



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:11 AM UTC

PDB ID : 7KHC / pdb_00007khc
EMDB ID : EMD-21879
Title : Escherichia coli RNA polymerase and rrnBP1 promoter closed complex
Authors : Shin, Y.; Qayyum, M.Z.; Murakami, K.S.
Deposited on : 2020-10-20
Resolution : 4.14 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

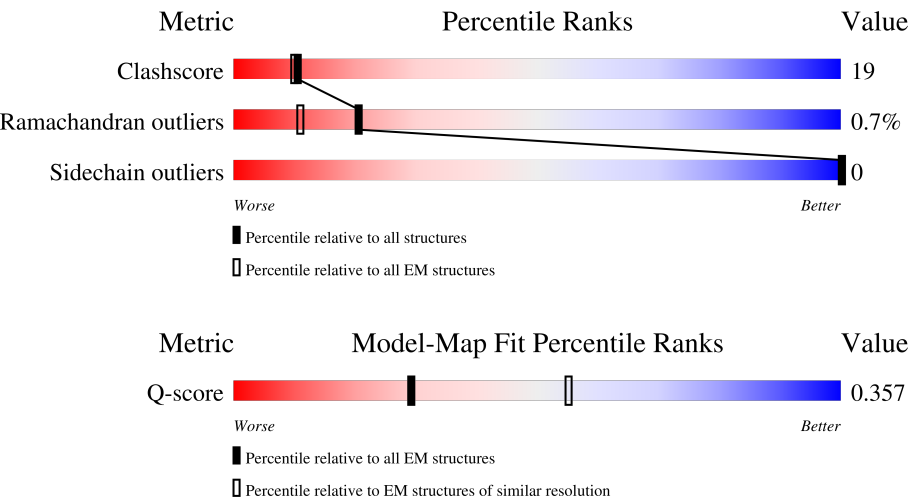
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.14 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	5577 (3.64 - 4.64)

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	329	17% 59% 33% 6%
1	B	329	22% 57% 39%
2	C	1342	65% 34%
3	D	1407	5% 59% 36% 5%

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Mol	Chain	Length	Quality of chain
4	E	91	
5	F	613	
6	X	63	
7	Y	63	
8	O	18	
9	P	18	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 33509 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total	C	N	O	S	0	0
			2407	1504	424	472	7		
1	B	316	Total	C	N	O	S	0	0
			2472	1545	436	483	8		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1342	Total	C	N	O	S	0	0
			10396	6530	1852	1965	49		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	447	Total	C	N	O	S	0	0
			3640	2283	648	689	20		

- Molecule 6 is DNA/RNA hybrid called DNA/RNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	63	Total	C	N	O	P	0	0
			1278	613	224	378	63		

- Molecule 7 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	63	Total	C	N	O	P	0	0
			1305	622	242	378	63		

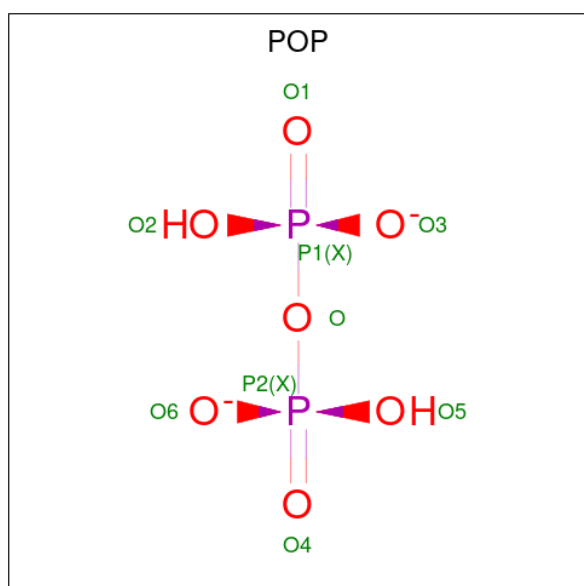
- Molecule 8 is a DNA chain called DNA (18 MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	18	Total	C	N	O	P	0	0
			370	175	71	106	18		

- Molecule 9 is a DNA chain called DNA (18 MER).

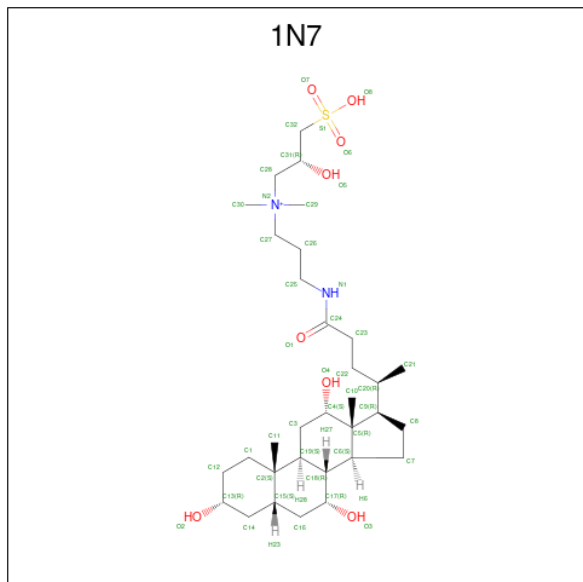
Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	18	Total	C	N	O	P	0	0
			368	175	65	110	18		

- Molecule 10 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	C	1	Total	O	P	0
			9	7	2	

- Molecule 11 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	S	0
			43	32	2	8	1	
11	C	1	Total	C	N	O	S	0
			43	32	2	8	1	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total	Mg	0
			1	1	

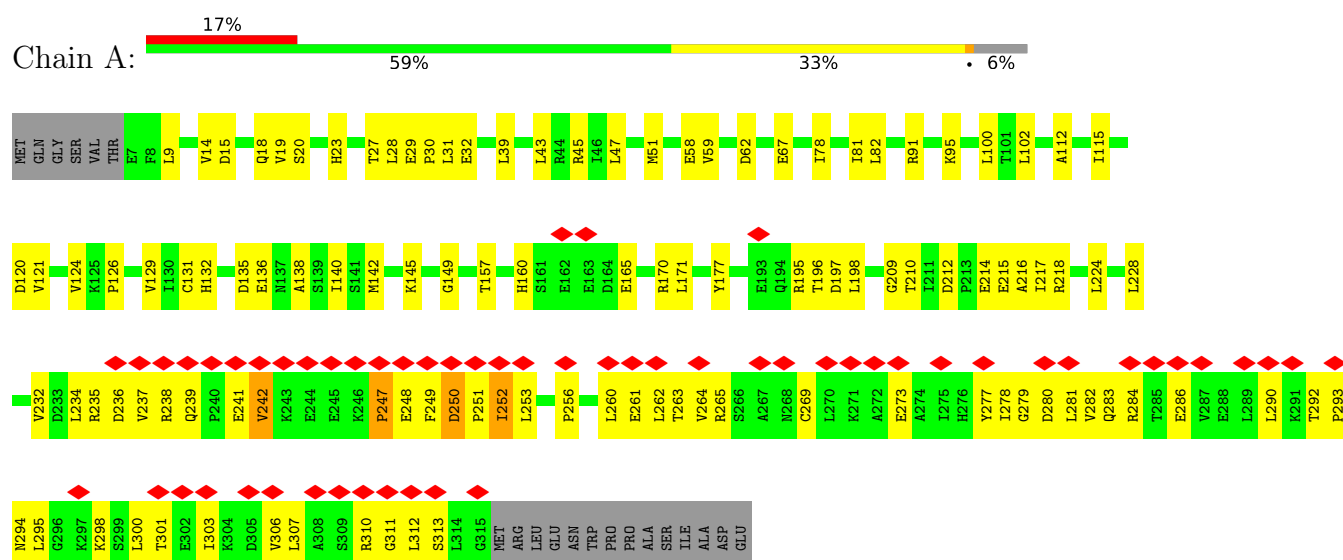
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	D	2	Total	Zn	0
			2	2	

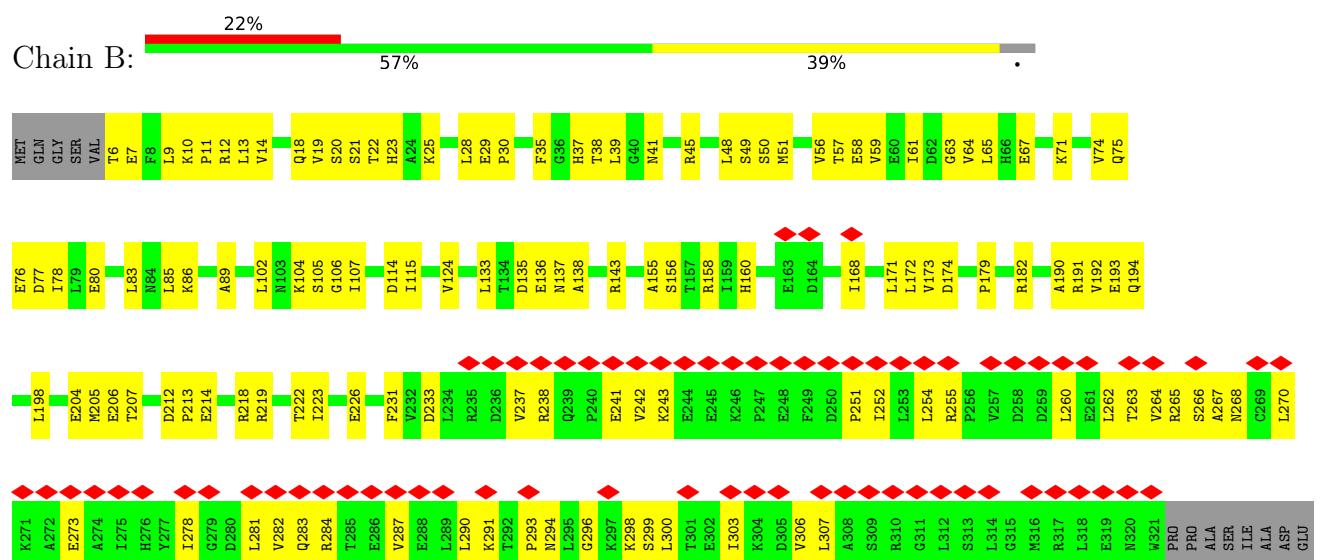
3 Residue-property plots

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.

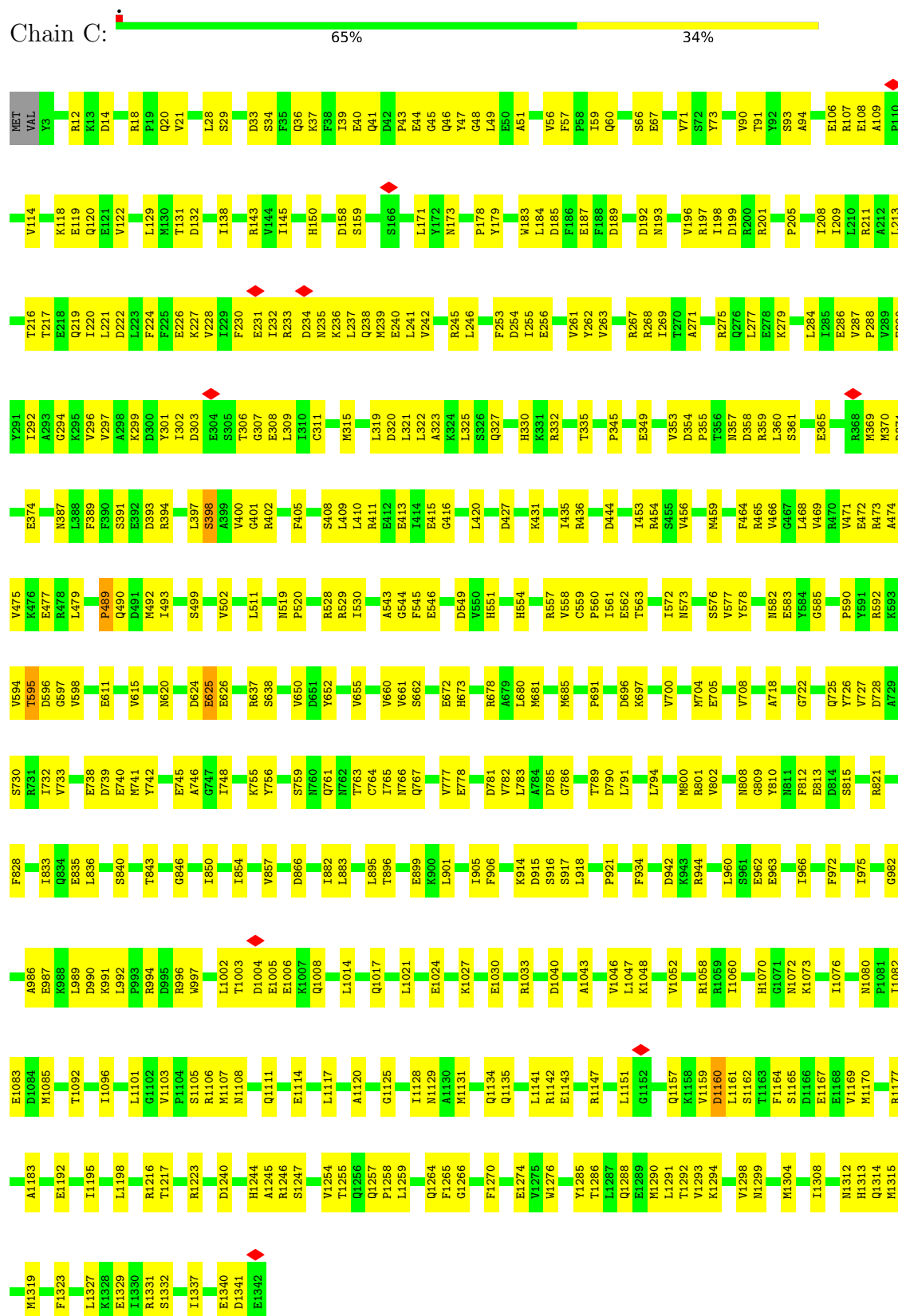
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



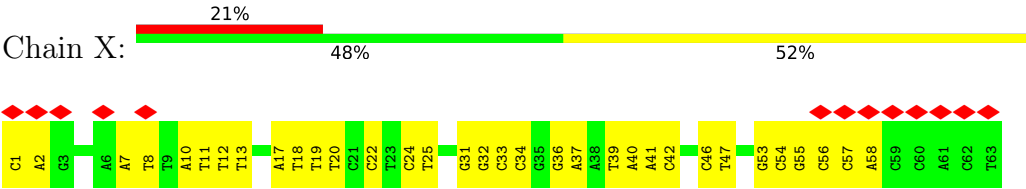
• Molecule 2: DNA-directed RNA polymerase subunit beta



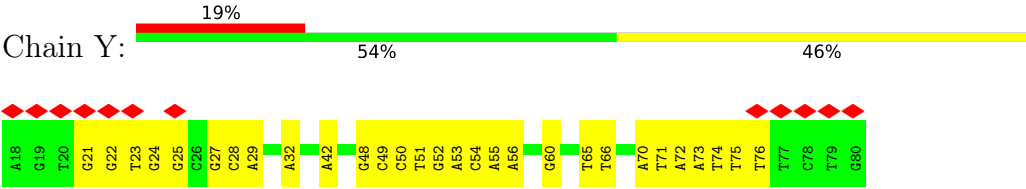
• Molecule 3: DNA-directed RNA polymerase subunit beta'



V1226	F1145	E1015	PHE	V831	C608	V506	G358	V272	G173	E91	MET
H1227	E1146	T1016	HIS	R832	L612	L510	P359	I273	D174	V92	LYS
A1228	A1079	V1017	ILE	R833	L737	L510	G367	R274	E175	R99	ASP
V1229	R1148	A1018	GLY	E833	Q738	T514	G370	R275	D176	E100	LEU
T1230	V1081	N1019	GLY	P834	Q739	R515	K370	R278	F177	R101	LYS
E1236	D1082	W1020	ALA	D837	V639	M525	K371	L285	M180	W102	PHE
	K1151	D1021	ALA	R838	G640	V526	K372	L286	S191	G103	LEU
E1152	A1083	H1084	SER	T844	D642	L527	A373	D289	E197	H104	GLN
	A1083	P1022	ARG	V848	D643	T528	E375	I290	L107	L107	ALA
A1157	G1085	H1023	ALA	T844	M644	G529	L376	I291	T111	T111	THR
E1158	G1086	T1024	A945	V848	P750	K531	F377	V292	A112	A112	LYS
S1160	D1087	V1027	S949	L849	S753	E532	K378	R293	H113	H113	T14
G1161	V1088	T1028	N954	R850	P758	A533	V407	N294	W115	W115	D18
V1163	L1089	E1030	N954	P851	T759	E534	M298	E204			A19
	T1090	V1031	S957	G852	I760	R535	E301	S210			I20
G1166	G1091	S1032	I953	D855	S655	R535	A302	R214			M29
K1167	G1092	G1033	R959	V858	A657	L536	V303	K215			S34
E1168	G1092	F1034	L960	P859	A657	E658	V302	K216			V38
T1169	T1093	V1035	S961	R860	N762		G313	K217			K39
K1170	D1094	R1036	N962	R861	F763		V303	L217			K40
K1172	M1095	F1037	N962	N861	N764		G313	K218			P41
R1173	P1096	T1038	K964	L864	T674		R312	K219			V38
G1174	P1102	D1039	S965	R864	V769		R314	R220			K39
L1175	G1103	M1040	V966	R883	L770		A315	R221			K40
V1176	G1103	I1041	V967	S884	Q771		I316	K222			E42
T1177	K1104	D1042	N968	V885	F772		D304	L217			P41
T1178	A1105	G1043	S969	N885	F773		E414	G125			T43
P1179		G1043	S969	F892	I774		R312	G126			I44
V1180	Q1108	Q1044	K972	C895	S775		R322	I135			N45
D1181	L1109	T1045	L973	C895	H777		P323	E136			Y46
G1182	E1110	I1046	V974	C898	R780		L324	R137			R47
D1184		T1047	I975	T976	R780		K325	Y140			T48
P1185	V1113	Q1049	T976	D902	D691		S326	F141			F49
	Q1114	T1050	R979	L903	R692		E443	E142			R53
I1115	I1115	D1051	N979	D902	V693		Q448	E143			D54
S1116	S1116	E1052	T980	L903	S694		C454	T240			C58
G1118	D1119	L1053	E981	K911	M697		M466	V244			A59
T1120	T1120	T1054	L984	G912	E704		T473	E148			I61
L1121	L1121	L1055	D985	E913	T705		L474	M151			F62
A1122	R1123	S1057	S987	E914	V706		L474	E155			G73
		L1056	F988	I915	I707		A476	E156			Y75
Q1126	Q1126	L1059	G989	I918	N708		R481	R157			K76
GLU	GLU	V1060	Y999	E925	D710		A482	Q158			R77
SER	SER	V1061	G1000	P926	G809		S590	I159			L78
GLY	GLY	L1062	A1001	P926	T810		V347	L160			K79
THR	THR	D1063	V1002	G927	C814		Y348	T161			H80
LYS	LYS	S1064	L1003	T928	R820		M485	E162			R81
ASP	ASP	A1065	G1006	Q929	M821		M488	L265			
ILE	ILE	R1066	G1006	L930	M822		P502	N266			E86
T1135	T1135	R1067	E1009	T931	V825		S503	D267			K87
G1136	G1136	T1068	Q1010	MEI	R825		E1601	L268			C88
L1138	L1138	A1069	V1011	ARG	R826			Y269			
P1139	P1139	G1070		THR				L169			
R1140	R1140	G1071						E170			
		K1072									
D1143	D1143	D1073									
L1144	L1144	L1074									
		R1075									
K1286	V1180										
V1298	D1181										
G1299	G1182										
A1300	D1184										
T1301	P1185										
	M1189										
T1310	I1190										
S1313	P1191										
L1314	S1117										
A1315	G1118										
T1316	D1119										
E1317	T1120										
S1318	L1121										
	E1202										
A1323	V1204										
S1324	E1205										
F1325	R1206										
Q1326	G1207										
E1327	D1208										
V1331	P1214										
E1334	E1215										
	A1216										
R1341	D1219										
D1342	T1135										
E1343	G1136										



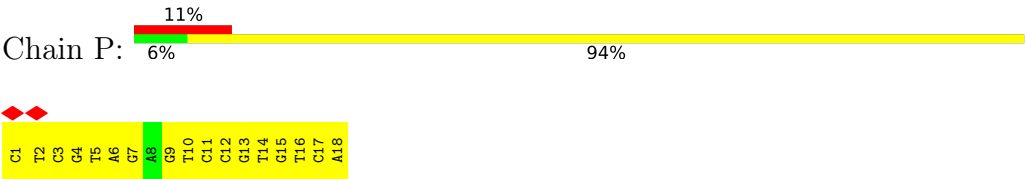
• Molecule 7: DNA (63-MER)



• Molecule 8: DNA (18 MER)



• Molecule 9: DNA (18 MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67187	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POP, MG, ZN, 1N7

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	0.22	0/2437	0.52	0/3301
1	B	0.20	0/2504	0.50	0/3392
2	C	0.25	1/10739 (0.0%)	0.49	2/14489 (0.0%)
3	D	0.23	0/10553	0.50	1/14253 (0.0%)
4	E	0.25	0/607	0.61	1/817 (0.1%)
5	F	0.23	0/3689	0.53	0/4958
6	X	0.32	0/1430	0.61	0/2201
7	Y	0.33	0/1466	0.58	0/2264
8	O	0.36	0/415	0.62	0/638
9	P	0.36	0/411	0.64	0/632
All	All	0.25	1/34251 (0.0%)	0.52	4/46945 (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
2	C	0	3
3	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	489	PRO	CG-CD	-7.38	1.25	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	489	PRO	N-CD-CG	-9.01	89.69	103.20
3	D	1189	MET	CB-CG-SD	7.57	135.41	112.70
2	C	489	PRO	CA-N-CD	-6.84	102.43	112.00
4	E	68	GLU	N-CA-CB	6.04	119.09	110.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2407	0	2463	90	0
1	B	2472	0	2525	105	0
2	C	10570	0	10582	379	0
3	D	10396	0	10583	401	0
4	E	605	0	612	29	0
5	F	3640	0	3705	220	0
6	X	1278	0	713	30	0
7	Y	1305	0	713	32	0
8	O	370	0	202	10	0
9	P	368	0	204	21	0
10	C	9	0	0	1	0
11	C	86	0	116	8	0
12	D	1	0	0	0	0
13	D	2	0	0	0	0
All	All	33509	0	32418	1234	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 19.

