



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:42 PM UTC

PDB ID : 6W2E / pdb_00006w2e
EMDB ID : EMD-21526
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-05
Resolution : 4.40 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:

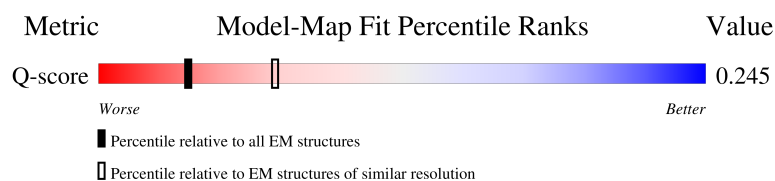
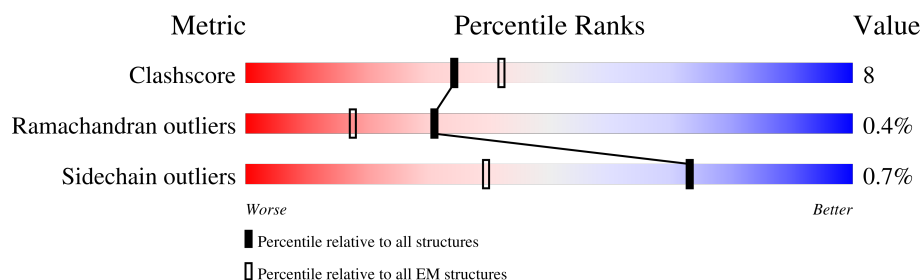
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 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	3132 (3.91 - 4.90)

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	J	1381	50% 77% 18% 6%
1	K	1381	54% 83% 16%
1	N	1381	60% 82% 16%
1	O	1381	53% 78% 16% 6%

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Mol	Chain	Length	Quality of chain
2	v	507	
3	w	570	
3	x	570	
4	y	3149	
4	z	3149	
5	Z	176	
5	a	176	
5	d	176	
5	e	176	
6	f	364	
6	h	364	
7	k	301	
7	m	301	
7	p	301	
7	r	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 62525 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	1305	Total	C	N	O	S	0	0
			10252	6507	1779	1908	58		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1299	Total	C	N	O	S	0	0
			10194	6468	1771	1895	60		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	293	Total	C	N	O	S	0	0
			2288	1472	398	407	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	w	68	Total	C	N	O	S	0	0
			549	332	106	108	3		
3	x	68	Total	C	N	O	S	0	0
			549	332	106	108	3		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	37	Total	C	N	O	0	0
			317	200	64	53		
4	z	37	Total	C	N	O	0	0
			317	200	64	53		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	253	Total	C	N	O	S	0	0
			1992	1291	333	361	7		
6	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

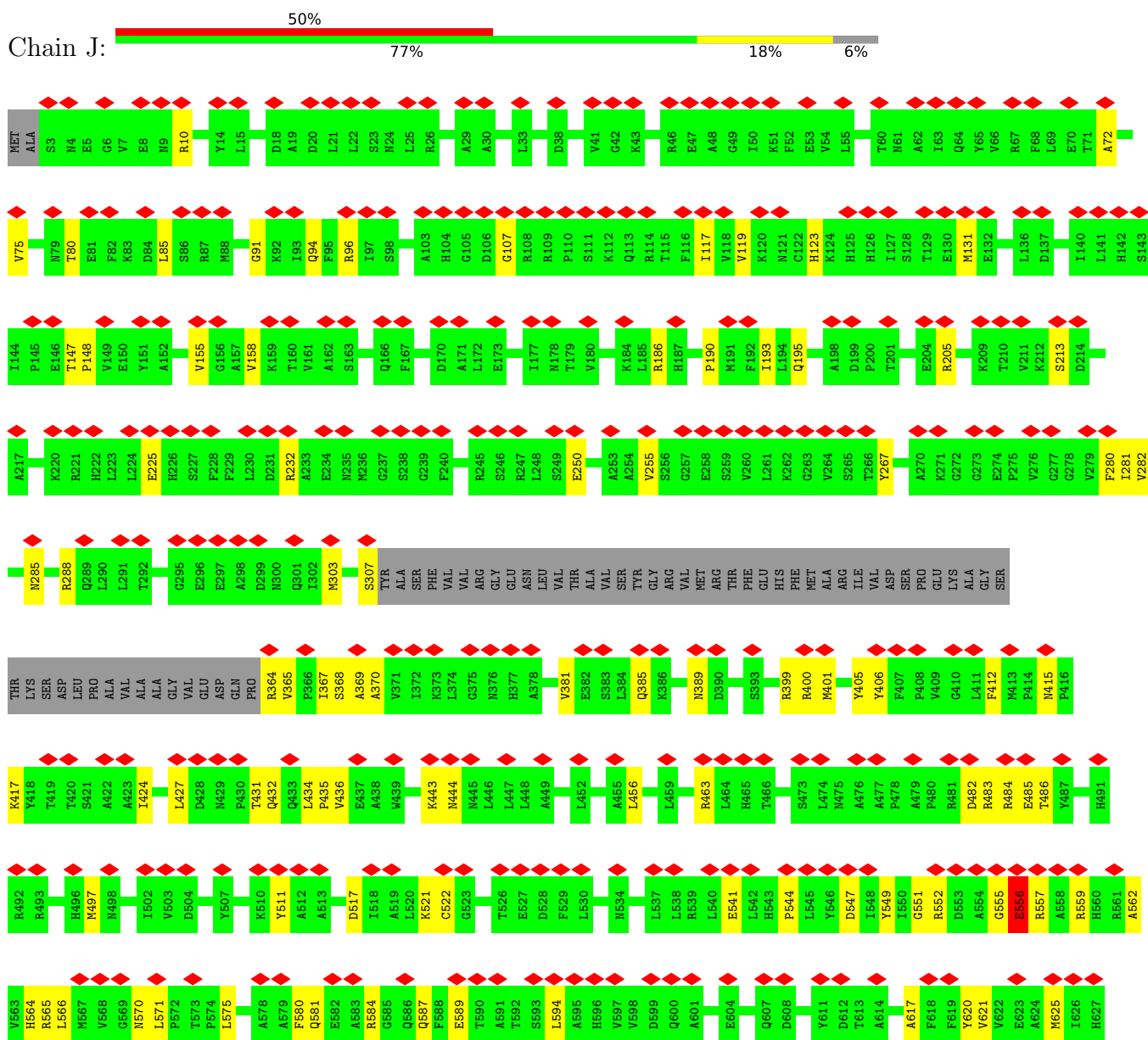
- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

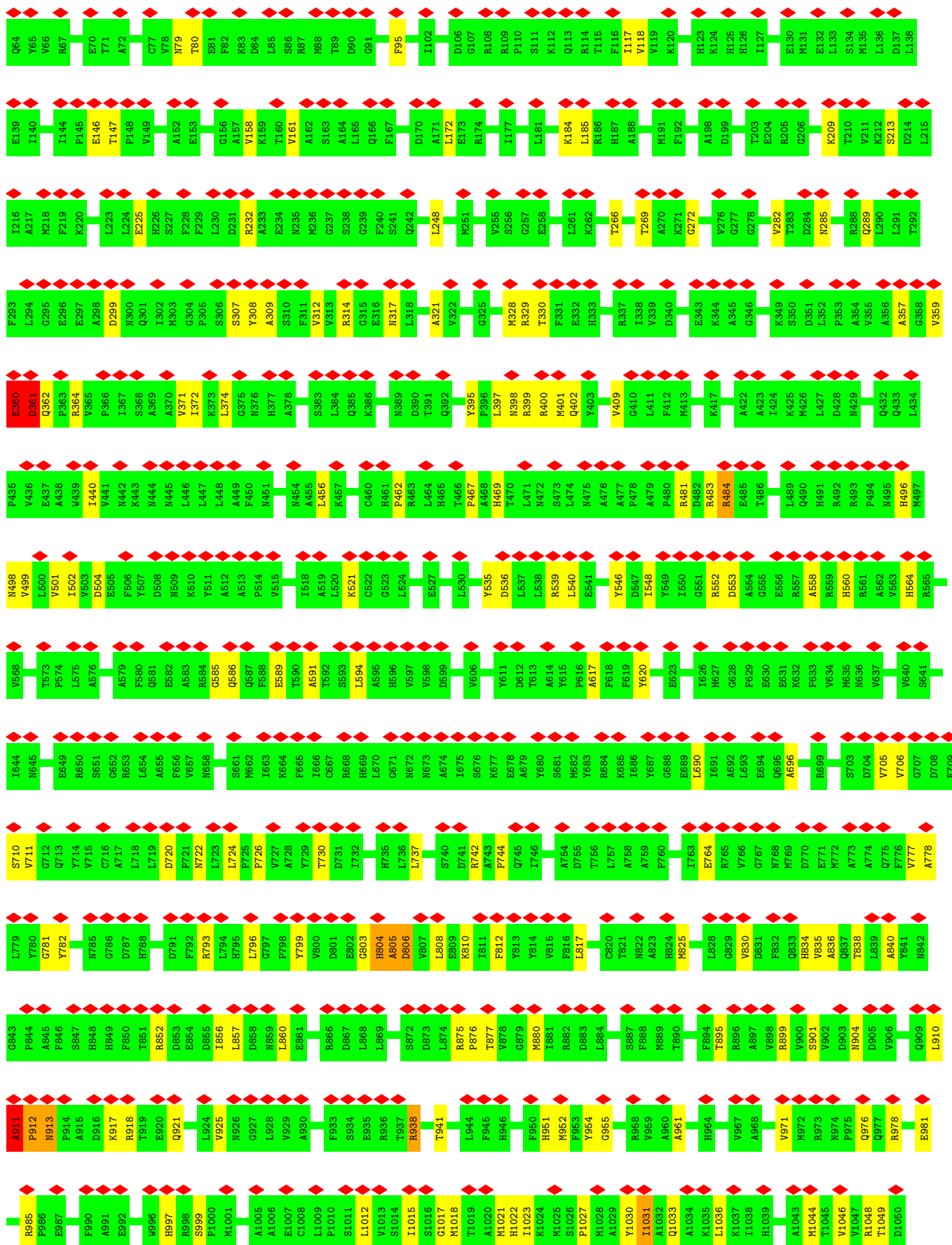
3 Residue-property plots

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.

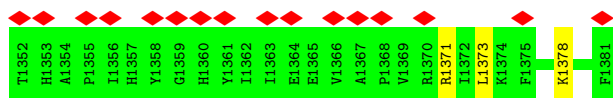
• Molecule 1: Major capsid protein



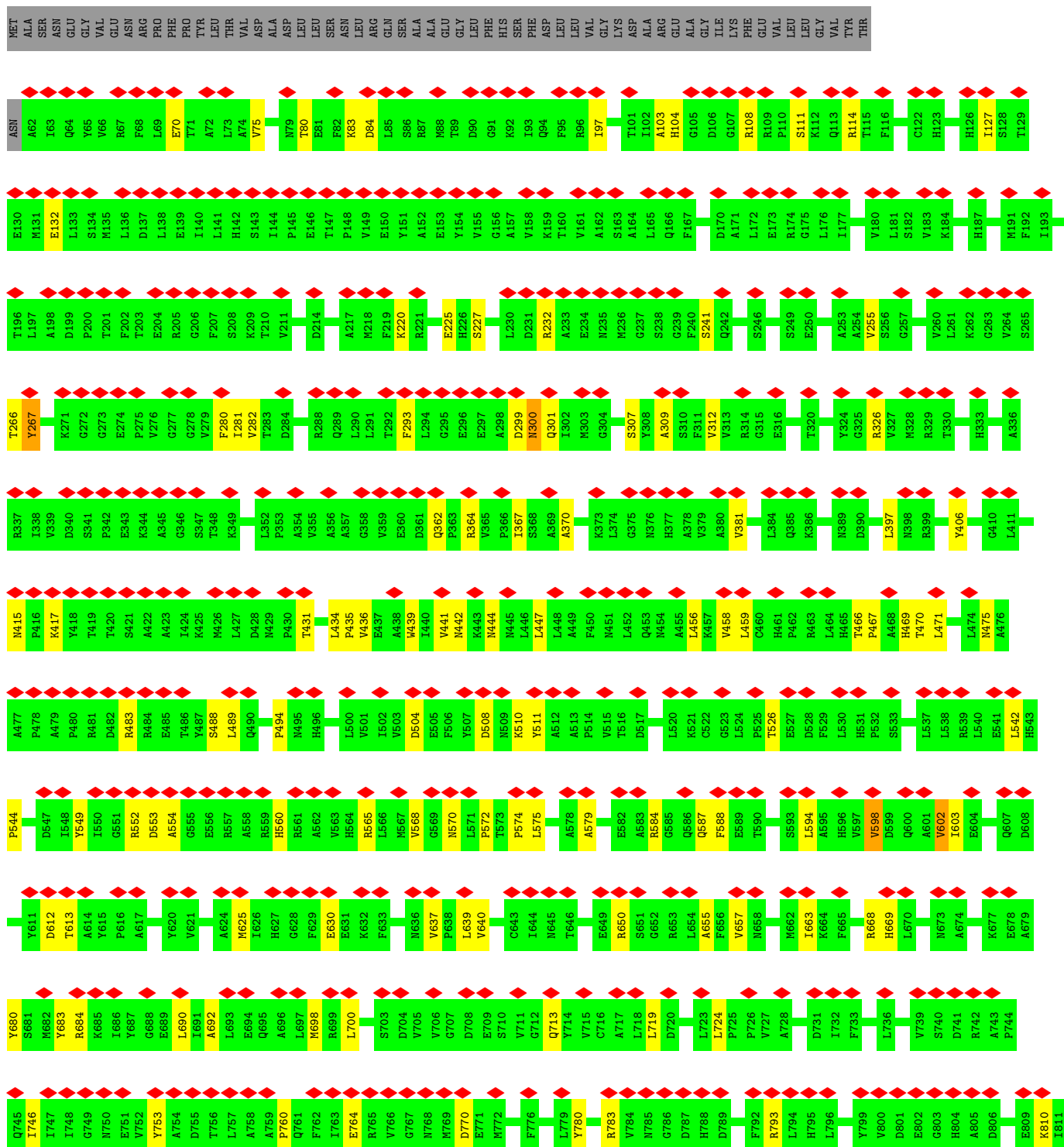
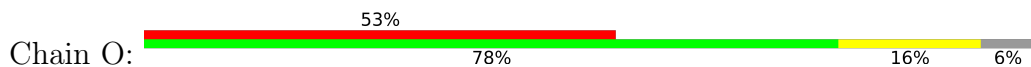


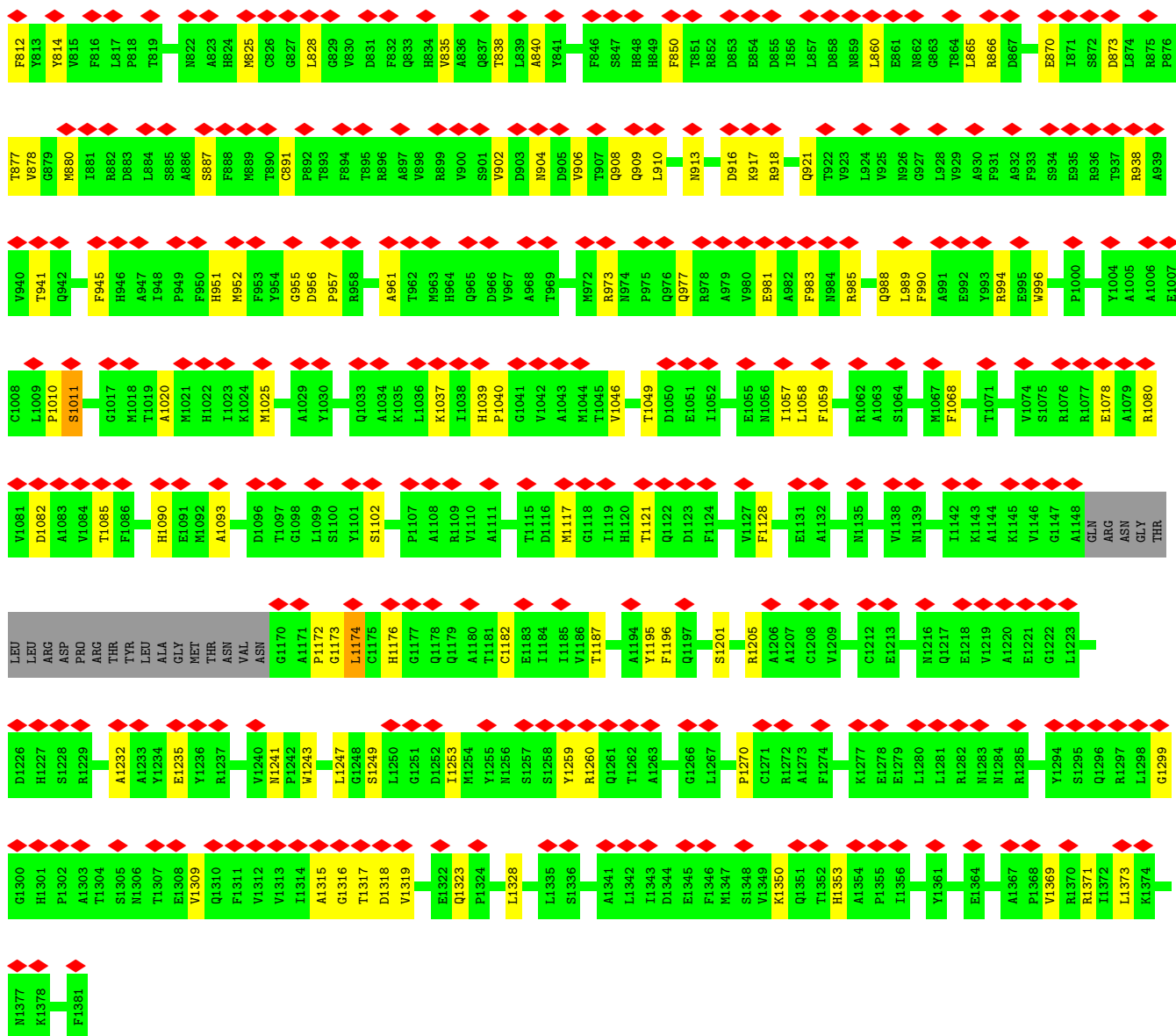


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E1218	V1219	L1220	E1221	G1222	L1223	L1224	Y1225	D1226	H1227	S1228	R1229	P1230	D1231	A1232	A1233	Y1234	E1235	H1236	G1237	S1238	P1242	W1243	A1244	S1245	Q1246	L1247	G1248	S1249	L1250	G1251	D1252	I1253	S1257	S1258	Y1259	R1260	Q1261	T1262	A1263	V1264	P1265	G1266	L1267	Y1268	S1269	P1270	C1271	R1272	I1273	A1274	F1275	N1276	K1277	S1278	E1279	L1280	L1281		
LEU	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	M1169	G1170	A1171	L1174	C1175	H1176	G1177	Q1178	Q1179	A1180	E1183	I1184	I1185	I1186	I1187	P1188	V1189	T1190	A1191	D1192	V1193	A1194	Y1195	S1199	M1200	S1201	P1202	R1203	G1204	R1205	A1206	A1207	C1208	V1209	V1210	S1211	C1212	E1213	M1214	Y1215	M1216	Q1217			
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Y954	G955	D956	P957	V959	A960	A961	T962	M963	Q964	Q965	D966	V967	A968	T969	F970	Y971	M972	R973	N974	P975	Q976	Q977	R978	A979	V980	E981	L982	F983	N984	R985	P986	E987	Q988	L989	F990	A991	E992	Y993	H996	H997	R998	S999	M1000	M1001	G1002	K1003	A1006	E1007	C1008	L1009	F1013	S1014	G1017						
A1020	M1021	H1022	I1023	K1024	P1027	Y1030	I1031	A1032	Q1033	A1034	K1035	L1036	K1037	I1038	H1039	P1040	G1041	V1042	A1043	M1044	T1045	T1049	D1050	A979	E1051	I1052	L1053	S1054	E1055	N1056	I1057	F1059	S1060	A1063	S1064	T1065	S1066	M1067	F1068	I1069	G1070	T1071	P1072	M1073	V1074	S1075	R1076	R1077	E1078	A1079	R1080	V1081	D1082	A1083					
F1086	E1087	V1088	H1089	H1090	E1091	M1092	A1093	S1094	I1095	D1096	L1099	S1100	Y1101	S1102	A1108	R1109	V1110	A1111	A1112	T1115	D1116	M1117	G1118	I1119	I1120	D1123	F1124	F1125	S1126	V1127	F1128	P1129	A1130	E1131	A1132	F1133	G1134	M1135	V1138	M1139	D1140	Y1141	I1142	K1143	A1144	K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY	THR					
LEU	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	M1169	G1170	A1171	L1174	C1175	H1176	G1177	Q1178	Q1179	A1180	E1183	I1184	I1185	I1186	I1187	P1188	V1189	T1190	A1191	D1192	V1193	A1194	Y1195	S1199	M1200	S1201	P1202	R1203	G1204	R1205	A1206	A1207	C1208	V1209	V1210	S1211	C1212	E1213	M1214	Y1215	M1216	Q1217			
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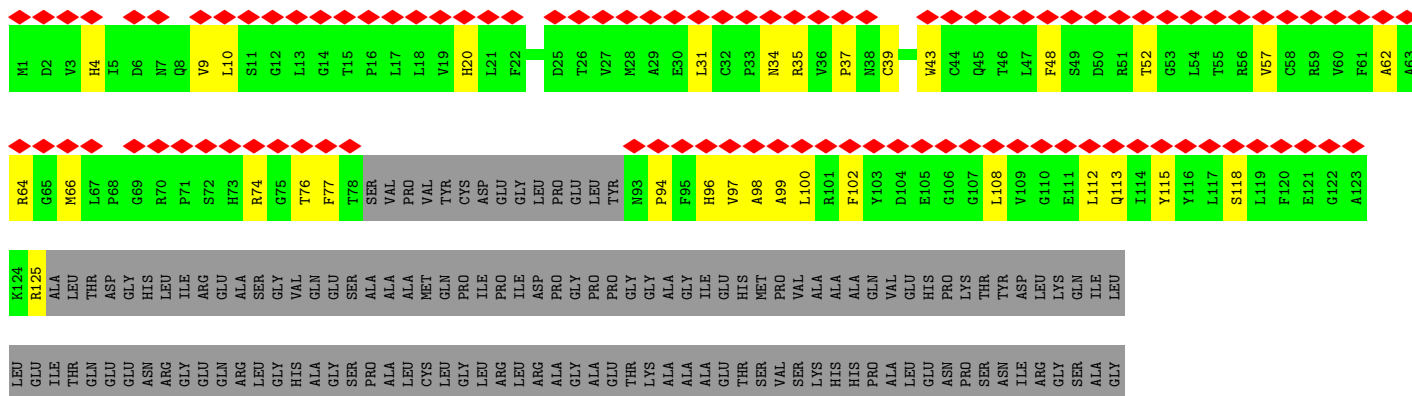
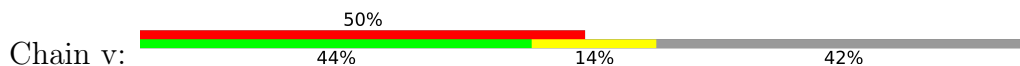


