



## Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 12:03 PM EDT

PDB ID : 7KHB / pdb\_00007khhb  
EMDB ID : EMD-21880  
Title : Escherichia coli RNA polymerase and rrnBP1 promoter open complex  
Authors : Shin, Y.; Qayyum, M.Z.; Murakami, K.S.  
Deposited on : 2020-10-20  
Resolution : 3.53 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

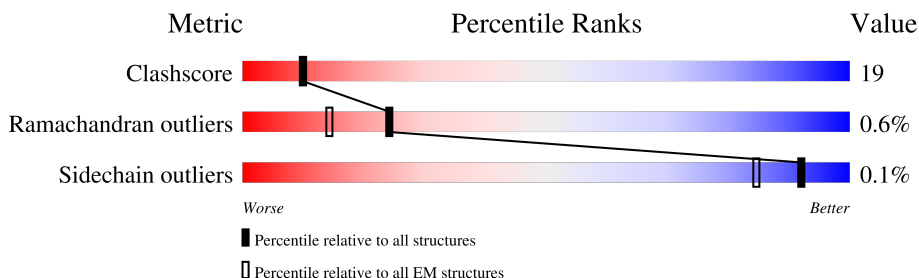
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.53 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	613	
6	X	64	
7	Y	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	D	2003	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 31608 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	231	Total	C	N	O	S	0	0
			1794	1117	318	353	6		
1	B	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		

- 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	1340	Total	C	N	O	S	0	0
			10382	6522	1849	1962	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	471	Total	C	N	O	S	0	0
			3836	2403	684	726	23		

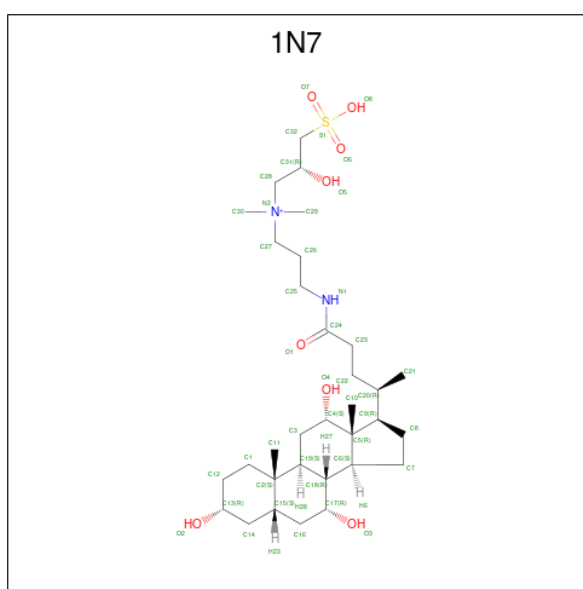
- Molecule 6 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	60	Total	C	N	O	P	0	0
			1221	582	219	360	60		

- Molecule 7 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	64	Total	C	N	O	P	0	0
			1325	628	248	385	64		

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula:  $C_{32}H_{59}N_2O_8S$ ) (labeled as "Ligand of Interest" by depositor).

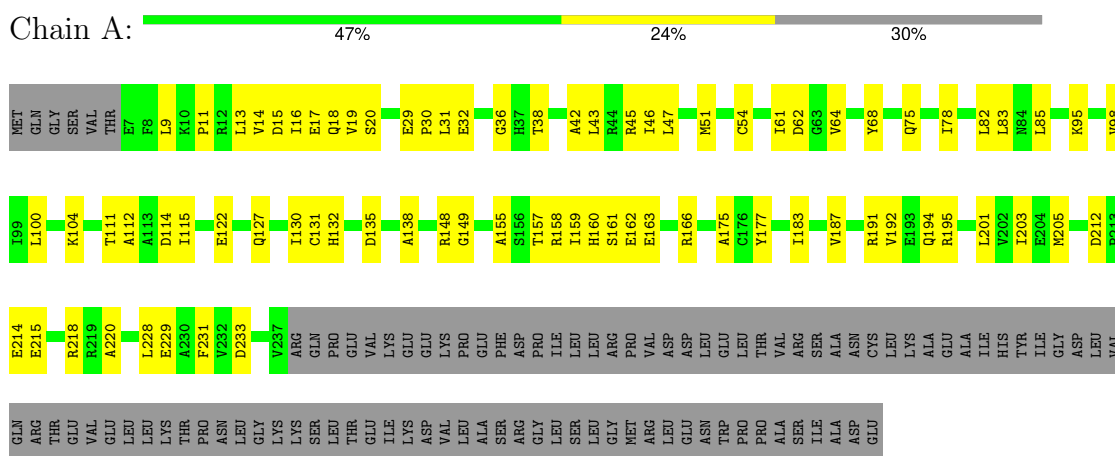


Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

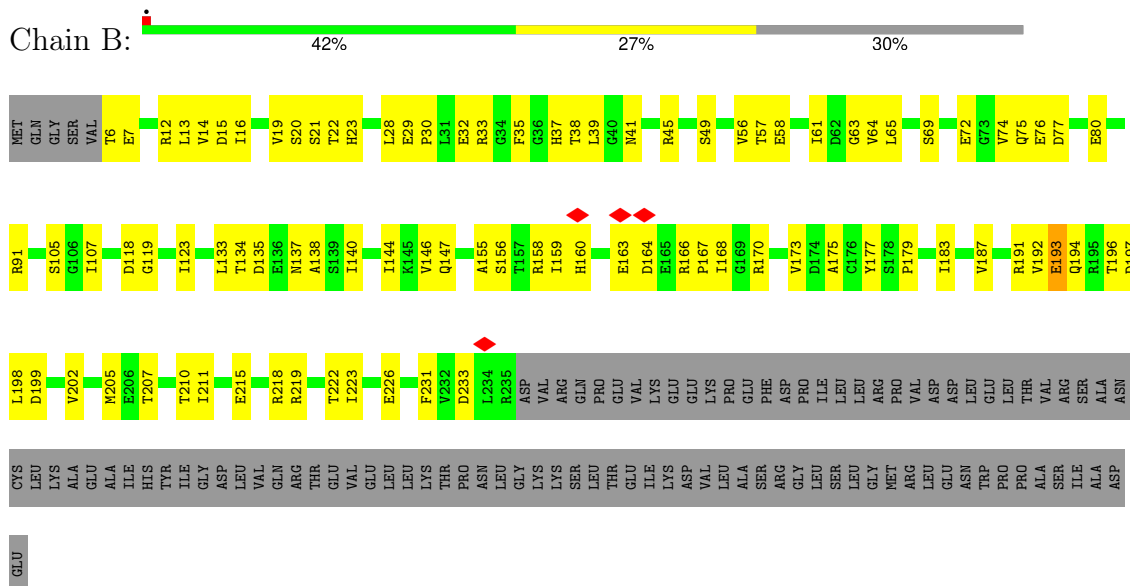
### 3 Residue-property plots

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



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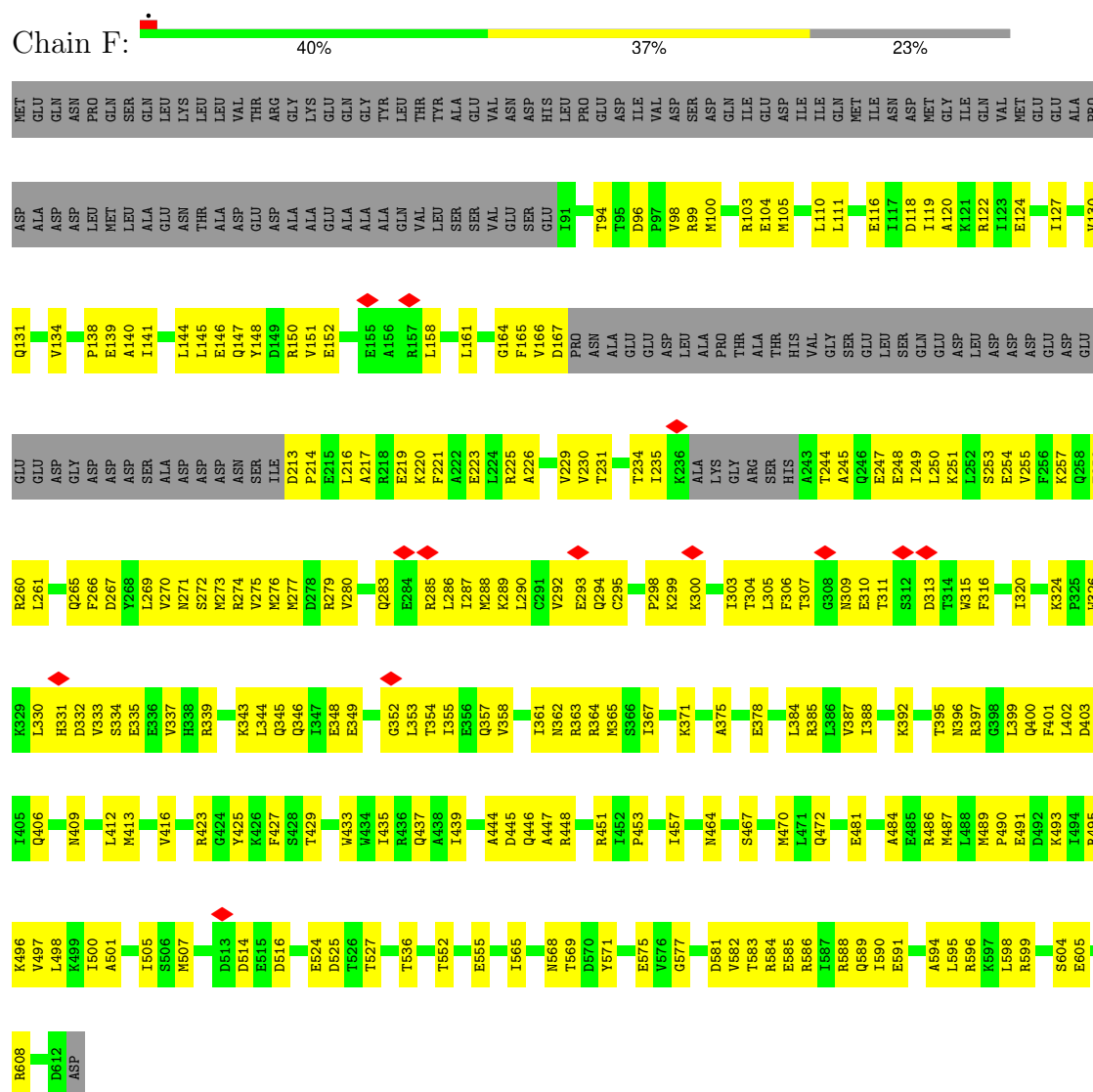