All (1234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:NH2	2:C:1165:SER:O	1.87	1.08
3:D:1344:LEU:O	3:D:1346:GLY:N	1.97	0.97
3:D:210:SER:OG	9:P:7:DG:OP1	1.83	0.97
2:C:905:ILE:O	5:F:599:ARG:NH1	1.99	0.95
1:B:296:GLY:N	6:X:11:DT:OP1	2.00	0.93
3:D:528:THR:N	3:D:532:GLU:OE2	2.04	0.90
5:F:348:GLU:O	5:F:352:GLY:N	2.06	0.88
3:D:218:THR:OG1	3:D:222:LYS:NZ	2.07	0.88
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.09	0.85
1:A:236:ASP:OD2	1:A:238:ARG:NH1	2.11	0.84
3:D:123:ARG:NH2	3:D:1334:GLU:OE1	2.11	0.84
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.10	0.83
1:A:280:ASP:OD2	1:A:284:ARG:NH1	2.11	0.83
2:C:1246:ARG:NH1	3:D:348:ASP:OD1	2.11	0.83
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.12	0.82
3:D:144:TYR:OH	3:D:293:ARG:NH2	2.12	0.82
5:F:355:ILE:O	5:F:358:VAL:N	2.11	0.82
2:C:813:GLU:OE2	3:D:504:GLN:NE2	2.12	0.82
3:D:337:ARG:O	3:D:340:GLN:N	2.12	0.82
1:A:294:ASN:ND2	7:Y:71:DT:O4'	2.13	0.82
2:C:187:GLU:OE2	2:C:197:ARG:NE	2.12	0.81
2:C:785:ASP:OD1	2:C:791:LEU:N	2.13	0.81
2:C:1143:GLU:OE2	2:C:1147:ARG:NH1	2.13	0.81
2:C:1329:GLU:O	2:C:1332:SER:OG	1.99	0.80
5:F:283:GLN:NE2	5:F:336:GLU:OE1	2.17	0.78
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.16	0.78
3:D:1172:LYS:HB2	3:D:1189:MET:HE3	1.66	0.78
3:D:278:ARG:NH2	5:F:403:ASP:OD1	2.17	0.77
1:A:218:ARG:NH1	1:B:231:PHE:O	2.16	0.77
2:C:678:ARG:NH1	2:C:681:MET:SD	2.57	0.77
5:F:132:CYS:O	5:F:253:SER:OG	2.02	0.77
4:E:69:ARG:O	4:E:73:GLN:NE2	2.17	0.76
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.66	0.76
3:D:892:PHE:N	3:D:1281:GLU:OE2	2.18	0.76
3:D:1029:THR:OG1	3:D:1119:ASP:OD1	2.03	0.76
1:A:18:GLN:NE2	1:A:20:SER:O	2.18	0.76
1:A:95:LYS:NZ	1:A:120:ASP:OD2	2.17	0.76
5:F:124:GLU:OE1	5:F:128:ASN:ND2	2.19	0.75
3:D:482:ALA:O	3:D:488:ASN:ND2	2.19	0.75
2:C:226:GLU:OE1	2:C:245:ARG:NH1	2.19	0.75
5:F:163:THR:OG1	5:F:260:ARG:NE	2.19	0.75
2:C:308:GLU:N	2:C:308:GLU:OE1	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:GLU:OE2	11:C:1403:1N7:N1	2.20	0.74
2:C:201:ARG:NH1	2:C:370:MET:SD	2.61	0.74
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.61	0.73
2:C:233:ARG:NH1	2:C:238:GLN:O	2.18	0.73
3:D:883:ARG:NH2	3:D:895:CYS:SG	2.61	0.73
2:C:60:GLN:NE2	2:C:67:GLU:OE1	2.21	0.73
2:C:197:ARG:NH1	2:C:201:ARG:O	2.22	0.72
2:C:398:SER:OG	11:C:1403:1N7:O3	2.06	0.72
5:F:303:ILE:O	5:F:307:THR:OG1	2.06	0.72
1:B:182:ARG:NH1	3:D:534:GLU:OE2	2.23	0.72
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.70	0.72
5:F:586:ARG:NH1	6:X:24:DC:OP2	2.22	0.72
2:C:469:VAL:O	2:C:472:GLU:HG3	1.91	0.71
1:A:58:GLU:OE2	1:A:170:ARG:NH1	2.22	0.71
1:A:157:THR:O	1:A:160:HIS:ND1	2.22	0.71
1:B:212:ASP:OD1	1:B:213:PRO:HD2	1.91	0.71
1:B:50:SER:O	1:B:51:MET:HE2	1.90	0.71
5:F:606:VAL:O	5:F:609:SER:OG	2.09	0.71
3:D:418:GLU:O	3:D:481:ARG:NH2	2.23	0.71
3:D:1148:ARG:NE	8:O:5:DA:OP1	2.24	0.71
2:C:490:GLN:O	5:F:472:GLN:NE2	2.25	0.70
2:C:20:GLN:N	2:C:20:GLN:OE1	2.25	0.70
2:C:557:ARG:NH2	2:C:611:GLU:OE1	2.25	0.70
5:F:490:PRO:O	5:F:491:GLU:HG2	1.91	0.70
3:D:1072:LYS:O	3:D:1075:ARG:NH1	2.25	0.69
5:F:317:ASN:O	5:F:321:ALA:N	2.25	0.69
3:D:1048:ARG:NH2	3:D:1110:GLU:OE1	2.24	0.69
2:C:866:ASP:OD2	2:C:944:ARG:NH1	2.26	0.69
1:B:77:ASP:OD1	1:B:78:ILE:N	2.25	0.68
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.25	0.68
1:A:234:LEU:O	1:B:218:ARG:NH2	2.26	0.67
1:A:265:ARG:NH2	1:A:294:ASN:O	2.27	0.67
1:A:14:VAL:HG22	1:A:15:ASP:H	1.60	0.67
3:D:1022:PRO:O	3:D:1126:GLN:NE2	2.27	0.67
5:F:133:SER:HB2	5:F:361:ILE:HG23	1.76	0.67
5:F:138:PRO:C	5:F:140:ALA:H	2.03	0.67
8:O:1:DT:H2''	8:O:2:DG:H5'	1.75	0.66
5:F:138:PRO:HG3	5:F:353:LEU:HB2	1.77	0.66
1:B:12:ARG:HG3	1:B:13:LEU:HD12	1.78	0.66
2:C:48:GLY:O	2:C:51:ALA:N	2.27	0.66
3:D:1219:ASP:OD2	3:D:1220:ILE:N	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:136:GLU:OE2	5:F:364:ARG:NH2	2.29	0.65
5:F:484:ALA:HB2	5:F:491:GLU:HB3	1.78	0.65
2:C:106:GLU:HB3	2:C:109:ALA:HB2	1.78	0.65
2:C:189:ASP:OD1	2:C:193:ASN:N	2.29	0.65
5:F:127:ILE:O	5:F:130:VAL:HG12	1.97	0.65
3:D:132:LEU:O	3:D:136:GLU:OE1	2.15	0.65
3:D:312:ARG:O	3:D:314:ARG:HD3	1.97	0.65
8:O:1:DT:H2'	8:O:2:DG:C8	2.32	0.65
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.30	0.64
3:D:1159:ILE:HD12	3:D:1179:PRO:HG3	1.80	0.64
5:F:354:THR:O	5:F:357:GLN:NE2	2.30	0.64
1:B:105:SER:HA	1:B:138:ALA:O	1.96	0.64
2:C:221:LEU:O	2:C:227:LYS:NZ	2.29	0.64
1:A:131:CYS:SG	1:A:132:HIS:N	2.71	0.64
3:D:1043:GLY:N	3:D:1046:ILE:O	2.20	0.64
1:B:23:HIS:ND1	1:B:206:GLU:OE2	2.31	0.64
4:E:65:ASP:HA	4:E:68:GLU:OE1	1.98	0.64
3:D:133:ARG:HE	3:D:137:ARG:HG3	1.63	0.64
3:D:973:LEU:HB2	3:D:1003:LEU:HB3	1.81	0.63
5:F:439:ILE:O	5:F:443:ILE:HD12	1.98	0.63
2:C:558:VAL:HG12	2:C:573:ASN:OD1	1.98	0.63
3:D:883:ARG:NH2	3:D:898:CYS:SG	2.66	0.63
5:F:121:LYS:O	5:F:124:GLU:HG3	1.98	0.63
2:C:1244:HIS:NE2	2:C:1265:PHE:O	2.31	0.63
5:F:415:ALA:O	5:F:419:PHE:N	2.32	0.63
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.80	0.62
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.05	0.62
4:E:65:ASP:HA	4:E:68:GLU:CD	2.24	0.62
2:C:582:ASN:OD1	2:C:583:GLU:N	2.30	0.62
2:C:987:GLU:OE1	2:C:987:GLU:N	2.24	0.62
2:C:267:ARG:NH1	2:C:268:ARG:O	2.32	0.62
3:D:337:ARG:O	3:D:339:ARG:N	2.32	0.62
2:C:231:GLU:HB2	2:C:233:ARG:HH11	1.63	0.62
1:B:192:VAL:O	1:B:194:GLN:N	2.29	0.61
1:B:273:GLU:O	1:B:284:ARG:NH2	2.32	0.61
3:D:424:ASN:OD1	3:D:425:ARG:N	2.33	0.61
5:F:317:ASN:HA	5:F:320:ILE:HG12	1.82	0.61
5:F:584:ARG:HG3	5:F:585:GLU:H	1.66	0.61
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.31	0.61
3:D:73:GLY:O	3:D:76:LYS:NZ	2.33	0.60
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:355:ILE:O	5:F:357:GLN:N	2.34	0.60
4:E:64:LEU:O	4:E:68:GLU:OE1	2.19	0.60
2:C:211:ARG:NH1	2:C:357:ASN:O	2.35	0.60
2:C:238:GLN:HA	2:C:287:VAL:HG12	1.83	0.60
5:F:565:ILE:O	5:F:566:ASP:OD1	2.19	0.60
5:F:277:MET:HE3	5:F:277:MET:O	2.02	0.60
3:D:712:GLN:OE1	3:D:713:GLU:O	2.20	0.59
3:D:1205:GLU:N	3:D:1208:ASP:OD2	2.31	0.59
5:F:308:GLY:N	5:F:356:GLU:OE2	2.29	0.59
2:C:549:ASP:OD2	3:D:777:HIS:NE2	2.35	0.59
3:D:1143:ASP:O	3:D:1147:ALA:N	2.35	0.59
1:B:20:SER:O	1:B:22:THR:N	2.35	0.59
3:D:1158:GLU:N	3:D:1158:GLU:OE2	2.33	0.59
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.35	0.59
3:D:174:ASP:OD2	5:F:362:ASN:ND2	2.36	0.59
3:D:298:MET:HE1	5:F:406:GLN:HG3	1.83	0.59
1:A:256:PRO:HA	1:A:277:TYR:HA	1.83	0.59
1:B:48:LEU:HD11	3:D:535:ARG:HD2	1.85	0.59
2:C:696:ASP:OD1	2:C:697:LYS:N	2.31	0.59
5:F:398:GLY:O	5:F:399:LEU:HD22	2.02	0.58
2:C:233:ARG:CZ	2:C:284:LEU:HD11	2.32	0.58
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.85	0.58
3:D:694:SER:HB2	3:D:738:ARG:HE	1.68	0.58
3:D:810:THR:O	3:D:911:LYS:NZ	2.31	0.58
5:F:127:ILE:O	5:F:131:GLN:HG2	2.03	0.58
5:F:401:PHE:HA	5:F:404:LEU:HD12	1.83	0.58
2:C:739:ASP:OD1	2:C:740:GLU:N	2.35	0.58
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.83	0.58
2:C:290:GLU:OE2	2:C:290:GLU:N	2.34	0.58
1:A:307:LEU:HA	1:A:310:ARG:HB2	1.85	0.58
3:D:201:LEU:HB3	3:D:217:LEU:HD11	1.86	0.58
1:A:9:LEU:N	1:A:32:GLU:OE2	2.36	0.58
2:C:528:ARG:NH2	2:C:576:SER:O	2.35	0.58
3:D:1036:ARG:NE	3:D:1081:VAL:HG21	2.18	0.58
2:C:233:ARG:NH2	2:C:238:GLN:HB2	2.18	0.57
3:D:140:TYR:OH	3:D:312:ARG:NE	2.38	0.57
3:D:301:GLU:HA	3:D:304:ASP:OD1	2.04	0.57
6:X:19:DT:H2"	6:X:20:DT:H71	1.86	0.57
7:Y:75:DT:H2"	7:Y:76:DT:H71	1.85	0.57
3:D:156:ARG:NH2	3:D:191:SER:OG	2.38	0.57
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ARG:NH2	3:D:413:ASP:OD2	2.38	0.57
2:C:558:VAL:CG1	2:C:573:ASN:OD1	2.52	0.57
3:D:849:LEU:HD12	3:D:855:ASP:H	1.70	0.57
3:D:1267:VAL:HG23	3:D:1301:THR:HG23	1.86	0.57
5:F:585:GLU:OE2	5:F:588:ARG:NH2	2.37	0.57
2:C:323:ALA:O	2:C:327:GLN:OE1	2.22	0.57
3:D:357:VAL:HG13	3:D:358:GLY:H	1.68	0.57
3:D:557:LYS:HA	3:D:562:GLU:O	2.05	0.57
3:D:1310:THR:O	3:D:1313:SER:OG	2.21	0.57
1:A:260:LEU:CD2	1:A:262:LEU:HD21	2.34	0.57
5:F:524:GLU:N	5:F:524:GLU:OE1	2.38	0.57
1:A:129:VAL:HG21	1:A:132:HIS:HE1	1.69	0.57
3:D:765:GLU:N	3:D:765:GLU:OE2	2.37	0.57
5:F:347:ILE:O	5:F:350:GLU:HG3	2.05	0.57
5:F:588:ARG:NH1	7:Y:53:DA:N7	2.52	0.57
1:A:247:PRO:HG2	1:A:250:ASP:HA	1.87	0.57
5:F:301:ASN:OD1	5:F:302:PHE:N	2.37	0.57
5:F:514:ASP:O	5:F:516:ASP:N	2.38	0.57
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.37	0.56
2:C:530:ILE:O	2:C:572:ILE:O	2.23	0.56
3:D:925:GLU:HG3	3:D:926:PRO:HD3	1.86	0.56
3:D:985:ILE:HG23	3:D:989:GLY:HA2	1.88	0.56
3:D:742:GLY:O	3:D:762:ASN:HB3	2.04	0.56
5:F:373:ARG:O	5:F:377:LYS:HG3	2.06	0.56
2:C:704:MET:HA	2:C:704:MET:HE2	1.86	0.56
4:E:32:VAL:O	4:E:34:GLY:N	2.34	0.56
5:F:529:GLU:OE2	5:F:534:SER:N	2.38	0.56
3:D:665:GLN:OE1	3:D:678:ARG:NH1	2.39	0.56
1:B:35:PHE:HA	1:B:38:THR:HG22	1.87	0.56
2:C:801:ARG:NH1	2:C:1092:THR:OG1	2.38	0.56
5:F:279:ARG:O	5:F:282:THR:OG1	2.19	0.56
2:C:843:THR:OG1	2:C:846:GLY:O	2.24	0.56
4:E:17:PHE:O	4:E:20:VAL:HG12	2.04	0.56
5:F:144:LEU:HD12	5:F:261:LEU:HD11	1.88	0.56
2:C:738:GLU:HA	2:C:741:MET:SD	2.46	0.56
3:D:961:SER:OG	3:D:981:GLU:HB3	2.06	0.56
5:F:347:ILE:O	5:F:351:THR:HG22	2.05	0.56
2:C:1006:GLU:OE1	2:C:1006:GLU:N	2.37	0.55
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.87	0.55
1:A:269:CYS:HB3	1:A:295:LEU:HD12	1.88	0.55
2:C:231:GLU:O	2:C:233:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:398:SER:HB3	2:C:401:GLY:H	1.71	0.55
2:C:473:ARG:O	2:C:477:GLU:OE1	2.24	0.55
2:C:595:THR:O	2:C:597:GLY:N	2.39	0.55
5:F:161:LEU:HA	5:F:260:ARG:O	2.06	0.55
1:B:80:GLU:OE2	3:D:551:ARG:NH2	2.40	0.55
1:B:156:SER:O	1:B:160:HIS:ND1	2.39	0.55
2:C:624:ASP:O	2:C:626:GLU:N	2.37	0.55
3:D:151:MET:HE3	5:F:277:MET:HE1	1.88	0.55
3:D:1216:ALA:O	3:D:1219:ASP:OD2	2.25	0.55
5:F:331:HIS:HA	5:F:334:SER:OG	2.06	0.55
1:A:273:GLU:OE1	1:A:292:THR:OG1	2.23	0.55
2:C:1312:ASN:OD1	2:C:1313:HIS:N	2.39	0.55
3:D:1252:HIS:O	3:D:1255:VAL:HG22	2.07	0.55
1:B:10:LYS:HG2	1:B:11:PRO:HD2	1.88	0.55
2:C:234:ASP:O	2:C:235:ASN:HB2	2.04	0.55
2:C:402:ARG:HG2	2:C:416:GLY:H	1.72	0.55
2:C:1290:MET:HA	2:C:1294:LYS:HG3	1.88	0.55
3:D:338:PHE:CE2	3:D:1324:SER:HB2	2.42	0.55
3:D:370:LYS:O	3:D:373:ALA:N	2.40	0.55
3:D:960:LEU:HB3	3:D:963:VAL:HG11	1.88	0.55
2:C:914:LYS:HD3	2:C:915:ASP:H	1.72	0.55
3:D:18:ASP:N	3:D:18:ASP:OD1	2.40	0.55
2:C:1285:TYR:CD2	3:D:475:GLU:HB3	2.43	0.55
1:A:252:ILE:HG22	1:A:252:ILE:O	2.07	0.54
2:C:296:VAL:O	2:C:335:THR:OG1	2.18	0.54
3:D:963:VAL:HB	3:D:980:THR:HG23	1.88	0.54
1:A:102:LEU:HD13	1:A:115:ILE:HA	1.90	0.54
1:B:237:VAL:HG22	1:B:238:ARG:H	1.71	0.54
2:C:238:GLN:HB3	2:C:286:GLU:HA	1.89	0.54
5:F:119:ILE:HG21	5:F:379:MET:HB2	1.88	0.54
5:F:567:MET:SD	5:F:568:ASN:N	2.81	0.54
1:B:135:ASP:OD1	1:B:136:GLU:N	2.40	0.54
1:B:251:PRO:O	1:B:254:LEU:HD22	2.08	0.54
2:C:420:LEU:HD12	2:C:420:LEU:O	2.06	0.54
2:C:915:ASP:OD1	2:C:916:SER:N	2.40	0.54
5:F:123:ILE:HD13	5:F:372:ALA:HB1	1.89	0.54
5:F:134:VAL:HG21	5:F:266:PHE:CE1	2.42	0.54
2:C:303:ASP:OD2	2:C:306:THR:OG1	2.26	0.54
2:C:722:GLY:N	2:C:777:VAL:O	2.41	0.54
5:F:131:GLN:CD	5:F:260:ARG:HA	2.32	0.54
4:E:65:ASP:HA	4:E:68:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:297:MET:SD	5:F:326:TRP:CZ2	3.01	0.54
7:Y:71:DT:H2''	7:Y:72:DA:C8	2.42	0.54
2:C:230:PHE:CE1	2:C:292:ILE:HG12	2.43	0.54
4:E:68:GLU:O	4:E:71:GLU:HG3	2.08	0.54
5:F:148:TYR:HD2	5:F:161:LEU:HD21	1.73	0.54
5:F:449:THR:HG21	5:F:504:PRO:HG3	1.89	0.54
2:C:895:LEU:HD12	2:C:899:GLU:HG3	1.89	0.54
3:D:45:ASN:O	3:D:47:ARG:N	2.41	0.54
1:A:250:ASP:O	1:A:253:LEU:N	2.41	0.54
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.08	0.54
2:C:696:ASP:O	2:C:697:LYS:HB3	2.08	0.53
3:D:978:ARG:HD3	3:D:999:TYR:HB2	1.88	0.53
5:F:314:THR:HA	5:F:317:ASN:OD1	2.07	0.53
2:C:271:ALA:O	2:C:275:ARG:HG3	2.08	0.53
5:F:166:VAL:H	5:F:258:GLN:HG2	1.73	0.53
5:F:595:LEU:O	5:F:599:ARG:HG2	2.08	0.53
2:C:233:ARG:CZ	2:C:238:GLN:HB2	2.38	0.53
2:C:1058:ARG:NE	2:C:1240:ASP:OD1	2.41	0.53
2:C:303:ASP:O	2:C:307:GLY:N	2.37	0.53
2:C:472:GLU:O	2:C:475:VAL:HG12	2.08	0.53
3:D:58:CYS:SG	3:D:60:ARG:HG2	2.47	0.53
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.26	0.53
2:C:986:ALA:HA	2:C:989:LEU:HB3	1.91	0.53
2:C:464:PHE:O	2:C:468:LEU:HD23	2.09	0.53
5:F:334:SER:HA	5:F:337:VAL:HG12	1.90	0.53
5:F:508:GLU:OE1	5:F:508:GLU:N	2.42	0.53
6:X:22:DC:O2	7:Y:60:DG:N2	2.42	0.53
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.09	0.53
3:D:29:MET:HE2	3:D:29:MET:HA	1.90	0.53
3:D:1323:ALA:HA	3:D:1331:VAL:HG21	1.91	0.53
1:A:294:ASN:HA	6:X:12:DT:H4'	1.90	0.53
2:C:36:GLN:NE2	2:C:40:GLU:OE1	2.34	0.53
2:C:120:GLN:OE1	2:C:120:GLN:N	2.39	0.53
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.89	0.53
2:C:1030:GLU:O	2:C:1033:ARG:HG2	2.09	0.53
3:D:789:LYS:NZ	3:D:929:GLN:O	2.39	0.53
5:F:157:ARG:HE	5:F:158:LEU:H	1.57	0.53
1:A:235:ARG:C	1:A:237:VAL:H	2.16	0.53
2:C:12:ARG:HD3	2:C:1183:ALA:HB2	1.91	0.53
2:C:205:PRO:O	2:C:208:ILE:HG22	2.08	0.53
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:N	1:B:174:ASP:OD1	2.32	0.52
5:F:291:CYS:SG	5:F:297:MET:HB3	2.48	0.52
2:C:41:GLN:NE2	2:C:73:TYR:O	2.42	0.52
2:C:475:VAL:HG23	2:C:492:MET:HB3	1.91	0.52
2:C:1101:LEU:HD12	3:D:505:ASP:OD1	2.08	0.52
3:D:233:LYS:HB3	3:D:235:GLU:OE1	2.10	0.52
3:D:1033:GLY:O	3:D:1115:ILE:HG12	2.10	0.52
3:D:475:GLU:OE1	3:D:475:GLU:N	2.35	0.52
3:D:582:ILE:HD11	3:D:627:THR:HG21	1.91	0.52
5:F:138:PRO:O	5:F:140:ALA:N	2.42	0.52
8:O:16:DG:H2''	8:O:17:DA:C8	2.44	0.52
3:D:514:THR:HG21	3:D:596:LEU:HB3	1.92	0.52
2:C:387:ASN:HA	2:C:391:SER:HB3	1.91	0.52
2:C:895:LEU:HB2	2:C:899:GLU:OE2	2.10	0.52
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.37	0.52
3:D:218:THR:HA	3:D:221:ILE:HG22	1.90	0.52
1:B:192:VAL:C	1:B:194:GLN:H	2.17	0.52
2:C:1131:MET:HE3	2:C:1141:LEU:HG	1.92	0.52
3:D:235:GLU:OE1	3:D:235:GLU:N	2.39	0.52
3:D:353:SER:OG	3:D:354:VAL:N	2.42	0.52
3:D:957:SER:HB3	3:D:985:ILE:HB	1.91	0.52
4:E:52:ARG:HH11	4:E:52:ARG:HG2	1.75	0.52
