HB3	7:W:1109:ARG:HG3	1.92	0.52
7:x:109:ARG:HH11	1:e:330:THR:HB	1.74	0.52
7:x:607:GLN:HA	7:x:821:THR:HG22	1.90	0.52
7:x:932:ALA:HA	7:x:959:VAL:HG23	1.91	0.52
2:7:284:LEU:HD11	2:7:298:CYS:HB2	1.92	0.52
7:S:877:THR:H	7:S:880:MET:HE3	1.73	0.52
7:T:726:PRO:HB3	7:T:950:PHE:HE2	1.73	0.52
7:W:553:ASP:OD1	7:W:553:ASP:N	2.40	0.52
7:W:731:ASP:HB3	7:W:799:TYR:HB2	1.90	0.52
7:T:742:ARG:NH1	7:T:904:ASN:O	2.43	0.52
7:T:903:ASP:HA	7:T:918:ARG:HA	1.91	0.52
7:x:953:PHE:HZ	7:x:1001:MET:HE3	1.74	0.52
7:x:961:ALA:HA	7:x:967:VAL:HG23	1.92	0.52
7:T:835:VAL:O	7:T:839:LEU:HB2	2.09	0.52
7:T:1073:ASN:O	7:T:1089:HIS:N	2.43	0.52
7:x:1011:SER:OG	7:x:1012:LEU:N	2.40	0.52
7:x:1372:ILE:HD12	7:x:1381:PHE:CE1	2.44	0.52
7:T:1230:PRO:HA	7:T:1238:SER:HA	1.90	0.52
7:x:815:VAL:O	7:x:819:THR:OG1	2.28	0.52
7:S:1257:SER:O	7:S:1261:GLN:NE2	2.43	0.52
7:W:788:HIS:C	7:W:790:HIS:H	2.18	0.52
7:x:567:MET:HA	7:x:1024:LYS:HA	1.91	0.52
7:T:395:TYR:CE1	7:T:397:LEU:CB	2.92	0.52
7:x:822:ASN:HB3	7:x:1006:ALA:HA	1.91	0.52
1:5:134:LEU:HD11	1:5:165:LEU:HB3	1.91	0.52
7:S:742:ARG:HB2	7:S:903:ASP:HB2	1.91	0.52
7:T:1071:THR:O	7:T:1073:ASN:ND2	2.43	0.52
7:x:986:PRO:HB2	7:x:989:LEU:HB3	1.92	0.52
7:S:458:VAL:HG11	7:S:1184:ILE:HB	1.92	0.52
7:T:395:TYR:HE1	7:T:397:LEU:CD1	2.23	0.52
7:W:79:ASN:ND2	7:W:308:TYR:CD1	2.77	0.52
7:W:139:GLU:OE1	1:e:218:ARG:NH1	2.42	0.52
7:W:893:THR:OG1	7:W:894:PHE:N	2.42	0.52
7:W:1056:ASN:ND2	7:W:1105:MET:SD	2.75	0.52
7:x:68:PHE:CZ	7:x:180:VAL:HG21	2.44	0.52
7:x:528:ASP:OD1	7:x:528:ASP:N	2.39	0.52
7:x:650:ARG:NH2	7:x:873:ASP:O	2.43	0.52
7:x:793:ARG:O	7:x:896:ARG:NH1	2.42	0.52
1:5:209:GLY:O	1:5:355:SER:N	2.41	0.51
2:6:266:VAL:HG13	2:6:267:MET:HE2	1.92	0.51
7:S:710:SER:OG	7:S:711:VAL:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:23:LEU:HD23	6:Z:51:LEU:HB3	1.92	0.51
7:T:79:ASN:CB	7:T:308:TYR:CD1	2.91	0.51
7:T:1212:CYS:HA	7:T:1223:LEU:HD12	1.91	0.51
7:W:132:GLU:O	7:x:113:GLN:NE2	2.42	0.51
1:e:343:SER:OG	1:e:344:SER:N	2.43	0.51
2:f:33:SER:OG	2:f:34:THR:N	2.43	0.51
2:7:123:VAL:HG23	2:7:132:ILE:HG13	1.92	0.51
7:S:706:VAL:HG11	7:S:1138:VAL:HG22	1.93	0.51
7:T:567:MET:HG3	7:T:1001:MET:HE1	1.92	0.51
7:W:326:ARG:HE	7:W:328:MET:HE1	1.74	0.51
2:f:247:ILE:HD11	2:g:214:THR:HG23	1.91	0.51
7:S:435:PRO:HB3	7:S:1338:SER:HB2	1.93	0.51
7:S:688:GLY:HA2	7:S:691:ILE:HD12	1.91	0.51
7:S:1272:ARG:HD3	7:S:1301:HIS:HE1	1.74	0.51
2:6:112:MET:HE3	2:6:113:PRO:HD2	1.92	0.51
7:S:513:ALA:O	7:S:977:GLN:NE2	2.44	0.51
2:f:16:ASP:OD1	2:f:16:ASP:N	2.43	0.51
4:C:7:ASN:ND2	4:C:60:VAL:HG12	2.25	0.51
7:W:804:HIS:HB3	7:W:807:VAL:HG12	1.91	0.51
2:f:217:PRO:HG3	2:f:264:MET:HE1	1.92	0.51
4:C:84:CYS:SG	4:C:116:TYR:OH	2.65	0.51
7:T:283:THR:OG1	7:T:385:GLN:OE1	2.28	0.51
7:T:1355:PRO:HA	7:T:1362:ILE:HG22	1.91	0.51
7:W:783:ARG:NH1	7:W:888:PHE:O	2.43	0.51
7:x:861:GLU:HB2	6:y:11:GLN:HE21	1.75	0.51
2:f:61:TYR:OH	2:f:112:MET:SD	2.64	0.51
1:5:309:GLN:HB3	4:C:266:ARG:HH12	1.76	0.51
7:W:973:ARG:HG3	7:W:974:ASN:HD22	1.75	0.51
2:6:199:LEU:HD23	2:6:202:LEU:HD12	1.93	0.51
2:7:228:ILE:HG23	2:7:229:ARG:HG2	1.93	0.51
7:S:1238:SER:OG	7:S:1239:THR:N	2.44	0.51
7:W:79:ASN:OD1	7:W:79:ASN:N	2.41	0.51
7:W:458:VAL:HG11	7:W:1184:ILE:HB	1.92	0.51
7:x:765:ARG:NH1	7:x:771:GLU:OE1	2.44	0.51
7:x:1133:PHE:CA	7:x:1139:ASN:ND2	2.69	0.51
2:f:279:ASN:OD1	2:f:283:ARG:NH2	2.44	0.51
6:Z:32:GLN:HB2	6:Z:35:LEU:HB3	1.93	0.51
7:T:1300:GLY:O	7:T:1323:GLN:NE2	2.43	0.51
1:5:223:VAL:HB	1:5:350:ILE:HB	1.92	0.50
2:6:233:HIS:HB2	2:6:236:LEU:HD13	1.93	0.50
7:S:748:ILE:HG21	7:S:794:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:781:GLY:O	7:S:785:ASN:HB3	2.11	0.50
7:T:230:LEU:HB3	7:T:1109:ARG:HB3	1.93	0.50
7:T:993:TYR:O	7:T:998:ARG:NH2	2.44	0.50
7:W:170:ASP:OD1	7:W:174:ARG:NH1	2.44	0.50
7:W:282:VAL:HG12	7:W:1057:ILE:HG12	1.93	0.50
7:W:371:VAL:HA	7:W:380:ALA:HA	1.93	0.50
7:W:1277:LYS:HA	7:W:1280:LEU:HD12	1.93	0.50
7:x:867:ASP:N	7:x:867:ASP:OD2	2.44	0.50
7:W:802:GLU:HG3	7:W:805:ALA:H	1.76	0.50
7:T:858:ASP:OD1	7:T:858:ASP:N	2.43	0.50
7:T:914:PRO:HA	7:T:917:LYS:HE3	1.93	0.50
4:C:25:ASP:H	4:C:73:HIS:HE1	1.58	0.50
7:T:395:TYR:HE1	7:T:397:LEU:HD12	1.76	0.50
7:x:644:ILE:HD11	7:x:675:ILE:HG12	1.94	0.50
1:e:304:ARG:NH1	1:e:315:GLU:O	2.44	0.50
2:f:20:LYS:HD2	2:f:123:VAL:HG12	1.94	0.50
2:g:151:LEU:HD21	2:g:205:LEU:HD23	1.94	0.50
2:7:254:ASP:OD1	2:7:254:ASP:N	2.45	0.50
7:T:471:LEU:HD21	7:T:562:ALA:HB2	1.94	0.50
2:6:232:HIS:NE2	2:6:236:LEU:O	2.45	0.50
6:2:10:LEU:HD11	7:W:838:THR:HA	1.93	0.50
7:S:450:PHE:HB2	7:S:1119:ILE:HD11	1.93	0.50
7:T:84:ASP:N	7:T:84:ASP:OD1	2.44	0.50
7:T:952:MET:HE2	7:T:999:SER:HA	1.93	0.50
7:W:913:ASN:ND2	7:W:916:ASP:OD2	2.41	0.50
3:K:24:TRP:N	4:C:372:ILE:O	2.43	0.50
3:K:56:ARG:NE	3:G:57:CYS:SG	2.75	0.50
4:C:38:ASN:HA	4:C:64:ARG:HD2	1.94	0.50
7:T:172:LEU:HD13	7:T:1090:HIS:HB2	1.93	0.50
4:C:477:LEU:HB2	4:C:481:PHE:HB2	1.94	0.50
7:S:127:ILE:HA	7:T:105:GLY:HA2	1.94	0.50
7:S:172:LEU:HD22	7:S:1090:HIS:HB2	1.93	0.50
6:Y:20:ASP:OD1	6:Y:20:ASP:N	2.42	0.50
6:2:8:PRO:HB2	6:2:10:LEU:HD13	1.92	0.50
7:S:1297:ARG:NH1	7:S:1317:THR:O	2.44	0.50
7:x:428:ASP:N	7:x:428:ASP:OD1	2.44	0.50
2:6:91:TYR:N	2:6:298:CYS:O	2.42	0.49
6:Y:49:VAL:HA	6:Y:52:THR:HG22	1.94	0.49
6:Z:13:ARG:HH21	6:Z:41:ARG:HD3	1.77	0.49
7:S:193:ILE:HG21	7:S:1291:VAL:HG11	1.94	0.49
7:T:270:ALA:N	7:T:299:ASP:OD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:903:ASP:OD1	7:T:909:GLN:NE2	2.45	0.49
7:W:625:MET:O	7:W:627:HIS:ND1	2.45	0.49
6:y:71:GLN:HA	6:y:74:ILE:HD12	1.94	0.49
2:f:109:LEU:N	2:f:284:LEU:O	2.45	0.49
7:S:77:CYS:SG	7:S:184:LYS:NZ	2.85	0.49
7:S:516:THR:OG1	7:S:517:ASP:N	2.45	0.49
7:T:764:GLU:HB2	7:T:795:HIS:HB3	1.94	0.49
7:T:95:PHE:HB2	7:T:118:VAL:HG13	1.94	0.49
7:x:1057:ILE:HG13	7:x:1108:ALA:HB2	1.94	0.49
4:C:7:ASN:ND2	4:C:61:PHE:O	2.45	0.49
7:S:824:HIS:CE1	7:S:958:ARG:HD3	2.47	0.49
7:W:657:VAL:HA	7:W:663:ILE:HD11	1.93	0.49
1:e:30:SER:OG	1:e:34:GLU:OE2	2.29	0.49
7:S:77:CYS:SG	7:S:1065:THR:OG1	2.68	0.49
7:S:463:ARG:NH1	7:S:1259:TYR:O	2.38	0.49
7:S:903:ASP:HA	7:S:918:ARG:HG2	1.93	0.49
7:W:532:PRO:HG2	7:W:1230:PRO:HB3	1.93	0.49
2:6:287:ALA:O	2:6:297:THR:OG1	2.30	0.49
4:C:410:ASN:HD22	4:C:494:ARG:HH11	1.61	0.49
7:x:1099:LEU:HD23	7:x:1100:SER:HB3	1.95	0.49
7:x:1133:PHE:C	7:x:1139:ASN:HD21	2.20	0.49
4:C:48:PHE:CE2	4:C:55:THR:HG21	2.48	0.49
4:C:463:VAL:HG22	4:C:478:PRO:HD3	1.95	0.49
7:S:1214:ASN:OD1	7:S:1214:ASN:N	2.43	0.49
7:S:1325:CYS:SG	7:S:1326:SER:N	2.85	0.49
7:T:1077:ARG:NH1	1:e:92:ASP:OD1	2.44	0.49
7:W:1339:SER:OG	7:W:1341:ALA:N	2.45	0.49
4:C:2:ASP:OD1	4:C:2:ASP:N	2.42	0.49
7:S:672:ASN:HA	7:T:650:ARG:HH11	1.78	0.49
7:T:598:VAL:HG13	7:T:602:VAL:HB	1.93	0.49
7:W:553:ASP:HA	7:W:558:ALA:HB2	1.94	0.49
2:f:279:ASN:HA	2:f:283:ARG:HH21	1.78	0.49
4:C:17:LEU:HD21	4:C:311:LEU:HD12	1.95	0.49
6:Y:31:ASN:ND2	6:Y:33:ASN:OD1	2.44	0.49
7:S:623:GLU:HB3	7:S:928:LEU:HD21	1.95	0.49
7:T:1238:SER:OG	7:T:1239:THR:N	2.43	0.49
7:W:131:MET:HE1	7:W:165:LEU:HA	1.94	0.49
7:x:881:ILE:HG13	7:x:884:LEU:HD12	1.94	0.49
4:C:424:HIS:O	4:C:463:VAL:N	2.43	0.49
7:S:464:LEU:HD12	7:S:1254:MET:HE3	1.94	0.49
7:S:619:PHE:HE1	7:S:643:CYS:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:916:ASP:OD1	7:S:916:ASP:N	2.32	0.49
7:W:11:PRO:HB3	7:W:47:GLU:HB3	1.95	0.49
7:W:510:LYS:O	7:W:973:ARG:NH2	2.39	0.49
7:W:1075:SER:OG	2:f:2:ASP:OD2	2.31	0.49
1:5:58:TRP:HZ3	7:x:1074:VAL:HG21	1.78	0.48
7:S:1011:SER:HG	7:S:1014:SER:H	1.60	0.48
7:T:543:HIS:HD2	7:T:545:LEU:H	1.61	0.48
7:T:1260:ARG:NH2	1:e:167:ASP:OD2	2.46	0.48
7:W:1213:GLU:O	7:W:1284:ASN:ND2	2.38	0.48
2:f:264:MET:SD	2:g:209:PHE:CZ	3.06	0.48
1:5:115:GLN:NE2	1:5:123:ASP:OD2	2.38	0.48
2:6:238:LEU:HD11	2:7:215:LEU:HD21	1.95	0.48
7:S:1039:HIS:ND1	7:S:1040:PRO:O	2.32	0.48
7:S:1241:ASN:OD1	7:S:1241:ASN:N	2.45	0.48
7:T:818:PRO:O	7:T:823:ALA:N	2.46	0.48
7:T:1009:LEU:O	7:T:1014:SER:OG	2.30	0.48
7:T:1204:GLY:HA2	7:T:1240:VAL:HG12	1.95	0.48
7:W:956:ASP:HB3	7:W:959:VAL:HG22	1.95	0.48
2:g:55:PRO:HB2	2:g:201:LEU:HD13	1.95	0.48
3:K:31:SER:O	3:K:33:ARG:NH1	2.47	0.48
7:S:181:LEU:HD11	7:S:281:ILE:HG21	1.95	0.48
1:e:358:SER:OG	1:e:359:ASP:N	2.46	0.48
2:6:98:GLN:NE2	2:6:120:HIS:O	2.46	0.48
7:S:89:ILE:O	7:S:124:LYS:NZ	2.45	0.48
7:S:371:VAL:HA	7:S:380:ALA:HA	1.95	0.48
7:S:815:VAL:HG23	7:S:1018:MET:HB3	1.95	0.48
7:S:877:THR:HG22	7:S:880:MET:HG2	1.94	0.48
7:T:268:THR:OG1	7:T:364:ARG:NH1	2.46	0.48
7:T:395:TYR:CE1	7:T:397:LEU:HD12	2.48	0.48
7:x:71:THR:OG1	7:x:72:ALA:N	2.46	0.48
7:S:390:ASP:N	7:S:390:ASP:OD1	2.46	0.48
7:T:61:ASN:OD1	7:T:61:ASN:N	2.44	0.48
7:T:125:HIS:HB2	7:T:1092:MET:HG3	1.95	0.48
7:T:955:GLY:HA3	7:T:985:ARG:HH21	1.78	0.48
7:T:1305:SER:OG	7:T:1306:ASN:N	2.46	0.48
7:W:468:ALA:O	7:W:472:ASN:ND2	2.47	0.48
7:S:488:SER:OG	7:S:992:GLU:N	2.37	0.48
7:S:622:VAL:HG12	7:S:884:LEU:HD11	1.96	0.48
7:S:838:THR:HG23	7:S:864:THR:HB	1.95	0.48
7:T:724:LEU:HD12	7:T:900:VAL:HG11	1.96	0.48
7:T:899:ARG:NH2	7:T:922:THR:OG1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:137:ASP:HA	7:W:140:ILE:HG22	1.95	0.48
7:W:901:SER:O	7:W:918:ARG:NH2	2.43	0.48
7:x:137:ASP:HB2	7:x:157:ALA:HB2	1.96	0.48
2:f:233:HIS:HB2	2:f:236:LEU:HG	1.94	0.48
7:x:1336:SER:OG	7:x:1337:ALA:N	2.47	0.48
2:f:207:LEU:HD11	2:g:236:LEU:HD23	1.95	0.48
2:6:112:MET:HB2	2:6:138:LEU:HD21	1.96	0.48
3:K:47:GLU:HA	3:K:50:ARG:HG2	1.95	0.48
7:T:1372:ILE:HD13	7:T:1381:PHE:CD1	2.38	0.48
7:W:852:ARG:HD2	7:W:879:GLY:HA2	1.96	0.48
7:x:94:GLN:HG2	7:x:119:VAL:HG12	1.96	0.48
7:x:852:ARG:O	7:x:877:THR:OG1	2.28	0.48
1:e:313:ILE:HB	2:f:215:LEU:HD22	1.96	0.48
2:7:49:TYR:OH	2:7:114:PRO:O	2.32	0.48
7:S:395:TYR:CE1	7:S:397:LEU:CA	2.90	0.48
7:W:884:LEU:O	7:W:887:SER:OG	2.32	0.48
7:x:935:GLU:OE2	7:x:965:GLN:NE2	2.47	0.48
2:g:87:PRO:HD3	2:g:300:LEU:HD23	1.95	0.48
1:5:258:CYS:O	1:5:283:SER:OG	2.32	0.48
1:5:327:PHE:HB3	1:5:353:PHE:HD1	1.78	0.48
7:S:497:MET:HE3	7:S:497:MET:HB3	1.81	0.48
7:T:895:THR:OG1	7:T:925:VAL:O	2.31	0.48
7:x:395:TYR:OH	7:x:397:LEU:HD23	2.14	0.48
7:x:1114:THR:OG1	7:x:1115:THR:N	2.47	0.48
1:5:174:ARG:NH1	1:5:178:ASP:OD2	2.47	0.47
7:T:1241:ASN:HD21	7:T:1244:ALA:HB3	1.79	0.47
7:W:81:GLU:N	7:W:309:ALA:O	2.42	0.47
7:W:129:THR:OG1	7:W:130:GLU:N	2.44	0.47
7:x:516:THR:HG23	7:x:519:ALA:H	1.79	0.47
4:C:7:ASN:ND2	4:C:60:VAL:CG1	2.77	0.47
7:T:230:LEU:HD23	7:T:1109:ARG:HD2	1.96	0.47
7:W:986:PRO:O	7:W:990:PHE:N	2.43	0.47
7:x:85:LEU:HD11	7:x:1068:PHE:HB3	1.96	0.47
7:x:155:VAL:HA	7:x:158:VAL:HG12	1.96	0.47
7:x:159:LYS:HD2	7:x:159:LYS:HA	1.65	0.47
6:y:59:GLU:O	6:y:63:ARG:NH2	2.47	0.47
2:g:29:LEU:HD12	2:g:44:GLY:H	1.79	0.47
2:g:33:SER:H	2:g:38:GLN:HE22	1.62	0.47
2:7:221:MET:HA	2:7:224:VAL:HG12	1.97	0.47
7:S:636:ASN:HB3	7:S:639:LEU:HD23	1.95	0.47
7:S:1118:GLY:H	7:S:1180:ALA:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:1236:TYR:OH	7:S:1237:ARG:NH2	2.40	0.47
7:T:1246:GLN:HB2	7:T:1249:SER:HB3	1.95	0.47
7:x:176:LEU:HD11	7:x:1069:ILE:CD1	2.43	0.47
6:Y:66:GLY:HA2	6:Y:69:ARG:HH12	1.78	0.47
7:S:566:LEU:HD21	7:S:919:THR:HG21	1.95	0.47
7:S:1231:ASP:OD1	7:S:1234:TYR:N	2.37	0.47
7:T:487:TYR:OH	7:T:985:ARG:N	2.47	0.47
7:x:631:GLU:OE2	7:x:769:MET:N	2.41	0.47
2:6:218:ARG:NH2	2:6:221:MET:SD	2.85	0.47
2:7:129:ASP:OD1	2:7:129:ASP:N	2.43	0.47
3:K:41:LEU:HA	3:K:44:ARG:HE	1.79	0.47
3:G:61:LEU:HB2	3:G:64:ARG:HH11	1.79	0.47
7:T:657:VAL:HA	7:T:663:ILE:HD11	1.96	0.47
2:7:237:ASN:HD22	2:7:240:GLN:HE21	1.62	0.47
2:7:249:ARG:NH1	4:C:9:VAL:O	2.47	0.47
4:C:342:LEU:HD13	4:C:398:SER:HB3	1.96	0.47
7:T:130:GLU:OE2	7:T:1077:ARG:NH2	2.44	0.47
7:x:1205:ARG:NH2	7:x:1223:LEU:O	2.35	0.47
1:e:261:ASP:OD1	1:e:261:ASP:N	2.42	0.47
4:C:48:PHE:HE2	4:C:55:THR:HG21	1.77	0.47
4:C:279:ARG:NH2	4:C:303:PRO:O	2.37	0.47
7:S:174:ARG:HB3	7:T:102:ILE:HG22	1.96	0.47
7:W:783:ARG:HG2	7:W:833:GLN:HE21	1.79	0.47
7:W:1276:ASN:OD1	7:W:1276:ASN:N	2.48	0.47
7:x:592:THR:HG21	7:x:696:ALA:HB1	1.97	0.47
7:x:742:ARG:HE	7:x:905:ASP:HA	1.80	0.47
7:x:821:THR:O	7:x:823:ALA:N	2.46	0.47
1:5:333:TRP:HZ3	1:5:335:ARG:HE	1.63	0.47
7:S:564:HIS:NE2	7:S:908:GLN:OE1	2.48	0.47
7:S:1067:MET:HE3	7:S:1069:ILE:HD11	1.96	0.47
7:x:922:THR:HG23	7:x:950:PHE:HD2	1.78	0.47
1:5:328:SER:OG	1:5:352:SER:OG	2.29	0.47
7:S:565:ARG:HB3	7:S:570:ASN:HB3	1.96	0.47
7:S:887:SER:O	7:S:887:SER:OG	2.33	0.47
7:T:1209:VAL:HG22	7:T:1210:VAL:HG13	1.96	0.47
7:T:1285:ARG:HE	7:T:1286:GLY:H	1.63	0.47
7:W:67:ARG:HB3	7:W:70:GLU:HB2	1.97	0.47
7:W:658:ASN:OD1	7:W:658:ASN:N	2.40	0.47
7:x:347:SER:N	7:x:350:SER:OG	2.44	0.47
7:x:670:LEU:HG	7:x:675:ILE:HD11	1.97	0.47
7:x:828:LEU:HD12	7:x:945:PHE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:179:VAL:HG23	2:7:186:TYR:HB2	1.97	0.47
4:C:63:ALA:O	4:C:76:THR:OG1	2.31	0.47
4:C:276:ARG:NH1	4:C:302:TYR:OH	2.47	0.47
7:S:461:HIS:CE1	7:S:1128:PHE:HB2	2.50	0.47