#### • Molecule 2: DNA-directed RNA polymerase subunit beta

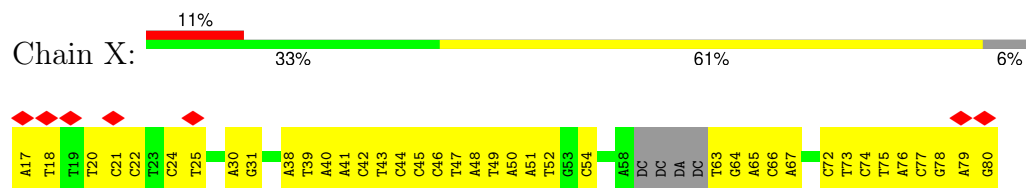




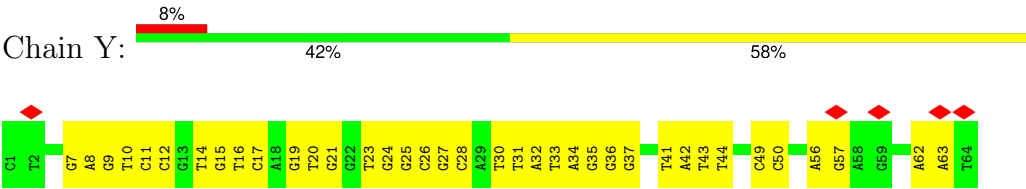
SER	Q1279	K1172	G1092	V1027	K953	H865	R764	E648	T528	K378	L291	M180	V92	MET
ALA	E1280	R1173	T1093	E1030	N954	E866	L767	K649	K531	Y382	I291	G181	V97	LYS
SER	E1281	R1174	D1094	E1031	K955	K867	L768	K650	E532	E295	E295	E183	V97	ASP
LEU	Y1282	V1176	M1095	V1032	G956	K868	V769	I654	E533	R388	M298	I185	E100	LEU
GLU	S1283	T1177	L1101	S1032	K959	D870	L770	E653	E534	K395	L299	L188	R101	LEU
LEU	E1284	T1178	L1102	F1034	L960	E871	Q771	E658	V548	V407	Q300	L196	M102	PHE
LEU	K1285	V1179	G1103	F1035	S961	L872	F772	E661	K549	E301	E301	E195	E106	LEU
ASN	K1286	V1180	K1104	T1038	S962	E873	F773	E662	E549	E302	E302	E196	G103	LEU
ALA	I1287	S1183	A1105	M1040	K963	E874	T774	E663	E552	I411	D304	Q196	H104	GLN
LEU	V1288	D1184	I1106	T1045	K964	N875	S775	E664	E553	I416	A305	E197	I105	THR
GLY	F1289	P1185	A1107	T1046	S965	S876	T776	E665	E554	R417	L306	C198	E106	LYS
GLY	F1290	Y1186	V1107	M1049	V966	S877	G782	E666	E555	E418	L307	E199	P110	THR
ASP	T1301	E1187	E1110	Q1044	N968	A879	T786	E667	K557	H419	R311	Q200	T111	LYS
ASN	S1313	E1188	T1045	T1045	N968	V880	T786	E667	K557	H419	R311	Q200	T111	LYS
GLU	L1314	M1189	T1046	T1046	N968	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLU	A1315	I1190	R1048	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	T1316	N1197	Q1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
ASP	E1317	V1198	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
ASN	S1318	F1199	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLU	A1319	E1200	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1320	G1201	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	F1321	E1202	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1322	R1203	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1323	E1204	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1324	E1205	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1325	R1206	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1326	G1207	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1327	D1208	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1328	E1215	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1329	A1216	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1330	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1331	H1227	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1332	E1215	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1333	A1216	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1334	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1335	H1227	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1336	E1215	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
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GLY	E1350	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
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GLY	E1353	A1216	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1354	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1355	H1227	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
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GLY	E1358	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
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GLY	E1389	A1216	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1390	E1220	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1391	H1227	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1392	E1215	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1393	A1216	T1049	Q1049	S977	K881	T786	E667	K557	H419	R311	Q200	T111	LYS
GLY	E1394	E1220	T1049	Q1049	S977	K88								



- Molecule 6: DNA (60-MER)



● Molecule 7: DNA (64-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	349752	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	0.104	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	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: 1N7, MG, ZN

