



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 03:20 PM EDT

PDB ID : 9OX8 / pdb_00009ox8
EMDB ID : EMD-70960
Title : NHEJ Short-range complex with Polymerase lambda
Authors : Vogt, A.; He, Y.
Deposited on : 2025-06-03
Resolution : 7.23 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:

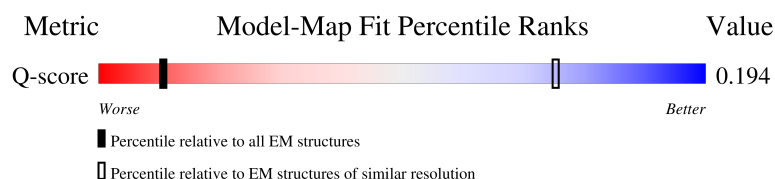
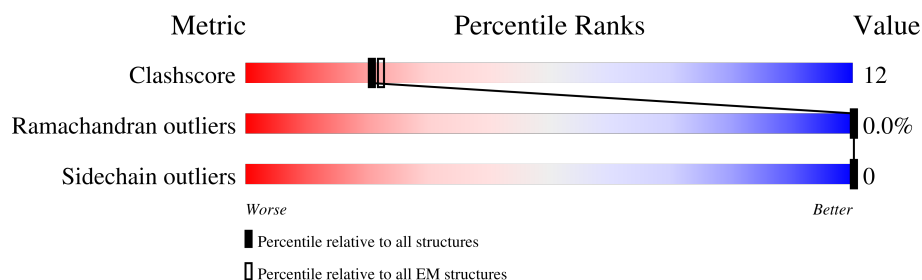
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.23 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.






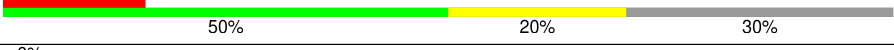


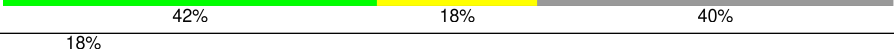
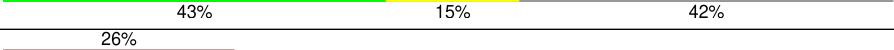
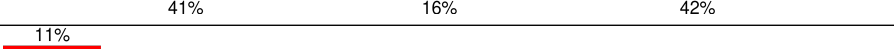
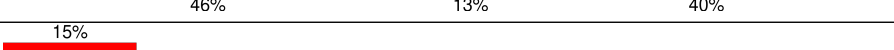

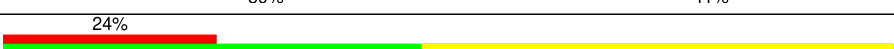




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	406 (6.73 - 7.70)

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	A	911	<div> <div>29%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>
1	X	911	<div> <div>8%</div> <div>22%</div> <div>5%</div> <div>72%</div> </div>
2	B	299	<div> <div>5%</div> <div>63%</div> <div>15%</div> <div>21%</div> </div>
2	I	299	<div> <div>58%</div> <div>21%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	600	
3	J	600	
4	D	732	
4	K	732	
5	E	575	
5	F	575	
6	G	336	
6	H	336	
6	O	336	
6	P	336	
7	L	34	
7	N	34	
8	M	34	
8	Q	34	
9	T	204	
9	U	204	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 77889 atoms, of which 38216 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 DNA ligase 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	816	Total	C	H	N	O	S	0	0
			11918	3948	5747	1049	1133	41		
1	X	254	Total	C	H	N	O	S	0	0
			4079	1314	2015	348	389	13		

- Molecule 2 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	237	Total	C	H	N	O	S	0	0
			3777	1202	1894	317	349	15		
2	I	237	Total	C	H	N	O	S	0	0
			3777	1202	1894	317	349	15		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	497	Total	C	H	N	O	S	0	0
			8124	2577	4103	680	746	18		
3	J	509	Total	C	H	N	O	S	0	0
			8310	2641	4189	694	767	19		

- Molecule 4 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	511	Total	C	H	N	O	S	0	0
			8240	2622	4141	686	768	23		
4	K	511	Total	C	H	N	O	S	0	0
			8240	2622	4141	686	768	23		

- Molecule 5 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	111	Total	C	H	N	O	S	0	0
			1781	561	902	165	150	3		
5	F	111	Total	C	H	N	O	S	0	0
			1780	561	901	165	150	3		

- Molecule 6 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	201	Total	C	H	N	O	S	0	0
			3248	1031	1620	278	312	7		
6	H	195	Total	C	H	N	O	S	0	0
			3188	1012	1593	272	304	7		
6	O	195	Total	C	H	N	O	S	0	0
			3189	1012	1594	272	304	7		
6	P	201	Total	C	H	N	O	S	0	0
			3248	1031	1620	278	312	7		

- Molecule 7 is a DNA chain called DNA (34-MER).

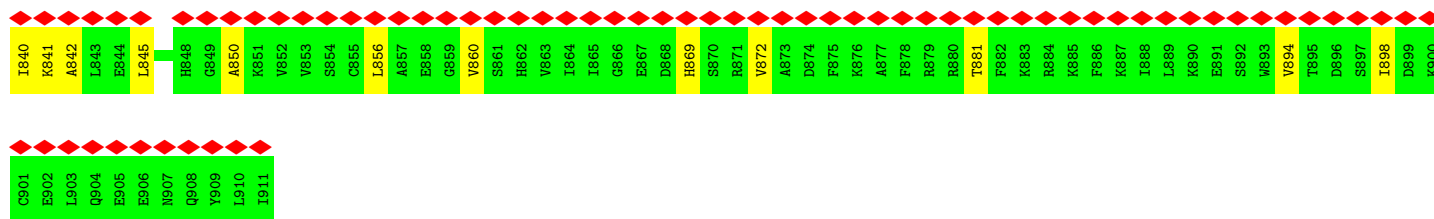
Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	34	Total	C	H	N	O	P	0	0
			1091	335	387	124	211	34		
7	N	34	Total	C	H	N	O	P	0	0
			1091	335	387	124	211	34		

- Molecule 8 is a DNA chain called DNA (34-MER).

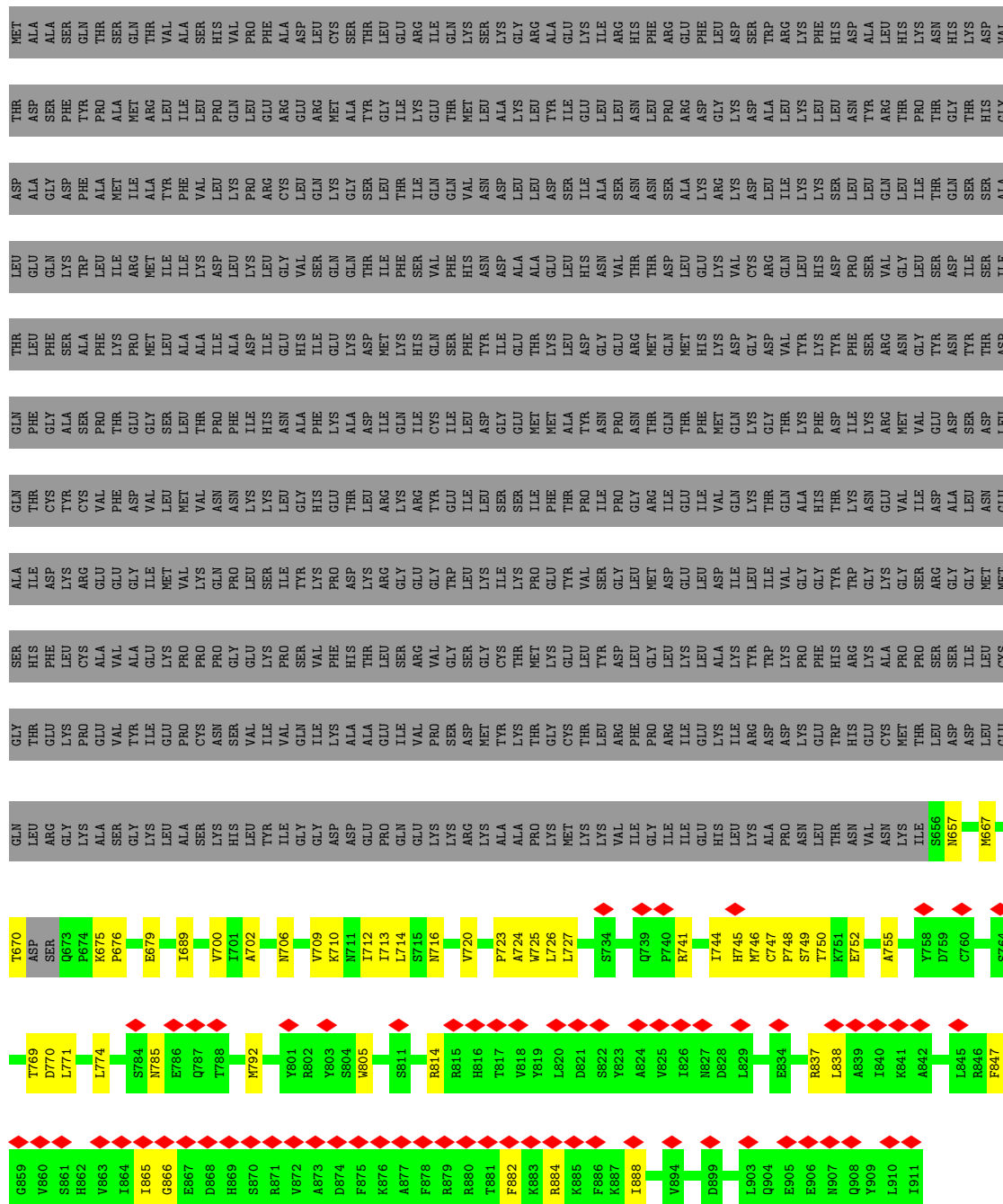
Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	34	Total	C	H	N	O	P	0	0
			1072	329	380	133	196	34		
8	Q	34	Total	C	H	N	O	P	0	0
			1060	329	368	133	196	34		

- Molecule 9 is a protein called Protein PAXX.

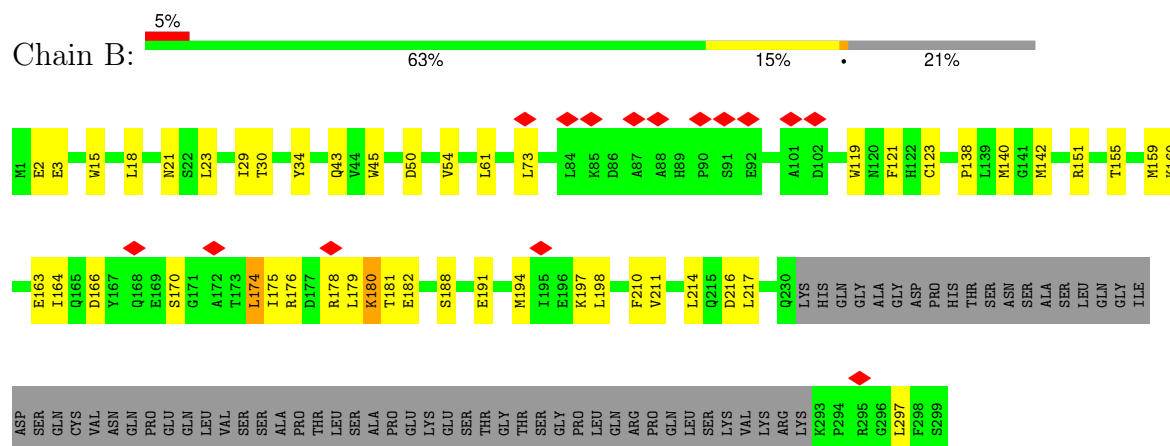
Mol	Chain	Residues	Atoms						AltConf	Trace
9	T	23	Total	C	H	N	O	S	0	0
			338	107	170	30	30	1		
9	U	23	Total	C	H	N	O	S	0	0
			338	107	170	30	30	1		



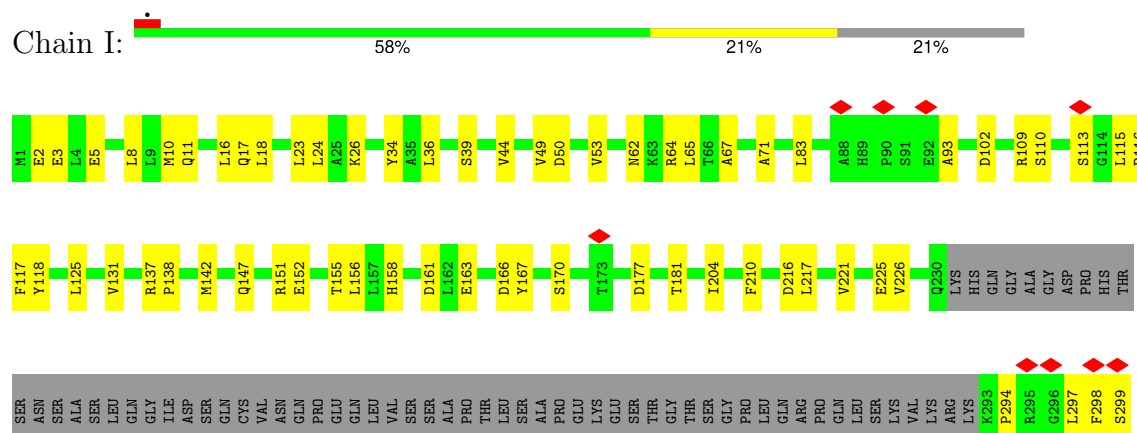
• Molecule 1: DNA ligase 4



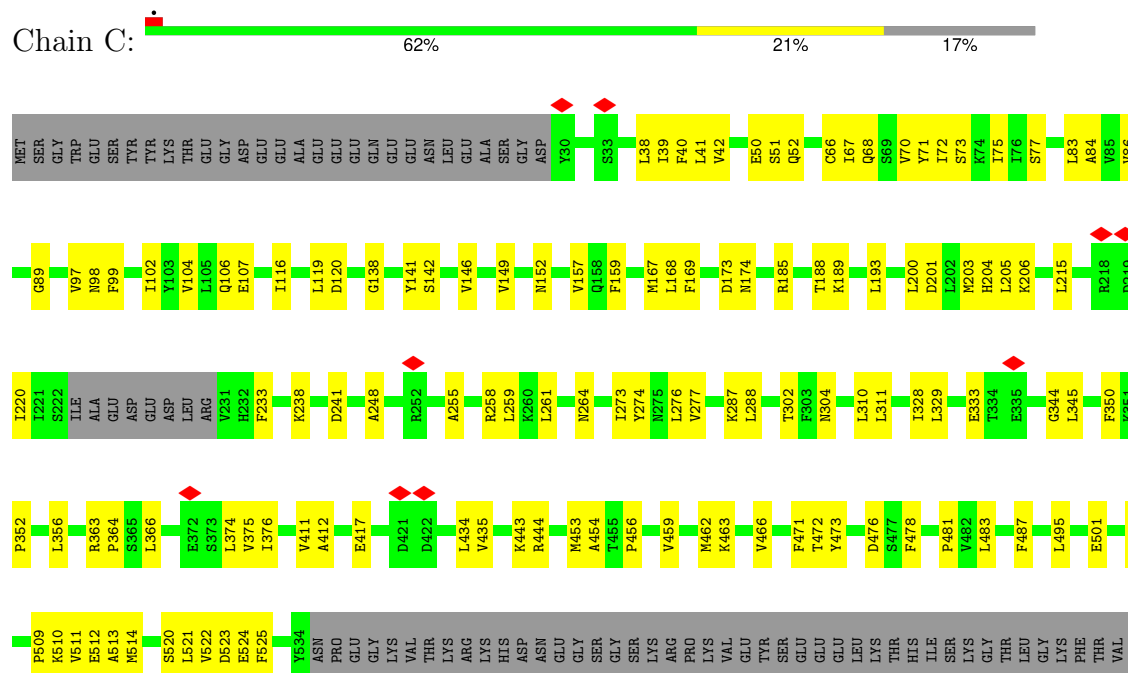
- Molecule 2: Non-homologous end-joining factor 1



- Molecule 2: Non-homologous end-joining factor 1



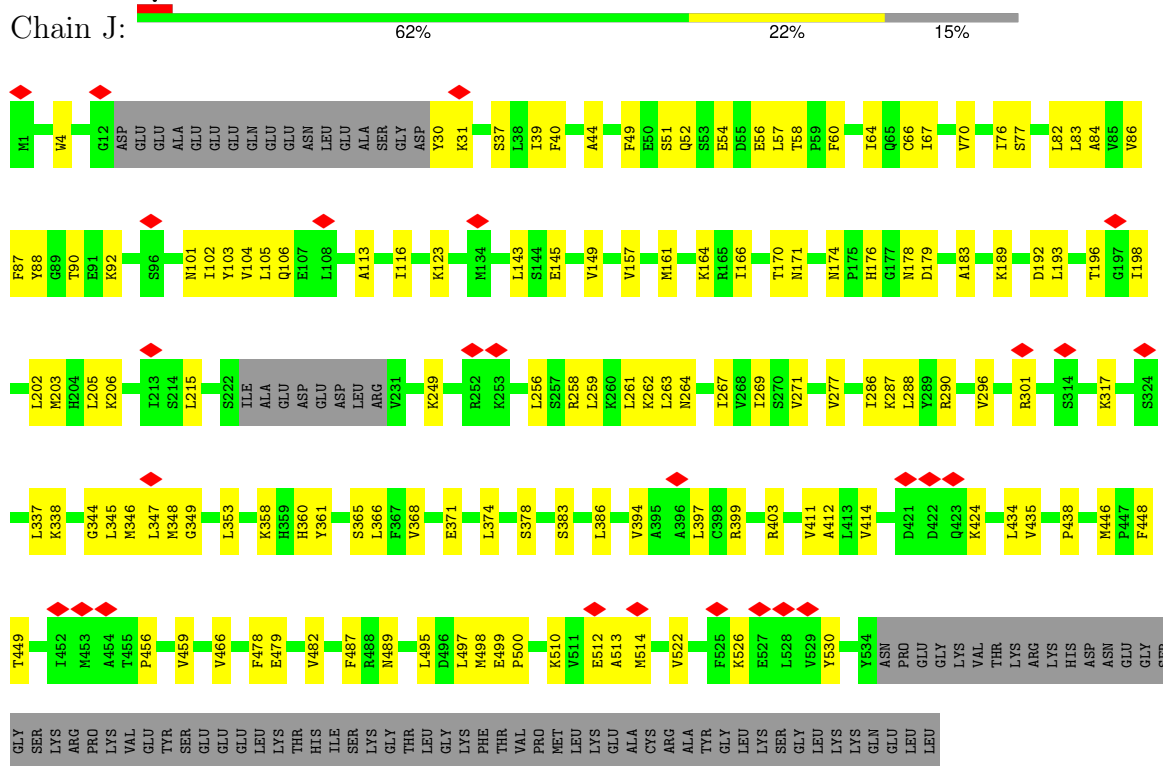
- Molecule 3: X-ray repair cross-complementing protein 6