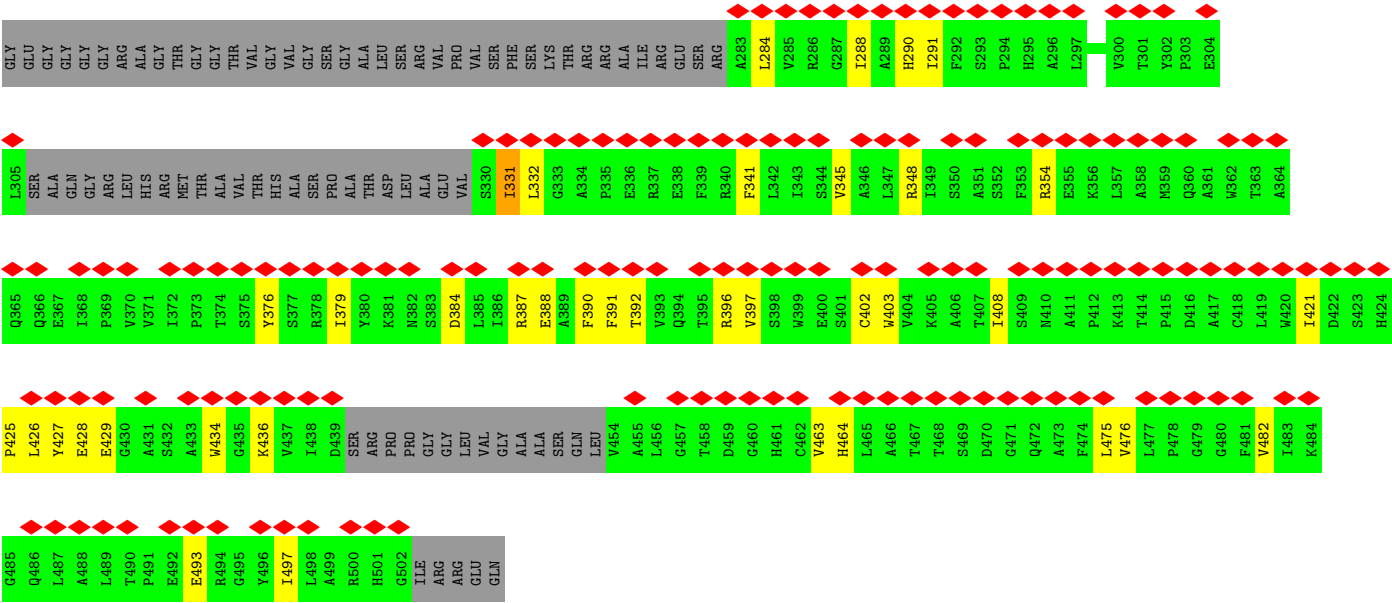
• Molecule 1: Major capsid protein



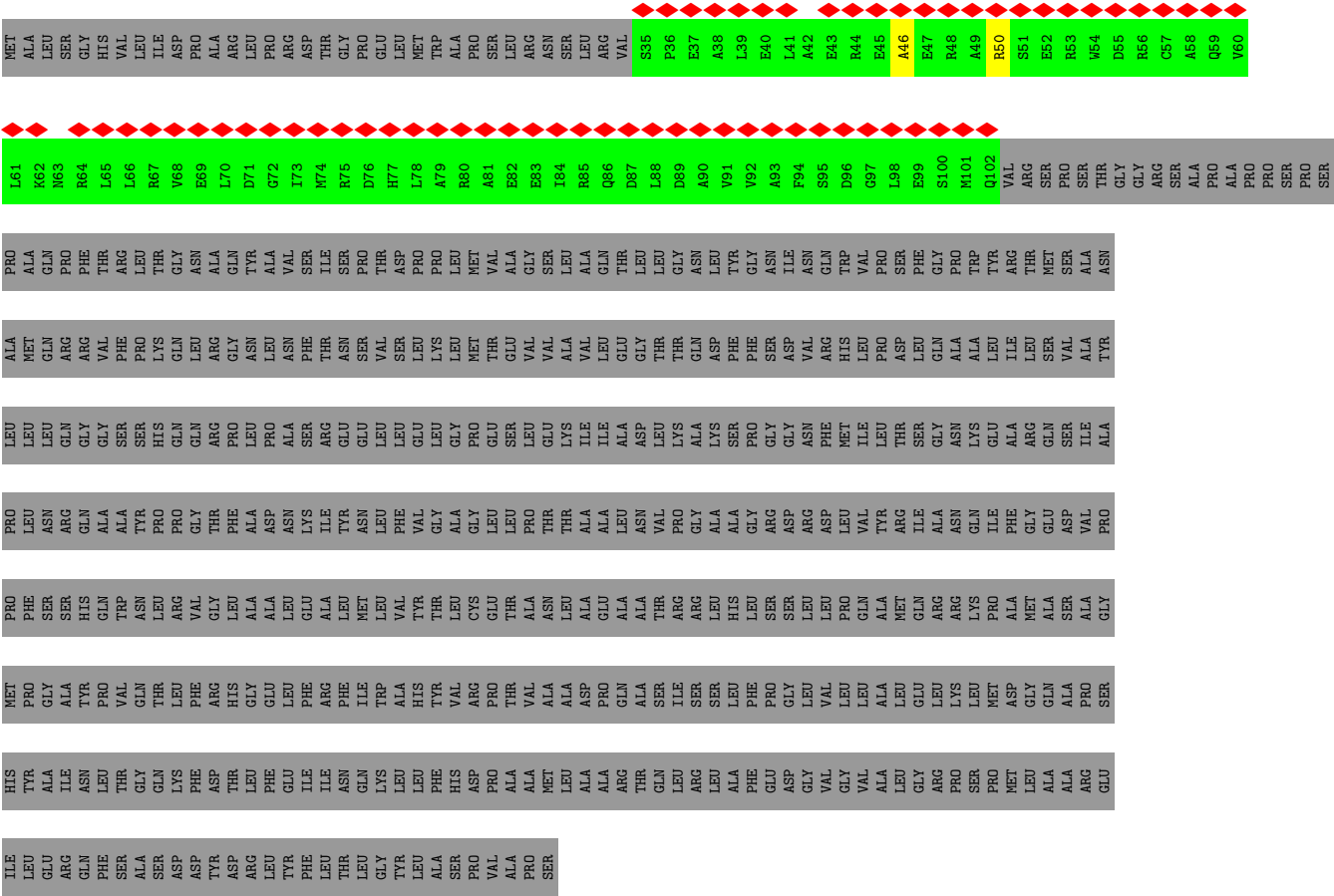


• Molecule 2: Capsid vertex component 1

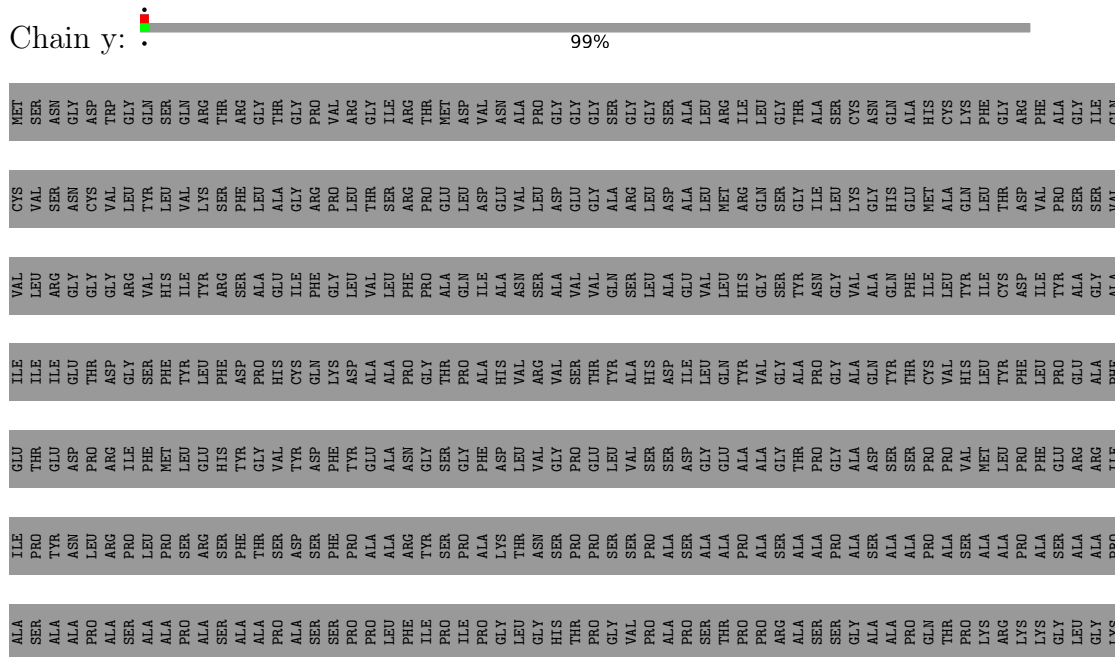




• Molecule 3: Capsid vertex component 2



• Molecule 3: Capsid vertex component 2







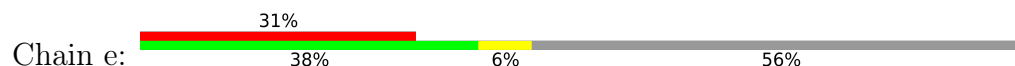
R3121	F3122	V3123	S3124	K3125	L3126	R3127	K3128	K3129	L3130	E3131	R3132	S3133	T3134	R3135	R3136	L3137	T3138	K3139	D3140	L3141	E3142	R3143	L3144	K3145	F3146	L3147	T3148	L3149
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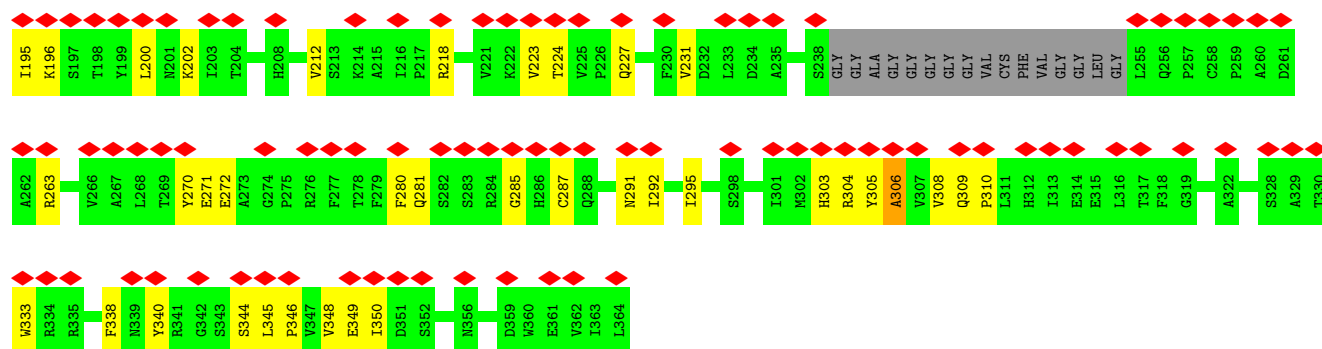
Chain z: 99%

SER	THR	THR	THR	HIS	ASP	ALA	ILE	GLU	ILE	VAL	CYS	MET
ASP	PRO	GLN	GLN	PRO	SER	SER	PRO	THR	ILE	LEU	VAL	SER
LEU	ALA	ALA	ALA	ALA	PRO	ALA	TYR	GLU	ILE	ARG	SER	ASN
GLU	PRO	GLN	GLN	PRO	HIS	ALA	ASN	ASP	GLU	GLY	ASN	GLY
PRO	PRO	PRO	PRO	SER	LYS	ALA	LEU	ARG	THR	GLY	CYS	ASP
PHE	ALA	GLN	GLN	THR	PRO	SER	ARG	ILE	ASP	ARG	VAL	TRP
LEU	GLN	ALA	ALA	ILE	THR	ALA	LEU	PHE	SER	VAL	LEU	GLN
MET	GLN	ALA	ALA	ALA	SER	ALA	PRO	MET	PHE	ILE	VAL	GLN
SER	PRO	PRO	PRO	SER	ARG	ALA	ARG	GLU	LEU	TVR	LYS	ARG
ASP	PRO	ALA	ALA	VAL	ARG	SER	SER	HIS	PHE	ARG	SER	THR
SER	SER	PRO	PRO	THR	LEU	ALA	PHE	TYR	ASP	SER	PHE	ARG
GLU	ALA	SER	SER	PRO	PRO	ALA	THR	GLY	PRO	ALA	LEU	GLY
GLU	THR	PRO	LEU	SER	LEU	PRO	SER	VAL	HIS	GLU	ALA	THR
ALA	THR	LEU	LEU	PRO	SER	ALA	ASP	TYR	CYS	ILE	GLY	PRO
GLU	LEU	GLU	LEU	ARG	SER	SER	SER	ASP	GLN	PHE	ARG	VAL
SER	GLU	PRO	GLU	LEU	THR	SER	PHE	PHE	LYS	GLY	PRO	VAL
ASP	PRO	GLN	GLN	PRO	THR	PRO	PRO	TYR	ASP	LEU	LEU	ARG
LEU	GLU	GLN	GLN	LEU	ASP	PRO	ALA	GLU	ALA	VAL	THR	GLY
ALA	LYS	GLN	GLN	GLN	THR	LEU	ALA	ALA	ALA	VAL	SER	ILE
ASN	ASN	PRO	ASN	ILE	GLU	PHE	ARG	ASN	ALA	PHE	ARG	ARG
ASP	HIS	THR	THR	PRO	ASP	ILE	TYR	GLY	GLY	PRO	PRO	THR
ILE	PRO	PRO	PRO	PRO	GLN	ILE	SER	GLY	VAL	ALA	GLU	MET
THR	ALA	ALA	ALA	LEU	LEU	PRO	ALA	PHE	HIS	ILE	ASP	ASP
GLU	ASP	PRO	PRO	ALA	THR	GLY	ASN	VAL	ARG	SER	LEU	PRO
GLU	ALA	PRO	ALA	ALA	HIS	HIS	SER	GLY	VAL	ALA	ASP	GLY
ASP	GLY	SER	ARG	ALA	PRO	PRO	PRO	PRO	HIS	LEU	LEU	GLY
GLU	PRO	GLN	ILE	PRO	PRO	ALA	ALA	SER	ASP	ALA	ALA	ALA
VAL	SER	GLN	PRO	PRO	PRO	PRO	SER	ASP	ILE	GLU	ALA	ALA
PHE	PRO	GLN	GLN	LEU	SER	THR	ALA	GLY	LEU	VAL	LEU	LEU
GLY	PRO	PRO	PRO	THR	ALA	THR	ALA	GLU	GLN	LEU	MET	ARG
ASN	PHE	PRO	PRO	THR	ALA	PRO	PRO	ALA	TYR	HIS	ARG	ILE
SER	GLY	PRO	SER	SER	ARG	PRO	ALA	ALA	VAL	GLY	GLN	LEU
LEU	GLN	SER	SER	SER	LEU	ARG	SER	GLY	GLY	SER	SER	GLY
GLU	GLN	ALA	ALA	PRO	PRO	ALA	ALA	THR	ALA	TYR	GLY	THR
GLU	PRO	ALA	ALA	SER	PRO	PRO	ALA	PRO	PRO	ASN	ILE	ALA
THR	ALA	LEU	LEU	ALA	PRO	GLN	PRO	PRO	CYS	ILE	MET	HIS
SER	SER	PRO	PRO	PRO	HIS	THR	ALA	PRO	VAL	LEU	ALA	CYS
PRO	GLY	GLY	GLY	THR	GLN	PRO	SER	VAL	THR	TVR	GLN	LEU
ILE	GLY	GLN	GLN	THR	SER	LYS	ALA	MET	ILE	ILE	THR	PHE
THR	SER	GLN	GLN	THR	PRO	ARG	ALA	LEU	TYR	CYS	THR	GLY
LEU	GLY	GLN	GLN	THR	PRO	LYS	PRO	PHE	PHE	ASP	ASP	ARG
ASP	LEU	PRO	PRO	THR	ALA	LYS	ALA	PHE	LEU	VAL	VAL	PHE
THR	LEU	LEU	LEU	SER	ALA	GLY	SER	GLU	LEU	TYR	PRO	ALA
ALA	THR	LEU	LEU	SER	PRO	THR	SER	ARG	PRO	GLY	SER	GLY
ALA	ARG	ALA	SER	PRO	PRO	GLY	ALA	ALA	GLU	ALA	GLY	ILE
ARG	THR	ALA	ALA	PRO	THR	LYS	PRO	PRO	PHE	GLY	VAL	THR

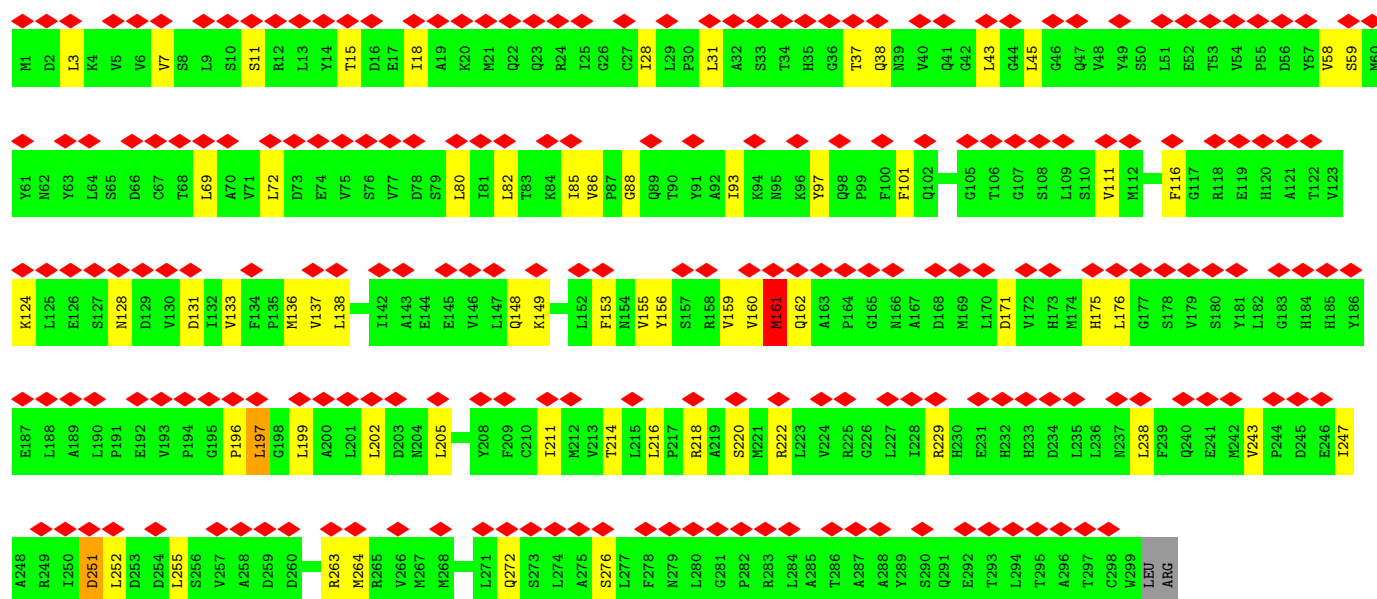
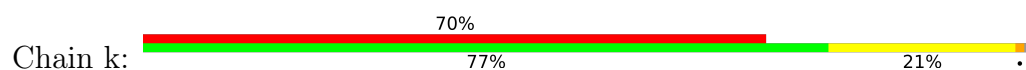