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	0.24	0/1816	0.46	0/2461
1	B	0.22	0/1808	0.51	0/2450
2	C	0.27	0/10739	0.49	0/14489
3	D	0.26	0/10539	0.52	1/14234 (0.0%)
4	E	0.17	0/607	0.43	0/817
5	F	0.22	0/3887	0.56	0/5224
6	X	0.33	0/1366	0.56	0/2101
7	Y	0.32	0/1488	0.57	0/2298
All	All	0.26	0/32250	0.52	1/44074 (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	2
3	D	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1203	ARG	CG-CD-NE	-5.89	99.04	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	Peptide
3	D	860	ARG	Peptide
3	D	901	ARG	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	1794	0	1819	62	0
1	B	1786	0	1813	73	0
2	C	10570	0	10582	389	0
3	D	10382	0	10571	447	0
4	E	605	0	612	24	0
5	F	3836	0	3907	198	0
6	X	1221	0	677	40	0
7	Y	1325	0	721	38	0
8	C	86	0	116	2	0
9	D	1	0	0	0	0
10	D	2	0	0	2	0
All	All	31608	0	30818	1195	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 (1195) 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)
5:F:277:MET:SD	5:F:362:ASN:ND2	2.28	1.07
3:D:816:THR:OG1	3:D:818:GLU:OE1	1.77	1.03
2:C:403:MET:SD	2:C:407:ARG:NH2	2.40	0.94
5:F:271:ASN:OD1	5:F:274:ARG:NH2	1.99	0.94
3:D:1344:LEU:O	3:D:1346:GLY:N	2.00	0.93
2:C:1246:ARG:NH1	3:D:348:ASP:OD1	2.02	0.92
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.04	0.91
5:F:164:GLY:O	5:F:260:ARG:NH2	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:528:THR:N	3:D:532:GLU:OE2	2.05	0.89
3:D:968:ASN:ND2	3:D:1117:SER:O	2.08	0.87
3:D:1061:VAL:O	3:D:1104:LYS:N	2.11	0.83
3:D:733:SER:OG	3:D:736:GLN:OE1	1.96	0.83
2:C:528:ARG:NH2	2:C:576:SER:O	2.12	0.82
1:A:214:GLU:OE2	1:A:218:ARG:NE	2.13	0.81
5:F:577:GLY:O	5:F:581:ASP:N	2.14	0.81
1:A:18:GLN:NE2	1:A:20:SER:O	2.14	0.80
5:F:586:ARG:NH1	6:X:24:DC:OP2	2.15	0.80
2:C:1146:GLN:NE2	2:C:1160:ASP:OD1	2.14	0.80
2:C:199:ASP:O	2:C:200:ARG:NE	2.13	0.79
5:F:445:ASP:OD1	5:F:446:GLN:N	2.16	0.78
3:D:337:ARG:O	3:D:340:GLN:N	2.16	0.77
1:A:157:THR:O	1:A:160:HIS:ND1	2.19	0.76
3:D:1106:ILE:N	3:D:1121:LEU:O	2.18	0.75
2:C:1312:ASN:ND2	2:C:1314:GLN:OE1	2.19	0.75
2:C:201:ARG:NH1	2:C:370:MET:SD	2.60	0.74
2:C:549:ASP:OD1	2:C:550:VAL:N	2.19	0.74
3:D:773:PHE:O	3:D:776:THR:OG1	2.06	0.74
5:F:605:GLU:N	5:F:605:GLU:OE1	2.20	0.74
3:D:874:GLU:OE1	3:D:875:ASN:ND2	2.21	0.73
3:D:395:LYS:NZ	5:F:536:THR:OG1	2.20	0.73
2:C:74:ARG:NH1	2:C:121:GLU:OE1	2.21	0.73
2:C:185:ASP:OD2	2:C:200:ARG:NH2	2.22	0.71
1:A:9:LEU:N	1:A:32:GLU:OE2	2.24	0.71
2:C:67:GLU:OE1	2:C:69:GLN:HG3	1.90	0.71
3:D:482:ALA:O	3:D:488:ASN:ND2	2.24	0.71
2:C:189:ASP:OD1	2:C:193:ASN:N	2.24	0.71
5:F:448:ARG:NH2	5:F:501:ALA:O	2.24	0.71
3:D:306:LEU:O	3:D:326:SER:OG	2.05	0.70
3:D:895:CYS:HG	10:D:2003:ZN:ZN	1.03	0.70
2:C:231:GLU:OE2	2:C:233:ARG:NH1	2.25	0.70
5:F:120:ALA:O	5:F:124:GLU:OE1	2.09	0.70
3:D:418:GLU:O	3:D:481:ARG:NH2	2.25	0.70
5:F:582:VAL:HG22	5:F:584:ARG:NE	2.07	0.70
3:D:818:GLU:OE1	3:D:818:GLU:N	2.26	0.68
5:F:348:GLU:O	5:F:352:GLY:N	2.26	0.68
7:Y:36:DG:H1'	7:Y:37:DG:H5'	1.76	0.68
3:D:980:THR:OG1	3:D:997:VAL:O	2.11	0.68
2:C:84:GLU:OE2	2:C:88:ARG:NH1	2.26	0.68
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1318:SER:OG	3:D:1342:ASP:OD1	2.10	0.68
7:Y:23:DT:H5'	7:Y:23:DT:C6	2.29	0.67
3:D:211:GLU:O	3:D:215:LYS:HD3	1.95	0.67
1:B:134:THR:HG22	1:B:135:ASP:H	1.60	0.67
1:B:163:GLU:N	1:B:163:GLU:OE1	2.29	0.66
2:C:1160:ASP:HB2	2:C:1162:SER:H	1.60	0.66
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.78	0.66
1:A:191:ARG:NH1	1:A:192:VAL:O	2.29	0.66
2:C:231:GLU:O	2:C:238:GLN:N	2.24	0.66
3:D:850:LYS:HD3	3:D:855:ASP:HB3	1.78	0.65
1:A:162:GLU:OE1	1:A:162:GLU:N	2.29	0.65
3:D:337:ARG:O	3:D:339:ARG:N	2.30	0.65
3:D:424:ASN:OD1	3:D:425:ARG:N	2.29	0.65
5:F:98:VAL:HG22	5:F:402:LEU:HD21	1.79	0.65
1:B:80:GLU:N	1:B:80:GLU:OE2	2.30	0.65
2:C:631:GLU:OE2	2:C:632:ASP:N	2.29	0.65
2:C:358:ASP:OD2	2:C:359:ARG:N	2.29	0.65
3:D:326:SER:N	3:D:329:ASP:OD1	2.29	0.65
6:X:63:DT:H2''	6:X:64:DG:H5'	1.79	0.65
5:F:267:ASP:O	5:F:271:ASN:ND2	2.30	0.64
5:F:332:ASP:OD2	5:F:333:VAL:N	2.30	0.64
5:F:309:ASN:OD1	5:F:310:GLU:N	2.31	0.64
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.27	0.64
3:D:1002:VAL:N	3:D:1019:ASN:O	2.30	0.64
3:D:1313:SER:HG	3:D:1325:PHE:HZ	1.45	0.64
5:F:145:LEU:HD22	5:F:225:ARG:HG3	1.79	0.64
2:C:397:LEU:O	2:C:398:SER:OG	2.15	0.64
2:C:895:LEU:HD12	2:C:899:GLU:OE1	1.99	0.64
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.80	0.64
3:D:127:LEU:O	3:D:220:ARG:NH1	2.31	0.63
2:C:357:ASN:OD1	2:C:358:ASP:N	2.30	0.63
7:Y:30:DT:H2''	7:Y:31:DT:H5''	1.80	0.63
3:D:665:GLN:OE1	3:D:669:GLN:NE2	2.32	0.63
2:C:942:ASP:OD2	2:C:943:LYS:N	2.31	0.63
2:C:841:ARG:N	2:C:848:GLU:OE2	2.31	0.63
7:Y:26:DC:H2''	7:Y:27:DG:H5'	1.80	0.63
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.81	0.62
3:D:826:ILE:HG22	3:D:831:VAL:HG12	1.81	0.62
2:C:1080:ASN:OD1	2:C:1081:PRO:HD2	1.98	0.62
3:D:1052:GLU:OE1	3:D:1052:GLU:N	2.28	0.62
3:D:895:CYS:SG	10:D:2003:ZN:ZN	1.87	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:925:GLU:HG3	3:D:926:PRO:HD3	1.80	0.62
3:D:956:GLY:HA3	3:D:984:LEU:HD11	1.81	0.62
3:D:850:LYS:HG3	3:D:857:LEU:HG	1.81	0.62
3:D:827:GLU:O	3:D:832:LYS:NZ	2.33	0.61
1:A:131:CYS:SG	1:A:132:HIS:N	2.73	0.61
2:C:696:ASP:OD1	2:C:697:LYS:N	2.32	0.61
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.82	0.61
3:D:789:LYS:NZ	3:D:930:LEU:O	2.32	0.61
3:D:19:ALA:HA	3:D:1342:ASP:O	2.00	0.61
2:C:1269:ARG:NH1	7:Y:21:DG:OP1	2.32	0.61
3:D:1203:ARG:HE	3:D:1203:ARG:HA	1.66	0.61
2:C:3:TYR:O	2:C:8:LYS:NZ	2.34	0.61