7:S:488:SER:OG	7:S:488:SER:O	2.26	0.47
7:W:977:GLN:NE2	7:W:982:ALA:O	2.47	0.47
7:x:1042:VAL:HG13	7:x:1186:VAL:HG13	1.96	0.47
2:f:73:ASP:OD1	2:f:73:ASP:N	2.47	0.47
2:g:109:LEU:N	2:g:284:LEU:O	2.40	0.47
7:S:720:ASP:O	7:S:810:LYS:NZ	2.34	0.46
7:S:843:GLY:HA3	7:S:844:PRO:HD3	1.82	0.46
7:W:906:VAL:HG11	7:W:1135:ASN:HB2	1.97	0.46
7:x:269:THR:HG23	7:x:273:GLY:H	1.80	0.46
7:x:349:LYS:HA	7:x:352:LEU:HD23	1.97	0.46
7:x:934:SER:OG	7:x:935:GLU:N	2.47	0.46
3:G:51:SER:HA	3:G:54:TRP:HD1	1.79	0.46
7:S:543:HIS:CD2	7:S:545:LEU:H	2.31	0.46
7:T:395:TYR:CE1	7:T:397:LEU:CG	2.88	0.46
7:T:876:PRO:HG2	7:T:881:ILE:HD11	1.96	0.46
7:T:1064:SER:OG	7:T:1065:THR:N	2.48	0.46
7:W:948:ILE:HG22	7:W:950:PHE:HB3	1.96	0.46
7:x:618:PHE:HA	7:x:621:VAL:HG12	1.97	0.46
7:x:835:VAL:HG12	7:x:944:LEU:HD12	1.97	0.46
1:e:107:GLY:O	1:e:224:THR:N	2.35	0.46
2:g:172:VAL:HB	2:g:176:LEU:HD12	1.98	0.46
6:Y:11:GLN:NE2	7:S:862:ASN:O	2.48	0.46
6:Z:5:LEU:HD22	7:T:500:LEU:HD22	1.97	0.46
7:S:395:TYR:CD1	7:S:397:LEU:CB	2.80	0.46
7:T:1012:LEU:HA	7:T:1015:ILE:HD12	1.97	0.46
7:W:494:PRO:O	7:W:750:ASN:ND2	2.46	0.46
7:W:536:ASP:N	7:W:536:ASP:OD1	2.40	0.46
7:x:713:GLN:HB2	7:x:720:ASP:HA	1.98	0.46
7:x:904:ASN:ND2	7:x:917:LYS:O	2.48	0.46
1:e:180:ARG:HH12	2:f:265:ARG:HB3	1.80	0.46
4:C:21:LEU:HD12	4:C:299:VAL:HA	1.98	0.46
7:T:1044:MET:SD	7:T:1044:MET:N	2.88	0.46
7:W:565:ARG:HG3	7:W:998:ARG:HH12	1.80	0.46
7:x:134:SER:HA	7:x:1083:ALA:HA	1.97	0.46
7:x:832:PHE:HA	7:x:835:VAL:HG22	1.97	0.46
7:x:913:ASN:HB3	7:x:916:ASP:HB2	1.97	0.46
2:6:148:GLN:HE22	2:7:265:ARG:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:646:THR:HG21	7:W:874:LEU:HD22	1.97	0.46
7:W:1239:THR:OG1	7:W:1240:VAL:N	2.48	0.46
7:x:256:SER:OG	7:x:1100:SER:OG	2.29	0.46
7:x:283:THR:OG1	7:x:385:GLN:OE1	2.33	0.46
7:x:385:GLN:HE21	7:x:389:ASN:HD21	1.64	0.46
7:x:395:TYR:CD1	7:x:395:TYR:C	2.94	0.46
7:x:898:VAL:HG13	7:x:923:VAL:HG13	1.97	0.46
2:6:149:LYS:HZ2	2:6:176:LEU:HG	1.79	0.46
2:f:49:TYR:HE1	2:f:55:PRO:HB3	1.80	0.46
2:g:168:ASP:HB3	2:g:171:ASP:HB2	1.98	0.46
2:6:216:LEU:HD12	2:7:213:VAL:HB	1.98	0.46
4:C:471:GLY:HA2	4:C:487:LEU:HD22	1.98	0.46
6:Y:23:LEU:HD13	6:Y:51:LEU:HB3	1.97	0.46
7:S:840:ALA:HB2	7:S:885:SER:HB2	1.96	0.46
7:W:1044:MET:SD	7:W:1044:MET:N	2.88	0.46
2:f:212:MET:HE1	2:f:270:TYR:HB3	1.97	0.46
2:6:211:ILE:O	2:6:214:THR:OG1	2.33	0.46
7:S:956:ASP:OD1	7:S:959:VAL:N	2.48	0.46
7:T:1277:LYS:HA	7:T:1280:LEU:HB2	1.98	0.46
7:W:567:MET:H	7:W:570:ASN:HD22	1.63	0.46
7:x:172:LEU:HD13	7:x:172:LEU:HA	1.76	0.46
4:C:38:ASN:HB2	4:C:104:ASP:HB3	1.98	0.46
4:C:49:SER:O	4:C:337:ARG:NH1	2.49	0.46
7:S:195:GLN:HE22	7:S:226:HIS:CG	2.33	0.46
7:T:631:GLU:HA	7:T:634:VAL:HG12	1.98	0.46
7:T:1079:ALA:HA	7:T:1084:VAL:HG23	1.98	0.46
7:W:822:ASN:HB2	7:W:824:HIS:HD2	1.80	0.46
2:f:108:SER:O	2:f:140:THR:OG1	2.33	0.46
2:g:56:ASP:H	2:g:60:MET:HE3	1.81	0.46
2:6:216:LEU:HD11	2:7:216:LEU:HD22	1.98	0.45
2:6:232:HIS:CE1	2:6:241:GLU:H	2.35	0.45
3:G:64:ARG:HG2	3:G:67:ARG:HH21	1.81	0.45
6:2:49:VAL:HG21	7:W:836:ALA:HB1	1.98	0.45
7:S:666:ILE:HG23	7:S:670:LEU:HD23	1.97	0.45
7:x:323:SER:OG	7:x:324:TYR:N	2.49	0.45
2:6:274:LEU:HD21	2:7:271:LEU:HD13	1.98	0.45
7:T:969:THR:O	7:T:973:ARG:NE	2.35	0.45
7:T:1192:ASP:OD1	7:T:1195:TYR:N	2.50	0.45
7:W:518:ILE:HG13	7:W:993:TYR:HE1	1.78	0.45
7:W:593:SER:O	7:W:593:SER:OG	2.32	0.45
7:W:772:MET:N	7:W:772:MET:SD	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:402:GLN:HE21	7:x:1321:LEU:HD11	1.80	0.45
7:x:485:GLU:N	7:x:485:GLU:OE1	2.49	0.45
7:x:795:HIS:HB2	7:x:892:PRO:HB3	1.98	0.45
1:e:133:ILE:HD11	1:e:165:LEU:HD12	1.99	0.45
4:C:52:THR:HG23	4:C:337:ARG:HH21	1.79	0.45
7:W:1008:CYS:SG	7:W:1009:LEU:N	2.90	0.45
6:Y:8:PRO:HD3	7:S:834:HIS:HD2	1.82	0.45
7:S:1230:PRO:HA	7:S:1238:SER:HA	1.98	0.45
7:W:724:LEU:O	7:W:921:GLN:NE2	2.49	0.45
1:5:157:LEU:HD11	1:5:342:GLY:HA3	1.98	0.45
2:7:106:THR:O	2:7:286:THR:OG1	2.34	0.45
5:O:3134:THR:HA	5:O:3137:LEU:HD12	1.99	0.45
7:S:127:ILE:HB	7:S:1090:HIS:HB3	1.99	0.45
7:W:1294:TYR:OH	7:W:1322:GLU:OE1	2.27	0.45
7:x:395:TYR:OH	7:x:397:LEU:CG	2.64	0.45
7:x:395:TYR:OH	7:x:397:LEU:HG	2.17	0.45
7:W:598:VAL:HG13	7:W:602:VAL:HB	1.98	0.45
7:W:742:ARG:NH2	7:W:905:ASP:OD1	2.49	0.45
7:x:1133:PHE:CB	7:x:1139:ASN:CG	2.66	0.45
2:f:274:LEU:HD21	2:g:271:LEU:HD21	1.98	0.45
1:5:290:MET:HE2	1:5:290:MET:HB3	1.81	0.45
2:6:275:ALA:HB2	2:7:275:ALA:HB1	1.99	0.45
4:C:117:LEU:O	4:C:121:GLU:HB2	2.17	0.45
7:S:24:ASN:ND2	7:x:203:THR:O	2.46	0.45
7:T:211:VAL:O	7:T:215:LEU:HB2	2.17	0.45
7:T:716:CYS:SG	7:T:719:LEU:N	2.89	0.45
7:W:891:CYS:HA	7:W:892:PRO:HD3	1.86	0.45
7:W:947:ALA:HB2	7:W:963:MET:HB3	1.98	0.45
7:W:1208:CYS:SG	7:W:1211:SER:HB3	2.57	0.45
7:W:1343:ILE:HD13	7:W:1362:ILE:HD11	1.98	0.45
7:x:768:ASN:OD1	7:x:771:GLU:N	2.50	0.45
6:y:31:ASN:ND2	6:y:34:ASN:OD1	2.50	0.45
7:S:868:LEU:HD23	7:S:868:LEU:HA	1.78	0.45
7:T:450:PHE:HB2	7:T:1119:ILE:HG13	1.99	0.45
7:W:970:PHE:HZ	7:W:984:ASN:HD22	1.62	0.45
1:5:298:SER:HA	1:5:301:ILE:HG12	1.98	0.45
1:5:313:ILE:HG12	2:6:215:LEU:HD21	1.98	0.45
2:6:228:ILE:HG22	2:6:229:ARG:HD2	1.99	0.45
3:G:78:LEU:HD12	3:G:81:ALA:HB3	1.99	0.45
7:S:1182:CYS:HA	7:S:1270:PRO:HG2	1.98	0.45
7:W:184:LYS:HD3	7:W:184:LYS:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:407:PHE:HB2	7:W:1336:SER:HB3	1.98	0.45
1:e:271:GLU:HG3	1:e:273:ALA:H	1.82	0.45
7:W:421:SER:HB2	7:W:1354:ALA:HB2	1.99	0.45
7:W:538:LEU:HD11	7:W:1242:PRO:HB3	1.99	0.45
7:x:420:THR:HG21	7:x:1355:PRO:HD2	1.99	0.45
2:f:39:ASN:OD1	2:f:39:ASN:N	2.42	0.45
2:f:226:GLY:O	2:f:230:HIS:HB2	2.17	0.45
2:g:69:LEU:HB2	2:g:85:ILE:HD11	1.98	0.45
2:6:69:LEU:HD23	2:6:69:LEU:HA	1.88	0.44
2:6:227:LEU:HD23	2:6:227:LEU:HA	1.84	0.44
4:C:474:PHE:HE1	4:C:484:LYS:HG2	1.82	0.44
7:S:1056:ASN:ND2	7:S:1105:MET:SD	2.89	0.44
7:S:1268:TYR:HD2	7:S:1312:VAL:HG22	1.81	0.44
7:W:471:LEU:HD21	7:W:562:ALA:HB2	1.99	0.44
7:W:639:LEU:HD21	7:W:884:LEU:HD22	1.99	0.44
7:x:68:PHE:HE1	7:x:180:VAL:HG21	1.82	0.44
7:x:637:VAL:HG13	7:x:638:PRO:HD3	1.99	0.44
7:x:770:ASP:OD1	6:y:57:TYR:OH	2.31	0.44
7:x:1026:SER:OG	7:x:1029:ALA:N	2.41	0.44
2:f:155:VAL:HG13	2:f:156:TYR:HD1	1.82	0.44
2:f:177:GLY:HA3	2:f:190:LEU:HD11	1.98	0.44
2:g:13:LEU:HD13	2:g:17:GLU:HB3	1.99	0.44
4:C:90:GLU:HA	4:C:314:MET:HG2	1.99	0.44
7:T:269:THR:OG1	7:T:272:GLY:O	2.34	0.44
7:T:1381:PHE:CD2	7:T:1381:PHE:O	2.70	0.44
2:g:184:HIS:HB3	2:g:186:TYR:CZ	2.53	0.44
2:6:38:GLN:HB3	2:6:39:ASN:H	1.64	0.44
4:C:305:LEU:O	4:C:309:GLY:N	2.50	0.44
6:Z:49:VAL:HA	6:Z:52:THR:HG22	1.99	0.44
7:S:255:VAL:HG11	7:S:1059:PHE:HE2	1.83	0.44
7:S:618:PHE:HA	7:S:621:VAL:HG22	1.98	0.44
7:S:1052:ILE:HG12	7:S:1113:ILE:HG23	2.00	0.44
7:T:335:MET:HB3	7:T:335:MET:HE2	1.79	0.44
7:T:815:VAL:HG21	7:T:1019:THR:HB	1.99	0.44
7:T:1039:HIS:ND1	7:T:1040:PRO:O	2.41	0.44
7:x:91:GLY:N	7:x:122:CYS:SG	2.84	0.44
7:x:632:LYS:HA	7:x:635:MET:HE2	1.99	0.44
2:f:22:GLN:HG2	2:f:75:VAL:HG13	1.98	0.44
2:6:154:ASN:HB2	2:6:194:PRO:HB3	2.00	0.44
6:2:10:LEU:HD21	7:W:837:GLN:HB3	2.00	0.44
7:S:465:HIS:CE1	7:S:1027:PRO:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:852:ARG:HG3	7:S:879:GLY:HA3	1.99	0.44
7:T:1335:LEU:HD21	7:T:1343:ILE:HD11	1.99	0.44
6:y:20:ASP:OD1	6:y:20:ASP:N	2.39	0.44
2:6:57:TYR:HE2	2:6:191:PRO:HD3	1.82	0.44
2:7:25:ILE:HD12	2:7:25:ILE:HA	1.90	0.44
4:C:35:ARG:HE	4:C:64:ARG:HH21	1.65	0.44
6:2:70:ARG:NH1	6:y:13:ARG:O	2.38	0.44
7:S:662:MET:HE2	7:S:666:ILE:HG13	2.00	0.44
7:T:143:SER:OG	7:T:144:ILE:N	2.50	0.44
7:W:720:ASP:OD2	7:W:1024:LYS:NZ	2.49	0.44
7:W:1123:ASP:OD2	7:W:1126:SER:N	2.51	0.44
7:x:68:PHE:O	7:x:68:PHE:CD2	2.70	0.44
7:x:447:LEU:HD12	7:x:447:LEU:HA	1.83	0.44
7:x:724:LEU:HD12	7:x:725:PRO:HD2	1.99	0.44
1:e:287:CYS:SG	1:e:288:GLN:N	2.90	0.44
7:S:967:VAL:HA	7:S:970:PHE:HB3	1.98	0.44
7:x:337:ARG:HA	7:x:337:ARG:HD3	1.85	0.44
2:7:156:TYR:HA	2:7:159:VAL:HG12	1.99	0.44
4:C:76:THR:HG1	4:C:77:PHE:H	1.65	0.44
6:Z:30:LEU:HG	6:Z:40:PHE:HE1	1.83	0.44
7:S:481:ARG:HH11	7:S:483:ARG:HE	1.65	0.44
7:S:592:THR:HG21	7:S:696:ALA:HB1	1.99	0.44
7:T:781:GLY:HA2	7:T:784:VAL:HG12	1.99	0.44
7:T:1123:ASP:OD1	7:T:1126:SER:N	2.51	0.44
7:W:831:ASP:HB3	7:W:834:HIS:HB2	2.00	0.44
2:f:227:LEU:HD12	2:f:227:LEU:HA	1.83	0.44
2:g:13:LEU:HD22	2:g:17:GLU:HG3	2.00	0.44
2:g:21:MET:HB3	2:g:75:VAL:HG21	1.99	0.44
7:W:587:GLN:NE2	7:W:1037:LYS:O	2.50	0.44
7:W:1277:LYS:HE3	7:W:1277:LYS:HB3	1.80	0.44
2:6:247:ILE:HA	2:6:250:ILE:HG12	1.99	0.44
7:S:570:ASN:HD21	7:S:998:ARG:NE	2.16	0.44
7:S:896:ARG:HB2	7:S:925:VAL:HB	1.98	0.44
7:T:724:LEU:O	7:T:814:TYR:OH	2.34	0.44
7:T:795:HIS:CE1	7:T:896:ARG:HH12	2.36	0.44
7:x:848:HIS:NE2	6:y:56:CYS:SG	2.88	0.44
7:S:665:PHE:O	7:S:669:HIS:HB2	2.17	0.43
7:T:1028:MET:SD	7:T:1028:MET:N	2.91	0.43
2:6:45:LEU:HB3	2:6:133:VAL:HG23	2.00	0.43
4:C:367:GLU:HB3	4:C:482:VAL:HG21	1.99	0.43
7:S:1186:VAL:HG12	7:S:1250:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:815:VAL:HG11	7:W:1019:THR:HB	1.99	0.43
7:x:485:GLU:HG2	7:x:489:LEU:HD21	2.00	0.43
1:e:137:HIS:CD2	1:e:162:PRO:HG3	2.54	0.43
1:e:359:ASP:OD1	2:g:283:ARG:NH2	2.52	0.43
2:f:25:ILE:HG23	2:f:73:ASP:HA	2.00	0.43
2:f:146:VAL:HG22	2:f:179:VAL:HG11	2.00	0.43
1:5:263:ARG:HG2	1:5:326:THR:HG22	1.99	0.43
2:7:242:MET:HE2	2:7:242:MET:HB3	1.96	0.43
2:7:259:ASP:OD1	2:7:259:ASP:N	2.50	0.43
4:C:114:ILE:HD12	4:C:114:ILE:HA	1.93	0.43
7:T:1133:PHE:C	7:T:1139:ASN:HD21	2.26	0.43
7:W:195:GLN:NE2	7:W:250:GLU:OE2	2.51	0.43
7:W:391:THR:HG21	7:x:102:ILE:HG13	2.00	0.43
7:W:1250:LEU:HD12	7:W:1250:LEU:HA	1.78	0.43
7:x:1064:SER:O	7:x:1097:THR:OG1	2.27	0.43
6:y:38:ASP:OD1	6:y:38:ASP:N	2.51	0.43
1:e:47:ALA:O	1:e:48:GLN:NE2	2.47	0.43
2:7:49:TYR:HA	2:7:55:PRO:HB3	2.01	0.43
7:S:229:PHE:HZ	7:S:1057:ILE:HD12	1.83	0.43
7:S:463:ARG:HG2	7:S:1254:MET:HE1	2.00	0.43
7:T:723:LEU:HB3	7:T:810:LYS:HD3	1.99	0.43
7:W:487:TYR:OH	7:W:985:ARG:N	2.50	0.43
7:W:828:LEU:HD12	7:W:945:PHE:HB3	1.99	0.43
1:5:196:LYS:HA	1:5:201:ASN:HD21	1.83	0.43
6:Z:4:ARG:HH22	7:T:833:GLN:HB2	1.83	0.43
7:T:1337:ALA:HB2	7:T:1343:ILE:HD13	1.99	0.43
7:x:660:PHE:CZ	7:x:808:LEU:HB3	2.53	0.43
2:f:106:THR:HG22	2:f:288:ALA:H	1.83	0.43
2:7:138:LEU:HD12	2:7:142:ILE:HG22	2.00	0.43
7:T:85:LEU:HD23	7:T:1091:GLU:HB2	2.01	0.43
7:T:737:LEU:HD23	7:T:737:LEU:HA	1.86	0.43
2:f:152:LEU:HA	2:f:155:VAL:HG12	2.00	0.43
1:5:151:LEU:HD21	1:5:228:GLU:HB3	2.00	0.43
2:6:84:LYS:HE3	2:6:84:LYS:HB2	1.88	0.43
4:C:1:MET:HB3	4:C:276:ARG:HE	1.84	0.43
7:S:182:SER:O	7:S:186:ARG:HB2	2.19	0.43
7:W:813:TYR:O	7:W:954:TYR:OH	2.30	0.43
7:x:705:VAL:HG12	7:x:710:SER:HA	2.01	0.43
7:T:172:LEU:HD23	7:T:172:LEU:HA	1.82	0.43
7:T:690:LEU:HD21	7:T:812:PHE:HD1	1.84	0.43
7:T:722:ASN:HD21	7:T:740:SER:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:136:MET:HE3	2:g:136:MET:HB3	1.90	0.43
1:5:207:VAL:HG11	2:7:287:ALA:HB1	2.01	0.43
1:5:311:LEU:HD12	4:C:266:ARG:HE	1.84	0.43
3:G:74:MET:HE2	5:O:3141:LEU:HB3	2.01	0.43
7:S:94:GLN:HB2	7:S:119:VAL:HG12	2.01	0.43
7:S:889:MET:HE3	7:S:889:MET:HB2	1.80	0.43
7:T:932:ALA:HA	7:T:959:VAL:HG13	2.01	0.43
7:W:921:GLN:HB2	7:W:996:TRP:CD1	2.53	0.43
7:x:385:GLN:HG2	7:x:389:ASN:HD21	1.84	0.43
7:x:1133:PHE:CB	7:x:1139:ASN:ND2	2.80	0.43
7:x:1328:LEU:HD12	7:x:1330:GLU:H	1.84	0.43
1:e:179:ARG:HG3	1:e:315:GLU:HA	2.00	0.43
2:g:68:THR:OG1	2:g:69:LEU:N	2.50	0.43
4:C:28:MET:HE2	4:C:28:MET:HB2	1.83	0.43
7:T:481:ARG:HH21	7:T:550:ILE:HG22	1.84	0.43
7:T:1223:LEU:HD23	7:T:1223:LEU:HA	1.87	0.43
7:T:1372:ILE:HD11	7:T:1381:PHE:CE1	2.53	0.43
7:W:186:ARG:HH11	7:W:1296:GLN:HB2	1.84	0.43
7:x:401:MET:SD	7:x:403:TYR:OH	2.68	0.43
7:x:1012:LEU:HD13	7:x:1012:LEU:HA	1.80	0.43
1:5:114:LYS:HE2	2:7:104:HIS:HB3	2.00	0.42
2:7:48:VAL:HG13	2:7:60:MET:HE2	2.01	0.42
7:S:291:LEU:HD23	7:S:291:LEU:HA	1.86	0.42
7:S:395:TYR:CD1	7:S:395:TYR:C	2.96	0.42
7:S:413:MET:HE1	7:S:1193:VAL:HG11	2.01	0.42
7:S:494:PRO:HD2	7:S:749:GLY:HA2	2.01	0.42
7:S:933:PHE:CD2	7:S:963:MET:HG2	2.54	0.42
7:T:728:ALA:HB3	7:T:925:VAL:HA	2.01	0.42
7:x:409:VAL:HG11	7:x:450:PHE:HE2	1.84	0.42
7:x:635:MET:HG3	6:y:60:TYR:CZ	2.54	0.42
7:x:638:PRO:HA	7:x:641:SER:HB3	2.01	0.42
2:6:215:LEU:HB3	2:6:263:ARG:HG2	2.01	0.42
7:S:411:LEU:HD23	7:S:411:LEU:HA	1.83	0.42
7:S:795:HIS:H	7:S:896:ARG:HH11	1.65	0.42
7:W:307:SER:OG	7:W:308:TYR:N	2.51	0.42
7:x:514:PRO:HD2	7:x:984:ASN:HD21	1.84	0.42
7:x:706:VAL:HG21	7:x:1138:VAL:HG22	2.01	0.42
7:x:941:THR:HA	7:x:944:LEU:HD23	2.01	0.42
2:g:102:GLN:HE22	2:g:291:GLN:HG3	1.84	0.42
1:5:109:PRO:HA	1:5:190:PRO:HA	2.01	0.42
1:5:351:ASP:OD1	1:5:351:ASP:N	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:64:ARG:HA	4:C:76:THR:HG1	1.83	0.42
6:2:56:CYS:HA	6:2:59:GLU:HG2	2.01	0.42
7:S:62:ALA:O	7:S:64:GLN:NE2	2.53	0.42
7:S:698:MET:HE3	7:T:978:ARG:HB2	2.01	0.42
7:S:715:VAL:HG23	7:S:1029:ALA:HA	2.00	0.42
7:S:1357:HIS:HD1	7:S:1358:TYR:H	1.66	0.42