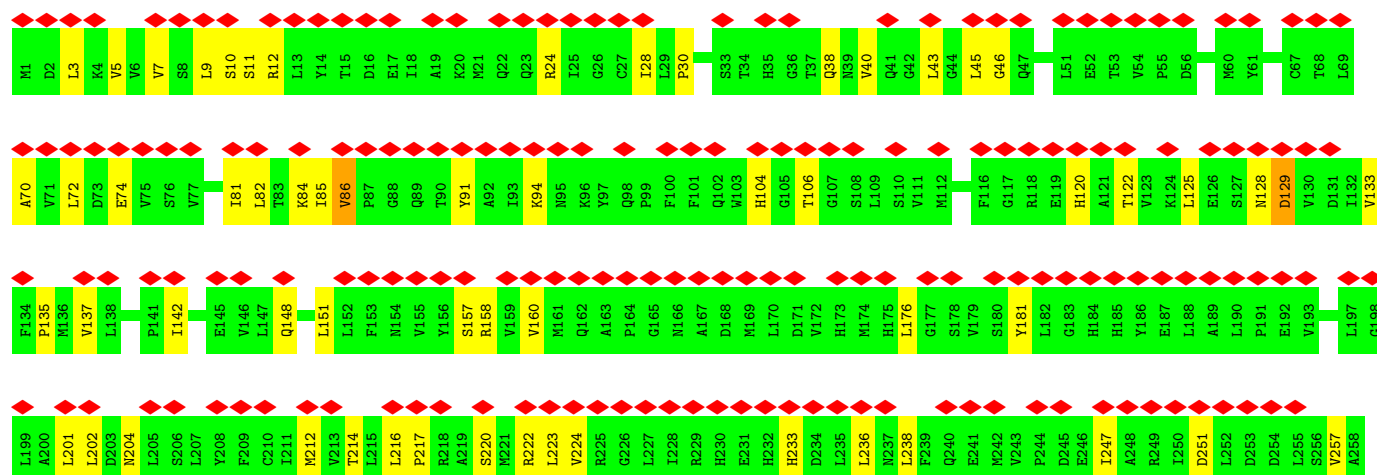
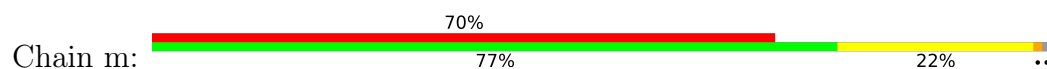


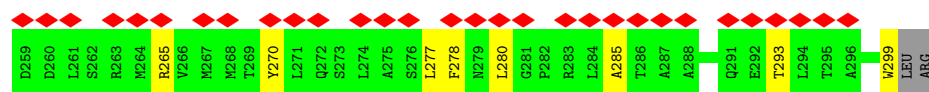


• Molecule 7: Triplex capsid protein 2

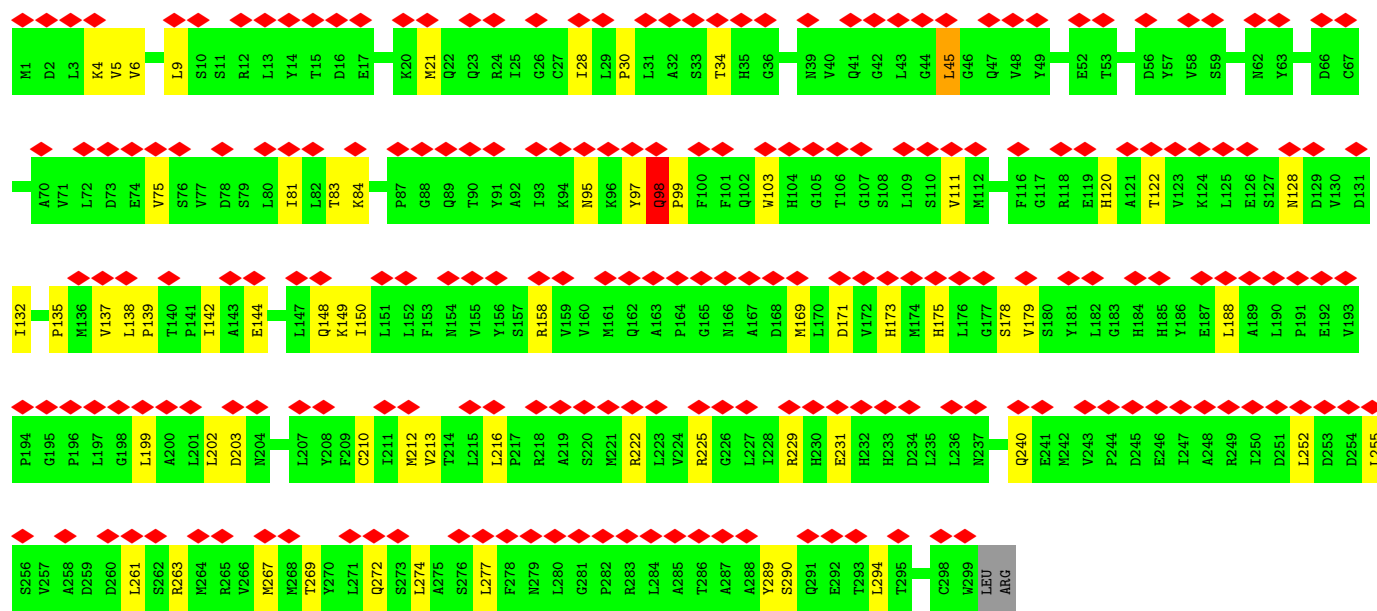
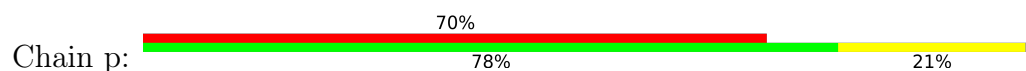


• Molecule 7: Triplex capsid protein 2

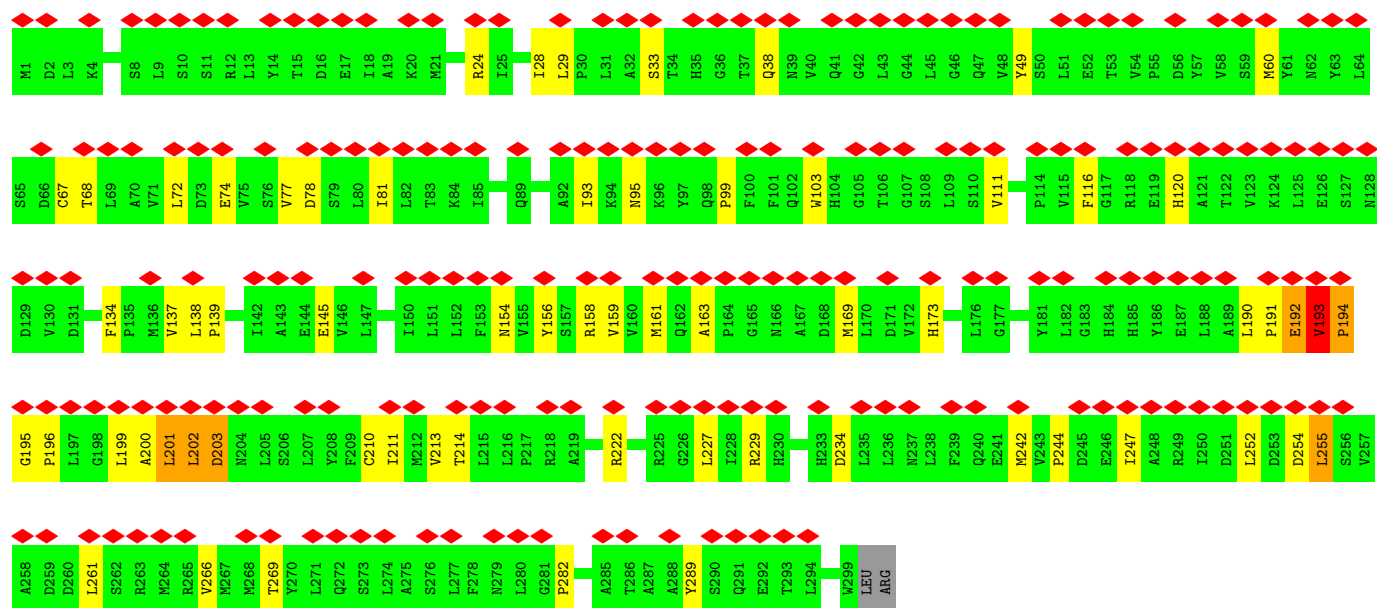
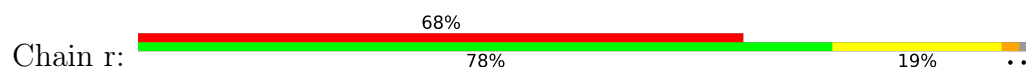




• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2305	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	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	J	0.27	0/10492	0.61	6/14259 (0.0%)
1	K	0.28	0/11085	0.63	6/15066 (0.0%)
1	N	0.28	0/10933	0.59	1/14858 (0.0%)
1	O	0.28	0/10435	0.60	2/14183 (0.0%)
2	v	0.31	0/2346	0.70	1/3190 (0.0%)
3	w	0.32	0/553	0.61	0/741
3	x	0.30	0/553	0.56	0/741
4	y	0.27	0/320	0.60	0/424
4	z	0.27	0/320	0.56	0/424
5	Z	0.31	0/664	0.67	0/896
5	a	0.29	0/664	1.04	2/896 (0.2%)
5	d	0.32	0/664	0.60	0/896
5	e	0.26	0/664	0.59	0/896
6	f	0.29	0/2049	0.88	2/2795 (0.1%)
6	h	0.28	0/2672	0.67	2/3635 (0.1%)
7	k	0.28	0/2388	0.60	2/3254 (0.1%)
7	m	0.29	0/2388	0.62	0/3254
7	p	0.27	0/2388	0.63	1/3254 (0.0%)
7	r	0.28	0/2388	0.64	1/3254 (0.0%)
All	All	0.28	0/63966	0.63	26/86916 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	161	SER	CA-C-N	-23.18	90.86	119.84
6	f	161	SER	C-N-CA	-23.18	90.86	119.84
5	a	18	PHE	CA-C-N	-16.47	99.25	119.84
5	a	18	PHE	C-N-CA	-16.47	99.25	119.84
1	N	483	ARG	N-CA-C	9.12	120.82	111.07
1	K	1264	VAL	CA-C-N	8.67	130.68	119.84
1	K	1264	VAL	C-N-CA	8.67	130.68	119.84
1	K	911	ALA	CA-C-N	7.95	129.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	911	ALA	C-N-CA	7.95	129.78	119.84
1	J	483	ARG	N-CA-C	7.41	120.29	111.02
1	J	706	VAL	N-CA-C	-6.84	106.06	112.83
2	v	428	GLU	N-CA-C	6.71	118.76	110.91
1	J	1264	VAL	CA-C-N	6.47	127.92	119.84
1	J	1264	VAL	C-N-CA	6.47	127.92	119.84
7	k	251	ASP	N-CA-C	6.46	120.17	112.93
7	p	45	LEU	N-CA-C	-6.28	105.56	112.72
6	h	105	ALA	CA-C-N	6.12	133.22	121.54
6	h	105	ALA	C-N-CA	6.12	133.22	121.54
7	r	195	GLY	N-CA-C	-5.73	100.65	112.34
1	J	91	GLY	CA-C-N	5.62	128.58	120.38
1	J	91	GLY	C-N-CA	5.62	128.58	120.38
7	k	252	LEU	N-CA-C	5.16	118.74	112.23
1	O	299	ASP	CA-C-N	5.09	131.27	121.54
1	O	299	ASP	C-N-CA	5.09	131.27	121.54
1	K	9	ASN	CA-C-N	5.01	127.78	120.51
1	K	9	ASN	C-N-CA	5.01	127.78	120.51

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10252	0	10074	165	0
1	K	10832	0	10655	186	0
1	N	10683	0	10500	153	0
1	O	10194	0	10022	147	0
2	v	2288	0	2273	60	0
3	w	549	0	540	5	0
3	x	549	0	540	23	0
4	y	317	0	341	6	0
4	z	317	0	341	5	0
5	Z	649	0	649	6	0
5	a	649	0	649	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	d	649	0	649	4	0
5	e	649	0	649	6	0
6	f	1992	0	1953	32	0
6	h	2604	0	2577	33	0
7	k	2338	0	2364	67	0
7	m	2338	0	2364	50	0
7	p	2338	0	2364	72	0
7	r	2338	0	2364	74	0
All	All	62525	0	61868	1008	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 8.