2:C:530:ILE:O	2:C:572:ILE:O	2.19	0.61
1:A:15:ASP:OD2	1:A:16:ILE:N	2.34	0.61
7:Y:23:DT:H4'	7:Y:23:DT:OP1	2.00	0.60
2:C:1024:GLU:HA	2:C:1027:LYS:HE2	1.83	0.60
5:F:586:ARG:HD2	5:F:590:ILE:HG12	1.83	0.60
1:B:20:SER:O	1:B:22:THR:N	2.34	0.60
3:D:514:THR:OG1	3:D:595:ALA:O	2.18	0.60
2:C:867:GLU:OE2	2:C:943:LYS:NZ	2.32	0.60
5:F:584:ARG:CZ	5:F:586:ARG:HB3	2.31	0.60
1:B:105:SER:HA	1:B:138:ALA:O	2.01	0.60
2:C:1017:GLN:O	2:C:1021:LEU:HD23	2.02	0.60
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.84	0.60
5:F:362:ASN:OD1	5:F:363:ARG:N	2.34	0.60
5:F:584:ARG:N	5:F:584:ARG:HD3	2.16	0.60
2:C:231:GLU:N	2:C:238:GLN:O	2.33	0.60
3:D:1044:GLN:O	3:D:1071:GLY:N	2.35	0.60
3:D:996:LYS:NZ	3:D:997:VAL:O	2.34	0.60
5:F:295:CYS:SG	5:F:326:TRP:NE1	2.75	0.60
7:Y:36:DG:H2''	7:Y:37:DG:OP2	2.02	0.59
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.67	0.59
3:D:1061:VAL:HB	3:D:1105:ALA:HB3	1.83	0.59
2:C:48:GLY:O	2:C:51:ALA:N	2.32	0.59
3:D:895:CYS:SG	3:D:898:CYS:SG	3.01	0.59
2:C:1297:ASP:OD2	2:C:1300:GLY:N	2.29	0.59
3:D:1027:VAL:HB	3:D:1121:LEU:HB2	1.85	0.59
3:D:215:LYS:HB3	3:D:219:LYS:NZ	2.18	0.59
5:F:279:ARG:NH1	5:F:283:GLN:OE1	2.34	0.59
3:D:1157:ALA:O	3:D:1207:GLY:N	2.35	0.58
3:D:1002:VAL:O	3:D:1019:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:LYS:HA	3:D:959:LYS:HE2	1.85	0.58
2:C:423:ASP:OD2	2:C:427:ASP:OD1	2.21	0.58
2:C:543:ALA:O	2:C:548:ARG:NH1	2.37	0.58
3:D:964:LYS:O	3:D:976:THR:OG1	2.21	0.58
2:C:1283:ALA:HA	3:D:479:GLU:OE1	2.03	0.58
6:X:44:DC:H2"	6:X:45:DC:H5"	1.85	0.58
2:C:1259:LEU:O	2:C:1266:GLY:HA2	2.04	0.58
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.30	0.58
3:D:1033:GLY:O	3:D:1115:ILE:N	2.29	0.58
5:F:279:ARG:NH1	5:F:280:VAL:HG12	2.19	0.58
2:C:985:GLU:OE1	2:C:988:LYS:N	2.36	0.57
3:D:1062:LEU:HB3	3:D:1066:GLU:HG3	1.86	0.57
3:D:304:ASP:OD1	3:D:305:ALA:N	2.37	0.57
2:C:59:ILE:HG23	2:C:476:LYS:HE3	1.86	0.57
1:B:137:ASN:OD1	1:B:138:ALA:N	2.33	0.57
5:F:248:GLU:HA	5:F:251:LYS:HD2	1.85	0.57
3:D:1033:GLY:HA3	3:D:1082:ASP:HA	1.87	0.57
6:X:63:DT:H2'	6:X:64:DG:C8	2.40	0.57
2:C:277:LEU:HD12	2:C:282:VAL:HG11	1.85	0.57
3:D:1149:ARG:HD3	3:D:1216:ALA:HB1	1.86	0.57
7:Y:20:DT:H2'	7:Y:21:DG:C8	2.39	0.57
5:F:283:GLN:O	5:F:287:ILE:HG12	2.05	0.57
2:C:472:GLU:OE1	2:C:473:ARG:N	2.38	0.57
3:D:831:VAL:HG23	3:D:831:VAL:O	2.05	0.57
3:D:450:HIS:NE2	3:D:625:MET:HE1	2.20	0.56
3:D:849:LEU:HD12	3:D:855:ASP:H	1.70	0.56
3:D:951:GLN:O	3:D:953:LYS:NZ	2.30	0.56
5:F:276:MET:O	5:F:280:VAL:HG13	2.05	0.56
5:F:327:SER:HA	5:F:330:LEU:HG	1.87	0.56
3:D:1203:ARG:HA	3:D:1203:ARG:NE	2.20	0.56
2:C:138:ILE:HG21	2:C:143:ARG:HD2	1.87	0.56
2:C:557:ARG:NH2	2:C:611:GLU:OE2	2.37	0.56
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.87	0.56
3:D:167:ASP:OD1	3:D:168:ALA:N	2.37	0.56
1:B:158:ARG:NH2	1:B:173:VAL:O	2.39	0.56
2:C:179:TYR:HB2	2:C:397:LEU:O	2.05	0.56
2:C:826:ASP:OD1	2:C:829:THR:OG1	2.13	0.56
3:D:749:LYS:HB2	3:D:750:PRO:HD2	1.88	0.56
3:D:1044:GLN:N	3:D:1044:GLN:OE1	2.39	0.56
5:F:293:GLU:OE1	5:F:294:GLN:HG3	2.06	0.56
3:D:1162:ILE:CD1	3:D:1203:ARG:HH22	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:588:ARG:O	5:F:591:GLU:HG3	2.05	0.56
3:D:311:ARG:O	3:D:312:ARG:HD3	2.06	0.56
3:D:1172:LYS:HB2	3:D:1189:MET:HE3	1.87	0.56
5:F:395:THR:O	5:F:397:ARG:N	2.39	0.56
2:C:304:GLU:OE1	2:C:330:HIS:NE2	2.38	0.56
2:C:1140:LYS:O	2:C:1143:GLU:HG3	2.06	0.56
2:C:412:GLU:OE1	2:C:412:GLU:N	2.39	0.56
2:C:960:LEU:O	2:C:963:GLU:HG3	2.06	0.56
3:D:167:ASP:O	3:D:171:GLU:HG3	2.06	0.56
5:F:279:ARG:HH12	5:F:280:VAL:HG12	1.71	0.56
3:D:475:GLU:OE2	3:D:475:GLU:N	2.34	0.56
3:D:768:ASN:OD1	3:D:771:GLN:OE1	2.23	0.55
2:C:582:ASN:OD1	2:C:583:GLU:N	2.34	0.55
2:C:742:TYR:O	2:C:974:ARG:NH2	2.38	0.55
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.39	0.55
3:D:215:LYS:HB3	3:D:219:LYS:HZ1	1.72	0.55
3:D:742:GLY:O	3:D:762:ASN:HB3	2.06	0.55
3:D:1148:ARG:NH1	6:X:67:DA:OP1	2.40	0.55
3:D:1189:MET:O	3:D:1190:ILE:HD13	2.06	0.55
2:C:393:ASP:OD2	2:C:394:ARG:N	2.39	0.55
2:C:1236:ASN:O	2:C:1236:ASN:ND2	2.33	0.55
5:F:584:ARG:HH22	5:F:586:ARG:NE	2.05	0.55
3:D:79:LYS:O	3:D:81:ARG:NH1	2.40	0.55
2:C:7:GLU:OE2	2:C:7:GLU:N	2.39	0.55
2:C:624:ASP:O	2:C:626:GLU:N	2.40	0.55
3:D:1110:GLU:HG2	3:D:1111:ASP:H	1.72	0.55
5:F:266:PHE:O	5:F:270:VAL:HG13	2.06	0.55
5:F:584:ARG:HG2	5:F:586:ARG:H	1.72	0.55
6:X:45:DC:H5'	6:X:46:DC:OP2	2.07	0.55
3:D:337:ARG:O	3:D:338:PHE:C	2.50	0.55
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.88	0.55
2:C:519:ASN:ND2	2:C:796:LEU:HD22	2.22	0.55
5:F:145:LEU:HD23	5:F:221:PHE:HD2	1.71	0.55
2:C:675:ASP:OD2	2:C:676:ALA:N	2.39	0.55
2:C:1119:MET:HE2	2:C:1228:GLY:HA2	1.89	0.55
5:F:584:ARG:NH1	5:F:586:ARG:HB3	2.21	0.55
5:F:490:PRO:O	5:F:491:GLU:HG2	2.06	0.54
2:C:415:GLU:N	2:C:415:GLU:OE1	2.40	0.54
2:C:590:PRO:HB3	2:C:605:TYR:CE2	2.43	0.54
2:C:1007:LYS:O	2:C:1011:LEU:HD23	2.07	0.54
2:C:1285:TYR:HB2	3:D:479:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:ILE:HD11	3:D:570:LYS:HG3	1.88	0.54
3:D:1021:ASP:HB3	3:D:1024:THR:HB	1.89	0.54
7:Y:32:DA:H2"	7:Y:34:DA:OP2	2.07	0.54
2:C:696:ASP:O	2:C:697:LYS:HB3	2.06	0.54
3:D:144:TYR:CE1	3:D:180:MET:SD	3.00	0.54
3:D:865:HIS:ND1	3:D:867:GLN:OE1	2.40	0.54
1:A:43:LEU:O	1:A:47:LEU:HD13	2.08	0.54
2:C:341:LEU:HD23	2:C:342:ASP:OD1	2.07	0.54
3:D:164:GLN:O	3:D:167:ASP:OD1	2.26	0.54
5:F:409:ASN:O	5:F:413:MET:HG3	2.07	0.54
2:C:60:GLN:OE1	2:C:60:GLN:N	2.39	0.54
3:D:210:SER:HB2	3:D:213:LYS:HE2	1.90	0.54
3:D:407:VAL:O	3:D:411:ILE:HG12	2.07	0.54