2:f:24:ARG:NH2	2:f:98:GLN:OE1	2.48	0.42
1:5:153:ARG:HG3	1:5:154:MET:HE2	2.01	0.42
1:5:294:ARG:O	1:5:298:SER:OG	2.34	0.42
2:6:225:ARG:HH12	2:6:248:ALA:HA	1.84	0.42
7:S:43:LYS:H	7:S:43:LYS:HG2	1.69	0.42
7:S:130:GLU:HG3	7:T:112:LYS:HE3	2.01	0.42
7:T:328:MET:HE2	7:T:328:MET:HB3	1.89	0.42
7:T:567:MET:HB2	7:T:569:GLY:H	1.84	0.42
7:T:715:VAL:HA	7:T:1029:ALA:HB2	2.01	0.42
7:T:1347:MET:HE1	7:T:1373:LEU:HD23	2.00	0.42
7:W:832:PHE:HA	7:W:835:VAL:HG12	2.02	0.42
7:W:933:PHE:HB2	7:W:962:THR:HG23	2.01	0.42
7:W:1179:GLN:NE2	7:W:1308:GLU:CD	2.78	0.42
7:W:1335:LEU:N	7:W:1365:GLU:OE2	2.52	0.42
7:x:451:ASN:OD1	7:x:454:ASN:N	2.46	0.42
1:5:128:PRO:HA	1:5:131:LEU:HB3	2.01	0.42
7:S:143:SER:OG	7:S:144:ILE:N	2.53	0.42
7:T:522:CYS:HB3	7:T:1000:PRO:HG3	2.02	0.42
7:T:532:PRO:HG3	7:T:1238:SER:HB3	2.01	0.42
7:x:520:LEU:HD23	7:x:520:LEU:HA	1.87	0.42
7:x:654:LEU:HD12	7:x:683:TYR:CZ	2.54	0.42
7:x:1037:LYS:HD3	7:x:1037:LYS:HA	1.83	0.42
7:x:1064:SER:OG	7:x:1065:THR:N	2.53	0.42
2:f:29:LEU:HD23	2:f:29:LEU:HA	1.93	0.42
2:f:112:MET:HE2	2:f:112:MET:HB2	1.84	0.42
2:g:24:ARG:NH2	2:g:98:GLN:OE1	2.41	0.42
1:5:101:ASN:HB2	1:5:159:TYR:HE1	1.84	0.42
4:C:100:LEU:HB2	4:C:112:LEU:HB3	2.02	0.42
7:T:402:GLN:NE2	7:T:1051:GLU:OE1	2.53	0.42
7:W:238:SER:O	7:W:238:SER:OG	2.37	0.42
7:W:629:PHE:HE2	7:W:632:LYS:HE3	1.84	0.42
7:W:856:ILE:HG22	7:W:860:LEU:HB2	2.01	0.42
7:W:911:ALA:O	7:W:917:LYS:NZ	2.48	0.42
6:2:63:ARG:NH1	7:W:883:ASP:OD1	2.53	0.42
7:S:1024:LYS:HB3	7:S:1024:LYS:HE2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:208:SER:OG	7:T:210:THR:OG1	2.37	0.42
7:T:725:PRO:HA	7:T:726:PRO:HD3	1.91	0.42
7:T:764:GLU:N	7:T:794:LEU:O	2.48	0.42
7:W:518:ILE:HG22	7:W:518:ILE:O	2.19	0.42
7:W:677:LYS:HG3	7:x:651:SER:HA	2.01	0.42
7:x:218:MET:HE3	7:x:218:MET:HB3	1.86	0.42
2:f:30:PRO:HD3	2:f:135:PRO:HG3	2.01	0.42
2:f:283:ARG:HG2	2:f:301:ARG:HH11	1.84	0.42
1:5:293:LEU:O	1:5:297:TYR:HB2	2.20	0.42
7:S:220:LYS:HB3	7:S:220:LYS:HE2	1.82	0.42
7:S:1195:TYR:OH	7:S:1203:ARG:O	2.29	0.42
7:S:1272:ARG:HD3	7:S:1301:HIS:CE1	2.55	0.42
7:T:67:ARG:HB2	7:T:70:GLU:HB2	2.02	0.42
7:T:600:GLN:HE22	7:T:1011:SER:HA	1.85	0.42
7:W:181:LEU:HD12	7:W:181:LEU:HA	1.86	0.42
7:W:495:ASN:HA	7:W:750:ASN:HD21	1.84	0.42
7:x:815:VAL:HG21	7:x:1019:THR:HB	2.01	0.42
1:e:154:MET:HE2	1:e:154:MET:HB2	1.78	0.42
2:6:120:HIS:NE2	2:6:136:MET:SD	2.85	0.42
2:6:283:ARG:HG3	2:6:301:ARG:HH11	1.85	0.42
3:G:88:LEU:HD22	5:O:3127:ARG:HG2	2.02	0.42
7:S:67:ARG:HB2	7:S:70:GLU:HB2	2.01	0.42
7:S:791:ASP:OD1	7:S:791:ASP:N	2.38	0.42
7:T:67:ARG:NE	7:T:70:GLU:OE1	2.50	0.42
7:x:181:LEU:HD12	7:x:181:LEU:HA	1.81	0.42
7:x:373:LYS:HE3	7:x:373:LYS:HB3	1.84	0.42
2:f:112:MET:N	2:f:136:MET:O	2.53	0.42
3:G:71:ASP:OD1	5:B:3145:LYS:NZ	2.53	0.42
7:S:11:PRO:HG2	7:T:322:VAL:HG23	2.02	0.42
7:S:185:LEU:HD13	7:S:399:ARG:HH11	1.83	0.42
7:S:591:ALA:HB1	7:S:1036:LEU:HG	2.01	0.42
7:W:53:GLU:HG2	7:x:90:ASP:HB3	2.02	0.42
7:W:212:LYS:HD2	7:W:1210:VAL:HB	2.02	0.42
7:W:531:HIS:HA	7:W:532:PRO:HD3	1.85	0.42
7:W:1054:SER:OG	7:W:1056:ASN:OD1	2.37	0.42
7:W:1179:GLN:HE21	7:W:1308:GLU:CD	2.28	0.42
7:x:182:SER:O	7:x:186:ARG:HB2	2.20	0.42
7:x:783:ARG:NH2	7:x:891:CYS:O	2.53	0.42
2:g:14:TYR:CZ	2:g:16:ASP:HB2	2.55	0.42
2:7:10:SER:OG	2:7:11:SER:N	2.53	0.41
6:Y:4:ARG:HH21	7:S:834:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:398:ASN:HB3	7:S:1053:LEU:HD11	2.01	0.41
7:S:727:VAL:HG22	7:S:813:TYR:HE2	1.85	0.41
7:S:804:HIS:HB3	7:S:807:VAL:HG12	2.02	0.41
7:T:828:LEU:HD12	7:T:945:PHE:HB3	2.01	0.41
7:x:471:LEU:HD21	7:x:562:ALA:HB2	2.01	0.41
7:x:1128:PHE:HZ	7:x:1260:ARG:HG2	1.85	0.41
2:g:252:LEU:HG	2:g:254:ASP:H	1.85	0.41
2:7:70:ALA:HA	2:7:84:LYS:HA	2.02	0.41
7:S:1187:THR:HG22	7:S:1241:ASN:HD22	1.85	0.41
7:T:1215:TYR:HD1	7:T:1215:TYR:HA	1.79	0.41
7:T:1352:THR:O	7:T:1352:THR:OG1	2.35	0.41
7:x:166:GLN:HA	7:x:169:VAL:HG12	2.02	0.41
7:x:282:VAL:HG12	7:x:1057:ILE:HG12	2.01	0.41
7:x:582:GLU:HB2	7:x:1013:VAL:HG22	2.02	0.41
7:x:1252:ASP:O	7:x:1256:ASN:N	2.53	0.41
2:6:109:LEU:HD12	2:6:109:LEU:HA	1.89	0.41
2:7:110:SER:OG	2:7:280:LEU:O	2.36	0.41
3:K:62:LYS:HA	3:K:62:LYS:HD3	1.87	0.41
3:G:43:GLU:HA	4:C:427:TYR:HD2	1.85	0.41
7:S:5:GLU:HB3	7:S:6:GLY:H	1.73	0.41
7:S:33:LEU:HD13	7:x:1288:TYR:HD1	1.85	0.41
7:S:68:PHE:HA	7:S:177:ILE:HD11	2.02	0.41
7:S:443:LYS:NZ	7:S:444:ASN:OD1	2.43	0.41
7:T:79:ASN:ND2	7:T:308:TYR:CE1	2.88	0.41
7:T:479:ALA:O	7:T:539:ARG:NH2	2.52	0.41
7:T:934:SER:HB3	7:T:937:THR:HG23	2.02	0.41
7:W:722:ASN:HD22	7:W:742:ARG:HH11	1.67	0.41
7:x:951:HIS:O	7:x:955:GLY:N	2.54	0.41
6:y:37:ASN:HD21	6:y:41:ARG:HH21	1.68	0.41
1:e:284:ARG:HB3	1:e:288:GLN:HB2	2.03	0.41
2:f:6:VAL:HG13	2:f:37:THR:HG22	2.03	0.41
2:6:293:THR:O	2:6:293:THR:OG1	2.36	0.41
2:7:38:GLN:HB3	2:7:39:ASN:H	1.71	0.41
3:K:75:ARG:HH11	4:C:125:ARG:HG3	1.85	0.41
7:T:264:VAL:O	7:T:1062:ARG:NH1	2.53	0.41
7:T:813:TYR:O	7:T:954:TYR:OH	2.35	0.41
7:T:961:ALA:HA	7:T:967:VAL:HG23	2.03	0.41
7:T:1044:MET:HE3	7:T:1044:MET:HB3	1.93	0.41
7:W:426:MET:HE1	7:W:1360:HIS:HD2	1.85	0.41
7:W:459:LEU:HA	7:W:464:LEU:HD12	2.03	0.41
7:W:1313:VAL:HG11	7:W:1319:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:x:474:LEU:HB3	7:x:560:HIS:CD2	2.55	0.41
2:6:264:MET:SD	2:7:209:PHE:CZ	3.14	0.41
2:7:11:SER:H	2:7:128:ASN:HD21	1.66	0.41
7:S:132:GLU:HB2	7:T:112:LYS:HD3	2.02	0.41
7:W:155:VAL:HG11	7:x:342:PRO:HB2	2.02	0.41
7:W:185:LEU:HA	7:W:185:LEU:HD23	1.86	0.41
7:W:743:ALA:O	7:W:918:ARG:NH2	2.53	0.41
7:x:358:GLY:O	7:x:362:GLN:HG2	2.20	0.41
2:f:261:LEU:HD21	2:g:176:LEU:HD21	2.03	0.41
3:G:67:ARG:HA	3:G:70:LEU:HG	2.03	0.41
7:S:165:LEU:HD23	7:S:165:LEU:HA	1.88	0.41
7:T:194:LEU:HD23	7:T:194:LEU:HA	1.89	0.41
7:T:838:THR:HG23	7:T:864:THR:HG23	2.02	0.41
7:T:1104:THR:OG1	7:T:1105:MET:N	2.53	0.41
7:W:788:HIS:O	7:W:789:ASP:C	2.64	0.41
1:e:359:ASP:N	1:e:359:ASP:OD2	2.48	0.41
2:7:62:ASN:HD22	2:7:62:ASN:HA	1.66	0.41
6:Z:60:TYR:CZ	7:T:635:MET:HG2	2.55	0.41
7:S:552:ARG:HA	7:S:552:ARG:HD2	1.81	0.41
7:T:1119:ILE:HD13	7:T:1119:ILE:HA	1.81	0.41
7:W:230:LEU:HD12	7:W:230:LEU:HA	1.89	0.41
7:W:619:PHE:HE1	7:W:643:CYS:HB2	1.86	0.41
7:W:710:SER:OG	7:W:711:VAL:N	2.54	0.41
2:g:144:GLU:OE1	2:g:148:GLN:NE2	2.53	0.41
2:6:29:LEU:HD23	2:6:29:LEU:HA	1.90	0.41
2:6:65:SER:HA	2:6:282:PRO:HD3	2.03	0.41
3:K:73:ILE:HG22	5:B:3141:LEU:HD23	2.02	0.41
4:C:111:GLU:OE1	4:C:500:ARG:NH1	2.48	0.41
7:S:67:ARG:NH1	7:S:70:GLU:OE1	2.54	0.41
7:S:223:LEU:HD12	7:S:223:LEU:HA	1.85	0.41
7:S:531:HIS:HD2	7:S:533:SER:HB3	1.86	0.41
7:T:637:VAL:HG13	7:T:638:PRO:HD3	2.03	0.41
7:T:899:ARG:NH1	7:T:991:ALA:H	2.18	0.41
7:W:481:ARG:O	7:W:484:ARG:NE	2.54	0.41
7:W:1252:ASP:N	7:W:1252:ASP:OD1	2.54	0.41
7:x:724:LEU:HD12	7:x:724:LEU:HA	1.84	0.41
7:x:736:LEU:HA	7:x:739:VAL:HG22	2.03	0.41
7:x:860:LEU:HD21	7:x:866:ARG:HD3	2.02	0.41
1:e:289:ILE:HD12	1:e:289:ILE:HA	1.79	0.41
2:6:256:SER:O	2:7:156:TYR:OH	2.36	0.41
2:6:264:MET:HG3	2:7:148:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:221:MET:HE2	2:7:252:LEU:HG	2.02	0.41
4:C:419:LEU:HD12	4:C:419:LEU:HA	1.85	0.41
4:C:490:THR:HG22	4:C:492:GLU:H	1.86	0.41
7:S:424:ILE:HD11	7:S:1341:ALA:HB1	2.03	0.41
7:S:568:VAL:HA	7:S:1025:MET:HE3	2.03	0.41
7:S:629:PHE:HB2	7:S:632:LYS:HB2	2.02	0.41
7:S:814:TYR:HD1	7:S:814:TYR:HA	1.78	0.41
7:S:842:ASN:OD1	7:S:861:GLU:N	2.50	0.41
7:S:1224:ILE:HG12	7:S:1280:LEU:HD21	2.02	0.41
7:W:172:LEU:HA	7:W:172:LEU:HD12	1.82	0.41
7:x:480:PRO:HB3	7:x:557:ARG:HH12	1.85	0.41
7:x:588:PHE:HB2	7:x:1038:ILE:HD11	2.02	0.41
2:f:264:MET:HE1	2:g:209:PHE:CZ	2.56	0.41
2:g:293:THR:OG1	2:g:295:THR:OG1	2.34	0.41
7:T:1213:GLU:OE1	7:T:1216:ASN:HB2	2.21	0.41
7:W:434:LEU:HD22	7:W:583:ALA:HB1	2.02	0.41
7:x:829:GLY:N	7:x:946:HIS:O	2.52	0.41
7:x:881:ILE:HA	7:x:884:LEU:HD12	2.03	0.41
1:e:86:ARG:NH1	2:g:88:GLY:O	2.54	0.41
1:e:102:ASN:HD22	1:e:194:ASN:HD21	1.68	0.41
5:O:3145:LYS:HE3	5:O:3149:LEU:HD22	2.02	0.40
7:T:620:TYR:OH	7:T:931:PHE:N	2.51	0.40
7:W:1287:LEU:HD12	7:W:1287:LEU:HA	1.95	0.40
7:x:603:ILE:HD13	7:x:603:ILE:HA	1.86	0.40
7:x:715:VAL:HG23	7:x:1029:ALA:HA	2.03	0.40
7:x:1229:ARG:HA	7:x:1230:PRO:HD3	1.96	0.40
1:5:284:ARG:HB2	1:5:289:ILE:HD13	2.02	0.40
2:6:161:MET:HE3	2:6:161:MET:HB3	1.88	0.40
2:7:24:ARG:HA	2:7:24:ARG:HD2	1.92	0.40
2:7:53:THR:HB	7:S:1265:PRO:HD3	2.02	0.40
4:C:279:ARG:HB3	4:C:284:LEU:HD11	2.02	0.40
7:T:387:MET:HE3	7:T:387:MET:HB3	1.98	0.40
7:T:547:ASP:HA	7:T:565:ARG:HH21	1.85	0.40
7:T:626:ILE:HD13	7:T:633:PHE:HA	2.03	0.40
7:W:55:LEU:HD23	7:x:328:MET:HG2	2.03	0.40
7:x:787:ASP:OD1	7:x:787:ASP:N	2.53	0.40
7:x:1028:MET:HE2	7:x:1028:MET:HB3	1.77	0.40
7:x:1195:TYR:OH	7:x:1203:ARG:O	2.38	0.40
2:g:86:VAL:N	2:g:91:TYR:OH	2.39	0.40
2:6:103:TRP:CD1	2:6:139:PRO:HG3	2.56	0.40
7:S:14:TYR:HA	7:W:58:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:1272:ARG:CZ	7:S:1276:ASN:HD21	2.34	0.40
7:S:1347:MET:HE3	7:S:1347:MET:HB3	1.90	0.40
7:T:180:VAL:HG13	7:T:1067:MET:HE1	2.04	0.40
7:T:657:VAL:HG12	7:T:663:ILE:HD11	2.04	0.40
7:T:789:ASP:OD1	7:T:790:HIS:N	2.54	0.40
7:W:266:THR:OG1	7:W:267:TYR:N	2.55	0.40
7:x:127:ILE:HD13	7:x:127:ILE:HA	1.89	0.40
1:e:86:ARG:HE	1:e:208:HIS:CE1	2.40	0.40
1:e:160:ASP:OD1	1:e:160:ASP:N	2.47	0.40
2:f:13:LEU:HA	2:f:13:LEU:HD12	1.90	0.40
2:g:188:LEU:HD13	2:g:190:LEU:HD21	2.04	0.40
1:5:68:VAL:O	7:S:142:HIS:NE2	2.34	0.40
1:5:120:SER:O	1:5:120:SER:OG	2.37	0.40
2:7:31:LEU:HD23	2:7:31:LEU:HA	1.87	0.40
7:S:566:LEU:HD11	7:S:919:THR:HG21	2.04	0.40
7:S:567:MET:HE2	7:S:567:MET:HB2	1.87	0.40
7:T:395:TYR:HD1	7:T:397:LEU:N	2.06	0.40
7:T:657:VAL:HG23	7:T:931:PHE:CZ	2.56	0.40
7:T:1347:MET:HE1	7:T:1373:LEU:HB3	2.03	0.40
7:W:541:GLU:OE1	7:W:565:ARG:NH2	2.54	0.40
7:W:722:ASN:ND2	7:W:742:ARG:HD3	2.37	0.40
7:W:1188:PRO:HD2	7:W:1241:ASN:HB2	2.03	0.40
7:W:1268:TYR:CZ	7:W:1303:ALA:HB2	2.56	0.40
1:e:274:GLY:HA2	1:e:275:PRO:HD3	1.91	0.40
2:f:222:ARG:HD2	2:f:222:ARG:HA	1.87	0.40
1:5:286:HIS:NE2	1:5:361:GLU:OE1	2.54	0.40
3:K:80:ARG:HH12	5:B:3137:LEU:HD23	1.86	0.40
4:C:46:THR:O	4:C:46:THR:OG1	2.39	0.40
6:Z:10:LEU:HD13	6:Z:10:LEU:HA	1.80	0.40
6:2:35:LEU:HD12	6:2:39:VAL:HG21	2.04	0.40
7:T:564:HIS:CD2	7:T:908:GLN:HG2	2.57	0.40
7:T:1246:GLN:HE21	7:T:1246:GLN:HB3	1.70	0.40
7:W:388:TYR:O	7:W:391:THR:OG1	2.35	0.40
7:x:405:TYR:HB3	7:x:1334:ALA:HB2	2.03	0.40
7:x:427:LEU:HD12	7:x:427:LEU:HA	1.84	0.40
7:x:498:ASN:OD1	7:x:498:ASN:N	2.54	0.40
7:x:756:THR:HA	7:x:759:ALA:HB2	2.04	0.40
2:f:29:LEU:HD23	2:f:135:PRO:HD2	2.03	0.40
2:g:49:TYR:HD1	2:g:60:MET:HE1	1.85	0.40
2:g:280:LEU:H	2:g:280:LEU:HG	1.51	0.40
2:g:289:TYR:HD1	2:g:296:ALA:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:298:CYS:SG	2:g:299:TRP:N	2.95	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	5	278/364 (76%)	260 (94%)	18 (6%)	0	100	100
1	e	311/364 (85%)	291 (94%)	20 (6%)	0	100	100
2	6	293/301 (97%)	276 (94%)	17 (6%)	0	100	100
2	7	281/301 (93%)	260 (92%)	21 (8%)	0	100	100
2	f	286/301 (95%)	270 (94%)	16 (6%)	0	100	100
2	g	282/301 (94%)	258 (92%)	24 (8%)	0	100	100
3	G	82/570 (14%)	76 (93%)	5 (6%)	1 (1%)	10	42
3	K	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
4	C	334/507 (66%)	301 (90%)	33 (10%)	0	100	100
5	B	33/3149 (1%)	32 (97%)	1 (3%)	0	100	100
5	O	27/3149 (1%)	27 (100%)	0	0	100	100
6	2	72/176 (41%)	60 (83%)	12 (17%)	0	100	100
6	Y	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
6	Z	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
6	y	72/176 (41%)	64 (89%)	8 (11%)	0	100	100
7	S	1286/1381 (93%)	1205 (94%)	81 (6%)	0	100	100
7	T	1301/1381 (94%)	1196 (92%)	105 (8%)	0	100	100
7	W	1320/1381 (96%)	1224 (93%)	95 (7%)	1 (0%)	48	82
7	x	1286/1381 (93%)	1196 (93%)	89 (7%)	1 (0%)	48	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7754/16105 (48%)	7193 (93%)	558 (7%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	789	ASP
7	x	509	ASN
3	G	15	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	234/289 (81%)	231 (99%)	3 (1%)	61	71
1	e	268/289 (93%)	267 (100%)	1 (0%)	84	82
2	6	264/267 (99%)	264 (100%)	0	100	100
2	7	256/267 (96%)	254 (99%)	2 (1%)	73	77
2	f	259/267 (97%)	256 (99%)	3 (1%)	63	73
2	g	256/267 (96%)	254 (99%)	2 (1%)	73	77
3	G	70/465 (15%)	69 (99%)	1 (1%)	59	70
3	K	59/465 (13%)	59 (100%)	0	100	100
4	C	288/400 (72%)	287 (100%)	1 (0%)	86	84
5	B	33/2539 (1%)	33 (100%)	0	100	100
5	O	27/2539 (1%)	27 (100%)	0	100	100
6	2	68/128 (53%)	66 (97%)	2 (3%)	37	58
6	Y	68/128 (53%)	67 (98%)	1 (2%)	57	70
6	Z	68/128 (53%)	67 (98%)	1 (2%)	57	70
6	y	68/128 (53%)	67 (98%)	1 (2%)	57	70
7	S	1101/1171 (94%)	1092 (99%)	9 (1%)	73	77
7	T	1111/1171 (95%)	1100 (99%)	11 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	W	1131/1171 (97%)	1122 (99%)	9 (1%)	73	77
7	x	1099/1171 (94%)	1085 (99%)	14 (1%)	61	71
All	All	6728/13250 (51%)	6667 (99%)	61 (1%)	68	75