PRO
MET
LEU
LYS
GLU
CYS
ALA
ARG
ALA
TYR
GLY
LEU
LYS
SER
GLY
LEU
LYS
LYS
GLN
GLU
LEU

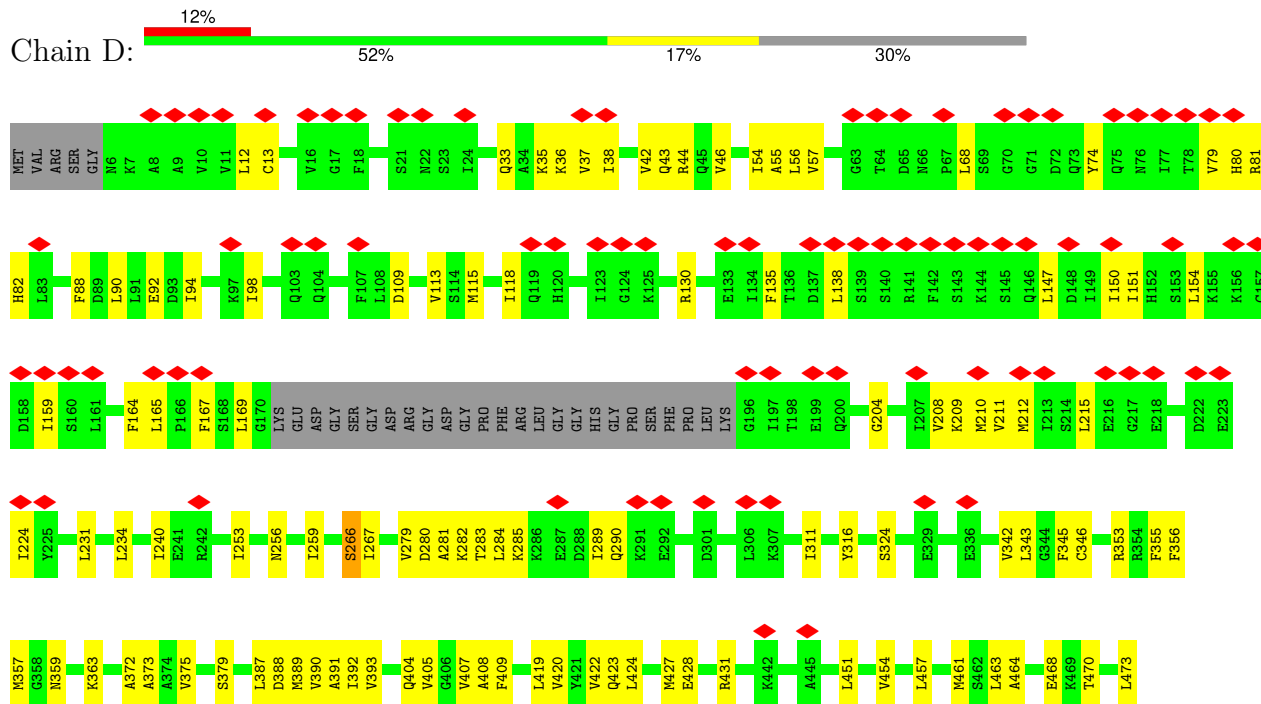
• Molecule 3: X-ray repair cross-complementing protein 6

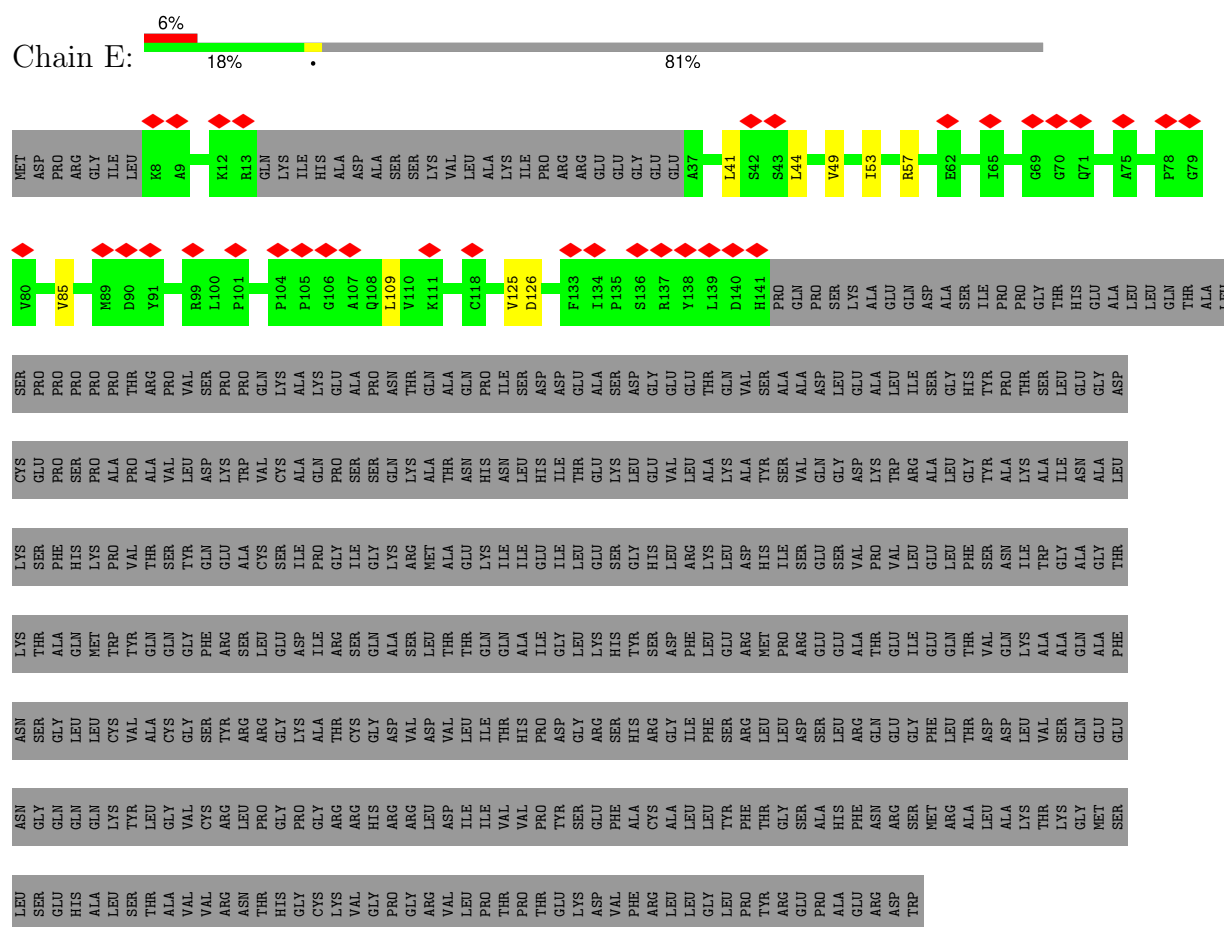
Chain J:



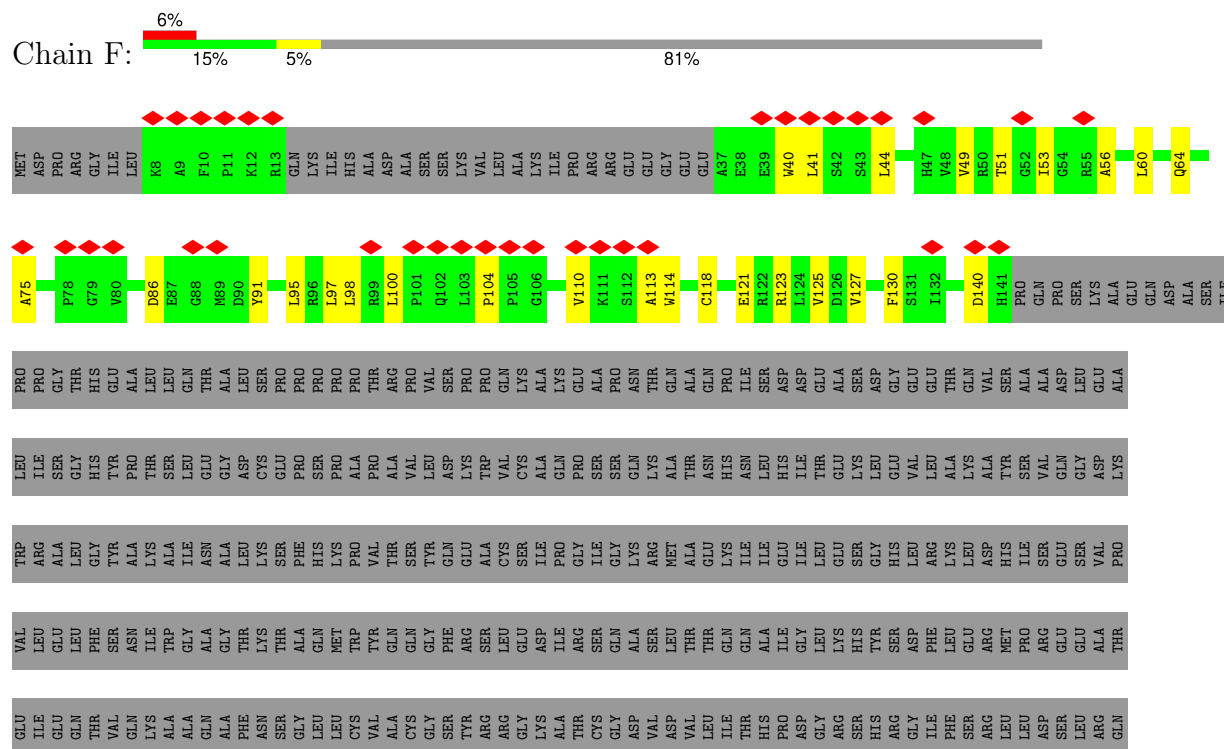
• Molecule 4: X-ray repair cross-complementing protein 5

Chain D:

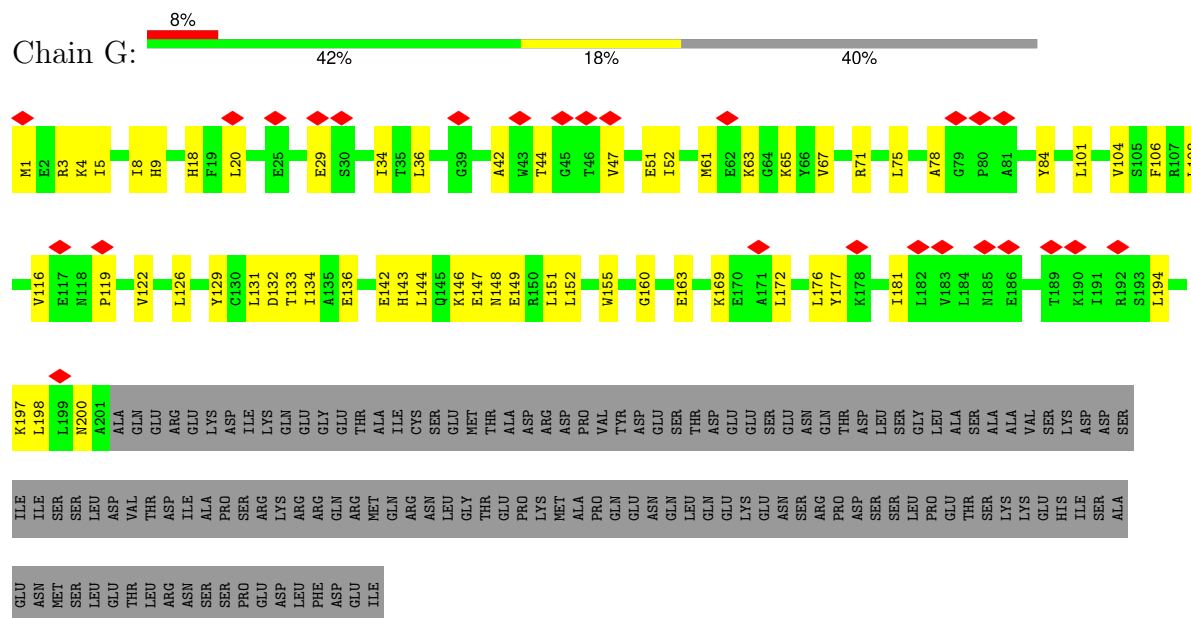




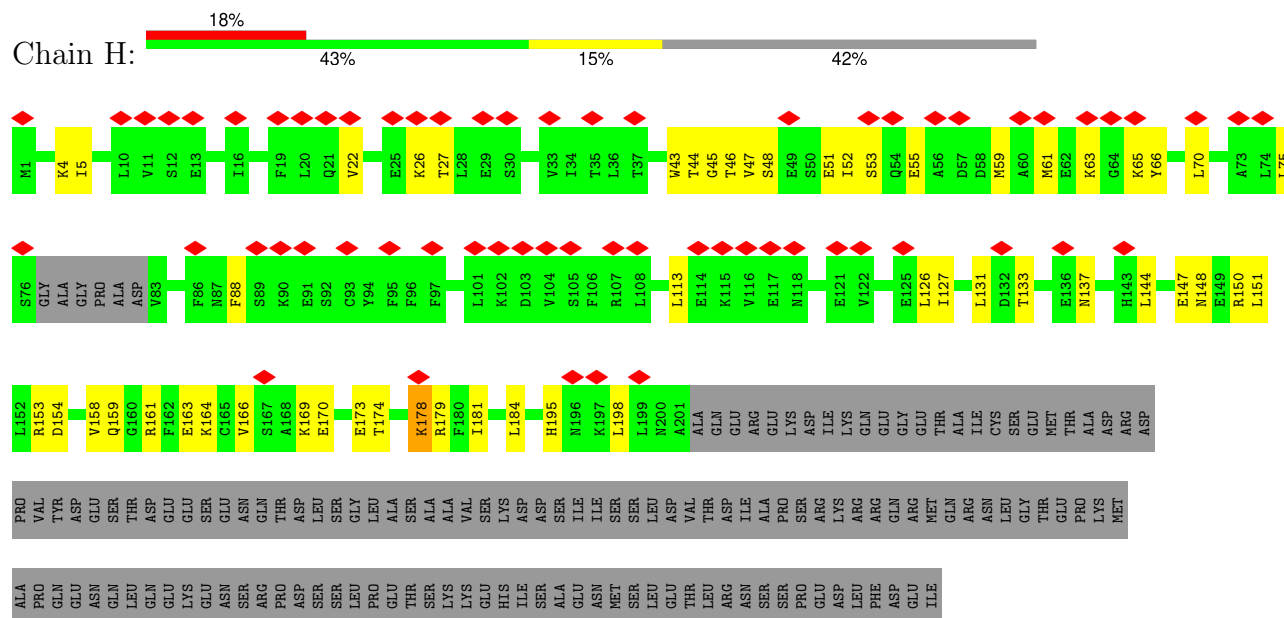
- Molecule 5: DNA polymerase lambda



- Molecule 6: DNA repair protein XRCC4



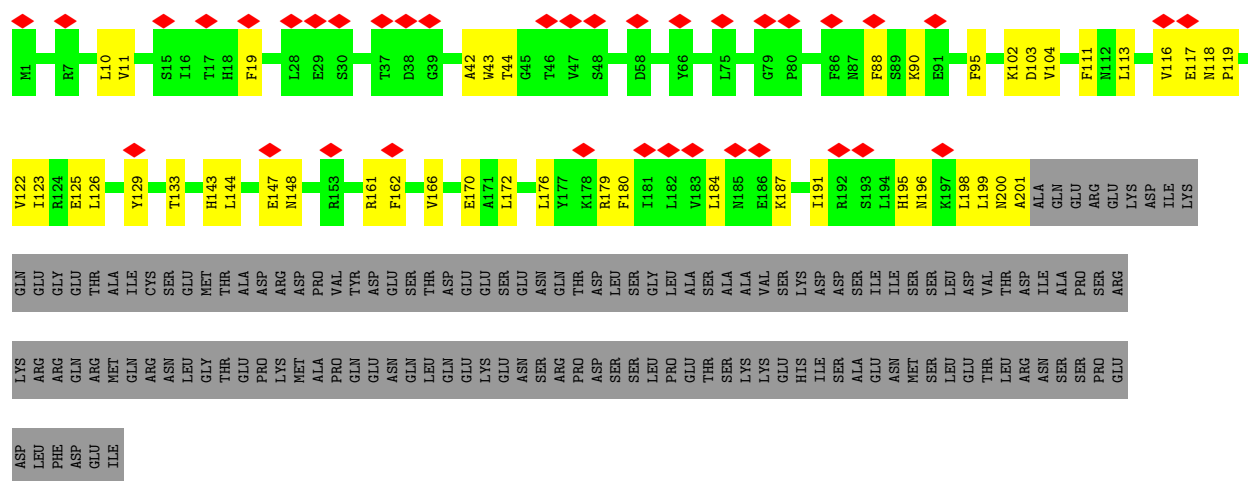
- Molecule 6: DNA repair protein XRCC4



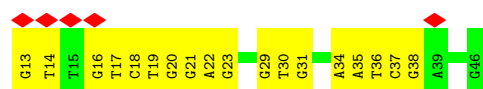
- Molecule 6: DNA repair protein XRCC4



- Molecule 6: DNA repair protein XRCC4

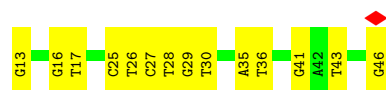


- Molecule 7: DNA (34-MER)



- Molecule 7: DNA (34-MER)

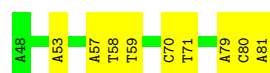




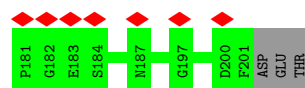
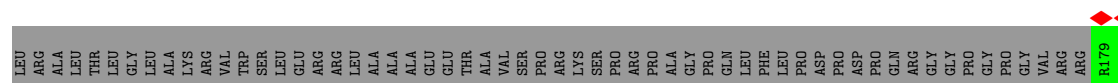
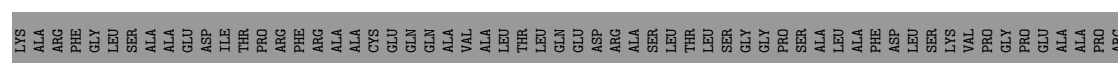
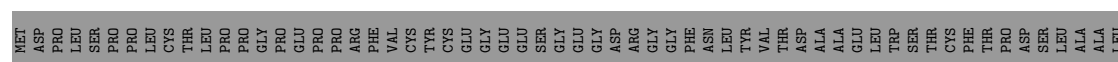
- Molecule 8: DNA (34-MER)