1:A:135:ASP:OD1	1:A:136:GLU:N	2.43	0.52
1:B:241:GLU:HG3	1:B:242:VAL:H	1.74	0.52
6:X:10:A:C2	7:Y:72:DA:C2	2.97	0.52
2:C:345:PRO:O	2:C:349:GLU:HG2	2.09	0.52
3:D:1006:GLY:N	3:D:1009:GLU:OE1	2.43	0.52
3:D:1172:LYS:HG2	3:D:1191:PRO:HA	1.92	0.52
1:A:29:GLU:HB2	1:A:30:PRO:HD3	1.90	0.52
1:B:86:LYS:HG2	1:B:173:VAL:CG1	2.40	0.52
3:D:45:ASN:HB3	3:D:48:THR:O	2.10	0.52
3:D:77:ARG:HG3	3:D:79:LYS:H	1.75	0.52
3:D:103:GLY:C	3:D:244:VAL:HG12	2.35	0.52
3:D:1157:ALA:O	3:D:1207:GLY:N	2.41	0.52
5:F:130:VAL:O	5:F:133:SER:OG	2.22	0.52
5:F:160:ASP:HB2	5:F:262:VAL:HG12	1.92	0.52
5:F:426:LYS:O	5:F:429:THR:HG22	2.10	0.52
1:B:242:VAL:HG12	1:B:243:LYS:H	1.75	0.52
2:C:179:TYR:HB2	2:C:397:LEU:O	2.10	0.52
3:D:285:LEU:HD23	5:F:413:MET:HE2	1.92	0.52
1:A:140:ILE:HD12	1:A:142:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:GLU:HB2	2:C:233:ARG:NH1	2.25	0.51
3:D:682:VAL:O	3:D:685:ILE:HG12	2.10	0.51
5:F:442:SER:HA	5:F:445:ASP:OD2	2.09	0.51
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.38	0.51
2:C:1244:HIS:CE1	2:C:1265:PHE:O	2.64	0.51
3:D:342:LEU:O	3:D:342:LEU:HD23	2.10	0.51
3:D:1166:GLY:O	3:D:1167:LYS:C	2.54	0.51
5:F:283:GLN:O	5:F:286:LEU:HG	2.10	0.51
1:A:19:VAL:HG23	1:A:23:HIS:HB3	1.91	0.51
2:C:33:ASP:O	2:C:37:LYS:HG2	2.10	0.51
2:C:727:VAL:HG23	2:C:732:ILE:CD1	2.40	0.51
3:D:337:ARG:HG3	3:D:338:PHE:H	1.74	0.51
5:F:492:ASP:O	5:F:496:LYS:HG3	2.10	0.51
1:A:58:GLU:HG2	1:A:145:LYS:HB3	1.91	0.51
2:C:611:GLU:OE2	2:C:637:ARG:NH2	2.43	0.51
3:D:1033:GLY:HA3	3:D:1082:ASP:HA	1.93	0.51
1:A:51:MET:HE1	1:A:216:ALA:HA	1.92	0.51
2:C:253:PHE:HB3	2:C:288:PRO:HG3	1.91	0.51
2:C:1106:ARG:NH2	10:C:1401:POP:O4	2.41	0.51
1:A:301:THR:HG21	1:B:291:LYS:HD2	1.93	0.51
1:A:303:ILE:O	1:A:307:LEU:HD13	2.10	0.51
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.92	0.51
3:D:860:ARG:HG2	3:D:861:ASN:H	1.76	0.51
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.92	0.51
3:D:975:ILE:O	3:D:1000:GLY:N	2.40	0.51
1:A:286:GLU:CD	1:A:300:LEU:HD21	2.35	0.51
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.39	0.51
3:D:166:LEU:O	3:D:169:LEU:HG	2.11	0.51
3:D:740:LEU:O	3:D:762:ASN:ND2	2.44	0.51
5:F:334:SER:O	5:F:337:VAL:HG12	2.11	0.51
2:C:465:ARG:HE	2:C:469:VAL:CG1	2.24	0.51
2:C:725:GLN:NE2	11:C:1402:1N7:H32	2.26	0.51
2:C:1120:ALA:HB1	2:C:1198:LEU:HD22	1.93	0.51
3:D:339:ARG:HE	3:D:798:ARG:NH1	2.09	0.51
1:A:279:GLY:O	1:A:283:GLN:HG3	2.11	0.51
2:C:119:GLU:OE1	2:C:489:PRO:HD2	2.11	0.51
2:C:761:GLN:N	2:C:761:GLN:OE1	2.43	0.51
2:C:990:ASP:OD1	2:C:991:LYS:N	2.44	0.51
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.25	0.51
4:E:49:ILE:HG22	4:E:53:GLU:OE2	2.11	0.51
5:F:601:PRO:O	5:F:602:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:798:ARG:HH22	3:D:1325:PHE:HB2	1.76	0.50
6:X:40:DA:C2	7:Y:42:DA:C2	2.99	0.50
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.92	0.50
1:B:9:LEU:HD21	1:B:30:PRO:HG2	1.93	0.50
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.93	0.50
3:D:326:SER:N	3:D:329:ASP:OD2	2.44	0.50
5:F:138:PRO:C	5:F:140:ALA:N	2.69	0.50
1:B:179:PRO:C	1:B:207:THR:HG1	2.19	0.50
2:C:233:ARG:NE	2:C:284:LEU:HD11	2.26	0.50
3:D:1057:SER:OG	3:D:1058:SER:N	2.44	0.50
5:F:357:GLN:O	5:F:361:ILE:HG13	2.10	0.50
6:X:19:DT:H2''	6:X:20:DT:C7	2.42	0.50
7:Y:48:DG:H2''	7:Y:49:DC:OP2	2.10	0.50
1:A:59:VAL:O	1:A:171:LEU:HB2	2.10	0.50
2:C:325:LEU:HD12	2:C:330:HIS:HB2	1.93	0.50
3:D:289:ASP:O	3:D:292:VAL:HG22	2.11	0.50
5:F:436:ARG:O	5:F:440:THR:HG22	2.12	0.50
2:C:1105:SER:OG	3:D:731:ARG:HB3	2.12	0.50
3:D:976:THR:HA	3:D:999:TYR:CE1	2.47	0.50
6:X:31:DG:H2''	6:X:32:DG:C8	2.46	0.50
2:C:962:GLU:O	2:C:966:ILE:HG13	2.12	0.50
5:F:316:PHE:O	5:F:320:ILE:HG12	2.11	0.50
2:C:854:ILE:O	2:C:857:VAL:HG22	2.11	0.50
2:C:1246:ARG:HD2	2:C:1266:GLY:C	2.37	0.50
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.47	0.50
1:B:14:VAL:HG12	1:B:28:LEU:HD13	1.92	0.50
1:B:262:LEU:HD13	1:B:266:SER:HB2	1.94	0.50
2:C:615:VAL:HG23	2:C:650:VAL:HA	1.94	0.50
2:C:1004:ASP:O	2:C:1005:GLU:HG3	2.11	0.50
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.44	0.50
3:D:697:MET:HE1	3:D:738:ARG:HA	1.93	0.50
3:D:967:VAL:HG22	3:D:973:LEU:HG	1.94	0.50
5:F:297:MET:HE2	5:F:302:PHE:CA	2.42	0.50
5:F:429:THR:OG1	7:Y:32:DA:OP2	2.25	0.50
8:O:2:DG:H1'	8:O:3:DA:C8	2.46	0.50
1:A:251:PRO:C	1:A:253:LEU:H	2.20	0.49
2:C:201:ARG:NH2	2:C:369:MET:O	2.44	0.49
2:C:228:VAL:HG22	2:C:245:ARG:CZ	2.42	0.49
2:C:358:ASP:OD1	2:C:359:ARG:N	2.43	0.49
2:C:562:GLU:O	2:C:562:GLU:OE1	2.29	0.49
2:C:850:ILE:HG22	2:C:850:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1048:ARG:HG2	3:D:1050:THR:OG1	2.11	0.49
5:F:133:SER:HB2	5:F:361:ILE:CG2	2.39	0.49
5:F:361:ILE:O	5:F:365:MET:HG3	2.12	0.49
2:C:405:PHE:O	2:C:408:SER:OG	2.28	0.49
3:D:826:ILE:HG13	3:D:826:ILE:O	2.10	0.49
5:F:125:ASP:OD1	5:F:166:VAL:HG12	2.12	0.49
5:F:419:PHE:HA	5:F:430:TYR:CE2	2.47	0.49
1:B:212:ASP:OD1	1:B:213:PRO:CD	2.59	0.49
2:C:691:PRO:HD2	2:C:763:THR:HG21	1.94	0.49
2:C:1106:ARG:O	2:C:1108:ASN:N	2.43	0.49
3:D:218:THR:C	3:D:222:LYS:HZ3	2.20	0.49
3:D:1178:THR:HG23	3:D:1184:ASP:CG	2.36	0.49
9:P:16:DT:H2''	9:P:17:DC:C5	2.47	0.49
1:A:224:LEU:O	1:A:228:LEU:HD23	2.12	0.49
2:C:409:LEU:C	2:C:410:LEU:HD23	2.37	0.49
2:C:813:GLU:C	2:C:815:SER:H	2.20	0.49
3:D:1344:LEU:C	3:D:1346:GLY:H	2.09	0.49
5:F:358:VAL:HA	5:F:361:ILE:HD12	1.94	0.49
7:Y:21:DG:H2''	7:Y:22:DG:C8	2.48	0.49
2:C:18:ARG:CZ	2:C:620:ASN:HA	2.43	0.49
2:C:786:GLY:N	2:C:789:THR:OG1	2.45	0.49
5:F:148:TYR:O	5:F:152:GLU:HG3	2.13	0.49
8:O:15:DC:H2''	8:O:16:DG:C8	2.48	0.49
2:C:413:GLU:OE2	2:C:415:GLU:N	2.43	0.49
2:C:1141:LEU:HD22	2:C:1170:MET:HE1	1.94	0.49
5:F:423:ARG:NH1	5:F:424:GLY:O	2.46	0.49
5:F:484:ALA:CB	5:F:491:GLU:HB3	2.41	0.49
2:C:896:THR:O	2:C:899:GLU:HG2	2.12	0.49
2:C:1340:GLU:CD	3:D:1341:ARG:HE	2.20	0.49
3:D:960:LEU:HB3	3:D:963:VAL:CG1	2.43	0.49
2:C:493:ILE:O	5:F:472:GLN:NE2	2.42	0.49
3:D:598:LYS:O	3:D:601:ILE:HG22	2.13	0.49
2:C:742:TYR:N	2:C:746:ALA:HB2	2.28	0.49
3:D:148:GLU:OE1	3:D:148:GLU:O	2.30	0.49
3:D:253:VAL:HG11	5:F:523:ILE:HG21	1.95	0.49
3:D:1060:VAL:O	3:D:1060:VAL:HG23	2.13	0.49
5:F:604:SER:O	5:F:608:ARG:N	2.40	0.49
1:A:14:VAL:HG21	1:A:29:GLU:OE2	2.11	0.49
1:A:249:PHE:O	1:A:253:LEU:HB3	2.13	0.49
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
3:D:244:VAL:HG23	3:D:269:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.95	0.49
3:D:772:TYR:O	3:D:773:PHE:C	2.55	0.49
1:B:287:VAL:O	1:B:291:LYS:HG2	2.13	0.48
2:C:199:ASP:N	2:C:199:ASP:OD1	2.45	0.48
2:C:755:LYS:O	2:C:756:TYR:C	2.56	0.48
2:C:960:LEU:O	2:C:963:GLU:HG3	2.13	0.48
2:C:1192:GLU:HA	2:C:1195:ILE:HD12	1.95	0.48
2:C:1264:GLN:O	2:C:1265:PHE:C	2.56	0.48
2:C:1274:GLU:HG3	3:D:428:THR:HG21	1.95	0.48
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.95	0.48
3:D:330:MET:O	3:D:337:ARG:HB2	2.12	0.48
3:D:338:PHE:CE2	3:D:1324:SER:HA	2.48	0.48
5:F:144:LEU:HD11	5:F:256:PHE:CZ	2.48	0.48
5:F:220:LYS:O	5:F:224:LEU:HD13	2.13	0.48
5:F:283:GLN:NE2	5:F:337:VAL:HA	2.28	0.48
9:P:2:DT:H2"	9:P:3:DC:C5	2.48	0.48
1:B:233:ASP:N	1:B:233:ASP:OD1	2.46	0.48
3:D:337:ARG:O	3:D:338:PHE:C	2.56	0.48
3:D:552:ILE:HD11	3:D:570:LYS:HG3	1.94	0.48
5:F:414:LYS:HA	5:F:417:ASP:OD1	2.13	0.48
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.94	0.48
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.94	0.48
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.47	0.48
3:D:680:ASN:O	3:D:683:ILE:HG22	2.13	0.48
3:D:1082:ASP:HB2	3:D:1088:VAL:CG1	2.43	0.48
5:F:344:LEU:O	5:F:348:GLU:HG3	2.13	0.48
5:F:493:LYS:O	5:F:497:VAL:HG23	2.13	0.48
1:A:239:GLN:HB2	1:A:241:GLU:OE1	2.13	0.48
1:B:278:ILE:O	1:B:282:VAL:HG22	2.13	0.48
2:C:320:ASP:OD1	2:C:321:LEU:HD12	2.13	0.48
3:D:316:ILE:HG22	3:D:317:THR:H	1.77	0.48
4:E:44:ASP:HB3	4:E:48:VAL:CG2	2.43	0.48
5:F:484:ALA:O	5:F:487:MET:O	2.32	0.48
2:C:577:VAL:HG13	2:C:578:TYR:N	2.29	0.48
5:F:317:ASN:HA	5:F:320:ILE:CG1	2.41	0.48
7:Y:54:DC:C2	7:Y:55:DA:N7	2.81	0.48
2:C:992:LEU:HD13	2:C:996:ARG:HB3	1.96	0.48
2:C:1101:LEU:CD2	3:D:725:MET:HG2	2.44	0.48
3:D:19:ALA:HA	3:D:1342:ASP:O	2.13	0.48
3:D:825:VAL:HG13	3:D:825:VAL:O	2.13	0.48
3:D:1036:ARG:CD	3:D:1081:VAL:CG2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:656:GLU:OE1	3:D:692:ARG:NH2	2.43	0.48
3:D:1062:LEU:HA	3:D:1103:GLY:HA2	1.96	0.48
3:D:1081:VAL:HA	3:D:1087:ASP:HA	1.96	0.48
5:F:213:ASP:N	5:F:213:ASP:OD1	2.47	0.48
5:F:319:ALA:HB1	5:F:327:SER:HB2	1.95	0.48
1:A:282:VAL:HG13	1:A:313:SER:O	2.13	0.48
2:C:840:SER:O	2:C:1047:LEU:N	2.47	0.48
3:D:1138:LEU:H	3:D:1139:PRO:CD	2.26	0.48
3:D:1178:THR:HG23	3:D:1184:ASP:OD1	2.14	0.48
5:F:560:ARG:NH1	5:F:566:ASP:OD2	2.46	0.48
7:Y:74:DT:H2''	7:Y:75:DT:H71	1.95	0.48
1:A:165:GLU:O	1:A:165:GLU:HG2	2.14	0.48
2:C:1107:MET:HE1	3:D:739:GLN:OE1	2.14	0.48
3:D:1150:PRO:C	3:D:1152:GLU:H	2.21	0.48
9:P:12:DC:C2	9:P:13:DG:C5	3.02	0.48
1:B:61:ILE:HG21	1:B:64:VAL:HG12	1.95	0.48
1:B:83:LEU:HD12	3:D:528:THR:HA	1.96	0.48
3:D:204:GLU:OE1	3:D:217:LEU:CD2	2.62	0.48
3:D:954:ASN:O	3:D:984:LEU:HD21	2.14	0.48
3:D:1314:LEU:HD12	3:D:1326:GLN:HE22	1.79	0.48
3:D:678:ARG:O	3:D:682:VAL:HG12	2.14	0.47
3:D:1032:SER:HA	3:D:1115:ILE:HG13	1.96	0.47
5:F:279:ARG:NH2	5:F:340:ALA:HA	2.29	0.47
1:A:241:GLU:O	1:A:242:VAL:C	2.57	0.47
1:B:19:VAL:O	1:B:20:SER:OG	2.32	0.47
2:C:563:THR:O	2:C:680:LEU:HD11	2.14	0.47
3:D:785:ASP:OD1	3:D:789:LYS:HE3	2.14	0.47
3:D:789:LYS:HE2	3:D:931:THR:HA	1.95	0.47
3:D:963:VAL:HG23	3:D:977:SER:HB2	1.96	0.47
1:A:39:LEU:O	1:A:43:LEU:HD23	2.14	0.47
2:C:46:GLN:O	2:C:51:ALA:HB2	2.14	0.47
2:C:238:GLN:HG2	2:C:286:GLU:HG3	1.97	0.47
2:C:905:ILE:HG22	2:C:906:PHE:CD1	2.49	0.47
2:C:1002:LEU:HB3	2:C:1008:GLN:OE1	2.15	0.47
2:C:1164:PHE:HE1	2:C:1167:GLU:HB3	1.78	0.47
3:D:407:VAL:O	3:D:411:ILE:HG12	2.13	0.47
3:D:586:GLY:HA3	3:D:612:LEU:HD11	1.97	0.47
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.15	0.47
9:P:17:DC:H5''	9:P:17:DC:H6	1.79	0.47
1:A:281:LEU:HD21	1:A:307:LEU:HD11	1.97	0.47
1:B:59:VAL:HA	1:B:143:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:SER:O	1:B:160:HIS:CG	2.67	0.47
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.14	0.47
2:C:211:ARG:NH2	2:C:217:THR:OG1	2.46	0.47
2:C:360:LEU:HD12	2:C:361:SER:N	2.29	0.47
2:C:840:SER:OG	2:C:1048:LYS:HG2	2.14	0.47
2:C:1255:THR:O	2:C:1257:GLN:N	2.41	0.47
3:D:146:VAL:HG22	3:D:158:GLN:O	2.14	0.47
3:D:252:LEU:O	3:D:252:LEU:HD23	2.14	0.47
3:D:591:ILE:HG13	3:D:592:VAL:N	2.29	0.47
3:D:850:LYS:C	3:D:852:GLY:H	2.22	0.47
3:D:958:ILE:HG13	3:D:1011:VAL:HG21	1.96	0.47
3:D:1150:PRO:O	3:D:1152:GLU:N	2.46	0.47
5:F:334:SER:O	5:F:338:HIS:CD2	2.67	0.47
2:C:231:GLU:HG2	2:C:332:ARG:HD3	1.96	0.47
2:C:1276:TRP:HH2	3:D:798:ARG:HG3	1.79	0.47
3:D:552:ILE:HD12	3:D:589:TYR:CD1	2.49	0.47
3:D:1036:ARG:CD	3:D:1081:VAL:HG22	2.45	0.47
3:D:1110:GLU:O	3:D:1113:VAL:HG22	2.14	0.47
5:F:131:GLN:OE1	5:F:266:PHE:CE2	2.67	0.47
5:F:600:HIS:HB2	5:F:603:ARG:NH2	2.29	0.47
2:C:106:GLU:HB2	2:C:114:VAL:CG2	2.44	0.47
2:C:1003:THR:HG1	2:C:1005:GLU:CD	2.23	0.47
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.97	0.47
3:D:151:MET:HE1	5:F:306:PHE:HE2	1.80	0.47
4:E:61:ASN:OD1	4:E:62:GLN:N	2.47	0.47
5:F:602:SER:H	5:F:605:GLU:HG2	1.79	0.47
1:B:63:GLY:HA3	1:B:71:LYS:HE2	1.97	0.47
1:B:158:ARG:HE	1:B:172:LEU:HD11	1.79	0.47
2:C:759:SER:HG	2:C:763:THR:N	2.12	0.47
2:C:1304:MET:HE1	2:C:1315:MET:HA	1.97	0.47
3:D:481:ARG:HA	3:D:485:MET:HE2	1.96	0.47
3:D:644:MET:HG2	3:D:644:MET:O	2.15	0.47
3:D:833:GLU:OE1	3:D:1242:ARG:NE	2.35	0.47
3:D:1239:ASP:HA	3:D:1242:ARG:HG2	1.97	0.47
4:E:60:ASN:H	4:E:63:ILE:HG22	1.80	0.47
5:F:132:CYS:HB2	5:F:257:LYS:HG3	1.95	0.47
6:X:41:DA:H2"	6:X:42:DC:C6	2.49	0.47
1:A:14:VAL:HG11	1:A:29:GLU:CD	2.40	0.47
1:B:303:ILE:O	1:B:306:VAL:HG22	2.15	0.47
2:C:185:ASP:HB2	2:C:197:ARG:HG3	1.97	0.47
2:C:237:LEU:CD1	2:C:322:LEU:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:848:VAL:H	3:D:858:VAL:HG22	1.80	0.47
4:E:47:THR:HG23	4:E:48:VAL:N	2.30	0.47
5:F:138:PRO:HG3	5:F:353:LEU:CB	2.43	0.47
1:B:74:VAL:HG12	1:B:133:LEU:HD23	1.97	0.47
2:C:728:ASP:O	2:C:730:SER:N	2.47	0.47
2:C:1258:PRO:CG	3:D:346:ARG:O	2.63	0.47
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.97	0.47
5:F:134:VAL:HG13	5:F:269:LEU:CD2	2.44	0.47
1:B:6:THR:OG1	1:B:7:GLU:N	2.48	0.47
3:D:215:LYS:O	3:D:218:THR:HG22	2.15	0.47
5:F:266:PHE:O	5:F:270:VAL:HG12	2.16	0.47
5:F:543:ALA:HA	5:F:546:ASP:OD1	2.14	0.47
5:F:567:MET:SD	5:F:568:ASN:O	2.73	0.47
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.97	0.46
1:B:75:GLN:HG2	1:B:76:GLU:N	2.29	0.46
2:C:37:LYS:HB3	2:C:47:TYR:CD2	2.50	0.46
2:C:1060:ILE:HD11	2:C:1076:ILE:CD1	2.45	0.46
2:C:1340:GLU:HG2	2:C:1341:ASP:N	2.30	0.46
3:D:339:ARG:HE	3:D:798:ARG:CZ	2.28	0.46
5:F:476:ARG:O	5:F:477:GLU:HB2	2.15	0.46
7:Y:24:DG:H2''	7:Y:25:DG:C8	2.51	0.46
2:C:37:LYS:HB3	2:C:47:TYR:CE2	2.49	0.46
2:C:766:ASN:OD1	2:C:767:GLN:N	2.48	0.46
3:D:45:ASN:O	3:D:46:TYR:CG	2.68	0.46
3:D:214:ARG:O	3:D:218:THR:HG22	2.16	0.46
5:F:466:ILE:HG23	5:F:486:ARG:HG2	1.97	0.46
7:Y:70:DA:H2''	7:Y:71:DT:C5	2.50	0.46
7:Y:73:DA:H2''	7:Y:74:DT:H71	1.96	0.46
9:P:1:DC:H2''	9:P:2:DT:H71	1.97	0.46
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.97	0.46
2:C:561:ILE:O	2:C:680:LEU:HD13	2.15	0.46
2:C:624:ASP:C	2:C:625:GLU:HG3	2.40	0.46
2:C:918:LEU:HD23	2:C:918:LEU:O	2.14	0.46
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.97	0.46
3:D:1136:GLY:HA2	3:D:1140:ARG:HB2	1.97	0.46
6:X:7:DA:H2''	6:X:8:DT:OP2	2.14	0.46
3:D:1145:PHE:HA	3:D:1260:MET:HE1	1.98	0.46
5:F:379:MET:O	5:F:379:MET:HG3	2.16	0.46
1:B:252:ILE:O	1:B:255:ARG:NH1	2.49	0.46
1:B:263:THR:HG23	1:B:266:SER:H	1.81	0.46
2:C:728:ASP:C	2:C:730:SER:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1151:LEU:HD22	2:C:1198:LEU:HD12	1.97	0.46
3:D:1027:VAL:O	3:D:1121:LEU:N	2.42	0.46
5:F:439:ILE:O	5:F:443:ILE:CD1	2.63	0.46