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	68	VAL
1	5	277	PHE
1	5	357	VAL
2	7	41	GLN
2	7	133	VAL
3	G	39	LEU
4	C	3	VAL
6	Y	67	VAL
6	Z	62	GLN
6	2	10	LEU
6	2	67	VAL
7	S	436	VAL
7	S	542	LEU
7	S	658	ASN
7	S	815	VAL
7	S	867	ASP
7	S	893	THR
7	S	1110	VAL
7	S	1214	ASN
7	S	1307	THR
7	T	54	VAL
7	T	61	ASN
7	T	118	VAL
7	T	258	GLU
7	T	637	VAL
7	T	704	ASP
7	T	815	VAL
7	T	904	ASN
7	T	1209	VAL
7	T	1317	THR
7	T	1369	VAL
7	W	327	VAL
7	W	415	ASN
7	W	545	LEU

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Mol	Chain	Res	Type
7	W	788	HIS
7	W	929	VAL
7	W	1015	ILE
7	W	1038	ILE
7	W	1304	THR
7	W	1380	VAL
7	x	464	LEU
7	x	524	LEU
7	x	547	ASP
7	x	597	VAL
7	x	637	VAL
7	x	675	ILE
7	x	815	VAL
7	x	819	THR
7	x	898	VAL
7	x	923	VAL
7	x	1028	MET
7	x	1190	THR
7	x	1240	VAL
7	x	1369	VAL
6	y	9	THR
1	e	362	VAL
2	f	51	LEU
2	f	75	VAL
2	f	192	GLU
2	g	138	LEU
2	g	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	96	HIS
1	5	156	ASN
1	5	183	ASN
1	5	208	HIS
1	5	312	HIS
2	6	22	GLN
2	6	148	GLN
2	6	154	ASN
2	6	204	ASN
2	6	230	HIS
2	6	279	ASN