All (1008) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:857:LEU:HD12	1:K:875:ARG:CD	1.20	1.58
1:J:1264:VAL:CG1	1:J:1265:PRO:HD2	1.34	1.52
1:K:1264:VAL:HB	1:K:1265:PRO:CD	1.09	1.44
7:r:193:VAL:HB	7:r:194:PRO:CD	1.33	1.43
1:K:1264:VAL:CB	1:K:1265:PRO:HD2	1.45	1.42
1:K:467:PRO:CG	1:K:912:PRO:HG3	1.59	1.33
1:O:483:ARG:NH2	1:O:553:ASP:OD2	1.62	1.32
1:K:857:LEU:CD1	1:K:875:ARG:CD	2.08	1.29
7:r:193:VAL:CB	7:r:194:PRO:HD3	1.64	1.28
1:K:1264:VAL:CB	1:K:1265:PRO:CD	2.02	1.28
1:K:803:GLY:O	1:K:804:HIS:CD2	1.86	1.27
1:K:857:LEU:CD1	1:K:875:ARG:HD3	1.65	1.27
1:K:803:GLY:C	1:K:804:HIS:CD2	2.16	1.23
1:K:484:ARG:CD	1:K:552:ARG:HA	1.68	1.23
1:J:1264:VAL:CG1	1:J:1265:PRO:CD	2.20	1.18
1:J:1264:VAL:HG13	1:J:1265:PRO:CD	1.74	1.18
1:N:670:LEU:CG	1:N:671:GLY:H	1.54	1.18
1:J:871:ILE:HD13	1:J:936:ARG:NH2	1.57	1.17
1:K:1264:VAL:HB	1:K:1265:PRO:HD3	1.16	1.15
1:K:803:GLY:O	1:K:804:HIS:CG	1.98	1.15
1:N:670:LEU:HG	1:N:671:GLY:N	1.30	1.14
1:J:85:LEU:HD11	1:J:1070:GLY:HA2	1.29	1.12
6:h:287:CYS:SG	7:m:280:LEU:HG	1.89	1.12
7:p:97:TYR:O	7:p:98:GLN:HB2	1.43	1.09
2:v:354:ARG:CD	3:x:39:LEU:HD21	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:857:LEU:HD12	1:K:875:ARG:HD2	1.29	1.07
5:a:18:PHE:HD2	5:a:19:PRO:HG3	1.19	1.07
1:J:85:LEU:CD1	1:J:1070:GLY:HA2	1.84	1.07
7:k:161:MET:CG	7:k:162:GLN:H	1.68	1.07
7:r:77:VAL:O	7:r:78:ASP:OD1	1.73	1.07
5:a:18:PHE:CD2	5:a:19:PRO:HG3	1.91	1.06
7:r:193:VAL:CB	7:r:194:PRO:CD	2.23	1.05
1:J:1264:VAL:HG12	1:J:1265:PRO:HD2	1.35	1.05
7:r:192:GLU:O	7:r:193:VAL:HG23	1.57	1.04
1:K:484:ARG:HD3	1:K:552:ARG:CA	1.88	1.02
1:K:857:LEU:HD11	1:K:875:ARG:HG2	1.37	1.02
1:K:1252:ASP:OD1	1:K:1256:ASN:ND2	1.92	1.02
7:k:161:MET:HG2	7:k:162:GLN:N	1.40	1.00
1:K:467:PRO:HG2	1:K:912:PRO:CG	1.92	1.00
1:K:1264:VAL:CG2	1:K:1265:PRO:HD2	1.90	0.99
1:K:467:PRO:CG	1:K:912:PRO:CG	2.40	0.99
1:J:556:GLU:HG2	1:J:557:ARG:H	1.27	0.97
7:k:161:MET:CG	7:k:162:GLN:N	2.24	0.97
1:K:467:PRO:HG2	1:K:912:PRO:HG3	0.96	0.95
1:K:484:ARG:HD3	1:K:552:ARG:HA	0.95	0.94
1:N:731:ASP:HA	1:N:796:LEU:HD21	1.45	0.94
1:J:72:ALA:HB2	1:J:369:ALA:HB2	1.50	0.93
1:K:857:LEU:CD1	1:K:875:ARG:CG	2.46	0.92
5:a:18:PHE:HD2	5:a:19:PRO:CG	1.82	0.92
5:a:18:PHE:HB3	5:a:19:PRO:HD3	1.52	0.92
1:O:483:ARG:HE	1:O:553:ASP:CG	1.80	0.90
1:O:483:ARG:CZ	1:O:553:ASP:OD2	2.20	0.89
7:m:277:LEU:O	7:m:280:LEU:HD11	1.72	0.89
1:K:857:LEU:CD1	1:K:875:ARG:HG2	2.03	0.88
7:r:199:LEU:HB2	7:r:202:LEU:O	1.73	0.87
2:v:354:ARG:HD3	3:x:39:LEU:HD21	1.53	0.87
1:J:1264:VAL:HG12	1:J:1265:PRO:CD	1.98	0.87
1:O:1010:PRO:O	1:O:1011:SER:O	1.92	0.86
1:J:1264:VAL:HG13	1:J:1265:PRO:HD2	0.87	0.86
7:p:98:GLN:HB3	7:p:120:HIS:NE2	1.91	0.85
7:k:156:TYR:CE2	7:p:261:LEU:HG	2.10	0.85
1:N:265:SER:O	1:N:266:THR:O	1.93	0.85
1:J:871:ILE:HD13	1:J:936:ARG:HH21	1.37	0.84
1:J:556:GLU:CG	1:J:557:ARG:N	2.41	0.84
1:K:857:LEU:HD11	1:K:875:ARG:CG	2.07	0.84
1:J:556:GLU:HG2	1:J:557:ARG:N	1.87	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HH11	1:N:484:ARG:HG2	1.41	0.83
1:N:619:PHE:HE1	1:N:874:LEU:HD23	1.41	0.83
7:r:254:ASP:O	7:r:255:LEU:HG	1.78	0.83
1:K:1252:ASP:CG	1:K:1256:ASN:ND2	2.38	0.82
2:v:354:ARG:HD3	3:x:39:LEU:CD2	2.09	0.82
1:N:670:LEU:CG	1:N:671:GLY:N	2.20	0.81
1:K:857:LEU:HD12	1:K:875:ARG:HD3	0.82	0.81
2:v:354:ARG:NE	3:x:39:LEU:HD21	1.96	0.81
6:f:160:ASP:O	6:f:161:SER:HB2	1.81	0.80
1:K:1256:ASN:OD1	1:K:1275:PHE:O	2.00	0.80
1:K:1264:VAL:HB	1:K:1265:PRO:HD2	0.80	0.80
1:K:1252:ASP:CG	1:K:1256:ASN:HD21	1.89	0.79
7:p:138:LEU:HD21	7:p:142:ILE:HG22	1.64	0.79
1:J:482:ASP:HB2	1:J:484:ARG:NH1	1.97	0.78
7:r:192:GLU:C	7:r:193:VAL:CG2	2.57	0.78
1:N:825:MET:HA	1:N:930:ALA:O	1.84	0.77
7:p:188:LEU:HD12	7:p:188:LEU:O	1.85	0.77
1:N:899:ARG:NH1	1:N:922:THR:HG23	1.99	0.76
6:f:187:PRO:HB2	6:f:357:VAL:CG1	2.15	0.76
7:r:202:LEU:O	7:r:203:ASP:HB3	1.85	0.75
6:h:272:GLU:HG3	6:h:304:ARG:HG2	1.69	0.75
7:r:201:LEU:N	7:r:201:LEU:HD22	2.02	0.74
1:O:483:ARG:NE	1:O:553:ASP:CG	2.44	0.74
1:J:828:LEU:HB3	1:J:928:LEU:O	1.87	0.74
5:a:18:PHE:CD2	5:a:19:PRO:CG	2.64	0.74
7:r:199:LEU:CD1	7:r:202:LEU:O	2.35	0.74
7:k:156:TYR:HD2	7:p:261:LEU:HD21	1.51	0.73
5:a:20:ASP:N	5:a:20:ASP:OD1	2.21	0.73
7:r:192:GLU:O	7:r:193:VAL:CG2	2.36	0.73
1:K:467:PRO:HG3	1:K:912:PRO:HG3	1.67	0.72
7:p:98:GLN:HB3	7:p:99:PRO:HD3	1.71	0.72
7:p:98:GLN:HG3	7:p:120:HIS:CE1	2.25	0.72
1:J:936:ARG:HD3	1:O:669:HIS:CD2	2.25	0.72
1:J:85:LEU:HD11	1:J:1070:GLY:CA	2.16	0.72
1:K:617:ALA:O	1:K:620:TYR:HB2	1.90	0.72
7:r:199:LEU:CB	7:r:202:LEU:O	2.36	0.72
2:v:62:ALA:HA	2:v:77:PHE:O	1.89	0.71
1:N:543:HIS:HD2	1:N:546:TYR:H	1.36	0.71
1:N:619:PHE:CE1	1:N:874:LEU:HD23	2.25	0.71
7:p:98:GLN:CB	7:p:99:PRO:CD	2.69	0.71
1:K:360:GLU:O	1:K:362:GLN:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:ARG:HD3	1:N:550:ILE:HG22	1.72	0.71
1:O:860:LEU:HD22	1:O:866:ARG:HG2	1.72	0.71
1:J:1067:MET:HE2	1:J:1092:MET:HE2	1.72	0.71
6:f:187:PRO:HB2	6:f:357:VAL:HG11	1.72	0.70
6:h:305:TYR:O	6:h:306:ALA:O	2.09	0.70
1:K:456:LEU:HD11	1:K:1031:ILE:HG13	1.74	0.70
1:K:1252:ASP:CB	1:K:1256:ASN:ND2	2.54	0.70
1:N:899:ARG:HH11	1:N:922:THR:CG2	2.05	0.70
1:J:871:ILE:HD13	1:J:936:ARG:HH22	1.54	0.70
7:k:156:TYR:HE2	7:p:261:LEU:HG	1.56	0.69
1:K:804:HIS:HE1	1:K:808:LEU:HD11	1.57	0.69
5:a:18:PHE:HD2	5:a:19:PRO:CD	2.04	0.69
7:k:222:ARG:CD	7:k:251:ASP:OD1	2.40	0.69
7:r:193:VAL:HB	7:r:194:PRO:HD2	1.65	0.69
7:p:138:LEU:HG	7:p:139:PRO:HD2	1.75	0.69
1:J:96:ARG:HG2	1:J:117:ILE:HG12	1.75	0.68
1:K:805:ALA:O	1:K:806:ASP:OD1	2.11	0.68
1:K:722:ASN:HD22	1:K:742:ARG:HH21	1.40	0.68
7:r:193:VAL:HB	7:r:194:PRO:HD3	0.68	0.68
1:K:912:PRO:O	1:K:913:ASN:HB3	1.93	0.68
7:m:5:VAL:HB	7:m:82:LEU:O	1.94	0.67
6:h:227:GLN:HG2	6:h:348:VAL:HG13	1.76	0.67
1:K:803:GLY:C	1:K:804:HIS:HD2	1.96	0.67
1:K:1252:ASP:CB	1:K:1256:ASN:HD22	2.07	0.67
1:K:1256:ASN:OD1	1:K:1275:PHE:HB3	1.95	0.67
1:O:241:SER:HA	1:O:293:PHE:HZ	1.58	0.67
1:J:856:ILE:HG13	1:J:881:ILE:HD12	1.76	0.67
1:K:852:ARG:HD3	5:a:63:ARG:HH11	1.59	0.67
1:O:639:LEU:HD12	1:O:880:MET:HB3	1.76	0.66
7:p:97:TYR:O	7:p:98:GLN:CB	2.29	0.66
1:N:1068:PHE:HB2	1:N:1093:ALA:HB3	1.78	0.66
1:J:436:VAL:HG11	1:J:587:GLN:HE22	1.59	0.66
1:J:456:LEU:HD21	1:J:1031:ILE:HG13	1.77	0.66
1:K:912:PRO:O	1:K:913:ASN:CB	2.44	0.66
7:r:192:GLU:C	7:r:193:VAL:HG23	2.19	0.66
7:m:277:LEU:O	7:m:280:LEU:CD1	2.44	0.66
1:J:401:MET:O	1:J:1051:GLU:HA	1.96	0.65
1:O:565:ARG:O	1:O:570:ASN:ND2	2.27	0.65
7:p:98:GLN:HB3	7:p:99:PRO:CD	2.26	0.65
7:r:161:MET:HG3	7:r:194:PRO:CG	2.26	0.65
1:N:650:ARG:NE	1:N:873:ASP:OD2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1117:MET:SD	1:O:1371:ARG:NH1	2.70	0.65
1:O:1068:PHE:HB2	1:O:1093:ALA:HB3	1.77	0.65
7:k:161:MET:HG2	7:k:162:GLN:H	0.72	0.65
1:O:568:VAL:HA	1:O:1025:MET:HE3	1.77	0.65
7:r:154:ASN:HB2	7:r:202:LEU:HG	1.78	0.65
1:N:899:ARG:HH11	1:N:922:THR:HG23	1.60	0.65
1:K:467:PRO:HG3	1:K:912:PRO:CG	2.22	0.65
5:a:18:PHE:CB	5:a:19:PRO:HD3	2.26	0.65
7:k:247:ILE:O	7:k:251:ASP:HB2	1.96	0.64
1:K:901:SER:HB3	1:K:918:ARG:HD2	1.80	0.64
1:K:911:ALA:HB3	1:K:912:PRO:CD	2.28	0.64
1:N:129:THR:HG22	1:O:103:ALA:HB2	1.80	0.64
1:O:104:HIS:HE1	1:O:108:ARG:HB2	1.62	0.64
1:J:1192:ASP:OD2	1:J:1237:ARG:NH2	2.31	0.64
6:f:195:ILE:HB	6:f:202:LYS:HB3	1.80	0.64
1:J:828:LEU:HD11	1:J:945:PHE:HB3	1.80	0.64
1:O:594:LEU:HD11	1:O:692:ALA:HB1	1.79	0.64
1:K:857:LEU:CD1	1:K:875:ARG:HD2	2.06	0.64
1:J:72:ALA:CB	1:J:369:ALA:HB2	2.26	0.64
5:a:21:SER:HB3	5:a:24:LEU:HD23	1.79	0.64
7:k:59:SER:HB2	7:k:197:LEU:HG	1.79	0.63
1:N:409:VAL:HG13	1:N:1044:MET:HG3	1.80	0.63
7:k:222:ARG:HD2	7:k:251:ASP:OD1	1.97	0.63
7:r:200:ALA:HB3	7:r:201:LEU:HD22	1.79	0.63
1:N:718:LEU:HD13	1:N:811:ILE:HG12	1.81	0.63
1:O:764:GLU:OE1	1:O:793:ARG:NH1	2.32	0.63
2:v:354:ARG:CD	3:x:39:LEU:CD2	2.67	0.63
2:v:354:ARG:HH12	3:x:43:GLU:HG3	1.63	0.63
2:v:354:ARG:CG	3:x:39:LEU:HD21	2.28	0.63
6:f:323:CYS:H	6:f:358:SER:HB3	1.64	0.63
3:w:46:ALA:O	3:w:50:ARG:HB2	1.98	0.63
1:N:1192:ASP:OD2	1:N:1237:ARG:NH2	2.31	0.63
7:k:156:TYR:CD2	7:p:261:LEU:HD21	2.34	0.63
1:K:764:GLU:HG3	1:K:793:ARG:HH11	1.64	0.62
1:K:1252:ASP:HB3	1:K:1256:ASN:HD22	1.63	0.62
1:J:399:ARG:HG3	1:J:1105:MET:HE1	1.80	0.62
1:K:804:HIS:CE1	1:K:808:LEU:HD11	2.35	0.62
1:K:1195:TYR:O	1:K:1200:ASN:ND2	2.31	0.62
1:N:804:HIS:CD2	1:N:808:LEU:HD11	2.35	0.62
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.65	0.62
7:k:156:TYR:CD2	7:p:261:LEU:CD2	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:817:LEU:HB3	1:N:825:MET:HE1	1.81	0.62
2:v:99:ALA:HA	2:v:112:LEU:O	2.00	0.62
7:k:220:SER:OG	7:p:210:CYS:SG	2.57	0.62
3:x:91:VAL:HG22	4:y:3122:PHE:HB3	1.81	0.62
1:J:783:ARG:NH2	1:J:891:CYS:O	2.33	0.61
7:m:9:LEU:HD13	7:m:40:VAL:HG11	1.80	0.61
1:J:72:ALA:HB2	1:J:369:ALA:CB	2.27	0.61
1:J:225:GLU:O	1:J:232:ARG:NH2	2.33	0.61
1:K:400:ARG:NE	1:K:1051:GLU:OE2	2.30	0.61
1:N:747:ILE:HB	1:N:899:ARG:HB2	1.81	0.61
1:N:1246:GLN:HB2	1:N:1249:SER:HB3	1.82	0.61
7:k:222:ARG:HD3	7:k:251:ASP:OD1	2.00	0.61
1:N:362:GLN:O	1:N:364:ARG:NH1	2.34	0.61
1:K:285:ASN:O	1:K:289:GLN:NE2	2.32	0.61
1:K:1252:ASP:HA	1:K:1256:ASN:ND2	2.15	0.61
1:N:53:GLU:OE2	1:O:326:ARG:NH1	2.33	0.61
1:O:225:GLU:O	1:O:232:ARG:NH1	2.34	0.61
3:x:76:ASP:HB3	4:y:3136:ARG:HE	1.65	0.61
1:K:184:LYS:NZ	1:K:1064:SER:OG	2.34	0.61
1:N:93:ILE:HD12	1:N:1095:ILE:HG21	1.82	0.60
1:N:439:TRP:HB2	1:N:1337:ALA:HB3	1.83	0.60
2:v:37:PRO:HG2	2:v:102:PHE:HZ	1.67	0.60
1:J:10:ARG:NH1	1:K:321:ALA:O	2.32	0.60
1:N:484:ARG:HG2	1:N:484:ARG:NH1	2.14	0.60
1:K:817:LEU:HB3	1:K:825:MET:HE1	1.84	0.60
1:N:737:LEU:HD23	1:N:744:PRO:HG2	1.82	0.60
6:f:193:GLU:HB2	6:f:204:THR:HB	1.84	0.60
1:N:619:PHE:CE1	1:N:874:LEU:CD2	2.84	0.60
2:v:464:HIS:HB3	2:v:476:VAL:HB	1.83	0.60
7:k:171:ASP:CB	7:p:261:LEU:HD11	2.31	0.60
1:K:1068:PHE:HB2	1:K:1093:ALA:HB3	1.83	0.60
7:m:7:VAL:HG22	7:m:38:GLN:HB2	1.84	0.60
1:J:431:THR:HG23	1:J:432:GLN:HG3	1.84	0.59
1:N:783:ARG:HA	1:N:788:HIS:HE1	1.66	0.59
6:f:179:ARG:NH1	6:f:315:GLU:OE2	2.35	0.59
6:f:304:ARG:NH1	6:f:315:GLU:O	2.35	0.59
1:K:484:ARG:CD	1:K:552:ARG:CA	2.63	0.59
1:N:184:LYS:NZ	1:N:1064:SER:OG	2.36	0.59
1:O:783:ARG:NH2	1:O:891:CYS:O	2.34	0.59
2:v:426:LEU:O	3:w:50:ARG:NH2	2.35	0.59
1:J:1374:LYS:HG2	1:J:1379:VAL:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:484:ARG:HD2	1:K:552:ARG:HA	1.76	0.59
1:O:301:GLN:HA	1:O:367:ILE:O	2.01	0.59
1:N:484:ARG:HD2	1:N:551:GLY:O	2.02	0.59
7:k:161:MET:HG3	7:k:162:GLN:OE1	2.02	0.59
7:p:4:LYS:HG2	7:p:83:THR:HG22	1.83	0.59
7:p:45:LEU:HG	7:p:45:LEU:O	2.03	0.59
7:r:199:LEU:HD12	7:r:202:LEU:O	2.00	0.59
1:K:409:VAL:HG13	1:K:1044:MET:HG3	1.85	0.59
7:p:149:LYS:NZ	7:p:178:SER:O	2.33	0.59
1:O:913:ASN:OD1	2:v:34:ASN:HA	2.02	0.59
7:m:265:ARG:NH1	7:r:145:GLU:OE2	2.36	0.59
7:m:3:LEU:HD21	7:m:86:VAL:HG23	1.83	0.59
1:K:548:ILE:HD11	1:K:560:HIS:HB3	1.85	0.59
1:N:1074:VAL:HG22	1:N:1088:VAL:HG22	1.84	0.59
7:k:272:GLN:NE2	7:p:144:GLU:OE2	2.36	0.58
1:O:850:PHE:HE2	1:O:878:VAL:HG21	1.68	0.58
7:p:138:LEU:HG	7:p:139:PRO:CD	2.32	0.58
1:K:877:THR:H	1:K:880:MET:HE2	1.68	0.58
1:J:936:ARG:HD3	1:O:669:HIS:HD2	1.68	0.58
1:N:942:GLN:NE2	1:N:943:CYS:SG	2.76	0.58
5:a:18:PHE:CD2	5:a:19:PRO:HD3	2.38	0.58
7:k:11:SER:OG	7:k:128:ASN:ND2	2.37	0.58
1:K:317:ASN:ND2	1:K:328:MET:O	2.36	0.58
1:J:551:GLY:HA3	1:J:559:ARG:HH11	1.67	0.58
1:K:724:LEU:O	1:K:921:GLN:NE2	2.36	0.58
1:K:910:LEU:C	1:K:912:PRO:HD2	2.29	0.58
1:N:185:LEU:HD13	1:N:399:ARG:HH21	1.69	0.58
1:J:463:ARG:HH22	1:J:1259:TYR:HB3	1.68	0.58
1:J:720:ASP:OD1	1:J:742:ARG:NH2	2.37	0.58
1:K:496:HIS:HE1	1:K:502:ILE:HG13	1.68	0.58
1:N:803:GLY:O	1:N:804:HIS:HB2	2.03	0.58
7:m:24:ARG:NH1	7:m:120:HIS:O	2.36	0.58
1:N:1195:TYR:O	1:N:1200:ASN:ND2	2.37	0.58
7:m:247:ILE:O	7:m:251:ASP:HB2	2.04	0.58
1:K:185:LEU:HD13	1:K:399:ARG:HH21	1.68	0.58
1:N:997:HIS:HE1	1:N:1022:HIS:HE1	1.52	0.58
1:O:406:TYR:HA	1:O:1046:VAL:O	2.03	0.58
6:f:320:ALA:HB1	6:f:360:TRP:HB3	1.85	0.58
7:k:156:TYR:CE2	7:p:261:LEU:CG	2.85	0.58
7:m:10:SER:OG	7:m:128:ASN:ND2	2.35	0.57
1:O:549:TYR:OH	1:O:994:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:202:LEU:O	7:r:203:ASP:CB	2.52	0.57
1:N:80:THR:HG22	1:N:309:ALA:HB3	1.87	0.57
1:O:904:ASN:ND2	1:O:908:GLN:O	2.37	0.57
2:v:384:ASP:OD1	2:v:387:ARG:NH1	2.37	0.57
6:f:236:TRP:HE3	6:f:237:LEU:HD23	1.70	0.57
1:K:359:VAL:O	1:K:360:GLU:O	2.22	0.57
1:K:496:HIS:ND1	1:K:498:ASN:OD1	2.37	0.57
1:N:401:MET:O	1:N:1051:GLU:HA	2.04	0.57
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	1.85	0.57
5:e:23:LEU:HD13	5:e:51:LEU:HB3	1.86	0.57
7:k:28:ILE:HD12	7:k:137:VAL:HG11	1.86	0.57
7:r:161:MET:HG3	7:r:194:PRO:HG2	1.85	0.57
1:K:586:GLN:NE2	1:K:589:GLU:OE2	2.36	0.57
1:O:439:TRP:HB3	1:O:447:LEU:HD11	1.87	0.57
1:J:406:TYR:HA	1:J:1046:VAL:O	2.05	0.57
1:N:742:ARG:HB3	1:N:903:ASP:HB2	1.85	0.57
2:v:396:ARG:HD3	2:v:434:TRP:HE1	1.69	0.57
1:K:594:LEU:HD13	1:K:696:ALA:HB2	1.87	0.57
2:v:463:VAL:CG1	2:v:475:LEU:HD11	2.35	0.57
1:O:282:VAL:HG12	1:O:1057:ILE:HG12	1.86	0.56
1:J:995:GLU:O	1:J:998:ARG:NH2	2.38	0.56
2:v:387:ARG:HD3	3:x:38:ALA:HB1	1.86	0.56
5:a:18:PHE:HD2	5:a:19:PRO:HD3	1.69	0.56
7:k:218:ARG:HG2	7:k:263:ARG:HH12	1.69	0.56
1:J:85:LEU:CD1	1:J:1070:GLY:CA	2.74	0.56
1:J:1264:VAL:HG12	1:J:1265:PRO:N	2.15	0.56
1:O:584:ARG:NH1	1:O:1020:ALA:O	2.35	0.56
1:O:650:ARG:NH1	1:O:873:ASP:O	2.39	0.56
6:h:195:ILE:HB	6:h:202:LYS:HB3	1.86	0.56
1:K:585:GLY:HA3	1:K:1017:GLY:HA2	1.88	0.56
1:N:133:LEU:HD13	1:N:138:LEU:HD21	1.87	0.56
1:N:731:ASP:CA	1:N:796:LEU:HD21	2.26	0.56
7:m:212:MET:HE2	7:m:270:TYR:HB3	1.87	0.56
1:J:443:LYS:HD3	1:J:1116:ASP:HA	1.88	0.56
1:N:673:ASN:HB3	1:O:650:ARG:HH22	1.71	0.56
1:J:497:MET:HE3	1:J:792:PHE:HA	1.86	0.56
1:N:567:MET:SD	1:N:1022:HIS:ND1	2.77	0.56
7:p:30:PRO:HG3	7:p:45:LEU:HB2	1.86	0.56
7:k:59:SER:N	7:k:197:LEU:HD12	2.21	0.56
1:J:584:ARG:NH1	1:J:1020:ALA:O	2.38	0.56
1:K:1246:GLN:HB2	1:K:1249:SER:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:SER:OG	1:O:114:ARG:NH2	2.39	0.56
2:v:118:SER:HB2	2:v:288:ILE:HB	1.87	0.56
7:p:28:ILE:HD12	7:p:137:VAL:HG21	1.87	0.56
1:J:555:GLY:O	1:J:557:ARG:N	2.39	0.56
1:J:666:ILE:HA	1:J:670:LEU:HD12	1.87	0.56
1:N:230:LEU:HD21	1:N:289:GLN:HG2	1.86	0.56
1:N:670:LEU:HG	1:N:671:GLY:H	0.62	0.56
1:J:400:ARG:NH2	1:J:1051:GLU:OE1	2.38	0.55
1:K:266:THR:O	1:K:364:ARG:NH1	2.34	0.55
1:O:127:ILE:HB	1:O:1090:HIS:O	2.06	0.55
1:O:1080:ARG:HE	1:O:1082:ASP:HB2	1.71	0.55
6:h:94:LEU:HD21	6:h:200:LEU:HD13	1.88	0.55
1:K:307:SER:OG	1:K:362:GLN:NE2	2.39	0.55
1:K:938:ARG:HA	1:K:941:THR:HB	1.88	0.55
1:N:783:ARG:HE	1:N:893:THR:HG22	1.71	0.55
7:r:49:TYR:HD2	7:r:60:MET:HE1	1.69	0.55
5:a:18:PHE:CD2	5:a:19:PRO:CD	2.86	0.55
6:h:129:LEU:HD22	6:h:158:LEU:HD12	1.87	0.55
7:k:28:ILE:HD11	7:k:93:ILE:HD11	1.87	0.55
1:K:911:ALA:N	1:K:912:PRO:HD2	2.22	0.55
1:N:269:THR:HG22	1:N:271:LYS:H	1.72	0.55
1:J:746:ILE:HB	1:J:753:TYR:HB3	1.87	0.55
1:J:763:ILE:HG12	1:J:794:LEU:HD11	1.89	0.55
1:K:269:THR:OG1	1:K:272:GLY:O	2.23	0.55
3:x:71:ASP:OD1	4:z:3145:LYS:NZ	2.38	0.55
7:k:156:TYR:O	7:k:160:VAL:HG22	2.07	0.55
1:N:856:ILE:HD12	1:N:876:PRO:HG2	1.89	0.55
1:N:857:LEU:HD12	1:N:875:ARG:HG2	1.88	0.55
7:r:199:LEU:HD12	7:r:203:ASP:HB3	1.88	0.55
1:J:935:GLU:OE1	1:O:668:ARG:NH1	2.38	0.55
1:J:955:GLY:HA3	1:J:985:ARG:HE	1.72	0.55
1:O:814:TYR:OH	1:O:921:GLN:NE2	2.40	0.55
7:r:95:ASN:ND2	7:r:289:TYR:OH	2.40	0.55