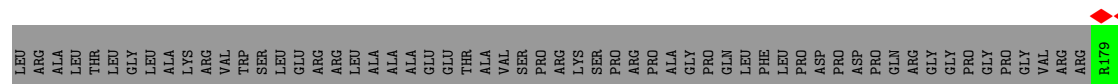
- Molecule 8: DNA (34-MER)



- Molecule 9: Protein PAXX



- Molecule 9: Protein PAXX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179057	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	19.506	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	439.296, 439.296, 439.296	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.056, 1.056, 1.056	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	A	0.14	0/6306	0.33	0/8552
1	X	0.14	0/2112	0.34	0/2851
2	B	0.28	1/1921 (0.1%)	0.50	3/2601 (0.1%)
2	I	0.17	0/1921	0.37	0/2601
3	C	0.17	0/4101	0.36	0/5523
3	J	0.14	0/4204	0.34	0/5660
4	D	0.14	0/4180	0.35	0/5640
4	K	0.14	0/4180	0.37	0/5640
5	E	0.09	0/898	0.25	0/1213
5	F	0.12	0/898	0.50	2/1213 (0.2%)
6	G	0.16	0/1657	0.37	0/2228
6	H	0.16	0/1622	0.41	0/2178
6	O	0.18	0/1622	0.47	0/2178
6	P	0.19	0/1657	0.40	0/2228
7	L	0.25	0/788	0.51	0/1217
7	N	0.25	0/788	0.93	3/1217 (0.2%)
8	M	0.40	0/777	0.56	0/1194
8	Q	0.24	0/777	0.44	0/1194
9	T	0.20	0/172	0.32	0/229
9	U	0.18	0/172	0.36	0/229
All	All	0.17	1/40753 (0.0%)	0.40	8/55586 (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	A	0	1
2	B	0	1
4	D	0	1
4	K	0	1
6	O	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	LYS	C-N	-5.21	1.23	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	46	DG	C2'-C3'-O3'	-18.58	83.62	111.50
7	N	46	DG	C4'-C3'-O3'	15.21	132.81	110.00
7	N	46	DG	C4'-C3'-C2'	-13.37	82.35	102.40
5	F	140	ASP	CA-C-N	9.92	139.56	121.70
5	F	140	ASP	C-N-CA	9.92	139.56	121.70
2	B	180	LYS	CA-C-N	-9.75	107.53	123.04
2	B	180	LYS	C-N-CA	-9.75	107.53	123.04
2	B	180	LYS	N-CA-C	-5.58	98.91	110.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	LYS	Peptide
2	B	174	LEU	Peptide
4	D	266	SER	Peptide
4	K	266	SER	Peptide
6	O	161	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6171	5747	5739	121	0
1	X	2064	2015	2012	43	0
2	B	1883	1894	1893	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1883	1894	1893	57	0
3	C	4021	4103	4100	112	0
3	J	4121	4189	4187	108	0
4	D	4099	4141	4139	110	0
4	K	4099	4141	4139	135	0
5	E	879	902	899	6	0
5	F	879	901	899	20	0
6	G	1628	1620	1620	56	0
6	H	1595	1593	1592	51	0
6	O	1595	1594	1592	55	0
6	P	1628	1620	1620	54	0
7	L	704	387	387	25	0
7	N	704	387	387	11	0
8	M	692	380	380	38	0
8	Q	692	368	380	11	0
9	T	168	170	169	0	0
9	U	168	170	169	4	0
All	All	39673	38216	38196	937	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 12.