3:D:846:GLU:OE1	3:D:847:ASP:O	2.26	0.54
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.37	0.54
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.35	0.54
3:D:982:LEU:O	3:D:982:LEU:HD12	2.07	0.54
2:C:899:GLU:OE2	2:C:903:ARG:CZ	2.55	0.54
3:D:1158:GLU:HG3	3:D:1186:TYR:CZ	2.43	0.54
3:D:952:VAL:HG13	3:D:984:LEU:HD22	1.89	0.54
1:B:192:VAL:O	1:B:194:GLN:N	2.39	0.54
2:C:4:SER:HB3	2:C:7:GLU:OE2	2.08	0.54
2:C:987:GLU:HG3	2:C:988:LYS:H	1.73	0.54
3:D:147:ILE:HD11	3:D:179:LYS:CE	2.38	0.54
3:D:149:GLY:O	3:D:152:THR:HG22	2.09	0.53
2:C:260:LYS:NZ	2:C:276:GLN:OE1	2.39	0.53
1:A:95:LYS:HE2	1:A:98:VAL:HG12	1.91	0.53
2:C:1164:PHE:HE2	2:C:1167:GLU:H	1.53	0.53
3:D:1061:VAL:HG13	3:D:1076:PRO:HG2	1.90	0.53
3:D:1205:GLU:OE1	3:D:1206:ARG:O	2.26	0.53
5:F:496:LYS:O	5:F:500:ILE:HG12	2.08	0.53
1:A:62:ASP:OD1	1:A:62:ASP:N	2.42	0.53
3:D:195:GLU:OE1	3:D:195:GLU:N	2.33	0.53
3:D:1151:LYS:HG3	3:D:1152:GLU:OE1	2.08	0.53
5:F:138:PRO:C	5:F:140:ALA:H	2.17	0.53
5:F:141:ILE:HA	5:F:144:LEU:HD12	1.90	0.53
5:F:361:ILE:HG22	5:F:364:ARG:NH2	2.23	0.53
7:Y:17:DC:H5"	7:Y:17:DC:H6	1.72	0.53
2:C:12:ARG:NH1	2:C:1182:ILE:O	2.38	0.53
3:D:298:MET:SD	5:F:402:LEU:HB3	2.48	0.53
2:C:379:GLU:OE2	2:C:379:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:847:ASP:N	3:D:847:ASP:OD1	2.41	0.53
4:E:42:GLU:OE1	4:E:42:GLU:N	2.42	0.53
5:F:594:ALA:O	5:F:598:LEU:HD23	2.09	0.53
5:F:147:GLN:HA	5:F:150:ARG:HE	1.74	0.53
2:C:206:ALA:O	2:C:209:ILE:HG22	2.09	0.53
2:C:850:ILE:HG22	2:C:850:ILE:O	2.08	0.53
2:C:897:PRO:O	2:C:900:LYS:HB2	2.08	0.53
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.09	0.53
3:D:62:PHE:O	3:D:101:ARG:HD3	2.09	0.53
3:D:266:ASN:O	3:D:270:ARG:HG3	2.09	0.53
3:D:514:THR:HG21	3:D:596:LEU:HD12	1.91	0.53
3:D:1267:VAL:O	3:D:1274:PHE:CE1	2.62	0.53
5:F:361:ILE:HG13	5:F:362:ASN:N	2.24	0.52
2:C:106:GLU:HB3	2:C:109:ALA:HB2	1.91	0.52
2:C:479:LEU:HD21	2:C:492:MET:HE1	1.90	0.52
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.09	0.52
3:D:1031:VAL:HG22	3:D:1080:ILE:HD12	1.91	0.52
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.90	0.52
5:F:489:MET:SD	5:F:489:MET:N	2.83	0.52
2:C:158:ASP:OD1	2:C:159:SER:N	2.42	0.52
3:D:867:GLN:HA	3:D:870:ASP:OD2	2.09	0.52
5:F:595:LEU:HB3	5:F:599:ARG:HH12	1.74	0.52
2:C:75:LEU:HD21	2:C:127:ILE:HD11	1.91	0.52
2:C:575:LEU:HD21	2:C:579:ALA:HB3	1.92	0.52
2:C:660:VAL:HG21	3:D:769:VAL:CG1	2.40	0.52
2:C:522:SER:OG	2:C:687:ARG:O	2.27	0.52
5:F:300:LYS:O	5:F:304:THR:HG23	2.10	0.52
5:F:571:TYR:HB3	5:F:575:GLU:HB2	1.90	0.52
1:B:61:ILE:HG22	1:B:63:GLY:H	1.75	0.52
2:C:595:THR:O	2:C:597:GLY:N	2.43	0.52
3:D:901:ARG:HD2	3:D:906:GLY:O	2.10	0.52
1:A:183:ILE:HD13	1:A:205:MET:HB2	1.91	0.52
3:D:860:ARG:HG2	3:D:861:ASN:H	1.74	0.52
1:B:155:ALA:HA	1:B:158:ARG:HH21	1.74	0.51
2:C:1164:PHE:HE2	2:C:1167:GLU:HB3	1.76	0.51
3:D:213:LYS:O	3:D:217:LEU:HD23	2.10	0.51
6:X:24:DC:H2"	6:X:25:DT:OP2	2.08	0.51
2:C:14:ASP:HB3	2:C:1157:GLN:OE1	2.10	0.51
2:C:18:ARG:O	2:C:1156:ARG:NH1	2.42	0.51
2:C:36:GLN:O	2:C:40:GLU:HB2	2.10	0.51
5:F:505:ILE:HD11	7:Y:28:DC:N4	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:HD22	2:C:1217:THR:HA	1.75	0.51
3:D:218:THR:HA	3:D:221:ILE:HG22	1.92	0.51
3:D:709:ARG:HG3	3:D:710:ASP:H	1.75	0.51
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.24	0.51
2:C:494:ASN:OD1	2:C:496:LYS:HB2	2.11	0.51
2:C:542:ARG:NH1	6:X:63:DT:OP1	2.43	0.51
2:C:1023:HIS:O	2:C:1026:GLU:HG3	2.09	0.51
5:F:320:ILE:HG12	5:F:327:SER:O	2.11	0.51
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.45	0.51
2:C:765:ILE:HG23	2:C:765:ILE:O	2.10	0.51
2:C:990:ASP:OD1	2:C:991:LYS:HG3	2.10	0.51
5:F:289:LYS:O	5:F:293:GLU:HG3	2.10	0.51
1:A:45:ARG:HG2	1:B:38:THR:OG1	2.11	0.51
2:C:398:SER:HB2	2:C:401:GLY:H	1.76	0.51
3:D:125:GLY:HA2	3:D:135:ILE:HD11	1.93	0.51
3:D:1048:ARG:HH11	3:D:1048:ARG:HG2	1.75	0.51
5:F:105:MET:HE3	5:F:384:LEU:C	2.36	0.51
1:B:13:LEU:O	1:B:13:LEU:HD23	2.10	0.51
3:D:126:LEU:CD1	3:D:223:LEU:HD13	2.41	0.51
1:A:175:ALA:HB1	1:A:177:TYR:CE2	2.46	0.51
5:F:387:VAL:HG11	5:F:409:ASN:OD1	2.10	0.51
2:C:979:LEU:HD22	2:C:989:LEU:HD22	1.93	0.51
3:D:677:GLU:OE1	3:D:677:GLU:HA	2.11	0.51
5:F:105:MET:CE	5:F:385:ARG:HA	2.41	0.51
5:F:216:LEU:O	5:F:219:GLU:HG3	2.11	0.51
1:A:29:GLU:HB2	1:A:30:PRO:HD3	1.92	0.51
1:B:64:VAL:CG2	1:B:69:SER:HB3	2.41	0.51
2:C:903:ARG:NH1	2:C:910:ALA:HB2	2.26	0.51
2:C:1291:LEU:HD11	3:D:1351:VAL:HG13	1.93	0.51
3:D:949:SER:HB2	3:D:1016:THR:HG23	1.93	0.51
1:B:118:ASP:OD2	1:B:119:GLY:N	2.39	0.50
1:B:123:ILE:O	1:B:123:ILE:HG13	2.11	0.50
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.10	0.50
5:F:295:CYS:HB2	5:F:326:TRP:CD1	2.46	0.50
2:C:230:PHE:HE2	2:C:335:THR:HG21	1.76	0.50
3:D:1062:LEU:HD12	3:D:1066:GLU:HG3	1.93	0.50
5:F:279:ARG:NH1	5:F:344:LEU:CD2	2.75	0.50
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.47	0.50
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.77	0.50
2:C:601:ASP:O	2:C:601:ASP:OD2	2.29	0.50
3:D:418:GLU:HB2	4:E:45:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:424:ASN:OD1	3:D:424:ASN:C	2.55	0.50
3:D:478:LEU:CD2	4:E:51:LEU:HD11	2.40	0.50
3:D:648:GLU:OE1	3:D:649:LYS:HD3	2.11	0.50
5:F:217:ALA:O	5:F:221:PHE:HD1	1.94	0.50
5:F:493:LYS:HA	5:F:496:LYS:HD3	1.93	0.50
2:C:987:GLU:O	2:C:991:LYS:NZ	2.32	0.50
2:C:1155:VAL:O	2:C:1158:LYS:NZ	2.38	0.50
3:D:45:ASN:O	3:D:46:TYR:CD1	2.65	0.50
3:D:357:VAL:O	3:D:449:LEU:O	2.30	0.50
5:F:99:ARG:O	5:F:103:ARG:HG3	2.12	0.50
1:B:199:ASP:OD1	1:B:199:ASP:N	2.43	0.50