1:J:1135:ASN:HB3	1:J:1138:VAL:HG12	1.89	0.55
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.36	0.55
7:k:45:LEU:HB3	7:k:133:VAL:HB	1.88	0.55
1:N:267:TYR:HD1	1:N:267:TYR:N	2.05	0.54
1:J:1174:LEU:O	1:K:213:SER:OG	2.21	0.54
1:J:1308:GLU:HG3	1:J:1309:VAL:HG13	1.88	0.54
1:K:40:LEU:HD22	1:K:44:ASP:HB3	1.88	0.54
1:K:1117:MET:SD	1:K:1371:ARG:NH2	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:GLN:NE2	1:J:250:GLU:OE2	2.40	0.54
1:K:361:ASP:O	1:K:362:GLN:C	2.49	0.54
1:J:871:ILE:CD1	1:J:936:ARG:HH21	2.14	0.54
1:K:591:ALA:HB1	1:K:1036:LEU:HD12	1.88	0.54
1:K:952:MET:HA	1:K:985:ARG:HH22	1.71	0.54
2:v:476:VAL:HG22	2:v:482:VAL:HG22	1.90	0.54
7:m:148:GLN:HE22	7:r:269:THR:HG23	1.72	0.54
1:J:303:MET:O	1:J:364:ARG:N	2.41	0.54
1:K:95:PHE:HB2	1:K:118:VAL:HB	1.90	0.54
1:N:287:LEU:HD13	1:N:383:SER:HB3	1.90	0.54
1:N:844:PRO:O	1:N:882:ARG:NH2	2.36	0.54
5:d:23:LEU:HD22	5:d:51:LEU:HB3	1.89	0.54
1:K:720:ASP:O	1:K:810:LYS:NZ	2.40	0.54
1:K:997:HIS:HE1	1:K:1022:HIS:HE1	1.54	0.54
1:N:1119:ILE:HD11	1:O:1235:GLU:HB3	1.90	0.54
1:N:1298:LEU:HD21	1:N:1302:PRO:HG3	1.90	0.54
1:O:417:LYS:NZ	1:O:431:THR:O	2.40	0.54
1:N:572:PRO:HG2	1:N:575:LEU:HD12	1.90	0.54
4:y:3131:GLU:O	4:y:3135:HIS:ND1	2.39	0.54
6:h:224:THR:HG22	6:h:349:GLU:HG2	1.90	0.54
7:k:156:TYR:CE2	7:p:261:LEU:CD2	2.91	0.54
7:k:222:ARG:HG3	7:k:255:LEU:HD11	1.90	0.54
1:N:1053:LEU:HD12	1:N:1112:ALA:HB3	1.90	0.54
1:O:1299:GLY:O	1:O:1323:GLN:NE2	2.41	0.54
6:f:192:VAL:HG12	6:f:193:GLU:HG3	1.90	0.54
7:p:171:ASP:O	7:p:175:HIS:ND1	2.33	0.54
7:r:254:ASP:O	7:r:255:LEU:CG	2.55	0.54
1:J:400:ARG:HH22	1:J:1114:THR:HG21	1.72	0.53
2:v:396:ARG:HH21	2:v:434:TRP:HE1	1.56	0.53
5:a:65:PHE:HE2	5:a:68:PRO:HB3	1.73	0.53
1:K:911:ALA:CB	1:K:912:PRO:CD	2.86	0.53
1:J:617:ALA:HA	1:J:620:TYR:HD2	1.73	0.53
1:K:329:ARG:HG2	1:K:330:THR:HG23	1.90	0.53
1:J:565:ARG:O	1:J:570:ASN:ND2	2.35	0.53
1:J:589:GLU:HG2	1:J:594:LEU:HD12	1.90	0.53
1:K:312:VAL:HG12	1:K:314:ARG:H	1.73	0.53
1:K:1264:VAL:HG23	1:K:1265:PRO:HD2	1.88	0.53
1:N:282:VAL:HG12	1:N:1057:ILE:HG12	1.90	0.53
1:N:532:PRO:HB3	1:N:1238:SER:HB2	1.90	0.53
1:O:598:VAL:HG13	1:O:602:VAL:HG13	1.89	0.53
1:J:399:ARG:HD3	1:J:1320:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1326:SER:O	1:J:1329:GLN:NE2	2.42	0.53
6:h:46:HIS:CE1	6:h:71:ALA:H	2.27	0.53
7:k:211:ILE:O	7:k:214:THR:OG1	2.25	0.53
7:m:74:GLU:HB3	7:m:81:ILE:HB	1.90	0.53
7:m:122:THR:HG22	7:m:133:VAL:HA	1.90	0.53
7:p:98:GLN:CB	7:p:99:PRO:HD3	2.34	0.53
1:J:85:LEU:HD13	1:J:1070:GLY:HA2	1.85	0.53
1:K:690:LEU:HD11	1:K:812:PHE:HB2	1.91	0.53
1:K:803:GLY:O	1:K:804:HIS:NE2	2.40	0.53
1:K:804:HIS:HE1	1:K:808:LEU:CD1	2.20	0.53
1:O:307:SER:OG	1:O:362:GLN:OE1	2.27	0.53
1:J:427:LEU:O	1:J:427:LEU:HD23	2.09	0.53
1:K:535:TYR:HE2	1:K:539:ARG:HH21	1.57	0.53
7:m:214:THR:HG22	7:r:244:PRO:HD3	1.91	0.53
7:r:201:LEU:HD22	7:r:201:LEU:H	1.73	0.53
1:J:281:ILE:HD12	1:J:1058:LEU:HD23	1.90	0.53
1:K:225:GLU:O	1:K:232:ARG:NH2	2.38	0.53
6:f:237:LEU:O	6:f:237:LEU:HD12	2.08	0.53
7:r:158:ARG:HH22	7:r:196:PRO:HA	1.74	0.53
1:O:625:MET:SD	1:O:887:SER:OG	2.61	0.52
7:k:156:TYR:HE2	7:p:261:LEU:CG	2.20	0.52
1:K:840:ALA:HB3	5:a:49:VAL:HG22	1.90	0.52
1:O:504:ASP:O	1:O:508:ASP:HB2	2.09	0.52
4:z:3114:GLN:OE1	4:z:3117:ARG:NH1	2.42	0.52
1:N:484:ARG:HH11	1:N:484:ARG:CG	2.16	0.52
1:O:510:LYS:O	1:O:973:ARG:NH2	2.42	0.52
1:J:904:ASN:ND2	1:J:919:THR:OG1	2.33	0.52
1:O:921:GLN:HB2	1:O:996:TRP:CD1	2.44	0.52
2:v:39:CYS:HB2	2:v:62:ALA:HB3	1.91	0.52
1:J:367:ILE:O	1:J:368:SER:OG	2.21	0.52
1:O:835:VAL:O	1:O:838:THR:OG1	2.26	0.52
5:a:32:GLN:HG2	5:a:33:ASN:H	1.75	0.52
6:f:179:ARG:HH11	6:f:304:ARG:HH11	1.58	0.52
6:h:154:MET:HE1	6:h:340:TYR:HB3	1.90	0.52
7:m:72:LEU:HA	7:m:82:LEU:HG	1.92	0.52
1:O:902:VAL:O	1:O:918:ARG:HA	2.09	0.52
7:r:161:MET:HG3	7:r:194:PRO:HG3	1.92	0.52
1:N:267:TYR:N	1:N:267:TYR:CD1	2.76	0.52
1:N:835:VAL:O	1:N:838:THR:OG1	2.25	0.52
1:N:840:ALA:HB3	5:d:49:VAL:HG22	1.91	0.52
1:O:1128:PHE:HZ	1:O:1260:ARG:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:803:GLY:CA	1:K:804:HIS:CD2	2.92	0.52
1:N:513:ALA:HB1	1:N:984:ASN:HD22	1.75	0.52
1:N:1115:THR:HG22	1:N:1180:ALA:HB2	1.92	0.52
1:N:1299:GLY:HA3	1:N:1323:GLN:HE21	1.74	0.52
6:f:223:VAL:HG13	6:f:350:ILE:HG13	1.91	0.52
6:h:154:MET:HG2	6:h:345:LEU:HD22	1.92	0.52
7:k:171:ASP:HA	7:p:261:LEU:CD1	2.40	0.52
7:p:111:VAL:HG22	7:p:137:VAL:HG22	1.92	0.52
1:K:553:ASP:HB3	1:K:558:ALA:HB2	1.91	0.51
1:O:266:THR:O	1:O:364:ARG:NH1	2.41	0.51
1:J:731:ASP:HB3	1:J:799:TYR:HB2	1.92	0.51
1:K:401:MET:O	1:K:1051:GLU:HA	2.11	0.51
1:K:1203:ARG:HE	1:K:1245:SER:HA	1.75	0.51
7:p:95:ASN:ND2	7:p:289:TYR:OH	2.44	0.51
1:J:855:ASP:OD2	1:J:875:ARG:NH2	2.39	0.51
1:K:359:VAL:C	1:K:360:GLU:O	2.53	0.51
1:K:1205:ARG:HG2	1:K:1231:ASP:HB3	1.93	0.51
1:N:587:GLN:NE2	1:N:1037:LYS:O	2.44	0.51
1:N:952:MET:HE2	1:N:999:SER:HA	1.91	0.51
1:O:603:ILE:HD13	1:O:1011:SER:O	2.11	0.51
1:O:639:LEU:HA	1:O:880:MET:HE3	1.93	0.51
1:J:1176:HIS:HE1	1:K:1233:ALA:HA	1.76	0.51
1:O:406:TYR:HE2	1:O:1196:PHE:HD1	1.58	0.51
6:h:281:GLN:OE1	6:h:333:TRP:NE1	2.36	0.51
7:p:6:VAL:HG22	7:p:81:ILE:HG12	1.92	0.51
1:J:1123:ASP:N	1:J:1123:ASP:OD1	2.43	0.51
1:K:1252:ASP:CA	1:K:1256:ASN:ND2	2.74	0.51
1:N:637:VAL:HG23	1:N:638:PRO:HD3	1.92	0.51
7:k:171:ASP:HB3	7:p:261:LEU:HD11	1.92	0.51
7:p:21:MET:HB3	7:p:75:VAL:HG21	1.91	0.51
1:O:456:LEU:HA	1:O:459:LEU:HB2	1.91	0.51
1:J:587:GLN:NE2	1:J:1037:LYS:O	2.44	0.51
1:K:521:LYS:NZ	1:K:540:LEU:O	2.44	0.51
1:K:1027:PRO:HA	1:K:1030:TYR:HD2	1.74	0.51
1:N:670:LEU:O	1:N:671:GLY:C	2.54	0.51
1:O:770:ASP:OD1	5:e:57:TYR:OH	2.29	0.51
1:O:1315:ALA:HB1	1:O:1317:THR:HG23	1.92	0.51
1:K:1159:ARG:NH2	1:K:1317:THR:OG1	2.44	0.51
1:J:581:GLN:HE21	1:J:1021:MET:HG2	1.76	0.50
1:O:434:LEU:HD12	1:O:435:PRO:HD2	1.93	0.50
5:a:61:VAL:O	5:a:64:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:564:HIS:HD2	1:J:566:LEU:HD23	1.76	0.50
1:K:971:VAL:HG13	1:K:978:ARG:HE	1.77	0.50
1:N:122:CYS:O	7:m:12:ARG:NH2	2.45	0.50
1:J:482:ASP:HB2	1:J:484:ARG:HH12	1.75	0.50
1:K:777:VAL:O	1:K:781:GLY:N	2.42	0.50
1:O:554:ALA:HB1	2:v:425:PRO:HG3	1.94	0.50
6:h:16:ILE:O	6:h:20:LEU:HB2	2.12	0.50
7:m:7:VAL:HG21	7:m:43:LEU:HD13	1.93	0.50
7:p:150:ILE:HD12	7:p:202:LEU:HD21	1.92	0.50
1:J:978:ARG:HB2	1:O:698:MET:HE3	1.92	0.50
1:K:805:ALA:O	1:K:806:ASP:CG	2.55	0.50
1:N:673:ASN:ND2	1:O:873:ASP:OD2	2.44	0.50
1:O:655:ALA:O	1:O:683:TYR:OH	2.28	0.50
7:k:111:VAL:HG22	7:k:137:VAL:HG12	1.92	0.50
1:J:72:ALA:CB	1:J:369:ALA:CB	2.89	0.50
1:K:440:ILE:HG21	1:K:1048:ARG:HH22	1.77	0.50
1:O:470:THR:HG22	1:O:1253:ILE:HG13	1.94	0.50
2:v:115:TYR:HD2	2:v:291:ILE:HB	1.76	0.50
2:v:354:ARG:HG2	3:x:39:LEU:HD21	1.92	0.50
6:f:236:TRP:CE3	6:f:237:LEU:HD23	2.47	0.50
1:K:1350:LYS:O	1:K:1353:HIS:ND1	2.45	0.50
1:N:230:LEU:HD22	1:N:1109:ARG:HD2	1.94	0.50
1:N:484:ARG:CD	1:N:551:GLY:O	2.60	0.50
1:O:1350:LYS:O	1:O:1353:HIS:ND1	2.36	0.50
2:v:331:ILE:HG23	2:v:332:LEU:HG	1.93	0.50
3:x:74:MET:HE1	4:z:3138:ILE:HG12	1.94	0.50
6:f:94:LEU:HD23	6:f:200:LEU:HD13	1.93	0.50
7:p:30:PRO:HD3	7:p:135:PRO:HD3	1.94	0.50
1:J:75:VAL:HG22	1:J:267:TYR:HD2	1.75	0.50
1:J:131:MET:O	1:J:1085:THR:HA	2.12	0.50
1:J:1197:GLN:NE2	1:J:1364:GLU:OE1	2.44	0.50
2:v:427:TYR:HB3	3:w:50:ARG:HD3	1.92	0.50
5:a:18:PHE:CE2	5:a:19:PRO:HG3	2.42	0.50
6:f:261:ASP:O	6:f:263:ARG:NH2	2.45	0.50
7:k:153:PHE:HA	7:k:176:LEU:HD13	1.93	0.50
7:m:151:LEU:HB3	7:m:202:LEU:HD21	1.93	0.50
2:v:98:ALA:O	2:v:113:GLN:HA	2.12	0.49
7:r:192:GLU:C	7:r:193:VAL:HG22	2.35	0.49
1:O:70:GLU:HA	1:O:367:ILE:HD12	1.95	0.49
6:h:223:VAL:HG13	6:h:350:ILE:HB	1.93	0.49
1:J:908:GLN:NE2	1:J:1026:SER:OG	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:518:ILE:HA	1:N:521:LYS:HB2	1.94	0.49
1:N:548:ILE:HA	1:N:561:ARG:O	2.12	0.49
1:O:724:LEU:O	1:O:814:TYR:OH	2.29	0.49
1:O:877:THR:OG1	1:O:880:MET:SD	2.67	0.49
2:v:354:ARG:NE	3:x:39:LEU:CD2	2.73	0.49
7:m:176:LEU:HD21	7:r:261:LEU:HD11	1.93	0.49
5:Z:61:VAL:O	5:Z:64:THR:OG1	2.27	0.49
7:m:238:LEU:HD11	7:r:266:VAL:HG21	1.94	0.49
7:r:138:LEU:HD12	7:r:139:PRO:HD2	1.94	0.49
1:N:829:GLY:HA2	1:N:895:THR:HG21	1.95	0.49
1:O:780:TYR:O	1:O:783:ARG:HB2	2.12	0.49
1:O:825:MET:N	1:O:956:ASP:OD2	2.43	0.49
2:v:354:ARG:CZ	3:x:39:LEU:HG	2.43	0.49
7:p:122:THR:OG1	7:p:132:ILE:O	2.24	0.49
1:J:123:HIS:O	1:J:1093:ALA:HA	2.12	0.49
1:J:213:SER:OG	1:O:1174:LEU:O	2.22	0.49
1:N:481:ARG:O	1:N:484:ARG:NH1	2.45	0.49
1:O:657:VAL:HA	1:O:663:ILE:HD11	1.94	0.49
2:v:345:VAL:HG22	2:v:348:ARG:HH11	1.77	0.49
7:p:158:ARG:NH2	7:p:203:ASP:OD2	2.45	0.49
1:J:571:LEU:HB3	1:J:575:LEU:HD23	1.95	0.49
2:v:429:GLU:H	3:w:50:ARG:HH21	1.61	0.49
1:J:1350:LYS:O	1:J:1353:HIS:ND1	2.45	0.49
1:N:804:HIS:CG	1:N:808:LEU:HD11	2.48	0.49
2:v:48:PHE:HA	2:v:96:HIS:HB2	1.95	0.49
7:p:9:LEU:HB3	7:p:128:ASN:HD21	1.78	0.49
1:K:911:ALA:HB3	1:K:912:PRO:HD3	1.95	0.49
1:O:625:MET:HE2	1:O:835:VAL:HG12	1.94	0.49
1:O:526:THR:HG22	1:O:574:PRO:HA	1.94	0.49
7:r:28:ILE:HD11	7:r:93:ILE:HD13	1.95	0.49
1:K:1264:VAL:CB	1:K:1265:PRO:HD3	2.04	0.48
1:N:951:HIS:HA	1:N:990:PHE:HE1	1.77	0.48
1:N:1347:MET:HE2	1:N:1378:LYS:HG3	1.95	0.48
1:O:1010:PRO:O	1:O:1011:SER:C	2.55	0.48
2:v:35:ARG:HB3	2:v:37:PRO:HD3	1.95	0.48
6:h:291:ASN:HD21	7:m:204:ASN:HD21	1.61	0.48
1:N:312:VAL:HG11	1:N:314:ARG:HH11	1.79	0.48
1:O:724:LEU:O	1:O:921:GLN:NE2	2.33	0.48
7:k:216:LEU:HD22	7:p:213:VAL:HG23	1.94	0.48
1:K:1347:MET:HE2	1:K:1375:PHE:HB2	1.93	0.48
1:N:73:LEU:HD13	1:N:177:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:403:TYR:O	1:N:1049:THR:HA	2.12	0.48
1:N:518:ILE:HG22	1:N:521:LYS:HD2	1.95	0.48
3:w:46:ALA:HB1	3:w:50:ARG:HD2	1.94	0.48
6:h:305:TYR:OH	7:r:242:MET:SD	2.67	0.48
7:k:97:TYR:HE2	7:k:137:VAL:HG22	1.77	0.48
7:p:274:LEU:HA	7:p:277:LEU:HD12	1.94	0.48
1:J:549:TYR:OH	1:J:994:ARG:NH1	2.35	0.48
1:K:440:ILE:HD12	1:K:1119:ILE:HG22	1.95	0.48
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.78	0.48
1:O:1121:THR:HA	1:O:1182:CYS:HB2	1.96	0.48
2:v:35:ARG:HH21	2:v:108:LEU:HB2	1.79	0.48
2:v:390:PHE:CE2	3:x:39:LEU:HD11	2.49	0.48
1:J:1049:THR:HG23	1:J:1270:PRO:HB3	1.96	0.48
1:N:1039:HIS:ND1	1:N:1040:PRO:O	2.45	0.48
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.96	0.48
1:O:467:PRO:HB2	1:O:471:LEU:HD23	1.94	0.48
1:O:985:ARG:HH21	1:O:990:PHE:HZ	1.61	0.48
2:v:10:LEU:O	7:p:225:ARG:NH1	2.36	0.48
7:m:85:ILE:HA	7:m:91:TYR:HE2	1.78	0.48
7:r:193:VAL:CG2	7:r:194:PRO:CD	2.90	0.48
1:J:186:ARG:NH2	1:J:1296:GLN:O	2.46	0.48
1:J:1205:ARG:HG3	1:J:1239:THR:HG23	1.95	0.48
1:N:731:ASP:HA	1:N:796:LEU:CD2	2.32	0.48
1:O:840:ALA:HB3	5:e:49:VAL:HG13	1.95	0.48
2:v:341:PHE:HE1	2:v:493:GLU:HG2	1.79	0.48
1:J:1173:GLY:HA2	1:K:209:LYS:HD3	1.96	0.48
1:K:1290:MET:HB3	1:K:1290:MET:HE3	1.73	0.48
6:h:345:LEU:HD12	6:h:346:PRO:HD2	1.96	0.48
7:p:99:PRO:HD3	7:p:120:HIS:NE2	2.28	0.48
1:J:205:ARG:NH1	1:O:1318:ASP:O	2.46	0.48
1:J:424:ILE:HD11	1:J:1345:GLU:HG2	1.96	0.48
1:J:835:VAL:O	1:J:838:THR:OG1	2.31	0.48
2:v:31:LEU:HD11	2:v:112:LEU:HB2	1.94	0.48
7:k:171:ASP:OD1	7:p:261:LEU:HD12	2.14	0.48
7:p:138:LEU:HD21	7:p:142:ILE:CG2	2.40	0.48
1:J:1121:THR:HA	1:J:1182:CYS:HB2	1.96	0.47
1:K:360:GLU:OE1	1:K:360:GLU:HA	2.11	0.47
1:O:220:LYS:HZ3	1:O:1328:LEU:HB3	1.79	0.47
1:O:690:LEU:HD21	1:O:812:PHE:HB2	1.96	0.47
1:J:522:CYS:HB3	1:J:1000:PRO:HG3	1.97	0.47
1:J:1068:PHE:HB2	1:J:1093:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:300:ASN:HA	1:O:370:ALA:HA	1.96	0.47
1:O:760:PRO:HB2	4:z:3146:PHE:CZ	2.49	0.47
6:f:156:ASN:O	6:f:160:ASP:OD1	2.32	0.47
1:J:511:TYR:HD1	1:J:973:ARG:HH12	1.61	0.47
7:r:67:CYS:SG	7:r:68:THR:N	2.87	0.47
1:K:804:HIS:CE1	1:K:808:LEU:CD1	2.97	0.47
1:N:794:LEU:HD11	1:N:925:VAL:HG21	1.97	0.47
1:N:947:ALA:H	1:N:964:HIS:HE1	1.62	0.47
1:O:588:PHE:HE1	1:O:700:LEU:HG	1.79	0.47
7:m:257:VAL:HG13	7:r:156:TYR:HE2	1.79	0.47
7:p:34:THR:O	7:p:84:LYS:NZ	2.42	0.47
7:r:169:MET:HE3	7:r:173:HIS:HE1	1.79	0.47
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.79	0.47
1:N:484:ARG:NH1	1:N:484:ARG:CG	2.74	0.47
1:N:684:ARG:HH22	1:O:613:THR:H	1.63	0.47
6:h:291:ASN:HD21	7:m:204:ASN:ND2	2.13	0.47
7:m:46:GLY:HA2	7:m:133:VAL:HG23	1.96	0.47
1:O:793:ARG:NH2	4:z:3146:PHE:O	2.48	0.47
1:J:1233:ALA:HA	1:O:1176:HIS:HE1	1.80	0.47
1:K:730:THR:HB	1:K:799:TYR:HA	1.97	0.47
1:K:835:VAL:O	1:K:838:THR:OG1	2.30	0.47
1:K:857:LEU:CG	1:K:875:ARG:HD2	2.44	0.47
1:N:395:TYR:CE2	1:N:397:LEU:HB2	2.49	0.47
1:N:705:VAL:HG12	1:N:710:SER:HA	1.96	0.47
1:O:1316:GLY:HA2	1:O:1319:VAL:HB	1.97	0.47
5:Z:20:ASP:HA	5:Z:24:LEU:HD11	1.96	0.47
7:p:216:LEU:HA	7:p:267:MET:HE3	1.96	0.47
2:v:396:ARG:HD3	2:v:434:TRP:NE1	2.30	0.47
2:v:421:ILE:HD11	2:v:436:LYS:HD3	1.97	0.47
7:k:124:LYS:HG2	7:k:131:ASP:HB3	1.95	0.47
7:p:222:ARG:HE	7:p:252:LEU:HD13	1.80	0.47
7:r:154:ASN:CB	7:r:202:LEU:HG	2.45	0.47
7:r:200:ALA:C	7:r:201:LEU:HD13	2.40	0.47
1:J:747:ILE:HG12	1:J:752:VAL:HG12	1.97	0.47
1:N:128:SER:HA	1:N:1088:VAL:O	2.15	0.47
1:O:442:ASN:O	1:O:1371:ARG:NH2	2.45	0.47
7:p:138:LEU:CG	7:p:139:PRO:HD2	2.43	0.47
7:r:24:ARG:HD3	7:r:134:PHE:CE2	2.50	0.47
1:O:281:ILE:HD12	1:O:1058:LEU:HD23	1.96	0.46
2:v:402:CYS:SG	2:v:403:TRP:N	2.87	0.46
6:f:301:ILE:HG23	6:f:305:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:874:LEU:O	1:N:876:PRO:HD3	2.15	0.46
1:N:456:LEU:HD23	1:N:1146:VAL:HG23	1.97	0.46
1:O:957:PRO:O	1:O:961:ALA:HB2	2.15	0.46
7:k:7:VAL:HG22	7:k:38:GLN:HB2	1.96	0.46
7:r:193:VAL:CB	7:r:194:PRO:HD2	2.34	0.46
1:K:961:ALA:HB2	1:K:971:VAL:HG21	1.98	0.46
1:K:1195:TYR:OH	1:K:1203:ARG:O	2.33	0.46
7:r:74:GLU:HB3	7:r:81:ILE:HD12	1.96	0.46
7:r:193:VAL:CG2	7:r:194:PRO:HD2	2.46	0.46
1:J:282:VAL:HG12	1:J:1057:ILE:HG12	1.96	0.46
1:J:1074:VAL:HG22	1:J:1088:VAL:HG22	1.97	0.46
1:K:1204:GLY:HA3	1:K:1240:VAL:H	1.81	0.46
1:N:440:ILE:HD12	1:N:1119:ILE:HG22	1.97	0.46
1:J:412:PHE:HB2	1:J:1189:VAL:HG12	1.98	0.46
1:J:434:LEU:HD12	1:J:435:PRO:HD2	1.98	0.46
1:J:1215:TYR:HE1	1:J:1285:ARG:HG2	1.80	0.46
1:N:298:ALA:HB3	1:N:371:VAL:HG23	1.97	0.46
1:J:806:ASP:HB3	1:J:810:LYS:HE3	1.98	0.46
1:K:706:VAL:HG23	1:K:711:VAL:HG12	1.98	0.46
1:N:499:VAL:HA	1:N:502:ILE:HD12	1.98	0.46
1:N:584:ARG:NH1	1:N:1020:ALA:O	2.44	0.46
6:f:187:PRO:HB2	6:f:357:VAL:HG12	1.97	0.46
7:k:216:LEU:HD21	7:p:216:LEU:HD23	1.97	0.46
1:J:862:ASN:ND2	5:e:65:PHE:O	2.43	0.46
1:K:79:ASN:HB3	1:K:308:TYR:CD1	2.51	0.46
1:N:619:PHE:HE1	1:N:874:LEU:CD2	2.15	0.46
7:r:191:PRO:O	7:r:193:VAL:N	2.49	0.46
1:J:544:PRO:HG3	1:J:1243:TRP:CD2	2.51	0.46
1:K:1263:ALA:O	1:K:1264:VAL:O	2.33	0.46
1:O:544:PRO:HG3	1:O:1243:TRP:CD2	2.51	0.46
1:O:985:ARG:HD2	1:O:990:PHE:CE1	2.51	0.46
1:J:280:PHE:HB2	1:J:381:VAL:HG22	1.97	0.46
1:N:279:VAL:O	1:N:1059:PHE:HA	2.15	0.46
2:v:115:TYR:CD2	2:v:291:ILE:HB	2.51	0.46
7:k:3:LEU:HD11	7:k:86:VAL:HG23	1.97	0.46
7:m:220:SER:OG	7:r:210:CYS:SG	2.63	0.46
7:m:278:PHE:C	7:m:280:LEU:HD12	2.41	0.46
7:p:179:VAL:HG21	7:p:188:LEU:HD21	1.98	0.46
1:K:80:THR:HG22	1:K:309:ALA:HB3	1.98	0.45
1:N:302:ILE:HG13	1:N:367:ILE:HB	1.98	0.45
1:O:281:ILE:HG22	1:O:397:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:138:LEU:HG	7:p:139:PRO:N	2.30	0.45
1:J:486:THR:HG21	1:J:552:ARG:HB2	1.99	0.45
1:O:860:LEU:HD11	1:O:865:LEU:HB3	1.97	0.45
7:m:223:LEU:HD12	7:r:159:VAL:HG23	1.99	0.45
7:p:169:MET:O	7:p:173:HIS:ND1	2.37	0.45
1:J:190:PRO:HD2	1:J:193:ILE:HD12	1.98	0.45