All (937) 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)
6:G:194:LEU:HD21	6:H:198:LEU:HD11	1.61	0.82
4:K:12:LEU:HD21	4:K:38:ILE:HD11	1.60	0.81
3:J:86:VAL:HG13	3:J:103:TYR:O	1.80	0.81
3:C:116:ILE:HG21	3:C:495:LEU:HD13	1.61	0.80
1:A:768:ASP:O	1:A:769:THR:C	2.29	0.76
5:E:85:VAL:HG21	5:E:109:LEU:HD11	1.68	0.75
8:Q:80:DC:H2''	8:Q:81:DA:H3'	1.67	0.75
1:X:744:ILE:HG22	1:X:745:HIS:H	1.52	0.74
6:G:129:TYR:O	6:G:133:THR:HG23	1.88	0.74
3:J:174:ASN:HB2	3:J:215:LEU:HD21	1.69	0.73
4:K:356:PHE:CD2	4:K:422:VAL:HG11	2.24	0.73
6:G:61:MET:HE2	2:I:116:PRO:HG3	1.71	0.72
2:B:175:ILE:HD12	2:I:166:ASP:OD2	1.90	0.72
3:C:248:ALA:HB2	4:D:427:MET:HE1	1.72	0.72
6:H:47:VAL:CG1	6:H:51:GLU:HB2	2.20	0.71
6:G:198:LEU:HD13	6:H:198:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ILE:HD11	2:I:170:SER:OG	1.90	0.71
3:J:86:VAL:HG22	3:J:104:VAL:HA	1.73	0.70
6:H:47:VAL:HG11	6:H:51:GLU:HB2	1.73	0.69
4:K:258:SER:O	4:K:259:ILE:HD13	1.92	0.69
3:J:189:LYS:O	3:J:193:LEU:HD23	1.93	0.68
4:D:165:LEU:HD13	4:D:167:PHE:CZ	2.28	0.68
1:A:388:ILE:O	1:A:392:ILE:HG23	1.93	0.67
4:K:531:SER:O	4:K:535:THR:HG23	1.94	0.67
2:I:93:ALA:HA	2:I:110:SER:HB3	1.76	0.67
6:P:196:ASN:HA	6:P:199:LEU:HD12	1.77	0.67
2:I:110:SER:HG	2:I:117:PHE:HE1	1.39	0.67
2:B:30:THR:O	2:B:73:LEU:HD13	1.94	0.67
3:C:478:PHE:CD2	4:D:405:VAL:HG11	2.30	0.67
3:C:174:ASN:HB2	3:C:215:LEU:HD21	1.77	0.66
3:C:483:LEU:HD23	4:D:428:GLU:OE2	1.94	0.66
8:M:57:DA:C6	8:M:58:DT:C4	2.84	0.66
1:A:82:TYR:CZ	1:A:152:LEU:HD22	2.31	0.66
1:A:250:LEU:HD13	1:A:443:ARG:NH2	2.11	0.66
4:K:343:LEU:HD21	9:U:199:VAL:HG22	1.78	0.66
6:P:195:HIS:CD2	6:P:199:LEU:HD11	2.31	0.66
4:D:457:LEU:HD22	4:D:533:ILE:HD11	1.78	0.65
4:D:520:ALA:O	4:D:524:THR:HG23	1.97	0.65
3:C:329:LEU:HD23	3:C:333:GLU:CD	2.22	0.65
5:F:41:LEU:HD22	5:F:44:LEU:HD22	1.77	0.65
8:M:57:DA:C2	8:M:58:DT:C6	2.84	0.65
3:J:101:ASN:O	3:J:102:ILE:HD13	1.96	0.65
3:J:386:LEU:HD23	4:K:438:LEU:HD11	1.77	0.65
4:D:68:LEU:HD12	4:D:113:VAL:HG22	1.77	0.65
3:J:82:LEU:HD13	3:J:157:VAL:HG21	1.77	0.65
5:E:41:LEU:HD22	5:E:44:LEU:HD22	1.79	0.65
6:H:169:LYS:O	6:H:173:GLU:OE1	2.14	0.64
2:B:297:LEU:HD11	4:D:164:PHE:CE2	2.32	0.64
2:I:102:ASP:OD2	2:I:125:LEU:HD12	1.98	0.64
6:G:151:LEU:HD22	6:H:151:LEU:HB3	1.80	0.64
1:A:23:LEU:HD23	1:A:26:ILE:HD12	1.79	0.64
3:J:478:PHE:CD2	4:K:405:VAL:HG11	2.33	0.64
7:L:34:DA:H62	8:M:56:DG:H5'	1.61	0.64
4:K:241:GLU:HG3	8:M:74:DA:H61	1.63	0.64
1:A:740:PRO:HA	1:A:743:MET:HG2	1.79	0.63
3:C:102:ILE:HD11	3:C:146:VAL:HG22	1.79	0.63
4:D:36:LYS:NZ	4:D:231:LEU:HD11	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:221:VAL:HG12	2:I:225:GLU:OE2	1.99	0.63
5:F:91:TYR:CE2	5:F:95:LEU:HD11	2.33	0.63
6:H:133:THR:HG22	6:H:137:ASN:HD21	1.63	0.63
3:C:41:LEU:O	3:C:168:LEU:HD12	1.99	0.63
3:C:41:LEU:HD23	3:C:168:LEU:HD13	1.81	0.63
6:O:127:ILE:HD12	6:P:19:PHE:CE2	2.33	0.62
3:C:363:ARG:HG2	3:C:364:PRO:HD2	1.80	0.62
1:A:332:MET:HE1	1:A:364:TYR:CD1	2.34	0.62
6:P:129:TYR:O	6:P:133:THR:HG23	2.00	0.62
7:N:35:DA:H2'	7:N:36:DT:H72	1.82	0.62
1:A:768:ASP:O	1:A:768:ASP:OD1	2.17	0.62
2:I:23:LEU:HD23	2:I:24:LEU:N	2.14	0.62
3:C:71:TYR:CD1	3:C:83:LEU:HD23	2.34	0.62
3:C:310:LEU:HD21	5:E:57:ARG:CZ	2.30	0.62
6:H:88:PHE:CZ	6:H:113:LEU:HD12	2.35	0.62
1:A:767:ILE:HG23	1:A:767:ILE:O	1.99	0.61
3:C:102:ILE:HG21	3:C:149:VAL:HG21	1.82	0.61
2:I:297:LEU:C	4:K:41:PHE:HB2	2.25	0.61
3:J:92:LYS:HB3	3:J:103:TYR:OH	2.01	0.61
3:J:178:ASN:OD1	3:J:179:ASP:N	2.33	0.61
4:D:422:VAL:HG12	4:D:423:GLN:H	1.66	0.61
3:J:466:VAL:HG23	4:K:345:PHE:CD2	2.36	0.61
6:H:166:VAL:O	6:H:170:GLU:OE1	2.19	0.61
3:J:258:ARG:C	3:J:259:LEU:HD12	2.26	0.61
6:H:5:ILE:HD13	6:H:126:LEU:HG	1.83	0.60
3:C:273:ILE:CG2	3:C:366:LEU:HD23	2.31	0.60
4:K:407:VAL:H	4:K:424:LEU:HD23	1.66	0.60
6:G:134:ILE:HD11	6:H:137:ASN:ND2	2.16	0.60
4:D:266:SER:O	4:D:267:ILE:HG12	2.00	0.60
6:H:159:GLN:O	6:H:163:GLU:OE1	2.19	0.60
1:A:224:VAL:HG13	1:A:228:LEU:HD12	1.84	0.60
1:A:681:ARG:HH11	1:A:727:LEU:HD22	1.65	0.60
2:B:181:THR:O	2:B:181:THR:OG1	2.12	0.60
5:F:118:CYS:SG	5:F:125:VAL:HG22	2.42	0.60
3:C:364:PRO:O	3:C:366:LEU:HD12	2.01	0.59
6:H:174:THR:HG23	6:H:178:LYS:HD2	1.84	0.59
4:D:463:LEU:HD11	4:D:477:PHE:CE2	2.37	0.59
6:G:144:LEU:HD11	6:H:148:ASN:ND2	2.16	0.59
1:A:70:LEU:HB3	1:A:189:MET:HE3	1.84	0.59
1:A:332:MET:HE1	1:A:364:TYR:HD1	1.67	0.59
6:H:48:SER:O	6:H:52:ILE:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:104:VAL:O	3:J:104:VAL:HG13	2.01	0.59
4:K:81:ARG:HD3	4:K:84:MET:HE2	1.85	0.59
3:J:482:VAL:HG21	4:K:402:ASN:HD22	1.66	0.59
1:A:279:MET:HB3	1:A:332:MET:HE3	1.84	0.59
2:B:164:ILE:HG21	2:B:181:THR:OG1	2.02	0.59
8:M:75:DG:H2''	8:M:76:DA:O5'	2.02	0.59
6:P:88:PHE:HD1	6:P:95:PHE:HB3	1.68	0.59
4:D:147:LEU:HD23	4:D:150:ILE:HD11	1.85	0.59
4:D:422:VAL:HG12	4:D:423:GLN:N	2.18	0.58
4:K:209:LYS:HA	4:K:212:MET:HE2	1.85	0.58
3:C:86:VAL:HG23	3:C:104:VAL:HA	1.85	0.58
6:H:88:PHE:CE1	6:H:113:LEU:HD12	2.38	0.58
5:F:60:LEU:O	5:F:64:GLN:OE1	2.22	0.58
3:C:261:LEU:HD13	3:C:345:LEU:HB3	1.86	0.58
4:D:493:CYS:SG	4:D:505:LEU:HD11	2.44	0.58
6:G:132:ASP:O	6:G:136:GLU:OE1	2.21	0.58
1:A:429:ILE:HG22	1:A:430:MET:H	1.68	0.58
3:J:40:PHE:CZ	3:J:70:VAL:HG21	2.38	0.58
4:K:266:SER:O	4:K:267:ILE:HG12	2.03	0.58
2:B:180:LYS:O	2:B:181:THR:HG22	2.04	0.57
6:H:181:ILE:HG23	6:H:184:LEU:HD23	1.86	0.57
2:I:62:ASN:HB3	2:I:65:LEU:HD23	1.86	0.57
4:K:240:ILE:CD1	4:K:270:GLU:CD	2.78	0.57
1:A:739:GLN:N	1:A:740:PRO:CD	2.68	0.57
4:D:57:VAL:O	4:D:57:VAL:HG13	2.05	0.57
6:G:101:LEU:HD12	2:I:113:SER:HA	1.86	0.57
6:P:195:HIS:O	6:P:199:LEU:HG	2.05	0.57
1:A:263:MET:HE2	1:A:263:MET:N	2.19	0.57
4:D:169:LEU:HD13	4:D:224:ILE:HD13	1.87	0.57
6:H:43:TRP:O	6:H:113:LEU:HD13	2.04	0.57
1:A:818:VAL:HG11	1:A:845:LEU:HD21	1.87	0.57
3:C:435:VAL:HG13	3:C:435:VAL:O	2.04	0.57
3:J:424:LYS:O	3:J:424:LYS:HD3	2.05	0.57
4:D:151:ILE:HG23	4:D:215:LEU:HD23	1.86	0.57
6:O:144:LEU:HD11	6:P:148:ASN:OD1	2.04	0.57
6:H:51:GLU:O	6:H:55:GLU:HG2	2.05	0.56
1:A:666:VAL:HG22	1:A:675:LYS:NZ	2.20	0.56
3:J:58:THR:HG21	3:J:60:PHE:CZ	2.41	0.56
4:K:40:MET:HE1	4:K:44:ARG:HD2	1.88	0.56
4:K:151:ILE:HG23	4:K:215:LEU:HD23	1.87	0.56
5:F:98:LEU:HD21	5:F:100:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:522:VAL:HG21	4:K:256:ASN:HB2	1.87	0.56
6:O:45:GLY:N	6:O:113:LEU:HD23	2.21	0.56
3:C:520:SER:O	3:C:523:ASP:OD2	2.23	0.56
6:G:61:MET:HE3	6:G:65:LYS:HD2	1.88	0.56
6:O:151:LEU:O	6:O:154:ASP:OD1	2.23	0.56
3:J:261:LEU:HD13	3:J:345:LEU:HB3	1.87	0.56
2:B:15:TRP:HB2	2:B:211:VAL:HG21	1.87	0.55
2:B:151:ARG:O	2:B:155:THR:HG23	2.05	0.55
6:H:66:TYR:CE1	6:H:70:LEU:HD11	2.40	0.55
2:I:93:ALA:CA	2:I:110:SER:HB3	2.37	0.55
3:J:287:LYS:HD3	3:J:296:VAL:HG21	1.86	0.55
6:P:88:PHE:CZ	6:P:113:LEU:HD23	2.42	0.55
4:K:304:GLU:OE2	4:K:305:VAL:HG22	2.06	0.55
6:P:42:ALA:HB3	6:P:119:PRO:HB3	1.88	0.55
1:A:198:VAL:O	1:A:198:VAL:HG13	2.06	0.55
3:J:344:GLY:C	3:J:345:LEU:HD22	2.32	0.55
3:C:41:LEU:HD12	3:C:86:VAL:HG13	1.88	0.55
6:H:195:HIS:HA	6:H:198:LEU:HD12	1.89	0.55
2:I:39:SER:HB2	2:I:44:VAL:HG12	1.88	0.55
3:C:104:VAL:HG11	3:C:107:GLU:OE1	2.07	0.55
8:M:57:DA:C2	8:M:58:DT:C2	2.94	0.55
2:I:34:TYR:CE2	2:I:49:VAL:HG22	2.42	0.55
4:K:245:ILE:HG23	8:M:75:DG:N7	2.21	0.55
1:A:720:VAL:HG12	1:A:745:HIS:O	2.07	0.55
4:D:38:ILE:O	4:D:42:VAL:HG23	2.07	0.55
3:J:366:LEU:HB3	3:J:434:LEU:HD12	1.89	0.55
6:O:31:GLY:HA2	6:O:48:SER:HA	1.89	0.55
1:A:127:MET:HE2	1:A:127:MET:N	2.22	0.55
3:J:349:GLY:HA2	4:K:461:MET:HE1	1.87	0.55
3:C:40:PHE:CD2	3:C:67:ILE:HD12	2.41	0.55
4:D:540:ILE:HD12	4:D:540:ILE:H	1.72	0.55
5:F:51:THR:HG23	4:K:302:GLU:HA	1.88	0.55
3:J:365:SER:OG	3:J:435:VAL:HG22	2.07	0.55
6:P:200:ASN:OD1	6:P:200:ASN:O	2.25	0.55
1:X:713:ILE:HD13	1:X:720:VAL:HG21	1.89	0.55
5:F:56:ALA:O	5:F:60:LEU:HD23	2.07	0.54
7:L:17:DT:OP2	7:L:17:DT:H73	2.06	0.54
3:C:255:ALA:HB2	3:C:274:TYR:HE1	1.73	0.54
4:D:387:LEU:O	4:D:388:ASP:OD1	2.25	0.54
1:A:422:ILE:HD11	1:A:452:PRO:HG3	1.90	0.54
4:D:38:ILE:HG22	4:D:135:PHE:HE2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:51:GLU:H	6:O:51:GLU:CD	2.15	0.54
1:A:881:THR:HG22	1:A:881:THR:O	2.08	0.54
4:D:36:LYS:HZ1	4:D:231:LEU:HD11	1.72	0.54
4:K:68:LEU:HD12	4:K:113:VAL:HG22	1.90	0.54
3:C:205:LEU:HD12	3:C:206:LYS:N	2.23	0.54
4:K:339:CYS:SG	4:K:396:ALA:HB3	2.48	0.54
1:A:845:LEU:CD1	1:A:894:VAL:HG21	2.38	0.54
2:B:176:ARG:O	2:B:179:LEU:N	2.41	0.54
2:B:181:THR:O	2:B:182:GLU:C	2.51	0.54
2:B:181:THR:HG21	2:I:163:GLU:HG2	1.90	0.54
2:B:159:MET:O	2:B:163:GLU:OE1	2.26	0.54
5:F:75:ALA:HB3	5:F:98:LEU:HD11	1.90	0.54
6:G:104:VAL:HG21	2:I:71:ALA:HB1	1.90	0.54
1:A:845:LEU:HB3	1:A:850:ALA:HB3	1.90	0.53
3:C:462:MET:HE2	3:C:525:PHE:CE2	2.43	0.53
3:C:328:ILE:C	3:C:329:LEU:HD12	2.32	0.53
4:K:399:LYS:O	4:K:400:ARG:HG2	2.08	0.53
6:O:127:ILE:HD12	6:P:19:PHE:CZ	2.43	0.53
6:O:159:GLN:HA	6:O:162:PHE:CE1	2.44	0.53
2:B:18:LEU:HD12	2:B:21:ASN:OD1	2.07	0.53
3:C:41:LEU:HD11	3:C:146:VAL:CG1	2.39	0.53
3:C:374:LEU:HG	3:C:375:VAL:HG23	1.89	0.53
8:Q:58:DT:H2'	8:Q:59:DT:H72	1.89	0.53
2:I:151:ARG:O	2:I:155:THR:HG23	2.07	0.53
4:K:396:ALA:HB2	4:K:403:PRO:HA	1.88	0.53
1:A:665:CYS:HB3	1:A:700:VAL:HG12	1.90	0.53
3:C:463:LYS:O	3:C:466:VAL:HG12	2.07	0.53
4:D:464:ALA:HB1	4:D:473:LEU:HB3	1.91	0.53
8:M:57:DA:N3	8:M:58:DT:C6	2.77	0.53
1:A:795:LEU:O	1:A:799:LEU:HD23	2.08	0.53
6:H:26:LYS:O	6:H:27:THR:HG23	2.08	0.53
6:O:48:SER:N	6:O:51:GLU:OE2	2.42	0.53
2:B:179:LEU:C	2:B:180:LYS:O	2.48	0.53
6:G:155:TRP:HE1	6:H:158:VAL:HG21	1.74	0.53
6:O:161:ARG:NH1	6:P:162:PHE:CG	2.77	0.53
1:X:667:MET:HE1	1:X:700:VAL:HG22	1.90	0.53
1:A:840:ILE:HD12	6:P:161:ARG:CZ	2.40	0.52
4:D:81:ARG:NH2	4:D:90:LEU:HD22	2.24	0.52
3:J:478:PHE:CE2	4:K:405:VAL:HG11	2.44	0.52
8:M:57:DA:C2	8:M:58:DT:N1	2.78	0.52
4:D:468:GLU:OE1	4:D:470:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:187:ASN:OD1	9:U:187:ASN:O	2.27	0.52
3:J:58:THR:HG21	3:J:60:PHE:CE2	2.44	0.52
3:J:82:LEU:CD1	3:J:157:VAL:HG21	2.39	0.52
4:K:212:MET:HE1	4:K:221:LEU:HD23	1.91	0.52
8:M:57:DA:N1	8:M:58:DT:C4	2.78	0.52
6:H:61:MET:HE1	6:H:65:LYS:HG3	1.92	0.52
7:L:19:DT:C2	7:L:20:DG:C5	2.97	0.52
1:A:14:VAL:HG12	3:J:4:TRP:CZ2	2.45	0.52
6:H:46:THR:O	6:H:47:VAL:HG23	2.09	0.52
7:L:34:DA:C4'	8:M:60:DG:H22	2.23	0.52
2:I:64:ARG:C	2:I:65:LEU:HD22	2.34	0.52
3:J:403:ARG:HE	7:L:31:DG:C5'	2.23	0.52
2:B:176:ARG:O	2:B:179:LEU:C	2.52	0.52
6:G:42:ALA:O	6:G:116:VAL:HG22	2.10	0.52
3:J:347:LEU:HD12	3:J:397:LEU:O	2.10	0.52
1:X:657:ASN:O	1:X:657:ASN:OD1	2.27	0.52
3:C:363:ARG:CG	3:C:364:PRO:HD2	2.40	0.52
3:J:277:VAL:HG22	4:K:357:MET:HE1	1.90	0.52
4:K:253:ILE:HD13	4:K:342:VAL:HB	1.91	0.52
1:A:220:ASP:O	1:A:224:VAL:HG23	2.10	0.52
4:K:136:THR:O	4:K:165:LEU:HD13	2.10	0.52
6:G:4:LYS:HG2	6:G:75:LEU:HD12	1.91	0.51
6:O:154:ASP:O	6:O:157:ASP:OD1	2.28	0.51
1:A:667:MET:HE3	1:A:708:ARG:NH2	2.25	0.51
8:Q:80:DC:H2''	8:Q:81:DA:H5'	1.92	0.51
1:A:224:VAL:HG13	1:A:228:LEU:CD1	2.39	0.51
3:C:302:THR:HG23	4:D:290:GLN:O	2.10	0.51
6:H:4:LYS:HB3	6:H:75:LEU:HD22	1.91	0.51
6:H:169:LYS:HE2	6:H:173:GLU:OE2	2.10	0.51
4:K:269:GLN:O	4:K:269:GLN:CD	2.53	0.51
8:M:58:DT:H3'	8:M:59:DT:O2	2.10	0.51
1:A:71:ILE:HG23	1:A:72:LEU:CD1	2.40	0.51
1:A:71:ILE:HG23	1:A:72:LEU:HD12	1.92	0.51
4:D:130:ARG:HB3	4:D:159:ILE:HD12	1.93	0.51
4:K:412:ILE:HG23	4:K:417:GLU:OE2	2.10	0.51
8:Q:57:DA:H2'	8:Q:58:DT:H71	1.93	0.51
2:B:174:LEU:HD12	2:B:180:LYS:NZ	2.25	0.51
3:C:41:LEU:HD21	3:C:146:VAL:CG1	2.41	0.51
4:D:390:VAL:HG22	4:D:391:ALA:N	2.26	0.51
3:J:166:ILE:HD11	3:J:198:ILE:HD11	1.93	0.51
4:K:16:VAL:HG21	4:K:61:THR:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:O	3:C:98:ASN:OD1	2.29	0.51
4:D:43:GLN:HA	4:D:46:VAL:HG12	1.92	0.51
6:G:131:LEU:O	6:G:134:ILE:HG22	2.11	0.51
3:J:145:GLU:O	3:J:149:VAL:HG23	2.10	0.51
6:P:143:HIS:O	6:P:147:GLU:OE1	2.29	0.51
1:X:744:ILE:HG22	1:X:745:HIS:N	2.22	0.51
6:G:8:ILE:HG22	6:G:9:HIS:N	2.26	0.51
2:I:10:MET:HE2	2:I:226:VAL:HG21	1.92	0.51
1:X:676:PRO:O	1:X:679:GLU:HB3	2.10	0.51
1:A:467:VAL:HG21	1:A:486:ALA:HB2	1.92	0.51
1:A:894:VAL:HG22	1:A:898:ILE:CD1	2.40	0.51
4:K:361:VAL:HG22	4:K:422:VAL:HG22	1.93	0.51
3:C:276:LEU:O	3:C:276:LEU:HD23	2.12	0.50
4:K:35:LYS:HD3	4:K:98:ILE:HD13	1.93	0.50
6:P:200:ASN:O	6:P:201:ALA:HB2	2.10	0.50
1:A:565:VAL:HG12	1:A:577:ARG:NH2	2.26	0.50
4:D:80:HIS:CD2	4:D:90:LEU:HD11	2.46	0.50
4:D:356:PHE:CD2	4:D:422:VAL:HG11	2.45	0.50
4:K:464:ALA:HB1	4:K:473:LEU:HB3	1.93	0.50
1:A:694:GLY:O	1:A:697:THR:HG22	2.11	0.50
4:D:33:GLN:O	4:D:37:VAL:HG23	2.11	0.50
6:H:133:THR:HG22	6:H:137:ASN:ND2	2.26	0.50
3:J:361:TYR:O	4:K:267:ILE:HG21	2.11	0.50
8:M:57:DA:C4	8:M:58:DT:C5	3.00	0.50
3:J:317:LYS:HZ2	4:K:281:ALA:HB2	1.75	0.50
8:Q:80:DC:H1'	8:Q:81:DA:H5'	1.93	0.50
1:A:389:LEU:HD12	1:A:392:ILE:HD11	1.94	0.50
4:D:209:LYS:HA	4:D:212:MET:HE2	1.93	0.50
3:J:261:LEU:O	3:J:269:ILE:HG12	2.11	0.50
1:A:856:LEU:HA	1:A:860:VAL:HG21	1.92	0.50
4:D:451:LEU:O	4:D:454:VAL:HG12	2.12	0.50
4:D:477:PHE:CZ	4:D:519:PRO:HD2	2.47	0.50
3:J:264:ASN:HB2	4:K:530:LEU:HD22	1.94	0.50
1:A:328:LEU:HD12	1:A:366:VAL:HG21	1.94	0.50
1:A:741:ARG:HD2	1:A:764:SER:HA	1.92	0.50
2:B:214:LEU:HD21	2:I:147:GLN:HB2	1.93	0.50
3:C:102:ILE:CD1	3:C:146:VAL:HG22	2.41	0.50
6:G:20:LEU:CD1	6:G:34:ILE:HD11	2.42	0.50
6:G:108:LEU:CD2	2:I:115:LEU:HD13	2.42	0.50
3:J:37:SER:HB3	3:J:161:MET:HE1	1.93	0.50
3:J:164:LYS:HB3	3:J:198:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:240:ILE:HG12	4:K:241:GLU:N	2.27	0.50
6:O:47:VAL:HG23	6:O:47:VAL:O	2.11	0.50
1:X:679:GLU:OE2	1:X:689:ILE:HD12	2.12	0.50
4:K:246:HIS:H	8:M:73:DC:H2"	1.77	0.50
6:P:43:TRP:HB2	6:P:113:LEU:HD21	1.92	0.50
6:G:142:GLU:HG3	6:G:146:LYS:HE3	1.94	0.49
4:K:132:ILE:HG23	4:K:161:LEU:HA	1.94	0.49
4:K:438:LEU:HD23	4:K:438:LEU:H	1.77	0.49
6:P:88:PHE:CD1	6:P:95:PHE:HB3	2.47	0.49
1:X:675:LYS:HB2	1:X:676:PRO:HD3	1.94	0.49
1:A:23:LEU:HA	1:A:26:ILE:HD12	1.94	0.49
2:B:18:LEU:HD11	2:B:23:LEU:HG	1.94	0.49
3:C:411:VAL:HG21	3:C:434:LEU:HD22	1.93	0.49
3:C:453:MET:O	4:D:375:VAL:HG23	2.11	0.49
4:K:408:ALA:HB1	4:K:419:LEU:HD21	1.93	0.49
3:C:483:LEU:HD11	3:C:487:PHE:CZ	2.48	0.49
4:D:165:LEU:HD13	4:D:167:PHE:HZ	1.73	0.49
6:O:154:ASP:O	6:O:158:VAL:HG23	2.13	0.49
6:P:118:ASN:N	6:P:119:PRO:CD	2.75	0.49
3:C:38:LEU:HD11	3:C:167:MET:HG3	1.94	0.49
6:G:44:THR:OG1	6:G:116:VAL:HG11	2.13	0.49