3:D:147:ILE:HG13	3:D:147:ILE:O	2.12	0.50
3:D:706:VAL:O	3:D:706:VAL:HG23	2.12	0.50
5:F:231:THR:HG23	5:F:248:GLU:HB2	1.94	0.50
1:A:14:VAL:HG21	1:A:29:GLU:HG2	1.94	0.49
3:D:1204:VAL:HB	3:D:1208:ASP:OD1	2.12	0.49
5:F:225:ARG:O	5:F:229:VAL:HG12	2.12	0.49
5:F:251:LYS:O	5:F:255:VAL:HG13	2.12	0.49
2:C:782:VAL:HG13	2:C:782:VAL:O	2.12	0.49
3:D:961:SER:OG	3:D:981:GLU:HB3	2.12	0.49
3:D:1344:LEU:C	3:D:1346:GLY:H	2.13	0.49
5:F:358:VAL:HA	5:F:361:ILE:HG12	1.95	0.49
2:C:91:THR:HB	2:C:138:ILE:O	2.12	0.49
2:C:262:TYR:OH	2:C:280:ASP:OD2	2.21	0.49
2:C:273:HIS:O	2:C:277:LEU:HD23	2.12	0.49
2:C:683:ALA:O	2:C:687:ARG:HG3	2.13	0.49
2:C:1072:ASN:HD21	2:C:1230:MET:HE1	1.76	0.49
3:D:103:GLY:C	3:D:244:VAL:HG22	2.38	0.49
3:D:553:THR:O	3:D:553:THR:OG1	2.30	0.49
1:B:32:GLU:HB3	1:B:35:PHE:CD1	2.47	0.49
2:C:46:GLN:OE1	2:C:46:GLN:HA	2.11	0.49
2:C:1010:GLN:O	2:C:1014:LEU:HG	2.13	0.49
3:D:515:ARG:HH12	3:D:717:VAL:HG23	1.77	0.49
3:D:1313:SER:OG	3:D:1325:PHE:HZ	1.95	0.49
5:F:348:GLU:HB3	5:F:353:LEU:O	2.12	0.49
5:F:401:PHE:HA	5:F:404:LEU:HD12	1.94	0.49
5:F:413:MET:O	5:F:416:VAL:HG12	2.11	0.49
1:A:161:SER:O	1:A:163:GLU:HG2	2.12	0.49
1:B:12:ARG:O	1:B:29:GLU:O	2.31	0.49
2:C:43:PRO:HG2	2:C:44:GLU:OE2	2.13	0.49
3:D:18:ASP:N	3:D:18:ASP:OD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:THR:OG1	3:D:153:ASN:N	2.46	0.49
3:D:1215:GLU:OE1	3:D:1215:GLU:N	2.41	0.49
5:F:495:ARG:HA	5:F:498:LEU:HD12	1.93	0.49
1:B:222:THR:O	1:B:226:GLU:HG2	2.12	0.49
2:C:46:GLN:O	2:C:51:ALA:HB2	2.12	0.49
2:C:207:THR:OG1	2:C:354:ASP:OD1	2.26	0.49
2:C:275:ARG:C	2:C:275:ARG:HD2	2.37	0.49
3:D:710:ASP:OD1	3:D:711:GLY:N	2.44	0.49
4:E:68:GLU:OE2	4:E:69:ARG:HG3	2.13	0.49
5:F:344:LEU:O	5:F:348:GLU:HG2	2.12	0.49
5:F:437:GLN:OE1	7:Y:34:DA:N6	2.45	0.49
1:A:17:GLU:OE1	1:A:19:VAL:HG23	2.12	0.49
2:C:126:GLU:HA	2:C:126:GLU:OE1	2.12	0.49
3:D:662:ALA:O	3:D:665:GLN:HG3	2.12	0.49
3:D:1084:GLN:OE1	3:D:1084:GLN:N	2.40	0.49
5:F:565:ILE:HD12	5:F:565:ILE:H	1.76	0.49
1:A:45:ARG:HD2	2:C:1083:GLU:HG3	1.94	0.49
2:C:1030:GLU:OE1	2:C:1034:ARG:NH1	2.45	0.49
6:X:30:DA:H2"	6:X:31:DG:C8	2.47	0.49
2:C:37:LYS:HB3	2:C:47:TYR:CD2	2.48	0.49
2:C:161:LYS:HB2	2:C:170:VAL:HG12	1.95	0.49
2:C:374:GLU:OE1	5:F:99:ARG:NH1	2.46	0.49
2:C:1240:ASP:OD1	2:C:1241:ASP:N	2.45	0.49
3:D:1166:GLY:O	3:D:1167:LYS:C	2.56	0.49
3:D:69:GLU:OE1	3:D:70:CYS:O	2.31	0.48
5:F:305:LEU:HD12	5:F:306:PHE:N	2.28	0.48
3:D:388:ARG:HG3	3:D:388:ARG:HH11	1.78	0.48
3:D:782:GLY:O	3:D:786:THR:HG23	2.14	0.48
3:D:821:MET:CE	3:D:879:ALA:HB1	2.43	0.48
3:D:1162:ILE:HD13	3:D:1203:ARG:HH22	1.78	0.48
5:F:357:GLN:NE2	5:F:358:VAL:HG23	2.28	0.48
2:C:826:ASP:OD1	2:C:829:THR:CB	2.61	0.48
1:B:219:ARG:O	1:B:223:ILE:HG13	2.13	0.48
2:C:987:GLU:HG3	2:C:988:LYS:N	2.28	0.48
2:C:996:ARG:C	2:C:997:TRP:HD1	2.21	0.48
3:D:515:ARG:NH1	3:D:717:VAL:HG23	2.29	0.48
3:D:1160:SER:OG	3:D:1205:GLU:HA	2.12	0.48
5:F:105:MET:SD	5:F:388:ILE:HD12	2.54	0.48
2:C:61:SER:O	2:C:63:SER:N	2.47	0.48
5:F:96:ASP:C	5:F:96:ASP:OD1	2.56	0.48
5:F:604:SER:OG	5:F:608:ARG:NH1	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:VAL:HG23	2:C:170:VAL:O	2.13	0.48
3:D:198:CYS:SG	3:D:202:ARG:NH2	2.86	0.48
3:D:972:LYS:HE3	3:D:1003:LEU:N	2.29	0.48
3:D:977:SER:HB2	3:D:980:THR:CG2	2.44	0.48
5:F:118:ASP:O	5:F:122:ARG:HG2	2.13	0.48
7:Y:49:DC:H2"	7:Y:50:DC:OP2	2.14	0.48
1:A:111:THR:HG22	1:A:112:ALA:N	2.28	0.48
1:A:155:ALA:O	1:A:159:ILE:HG12	2.14	0.48
2:C:198:ILE:O	2:C:200:ARG:N	2.47	0.48
2:C:496:LYS:HB2	2:C:497:PRO:HD3	1.96	0.48
2:C:337:PHE:CZ	2:C:339:ASN:HB2	2.48	0.48
2:C:1258:PRO:CG	3:D:346:ARG:O	2.62	0.48
3:D:528:THR:HG22	3:D:532:GLU:CD	2.37	0.48
3:D:972:LYS:HE3	3:D:1003:LEU:H	1.79	0.48
6:X:20:DT:H2"	6:X:21:DC:C5	2.49	0.48
1:A:78:ILE:O	1:A:82:LEU:HD13	2.14	0.48
2:C:407:ARG:HH11	2:C:407:ARG:HG3	1.78	0.48
2:C:558:VAL:HG11	2:C:573:ASN:HB3	1.96	0.48
3:D:513:MET:HE2	3:D:631:TYR:CG	2.49	0.48
3:D:982:LEU:HD23	3:D:997:VAL:HB	1.95	0.48
2:C:813:GLU:C	2:C:815:SER:H	2.21	0.47
3:D:1047:THR:OG1	3:D:1049:GLN:OE1	2.30	0.47
2:C:318:SER:OG	2:C:321:LEU:HD23	2.14	0.47
2:C:975:ILE:HA	2:C:978:VAL:HG12	1.96	0.47
3:D:179:LYS:HB3	3:D:183:GLU:OE2	2.15	0.47
3:D:316:ILE:HG22	3:D:317:THR:N	2.29	0.47
4:E:28:ARG:O	4:E:32:VAL:HG22	2.14	0.47
5:F:588:ARG:HG2	5:F:588:ARG:HH11	1.79	0.47
1:A:42:ALA:O	1:A:46:ILE:HG12	2.15	0.47
1:A:111:THR:HG22	1:A:112:ALA:H	1.79	0.47
1:B:64:VAL:HG23	1:B:69:SER:HB3	1.95	0.47
2:C:1002:LEU:HD23	2:C:1003:THR:N	2.30	0.47
3:D:1045:THR:HG21	3:D:1076:PRO:HD3	1.97	0.47
3:D:1266:ILE:HD11	3:D:1300:ALA:HB1	1.95	0.47
5:F:151:VAL:HG11	5:F:158:LEU:HA	1.96	0.47
5:F:213:ASP:OD1	5:F:214:PRO:HD2	2.14	0.47
1:A:127:GLN:OE1	1:A:127:GLN:N	2.42	0.47
2:C:466:VAL:O	2:C:469:VAL:HG22	2.14	0.47
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.96	0.47
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.80	0.47
3:D:1045:THR:O	3:D:1046:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:74:DC:C6	6:X:75:DT:H72	2.49	0.47
2:C:122:VAL:HG21	2:C:493:ILE:CG2	2.45	0.47
3:D:1002:VAL:HB	3:D:1019:ASN:HB2	1.96	0.47
3:D:1250:ASP:OD2	3:D:1251:LYS:N	2.47	0.47
4:E:7:GLN:O	4:E:10:VAL:HG12	2.14	0.47
5:F:375:ALA:HA	5:F:378:GLU:OE2	2.15	0.47
5:F:514:ASP:OD1	5:F:516:ASP:OD2	2.33	0.47
2:C:60:GLN:O	2:C:476:LYS:HE2	2.15	0.47
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.15	0.47
2:C:616:ILE:O	2:C:636:CYS:HB3	2.13	0.47
2:C:972:PHE:CZ	2:C:1018:TYR:CE2	3.03	0.47
3:D:45:ASN:O	3:D:47:ARG:N	2.46	0.47
3:D:97:VAL:HG22	3:D:101:ARG:CD	2.45	0.47