1:J:255:VAL:HG13	1:J:1102:SER:HA	1.99	0.45
1:J:1350:LYS:HD3	1:J:1380:VAL:HG13	1.98	0.45
7:m:94:LYS:NZ	7:m:293:THR:O	2.47	0.45
7:p:202:LEU:HB3	7:p:203:ASP:H	1.61	0.45
1:N:267:TYR:HD1	1:N:267:TYR:H	1.64	0.45
1:N:953:PHE:HZ	1:N:1001:MET:HE3	1.81	0.45
1:N:1146:VAL:HG13	1:N:1148:ALA:H	1.80	0.45
1:O:951:HIS:O	1:O:955:GLY:N	2.49	0.45
1:O:1187:THR:HG23	1:O:1241:ASN:HB3	1.99	0.45
5:a:23:LEU:HD11	5:a:55:PHE:HB2	1.97	0.45
7:m:224:VAL:HG11	7:r:214:THR:HG21	1.98	0.45
1:J:155:VAL:HA	1:J:158:VAL:HG22	1.98	0.45
1:J:814:TYR:OH	1:J:921:GLN:NE2	2.49	0.45
1:K:402:GLN:HB2	1:K:1323:GLN:HB3	1.99	0.45
1:N:61:ASN:HD22	1:O:97:ILE:HG23	1.82	0.45
1:N:947:ALA:H	1:N:964:HIS:CE1	2.34	0.45
1:O:441:VAL:HG11	1:O:1373:LEU:HD22	1.97	0.45
2:v:390:PHE:CE2	3:x:39:LEU:CD1	3.00	0.45
7:m:11:SER:H	7:m:128:ASN:HD21	1.62	0.45
7:r:222:ARG:HH11	7:r:252:LEU:HD23	1.82	0.45
1:N:630:GLU:OE2	1:N:668:ARG:NH2	2.50	0.45
6:f:151:LEU:HD23	6:f:345:LEU:HD11	1.99	0.45
7:m:28:ILE:HA	7:m:70:ALA:O	2.15	0.45
1:J:1377:ASN:N	1:K:1364:GLU:OE1	2.40	0.45
1:K:955:GLY:O	1:K:985:ARG:NH2	2.49	0.45
1:K:1023:ILE:HG21	1:K:1033:GLN:HE21	1.81	0.45
1:N:612:ASP:OD2	1:N:647:TYR:OH	2.33	0.45
2:v:376:TYR:HB2	2:v:379:ILE:HB	1.99	0.45
7:p:290:SER:O	7:p:294:LEU:N	2.50	0.45
1:N:591:ALA:HB1	1:N:1036:LEU:HD12	1.99	0.45
1:N:828:LEU:HD11	1:N:945:PHE:HB3	1.97	0.45
6:h:102:ASN:HD21	6:h:196:LYS:HG2	1.81	0.45
1:J:986:PRO:O	1:J:990:PHE:N	2.48	0.45
1:K:499:VAL:HA	1:K:502:ILE:HD12	1.99	0.45
1:K:1276:ASN:HB3	1:K:1279:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:r:199:LEU:HD13	7:r:202:LEU:O	2.14	0.45
1:O:552:ARG:NH2	2:v:429:GLU:OE2	2.50	0.45
6:h:174:ARG:NE	6:h:178:ASP:OD2	2.50	0.45
6:h:338:PHE:O	6:h:344:SER:HA	2.17	0.45
7:p:144:GLU:O	7:p:148:GLN:HG2	2.16	0.45
7:r:95:ASN:HD22	7:r:103:TRP:CD1	2.35	0.45
1:K:481:ARG:NH1	1:K:536:ASP:OD2	2.51	0.44
1:K:796:LEU:HD21	1:K:925:VAL:HG13	1.99	0.44
1:K:951:HIS:O	1:K:955:GLY:N	2.50	0.44
1:O:132:GLU:HG2	1:O:1085:THR:HG22	1.98	0.44
1:O:572:PRO:HD2	1:O:575:LEU:HD12	1.99	0.44
1:O:637:VAL:HA	1:O:640:VAL:HG22	1.99	0.44
7:p:255:LEU:HD21	7:p:263:ARG:HG3	1.99	0.44
1:J:94:GLN:HG2	1:J:119:VAL:HG22	1.99	0.44
1:N:619:PHE:CZ	1:N:874:LEU:HD22	2.52	0.44
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.50	0.44
1:O:680:TYR:OH	1:O:684:ARG:NH1	2.50	0.44
2:v:125:ARG:HG3	2:v:284:LEU:HD22	1.98	0.44
1:N:609:THR:HG22	1:N:653:ARG:HB3	1.98	0.44
1:N:1348:SER:OG	1:N:1349:VAL:N	2.51	0.44
6:f:216:ILE:HG13	6:f:217:PRO:HD2	2.00	0.44
6:h:271:GLU:HA	6:h:304:ARG:HG3	1.99	0.44
1:N:564:HIS:HD2	1:N:566:LEU:HD23	1.82	0.44
1:N:571:LEU:HD12	1:N:572:PRO:HD2	2.00	0.44
4:y:3131:GLU:O	4:y:3134:THR:OG1	2.33	0.44
7:k:72:LEU:HA	7:k:82:LEU:HD23	1.99	0.44
7:k:199:LEU:HD23	7:k:202:LEU:HD12	1.98	0.44
7:k:238:LEU:HD21	7:p:263:ARG:HD3	1.98	0.44
7:m:7:VAL:HG11	7:m:43:LEU:HD22	1.99	0.44
7:r:244:PRO:HD2	7:r:247:ILE:HD12	1.99	0.44
1:J:1061:SER:HG	1:J:1064:SER:HG	1.62	0.44
1:K:359:VAL:O	1:K:360:GLU:C	2.60	0.44
1:N:598:VAL:HB	1:N:689:GLU:HB2	2.00	0.44
5:d:61:VAL:O	5:d:64:THR:OG1	2.32	0.44
7:p:229:ARG:HH22	7:p:231:GLU:HB2	1.82	0.44
1:K:395:TYR:CE2	1:K:397:LEU:HB2	2.53	0.44
1:K:856:ILE:HD12	1:K:876:PRO:HG2	2.00	0.44
1:N:706:VAL:HG23	1:N:711:VAL:HG12	1.99	0.44
1:O:469:HIS:HB2	1:O:1259:TYR:HE2	1.82	0.44
1:J:1223:LEU:HD11	1:O:1173:GLY:HA3	1.98	0.44
1:K:483:ARG:O	1:K:483:ARG:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:720:ASP:O	1:N:810:LYS:NZ	2.51	0.44
5:e:43:ALA:O	5:e:46:SER:OG	2.31	0.44
7:k:148:GLN:NE2	7:p:272:GLN:OE1	2.50	0.44
7:k:171:ASP:HA	7:p:261:LEU:HD11	2.00	0.44
7:m:233:HIS:H	7:m:236:LEU:HB2	1.82	0.44
1:J:544:PRO:O	1:J:565:ARG:NH1	2.51	0.44
1:K:834:HIS:HD2	5:a:7:LYS:HA	1.83	0.44
1:N:639:LEU:HD12	1:N:880:MET:HB3	2.00	0.44
1:O:746:ILE:HB	1:O:753:TYR:HB3	1.98	0.44
7:k:7:VAL:HG11	7:k:43:LEU:HD22	2.00	0.44
7:r:201:LEU:N	7:r:201:LEU:CD2	2.74	0.44
1:N:959:VAL:HG12	1:N:963:MET:HE3	2.00	0.43
1:O:663:ILE:HG23	1:O:683:TYR:HD1	1.83	0.43
2:v:43:TRP:CE3	2:v:57:VAL:HG12	2.52	0.43
2:v:390:PHE:CZ	3:x:39:LEU:HD11	2.53	0.43
1:J:307:SER:OG	1:J:364:ARG:NH1	2.50	0.43
1:J:485:GLU:HB3	1:J:517:ASP:HB2	2.00	0.43
1:J:698:MET:HE2	1:J:698:MET:HB3	1.84	0.43
1:N:158:VAL:HA	1:N:161:VAL:HG12	2.00	0.43
1:N:956:ASP:HA	1:N:957:PRO:HD3	1.86	0.43
4:y:3129:LYS:HG2	4:y:3132:ARG:HE	1.83	0.43
7:m:30:PRO:HD3	7:m:135:PRO:HG3	2.00	0.43
1:J:668:ARG:HH11	1:J:669:HIS:CE1	2.37	0.43
1:N:857:LEU:HD23	1:N:860:LEU:HD12	1.98	0.43
1:O:227:SER:O	1:O:232:ARG:NH2	2.49	0.43
1:O:866:ARG:O	1:O:870:GLU:HB2	2.18	0.43
1:O:952:MET:HE1	1:O:981:GLU:HA	2.00	0.43
7:k:72:LEU:HD11	7:k:80:LEU:HD22	1.99	0.43
7:m:128:ASN:O	7:m:129:ASP:OD1	2.36	0.43
7:m:222:ARG:HG2	7:m:251:ASP:OD1	2.19	0.43
1:J:497:MET:HE1	1:J:748:ILE:HG22	2.00	0.43
1:J:737:LEU:HG	1:J:744:PRO:HG2	2.01	0.43
1:N:412:PHE:HD1	1:N:1189:VAL:HG12	1.83	0.43
2:v:354:ARG:HD3	3:x:39:LEU:HD23	1.97	0.43
7:k:31:LEU:HD21	7:k:38:GLN:HG3	2.01	0.43
1:J:704:ASP:O	1:K:976:GLN:NE2	2.47	0.43
1:K:1255:TYR:HB2	1:K:1275:PHE:HD2	1.83	0.43
1:N:474:LEU:HG	1:N:560:HIS:CE1	2.53	0.43
5:e:32:GLN:O	5:e:34:ASN:N	2.51	0.43
6:f:327:PHE:HB3	6:f:353:PHE:HD1	1.83	0.43
7:r:111:VAL:HG22	7:r:137:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:VAL:HG12	1:K:1057:ILE:HG12	2.00	0.43
1:N:77:CYS:SG	1:N:1065:THR:OG1	2.72	0.43
1:O:75:VAL:HG23	1:O:267:TYR:CG	2.54	0.43
1:O:83:LYS:HG3	1:O:312:VAL:HG23	1.99	0.43
3:x:102:GLN:HA	4:y:3114:GLN:HG3	2.00	0.43
6:h:308:VAL:HG12	6:h:309:GLN:HE21	1.83	0.43
7:k:149:LYS:NZ	7:k:175:HIS:O	2.50	0.43
7:p:138:LEU:CD1	7:p:139:PRO:HD2	2.49	0.43
7:p:229:ARG:HH12	7:p:231:GLU:HB2	1.84	0.43
7:r:227:LEU:HD23	7:r:227:LEU:HA	1.87	0.43
1:J:1335:LEU:HG	1:J:1365:GLU:HB2	2.00	0.43
1:K:777:VAL:HG22	5:a:50:PHE:HZ	1.83	0.43
1:K:904:ASN:ND2	1:K:917:LYS:O	2.52	0.43
1:N:139:GLU:HB3	6:h:47:ALA:HB2	1.99	0.43
1:N:1117:MET:SD	1:N:1371:ARG:NH1	2.91	0.43
1:O:587:GLN:NE2	1:O:1037:LYS:O	2.52	0.43
2:v:426:LEU:HD21	2:v:463:VAL:HG23	2.00	0.43
6:f:179:ARG:HG3	6:f:270:TYR:CE2	2.53	0.43
7:m:216:LEU:HD22	7:r:213:VAL:HG23	2.01	0.43
1:K:95:PHE:O	1:K:117:ILE:HA	2.19	0.43
1:N:317:ASN:HD21	1:N:331:PHE:HB2	1.82	0.43
6:f:178:ASP:O	6:f:180:ARG:NH2	2.52	0.43
6:h:40:ARG:HA	6:h:43:VAL:HB	2.01	0.43
7:k:229:ARG:HH22	7:k:243:VAL:HG12	1.84	0.43
7:m:142:ILE:HD12	7:m:181:TYR:HE2	1.83	0.43
1:K:546:TYR:HA	1:K:564:HIS:HA	2.01	0.43
1:K:952:MET:HE2	1:K:999:SER:HA	2.00	0.43
1:K:1049:THR:HG23	1:K:1270:PRO:HB3	2.01	0.43
1:O:280:PHE:HB2	1:O:381:VAL:HG22	2.00	0.43
1:O:444:ASN:HD22	1:O:1176:HIS:CD2	2.36	0.43
1:O:913:ASN:HD22	1:O:916:ASP:CG	2.26	0.43
7:r:77:VAL:O	7:r:78:ASP:CG	2.58	0.43
7:r:154:ASN:HD22	7:r:202:LEU:HD12	1.84	0.43
1:J:668:ARG:HH11	1:J:669:HIS:HE1	1.67	0.43
1:K:856:ILE:HG22	1:K:860:LEU:HB2	2.01	0.43
1:K:1217:GLN:HE22	1:K:1281:LEU:HD23	1.84	0.43
2:v:43:TRP:O	2:v:100:LEU:HA	2.19	0.43
7:r:29:LEU:HD12	7:r:72:LEU:HD11	2.00	0.43
7:r:33:SER:H	7:r:38:GLN:NE2	2.17	0.43
1:J:639:LEU:HD12	1:J:880:MET:HB3	2.00	0.42
1:J:1313:VAL:HG21	1:J:1319:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:810:LYS:O	1:O:814:TYR:HB2	2.19	0.42
2:v:4:HIS:CE1	2:v:20:HIS:HB3	2.54	0.42
6:h:131:LEU:HG	6:h:135:MET:HE2	2.01	0.42
7:p:212:MET:HE3	7:p:212:MET:HB3	1.98	0.42
1:J:400:ARG:NE	1:J:1305:SER:OG	2.52	0.42
1:J:547:ASP:O	1:J:562:ALA:HA	2.20	0.42
1:K:172:LEU:HD11	1:K:1090:HIS:HB2	2.01	0.42
1:N:705:VAL:HA	1:N:711:VAL:HG13	2.00	0.42
6:h:46:HIS:HE1	6:h:70:VAL:HA	1.83	0.42
6:h:212:VAL:HG13	6:h:218:ARG:HH22	1.84	0.42
7:k:69:LEU:HB2	7:k:85:ILE:HD12	2.01	0.42
1:J:285:ASN:HD22	1:J:288:ARG:HH22	1.68	0.42
1:K:501:VAL:HA	1:K:504:ASP:HB2	2.00	0.42
1:N:764:GLU:HB2	1:N:793:ARG:HD3	2.02	0.42
1:N:856:ILE:HG22	1:N:860:LEU:HG	2.01	0.42
1:O:415:ASN:HD21	1:O:579:ALA:HB2	1.85	0.42
1:O:1039:HIS:ND1	1:O:1040:PRO:O	2.53	0.42
6:h:263:ARG:HH12	6:h:285:GLY:HA2	1.84	0.42
7:m:285:ALA:HB3	7:m:299:TRP:HE3	1.84	0.42
1:J:1124:PHE:HA	1:J:1127:VAL:HG12	2.01	0.42
2:v:408:ILE:HD11	2:v:497:ILE:HG22	2.02	0.42
1:J:952:MET:HE2	1:J:999:SER:HA	2.01	0.42
1:K:467:PRO:HG3	1:K:912:PRO:HG2	2.01	0.42
1:K:737:LEU:HD23	1:K:744:PRO:HG2	2.01	0.42
6:f:358:SER:OG	6:f:359:ASP:N	2.51	0.42
1:J:385:GLN:HG2	1:J:389:ASN:HD21	1.83	0.42
1:J:405:TYR:O	1:J:1047:VAL:HA	2.20	0.42
1:J:690:LEU:HD21	1:J:812:PHE:HB2	2.01	0.42
1:J:724:LEU:HD12	1:J:900:VAL:HG21	2.01	0.42
1:J:905:ASP:OD1	1:J:906:VAL:N	2.51	0.42
1:K:778:ALA:O	1:K:782:TYR:N	2.51	0.42
1:K:1012:LEU:HA	1:K:1015:ILE:HD12	2.01	0.42
2:v:66:MET:SD	2:v:74:ARG:NH2	2.92	0.42
3:x:74:MET:HE3	3:x:74:MET:HB3	1.90	0.42
6:h:303:HIS:O	6:h:306:ALA:HB3	2.20	0.42
7:k:80:LEU:HD23	7:k:80:LEU:HA	1.86	0.42
1:J:415:ASN:OD1	1:J:417:LYS:NZ	2.39	0.42
1:J:621:VAL:O	1:J:625:MET:HG2	2.20	0.42
1:J:788:HIS:O	1:J:896:ARG:NH1	2.53	0.42
1:K:952:MET:HE1	1:K:981:GLU:HA	2.01	0.42
1:N:155:VAL:HA	1:N:158:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1049:THR:HG23	1:O:1270:PRO:HB3	2.02	0.42
5:Z:49:VAL:O	5:Z:52:THR:OG1	2.34	0.42
7:m:3:LEU:HD23	7:m:84:LYS:HB3	2.01	0.42
7:r:29:LEU:HD23	7:r:29:LEU:HA	1.86	0.42
1:J:369:ALA:O	1:J:370:ALA:C	2.62	0.42
1:J:748:ILE:HG13	1:J:898:VAL:HG13	2.02	0.42
1:J:1269:SER:HB2	1:J:1272:ARG:HB2	2.01	0.42
1:K:1146:VAL:HG13	1:K:1148:ALA:H	1.85	0.42
1:K:1225:TYR:CE2	1:K:1277:LYS:HE2	2.55	0.42
1:N:312:VAL:HG12	1:N:314:ARG:H	1.84	0.42
1:O:84:ASP:OD1	1:O:84:ASP:N	2.49	0.42
1:O:828:LEU:HD11	1:O:945:PHE:HB3	2.01	0.42
6:f:361:GLU:OE2	7:k:276:SER:OG	2.36	0.42
7:r:111:VAL:HB	7:r:282:PRO:HB2	2.02	0.42
7:r:234:ASP:OD1	7:r:234:ASP:N	2.53	0.42
1:J:521:LYS:NZ	1:J:541:GLU:OE2	2.40	0.42
1:K:158:VAL:HA	1:K:161:VAL:HG12	2.01	0.42
1:N:834:HIS:CD2	5:d:7:LYS:HD3	2.54	0.42
1:O:494:PRO:HB3	1:O:988:GLN:HG2	2.01	0.42
7:k:202:LEU:HD23	7:k:205:LEU:HD12	2.00	0.42
1:J:843:GLY:HA2	1:J:846:PHE:HB3	2.02	0.42
1:J:856:ILE:HD11	1:J:878:VAL:HA	2.02	0.42
1:K:726:PRO:HG3	1:K:954:TYR:HE2	1.85	0.42
1:K:1018:MET:HB2	1:K:1018:MET:HE3	1.78	0.42
1:N:638:PRO:HG2	1:N:880:MET:SD	2.59	0.42
1:N:828:LEU:HB3	1:N:928:LEU:O	2.20	0.42
6:f:109:PRO:HA	6:f:190:PRO:HA	2.01	0.42
1:N:1175:CYS:H	1:O:1232:ALA:HB1	1.85	0.41
1:O:906:VAL:HA	1:O:909:GLN:HB2	2.02	0.41
1:K:705:VAL:HG12	1:K:710:SER:HA	2.00	0.41
1:N:626:ILE:HG22	1:N:628:GLY:H	1.85	0.41
1:N:684:ARG:NH2	1:O:612:ASP:HA	2.35	0.41
1:O:909:GLN:HE21	1:O:917:LYS:HD3	1.85	0.41
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.85	0.41
6:f:176:VAL:O	6:f:179:ARG:NH2	2.53	0.41
1:K:830:VAL:H	1:K:895:THR:HG21	1.86	0.41
1:O:466:THR:HB	1:O:910:LEU:HD13	2.02	0.41
6:f:340:TYR:HB3	6:f:343:SER:HB3	2.02	0.41
1:J:80:THR:HG21	1:J:1068:PHE:HE1	1.85	0.41
1:O:713:GLN:NE2	1:O:719:LEU:O	2.44	0.41
1:O:1195:TYR:OH	1:O:1201:SER:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:v:388:GLU:HA	2:v:391:PHE:HB2	2.03	0.41
2:v:390:PHE:HB2	3:x:42:ALA:HB1	2.02	0.41
6:h:292:ILE:HA	6:h:295:ILE:HG12	2.02	0.41
7:m:157:SER:HA	7:m:160:VAL:HG12	2.01	0.41
1:K:299:ASP:HB2	1:K:371:VAL:HG21	2.03	0.41
1:O:955:GLY:HA3	1:O:985:ARG:NE	2.36	0.41
2:v:97:VAL:HG13	2:v:115:TYR:HE1	1.86	0.41
1:J:107:GLY:HA2	7:k:37:THR:HB	2.03	0.41
1:J:444:ASN:HD22	1:J:1176:HIS:HD2	1.69	0.41
1:J:852:ARG:NH2	5:Z:63:ARG:HD3	2.35	0.41
1:N:724:LEU:HD23	1:N:724:LEU:HA	1.85	0.41
2:v:64:ARG:HA	2:v:76:THR:HA	2.02	0.41
7:k:155:VAL:O	7:k:159:VAL:HG23	2.20	0.41
7:k:171:ASP:CA	7:p:261:LEU:HD11	2.51	0.41
7:m:45:LEU:HB3	7:m:133:VAL:HB	2.03	0.41
7:m:201:LEU:HA	7:m:204:ASN:HD22	1.84	0.41
1:K:1285:ARG:NH2	1:K:1293:GLU:OE1	2.54	0.41
1:O:989:LEU:HD23	1:O:989:LEU:HA	1.75	0.41
7:r:99:PRO:HG3	7:r:116:PHE:HD2	1.85	0.41
1:J:147:THR:HA	1:J:148:PRO:HD3	1.96	0.41
1:J:871:ILE:HD12	1:J:871:ILE:HA	1.89	0.41
1:K:1157:ASP:HA	1:K:1158:PRO:HD3	1.95	0.41
6:f:269:THR:O	6:f:275:PRO:HA	2.21	0.41
7:k:148:GLN:HE22	7:p:269:THR:HA	1.86	0.41
7:k:196:PRO:O	7:k:197:LEU:CB	2.68	0.41
7:m:104:HIS:HB2	7:m:106:THR:HG22	2.02	0.41
7:m:125:LEU:O	7:m:129:ASP:N	2.53	0.41
1:K:1046:VAL:HG22	1:K:1184:ILE:HG13	2.02	0.41
1:K:1077:ARG:O	1:K:1085:THR:OG1	2.30	0.41
1:N:268:THR:HG22	1:N:275:PRO:HB3	2.03	0.41
1:N:336:ALA:HA	1:N:340:ASP:HB2	2.03	0.41
1:O:255:VAL:HG13	1:O:1102:SER:HA	2.02	0.41
1:O:1201:SER:OG	1:O:1205:ARG:O	2.36	0.41
2:v:9:VAL:HG21	7:p:240:GLN:HB3	2.03	0.41
6:f:265:TYR:CZ	6:f:289:ILE:HG21	2.56	0.41
6:h:231:VAL:HB	6:h:280:PHE:HE1	1.86	0.41
7:k:264:MET:HG3	7:p:148:GLN:NE2	2.36	0.41
7:m:217:PRO:HD2	7:r:213:VAL:HG21	2.02	0.41
7:p:95:ASN:HD22	7:p:103:TRP:CD1	2.38	0.41
7:p:199:LEU:HG	7:p:203:ASP:HB2	2.01	0.41
7:r:99:PRO:HD3	7:r:120:HIS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1128:PHE:CE1	1:N:1263:ALA:HB2	2.56	0.41
6:h:179:ARG:HG3	6:h:270:TYR:CD2	2.56	0.41
7:k:101:PHE:HD2	7:k:138:LEU:HD22	1.86	0.41
7:k:116:PHE:HD2	7:k:136:MET:HE3	1.86	0.41
1:J:255:VAL:HG11	1:J:1061:SER:HB3	2.03	0.40
1:J:835:VAL:HG22	1:J:944:LEU:HD22	2.02	0.40
3:x:50:ARG:HH11	3:x:50:ARG:HD2	1.74	0.40
7:k:15:THR:HA	7:k:18:ILE:HG22	2.02	0.40
7:r:33:SER:H	7:r:38:GLN:HE22	1.68	0.40
1:J:1057:ILE:HB	1:J:1106:THR:HG22	2.03	0.40
1:K:836:ALA:HB1	5:a:49:VAL:HG11	2.03	0.40
1:K:899:ARG:HA	1:K:899:ARG:HD2	1.83	0.40
1:K:1018:MET:HA	1:K:1021:MET:HG3	2.04	0.40
1:N:575:LEU:HD13	1:N:1243:TRP:HH2	1.87	0.40
1:N:750:ASN:H	1:N:792:PHE:HE1	1.68	0.40
1:O:511:TYR:HA	1:O:973:ARG:HH12	1.86	0.40
1:O:542:LEU:HB3	1:O:1249:SER:HA	2.03	0.40
2:v:388:GLU:OE2	2:v:392:THR:OG1	2.39	0.40
1:J:580:PHE:CE1	1:J:1189:VAL:HG11	2.57	0.40
1:K:469:HIS:HB2	1:K:1253:ILE:HD12	2.03	0.40
1:O:255:VAL:HG21	1:O:1059:PHE:HD2	1.86	0.40
1:O:1078:GLU:H	1:O:1085:THR:HG1	1.70	0.40
7:k:58:VAL:C	7:k:197:LEU:HD12	2.47	0.40
7:k:86:VAL:HG12	7:k:88:GLY:H	1.86	0.40
7:p:179:VAL:HG21	7:p:188:LEU:CD2	2.52	0.40
1:K:146:GLU:HG3	1:K:147:THR:HG23	2.02	0.40
1:K:248:LEU:HB3	1:K:374:LEU:HD21	2.02	0.40
1:K:462:PRO:HG2	1:K:1131:GLU:HB3	2.03	0.40
7:m:158:ARG:NH2	7:r:229:ARG:HG3	2.37	0.40
7:r:95:ASN:HD22	7:r:103:TRP:HD1	1.70	0.40
7:r:159:VAL:O	7:r:163:ALA:N	2.55	0.40
1:J:1229:ARG:HD3	1:O:1172:PRO:HD3	2.04	0.40
1:K:395:TYR:HB3	1:K:398:ASN:ND2	2.36	0.40
1:K:1174:LEU:HD23	1:K:1174:LEU:HA	1.97	0.40
1:N:269:THR:HG22	1:N:271:LYS:N	2.35	0.40
1:O:938:ARG:HA	1:O:941:THR:HG22	2.03	0.40
1:O:1247:LEU:HD23	1:O:1247:LEU:HA	1.91	0.40
5:Z:68:PRO:HG2	5:Z:71:GLN:HB3	2.02	0.40
5:a:27:PHE:HZ	5:a:44:GLN:HB2	1.87	0.40
7:k:124:LYS:HA	7:k:131:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	J	1299/1381 (94%)	1225 (94%)	73 (6%)	1 (0%)	48	83
1	K	1379/1381 (100%)	1313 (95%)	56 (4%)	10 (1%)	18	55
1	N	1358/1381 (98%)	1305 (96%)	49 (4%)	4 (0%)	36	71
1	O	1295/1381 (94%)	1239 (96%)	52 (4%)	4 (0%)	36	71
2	v	283/507 (56%)	260 (92%)	22 (8%)	1 (0%)	30	66
3	w	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
3	x	66/570 (12%)	66 (100%)	0	0	100	100
4	y	35/3149 (1%)	35 (100%)	0	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	71 (95%)	4 (5%)	0	100	100
5	a	75/176 (43%)	71 (95%)	3 (4%)	1 (1%)	9	41
5	d	75/176 (43%)	73 (97%)	2 (3%)	0	100	100
5	e	75/176 (43%)	73 (97%)	1 (1%)	1 (1%)	9	41
6	f	247/364 (68%)	224 (91%)	21 (8%)	2 (1%)	16	52
6	h	330/364 (91%)	308 (93%)	20 (6%)	2 (1%)	21	58
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	36	71
7	m	297/301 (99%)	281 (95%)	15 (5%)	1 (0%)	36	71
7	p	297/301 (99%)	285 (96%)	11 (4%)	1 (0%)	36	71
7	r	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	7	35
All	All	7881/16105 (49%)	7492 (95%)	355 (4%)	34 (0%)	31	66