2:I:110:SER:OG	2:I:117:PHE:HE1	1.96	0.49
3:J:269:ILE:HB	3:J:378:SER:HB2	1.95	0.49
3:C:238:LYS:O	3:C:241:ASP:OD1	2.29	0.49
4:K:9:ALA:HB3	4:K:130:ARG:HG3	1.94	0.49
7:N:16:DG:C2'	7:N:17:DT:H72	2.43	0.49
1:X:706:ASN:OD1	1:X:709:VAL:HG23	2.12	0.49
1:A:752:GLU:HA	1:A:755:ALA:HB3	1.94	0.49
2:B:50:ASP:O	2:B:54:VAL:HG23	2.12	0.49
3:J:64:ILE:HD12	3:J:123:LYS:HA	1.93	0.49
6:P:166:VAL:O	6:P:170:GLU:OE1	2.29	0.49
6:G:143:HIS:O	6:G:147:GLU:OE1	2.30	0.49
4:D:55:ALA:C	4:D:56:LEU:HD22	2.38	0.49
4:K:468:GLU:O	4:K:468:GLU:HG3	2.12	0.49
6:P:102:LYS:O	6:P:103:ASP:OD1	2.30	0.49
1:X:723:PRO:O	1:X:726:LEU:HD23	2.13	0.49
3:C:75:ILE:HD13	4:D:316:TYR:CE1	2.48	0.49
3:C:376:ILE:HB	4:D:540:ILE:HD13	1.94	0.48
3:C:478:PHE:CE2	4:D:405:VAL:HG11	2.48	0.48
4:D:88:PHE:O	4:D:92:GLU:OE1	2.31	0.48
4:D:280:ASP:H	4:D:289:ILE:HD11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:GLN:C	2:I:18:LEU:HD22	2.38	0.48
4:K:306:LEU:O	4:K:310:ILE:HD13	2.13	0.48
4:K:380:LEU:HD23	4:K:384:LEU:HD13	1.95	0.48
8:M:54:DT:H72	8:M:56:DG:H22	1.77	0.48
8:M:57:DA:C2	8:M:58:DT:C5	3.01	0.48
6:O:56:ALA:HB2	6:O:63:LYS:HE2	1.93	0.48
3:C:167:MET:HB3	3:C:203:MET:HE1	1.94	0.48
4:K:244:SER:O	8:M:74:DA:C8	2.66	0.48
1:A:738:TRP:HB3	1:A:768:ASP:HB3	1.94	0.48
3:C:72:ILE:HD13	3:C:116:ILE:HD12	1.95	0.48
6:H:55:GLU:O	6:H:59:MET:HE1	2.13	0.48
6:H:66:TYR:HE1	6:H:70:LEU:HD11	1.78	0.48
6:O:32:PHE:HE2	6:O:52:ILE:HD12	1.78	0.48
1:A:219:THR:HG22	1:A:219:THR:O	2.14	0.48
3:C:258:ARG:C	3:C:259:LEU:HD22	2.38	0.48
6:G:29:GLU:OE1	6:G:67:VAL:HG21	2.13	0.48
3:J:66:CYS:O	3:J:70:VAL:HG22	2.13	0.48
3:J:105:LEU:HD23	3:J:106:GLN:HG3	1.95	0.48
6:O:182:LEU:HD12	6:O:182:LEU:C	2.37	0.48
1:A:61:THR:HG23	1:A:62:ASP:N	2.27	0.48
1:A:818:VAL:HG11	1:A:845:LEU:CD2	2.44	0.48
1:A:894:VAL:HG22	1:A:898:ILE:HD11	1.93	0.48
4:D:36:LYS:NZ	4:D:231:LEU:HD21	2.28	0.48
2:I:158:HIS:O	2:I:161:ASP:OD1	2.30	0.48
3:J:192:ASP:O	3:J:196:THR:HG23	2.13	0.48
4:K:342:VAL:HG22	4:K:393:VAL:HG22	1.95	0.48
1:A:744:ILE:O	1:A:746:MET:HG3	2.13	0.48
3:C:42:VAL:HG22	3:C:169:PHE:HB2	1.95	0.48
4:D:204:GLY:O	4:D:208:VAL:HG23	2.14	0.48
6:H:45:GLY:CA	6:H:113:LEU:HD22	2.44	0.48
4:K:461:MET:O	4:K:461:MET:SD	2.70	0.48
8:M:57:DA:N1	8:M:58:DT:N3	2.61	0.48
6:O:187:LYS:HE2	6:P:184:LEU:HD12	1.94	0.48
6:H:161:ARG:O	6:H:164:LYS:HG3	2.13	0.48
3:J:259:LEU:HD23	3:J:344:GLY:N	2.29	0.48
3:J:371:GLU:OE1	3:J:374:LEU:HD13	2.14	0.48
4:K:305:VAL:O	4:K:310:ILE:HD11	2.13	0.48
4:K:538:PRO:C	4:K:539:LEU:HD12	2.38	0.48
1:A:176:THR:HG23	3:C:99:PHE:HE1	1.79	0.48
5:F:49:VAL:HG21	5:F:97:LEU:HD23	1.96	0.48
6:P:117:GLU:C	6:P:119:PRO:HD2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASP:C	1:A:661:ASP:OD1	2.57	0.48
4:D:212:MET:HE1	4:D:224:ILE:CG1	2.44	0.48
6:G:104:VAL:HG21	2:I:71:ALA:CB	2.44	0.48
6:H:133:THR:O	6:H:137:ASN:ND2	2.47	0.48
8:M:59:DT:O2	8:M:59:DT:O4'	2.32	0.48
6:O:193:SER:O	6:O:197:LYS:HG2	2.12	0.48
1:X:771:LEU:O	1:X:774:LEU:HD23	2.12	0.48
1:A:690:VAL:HG13	3:J:290:ARG:NH1	2.28	0.47
3:J:90:THR:HG21	3:J:103:TYR:CE2	2.49	0.47
6:O:155:TRP:O	6:O:159:GLN:HG2	2.13	0.47
1:X:716:ASN:OD1	1:X:716:ASN:O	2.32	0.47
2:B:140:MET:HE2	2:I:210:PHE:CG	2.49	0.47
2:B:180:LYS:C	2:B:181:THR:CG2	2.85	0.47
3:C:356:LEU:HD11	3:C:412:ALA:HB1	1.96	0.47
6:G:198:LEU:HD22	6:H:198:LEU:HD21	1.95	0.47
7:L:17:DT:O2	7:L:18:DC:C5	2.67	0.47
1:A:14:VAL:HG23	1:A:145:ILE:HG12	1.95	0.47
4:D:457:LEU:CD2	4:D:533:ILE:HD11	2.44	0.47
2:I:44:VAL:O	2:I:125:LEU:HD23	2.15	0.47
2:I:50:ASP:OD1	2:I:53:VAL:HG23	2.15	0.47
3:J:90:THR:HG21	3:J:103:TYR:CD2	2.50	0.47
1:X:792:MET:HE2	1:X:792:MET:HA	1.96	0.47
1:A:279:MET:CB	1:A:332:MET:HE3	2.44	0.47
1:A:741:ARG:HD3	1:A:766:PHE:O	2.15	0.47
1:A:845:LEU:HD12	1:A:894:VAL:HG21	1.95	0.47
3:C:476:ASP:OD1	3:C:476:ASP:C	2.57	0.47
6:P:102:LYS:O	6:P:104:VAL:HG23	2.15	0.47
5:F:98:LEU:CD2	5:F:100:LEU:HD12	2.43	0.47
4:D:35:LYS:HE3	4:D:98:ILE:HG21	1.97	0.47
3:J:64:ILE:HA	3:J:67:ILE:HG22	1.96	0.47
4:K:118:ILE:HD13	4:K:159:ILE:HG21	1.95	0.47
4:K:130:ARG:HB3	4:K:159:ILE:HG22	1.96	0.47
4:K:435:PHE:O	4:K:436:SER:C	2.57	0.47
1:A:19:LEU:HD12	1:A:145:ILE:HD11	1.96	0.47
4:D:55:ALA:O	4:D:56:LEU:HD22	2.14	0.47
4:D:392:ILE:HG22	4:D:393:VAL:N	2.30	0.47
5:F:51:THR:OG1	5:F:97:LEU:HD21	2.14	0.47
2:I:23:LEU:HD23	2:I:24:LEU:H	1.80	0.47
2:I:216:ASP:OD2	2:I:217:LEU:N	2.48	0.47
3:C:454:ALA:HB1	4:D:379:SER:OG	2.14	0.47
5:F:110:VAL:HG12	5:F:127:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:332:LYS:HG3	4:K:333:TYR:H	1.80	0.47
3:C:50:GLU:O	3:C:52:GLN:HG3	2.15	0.47
3:C:73:SER:O	3:C:77:SER:HB3	2.15	0.47
3:J:277:VAL:CG2	4:K:357:MET:HE1	2.44	0.47
3:C:363:ARG:HG2	3:C:364:PRO:CD	2.44	0.47
5:E:49:VAL:O	5:E:53:ILE:HD12	2.15	0.47
6:O:124:ARG:HA	6:O:127:ILE:HD11	1.97	0.46
1:X:670:THR:HG21	1:X:675:LYS:HG3	1.97	0.46
3:C:443:LYS:O	3:C:444:ARG:C	2.57	0.46
7:L:22:DA:H1'	7:L:23:DG:C8	2.50	0.46
6:P:10:LEU:HD12	6:P:11:VAL:N	2.29	0.46
4:K:461:MET:O	4:K:462:SER:C	2.59	0.46
2:B:45:TRP:HB3	2:B:123:CYS:HB3	1.98	0.46
4:D:138:LEU:HD22	4:D:204:GLY:HA3	1.97	0.46
6:G:3:ARG:HH11	6:G:5:ILE:HD12	1.81	0.46
6:H:47:VAL:HG11	6:H:51:GLU:CB	2.42	0.46
3:J:205:LEU:HD12	3:J:206:LYS:N	2.30	0.46
3:J:256:LEU:HD11	8:M:64:DC:H4'	1.97	0.46
4:K:453:ALA:O	4:K:457:LEU:HD23	2.16	0.46
6:O:159:GLN:O	6:O:163:GLU:HG2	2.15	0.46
6:O:162:PHE:O	6:O:166:VAL:HG23	2.15	0.46
6:O:201:ALA:HB1	6:P:201:ALA:HB3	1.98	0.46
1:A:16:PHE:HZ	1:A:148:VAL:HG22	1.80	0.46
2:I:44:VAL:HG21	2:I:131:VAL:HG22	1.98	0.46
3:J:526:LYS:HA	3:J:530:TYR:HB2	1.97	0.46
4:K:16:VAL:HG11	4:K:58:LEU:HD13	1.96	0.46
6:O:148:ASN:ND2	6:P:144:LEU:HD11	2.31	0.46
8:Q:70:DC:H2'	8:Q:71:DT:H71	1.97	0.46
2:B:159:MET:HE1	2:I:181:THR:HG22	1.96	0.46
6:G:18:HIS:HB3	6:G:36:LEU:HD11	1.98	0.46
6:G:67:VAL:O	6:G:71:ARG:HG2	2.16	0.46
1:X:720:VAL:HG12	1:X:744:ILE:HD12	1.98	0.46
1:A:738:TRP:O	1:A:768:ASP:OD2	2.32	0.46
4:D:404:GLN:HB3	4:D:423:GLN:OE1	2.15	0.46
4:K:407:VAL:HG12	4:K:408:ALA:N	2.30	0.46
1:A:240:ILE:HG22	1:A:241:THR:N	2.31	0.46
3:C:40:PHE:CG	3:C:67:ILE:HD12	2.51	0.46
3:C:200:LEU:HD22	3:C:220:ILE:HG22	1.98	0.46
3:C:473:TYR:HB2	4:D:346:CYS:SG	2.56	0.46
6:O:191:ILE:HD13	6:P:191:ILE:HD11	1.97	0.46
6:P:44:THR:C	6:P:113:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:198:LEU:O	6:P:201:ALA:C	2.59	0.46
1:A:464:ILE:HD12	1:A:485:CYS:CB	2.46	0.46
4:D:390:VAL:CG2	4:D:407:VAL:HG13	2.46	0.46
3:J:105:LEU:HD23	3:J:105:LEU:C	2.41	0.46
3:J:288:LEU:HD23	4:K:313:GLY:HA3	1.98	0.46
3:J:403:ARG:HE	7:L:31:DG:H5'	1.81	0.46
3:C:356:LEU:HD11	3:C:412:ALA:CB	2.46	0.46
6:G:106:PHE:CD1	2:I:65:LEU:HD13	2.51	0.46
2:I:152:GLU:O	2:I:156:LEU:HG	2.16	0.46
3:J:170:THR:HG22	3:J:171:ASN:N	2.31	0.46
4:K:240:ILE:HD13	4:K:270:GLU:CD	2.40	0.46
4:K:536:LEU:O	4:K:536:LEU:HG	2.16	0.46
1:X:716:ASN:OD1	1:X:748:PRO:HD3	2.16	0.46
1:A:382:LEU:O	1:A:382:LEU:HD23	2.15	0.45
1:A:713:ILE:HD11	1:A:720:VAL:HG11	1.97	0.45
2:B:180:LYS:O	2:B:181:THR:CG2	2.64	0.45
4:D:38:ILE:HD12	4:D:94:ILE:HG12	1.98	0.45
4:D:80:HIS:HD2	4:D:90:LEU:HD11	1.81	0.45
6:G:151:LEU:C	6:G:151:LEU:HD23	2.41	0.45
2:I:93:ALA:HA	2:I:109:ARG:O	2.16	0.45
4:K:245:ILE:HB	8:M:73:DC:H1'	1.98	0.45
6:O:137:ASN:OD1	6:O:138:GLN:N	2.48	0.45
6:O:181:ILE:HG22	6:O:181:ILE:O	2.16	0.45
6:P:88:PHE:CE2	6:P:90:LYS:HA	2.50	0.45
1:A:85:LYS:HB2	7:N:43:DT:P	2.56	0.45
1:A:813:PHE:HB3	1:A:850:ALA:HB2	1.97	0.45
4:D:279:VAL:HG11	4:D:284:LEU:HA	1.99	0.45
4:K:245:ILE:HD13	8:M:73:DC:H1'	1.98	0.45
3:J:143:LEU:HD12	3:J:143:LEU:O	2.16	0.45
6:P:180:PHE:O	6:P:184:LEU:HD23	2.17	0.45
2:B:197:LYS:CE	2:I:152:GLU:OE2	2.65	0.45
3:C:185:ARG:HA	3:C:188:THR:HG22	1.99	0.45
3:C:363:ARG:O	3:C:364:PRO:C	2.58	0.45
4:D:109:ASP:OD1	4:D:109:ASP:C	2.59	0.45
5:F:100:LEU:HD13	5:F:104:PRO:HD3	1.98	0.45
2:B:194:MET:HA	2:B:198:LEU:HB2	1.99	0.45
6:H:166:VAL:O	6:H:169:LYS:HB3	2.16	0.45
4:K:56:LEU:HB2	4:K:80:HIS:HB2	1.98	0.45
4:K:457:LEU:HG	4:K:533:ILE:HD11	1.98	0.45
7:L:17:DT:O2	7:L:18:DC:C6	2.69	0.45
7:L:38:DG:C2	8:M:57:DA:H1'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HA	1:A:190:ILE:HG22	1.98	0.45
8:M:74:DA:H2'	8:M:75:DG:O5'	2.15	0.45
1:A:707:ILE:HD12	1:A:707:ILE:N	2.32	0.45
1:A:716:ASN:O	1:A:747:CYS:HB3	2.16	0.45
3:J:271:VAL:CG2	3:J:368:VAL:HG13	2.46	0.45
4:K:164:PHE:C	4:K:165:LEU:HD22	2.42	0.45
6:O:32:PHE:CE2	6:O:52:ILE:HD12	2.51	0.45
6:O:150:ARG:HA	6:O:153:ARG:CD	2.47	0.45
6:P:10:LEU:HD12	6:P:11:VAL:H	1.80	0.45
3:C:142:SER:O	3:C:146:VAL:HG23	2.16	0.45
3:C:329:LEU:HD23	3:C:333:GLU:OE2	2.17	0.45
1:A:64:PHE:CZ	1:A:68:MET:HE3	2.52	0.45
1:A:382:LEU:HD23	1:A:382:LEU:C	2.42	0.45
1:A:826:ILE:CG2	1:A:856:LEU:HD12	2.46	0.45
3:C:435:VAL:HG21	4:D:353:ARG:NH2	2.31	0.45
4:D:463:LEU:CD1	4:D:477:PHE:CE2	2.99	0.45
3:J:82:LEU:C	3:J:83:LEU:HD22	2.41	0.45
4:K:423:GLN:O	4:K:424:LEU:HD22	2.17	0.45
1:X:805:TRP:O	1:X:805:TRP:CD2	2.70	0.45
1:A:565:VAL:HG12	1:A:577:ARG:HH21	1.82	0.45
3:C:189:LYS:O	3:C:193:LEU:HD23	2.17	0.45
4:D:427:MET:SD	4:D:427:MET:C	3.00	0.45
6:H:150:ARG:HA	6:H:153:ARG:NE	2.32	0.45
6:O:161:ARG:HD2	6:O:161:ARG:C	2.42	0.45
2:B:174:LEU:HD12	2:B:180:LYS:HZ3	1.81	0.44
4:D:283:THR:O	4:D:284:LEU:HG	2.17	0.44
3:J:176:HIS:NE2	3:J:179:ASP:O	2.50	0.44
8:M:72:DC:H1'	8:M:73:DC:C4	2.52	0.44
6:O:118:ASN:C	6:O:118:ASN:HD22	2.25	0.44
6:O:159:GLN:HA	6:O:162:PHE:CD1	2.51	0.44
1:A:194:LEU:O	1:A:194:LEU:HD23	2.17	0.44
1:A:422:ILE:HD13	1:A:578:PHE:HD1	1.81	0.44
1:A:738:TRP:HA	1:A:740:PRO:HD2	1.99	0.44
3:C:72:ILE:O	3:C:75:ILE:HG22	2.17	0.44
4:D:68:LEU:O	4:D:74:TYR:HB2	2.17	0.44
2:I:177:ASP:O	2:I:177:ASP:OD2	2.35	0.44
3:J:514:MET:HE2	4:K:254:GLY:CA	2.48	0.44
1:X:723:PRO:O	1:X:727:LEU:HG	2.17	0.44
1:A:70:LEU:HD22	1:A:189:MET:CE	2.47	0.44
3:C:173:ASP:HB2	3:C:215:LEU:HD23	1.98	0.44
3:C:350:PHE:H	4:D:463:LEU:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:52:ILE:HG23	6:H:53:SER:N	2.32	0.44
1:X:837:ARG:NE	1:X:837:ARG:HA	2.32	0.44
2:B:29:ILE:HD13	2:B:34:TYR:HB2	2.00	0.44
3:C:200:LEU:HD23	3:C:201:ASP:N	2.32	0.44
3:C:512:GLU:HG2	3:C:513:ALA:N	2.33	0.44
3:J:366:LEU:CB	3:J:434:LEU:HD12	2.47	0.44
6:P:118:ASN:O	6:P:119:PRO:C	2.61	0.44
6:P:172:LEU:O	6:P:176:LEU:HG	2.17	0.44
1:A:16:PHE:CZ	1:A:148:VAL:HG13	2.52	0.44
3:C:41:LEU:HD21	3:C:146:VAL:HG11	1.99	0.44
3:C:481:PRO:HA	3:C:505:ASP:OD2	2.17	0.44
4:D:240:ILE:HG23	4:D:240:ILE:O	2.16	0.44
5:E:125:VAL:HG12	5:E:126:ASP:N	2.33	0.44
1:A:327:ILE:C	1:A:328:LEU:HD22	2.42	0.44
1:A:675:LYS:HB3	1:A:676:PRO:HD3	2.00	0.44
1:A:841:LYS:O	1:A:845:LEU:HD13	2.17	0.44
6:H:44:THR:O	6:H:113:LEU:HB3	2.17	0.44
2:I:62:ASN:HB3	2:I:65:LEU:CD2	2.47	0.44
2:I:93:ALA:CB	2:I:110:SER:HB3	2.47	0.44
3:J:39:ILE:CD1	3:J:84:ALA:HB3	2.48	0.44
3:J:77:SER:HA	3:J:249:LYS:HA	2.00	0.44
7:L:18:DC:C6	7:L:19:DT:C2	3.05	0.44
6:O:139:ALA:O	6:O:143:HIS:ND1	2.38	0.44
8:Q:79:DA:C2	8:Q:80:DC:C2	3.06	0.44
1:A:746:MET:HB2	1:A:750:THR:OG1	2.17	0.44
3:C:116:ILE:HG22	3:C:120:ASP:OD2	2.17	0.44
3:C:411:VAL:HG22	3:C:412:ALA:N	2.33	0.44
6:G:194:LEU:HD21	6:H:198:LEU:CD1	2.40	0.44
3:J:76:ILE:HG23	3:J:487:PHE:CE1	2.53	0.44
4:K:387:LEU:O	4:K:388:ASP:OD1	2.35	0.44
7:L:13:DG:H2'	7:L:14:DT:H72	1.99	0.44
7:L:19:DT:C2	7:L:20:DG:N7	2.86	0.44
7:L:20:DG:H1'	7:L:21:DG:C5'	2.48	0.44
1:A:660:GLU:O	1:A:661:ASP:OD1	2.36	0.44
3:C:102:ILE:HG21	3:C:149:VAL:HG11	2.00	0.44
4:D:311:ILE:HD11	4:D:324:SER:HA	1.99	0.44
4:D:387:LEU:O	4:D:389:MET:HG2	2.18	0.44
3:J:51:SER:O	3:J:52:GLN:C	2.61	0.44
6:P:122:VAL:HA	6:P:125:GLU:HG3	1.99	0.44
3:C:52:GLN:CD	3:C:52:GLN:O	2.61	0.44
3:C:204:HIS:CD2	3:C:233:PHE:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:144:LEU:HA	6:H:147:GLU:HG3	1.99	0.44
2:I:16:LEU:HD11	2:I:83:LEU:HD21	1.99	0.44
4:K:457:LEU:HD13	4:K:529:PRO:CB	2.48	0.44
1:A:19:LEU:HD12	1:A:145:ILE:CD1	2.48	0.43
1:A:198:VAL:HG23	1:A:201:GLN:HE21	1.83	0.43
4:D:35:LYS:HD3	4:D:38:ILE:HD11	1.99	0.43
6:G:1:MET:SD	6:G:1:MET:C	3.01	0.43
6:G:169:LYS:HA	6:G:172:LEU:HD23	2.00	0.43
7:N:28:DT:H2"	7:N:29:DG:C8	2.54	0.43
6:P:102:LYS:O	6:P:102:LYS:HG3	2.18	0.43
1:X:752:GLU:O	1:X:755:ALA:N	2.51	0.43
1:A:418:LEU:HA	1:A:429:ILE:HD11	1.99	0.43
3:C:287:LYS:C	3:C:288:LEU:HD22	2.43	0.43
6:G:104:VAL:CG1	2:I:67:ALA:HB2	2.48	0.43
3:J:49:PHE:O	3:J:60:PHE:CE2	2.70	0.43
3:J:87:PHE:HE2	3:J:105:LEU:HD13	1.82	0.43
3:J:394:VAL:O	3:J:394:VAL:HG13	2.18	0.43
4:K:240:ILE:CG1	4:K:241:GLU:N	2.81	0.43
4:K:259:ILE:HG22	4:K:373:ALA:HB1	1.98	0.43
6:P:117:GLU:C	6:P:119:PRO:CD	2.91	0.43
1:X:709:VAL:O	1:X:713:ILE:HG12	2.18	0.43
2:B:138:PRO:O	2:B:142:MET:HG3	2.18	0.43
4:D:407:VAL:HG23	4:D:424:LEU:CD2	2.48	0.43
4:K:519:PRO:O	4:K:522:VAL:HG12	2.18	0.43
7:L:36:DT:O2	8:M:58:DT:O4	2.36	0.43
1:A:690:VAL:HG12	1:A:692:ASN:O	2.19	0.43
4:D:409:PHE:O	4:D:419:LEU:HD12	2.18	0.43
6:H:174:THR:HG22	1:X:785:ASN:OD1	2.17	0.43
2:I:8:LEU:HA	2:I:11:GLN:HG2	2.01	0.43
6:P:162:PHE:CZ	6:P:166:VAL:HG21	2.54	0.43
1:A:364:TYR:HD2	1:A:400:ILE:HG13	1.84	0.43
2:B:216:ASP:OD1	2:B:217:LEU:N	2.52	0.43
4:D:210:MET:SD	4:D:210:MET:C	3.02	0.43
3:J:267:ILE:HD11	4:K:534:LYS:HG2	2.00	0.43
4:K:37:VAL:HG12	4:K:231:LEU:CD2	2.49	0.43
1:X:709:VAL:O	1:X:712:ILE:HG12	2.19	0.43
3:C:39:ILE:HG13	3:C:84:ALA:O	2.18	0.43
3:C:89:GLY:O	3:C:138:GLY:HA2	2.17	0.43
6:G:5:ILE:HA	6:G:20:LEU:O	2.18	0.43
3:J:176:HIS:NE2	3:J:183:ALA:HB2	2.34	0.43
3:J:301:ARG:HG2	4:K:292:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:479:GLU:HG3	4:K:427:MET:SD	2.59	0.43
4:K:37:VAL:HG12	4:K:231:LEU:HD23	2.01	0.43
4:K:393:VAL:HG12	4:K:394:ARG:N	2.33	0.43
8:M:70:DC:H2'	8:M:71:DT:H71	2.01	0.43
6:O:52:ILE:O	6:O:55:GLU:HB2	2.17	0.43
8:Q:80:DC:C2'	8:Q:81:DA:H5'	2.49	0.43
5:F:114:TRP:NE1	5:F:125:VAL:HG23	2.34	0.43
6:H:181:ILE:HG22	6:H:181:ILE:O	2.19	0.43
3:J:346:MET:HB3	3:J:348:MET:HE2	2.01	0.43
3:C:510:LYS:O	3:C:510:LYS:HG3	2.18	0.43
4:D:12:LEU:HD13	4:D:54:ILE:HD11	2.00	0.43
4:D:259:ILE:HD11	4:D:373:ALA:CA	2.49	0.43
4:D:478:PRO:C	4:D:480:THR:N	2.74	0.43
3:J:499:GLU:OE1	3:J:500:PRO:O	2.37	0.43
4:K:35:LYS:HA	4:K:38:ILE:HG22	2.00	0.43
4:K:245:ILE:O	8:M:74:DA:C2'	2.67	0.43
8:M:65:DA:H2'	8:M:66:DG:H8	1.82	0.43
6:O:48:SER:O	6:O:51:GLU:HG2	2.19	0.43
6:O:176:LEU:HD11	6:P:176:LEU:HD12	2.01	0.43
1:X:741:ARG:HD3	1:X:766:PHE:HB2	2.01	0.43
2:B:159:MET:HE1	2:I:181:THR:CG2	2.49	0.43
2:B:163:GLU:O	2:B:166:ASP:OD1	2.37	0.43