5:F:561:MET:HE2	5:F:571:TYR:HB2	1.98	0.46
1:B:65:LEU:HB3	1:B:168:ILE:CG2	2.46	0.46
2:C:299:LYS:HD3	2:C:301:TYR:CZ	2.51	0.46
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.50	0.46
2:C:989:LEU:HD11	2:C:997:TRP:CG	2.50	0.46
3:D:372:MET:O	3:D:376:LEU:HD23	2.16	0.46
3:D:743:MET:HE2	3:D:758:PRO:HB2	1.96	0.46
3:D:949:SER:HA	3:D:1018:ALA:O	2.16	0.46
3:D:1163:VAL:HG22	3:D:1175:LEU:HD22	1.97	0.46
3:D:1282:TYR:O	3:D:1286:LYS:HG2	2.16	0.46
5:F:139:GLU:OE1	5:F:350:GLU:O	2.33	0.46
5:F:355:ILE:O	5:F:356:GLU:C	2.59	0.46
9:P:14:DT:H2"	9:P:15:DG:H8	1.81	0.46
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.97	0.46
2:C:765:ILE:HG13	2:C:765:ILE:O	2.16	0.46
5:F:322:MET:HE2	5:F:322:MET:HA	1.97	0.46
5:F:332:ASP:OD1	5:F:333:VAL:N	2.49	0.46
2:C:595:THR:O	2:C:598:VAL:N	2.49	0.46
2:C:800:MET:SD	2:C:1096:ILE:HD11	2.56	0.46
2:C:1021:LEU:O	2:C:1024:GLU:HG3	2.15	0.46
3:D:107:LEU:HB3	3:D:240:THR:O	2.15	0.46
3:D:174:ASP:C	3:D:176:PHE:N	2.73	0.46
3:D:809:VAL:HG13	3:D:809:VAL:O	2.15	0.46
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.81	0.46
1:A:293:PRO:HA	6:X:13:DT:H5"	1.98	0.46
2:C:48:GLY:O	2:C:49:LEU:C	2.58	0.46
2:C:183:TRP:H	2:C:199:ASP:HB3	1.80	0.46
2:C:397:LEU:O	2:C:398:SER:HB2	2.15	0.46
2:C:400:VAL:HG23	11:C:1403:1N7:H7	1.97	0.46
2:C:778:GLU:N	2:C:781:ASP:OD2	2.34	0.46
5:F:297:MET:HE2	5:F:302:PHE:N	2.30	0.46
1:A:307:LEU:HB3	1:A:312:LEU:O	2.15	0.46
1:B:278:ILE:O	1:B:282:VAL:HG13	2.16	0.46
2:C:46:GLN:OE1	11:C:1403:1N7:H32	2.16	0.46
3:D:691:ASP:OD2	3:D:691:ASP:C	2.58	0.46
3:D:1108:GLN:HG2	3:D:1109:LEU:N	2.31	0.46
1:B:14:VAL:HG23	1:B:14:VAL:O	2.16	0.45
2:C:93:SER:OG	2:C:94:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:GLU:C	2:C:233:ARG:HH11	2.23	0.45
2:C:239:MET:SD	2:C:240:GLU:O	2.75	0.45
2:C:297:VAL:HG12	2:C:315:MET:O	2.16	0.45
2:C:1292:THR:HG23	2:C:1293:VAL:N	2.32	0.45
3:D:709:ARG:HG3	3:D:710:ASP:H	1.81	0.45
4:E:41:GLU:OE1	4:E:43:ASN:N	2.43	0.45
4:E:71:GLU:OE2	4:E:75:GLN:OE1	2.34	0.45
5:F:119:ILE:O	5:F:123:ILE:HG12	2.15	0.45
5:F:130:VAL:HA	5:F:133:SER:OG	2.16	0.45
5:F:299:LYS:O	5:F:303:ILE:HG12	2.16	0.45
5:F:322:MET:HB3	5:F:324:LYS:HE2	1.98	0.45
5:F:573:LEU:O	5:F:576:VAL:HG12	2.16	0.45
1:A:228:LEU:O	1:A:232:VAL:HG23	2.16	0.45
2:C:242:VAL:HB	2:C:245:ARG:HB2	1.98	0.45
2:C:594:VAL:HG23	2:C:652:TYR:HA	1.99	0.45
3:D:78:LEU:HB3	3:D:81:ARG:NH2	2.32	0.45
3:D:357:VAL:HG13	3:D:358:GLY:N	2.31	0.45
3:D:714:GLU:HG2	3:D:715:LYS:H	1.80	0.45
3:D:885:VAL:HG12	3:D:1254:GLU:HB3	1.97	0.45
5:F:138:PRO:CG	5:F:353:LEU:HB2	2.45	0.45
1:B:219:ARG:O	1:B:223:ILE:HG13	2.17	0.45
2:C:466:VAL:O	2:C:469:VAL:HG22	2.16	0.45
2:C:800:MET:HE1	2:C:828:PHE:CE2	2.52	0.45
3:D:47:ARG:HE	3:D:47:ARG:HA	1.82	0.45
3:D:525:MET:O	3:D:548:VAL:HG13	2.16	0.45
4:E:63:ILE:O	4:E:66:VAL:HG22	2.16	0.45
5:F:310:GLU:O	5:F:310:GLU:HG2	2.16	0.45
9:P:14:DT:C2	9:P:15:DG:N7	2.84	0.45
1:A:197:ASP:OD1	1:A:197:ASP:N	2.49	0.45
1:A:290:LEU:HD22	1:A:300:LEU:HD22	1.98	0.45
1:B:290:LEU:HD11	1:B:300:LEU:HD22	1.97	0.45
2:C:107:ARG:HA	2:C:108:GLU:HA	1.65	0.45
2:C:402:ARG:HG2	2:C:416:GLY:N	2.32	0.45
2:C:764:CYS:SG	2:C:833:ILE:HG13	2.56	0.45
2:C:1080:ASN:HB2	2:C:1085:MET:HE3	1.98	0.45
3:D:743:MET:HE3	3:D:760:THR:HA	1.97	0.45
3:D:915:ILE:O	3:D:918:ILE:HG12	2.16	0.45
3:D:1161:GLY:HA3	3:D:1178:THR:O	2.16	0.45
4:E:63:ILE:HA	4:E:66:VAL:HG22	1.99	0.45
5:F:449:THR:HG23	5:F:450:ILE:N	2.32	0.45
5:F:584:ARG:NE	5:F:584:ARG:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:51:DT:H2''	7:Y:52:DG:H8	1.81	0.45
1:A:14:VAL:HG12	1:A:27:THR:O	2.17	0.45
1:B:137:ASN:O	1:B:138:ALA:C	2.59	0.45
1:B:264:VAL:HG12	1:B:268:ASN:OD1	2.17	0.45
2:C:309:LEU:HD11	2:C:311:CYS:O	2.16	0.45
2:C:519:ASN:OD1	2:C:520:PRO:HD2	2.16	0.45
2:C:545:PHE:O	2:C:546:GLU:C	2.59	0.45
3:D:256:ASP:OD1	3:D:256:ASP:N	2.49	0.45
3:D:530:PRO:O	3:D:533:ALA:HB3	2.17	0.45
3:D:1050:THR:HA	3:D:1057:SER:HA	1.98	0.45
3:D:1181:ASP:OD1	3:D:1181:ASP:N	2.47	0.45
5:F:144:LEU:HD11	5:F:256:PHE:CE1	2.51	0.45
1:B:38:THR:HG23	1:B:39:LEU:N	2.32	0.45
1:B:104:LYS:NZ	1:B:114:ASP:OD2	2.50	0.45
2:C:1319:MET:HA	2:C:1319:MET:HE2	1.99	0.45
11:C:1403:1N7:H5	11:C:1403:1N7:H31	1.97	0.45
3:D:61:ILE:HG23	3:D:62:PHE:N	2.32	0.45
3:D:532:GLU:O	3:D:535:ARG:HB2	2.17	0.45
3:D:1003:LEU:HD12	3:D:1017:VAL:O	2.17	0.45
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.97	0.45
1:B:20:SER:HG	1:B:23:HIS:HB3	1.81	0.45
1:B:267:ALA:O	1:B:270:LEU:HG	2.16	0.45
3:D:807:LEU:HD21	3:D:1259:GLN:CD	2.42	0.45
4:E:34:GLY:O	4:E:35:LYS:HD2	2.16	0.45
5:F:445:ASP:OD1	5:F:446:GLN:N	2.49	0.45
2:C:901:LEU:O	2:C:905:ILE:HG13	2.17	0.45
2:C:972:PHE:HD2	2:C:994:ARG:HE	1.64	0.45
3:D:124:ILE:HG12	3:D:237:MET:HE2	1.97	0.45
3:D:146:VAL:O	3:D:156:ARG:O	2.35	0.45
3:D:210:SER:O	3:D:214:ARG:HG3	2.16	0.45
3:D:334:LYS:O	3:D:340:GLN:HB2	2.17	0.45
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.50	0.45
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	1.98	0.45
8:O:3:DA:H2''	8:O:4:DC:H5'	1.98	0.45
2:C:138:ILE:HG21	2:C:143:ARG:HD2	1.98	0.45
2:C:353:VAL:O	2:C:355:PRO:HD3	2.15	0.45
2:C:561:ILE:HD13	2:C:661:VAL:HG12	1.99	0.45
2:C:782:VAL:HG13	2:C:782:VAL:O	2.17	0.45
3:D:1080:ILE:HG22	3:D:1088:VAL:CG2	2.47	0.45
5:F:137:TYR:HB2	5:F:361:ILE:HD13	1.97	0.45
5:F:252:LEU:HA	5:F:255:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:CD1	1:A:303:ILE:HG12	2.47	0.45
1:B:190:ALA:O	1:B:198:LEU:HB2	2.17	0.45
2:C:813:GLU:O	2:C:815:SER:N	2.50	0.45
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.17	0.45
3:D:414:GLU:O	4:E:45:LYS:NZ	2.41	0.45
3:D:710:ASP:OD1	3:D:711:GLY:N	2.50	0.45
3:D:822:MET:SD	3:D:838:ARG:NH2	2.89	0.45
3:D:860:ARG:O	3:D:861:ASN:C	2.60	0.45
3:D:1146:GLU:OE2	3:D:1310:THR:HG23	2.17	0.45
5:F:305:LEU:HD12	5:F:306:PHE:N	2.31	0.45
5:F:612:ASP:OD1	5:F:612:ASP:N	2.49	0.45
9:P:16:DT:H2"	9:P:17:DC:C6	2.52	0.45
1:B:61:ILE:HG22	1:B:63:GLY:H	1.81	0.44
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.98	0.44
3:D:141:PHE:HA	3:D:180:MET:HG2	1.99	0.44
3:D:930:LEU:HD11	3:D:1244:GLN:HG2	1.98	0.44
3:D:1158:GLU:O	3:D:1206:ARG:HB2	2.17	0.44
3:D:1198:VAL:HG21	3:D:1204:VAL:CG1	2.47	0.44
4:E:70:GLN:O	4:E:74:GLU:HG3	2.16	0.44
5:F:161:LEU:O	5:F:260:ARG:N	2.49	0.44
5:F:166:VAL:HG11	5:F:257:LYS:HZ2	1.82	0.44
5:F:309:ASN:CG	5:F:310:GLU:H	2.25	0.44
1:B:102:LEU:CD2	1:B:115:ILE:HA	2.48	0.44
1:B:281:LEU:O	1:B:282:VAL:C	2.59	0.44
2:C:239:MET:HE1	2:C:241:LEU:HD12	1.99	0.44
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.44
2:C:615:VAL:HG12	2:C:638:SER:HB2	1.98	0.44
2:C:1254:VAL:HG13	2:C:1255:THR:N	2.32	0.44
3:D:45:ASN:C	3:D:47:ARG:H	2.24	0.44
3:D:1350:ASN:OD1	3:D:1358:PRO:HD3	2.17	0.44
4:E:51:LEU:O	4:E:55:GLU:HG3	2.18	0.44
5:F:250:LEU:O	5:F:254:GLU:HG2	2.16	0.44
1:B:57:THR:O	1:B:173:VAL:N	2.44	0.44
2:C:413:GLU:OE2	2:C:415:GLU:O	2.35	0.44
2:C:705:GLU:OE1	2:C:705:GLU:N	2.45	0.44
2:C:996:ARG:C	2:C:997:TRP:HD1	2.26	0.44
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	2.00	0.44
3:D:1254:GLU:O	3:D:1257:VAL:HG22	2.17	0.44
5:F:148:TYR:CE2	5:F:221:PHE:CD2	3.06	0.44
5:F:320:ILE:HG23	5:F:328:GLU:HG2	1.98	0.44
5:F:479:THR:O	5:F:482:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:583:THR:O	5:F:584:ARG:HB2	2.17	0.44
9:P:17:DC:H2'	9:P:18:DA:C8	2.52	0.44
2:C:246:LEU:HD12	2:C:246:LEU:H	1.81	0.44
2:C:1043:ALA:O	2:C:1046:VAL:HG22	2.17	0.44
3:D:38:VAL:O	3:D:38:VAL:HG13	2.17	0.44
3:D:473:THR:HG23	3:D:476:ALA:H	1.83	0.44
3:D:902:ASP:O	3:D:903:LEU:HG	2.17	0.44
5:F:380:VAL:O	5:F:381:GLU:C	2.59	0.44
2:C:267:ARG:HD3	2:C:268:ARG:O	2.17	0.44
2:C:296:VAL:O	2:C:335:THR:HA	2.18	0.44
2:C:685:MET:SD	2:C:1073:LYS:HD3	2.58	0.44
3:D:88:CYS:C	3:D:90:VAL:H	2.25	0.44
3:D:510:LEU:O	3:D:514:THR:HG22	2.18	0.44
3:D:831:VAL:O	3:D:831:VAL:HG13	2.17	0.44
3:D:1267:VAL:O	3:D:1274:PHE:CZ	2.70	0.44
5:F:133:SER:OG	5:F:365:MET:HG2	2.18	0.44
1:A:67:GLU:O	1:A:78:ILE:HB	2.18	0.44
1:A:195:ARG:HE	1:A:196:THR:H	1.66	0.44
2:C:184:LEU:HD11	2:C:389:PHE:CE1	2.53	0.44
2:C:511:LEU:HD23	2:C:511:LEU:H	1.83	0.44
2:C:1270:PHE:CE1	2:C:1274:GLU:HB3	2.53	0.44
3:D:235:GLU:H	3:D:235:GLU:CD	2.26	0.44
3:D:834:PRO:O	3:D:837:ASP:OD2	2.35	0.44
3:D:1105:ALA:HB1	3:D:1122:ALA:HB1	1.98	0.44
5:F:128:ASN:HB3	5:F:257:LYS:HG2	2.00	0.44
1:B:205:MET:HE3	1:B:213:PRO:HB3	2.00	0.44
2:C:230:PHE:CE1	2:C:239:MET:HB2	2.53	0.44
2:C:319:LEU:O	2:C:322:LEU:HG	2.18	0.44
3:D:322:ARG:NH1	5:F:510:PRO:HD2	2.33	0.44
3:D:587:LEU:HD21	3:D:608:CYS:HA	1.99	0.44
3:D:639:VAL:O	3:D:639:VAL:HG23	2.18	0.44
3:D:1067:ARG:HH12	3:D:1075:ARG:HG3	1.83	0.44
5:F:309:ASN:O	5:F:311:THR:HG23	2.18	0.44
5:F:423:ARG:HG2	5:F:423:ARG:HH21	1.83	0.44
5:F:596:ARG:HA	5:F:599:ARG:HG2	2.00	0.44
1:A:124:VAL:HG11	1:A:209:GLY:O	2.18	0.44
1:B:25:LYS:HD2	1:B:204:GLU:OE2	2.17	0.44
2:C:189:ASP:OD1	2:C:192:ASP:N	2.51	0.44
2:C:263:VAL:HG11	2:C:269:ILE:HG12	2.00	0.44
2:C:371:ARG:HB2	2:C:374:GLU:OE2	2.18	0.44
2:C:808:ASN:O	2:C:810:TYR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1160:ASP:HB2	2:C:1162:SER:H	1.82	0.44
3:D:355:ILE:HG21	3:D:466:MET:SD	2.57	0.44
3:D:769:VAL:HG23	3:D:770:LEU:H	1.82	0.44
1:A:235:ARG:C	1:A:237:VAL:N	2.75	0.44
2:C:120:GLN:H	2:C:120:GLN:CD	2.24	0.44
2:C:178:PRO:HD2	2:C:183:TRP:CD1	2.53	0.44
2:C:624:ASP:O	2:C:625:GLU:HG3	2.18	0.44
2:C:813:GLU:C	2:C:815:SER:N	2.75	0.44
2:C:1337:ILE:HD11	3:D:20:ILE:HG22	1.99	0.44
3:D:343:LEU:HD11	3:D:1352:ILE:CD1	2.48	0.44
3:D:416:ILE:CG2	3:D:439:PRO:HG2	2.48	0.44
1:B:12:ARG:O	1:B:29:GLU:O	2.35	0.43
2:C:90:VAL:HG12	2:C:91:THR:N	2.32	0.43
2:C:233:ARG:NH2	2:C:284:LEU:HD11	2.33	0.43
2:C:934:PHE:HB3	2:C:1040:ASP:OD2	2.18	0.43
2:C:1293:VAL:HG11	2:C:1304:MET:HE3	2.00	0.43
3:D:197:GLU:OE2	3:D:220:ARG:NH1	2.44	0.43
3:D:268:LEU:HD11	3:D:324:LEU:CD1	2.48	0.43
3:D:502:PRO:HB3	3:D:506:VAL:CG2	2.48	0.43
1:B:65:LEU:HB3	1:B:168:ILE:HG22	1.99	0.43
2:C:323:ALA:O	2:C:327:GLN:CD	2.61	0.43
3:D:1159:ILE:HG12	3:D:1177:ILE:HD12	1.99	0.43
5:F:496:LYS:O	5:F:500:ILE:HG12	2.18	0.43
7:Y:53:DA:C4	7:Y:54:DC:C5	3.05	0.43
1:A:91:ARG:HD2	1:A:210:THR:HA	2.01	0.43
1:B:107:ILE:HG12	1:B:135:ASP:HA	2.01	0.43
1:B:296:GLY:CA	6:X:11:DT:OP1	2.64	0.43
2:C:262:TYR:HB3	2:C:277:LEU:HD11	2.00	0.43
2:C:393:ASP:OD2	2:C:394:ARG:N	2.50	0.43
2:C:499:SER:HA	2:C:502:VAL:HG22	1.98	0.43
2:C:821:ARG:HB2	2:C:1082:ILE:HD13	1.99	0.43
2:C:1270:PHE:CE2	2:C:1290:MET:SD	3.11	0.43
3:D:225:GLU:HA	3:D:228:VAL:HG22	2.00	0.43
3:D:1011:VAL:HG12	3:D:1015:GLU:HB3	2.00	0.43
5:F:141:ILE:HD12	5:F:141:ILE:H	1.84	0.43
5:F:261:LEU:HB2	5:F:266:PHE:CD2	2.53	0.43
2:C:158:ASP:OD1	2:C:159:SER:N	2.51	0.43
2:C:254:ASP:OD1	2:C:254:ASP:N	2.51	0.43
2:C:474:ALA:HA	2:C:477:GLU:OE1	2.19	0.43
3:D:259:ARG:NE	5:F:505:ILE:HD11	2.34	0.43
3:D:316:ILE:HG22	3:D:317:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:714:GLU:HG2	3:D:715:LYS:N	2.33	0.43
3:D:1042:ASP:HB3	3:D:1048:ARG:HB2	2.00	0.43
5:F:140:ALA:O	5:F:144:LEU:HB2	2.18	0.43
5:F:400:GLN:O	5:F:401:PHE:C	2.60	0.43
1:A:242:VAL:HG23	1:A:242:VAL:O	2.18	0.43
1:A:262:LEU:CD2	1:A:306:VAL:HG21	2.48	0.43
1:A:298:LYS:HD3	6:X:12:DT:OP1	2.18	0.43
1:B:299:SER:O	1:B:303:ILE:HG12	2.18	0.43
2:C:106:GLU:HB2	2:C:114:VAL:HG21	1.98	0.43
2:C:320:ASP:OD1	2:C:320:ASP:N	2.51	0.43
2:C:836:LEU:HD21	2:C:921:PRO:HD3	2.00	0.43
2:C:1142:ARG:NH2	2:C:1169:VAL:HG21	2.33	0.43
3:D:571:ASP:OD1	3:D:571:ASP:N	2.43	0.43
3:D:654:ILE:O	3:D:658:GLU:HG3	2.18	0.43
3:D:1059:LEU:HD12	3:D:1110:GLU:OE2	2.18	0.43
5:F:313:ASP:OD1	5:F:341:LEU:HG	2.18	0.43
5:F:356:GLU:CD	5:F:356:GLU:H	2.27	0.43
5:F:360:ASP:O	5:F:364:ARG:NE	2.41	0.43
9:P:11:DC:H2"	9:P:12:DC:C6	2.53	0.43
9:P:11:DC:C2	9:P:12:DC:C4	3.06	0.43
1:A:129:VAL:HG21	1:A:132:HIS:CE1	2.51	0.43
1:B:182:ARG:NH1	3:D:581:MET:HE3	2.34	0.43
3:D:147:ILE:O	3:D:177:ASP:HB2	2.18	0.43
4:E:32:VAL:O	4:E:32:VAL:HG13	2.19	0.43
6:X:32:DG:H2"	6:X:33:DC:C5	2.54	0.43
1:A:278:ILE:O	1:A:282:VAL:HG23	2.19	0.43
2:C:71:VAL:HG21	2:C:118:LYS:NZ	2.34	0.43
2:C:209:ILE:O	2:C:213:LEU:HD13	2.19	0.43
2:C:708:VAL:HG21	2:C:794:LEU:HD22	1.99	0.43
2:C:1298:VAL:HG13	2:C:1299:ASN:N	2.34	0.43
3:D:348:ASP:O	3:D:349:TYR:C	2.62	0.43
3:D:416:ILE:O	3:D:417:ARG:C	2.62	0.43
3:D:1003:LEU:HA	3:D:1017:VAL:O	2.18	0.43
5:F:586:ARG:HH12	6:X:24:DC:P	2.38	0.43
3:D:271:ARG:HH12	3:D:315:ALA:HB1	1.83	0.43
3:D:502:PRO:HB3	3:D:506:VAL:HG21	2.01	0.43
3:D:649:LYS:HD2	3:D:649:LYS:N	2.34	0.43
3:D:844:THR:OG1	3:D:861:ASN:HA	2.19	0.43
3:D:1062:LEU:HB2	3:D:1067:ARG:HA	2.00	0.43
5:F:127:ILE:HA	5:F:130:VAL:HG12	2.00	0.43
5:F:302:PHE:O	5:F:306:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:55:DA:H2"	7:Y:56:DA:OP2	2.18	0.43
2:C:596:ASP:OD1	2:C:597:GLY:N	2.51	0.43
2:C:882:ILE:HG23	2:C:917:SER:OG	2.19	0.43
3:D:143:SER:HB2	3:D:160:LEU:O	2.19	0.43
3:D:844:THR:CG2	3:D:864:LEU:HD21	2.48	0.43
3:D:978:ARG:CZ	3:D:1197:ASN:O	2.67	0.43
5:F:119:ILE:HD13	5:F:379:MET:HG2	2.01	0.43
5:F:262:VAL:HG21	5:F:264:LYS:HE3	2.00	0.43
5:F:355:ILE:O	5:F:358:VAL:HG12	2.19	0.43
1:B:41:ASN:ND2	2:C:1217:THR:O	2.44	0.43
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.01	0.43
2:C:590:PRO:HB2	2:C:655:VAL:HG21	2.01	0.43
3:D:270:ARG:O	3:D:273:ILE:HG22	2.19	0.43
8:O:17:DA:H2"	8:O:18:DG:C8	2.54	0.43
9:P:3:DC:H2"	9:P:4:DG:C8	2.54	0.43
1:A:253:LEU:HD12	1:A:279:GLY:HA2	2.01	0.42
2:C:397:LEU:O	2:C:398:SER:CB	2.67	0.42
2:C:673:HIS:ND1	3:D:765:GLU:O	2.51	0.42
2:C:895:LEU:HB2	2:C:899:GLU:CD	2.44	0.42
3:D:92:VAL:O	3:D:92:VAL:HG13	2.19	0.42
3:D:173:GLY:CA	5:F:366:SER:HB3	2.49	0.42
3:D:567:THR:HG23	3:D:567:THR:O	2.19	0.42
3:D:909:ILE:HD11	3:D:913:GLU:HB3	2.01	0.42
5:F:326:TRP:O	5:F:330:LEU:HG	2.19	0.42
8:O:3:DA:C6	8:O:4:DC:C4	3.07	0.42
1:A:47:LEU:O	1:A:51:MET:HG2	2.19	0.42
1:B:251:PRO:O	1:B:254:LEU:CD2	2.67	0.42
1:B:296:GLY:HA3	6:X:11:DT:P	2.59	0.42
2:C:231:GLU:CB	2:C:233:ARG:HH11	2.31	0.42
2:C:745:GLU:OE1	2:C:1017:GLN:HG2	2.18	0.42