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Mol	Chain	Res	Type
2	7	62	ASN
2	7	173	HIS
2	7	237	ASN
3	G	30	ASN
4	C	38	ASN
4	C	73	HIS
4	C	410	ASN
4	C	424	HIS
4	C	486	GLN
6	Z	11	GLN
6	Z	33	ASN
6	2	37	ASN
7	S	64	GLN
7	S	166	GLN
7	S	195	GLN
7	S	398	ASN
7	S	402	GLN
7	S	465	HIS
7	S	469	HIS
7	S	495	ASN
7	S	534	ASN
7	S	543	HIS
7	S	560	HIS
7	S	596	HIS
7	S	600	GLN
7	S	636	ASN
7	S	745	GLN
7	S	750	ASN
7	S	761	GLN
7	S	790	HIS
7	S	921	GLN
7	S	1089	HIS
7	S	1137	GLN
7	S	1261	GLN
7	S	1276	ASN
7	S	1301	HIS
7	S	1306	ASN
7	S	1353	HIS
7	T	113	GLN
7	T	398	ASN
7	T	465	HIS
7	T	475	ASN

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Mol	Chain	Res	Type
7	T	543	HIS
7	T	586	GLN
7	T	788	HIS
7	T	834	HIS
7	T	904	ASN
7	T	965	GLN
7	T	1178	GLN
7	T	1217	GLN
7	T	1241	ASN
7	T	1246	GLN
7	T	1261	GLN
7	T	1276	ASN
7	T	1301	HIS
7	T	1306	ASN
7	T	1360	HIS
7	W	79	ASN
7	W	385	GLN
7	W	432	GLN
7	W	433	GLN
7	W	472	ASN
7	W	534	ASN
7	W	669	HIS
7	W	695	GLN
7	W	722	ASN
7	W	750	ASN
7	W	761	GLN
7	W	795	HIS
7	W	842	ASN
7	W	859	ASN
7	W	942	GLN
7	W	964	HIS
7	W	977	GLN
7	W	1090	HIS
7	W	1136	GLN
7	W	1139	ASN
7	W	1149	GLN
7	W	1179	GLN
7	W	1216	ASN
7	W	1217	GLN
7	W	1246	GLN
7	W	1296	GLN
7	W	1360	HIS