3:D:1082:ASP:HB3	3:D:1084:GLN:OE1	2.15	0.47
3:D:1216:ALA:O	3:D:1220:ILE:HD12	2.15	0.47
2:C:339:ASN:N	2:C:343:HIS:O	2.48	0.47
2:C:477:GLU:OE1	2:C:478:ARG:N	2.47	0.47
2:C:479:LEU:HD21	2:C:492:MET:CE	2.45	0.47
2:C:745:GLU:OE1	2:C:1017:GLN:NE2	2.47	0.47
2:C:840:SER:OG	2:C:1048:LYS:HG2	2.15	0.47
2:C:1264:GLN:O	2:C:1265:PHE:C	2.57	0.47
3:D:46:TYR:CZ	5:F:453:PRO:HD3	2.49	0.47
3:D:126:LEU:HD11	3:D:223:LEU:HD13	1.96	0.47
3:D:198:CYS:SG	3:D:202:ARG:NH1	2.87	0.47
3:D:1018:ALA:O	3:D:1019:ASN:OD1	2.32	0.47
5:F:131:GLN:O	5:F:134:VAL:HG22	2.15	0.47
5:F:265:GLN:O	5:F:269:LEU:HG	2.15	0.47
1:A:201:LEU:HG	1:A:203:ILE:HD11	1.95	0.47
2:C:151:ARG:HH11	2:C:445:ILE:HG21	1.79	0.47
2:C:689:ALA:HB2	2:C:1233:LEU:HD23	1.96	0.47
2:C:975:ILE:HG12	2:C:1014:LEU:HD12	1.96	0.47
2:C:1108:ASN:OD1	2:C:1108:ASN:O	2.33	0.47
3:D:852:GLY:O	3:D:855:ASP:HB2	2.15	0.47
4:E:69:ARG:O	4:E:73:GLN:OE1	2.33	0.47
1:A:51:MET:HE2	1:A:51:MET:HA	1.97	0.47
2:C:128:PRO:HG2	2:C:506:PHE:HD2	1.79	0.47
3:D:263:SER:N	5:F:507:MET:HE2	2.30	0.47
3:D:560:ASN:OD1	3:D:562:GLU:OE2	2.33	0.47
5:F:487:MET:HE2	5:F:489:MET:HE1	1.97	0.47
5:F:552:THR:OG1	5:F:555:GLU:HB2	2.14	0.47
1:B:57:THR:HG21	1:B:147:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:778:GLU:OE2	2:C:778:GLU:HA	2.15	0.47
3:D:119:SER:O	3:D:120:LEU:C	2.58	0.47
3:D:557:LYS:HA	3:D:562:GLU:O	2.15	0.47
3:D:955:LYS:HE3	3:D:1010:GLN:CB	2.45	0.47
3:D:1040:MET:HA	3:D:1076:PRO:HB3	1.97	0.47
3:D:1059:LEU:O	3:D:1106:ILE:HA	2.14	0.47
5:F:335:GLU:O	5:F:339:ARG:HG2	2.15	0.47
6:X:65:DA:H2''	6:X:66:DC:H5'	1.96	0.47
1:B:192:VAL:O	1:B:192:VAL:HG23	2.14	0.46
2:C:434:ASP:OD1	2:C:434:ASP:C	2.58	0.46
2:C:539:THR:HG22	2:C:542:ARG:HE	1.79	0.46
2:C:813:GLU:O	2:C:815:SER:N	2.48	0.46
3:D:318:GLY:O	3:D:319:SER:OG	2.27	0.46
3:D:821:MET:SD	3:D:881:LYS:HB2	2.56	0.46
1:B:57:THR:HG23	1:B:58:GLU:N	2.30	0.46
1:B:77:ASP:HB3	1:B:80:GLU:OE2	2.14	0.46
2:C:745:GLU:CD	2:C:1017:GLN:OE1	2.58	0.46
2:C:962:GLU:O	2:C:966:ILE:HG13	2.15	0.46
2:C:968:GLU:HA	2:C:968:GLU:OE1	2.14	0.46
3:D:826:ILE:HG13	3:D:826:ILE:O	2.15	0.46
3:D:1106:ILE:HG23	3:D:1106:ILE:O	2.15	0.46
2:C:180:ARG:NH2	2:C:393:ASP:O	2.46	0.46
2:C:685:MET:SD	2:C:1073:LYS:HD3	2.56	0.46
2:C:1124:ILE:HD11	2:C:1198:LEU:CD1	2.45	0.46
2:C:1134:GLN:O	2:C:1135:GLN:HG2	2.15	0.46
3:D:196:GLN:O	3:D:199:GLU:HG2	2.15	0.46
3:D:252:LEU:O	3:D:252:LEU:HD23	2.15	0.46
3:D:1197:ASN:OD1	3:D:1198:VAL:HG13	2.14	0.46
5:F:245:ALA:O	5:F:249:ILE:HG12	2.15	0.46
6:X:64:DG:H1'	6:X:65:DA:C8	2.51	0.46
7:Y:30:DT:H4'	7:Y:30:DT:OP1	2.14	0.46
2:C:577:VAL:HG23	2:C:661:VAL:O	2.15	0.46
3:D:515:ARG:HH11	3:D:719:PHE:HE1	1.63	0.46
3:D:1149:ARG:HD3	3:D:1216:ALA:CB	2.46	0.46
3:D:1283:SER:O	3:D:1287:ILE:HG12	2.16	0.46
5:F:100:MET:HA	5:F:103:ARG:HG3	1.96	0.46
2:C:296:VAL:O	2:C:335:THR:OG1	2.28	0.46
2:C:305:SER:OG	2:C:306:THR:N	2.48	0.46
2:C:1160:ASP:HB2	2:C:1162:SER:N	2.28	0.46
2:C:1312:ASN:OD1	2:C:1313:HIS:N	2.49	0.46
3:D:356:THR:HG22	3:D:357:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:639:VAL:HG13	3:D:639:VAL:O	2.15	0.46
3:D:1082:ASP:HB2	3:D:1088:VAL:HG23	1.97	0.46
3:D:1275:LEU:HD12	3:D:1275:LEU:C	2.40	0.46
7:Y:27:DG:H4'	7:Y:28:DC:C5	2.50	0.46
2:C:582:ASN:HA	2:C:588:GLU:OE2	2.16	0.46
2:C:624:ASP:HB2	2:C:625:GLU:OE1	2.16	0.46
3:D:44:ILE:HG22	3:D:45:ASN:N	2.31	0.46
3:D:80:HIS:HB3	3:D:83:VAL:CG2	2.45	0.46
3:D:223:LEU:HD21	3:D:227:PHE:CE2	2.51	0.46
3:D:474:LEU:HD12	4:E:28:ARG:HE	1.80	0.46
3:D:965:SER:CB	3:D:973:LEU:HG	2.46	0.46
3:D:1156:LEU:HD12	3:D:1207:GLY:C	2.41	0.46
3:D:1165:PHE:HB3	3:D:1168:GLU:OE1	2.16	0.46
3:D:1250:ASP:OD2	3:D:1250:ASP:C	2.57	0.46
4:E:36:ASP:OD1	4:E:37:PRO:HD2	2.16	0.46
4:E:65:ASP:O	4:E:68:GLU:HG3	2.15	0.46
5:F:250:LEU:O	5:F:254:GLU:HG3	2.16	0.46
6:X:78:DG:H2''	6:X:79:DA:C8	2.51	0.46
1:A:166:ARG:HD3	1:A:166:ARG:H	1.79	0.46
3:D:15:GLU:HA	3:D:15:GLU:OE1	2.15	0.46
3:D:166:LEU:O	3:D:169:LEU:HG	2.15	0.46
3:D:278:ARG:NH2	5:F:403:ASP:OD1	2.49	0.46
3:D:298:MET:HE2	5:F:406:GLN:HG3	1.98	0.46
1:B:72:GLU:H	1:B:72:GLU:CD	2.22	0.46
1:B:196:THR:HG21	3:D:443:GLU:HG3	1.97	0.46
2:C:90:VAL:HG22	2:C:91:THR:N	2.31	0.46
2:C:524:ILE:HD11	2:C:712:SER:HA	1.98	0.46
2:C:818:VAL:HG21	2:C:1076:ILE:CD1	2.46	0.46
3:D:1162:ILE:O	3:D:1178:THR:HB	2.16	0.46
2:C:131:THR:HG22	2:C:132:ASP:H	1.81	0.46
2:C:397:LEU:O	2:C:398:SER:CB	2.64	0.46
3:D:261:ALA:HA	5:F:505:ILE:O	2.15	0.46
3:D:825:VAL:HG13	3:D:825:VAL:O	2.16	0.46
5:F:326:TRP:O	5:F:330:LEU:HG	2.16	0.46
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.46	0.46
2:C:30:ILE:HD11	2:C:575:LEU:HD13	1.96	0.46
2:C:127:ILE:HG13	2:C:127:ILE:O	2.16	0.46
2:C:151:ARG:HH21	2:C:177:ILE:HD11	1.80	0.46
2:C:197:ARG:O	2:C:197:ARG:HG3	2.15	0.46
2:C:226:GLU:HA	2:C:226:GLU:OE2	2.15	0.46
3:D:304:ASP:OD1	3:D:304:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:392:LYS:HE2	6:X:54:DC:H3'	1.98	0.46
1:A:15:ASP:OD2	1:A:15:ASP:C	2.58	0.45
1:B:215:GLU:HG3	1:B:219:ARG:NH1	2.31	0.45
2:C:203:LYS:HG3	2:C:203:LYS:O	2.16	0.45
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.97	0.45
3:D:552:ILE:HD12	3:D:589:TYR:CD1	2.50	0.45
3:D:1177:ILE:HG22	3:D:1186:TYR:HB3	1.98	0.45
5:F:286:LEU:O	5:F:290:LEU:HG	2.16	0.45
5:F:303:ILE:O	5:F:307:THR:N	2.46	0.45
6:X:21:DC:H2''	6:X:22:DC:C6	2.51	0.45
1:B:133:LEU:HD11	1:B:140:ILE:HG22	1.98	0.45
2:C:840:SER:HB3	2:C:850:ILE:HD11	1.98	0.45
2:C:1085:MET:HE1	2:C:1097:VAL:HG23	1.97	0.45
3:D:45:ASN:O	3:D:46:TYR:CG	2.70	0.45
3:D:85:CYS:HB3	3:D:88:CYS:O	2.15	0.45
3:D:211:GLU:O	3:D:215:LYS:CD	2.62	0.45