2:C:812:PHE:HE2	3:D:454:CYS:HG	1.67	0.42
2:C:896:THR:HG23	2:C:899:GLU:HG2	2.01	0.42
2:C:989:LEU:O	2:C:992:LEU:HG	2.19	0.42
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.83	0.42
3:D:806:ASP:OD2	3:D:806:ASP:N	2.52	0.42
3:D:858:VAL:HG23	3:D:858:VAL:O	2.19	0.42
3:D:987:GLU:OE1	3:D:987:GLU:N	2.41	0.42
3:D:1171:GLY:O	3:D:1172:LYS:HG3	2.20	0.42
4:E:65:ASP:CA	4:E:68:GLU:OE1	2.66	0.42
7:Y:54:DC:H2"	7:Y:55:DA:H8	1.84	0.42
9:P:9:DG:C8	9:P:10:DT:H72	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:O	1:A:248:GLU:C	2.62	0.42
1:A:263:THR:O	1:A:264:VAL:C	2.62	0.42
1:B:23:HIS:HA	1:B:206:GLU:HG2	2.00	0.42
1:B:71:LYS:HB3	1:B:74:VAL:CG2	2.48	0.42
1:B:265:ARG:H	7:Y:74:DT:H5"	1.84	0.42
1:B:283:GLN:O	1:B:283:GLN:HG3	2.19	0.42
2:C:256:GLU:HB3	2:C:261:VAL:HA	2.01	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.01	0.42
2:C:883:LEU:HD21	2:C:1052:VAL:HG21	2.01	0.42
2:C:233:ARG:NH2	2:C:284:LEU:CD1	2.82	0.42
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.54	0.42
2:C:1285:TYR:CD1	3:D:1356:LEU:HD21	2.55	0.42
3:D:218:THR:O	3:D:221:ILE:HG22	2.19	0.42
3:D:265:LEU:HD11	3:D:330:MET:HE1	2.00	0.42
3:D:697:MET:HE2	3:D:741:ALA:HB3	2.00	0.42
5:F:425:TYR:CE2	5:F:429:THR:HG23	2.55	0.42
6:X:57:DC:H2"	6:X:58:DA:C8	2.54	0.42
7:Y:27:DG:C4	7:Y:28:DC:C4	3.07	0.42
1:A:212:ASP:OD1	1:A:215:GLU:HB3	2.20	0.42
1:B:192:VAL:HG23	1:B:198:LEU:HG	2.01	0.42
2:C:302:ILE:HA	2:C:309:LEU:HA	2.01	0.42
2:C:802:VAL:HG12	2:C:1096:ILE:HB	2.01	0.42
3:D:111:THR:HG21	3:D:303:VAL:HG11	2.00	0.42
3:D:1023:HIS:O	3:D:1024:THR:OG1	2.35	0.42
2:C:196:VAL:HG11	2:C:209:ILE:HG12	2.00	0.42
2:C:216:THR:OG1	2:C:219:GLN:HB2	2.19	0.42
2:C:464:PHE:CE2	2:C:468:LEU:HD21	2.55	0.42
2:C:1164:PHE:CE1	2:C:1167:GLU:N	2.85	0.42
11:C:1402:1N7:H18	11:C:1402:1N7:H24	2.00	0.42
3:D:45:ASN:O	3:D:46:TYR:CD1	2.72	0.42
3:D:74:LYS:NZ	3:D:86:GLU:OE1	2.50	0.42
5:F:339:ARG:HA	5:F:339:ARG:NE	2.35	0.42
5:F:473:GLU:CD	5:F:474:MET:N	2.77	0.42
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.19	0.42
7:Y:50:DC:H2"	7:Y:51:DT:C7	2.50	0.42
1:B:293:PRO:O	1:B:294:ASN:HB2	2.20	0.42
2:C:44:GLU:O	2:C:44:GLU:HG2	2.20	0.42
2:C:66:SER:O	2:C:479:LEU:HD21	2.19	0.42
2:C:835:GLU:C	2:C:836:LEU:HD12	2.45	0.42
2:C:905:ILE:HG23	5:F:598:LEU:CD1	2.49	0.42
2:C:975:ILE:HG13	2:C:1014:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1125:GLY:O	2:C:1128:ILE:HG22	2.19	0.42
2:C:1304:MET:HE1	2:C:1314:GLN:O	2.20	0.42
3:D:294:ASN:O	3:D:298:MET:HE2	2.19	0.42
3:D:342:LEU:C	3:D:343:LEU:HD12	2.45	0.42
3:D:704:GLU:O	3:D:706:VAL:HG23	2.19	0.42
3:D:749:LYS:HG2	3:D:753:SER:O	2.19	0.42
5:F:320:ILE:HD12	5:F:328:GLU:HA	2.01	0.42
3:D:45:ASN:C	3:D:46:TYR:CD1	2.98	0.42
3:D:162:GLU:O	3:D:166:LEU:HG	2.20	0.42
3:D:204:GLU:OE1	3:D:217:LEU:HD22	2.19	0.42
3:D:1144:LEU:HD11	3:D:1236:GLU:HG2	2.01	0.42
4:E:6:VAL:O	4:E:10:VAL:HG23	2.20	0.42
5:F:138:PRO:HG2	5:F:351:THR:OG1	2.19	0.42
5:F:344:LEU:HD21	5:F:355:ILE:HD11	2.01	0.42
5:F:360:ASP:HB3	5:F:364:ARG:NH2	2.34	0.42
6:X:53:DG:H2"	6:X:54:DC:C6	2.54	0.42
1:B:281:LEU:HD22	1:B:307:LEU:HD21	2.02	0.42
3:D:259:ARG:CZ	5:F:505:ILE:HD11	2.50	0.42
3:D:1316:THR:HG22	3:D:1317:GLU:N	2.35	0.42
5:F:333:VAL:HG22	5:F:333:VAL:O	2.19	0.42
5:F:393:LYS:HD3	5:F:393:LYS:C	2.45	0.42
1:A:295:LEU:O	6:X:13:DT:OP1	2.38	0.42
1:B:59:VAL:HG23	1:B:143:ARG:O	2.20	0.42
1:B:106:GLY:O	1:B:138:ALA:HB1	2.20	0.42
2:C:529:ARG:HD3	2:C:572:ILE:HG23	2.02	0.42
2:C:696:ASP:O	2:C:790:ASP:CB	2.68	0.42
2:C:982:GLY:HA3	2:C:1002:LEU:HD11	2.02	0.42
3:D:155:GLU:CD	3:D:157:GLN:H	2.27	0.42
3:D:370:LYS:HD2	3:D:443:GLU:OE2	2.19	0.42
3:D:793:SER:HB3	3:D:927:GLY:O	2.20	0.42
3:D:850:LYS:C	3:D:852:GLY:N	2.77	0.42
3:D:930:LEU:H	3:D:930:LEU:HD12	1.84	0.42
3:D:1002:VAL:HB	3:D:1019:ASN:HB2	2.01	0.42
4:E:6:VAL:HG22	4:E:9:ALA:HB3	2.01	0.42
5:F:279:ARG:NH1	5:F:343:LYS:HB3	2.34	0.42
5:F:487:MET:HG2	5:F:489:MET:HE2	2.02	0.42
5:F:552:THR:OG1	5:F:555:GLU:HB2	2.19	0.42
2:C:131:THR:HG22	2:C:132:ASP:H	1.85	0.41
2:C:489:PRO:HA	2:C:492:MET:HE2	2.02	0.41
2:C:595:THR:O	2:C:596:ASP:C	2.62	0.41
2:C:1083:GLU:OE1	2:C:1083:GLU:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.45	0.41
2:C:1164:PHE:HE1	2:C:1167:GLU:H	1.62	0.41
2:C:1245:ALA:HB1	3:D:376:LEU:HD22	2.02	0.41
2:C:1247:SER:HB3	3:D:375:GLU:O	2.20	0.41
3:D:641:ILE:O	3:D:644:MET:SD	2.77	0.41
3:D:1065:ALA:HB2	3:D:1173:ARG:HB2	2.02	0.41
3:D:1169:THR:HG23	3:D:1169:THR:O	2.20	0.41
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.44	0.41
4:E:47:THR:CG2	4:E:48:VAL:N	2.83	0.41
5:F:142:THR:HG22	5:F:146:GLU:OE2	2.20	0.41
5:F:224:LEU:HA	5:F:252:LEU:HD11	2.02	0.41
9:P:16:DT:C2	9:P:17:DC:C4	3.08	0.41
1:A:311:GLY:C	1:A:312:LEU:HD12	2.45	0.41
1:B:56:VAL:HG11	1:B:85:LEU:HD13	2.01	0.41
2:C:551:HIS:H	2:C:554:HIS:CE1	2.38	0.41
2:C:1120:ALA:HB1	2:C:1198:LEU:CD2	2.50	0.41
2:C:1255:THR:O	2:C:1255:THR:HG23	2.20	0.41
3:D:573:THR:HG1	3:D:576:ARG:H	1.67	0.41
3:D:674:THR:OG1	3:D:677:GLU:HG3	2.20	0.41
3:D:804:ALA:O	3:D:916:GLY:HA3	2.19	0.41
3:D:1159:ILE:H	3:D:1177:ILE:HD12	1.84	0.41
9:P:12:DC:H2''	9:P:13:DG:C8	2.55	0.41
1:A:214:GLU:O	1:A:217:ILE:HG22	2.20	0.41
1:B:48:LEU:CD1	3:D:535:ARG:HD2	2.49	0.41
2:C:292:ILE:C	2:C:294:GLY:H	2.29	0.41
2:C:560:PRO:HB2	3:D:776:THR:HG21	2.01	0.41
3:D:19:ALA:HA	3:D:1343:GLU:HA	2.02	0.41
3:D:641:ILE:O	3:D:764:ARG:NH1	2.53	0.41
3:D:708:ASN:HA	3:D:713:GLU:HA	2.02	0.41
3:D:1226:VAL:O	3:D:1229:VAL:HG12	2.20	0.41
5:F:335:GLU:O	5:F:339:ARG:HG2	2.20	0.41
5:F:415:ALA:HB2	5:F:434:TRP:HB2	2.01	0.41
5:F:573:LEU:HD23	7:Y:52:DG:OP2	2.21	0.41
7:Y:55:DA:C4	7:Y:56:DA:C8	3.09	0.41
2:C:595:THR:HB	2:C:598:VAL:HG13	2.02	0.41
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	2.02	0.41
3:D:126:LEU:HD21	3:D:220:ARG:HA	2.02	0.41
3:D:137:ARG:O	3:D:142:GLU:HB3	2.21	0.41
3:D:589:TYR:O	3:D:590:SER:C	2.61	0.41
6:X:1:DC:H2''	6:X:2:DA:C8	2.55	0.41
7:Y:74:DT:C2'	7:Y:75:DT:H71	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.02	0.41
2:C:14:ASP:HB3	2:C:1157:GLN:OE1	2.20	0.41
2:C:222:ASP:HA	2:C:227:LYS:CE	2.50	0.41
2:C:239:MET:SD	2:C:240:GLU:C	3.04	0.41
2:C:275:ARG:O	2:C:279:LYS:HG2	2.21	0.41
2:C:453:ILE:HG22	2:C:585:GLY:O	2.20	0.41
2:C:1002:LEU:HD12	2:C:1003:THR:H	1.86	0.41
3:D:43:THR:HG23	3:D:44:ILE:N	2.35	0.41
3:D:532:GLU:O	3:D:536:LEU:HD23	2.20	0.41
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.35	0.41
3:D:1036:ARG:CD	3:D:1081:VAL:HG21	2.51	0.41
3:D:1073:ASP:OD1	3:D:1073:ASP:N	2.47	0.41
5:F:123:ILE:O	5:F:127:ILE:HG12	2.20	0.41
5:F:148:TYR:CD2	5:F:161:LEU:HD21	2.54	0.41
1:A:28:LEU:HB3	1:A:31:LEU:HD21	2.03	0.41
1:A:78:ILE:O	1:A:82:LEU:HD13	2.21	0.41
1:B:83:LEU:HD21	3:D:526:VAL:CG1	2.50	0.41
1:B:205:MET:HE1	1:B:213:PRO:HA	2.03	0.41
2:C:122:VAL:HG21	2:C:493:ILE:HD11	2.02	0.41
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.82	0.41
2:C:809:GLY:O	3:D:359:PRO:HG3	2.20	0.41
2:C:1323:PHE:CZ	2:C:1327:LEU:HD11	2.56	0.41
3:D:167:ASP:O	3:D:170:GLU:HG3	2.19	0.41
3:D:262:THR:HB	3:D:266:ASN:OD1	2.21	0.41
3:D:557:LYS:HB3	3:D:563:LEU:HD23	2.01	0.41
7:Y:27:DG:H2''	7:Y:28:DC:C6	2.56	0.41
1:A:301:THR:HG21	1:B:291:LYS:CD	2.51	0.41
1:B:67:GLU:HG3	1:B:171:LEU:HD22	2.02	0.41
1:B:298:LYS:NZ	6:X:10:A:OP1	2.44	0.41
2:C:28:LEU:O	2:C:29:SER:C	2.63	0.41
2:C:56:VAL:HG13	2:C:57:PHE:N	2.36	0.41
3:D:1108:GLN:HG2	3:D:1109:LEU:H	1.86	0.41
5:F:291:CYS:O	5:F:296:LYS:N	2.48	0.41
5:F:595:LEU:O	5:F:598:LEU:HG	2.21	0.41
7:Y:28:DC:C2	7:Y:29:DA:C5	3.08	0.41
1:A:51:MET:CE	1:A:216:ALA:HA	2.51	0.41
1:B:222:THR:O	1:B:226:GLU:HG2	2.21	0.41
2:C:43:PRO:HG2	2:C:44:GLU:OE1	2.21	0.41
2:C:159:SER:O	2:C:171:LEU:O	2.39	0.41
2:C:321:LEU:O	2:C:325:LEU:HD23	2.20	0.41
2:C:560:PRO:O	3:D:780:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:726:TYR:HB3	2:C:733:VAL:HB	2.03	0.41
2:C:1105:SER:HA	3:D:736:GLN:OE1	2.21	0.41
11:C:1402:1N7:H14	11:C:1402:1N7:H29	1.83	0.41
3:D:53:ARG:HA	3:D:54:ASP:HA	1.77	0.41
3:D:62:PHE:O	3:D:101:ARG:HD2	2.20	0.41
3:D:377:PHE:O	3:D:378:LYS:C	2.64	0.41
3:D:572:THR:OG1	3:D:573:THR:N	2.54	0.41
3:D:643:ASP:O	3:D:720:ASN:ND2	2.46	0.41
3:D:770:LEU:HD12	3:D:771:GLN:N	2.36	0.41
3:D:809:VAL:HG13	3:D:912:GLY:H	1.86	0.41
3:D:966:VAL:HG23	3:D:974:VAL:CG1	2.49	0.41
5:F:400:GLN:O	5:F:403:ASP:N	2.53	0.41
6:X:36:DG:H2"	6:X:37:DA:C8	2.56	0.41
7:Y:71:DT:C4	7:Y:72:DA:N6	2.88	0.41
9:P:5:DT:C2	9:P:6:DA:C5	3.09	0.41
9:P:10:DT:H2"	9:P:11:DC:C6	2.55	0.41
1:A:78:ILE:HA	1:A:81:ILE:HD12	2.02	0.41
1:A:149:GLY:O	1:A:177:TYR:HB3	2.20	0.41
1:B:242:VAL:HG12	1:B:243:LYS:N	2.34	0.41
1:B:294:ASN:HA	6:X:11:DT:H5"	2.03	0.41
2:C:302:ILE:HG22	2:C:309:LEU:HD13	2.02	0.41
2:C:436:ARG:O	2:C:436:ARG:NH1	2.53	0.41
2:C:444:ASP:OD1	2:C:444:ASP:N	2.50	0.41
2:C:572:ILE:O	2:C:573:ASN:C	2.63	0.41
2:C:625:GLU:OE1	2:C:626:GLU:HG3	2.21	0.41
2:C:700:VAL:CG1	2:C:1117:LEU:HD22	2.50	0.41
2:C:759:SER:OG	2:C:763:THR:N	2.52	0.41
2:C:1340:GLU:HB3	3:D:19:ALA:O	2.20	0.41
3:D:334:LYS:NZ	9:P:18:DA:OP1	2.46	0.41
3:D:780:ARG:HG2	3:D:780:ARG:HH11	1.86	0.41
3:D:807:LEU:HD21	3:D:1259:GLN:OE1	2.21	0.41
3:D:1021:ASP:CG	3:D:1024:THR:HB	2.45	0.41
3:D:1036:ARG:HD3	3:D:1081:VAL:CG2	2.51	0.41
3:D:1172:LYS:O	3:D:1189:MET:SD	2.78	0.41
3:D:1298:VAL:N	3:D:1299:GLY:CA	2.84	0.41
4:E:63:ILE:HD12	4:E:66:VAL:CG2	2.51	0.41
5:F:256:PHE:CE1	5:F:259:PHE:HB2	2.55	0.41
5:F:289:LYS:HD2	5:F:290:LEU:HD22	2.02	0.41
5:F:292:VAL:HA	5:F:296:LYS:HA	2.02	0.41
5:F:402:LEU:HA	5:F:405:ILE:HG12	2.03	0.41
5:F:605:GLU:O	5:F:608:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:33:DC:H2''	6:X:34:DC:C6	2.55	0.41
1:A:252:ILE:HG22	1:A:312:LEU:CD1	2.51	0.41
1:A:279:GLY:O	1:A:280:ASP:C	2.64	0.41
1:A:286:GLU:OE1	1:A:300:LEU:HD21	2.21	0.41
2:C:59:ILE:HG21	2:C:475:VAL:CG1	2.51	0.41
2:C:233:ARG:HH21	2:C:284:LEU:HG	1.85	0.41
3:D:119:SER:O	3:D:120:LEU:C	2.62	0.41
3:D:125:GLY:HA2	3:D:135:ILE:CD1	2.51	0.41
3:D:528:THR:HG22	3:D:532:GLU:OE2	2.21	0.41
3:D:704:GLU:O	3:D:706:VAL:N	2.54	0.41
3:D:961:SER:OG	3:D:981:GLU:OE1	2.36	0.41
3:D:1170:LYS:O	3:D:1170:LYS:HG2	2.21	0.41
5:F:394:TYR:HA	5:F:397:ARG:NH1	2.36	0.41
6:X:46:DC:H2''	6:X:47:DT:H72	2.03	0.41
7:Y:27:DG:H2''	7:Y:28:DC:C5	2.56	0.41
7:Y:50:DC:C2'	7:Y:51:DT:H72	2.51	0.41
1:B:83:LEU:HD12	3:D:528:THR:CA	2.51	0.40
1:B:260:LEU:HD22	1:B:306:VAL:HB	2.02	0.40
2:C:91:THR:OG1	2:C:138:ILE:O	2.34	0.40
2:C:232:ILE:HD12	2:C:330:HIS:O	2.20	0.40
2:C:459:MET:SD	2:C:511:LEU:HD11	2.61	0.40
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.04	0.40
3:D:34:SER:CB	3:D:104:HIS:HB3	2.50	0.40
3:D:370:LYS:HE3	3:D:409:TRP:CZ3	2.56	0.40
3:D:709:ARG:CG	3:D:710:ASP:H	2.34	0.40
3:D:1044:GLN:HG3	3:D:1045:THR:H	1.85	0.40
3:D:1150:PRO:HG3	3:D:1214:PRO:HB2	2.03	0.40
5:F:276:MET:HG3	5:F:347:ILE:HG21	2.03	0.40
5:F:442:SER:O	5:F:446:GLN:HG2	2.21	0.40
1:A:253:LEU:CD1	1:A:279:GLY:HA2	2.51	0.40
1:B:18:GLN:CD	1:B:18:GLN:O	2.65	0.40
1:B:45:ARG:O	1:B:49:SER:OG	2.39	0.40
2:C:431:LYS:O	2:C:435:ILE:HG13	2.21	0.40
3:D:963:VAL:HG22	3:D:964:LYS:N	2.36	0.40
3:D:1327:GLU:HG3	9:P:16:DT:OP1	2.21	0.40
3:D:1353:VAL:O	3:D:1353:VAL:HG12	2.20	0.40
5:F:122:ARG:HG3	5:F:375:ALA:HB2	2.03	0.40
5:F:228:TYR:HB2	5:F:252:LEU:CD2	2.51	0.40
5:F:277:MET:O	5:F:280:VAL:HG22	2.21	0.40
5:F:326:TRP:CG	5:F:327:SER:N	2.89	0.40
5:F:508:GLU:HA	5:F:518:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:586:ARG:HB2	6:X:25:DT:C7	2.51	0.40
6:X:39:DT:OP2	6:X:39:DT:H2'	2.21	0.40
7:Y:65:DT:H2''	7:Y:66:DT:H72	2.02	0.40
8:O:7:DG:H2''	8:O:8:DG:C8	2.56	0.40
9:P:14:DT:H2''	9:P:15:DG:C8	2.55	0.40
2:C:33:ASP:OD1	2:C:34:SER:N	2.54	0.40
2:C:119:GLU:OE2	2:C:490:GLN:HB3	2.21	0.40
2:C:220:ILE:O	2:C:224:PHE:HD1	2.03	0.40
2:C:232:ILE:HG12	2:C:237:LEU:HD23	2.03	0.40
2:C:322:LEU:HD12	2:C:323:ALA:N	2.37	0.40
2:C:678:ARG:NH2	2:C:1106:ARG:HD3	2.35	0.40
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.61	0.40
2:C:800:MET:SD	2:C:1096:ILE:CD1	3.09	0.40
2:C:812:PHE:HA	3:D:505:ASP:OD2	2.21	0.40
2:C:1286:THR:HG22	3:D:476:ALA:HB1	2.03	0.40
2:C:1313:HIS:O	4:E:28:ARG:NH2	2.54	0.40
3:D:275:ARG:NH1	3:D:298:MET:O	2.54	0.40
3:D:342:LEU:HD22	3:D:1352:ILE:HD12	2.04	0.40
5:F:163:THR:HG21	5:F:260:ARG:HH21	1.87	0.40
5:F:261:LEU:HB2	5:F:266:PHE:HD2	1.86	0.40
5:F:576:VAL:HG13	5:F:587:ILE:HG12	2.03	0.40
6:X:17:DA:C8	6:X:18:DT:H72	2.57	0.40
6:X:55:DG:H2''	6:X:56:DC:C5	2.56	0.40
7:Y:23:DT:H2''	7:Y:24:DG:C8	2.57	0.40
2:C:1288:GLN:O	2:C:1292:THR:HG22	2.21	0.40
3:D:122:SER:CB	3:D:132:LEU:HD13	2.52	0.40
3:D:832:LYS:HG2	3:D:1242:ARG:HD3	2.02	0.40
3:D:930:LEU:HD11	3:D:1244:GLN:CG	2.51	0.40
3:D:1159:ILE:CG1	3:D:1177:ILE:HD12	2.52	0.40
5:F:235:ILE:HG23	5:F:236:LYS:N	2.37	0.40
5:F:508:GLU:O	5:F:509:THR:C	2.64	0.40
1:A:62:ASP:OD1	1:A:62:ASP:N	2.54	0.40
1:B:57:THR:HG23	1:B:58:GLU:H	1.86	0.40
1:B:264:VAL:O	1:B:265:ARG:C	2.65	0.40
2:C:211:ARG:NE	2:C:354:ASP:OD2	2.45	0.40
2:C:1103:VAL:HG22	2:C:1111:GLN:HE21	1.87	0.40
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.54	0.40
3:D:356:THR:O	3:D:448:GLN:HA	2.21	0.40
3:D:515:ARG:O	3:D:545:HIS:CB	2.69	0.40
3:D:770:LEU:O	3:D:774:ILE:HG12	2.21	0.40
3:D:1162:ILE:HD12	3:D:1202:GLU:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:148:TYR:OH	5:F:218:ARG:HA	2.22	0.40
5:F:161:LEU:CA	5:F:260:ARG:O	2.69	0.40
5:F:456:MET:SD	5:F:497:VAL:HG22	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/329 (93%)	255 (83%)	47 (15%)	5 (2%)	7	37
1	B	314/329 (95%)	271 (86%)	41 (13%)	2 (1%)	21	58
2	C	1338/1342 (100%)	1227 (92%)	105 (8%)	6 (0%)	30	65
3	D	1336/1407 (95%)	1210 (91%)	115 (9%)	11 (1%)	16	52
4	E	74/91 (81%)	69 (93%)	5 (7%)	0	100	100
5	F	441/613 (72%)	397 (90%)	41 (9%)	3 (1%)	18	54
All	All	3810/4111 (93%)	3429 (90%)	354 (9%)	27 (1%)	20	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
3	D	338	PHE
3	D	1345	ARG
5	F	139	GLU
5	F	356	GLU
1	A	242	VAL
1	B	21	SER
1	B	193	GLU
2	C	398	SER