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Mol	Chain	Res	Type
7	x	104	HIS
7	x	195	GLN
7	x	222	HIS
7	x	333	HIS
7	x	376	ASN
7	x	389	ASN
7	x	454	ASN
7	x	465	HIS
7	x	534	ASN
7	x	596	HIS
7	x	636	ASN
7	x	722	ASN
7	x	745	GLN
7	x	849	HIS
7	x	859	ASN
7	x	904	ASN
7	x	964	HIS
7	x	977	GLN
7	x	1033	GLN
7	x	1090	HIS
7	x	1120	HIS
7	x	1122	GLN
7	x	1139	ASN
7	x	1216	ASN
7	x	1217	GLN
7	x	1276	ASN
7	x	1289	ASN
7	x	1310	GLN
7	x	1351	GLN
6	y	11	GLN
1	e	96	HIS
1	e	102	ASN
1	e	112	GLN
1	e	137	HIS
1	e	227	GLN
1	e	281	GLN
1	e	291	ASN
2	f	89	GLN
2	f	120	HIS
2	f	173	HIS
2	g	38	GLN
2	g	62	ASN

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Mol	Chain	Res	Type
2	g	102	GLN
2	g	104	HIS
2	g	154	ASN
2	g	184	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

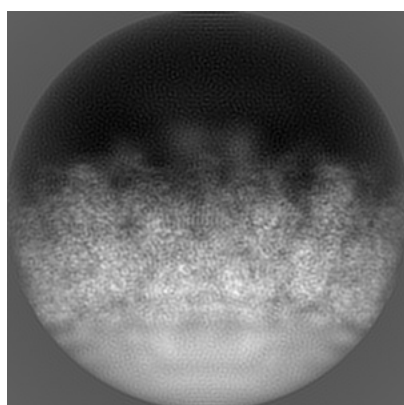
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30157. These allow visual inspection of the internal detail of the map and identification of artifacts.

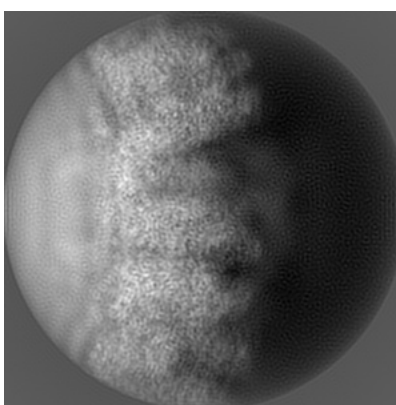
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

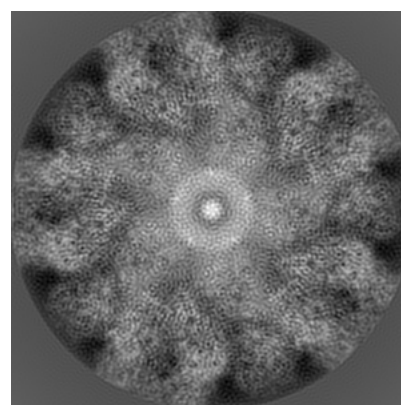
6.1.1 Primary map



X



Y

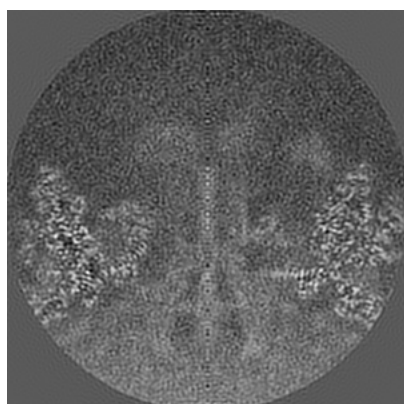


Z

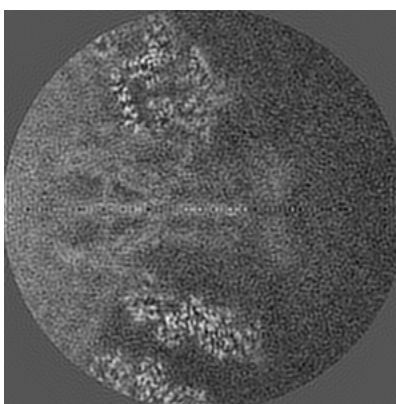
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

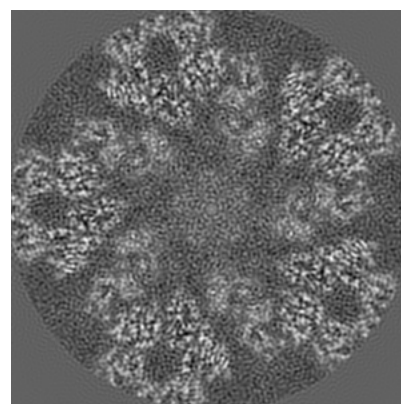
6.2.1 Primary map



X Index: 150



Y Index: 150

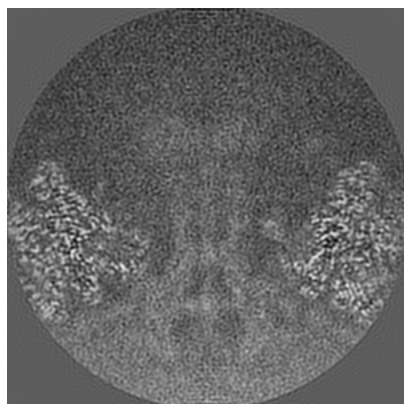


Z Index: 150

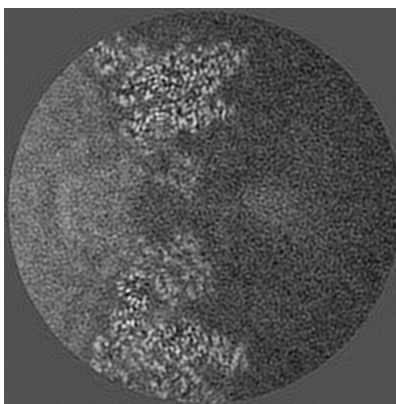
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

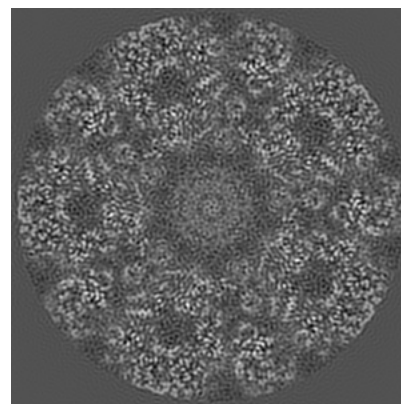
6.3.1 Primary map



X Index: 144



Y Index: 114

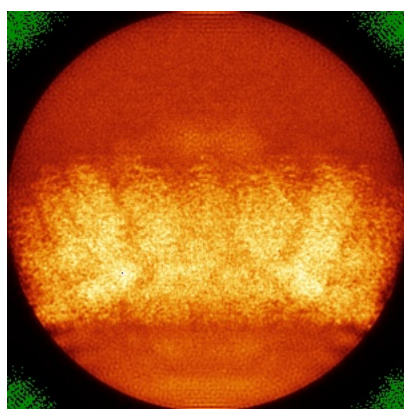


Z Index: 109

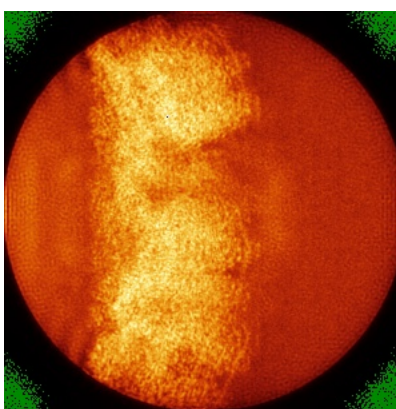
The images above show the largest variance slices of the map in three orthogonal directions.