3:C:417:GLU:N	3:C:417:GLU:OE2	2.52	0.43
4:D:355:PHE:O	4:D:356:PHE:C	2.62	0.43
4:D:422:VAL:CG1	4:D:423:GLN:H	2.32	0.43
3:J:58:THR:CG2	3:J:60:PHE:CE2	3.01	0.43
4:K:432:GLN:O	4:K:432:GLN:HG2	2.19	0.43
1:A:728:GLU:O	1:A:732:THR:HG23	2.17	0.43
3:C:75:ILE:HD13	4:D:316:TYR:HE1	1.83	0.43
3:C:344:GLY:C	3:C:345:LEU:HD22	2.43	0.43
3:C:352:PRO:HG2	4:D:473:LEU:HD22	2.01	0.43
4:D:38:ILE:HG22	4:D:135:PHE:CE2	2.52	0.43
4:D:281:ALA:O	4:D:282:LYS:HG2	2.18	0.43
6:O:191:ILE:CD1	6:P:191:ILE:HD11	2.49	0.43
1:X:710:LYS:NZ	1:X:714:LEU:HD21	2.34	0.43
1:A:820:LEU:CD1	1:A:842:ALA:HB2	2.49	0.42
2:B:43:GLN:HB2	2:B:45:TRP:CH2	2.54	0.42
6:G:3:ARG:NH1	6:G:5:ILE:HD12	2.34	0.42
8:M:55:DC:OP2	8:M:56:DG:N7	2.52	0.42
7:N:13:DG:C4	8:Q:81:DA:C6	3.07	0.42
7:N:27:DC:H2'	7:N:28:DT:H71	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:HD13	1:A:443:ARG:CZ	2.48	0.42
1:A:665:CYS:HA	1:A:690:VAL:O	2.18	0.42
1:A:739:GLN:HG3	1:A:743:MET:HE3	2.01	0.42
4:K:528:ILE:HB	4:K:529:PRO:HD3	2.00	0.42
6:O:55:GLU:HB3	6:O:66:TYR:CE2	2.54	0.42
6:P:44:THR:O	6:P:113:LEU:HD12	2.18	0.42
6:P:122:VAL:O	6:P:125:GLU:HG3	2.18	0.42
9:U:184:SER:HB3	9:U:192:SER:HA	2.01	0.42
1:X:723:PRO:O	1:X:724:ALA:C	2.63	0.42
1:X:838:LEU:HD21	1:X:866:GLY:HA3	2.01	0.42
1:A:31:GLY:O	1:A:32:ARG:C	2.61	0.42
1:A:840:ILE:HD12	6:P:161:ARG:NH1	2.34	0.42
3:C:116:ILE:HG21	3:C:495:LEU:CD1	2.40	0.42
6:G:119:PRO:HA	6:G:122:VAL:HG22	2.01	0.42
6:G:155:TRP:NE1	6:H:158:VAL:HG21	2.34	0.42
3:J:116:ILE:HG21	3:J:495:LEU:HD22	2.01	0.42
8:M:55:DC:H3'	8:M:56:DG:C4'	2.49	0.42
1:X:888:ILE:O	1:X:888:ILE:HG23	2.20	0.42
1:A:273:LYS:HA	1:A:430:MET:SD	2.59	0.42
1:A:422:ILE:HD13	1:A:578:PHE:CD1	2.54	0.42
4:D:266:SER:O	4:D:267:ILE:CG1	2.67	0.42
4:D:431:ARG:HG3	4:D:431:ARG:O	2.19	0.42
6:H:63:LYS:HA	6:H:66:TYR:HB3	2.01	0.42
3:J:54:GLU:HB3	3:J:56:GLU:OE1	2.19	0.42
4:K:41:PHE:CD1	4:K:41:PHE:C	2.97	0.42
4:K:356:PHE:CE2	4:K:422:VAL:HG21	2.55	0.42
7:L:29:DG:C8	7:L:30:DT:H72	2.54	0.42
7:N:41:DG:C2	8:Q:53:DA:C2	3.07	0.42
6:O:10:LEU:HD13	6:O:88:PHE:CD1	2.55	0.42
5:E:49:VAL:HG21	5:E:85:VAL:HG22	2.02	0.42
6:H:154:ASP:O	6:H:158:VAL:HG23	2.19	0.42
3:J:489:ASN:ND2	4:K:331:MET:HE2	2.34	0.42
4:K:430:LEU:HD11	9:U:193:LYS:NZ	2.35	0.42
6:P:95:PHE:CZ	6:P:111:PHE:HD2	2.38	0.42
2:B:119:TRP:CD1	2:B:121:PHE:CE1	3.07	0.42
3:C:68:GLN:O	3:C:72:ILE:HG12	2.19	0.42
3:C:264:ASN:ND2	4:D:530:LEU:HD12	2.34	0.42
3:C:521:LEU:HA	3:C:524:GLU:OE1	2.20	0.42
4:D:147:LEU:HD22	4:D:211:VAL:CG2	2.50	0.42
2:I:299:SER:O	4:K:41:PHE:HA	2.19	0.42
3:J:56:GLU:HG2	3:J:57:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:251:LEU:CD2	4:K:377:LEU:HD21	2.49	0.42
8:M:55:DC:H3'	8:M:56:DG:O4'	2.18	0.42
1:A:75:LEU:HD23	1:A:215:HIS:NE2	2.35	0.42
4:D:13:CYS:SG	4:D:57:VAL:HG12	2.60	0.42
5:F:53:ILE:N	5:F:53:ILE:HD12	2.34	0.42
5:F:98:LEU:HD12	5:F:98:LEU:O	2.19	0.42
3:J:456:PRO:HA	3:J:459:VAL:HG12	2.01	0.42
6:O:150:ARG:HA	6:O:153:ARG:NE	2.34	0.42
2:B:188:SER:O	2:B:191:GLU:HG3	2.19	0.42
4:D:359:ASN:OD1	4:D:359:ASN:C	2.63	0.42
3:J:202:LEU:HD12	3:J:203:MET:H	1.84	0.42
3:J:383:SER:CB	4:K:438:LEU:HD12	2.49	0.42
4:K:252:THR:OG1	4:K:341:SER:HA	2.20	0.42
6:P:118:ASN:O	6:P:118:ASN:OD1	2.38	0.42
6:G:177:TYR:N	6:G:177:TYR:CD1	2.86	0.42
6:G:181:ILE:HD13	1:X:771:LEU:HA	2.02	0.42
3:J:261:LEU:HD13	3:J:345:LEU:CB	2.49	0.42
4:K:209:LYS:O	4:K:213:ILE:HD12	2.19	0.42
1:X:667:MET:HE2	1:X:702:ALA:HB2	2.02	0.42
1:A:176:THR:HG23	3:C:99:PHE:CE1	2.55	0.42
2:B:180:LYS:HG3	2:B:181:THR:H	1.83	0.42
3:C:66:CYS:O	3:C:70:VAL:HG12	2.19	0.42
3:C:277:VAL:HG21	4:D:357:MET:HG3	2.02	0.42
5:F:40:TRP:CZ3	5:F:41:LEU:HD21	2.54	0.42
6:G:61:MET:HB2	2:I:116:PRO:HG2	2.02	0.42
2:I:294:PRO:HB3	2:I:298:PHE:HB3	2.02	0.42
2:I:297:LEU:CD1	4:K:56:LEU:HD11	2.50	0.42
3:J:411:VAL:HG22	3:J:412:ALA:N	2.34	0.42
3:J:512:GLU:HG2	3:J:513:ALA:N	2.34	0.42
4:K:240:ILE:CG1	4:K:241:GLU:H	2.33	0.42
6:P:176:LEU:HD22	6:P:179:ARG:NH2	2.35	0.42
1:X:814:ARG:HA	1:X:849:GLY:O	2.20	0.42
1:A:68:MET:HA	1:A:71:ILE:HG22	2.01	0.41
1:A:869:HIS:O	1:A:872:VAL:HG22	2.20	0.41
3:C:152:ASN:C	3:C:152:ASN:HD22	2.26	0.41
3:C:350:PHE:N	4:D:463:LEU:HB2	2.35	0.41
3:C:483:LEU:HD11	3:C:487:PHE:CE2	2.55	0.41
4:D:118:ILE:HD13	4:D:159:ILE:CD1	2.50	0.41
6:G:160:GLY:O	6:G:163:GLU:HG3	2.20	0.41
4:K:43:GLN:OE1	4:K:495:LEU:HD11	2.19	0.41
4:K:234:LEU:O	4:K:235:CYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:251:LEU:C	4:K:251:LEU:HD12	2.45	0.41
7:L:34:DA:N6	8:M:56:DG:H3'	2.36	0.41
7:L:37:DC:O2	7:L:37:DC:C2'	2.68	0.41
6:P:123:ILE:O	6:P:126:LEU:HG	2.20	0.41
1:X:670:THR:HG21	1:X:675:LYS:CG	2.50	0.41
1:X:882:PHE:HD2	1:X:884:ARG:O	2.02	0.41
1:A:262:ASP:C	1:A:263:MET:HE2	2.46	0.41
1:A:563:GLU:CB	1:A:577:ARG:NH1	2.82	0.41
1:A:766:PHE:CZ	1:A:768:ASP:HA	2.55	0.41
1:A:785:ASN:OD1	1:A:789:PRO:HB2	2.19	0.41
3:C:304:ASN:N	3:C:311:LEU:HD23	2.35	0.41
3:C:509:PRO:HA	4:D:343:LEU:CD2	2.50	0.41
6:G:198:LEU:HD13	6:H:198:LEU:CD2	2.46	0.41
6:H:127:ILE:O	6:H:131:LEU:HD23	2.20	0.41
3:J:337:LEU:HD12	3:J:338:LYS:HD3	2.02	0.41
3:J:510:LYS:O	3:J:514:MET:HG3	2.20	0.41
4:K:526:SER:O	4:K:530:LEU:HG	2.20	0.41
3:C:39:ILE:HG23	3:C:39:ILE:O	2.20	0.41
3:C:50:GLU:O	3:C:50:GLU:OE1	2.38	0.41
4:D:508:ILE:HD12	4:D:508:ILE:H	1.85	0.41
4:K:270:GLU:CD	4:K:271:ARG:N	2.78	0.41
6:O:45:GLY:HA3	6:O:113:LEU:HA	2.00	0.41
6:O:127:ILE:HD12	6:P:19:PHE:HE2	1.82	0.41
4:D:253:ILE:HD13	4:D:342:VAL:HG12	2.02	0.41
4:D:407:VAL:CG1	4:D:408:ALA:N	2.83	0.41
6:G:172:LEU:HD13	6:G:176:LEU:HD11	2.02	0.41
2:I:10:MET:CE	2:I:226:VAL:HG21	2.50	0.41
2:I:137:ARG:N	2:I:138:PRO:HD2	2.35	0.41
3:J:286:ILE:HD12	4:K:315:ARG:HG2	2.03	0.41
3:J:353:LEU:HD11	3:J:414:VAL:HG13	2.02	0.41
4:K:40:MET:HE1	4:K:44:ARG:CD	2.51	0.41
4:K:41:PHE:CZ	4:K:45:GLN:HG3	2.55	0.41
4:K:58:LEU:HD11	4:K:80:HIS:NE2	2.35	0.41
7:L:22:DA:H2''	7:L:23:DG:O5'	2.20	0.41
1:A:198:VAL:HG22	1:A:202:THR:OG1	2.20	0.41
2:B:170:SER:CB	2:I:167:TYR:OH	2.68	0.41
3:C:188:THR:HG23	3:C:189:LYS:N	2.35	0.41
3:C:472:THR:O	3:C:472:THR:HG23	2.20	0.41
5:F:113:ALA:HB3	5:F:130:PHE:CE1	2.55	0.41
2:I:2:GLU:HG2	2:I:3:GLU:N	2.35	0.41
2:I:138:PRO:O	2:I:142:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:44:ALA:HB3	3:J:88:TYR:O	2.20	0.41
3:J:446:MET:HE1	3:J:448:PHE:HA	2.03	0.41
8:M:66:DG:H2''	8:M:67:DA:C8	2.55	0.41
6:O:44:THR:HG22	6:O:45:GLY:N	2.36	0.41
6:O:161:ARG:O	6:O:164:LYS:HG2	2.21	0.41
1:X:865:ILE:CG1	1:X:888:ILE:HD11	2.51	0.41
2:B:178:ARG:HG3	2:B:179:LEU:H	1.86	0.41
3:C:51:SER:O	3:C:52:GLN:C	2.63	0.41
4:D:461:MET:HG3	4:D:522:VAL:HG22	2.02	0.41
6:H:179:ARG:CZ	1:X:792:MET:HE3	2.51	0.41
3:J:358:LYS:HG3	4:K:353:ARG:NE	2.35	0.41
3:J:446:MET:SD	3:J:446:MET:C	3.04	0.41
3:J:478:PHE:HZ	4:K:343:LEU:HD22	1.84	0.41
4:K:337:GLY:HA2	4:K:398:ASP:OD2	2.21	0.41
6:O:26:LYS:O	6:O:27:THR:HG23	2.21	0.41
6:P:187:LYS:O	6:P:191:ILE:HG12	2.20	0.41
1:A:31:GLY:O	1:A:35:LYS:HG2	2.20	0.41
3:J:349:GLY:CA	4:K:461:MET:HE1	2.50	0.41
4:K:43:GLN:CD	4:K:495:LEU:HD11	2.46	0.41
8:M:59:DT:O2	8:M:59:DT:O5'	2.38	0.41
7:N:25:DC:H2'	7:N:26:DT:H72	2.03	0.41
6:O:30:SER:C	6:O:49:GLU:HG3	2.45	0.41
6:O:126:LEU:HD12	6:O:127:ILE:HG23	2.03	0.41
6:O:145:GLN:HA	6:O:148:ASN:HD21	1.85	0.41
1:X:716:ASN:O	1:X:747:CYS:HB3	2.21	0.41
2:B:2:GLU:HG2	2:B:3:GLU:N	2.36	0.41
4:D:115:MET:HE1	4:D:159:ILE:HD13	2.01	0.41
6:G:148:ASN:ND2	6:H:148:ASN:HB3	2.36	0.41
4:K:31:PHE:CE2	4:K:100:PRO:HG3	2.56	0.41
7:L:16:DG:H2'	7:L:17:DT:C6	2.55	0.41
7:L:20:DG:H1'	7:L:21:DG:H5''	2.02	0.41
7:N:29:DG:C2'	7:N:30:DT:H72	2.51	0.41
1:X:725:TRP:CD1	1:X:725:TRP:C	2.98	0.41
1:X:748:PRO:O	1:X:749:SER:C	2.62	0.41
1:A:16:PHE:CZ	1:A:148:VAL:CG1	3.04	0.41
1:A:336:ASN:HB2	1:A:343:MET:SD	2.61	0.41
1:A:721:VAL:HG12	1:A:722:LYS:N	2.36	0.41
2:B:61:LEU:HD22	2:B:119:TRP:HA	2.02	0.41
3:C:471:PHE:CD1	3:C:471:PHE:C	2.99	0.41
3:C:522:VAL:HG21	4:D:256:ASN:HB2	2.03	0.41
4:D:538:PRO:C	4:D:539:LEU:HD22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:121:GLU:HG3	5:F:123:ARG:HB2	2.02	0.41
6:G:4:LYS:HD2	6:G:5:ILE:N	2.36	0.41
6:G:5:ILE:HG21	6:G:126:LEU:HD11	2.03	0.41
6:G:20:LEU:HD11	6:G:34:ILE:HD11	2.02	0.41
6:G:47:VAL:HG13	6:G:51:GLU:OE1	2.20	0.41
6:G:52:ILE:HG22	6:G:63:LYS:HE3	2.03	0.41
6:G:194:LEU:C	6:G:194:LEU:HD23	2.45	0.41
2:I:2:GLU:HA	2:I:5:GLU:OE1	2.21	0.41
2:I:62:ASN:HD21	2:I:118:TYR:H	1.67	0.41
3:J:30:TYR:CD1	3:J:31:LYS:N	2.89	0.41
3:J:263:LEU:HD22	3:J:347:LEU:CD2	2.51	0.41
3:J:360:HIS:HB3	3:J:438:PRO:HG3	2.02	0.41
3:J:497:LEU:O	3:J:498:MET:C	2.64	0.41
4:K:12:LEU:HD23	4:K:56:LEU:CD1	2.50	0.41
4:K:81:ARG:CD	4:K:84:MET:HE2	2.50	0.41
4:K:94:ILE:HG23	4:K:95:GLU:N	2.36	0.41
4:K:246:HIS:O	8:M:73:DC:C2'	2.69	0.41
4:K:266:SER:O	4:K:267:ILE:CG1	2.67	0.41
4:K:289:ILE:HG22	4:K:290:GLN:N	2.35	0.41
6:O:31:GLY:CA	6:O:48:SER:HA	2.50	0.41
6:O:162:PHE:CD2	6:O:162:PHE:C	2.99	0.41
6:O:172:LEU:O	6:O:176:LEU:CD2	2.68	0.41
6:P:88:PHE:HZ	6:P:113:LEU:HD23	1.85	0.41
6:P:116:VAL:HG23	6:P:119:PRO:HD3	2.03	0.41
6:P:119:PRO:HA	6:P:122:VAL:CG2	2.51	0.41
6:P:162:PHE:O	6:P:166:VAL:HG23	2.20	0.41
1:X:746:MET:HB3	1:X:750:THR:HG21	2.03	0.41
1:A:343:MET:HA	1:A:511:THR:O	2.21	0.41
3:C:456:PRO:HA	3:C:459:VAL:HG12	2.02	0.41
4:D:35:LYS:NZ	4:D:98:ILE:HG21	2.36	0.41
4:D:372:ALA:O	4:D:375:VAL:HG12	2.21	0.41
2:I:26:LYS:O	2:I:36:LEU:HD12	2.20	0.41
3:J:345:LEU:HD13	3:J:399:ARG:O	2.21	0.41
3:J:368:VAL:HG22	3:J:434:LEU:HD11	2.02	0.41
4:K:240:ILE:HG12	4:K:241:GLU:H	1.85	0.41
7:L:35:DA:C8	7:L:36:DT:N3	2.89	0.41
7:N:16:DG:H2''	7:N:17:DT:H72	2.02	0.41
6:O:13:GLU:O	6:O:13:GLU:HG2	2.20	0.41
1:A:194:LEU:HD23	1:A:194:LEU:C	2.47	0.40
1:A:666:VAL:HG22	1:A:675:LYS:HZ3	1.86	0.40
2:B:140:MET:HG2	2:I:204:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:466:VAL:HG23	4:D:345:PHE:CG	2.56	0.40
4:D:266:SER:OG	4:D:363:LYS:HD3	2.22	0.40
4:D:390:VAL:HG22	4:D:391:ALA:H	1.86	0.40
6:G:78:ALA:HB2	6:G:84:TYR:CE2	2.57	0.40
3:J:113:ALA:HA	3:J:116:ILE:HD12	2.02	0.40
3:J:448:PHE:O	3:J:449:THR:HG23	2.21	0.40
4:K:23:SER:OG	4:K:29:SER:HA	2.21	0.40
4:K:244:SER:OG	7:L:22:DA:H4'	2.21	0.40
4:K:294:VAL:O	4:K:294:VAL:HG13	2.22	0.40
6:O:63:LYS:O	6:O:63:LYS:HD3	2.21	0.40
6:O:131:LEU:HD11	6:P:19:PHE:CE1	2.56	0.40
6:O:188:LYS:O	6:O:192:ARG:HD2	2.22	0.40
1:X:770:ASP:CG	1:X:771:LEU:N	2.79	0.40
1:A:86:GLU:OE2	1:A:86:GLU:N	2.52	0.40
1:A:224:VAL:CG1	1:A:228:LEU:HD12	2.49	0.40
2:B:160:LYS:HA	2:B:163:GLU:OE1	2.20	0.40
2:B:188:SER:HA	2:B:191:GLU:HG3	2.03	0.40
3:C:89:GLY:HA2	3:C:141:TYR:HB3	2.03	0.40
3:C:501:GLU:N	3:C:501:GLU:OE1	2.54	0.40
4:D:150:ILE:O	4:D:154:LEU:HD13	2.20	0.40
4:D:408:ALA:HA	4:D:420:VAL:O	2.21	0.40
6:G:181:ILE:HG21	1:X:769:THR:O	2.21	0.40
4:K:150:ILE:O	4:K:154:LEU:HD13	2.22	0.40
4:K:244:SER:O	8:M:74:DA:H2'	2.21	0.40
4:K:278:VAL:HG12	4:K:279:VAL:N	2.36	0.40
7:L:20:DG:C2	7:L:21:DG:O4'	2.74	0.40
7:N:35:DA:C2'	7:N:36:DT:H72	2.50	0.40
1:A:128:ILE:O	1:A:132:VAL:HG23	2.21	0.40
1:A:788:THR:N	1:A:789:PRO:HD3	2.36	0.40
3:C:106:GLN:NE2	3:C:119:LEU:HD21	2.35	0.40
3:C:511:VAL:HA	3:C:514:MET:HE3	2.04	0.40
4:D:44:ARG:NH1	4:D:234:LEU:HD23	2.37	0.40
4:D:79:VAL:HG11	4:D:82:HIS:NE2	2.36	0.40
4:D:283:THR:O	4:D:285:LYS:HD3	2.22	0.40
5:F:53:ILE:HD11	5:F:86:ASP:N	2.35	0.40
6:H:4:LYS:O	6:H:22:VAL:HG12	2.20	0.40
2:I:297:LEU:HB2	4:K:12:LEU:HD22	2.04	0.40
4:K:240:ILE:CD1	4:K:270:GLU:OE1	2.70	0.40
4:K:270:GLU:OE2	4:K:271:ARG:O	2.38	0.40
1:X:675:LYS:CB	1:X:676:PRO:HD3	2.51	0.40
3:C:157:VAL:HG22	3:C:159:PHE:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:75:LEU:HG	6:G:75:LEU:O	2.21	0.40
6:G:149:GLU:O	6:G:152:LEU:HG	2.21	0.40
4:K:9:ALA:HB2	4:K:127:PHE:CE1	2.56	0.40
4:K:11:VAL:HG23	4:K:55:ALA:HB3	2.03	0.40
1:X:847:PHE:CD1	1:X:847:PHE:N	2.86	0.40
1:A:187:ILE:HG13	1:A:188:ARG:N	2.36	0.40
1:A:343:MET:SD	1:A:343:MET:N	2.95	0.40
1:A:424:LYS:O	1:A:425:ARG:HB2	2.22	0.40
2:B:210:PHE:HD1	2:B:214:LEU:HD12	1.87	0.40
3:C:97:VAL:O	3:C:99:PHE:CD1	2.75	0.40
4:D:36:LYS:HZ2	4:D:231:LEU:HD21	1.85	0.40
6:G:71:ARG:O	6:G:75:LEU:HB3	2.21	0.40
6:G:197:LYS:O	6:G:200:ASN:HB3	2.22	0.40
3:J:262:LYS:HG2	3:J:346:MET:HE1	2.03	0.40
3:J:287:LYS:CD	3:J:296:VAL:HG21	2.50	0.40
4:K:16:VAL:O	4:K:101:GLY:HA3	2.21	0.40
4:K:41:PHE:O	4:K:42:VAL:C	2.65	0.40
7:L:34:DA:N3	8:M:60:DG:N1	2.69	0.40
8:Q:79:DA:H2''	8:Q:80:DC:C6	2.57	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	A	800/911 (88%)	741 (93%)	59 (7%)	0	100	100
1	X	250/911 (27%)	224 (90%)	26 (10%)	0	100	100
2	B	233/299 (78%)	216 (93%)	17 (7%)	0	100	100
2	I	233/299 (78%)	227 (97%)	6 (3%)	0	100	100
3	C	493/600 (82%)	443 (90%)	50 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	503/600 (84%)	458 (91%)	45 (9%)	0	100	100
4	D	507/732 (69%)	460 (91%)	47 (9%)	0	100	100
4	K	507/732 (69%)	453 (89%)	54 (11%)	0	100	100
5	E	107/575 (19%)	105 (98%)	2 (2%)	0	100	100
5	F	107/575 (19%)	100 (94%)	7 (6%)	0	100	100
6	G	199/336 (59%)	194 (98%)	5 (2%)	0	100	100
6	H	191/336 (57%)	171 (90%)	19 (10%)	1 (0%)	24	63
6	O	191/336 (57%)	178 (93%)	13 (7%)	0	100	100
6	P	199/336 (59%)	191 (96%)	8 (4%)	0	100	100
9	T	21/204 (10%)	19 (90%)	2 (10%)	0	100	100
9	U	21/204 (10%)	19 (90%)	2 (10%)	0	100	100
All	All	4562/7986 (57%)	4199 (92%)	362 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	H	178	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/808 (74%)	602 (100%)	0	100	100
1	X	230/808 (28%)	230 (100%)	0	100	100
2	B	209/262 (80%)	209 (100%)	0	100	100
2	I	209/262 (80%)	209 (100%)	0	100	100
3	C	452/540 (84%)	452 (100%)	0	100	100
3	J	462/540 (86%)	462 (100%)	0	100	100
4	D	463/649 (71%)	463 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	K	463/649 (71%)	463 (100%)	0	100	100
5	E	92/480 (19%)	92 (100%)	0	100	100
5	F	92/480 (19%)	92 (100%)	0	100	100
6	G	180/303 (59%)	180 (100%)	0	100	100
6	H	178/303 (59%)	178 (100%)	0	100	100
6	O	178/303 (59%)	178 (100%)	0	100	100
6	P	180/303 (59%)	180 (100%)	0	100	100
9	T	18/160 (11%)	18 (100%)	0	100	100
9	U	18/160 (11%)	18 (100%)	0	100	100
All	All	4026/7010 (57%)	4026 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	691	GLN
2	B	62	ASN
3	C	360	HIS
3	C	489	ASN
4	D	33	GLN
4	D	43	GLN
4	D	131	HIS
4	D	146	GLN
4	D	256	ASN
5	F	68	HIS
5	F	82	HIS
5	F	108	GLN
6	G	18	HIS
6	H	40	HIS
6	H	185	ASN
6	H	200	ASN
3	J	137	HIS
3	J	416	GLN
3	J	426	GLN
3	J	489	ASN
4	K	76	ASN
4	K	146	GLN