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Mol	Chain	Res	Type
2	C	625	GLU
3	D	258	GLY
3	D	588	PRO
1	A	247	PRO
3	D	46	TYR
3	D	345	LYS
3	D	860	ARG
3	D	1138	LEU
3	D	1151	LYS
1	A	250	ASP
2	C	1160	ASP
3	D	337	ARG
5	F	396	ASN
3	D	49	PHE
2	C	39	ILE
1	A	252	ILE
2	C	45	GLY
2	C	1223	ARG

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	269/286 (94%)	269 (100%)	0	100	100
1	B	276/286 (96%)	276 (100%)	0	100	100
2	C	1155/1157 (100%)	1155 (100%)	0	100	100
3	D	1114/1168 (95%)	1114 (100%)	0	100	100
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	397/540 (74%)	397 (100%)	0	100	100
All	All	3276/3512 (93%)	3276 (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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	276	HIS
1	A	294	ASN
2	C	139	ASN
2	C	165	HIS
2	C	628	HIS
2	C	760	ASN
2	C	762	ASN
2	C	808	ASN
3	D	113	HIS
3	D	606	ASN
3	D	907	HIS
3	D	929	GLN
4	E	7	GLN
5	F	518	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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	1N7	C	1402	-	44,46,46	4.23	20 (45%)	69,72,72	2.39	22 (31%)
10	POP	C	1401	-	6,8,8	0.78	0	12,13,13	0.82	0
11	1N7	C	1403	-	44,46,46	4.15	19 (43%)	69,72,72	1.96	18 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1N7	C	1402	-	-	6/27/92/92	0/4/4/4
10	POP	C	1401	-	-	0/6/6/6	-
11	1N7	C	1403	-	-	6/27/92/92	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1402	1N7	C3-C4	-13.10	1.31	1.53
11	C	1403	1N7	C3-C4	-12.85	1.32	1.53
11	C	1402	1N7	C5-C9	-11.50	1.36	1.55
11	C	1403	1N7	C5-C9	-11.13	1.36	1.55
11	C	1402	1N7	C3-C19	-9.40	1.38	1.53
11	C	1403	1N7	C3-C19	-9.35	1.38	1.53
11	C	1402	1N7	C2-C19	7.49	1.69	1.56
11	C	1403	1N7	C2-C19	6.76	1.67	1.56
11	C	1403	1N7	C5-C4	6.76	1.64	1.54
11	C	1402	1N7	C5-C4	6.61	1.64	1.54
11	C	1403	1N7	C24-N1	6.39	1.48	1.33
11	C	1403	1N7	C7-C6	-6.31	1.41	1.54
11	C	1402	1N7	C24-N1	6.26	1.48	1.33
11	C	1402	1N7	C7-C6	-6.08	1.42	1.54
11	C	1402	1N7	C18-C19	-5.82	1.42	1.53
11	C	1403	1N7	C18-C19	-5.72	1.42	1.53
11	C	1402	1N7	C8-C7	5.44	1.68	1.54
11	C	1403	1N7	C8-C7	5.15	1.68	1.54
11	C	1403	1N7	C5-C6	4.89	1.63	1.55
11	C	1402	1N7	C5-C6	4.87	1.63	1.55
11	C	1402	1N7	C18-C6	4.56	1.62	1.53
11	C	1403	1N7	C18-C6	4.55	1.62	1.53
11	C	1402	1N7	C20-C9	4.34	1.61	1.54
11	C	1403	1N7	C2-C15	-4.27	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1403	1N7	C20-C9	3.37	1.60	1.54
11	C	1403	1N7	O3-C17	-3.28	1.36	1.43
11	C	1402	1N7	O3-C17	-3.20	1.36	1.43
11	C	1402	1N7	C2-C15	-3.13	1.50	1.55
11	C	1402	1N7	C8-C9	2.87	1.60	1.54
11	C	1403	1N7	C23-C24	2.76	1.56	1.51
11	C	1402	1N7	C23-C24	2.65	1.56	1.51
11	C	1402	1N7	O1-C24	-2.60	1.18	1.23
11	C	1403	1N7	O1-C24	-2.57	1.18	1.23
11	C	1402	1N7	O7-S1	2.52	1.52	1.45
11	C	1403	1N7	O7-S1	2.50	1.52	1.45
11	C	1403	1N7	C8-C9	2.25	1.59	1.54
11	C	1402	1N7	C14-C15	2.25	1.57	1.53
11	C	1402	1N7	O6-S1	2.15	1.51	1.45
11	C	1403	1N7	O6-S1	2.10	1.51	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1402	1N7	C5-C6-C18	-8.12	104.43	114.72
11	C	1402	1N7	C5-C9-C20	-7.56	110.33	119.48
11	C	1403	1N7	C5-C6-C18	-6.32	106.70	114.72
11	C	1403	1N7	C6-C5-C4	-5.51	102.38	107.42
11	C	1402	1N7	C16-C17-C18	-5.23	105.79	111.50
11	C	1402	1N7	C23-C22-C20	-4.93	105.25	114.46
11	C	1402	1N7	C8-C9-C20	4.72	119.32	112.18
11	C	1403	1N7	C5-C9-C20	-4.30	114.28	119.48
11	C	1402	1N7	C1-C2-C15	3.99	113.47	107.75
11	C	1402	1N7	C8-C7-C6	-3.90	97.51	105.14
11	C	1403	1N7	O6-S1-O7	-3.86	101.27	113.82
11	C	1402	1N7	O6-S1-O7	-3.73	101.71	113.82
11	C	1403	1N7	C8-C7-C6	-3.58	98.15	105.14
11	C	1403	1N7	C23-C22-C20	-3.34	108.22	114.46
11	C	1403	1N7	C3-C19-C2	-3.31	110.34	113.70
11	C	1402	1N7	C21-C20-C9	-3.30	107.93	112.88
11	C	1402	1N7	C11-C2-C15	-3.16	105.16	110.44
11	C	1403	1N7	O7-S1-C32	3.12	111.41	106.76
11	C	1403	1N7	O6-S1-C32	3.00	111.23	106.76
11	C	1402	1N7	C1-C12-C13	-2.99	106.53	110.48
11	C	1402	1N7	C22-C20-C9	2.94	116.42	110.33
11	C	1402	1N7	O6-S1-C32	2.93	111.12	106.76
11	C	1403	1N7	C6-C18-C17	-2.91	107.99	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1402	1N7	C16-C15-C14	-2.88	107.94	111.23
11	C	1402	1N7	C19-C2-C15	2.84	112.46	108.51
11	C	1403	1N7	C15-C14-C13	-2.83	108.43	112.71
11	C	1402	1N7	O7-S1-C32	2.80	110.94	106.76
11	C	1402	1N7	C2-C19-C18	-2.79	108.73	111.84
11	C	1403	1N7	C2-C19-C18	-2.78	108.74	111.84
11	C	1403	1N7	C14-C13-C12	-2.73	107.29	110.62
11	C	1403	1N7	C21-C20-C9	-2.64	108.92	112.88
11	C	1402	1N7	C9-C5-C4	-2.37	115.53	117.67
11	C	1402	1N7	C15-C16-C17	-2.31	111.66	114.40
11	C	1403	1N7	O8-S1-C32	2.25	110.32	105.97
11	C	1402	1N7	O8-S1-C32	2.22	110.26	105.97
11	C	1402	1N7	C16-C15-C2	2.22	115.02	112.66
11	C	1402	1N7	C19-C18-C17	-2.21	109.08	111.86
11	C	1403	1N7	C31-C28-N2	-2.21	112.86	116.69
11	C	1403	1N7	C26-C27-N2	-2.18	110.92	115.35
11	C	1403	1N7	C19-C3-C4	2.13	117.08	114.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1402	1N7	C21-C20-C9-C5
11	C	1402	1N7	C22-C20-C9-C5
11	C	1402	1N7	C22-C20-C9-C8
11	C	1402	1N7	N2-C28-C31-C32
11	C	1402	1N7	N2-C28-C31-O5
11	C	1403	1N7	N2-C28-C31-C32
11	C	1403	1N7	N2-C28-C31-O5
11	C	1402	1N7	C21-C20-C9-C8
11	C	1403	1N7	C9-C20-C22-C23
11	C	1403	1N7	C21-C20-C22-C23
11	C	1403	1N7	N1-C25-C26-C27
11	C	1403	1N7	C20-C22-C23-C24