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	556	GLU
1	K	360	GLU

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Mol	Chain	Res	Type
1	K	911	ALA
1	K	912	PRO
1	K	1264	VAL
1	K	1265	PRO
1	N	266	THR
1	O	488	SER
1	O	1011	SER
5	a	19	PRO
6	h	306	ALA
7	p	98	GLN
7	r	192	GLU
7	r	193	VAL
7	r	203	ASP
1	K	361	ASP
5	e	33	ASN
7	r	255	LEU
1	K	805	ALA
1	O	300	ASN
7	k	161	MET
7	m	129	ASP
1	K	806	ASP
1	K	913	ASN
1	O	489	LEU
6	f	161	SER
6	h	310	PRO
1	N	484	ARG
1	N	671	GLY
1	N	672	ASN
7	r	194	PRO
1	K	357	ALA
6	f	162	PRO
2	v	94	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	1110/1171 (95%)	1105 (100%)	5 (0%)	81	81
1	K	1171/1171 (100%)	1163 (99%)	8 (1%)	76	79
1	N	1155/1171 (99%)	1146 (99%)	9 (1%)	73	77
1	O	1103/1171 (94%)	1096 (99%)	7 (1%)	78	80
2	v	243/400 (61%)	239 (98%)	4 (2%)	55	69
3	w	57/465 (12%)	57 (100%)	0	100	100
3	x	57/465 (12%)	57 (100%)	0	100	100
4	y	35/2539 (1%)	35 (100%)	0	100	100
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	71 (100%)	0	100	100
5	a	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	d	71/128 (56%)	71 (100%)	0	100	100
5	e	71/128 (56%)	71 (100%)	0	100	100
6	f	218/289 (75%)	217 (100%)	1 (0%)	81	81
6	h	278/289 (96%)	278 (100%)	0	100	100
7	k	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	m	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	p	265/267 (99%)	263 (99%)	2 (1%)	73	77
7	r	265/267 (99%)	260 (98%)	5 (2%)	50	66
All	All	6806/13250 (51%)	6760 (99%)	46 (1%)	73	79

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	365	VAL
1	J	556	GLU
1	J	794	LEU
1	J	1031	ILE
1	J	1110	VAL
1	K	360	GLU
1	K	361	ASP
1	K	372	ILE
1	K	484	ARG
1	K	804	HIS
1	K	938	ARG
1	K	1031	ILE

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Mol	Chain	Res	Type
1	K	1264	VAL
1	N	266	THR
1	N	267	TYR
1	N	313	VAL
1	N	484	ARG
1	N	602	VAL
1	N	626	ILE
1	N	654	LEU
1	N	670	LEU
1	N	1031	ILE
1	O	267	TYR
1	O	458	VAL
1	O	598	VAL
1	O	602	VAL
1	O	1174	LEU
1	O	1309	VAL
1	O	1369	VAL
2	v	52	THR
2	v	290	HIS
2	v	331	ILE
2	v	397	VAL
5	a	20	ASP
6	f	237	LEU
7	k	161	MET
7	k	197	LEU
7	m	86	VAL
7	m	137	VAL
7	p	5	VAL
7	p	98	GLN
7	r	190	LEU
7	r	193	VAL
7	r	201	LEU
7	r	202	LEU
7	r	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	126	HIS
1	J	285	ASN
1	J	300	ASN
1	J	389	ASN

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Mol	Chain	Res	Type
1	J	444	ASN
1	J	445	ASN
1	J	465	HIS
1	J	560	HIS
1	J	581	GLN
1	J	587	GLN
1	J	596	HIS
1	J	669	HIS
1	J	834	HIS
1	J	904	ASN
1	J	908	GLN
1	J	909	GLN
1	J	921	GLN
1	J	1122	GLN
1	J	1176	HIS
1	J	1241	ASN
1	J	1360	HIS
1	K	113	GLN
1	K	123	HIS
1	K	125	HIS
1	K	301	GLN
1	K	317	ASN
1	K	362	GLN
1	K	385	GLN
1	K	389	ASN
1	K	402	GLN
1	K	543	HIS
1	K	658	ASN
1	K	788	HIS
1	K	790	HIS
1	K	795	HIS
1	K	804	HIS
1	K	824	HIS
1	K	849	HIS
1	K	997	HIS
1	K	1120	HIS
1	K	1197	GLN
1	K	1217	GLN
1	K	1227	HIS
1	K	1246	GLN
1	K	1301	HIS
1	K	1310	GLN

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Mol	Chain	Res	Type
1	N	121	ASN
1	N	123	HIS
1	N	125	HIS
1	N	289	GLN
1	N	317	ASN
1	N	362	GLN
1	N	432	GLN
1	N	444	ASN
1	N	496	HIS
1	N	543	HIS
1	N	564	HIS
1	N	587	GLN
1	N	672	ASN
1	N	735	HIS
1	N	788	HIS
1	N	804	HIS
1	N	926	ASN
1	N	942	GLN
1	N	964	HIS
1	N	976	GLN
1	N	997	HIS
1	N	1056	ASN
1	N	1090	HIS
1	N	1137	GLN
1	N	1284	ASN
1	N	1323	GLN
1	O	64	GLN
1	O	104	HIS
1	O	121	ASN
1	O	125	HIS
1	O	301	GLN
1	O	333	HIS
1	O	389	ASN
1	O	402	GLN
1	O	415	ASN
1	O	491	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	790	HIS
1	O	822	ASN
1	O	824	HIS

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Mol	Chain	Res	Type
1	O	997	HIS
1	O	1033	GLN
1	O	1090	HIS
1	O	1122	GLN
1	O	1176	HIS
1	O	1246	GLN
1	O	1360	HIS
1	O	1377	ASN
2	v	7	ASN
2	v	45	GLN
2	v	290	HIS
2	v	394	GLN
3	w	77	HIS
3	x	63	ASN
5	Z	33	ASN
5	Z	71	GLN
5	a	71	GLN
5	e	32	GLN
5	e	54	GLN
6	f	256	GLN
6	f	309	GLN
6	h	291	ASN
6	h	303	HIS
6	h	309	GLN
7	k	120	HIS
7	k	128	ASN
7	k	185	HIS
7	k	204	ASN
7	k	233	HIS
7	m	104	HIS
7	m	120	HIS
7	m	128	ASN
7	m	148	GLN
7	m	204	ASN
7	m	291	GLN
7	p	47	GLN
7	p	98	GLN
7	p	102	GLN
7	p	148	GLN
7	r	38	GLN
7	r	120	HIS
7	r	154	ASN

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Mol	Chain	Res	Type
7	r	204	ASN
7	r	233	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.

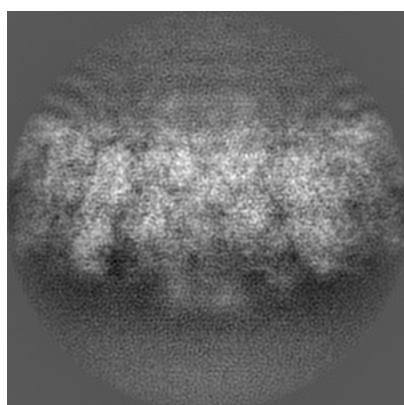
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21526. These allow visual inspection of the internal detail of the map and identification of artifacts.

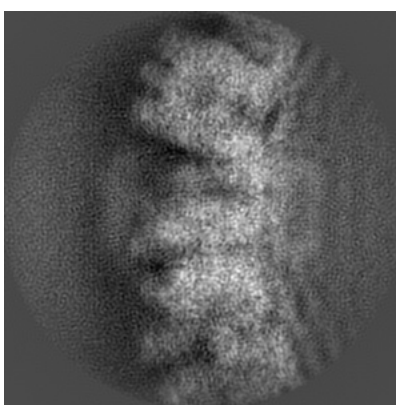
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

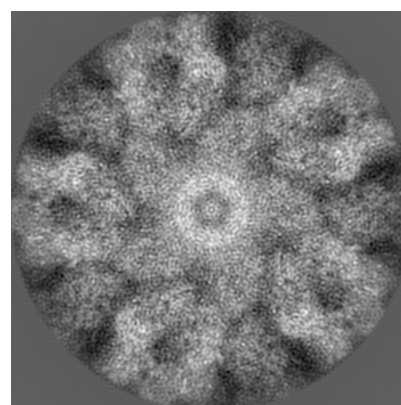
6.1.1 Primary map



X



Y

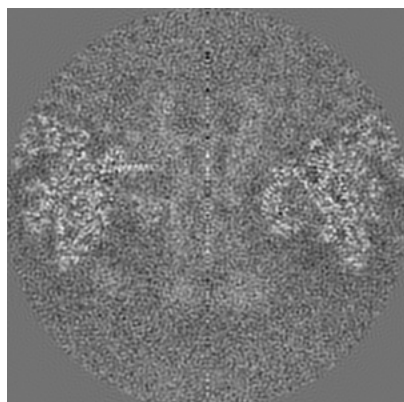


Z

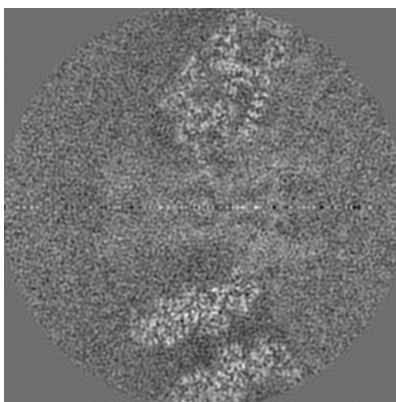
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

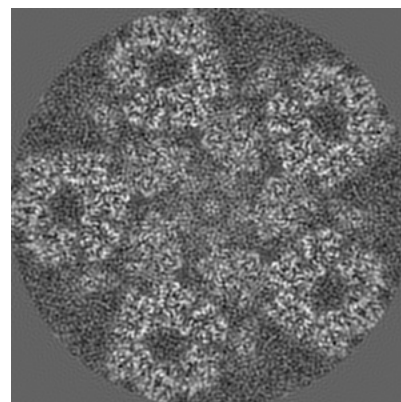
6.2.1 Primary map



X Index: 160



Y Index: 160

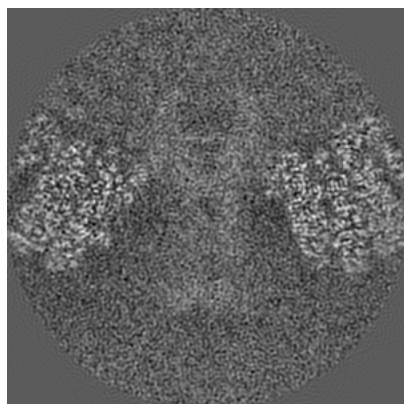


Z Index: 160

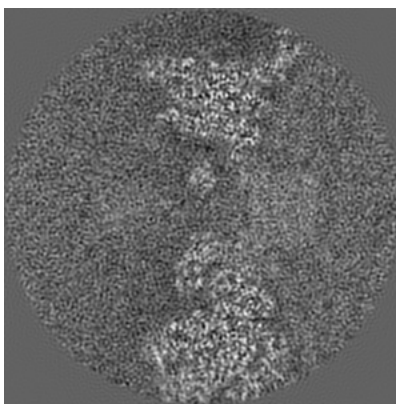
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

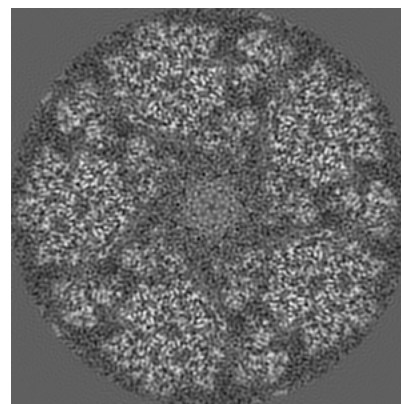
6.3.1 Primary map



X Index: 147



Y Index: 193

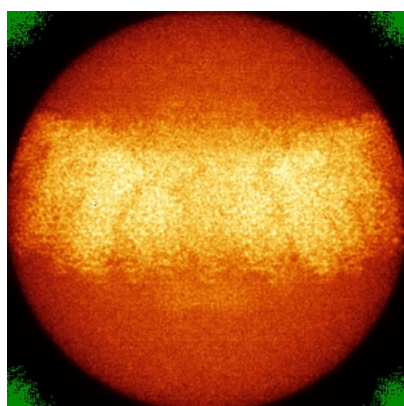


Z Index: 175

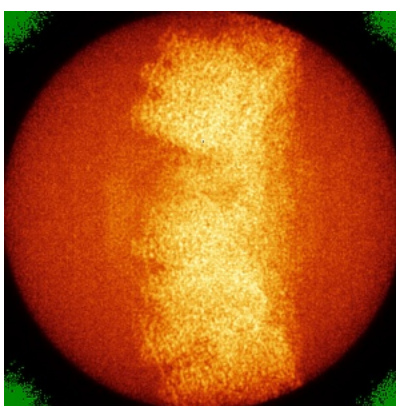
The images above show the largest variance slices of the map in three orthogonal directions.