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

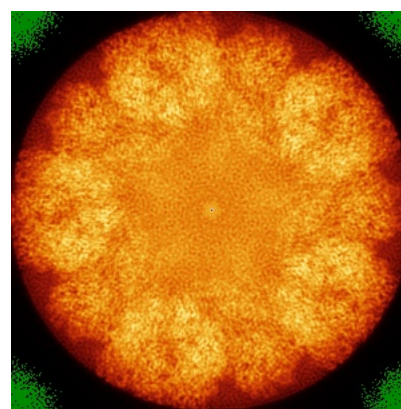
6.4.1 Primary map



X



Y

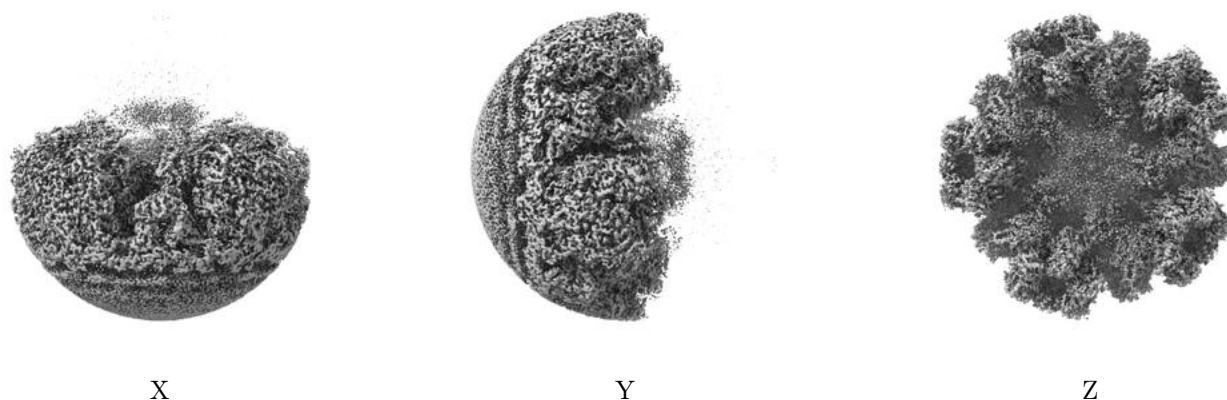


Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

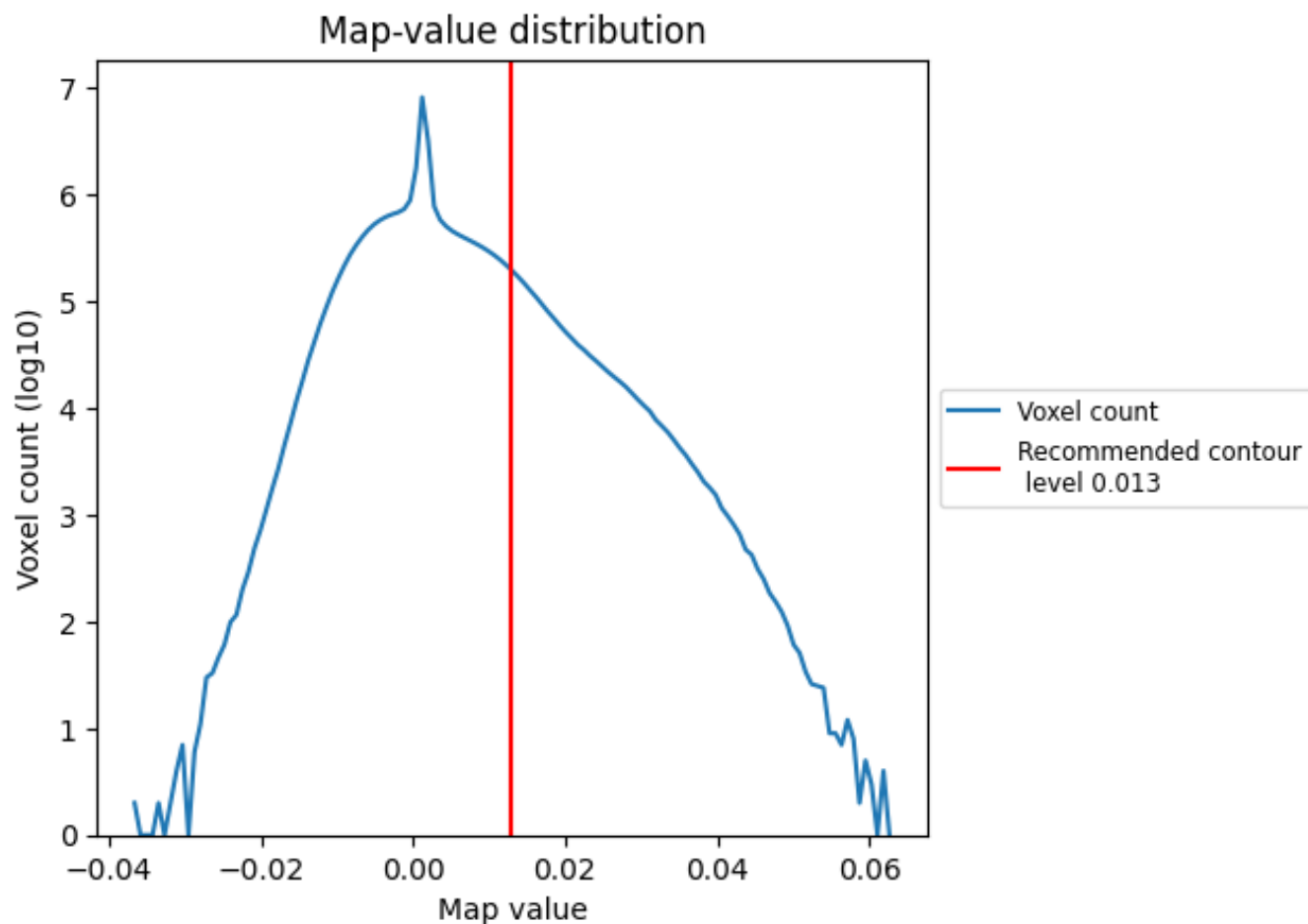
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

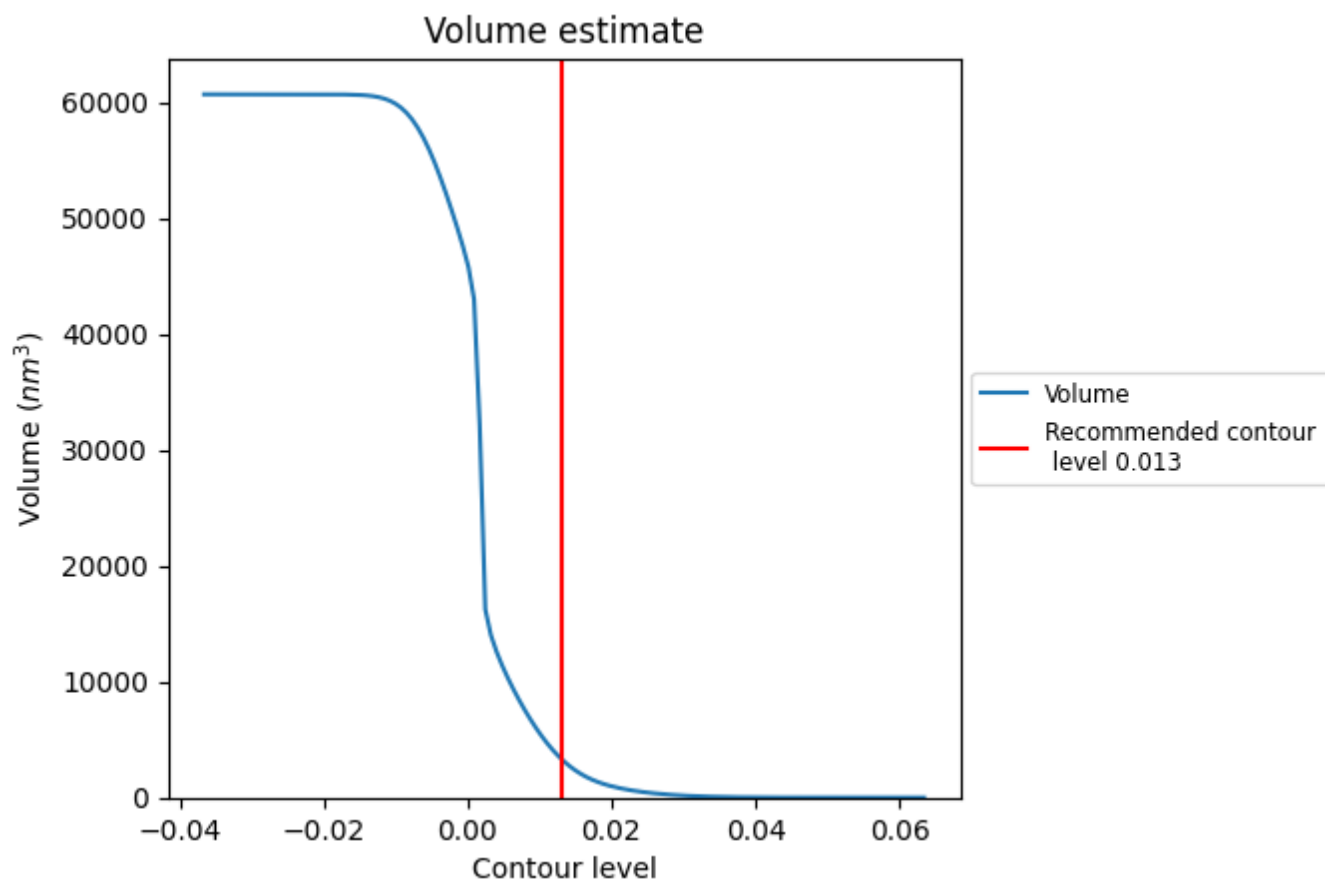
This section contains the results of statistical analysis of the map.

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.