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Mol	Chain	Res	Type
4	K	246	HIS
4	K	402	ASN
6	O	118	ASN
6	P	138	GLN
6	P	195	HIS
6	P	196	ASN
6	P	200	ASN
1	X	739	GLN
1	X	816	HIS
1	X	904	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

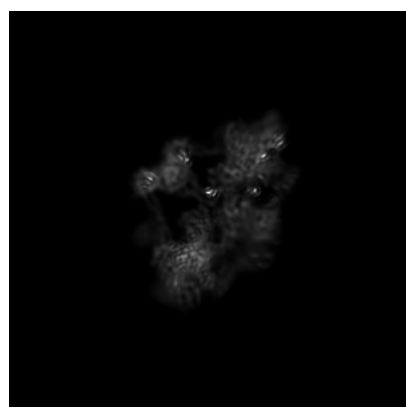
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70960. These allow visual inspection of the internal detail of the map and identification of artifacts.

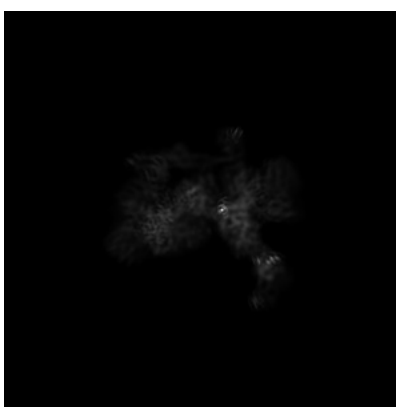
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

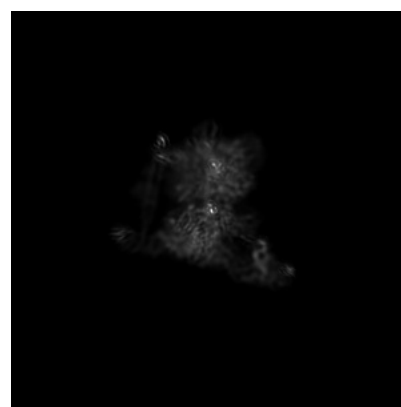
6.1.1 Primary map



X



Y

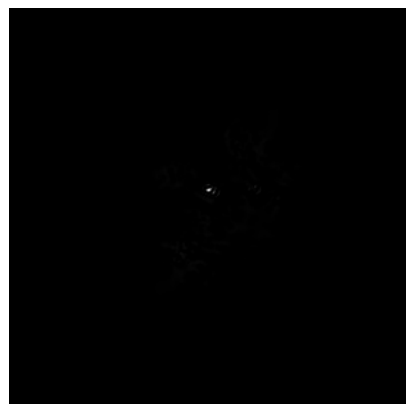


Z

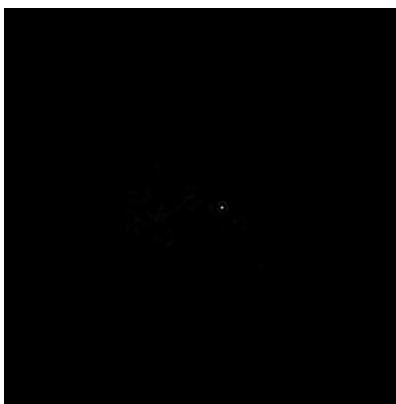
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

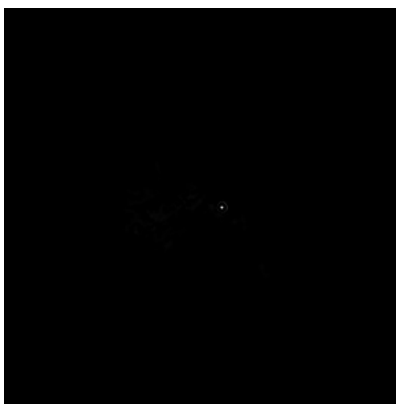
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

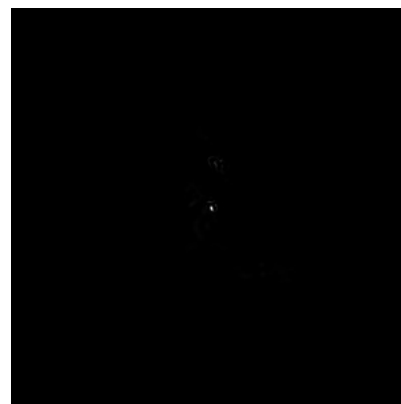
6.3.1 Primary map



X Index: 208



Y Index: 207

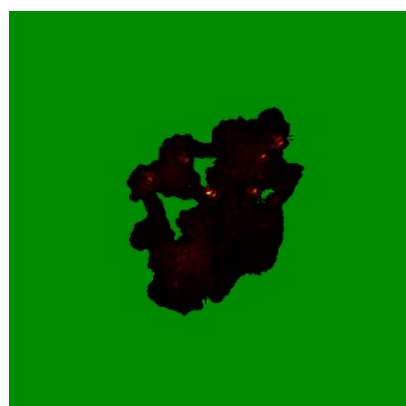


Z Index: 226

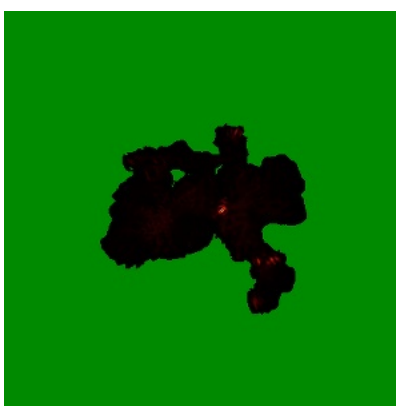
The images above show the largest variance slices of the map in three orthogonal directions.

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

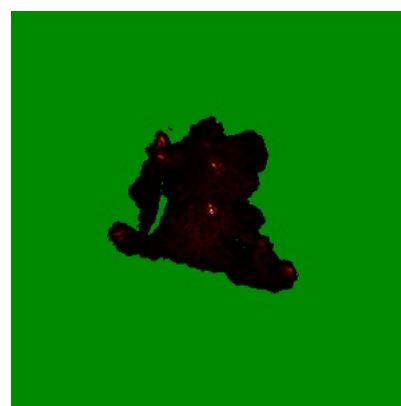
6.4.1 Primary map



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

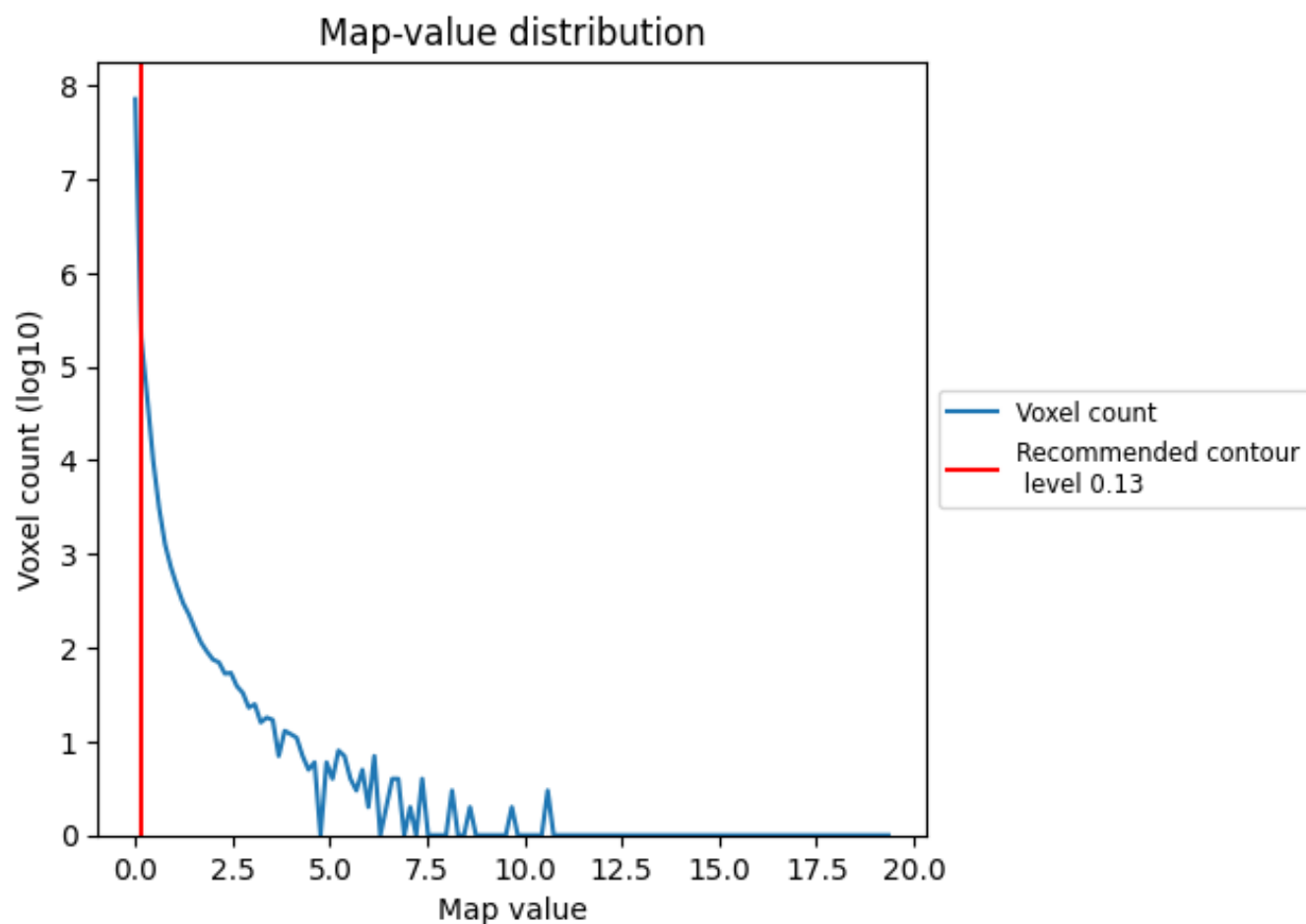
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