There are no ring outliers.

3 monomers are involved in 9 short contacts:

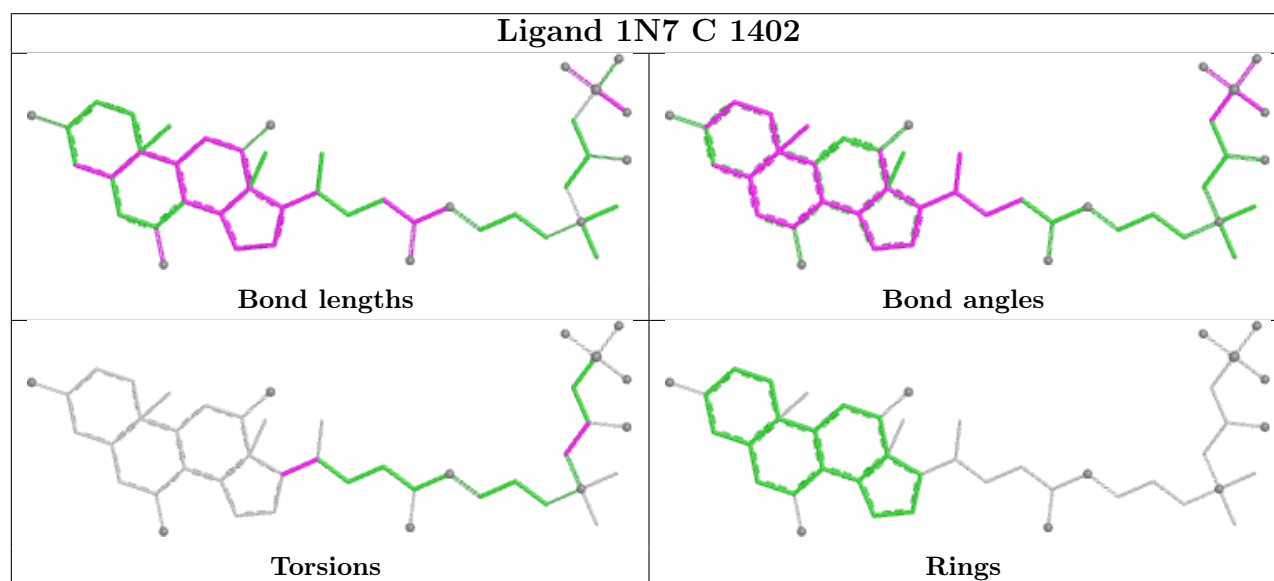
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1402	1N7	3	0
10	C	1401	POP	1	0

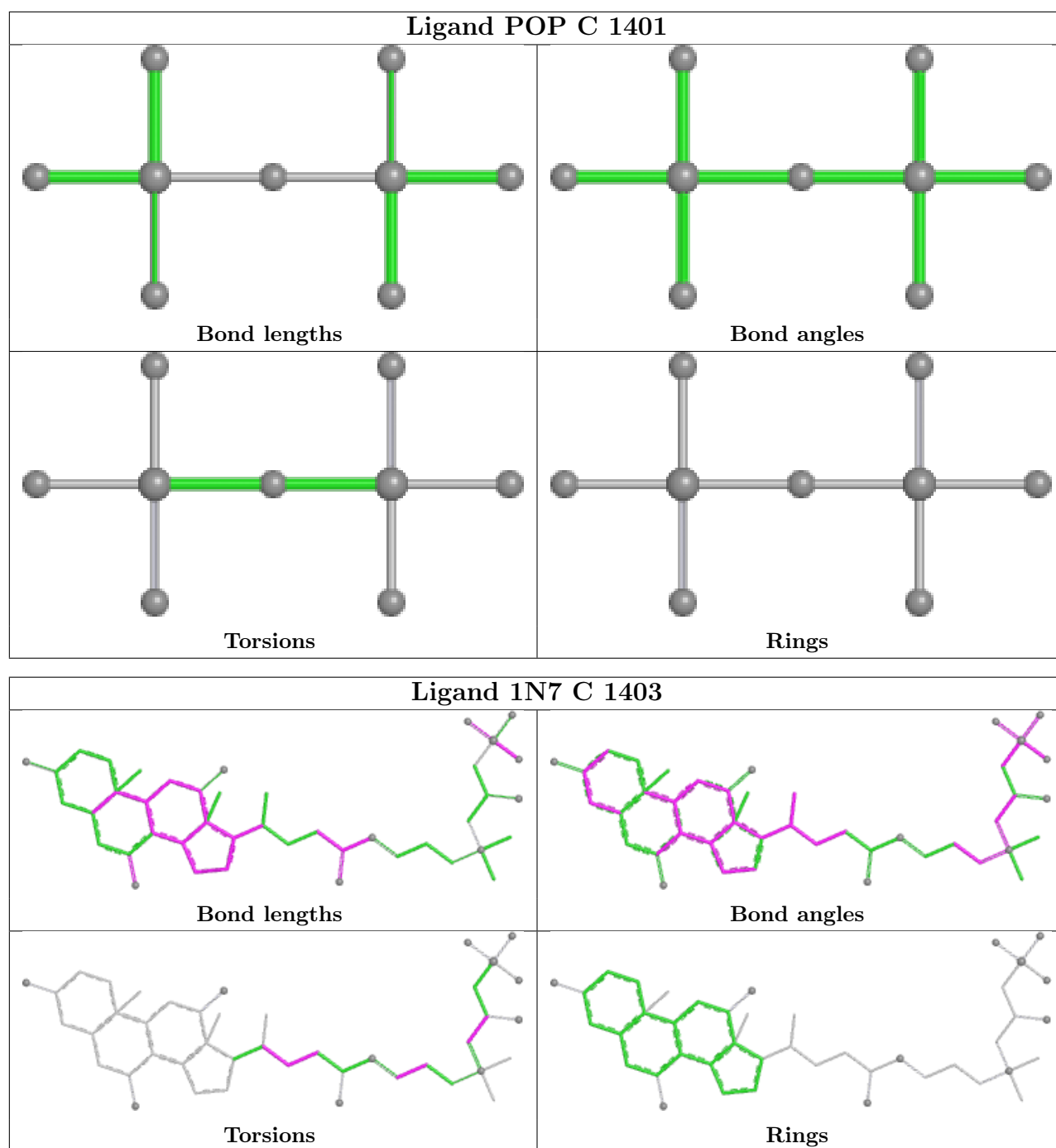
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1403	1N7	5	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

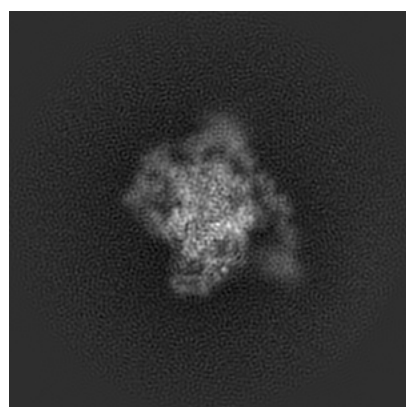
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21879. These allow visual inspection of the internal detail of the map and identification of artifacts.

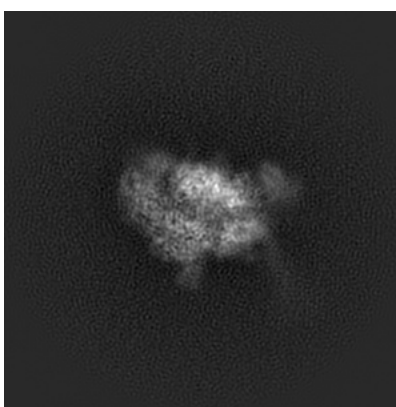
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

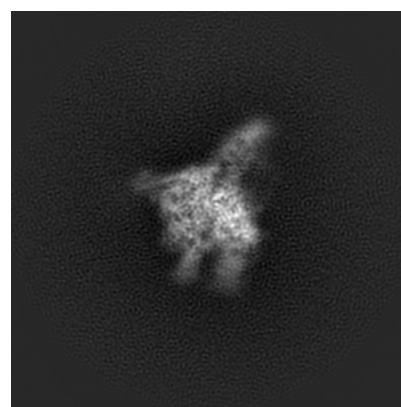
6.1.1 Primary map



X



Y

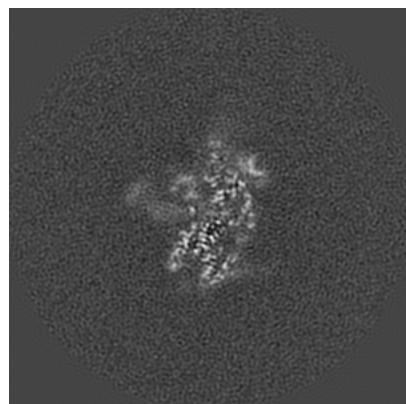


Z

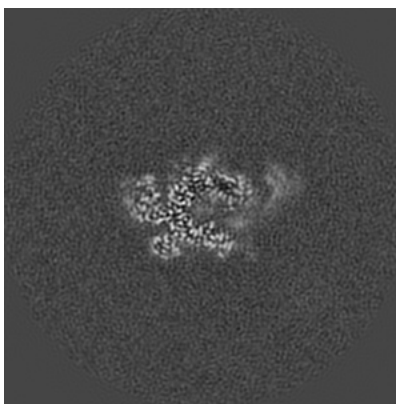
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

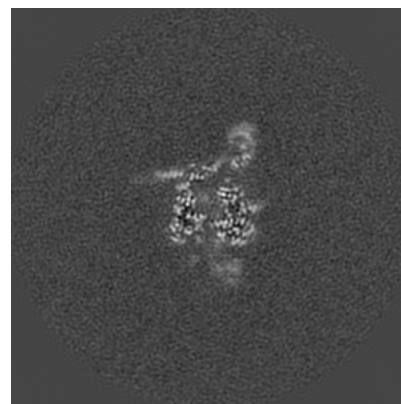
6.2.1 Primary map



X Index: 180



Y Index: 180

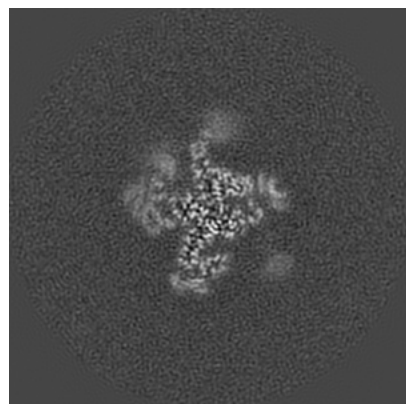


Z Index: 180

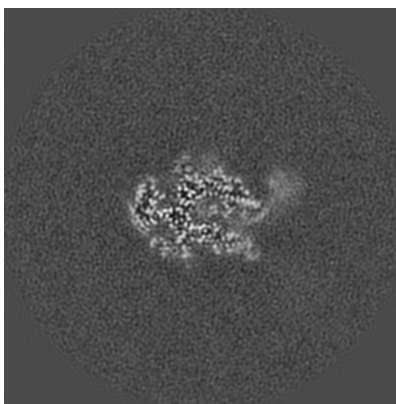
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

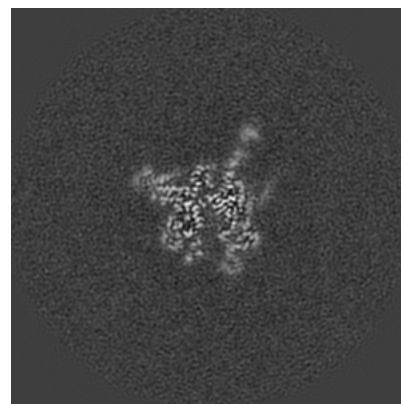
6.3.1 Primary map



X Index: 197



Y Index: 185

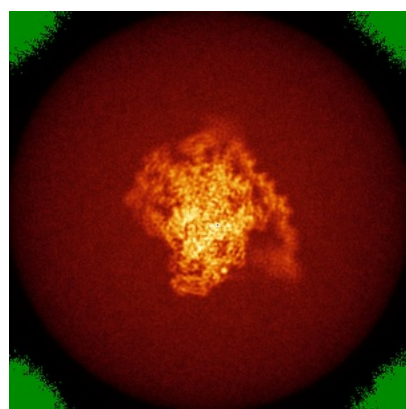


Z Index: 167

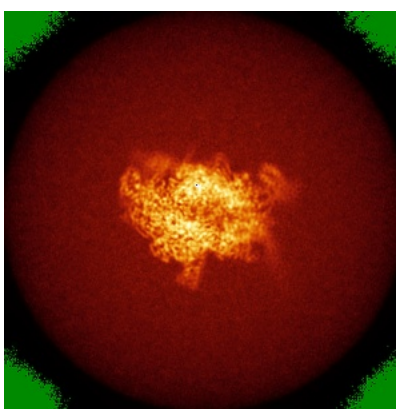
The images above show the largest variance slices of the map in three orthogonal directions.