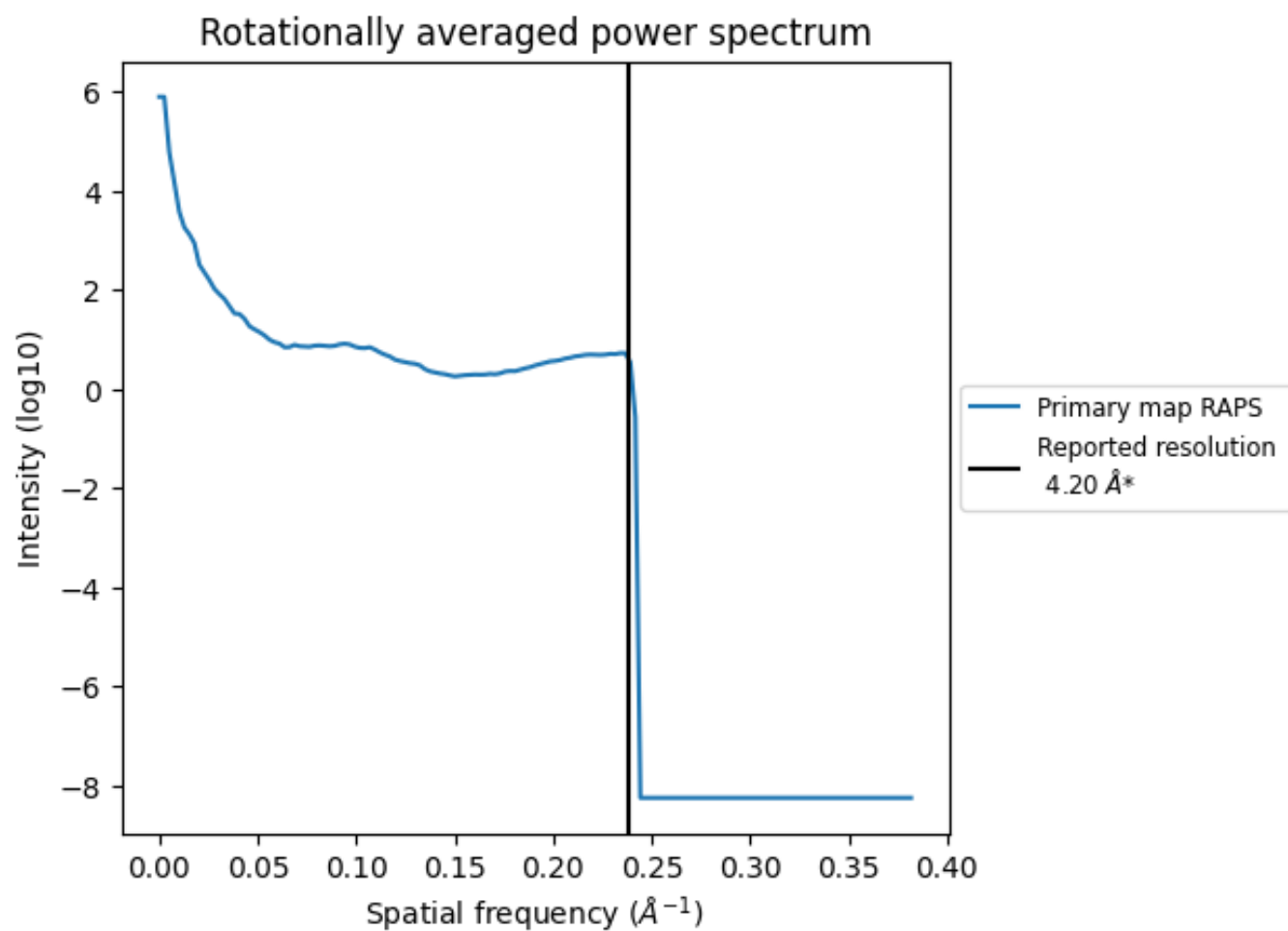
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3365 nm³; this corresponds to an approximate mass of 3040 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 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation ⓘ

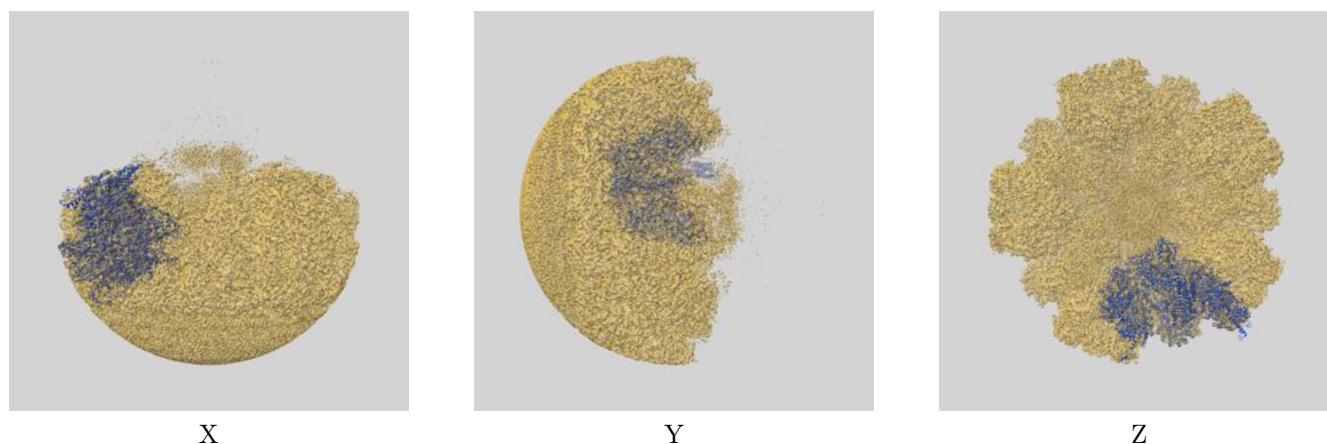
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

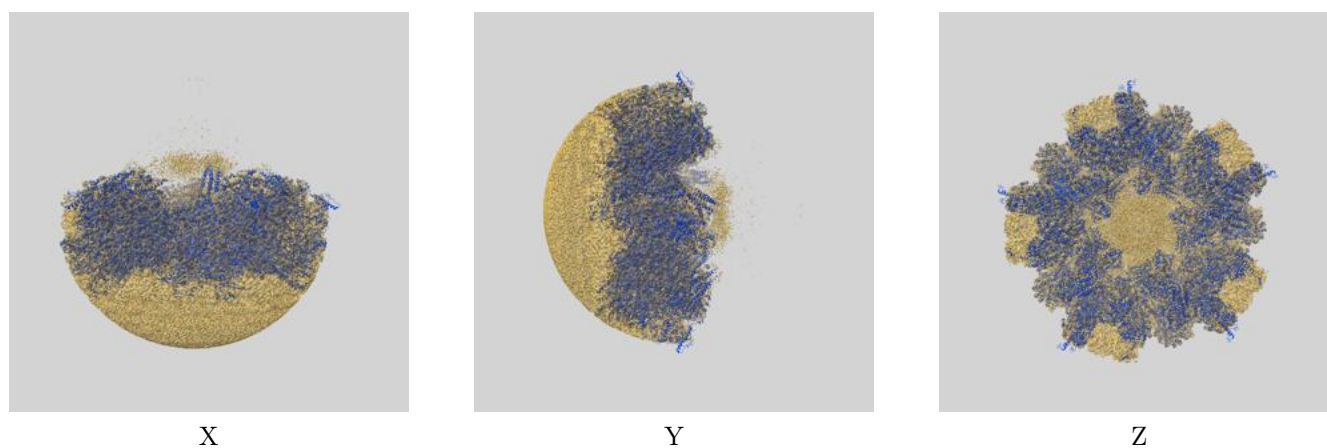
This section contains information regarding the fit between EMDB map EMD-30157 and PDB model 7BQX. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

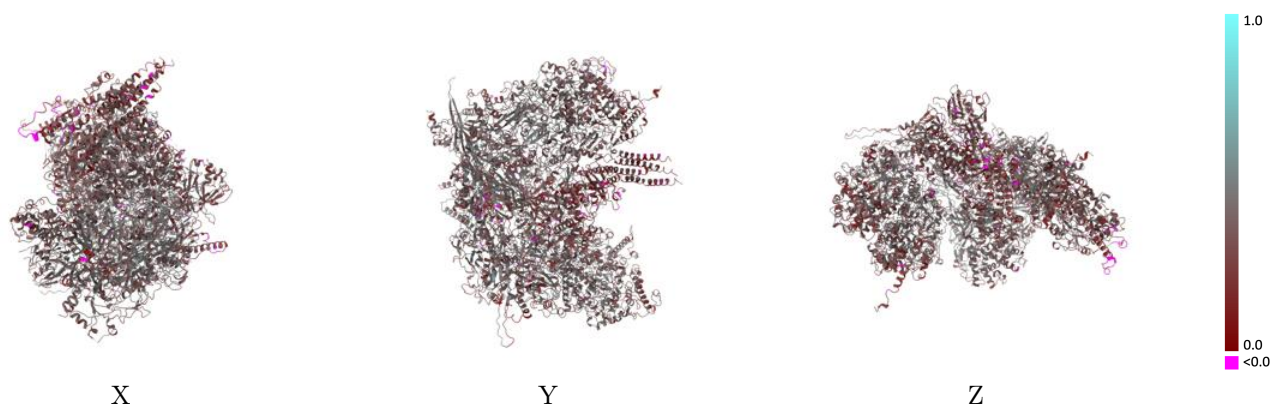


9.1.2 Map-model assembly overlay [i](#)



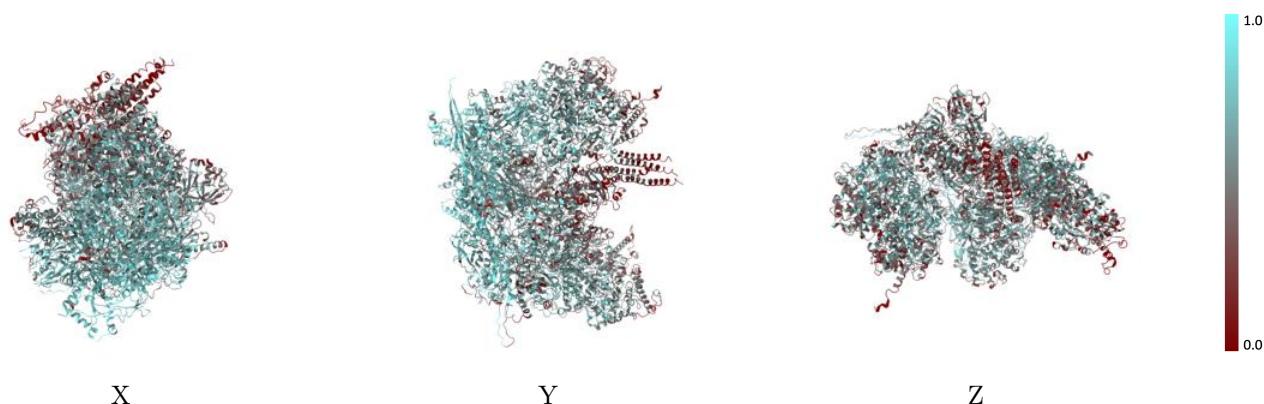
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



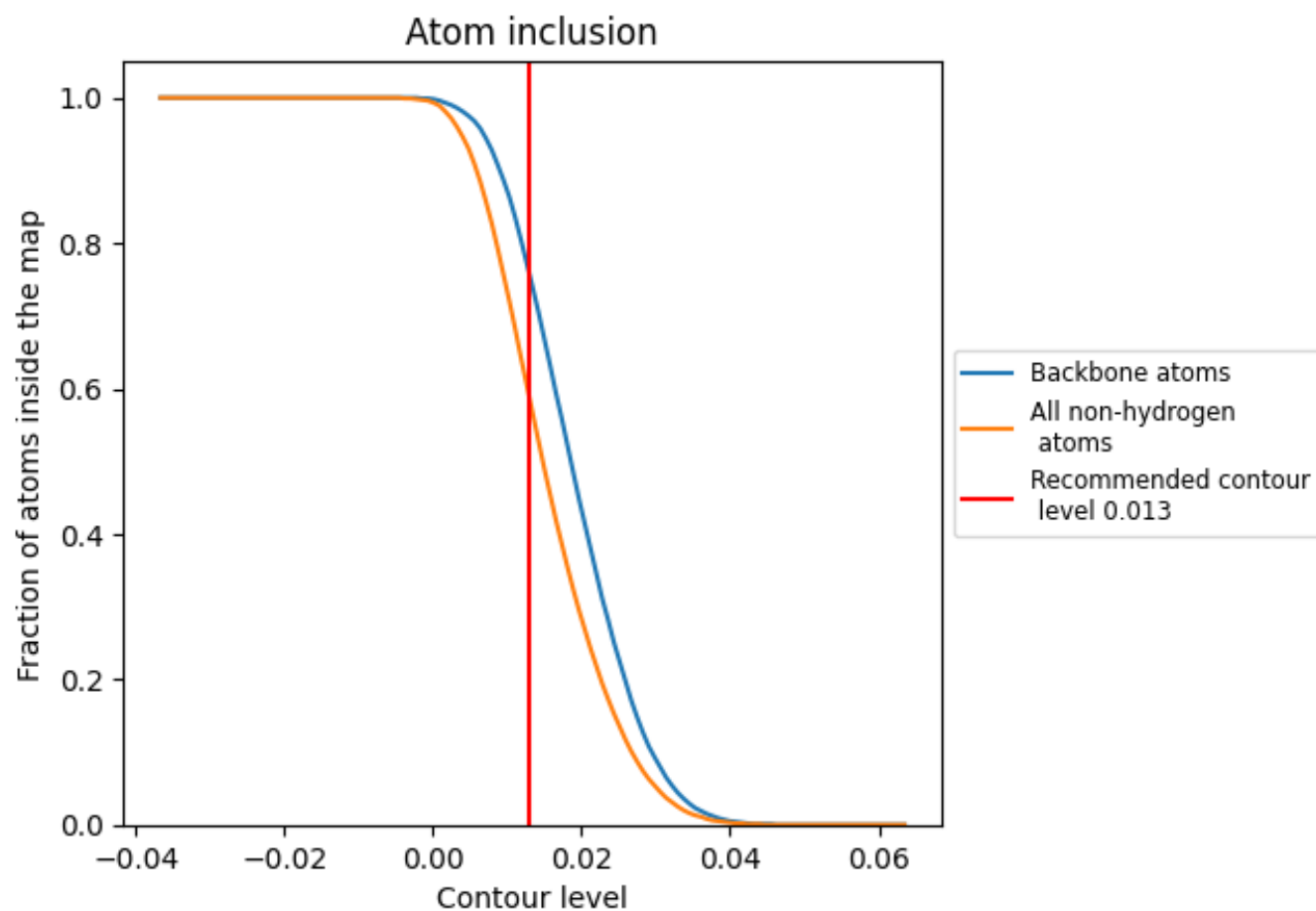
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 59% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.3650
2	 0.1330	 0.1500
5	 0.4500	 0.3030
6	 0.4870	 0.3080
7	 0.4880	 0.3280
B	 0.1820	 0.2560
C	 0.4060	 0.2870
G	 0.3640	 0.2950
K	 0.3990	 0.3100
O	 0.1370	 0.2440
S	 0.6200	 0.3830
T	 0.6580	 0.3980
W	 0.6290	 0.3780
Y	 0.3750	 0.3180
Z	 0.3150	 0.2840
e	 0.7130	 0.4020
f	 0.6290	 0.3720
g	 0.6380	 0.3760
x	 0.6270	 0.3830
y	 0.3170	 0.2980