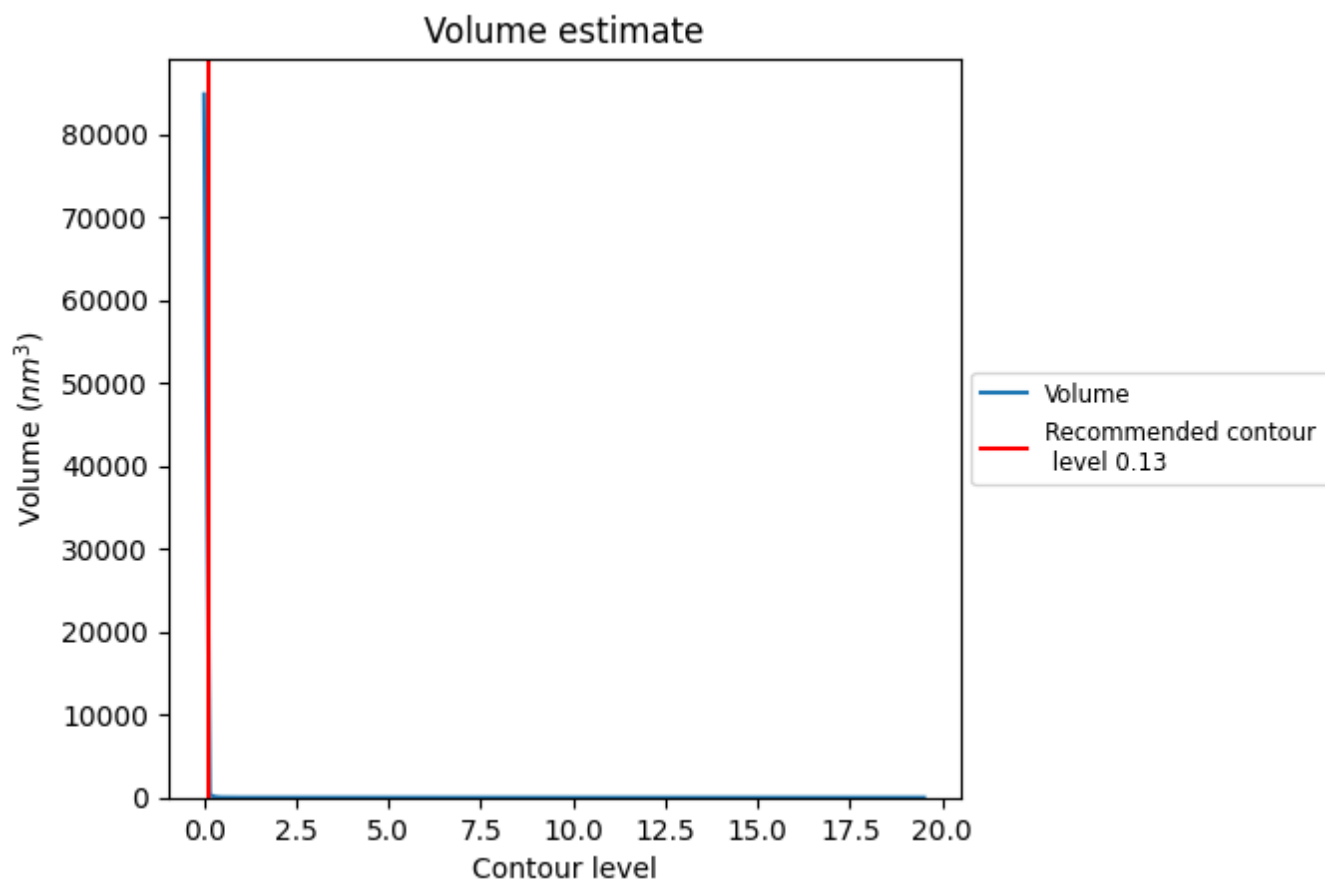
This section contains the results of statistical analysis of the map.

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.

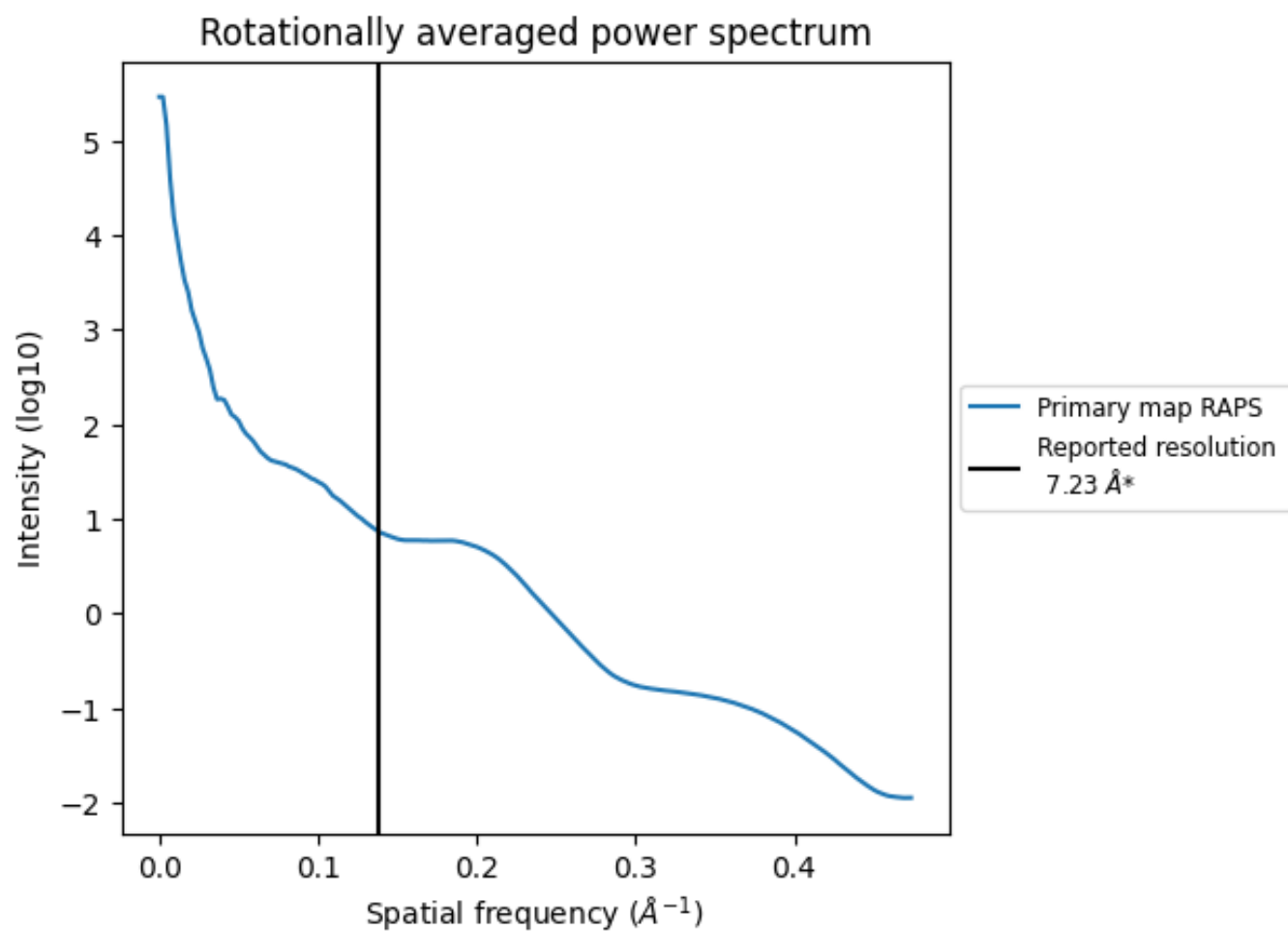
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 12730 nm^3 ; this corresponds to an approximate mass of 11499 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 0.138 Å⁻¹

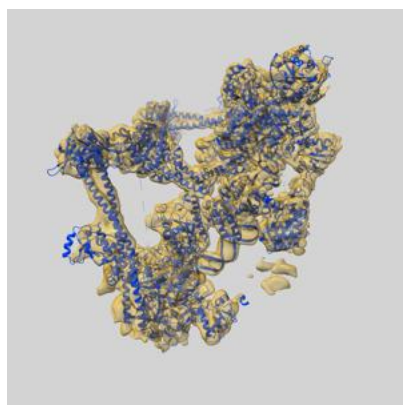
8 Fourier-Shell correlation ⓘ

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

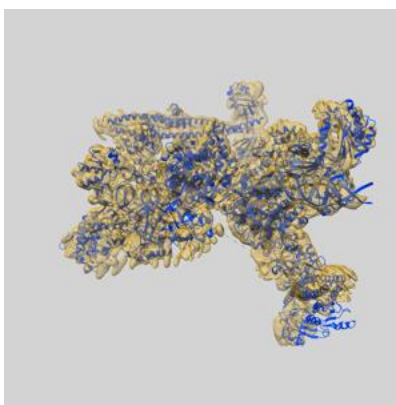
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70960 and PDB model 9OX8. Per-residue inclusion information can be found in section [3](#) on page [6](#).

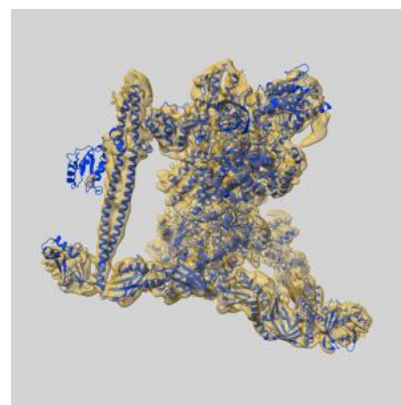
9.1 Map-model overlay [i](#)



X



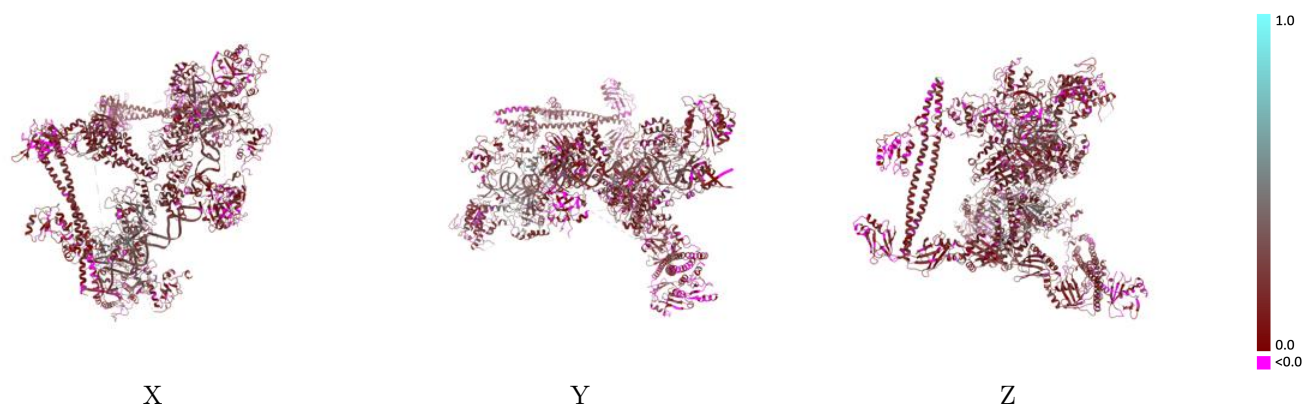
Y



Z

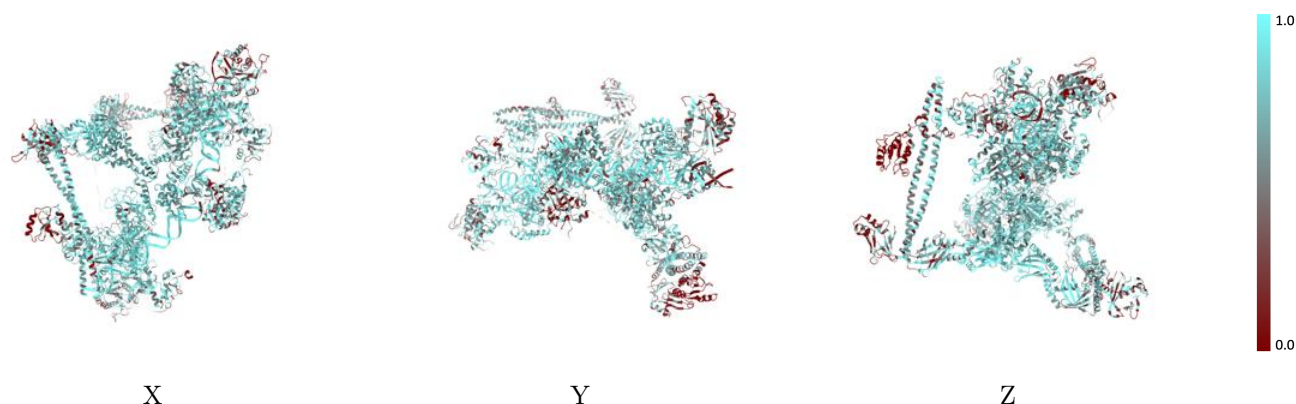
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



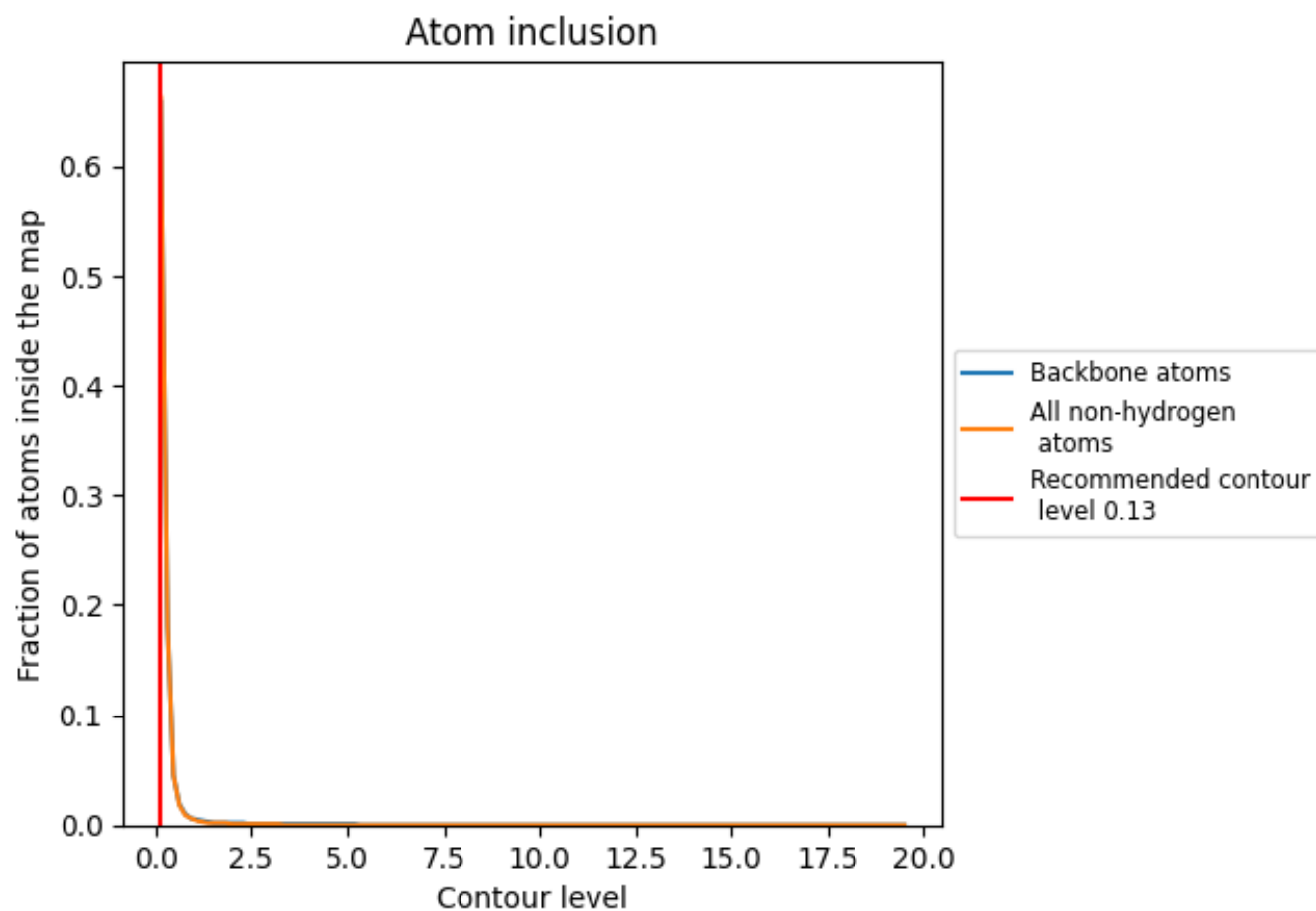
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6620	 0.1940
A	 0.5430	 0.1310
B	 0.7790	 0.1920
C	 0.8190	 0.3080
D	 0.6990	 0.2330
E	 0.5760	 0.1710
F	 0.5770	 0.1570
G	 0.7070	 0.1530
H	 0.5710	 0.1060
I	 0.7790	 0.1860
J	 0.7240	 0.2160
K	 0.6120	 0.1990
L	 0.7940	 0.2460
M	 0.7410	 0.2330
N	 0.9250	 0.2860
O	 0.4750	 0.0930
P	 0.6460	 0.1580
Q	 0.9350	 0.3040
T	 0.4400	 0.2790
U	 0.1810	 0.1470
X	 0.5550	 0.1750