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

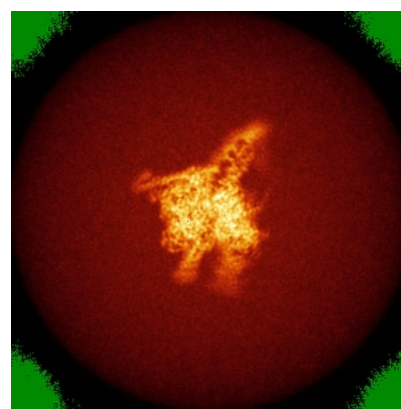
6.4.1 Primary map



X



Y

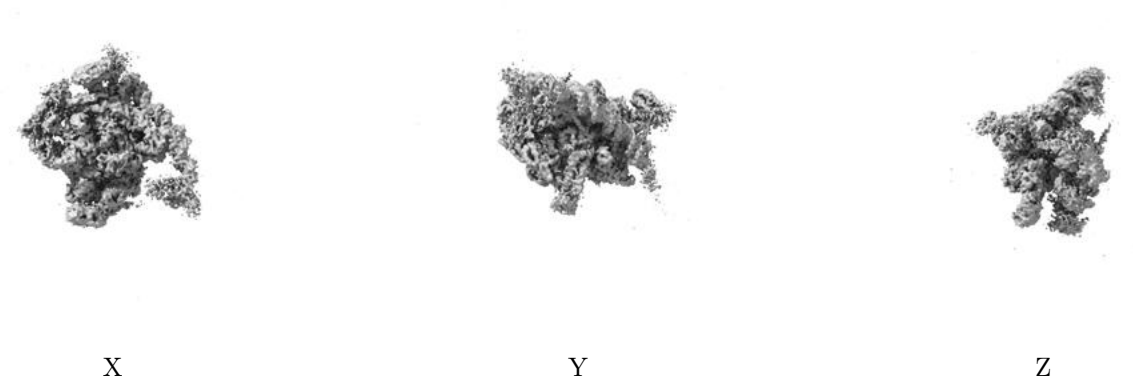


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

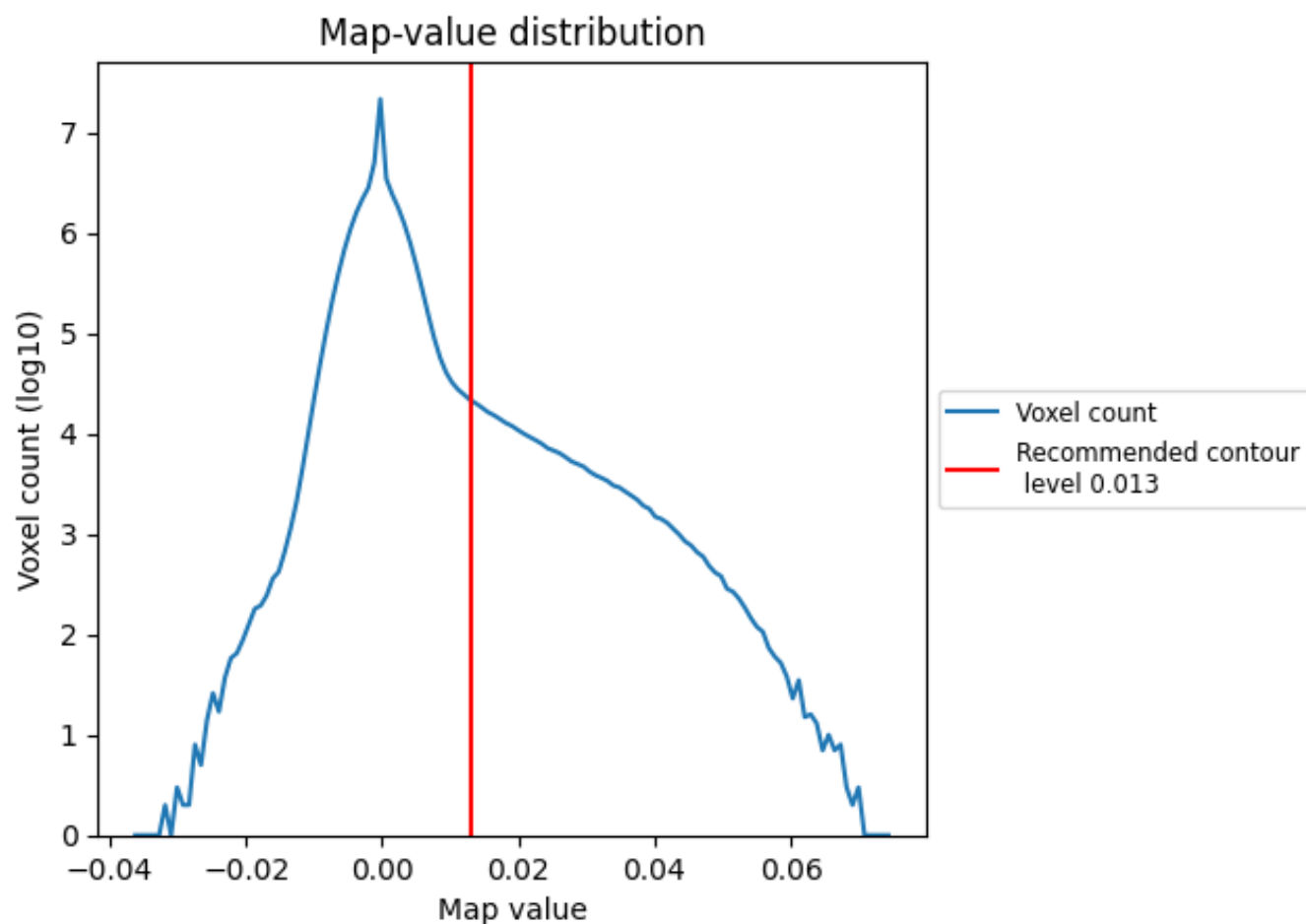
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

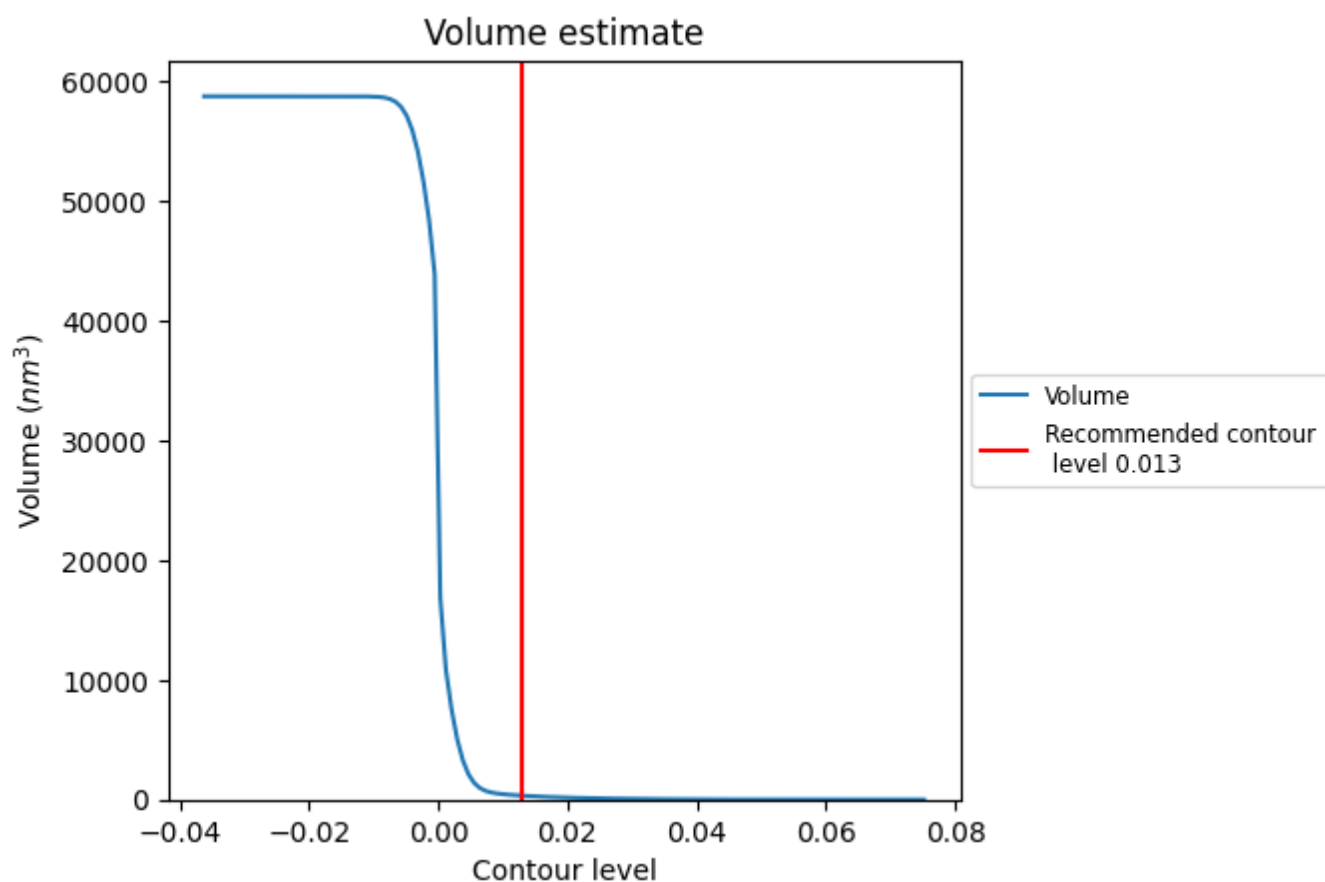
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

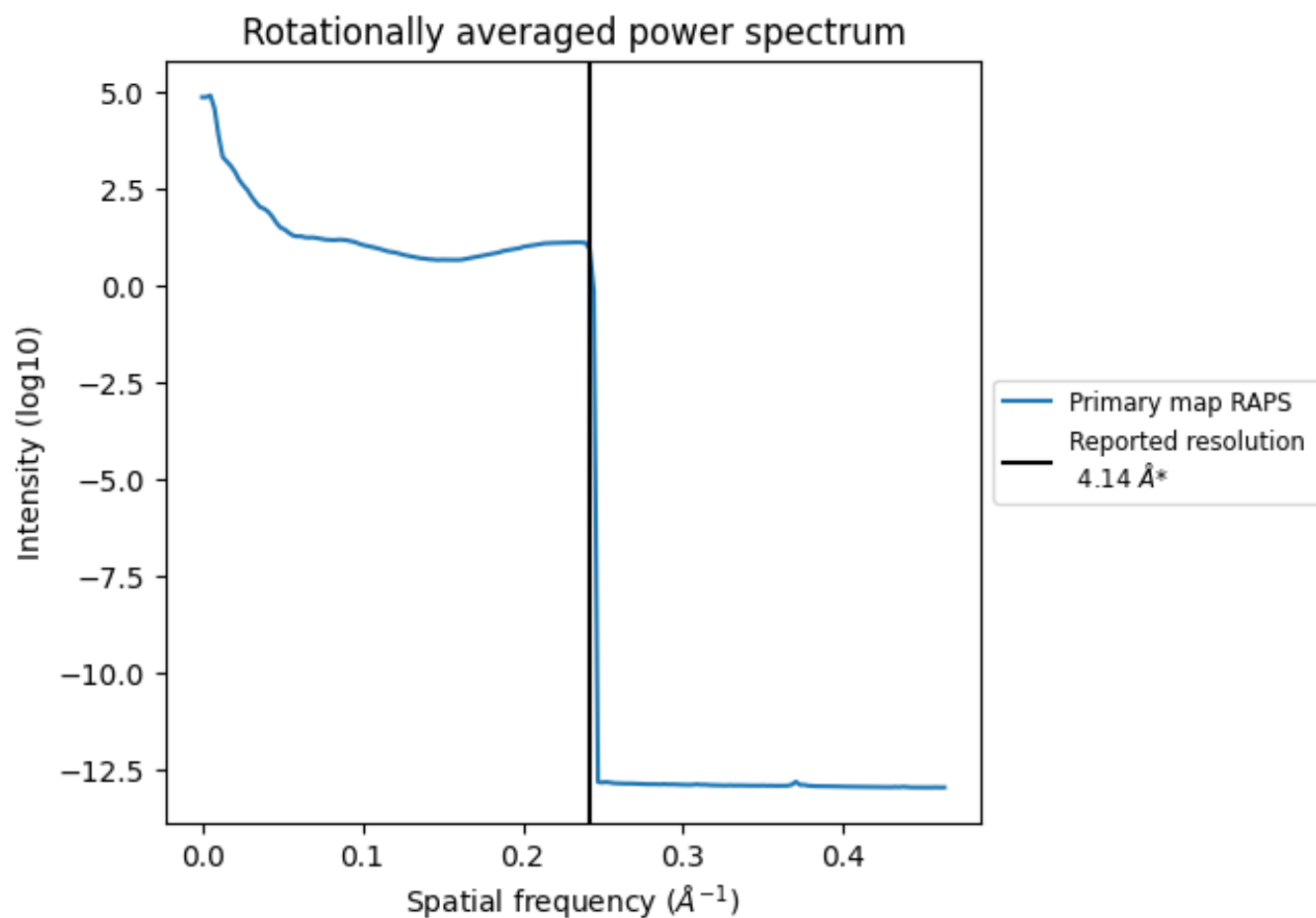
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 295 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 0.242 Å⁻¹

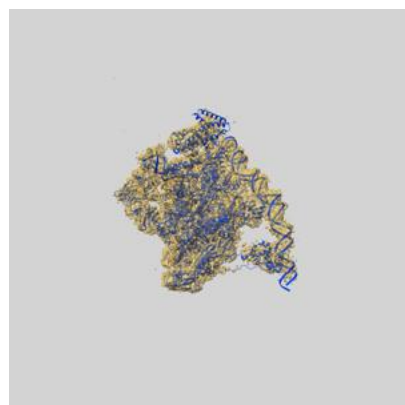
8 Fourier-Shell correlation ⓘ

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

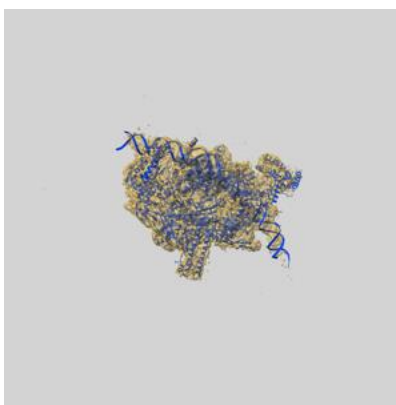
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21879 and PDB model 7KHC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

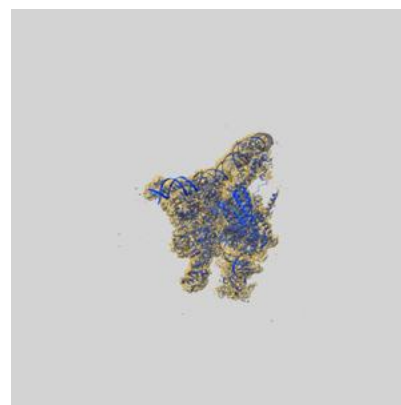
9.1 Map-model overlay [i](#)



X



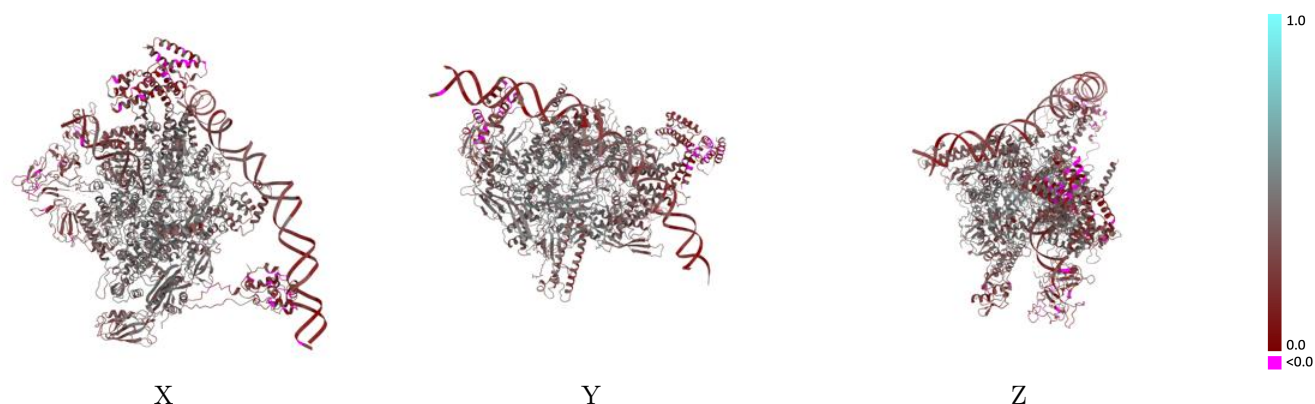
Y



Z

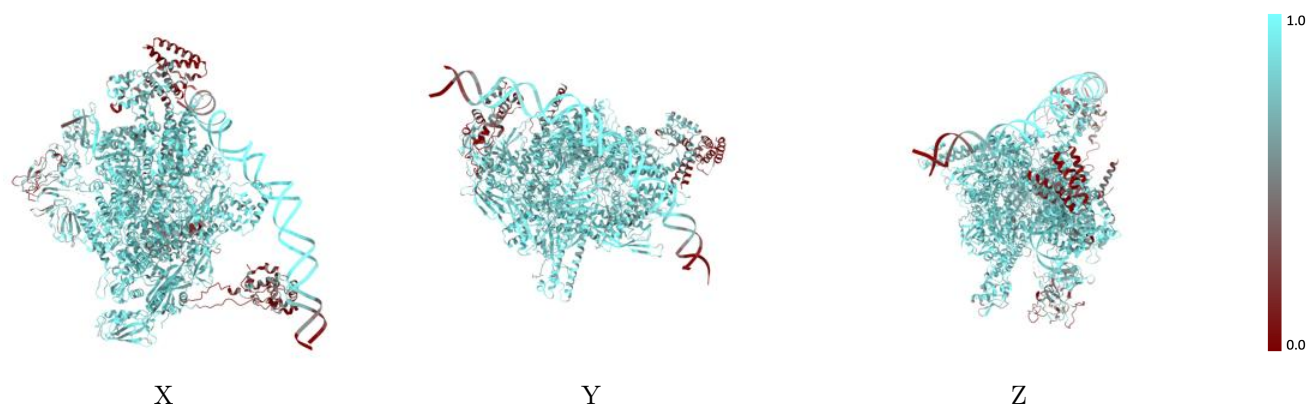
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



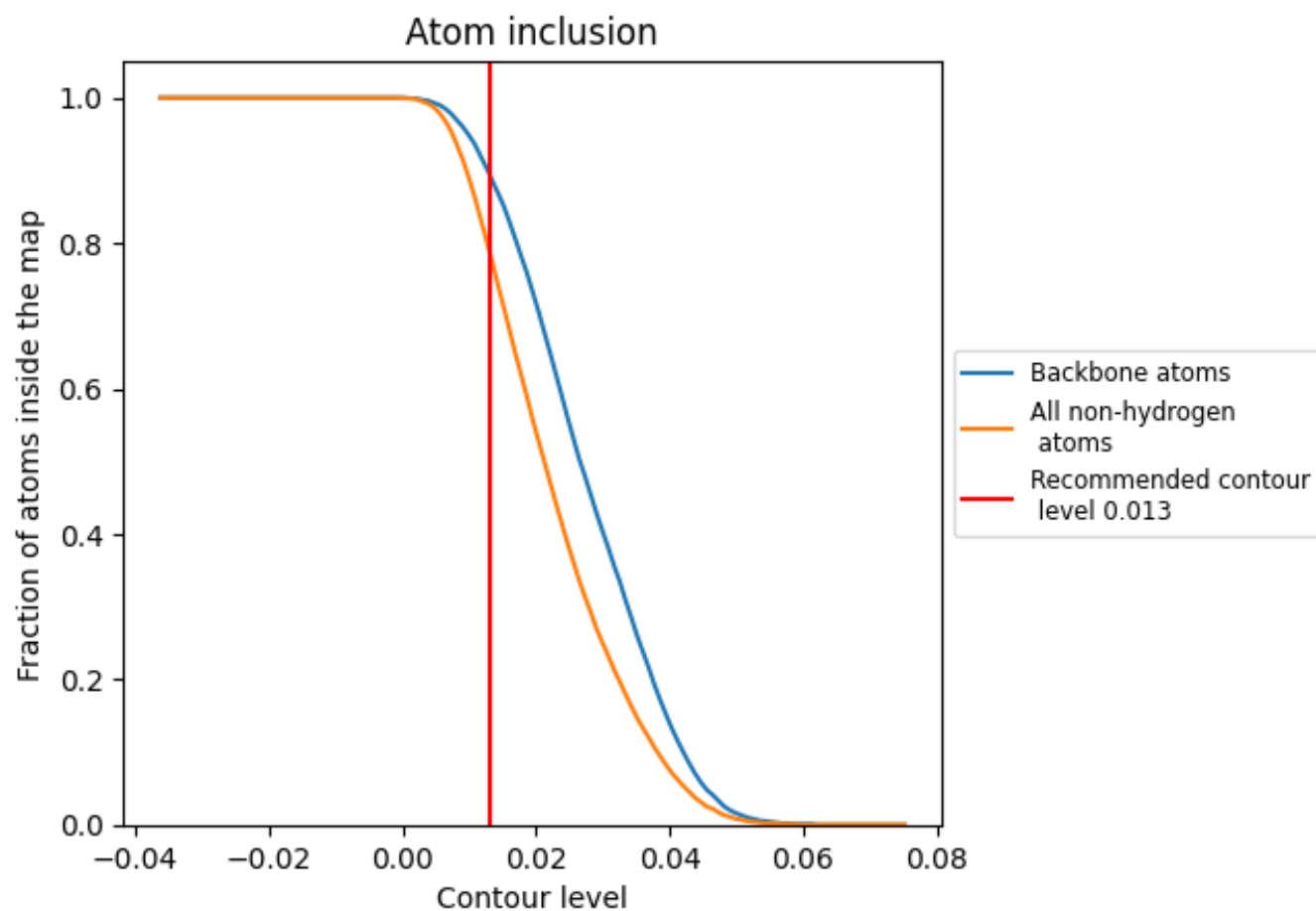
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.3570
A	0.7060	0.3580
B	0.6600	0.3310
C	0.8700	0.4070
D	0.8310	0.3870
E	0.5670	0.3720
F	0.6540	0.2600
O	0.8350	0.2130
P	0.8510	0.2720
X	0.7210	0.2050
Y	0.7340	0.2250

1.0

0.0

<0.0