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

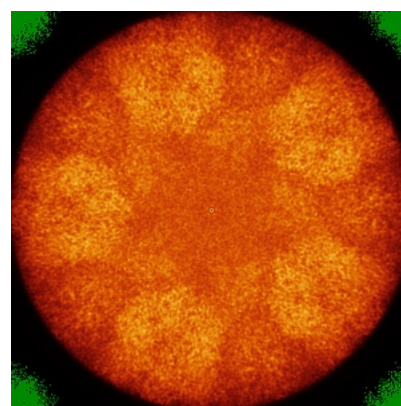
6.4.1 Primary map



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

This section was not generated.

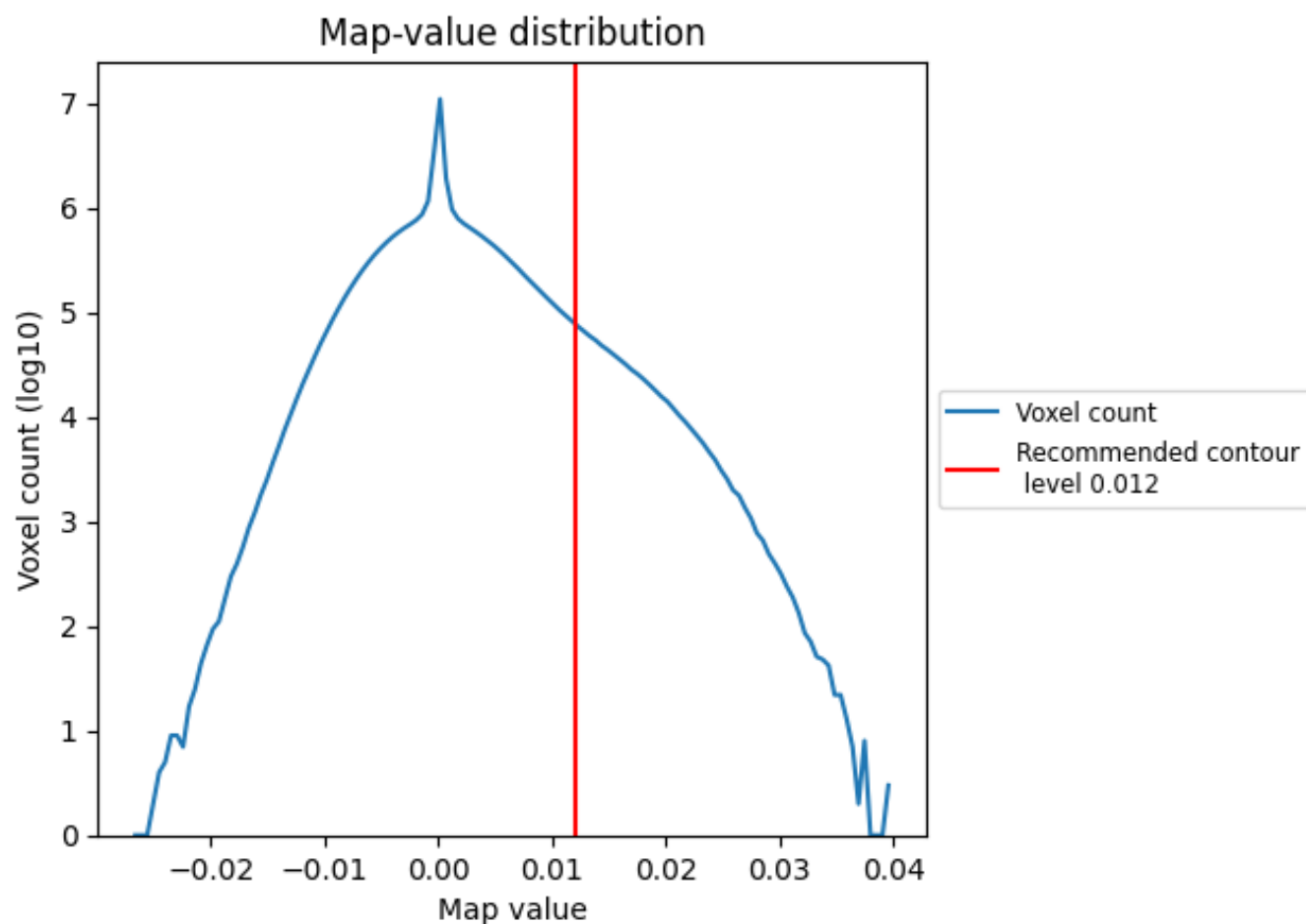
6.6 Mask visualisation

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

7 Map analysis [i](#)

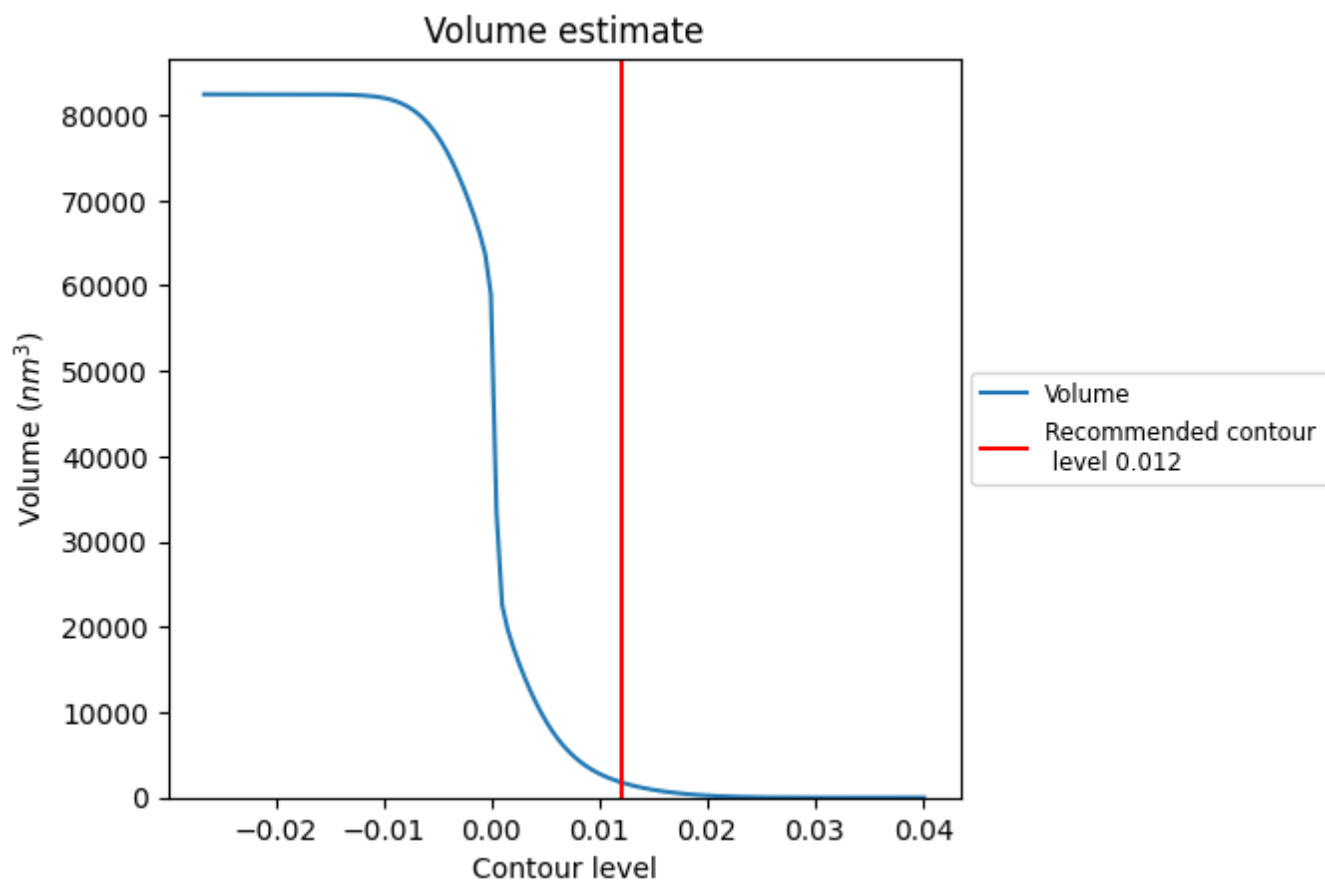
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

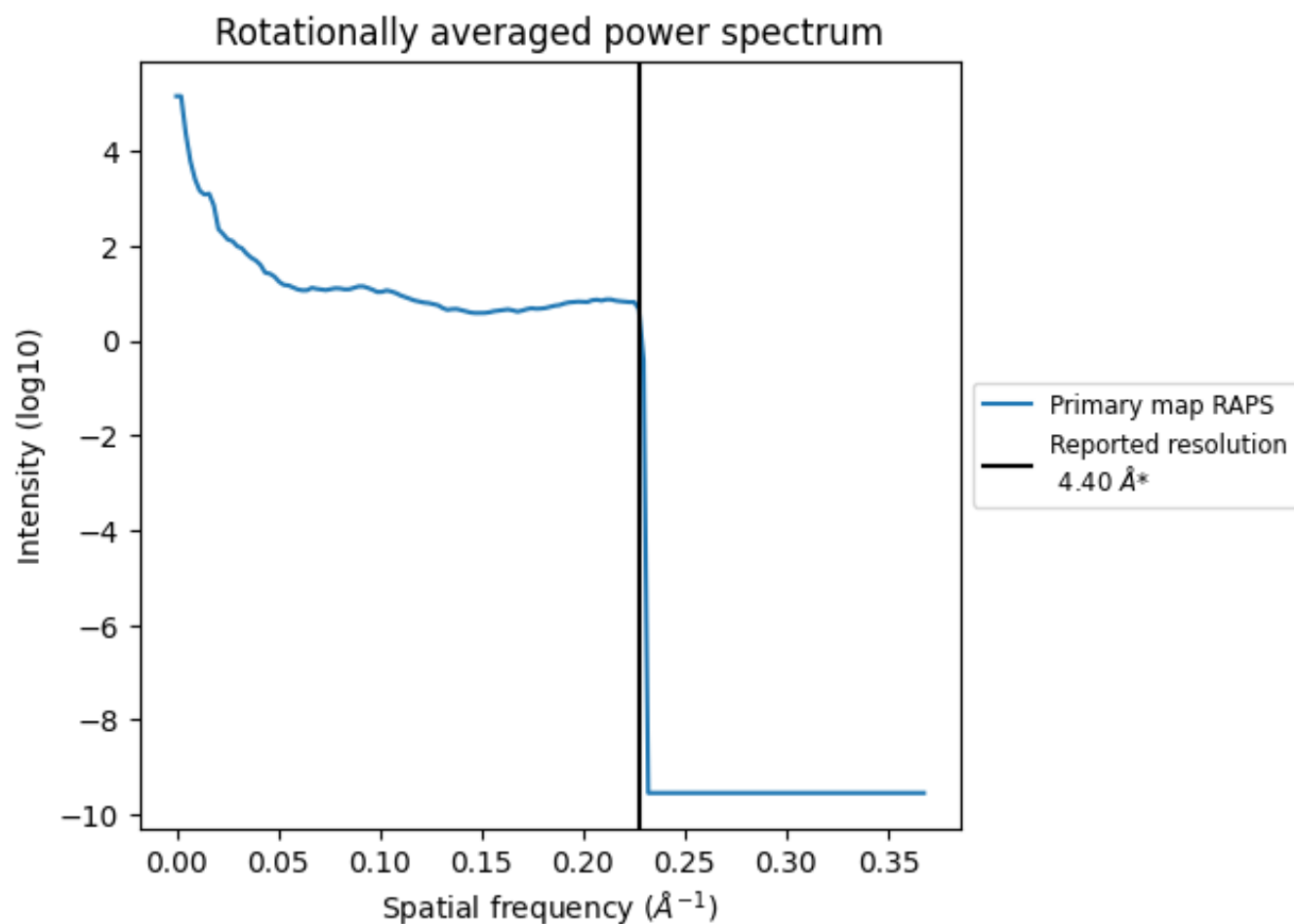
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1798 nm³; this corresponds to an approximate mass of 1624 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 0.227 $\text{\AA}^{-1}$

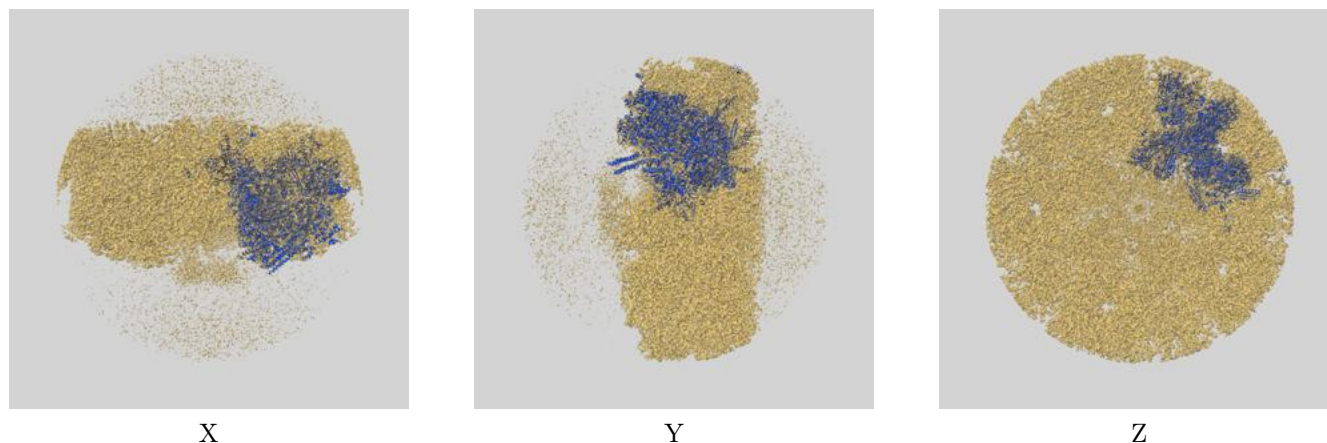
8 Fourier-Shell correlation ⓘ

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-21526 and PDB model 6W2E. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



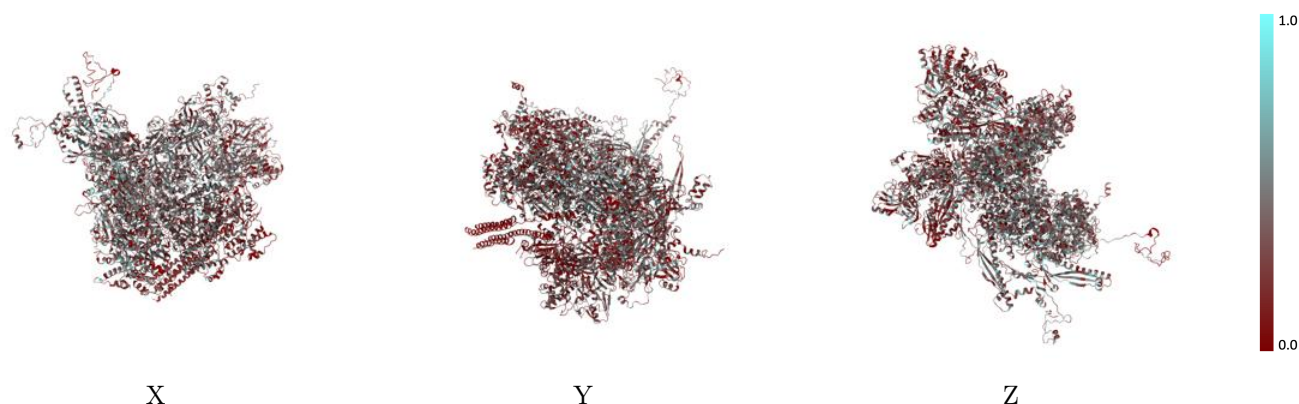
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



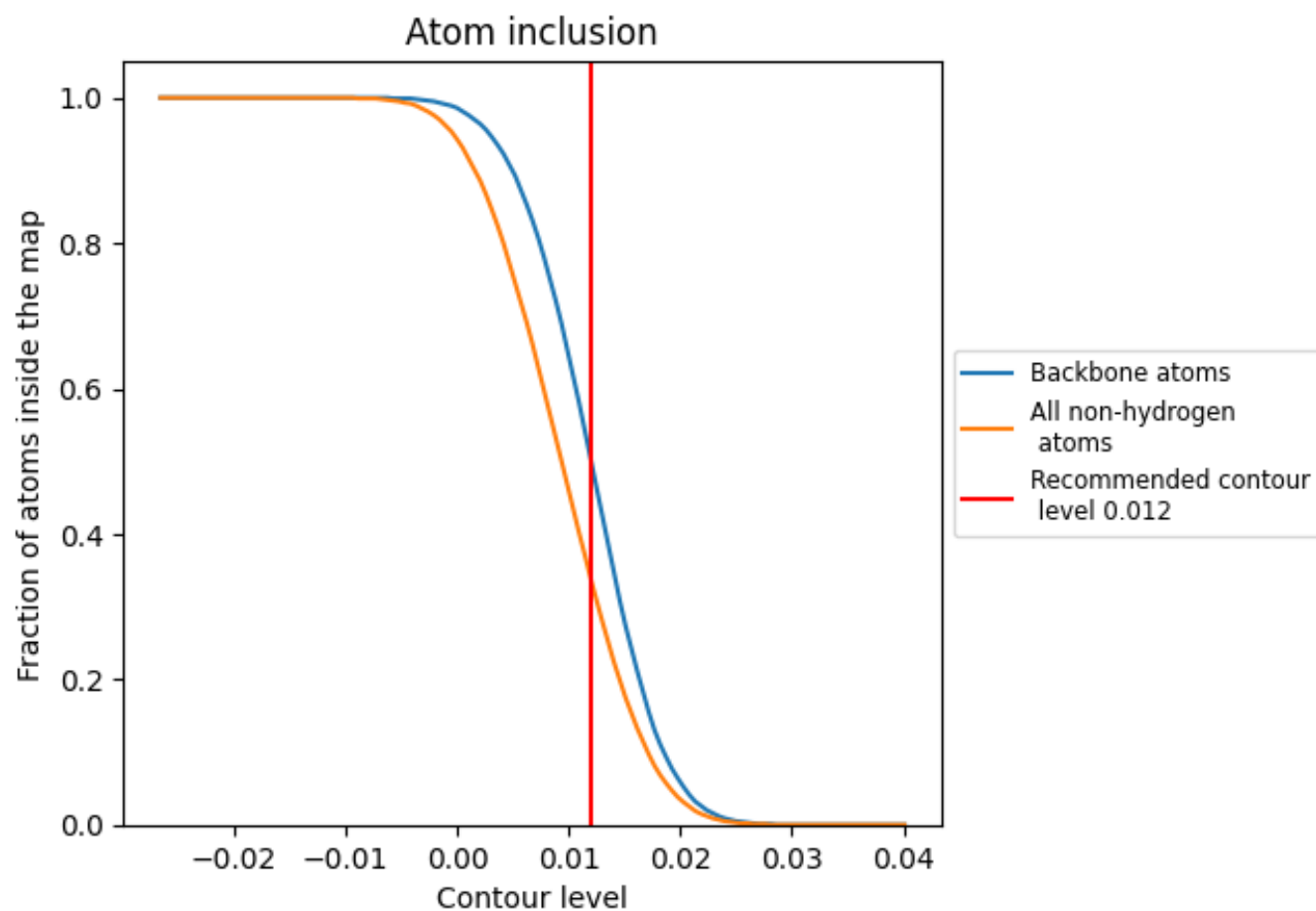
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 34% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3360	 0.2450
J	 0.3910	 0.2500
K	 0.3870	 0.2640
N	 0.3500	 0.2590
O	 0.3700	 0.2460
Z	 0.3000	 0.2300
a	 0.3100	 0.2180
d	 0.1720	 0.1880
e	 0.2860	 0.2230
f	 0.2490	 0.2260
h	 0.3450	 0.2610
k	 0.2780	 0.2310
m	 0.2860	 0.2490
p	 0.2910	 0.2330
r	 0.2990	 0.2550
v	 0.1690	 0.1870
w	 0.0720	 0.1710
x	 0.1170	 0.1700
y	 0.0630	 0.1150
z	 0.0500	 0.1040