3:D:1075:ARG:HE	3:D:1168:GLU:CD	2.23	0.45
3:D:1095:MET:O	3:D:1095:MET:SD	2.74	0.45
5:F:100:MET:O	5:F:104:GLU:HG2	2.16	0.45
2:C:198:ILE:O	2:C:199:ASP:C	2.60	0.45
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.56	0.45
2:C:878:THR:HG22	2:C:879:GLY:N	2.31	0.45
5:F:596:ARG:HG2	5:F:596:ARG:HH11	1.81	0.45
1:B:74:VAL:HG12	1:B:133:LEU:HD23	1.99	0.45
2:C:539:THR:CG2	2:C:542:ARG:HG3	2.47	0.45
2:C:741:MET:HG3	2:C:746:ALA:HB1	1.98	0.45
2:C:849:GLU:HG2	2:C:851:THR:H	1.81	0.45
3:D:146:VAL:HG23	3:D:146:VAL:O	2.16	0.45
3:D:964:LYS:O	3:D:964:LYS:HG3	2.15	0.45
3:D:1063:ASP:O	3:D:1067:ARG:N	2.50	0.45
5:F:219:GLU:OE2	5:F:220:LYS:NZ	2.42	0.45
5:F:361:ILE:HG22	5:F:364:ARG:HH21	1.81	0.45
1:B:193:GLU:HG2	1:B:194:GLN:HG2	1.97	0.45
2:C:199:ASP:OD2	2:C:200:ARG:N	2.46	0.45
2:C:434:ASP:OD1	2:C:439:LYS:HB2	2.17	0.45
2:C:755:LYS:O	2:C:757:THR:HG23	2.17	0.45
3:D:582:ILE:HG13	3:D:583:VAL:N	2.31	0.45
3:D:986:ASP:OD2	3:D:990:ARG:N	2.49	0.45
2:C:232:ILE:O	2:C:232:ILE:HG13	2.17	0.45
2:C:237:LEU:HD12	2:C:289:VAL:HG22	1.97	0.45
2:C:681:MET:O	2:C:685:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1013:GLN:O	2:C:1016:GLU:HG2	2.16	0.45
2:C:1122:LYS:HG2	2:C:1229:TYR:CE2	2.51	0.45
2:C:1142:ARG:NH1	2:C:1165:SER:O	2.49	0.45
2:C:1326:LEU:CD2	3:D:338:PHE:HE1	2.30	0.45
2:C:1340:GLU:HB2	3:D:19:ALA:O	2.17	0.45
3:D:26:SER:H	3:D:29:MET:HE3	1.81	0.45
3:D:45:ASN:HB3	3:D:48:THR:O	2.16	0.45
3:D:78:LEU:O	3:D:81:ARG:HD3	2.17	0.45
3:D:966:VAL:HG13	3:D:966:VAL:O	2.16	0.45
3:D:1060:VAL:O	3:D:1060:VAL:HG23	2.16	0.45
4:E:15:ASN:HB3	4:E:18:ASP:OD1	2.16	0.45
7:Y:9:DG:C8	7:Y:10:DT:H72	2.52	0.45
1:A:45:ARG:CD	2:C:1083:GLU:HG3	2.47	0.45
2:C:1232:MET:C	2:C:1233:LEU:HD12	2.41	0.45
3:D:963:VAL:HB	3:D:980:THR:HG22	1.97	0.45
5:F:130:VAL:O	5:F:134:VAL:HG13	2.16	0.45
5:F:288:MET:CE	5:F:299:LYS:HG3	2.47	0.45
5:F:586:ARG:HD2	5:F:586:ARG:O	2.17	0.45
6:X:38:DA:H2''	6:X:39:DT:H72	1.99	0.45
1:B:166:ARG:HB3	1:B:170:ARG:HG3	1.98	0.45
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.82	0.45
2:C:1298:VAL:HG23	2:C:1299:ASN:H	1.82	0.45
3:D:141:PHE:CB	3:D:180:MET:HE2	2.47	0.45
3:D:1170:LYS:HD3	3:D:1189:MET:HE1	1.97	0.45
5:F:96:ASP:OD1	5:F:98:VAL:N	2.49	0.45
5:F:313:ASP:OD1	5:F:316:PHE:HB3	2.16	0.45
5:F:397:ARG:NH2	7:Y:31:DT:H2'	2.32	0.45
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.47	0.45
2:C:1259:LEU:HD11	5:F:524:GLU:HB3	1.99	0.45
3:D:615:LYS:HE3	4:E:5:THR:HB	1.98	0.45
6:X:20:DT:H2''	6:X:21:DC:C6	2.52	0.45
2:C:678:ARG:NH2	2:C:1106:ARG:HG2	2.32	0.45
2:C:748:ILE:HD11	2:C:966:ILE:HG22	1.99	0.45
3:D:127:LEU:HD13	3:D:223:LEU:CD2	2.46	0.45
3:D:770:LEU:O	3:D:774:ILE:HG13	2.17	0.45
3:D:814:CYS:SG	3:D:816:THR:HG22	2.57	0.45
3:D:975:ILE:HG23	3:D:980:THR:HG21	1.98	0.45
3:D:1325:PHE:CZ	3:D:1326:GLN:HG3	2.52	0.45
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.45
1:B:37:HIS:NE2	1:B:187:VAL:HG11	2.33	0.44
2:C:188:PHE:HE2	2:C:436:ARG:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:VAL:HB	2:C:335:THR:CG2	2.47	0.44
2:C:371:ARG:HE	2:C:384:LEU:HD12	1.83	0.44
2:C:576:SER:OG	2:C:577:VAL:N	2.50	0.44
8:C:1401:1N7:H5	8:C:1401:1N7:H31	1.98	0.44
3:D:641:ILE:O	3:D:764:ARG:NH1	2.51	0.44
3:D:1045:THR:OG1	3:D:1071:GLY:HA3	2.17	0.44
3:D:1072:LYS:O	3:D:1075:ARG:NH1	2.49	0.44
3:D:1113:VAL:O	3:D:1115:ILE:HD13	2.17	0.44
3:D:1314:LEU:HB2	3:D:1326:GLN:HE22	1.81	0.44
3:D:1345:ARG:HG2	3:D:1345:ARG:HH11	1.80	0.44
5:F:148:TYR:O	5:F:152:GLU:HG3	2.17	0.44
5:F:333:VAL:HG22	5:F:333:VAL:O	2.16	0.44
7:Y:25:DG:H2'	7:Y:26:DC:C6	2.52	0.44
7:Y:56:DA:H2''	7:Y:57:DG:OP2	2.17	0.44
1:B:164:ASP:N	1:B:164:ASP:OD1	2.49	0.44
2:C:514:PHE:HE2	7:Y:26:DC:P	2.40	0.44
2:C:738:GLU:OE2	2:C:738:GLU:HA	2.17	0.44
3:D:215:LYS:O	3:D:218:THR:HG22	2.16	0.44
3:D:677:GLU:O	3:D:681:LYS:HG3	2.18	0.44
3:D:727:ASP:OD1	3:D:727:ASP:C	2.61	0.44
4:E:50:ALA:O	4:E:54:ILE:HG12	2.17	0.44
5:F:122:ARG:HE	5:F:371:LYS:HE2	1.81	0.44
5:F:605:GLU:N	5:F:608:ARG:NH1	2.65	0.44
2:C:505:PHE:CD2	2:C:506:PHE:CD1	3.05	0.44
2:C:1160:ASP:CB	2:C:1162:SER:H	2.29	0.44
3:D:148:GLU:N	3:D:148:GLU:OE2	2.51	0.44
3:D:682:VAL:HA	3:D:685:ILE:HG12	2.00	0.44
3:D:1239:ASP:OD2	3:D:1242:ARG:NH1	2.50	0.44
3:D:1323:ALA:HA	3:D:1331:VAL:HG21	1.99	0.44
5:F:451:ARG:NH2	6:X:42:DC:OP1	2.51	0.44
5:F:525:ASP:OD1	5:F:527:THR:HG22	2.18	0.44
7:Y:14:DT:H2''	7:Y:15:DG:C8	2.53	0.44
2:C:992:LEU:HD12	2:C:993:PRO:O	2.18	0.44
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.52	0.44
2:C:1290:MET:HG3	3:D:347:VAL:HG11	1.99	0.44
3:D:527:LEU:HD12	3:D:548:VAL:HG11	1.99	0.44
3:D:891:ASP:HA	3:D:1281:GLU:OE2	2.17	0.44
3:D:1080:ILE:O	3:D:1080:ILE:HG13	2.16	0.44
5:F:147:GLN:HA	5:F:150:ARG:NE	2.33	0.44
6:X:66:DC:H2''	6:X:67:DA:C8	2.52	0.44
1:A:160:HIS:O	1:A:162:GLU:OE1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:HD3	1:A:166:ARG:N	2.32	0.44
2:C:234:ASP:O	2:C:235:ASN:HB3	2.17	0.44
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.98	0.44
2:C:1271:GLY:N	2:C:1274:GLU:OE2	2.50	0.44
3:D:140:TYR:OH	3:D:312:ARG:CZ	2.65	0.44
3:D:579:LEU:O	3:D:582:ILE:HG12	2.17	0.44
3:D:747:MET:HG3	3:D:759:ILE:HD11	2.00	0.44
3:D:1089:LEU:HD12	3:D:1093:THR:O	2.17	0.44
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.42	0.44
3:D:1267:VAL:HG13	3:D:1301:THR:HG23	1.99	0.44
5:F:277:MET:O	5:F:280:VAL:HG22	2.18	0.44
5:F:585:GLU:OE2	5:F:588:ARG:NH2	2.51	0.44
1:A:13:LEU:CD2	1:A:16:ILE:HD11	2.47	0.44
2:C:106:GLU:HB2	2:C:114:VAL:CG2	2.47	0.44
2:C:545:PHE:O	2:C:546:GLU:C	2.61	0.44
2:C:866:ASP:HB3	2:C:872:TYR:CE1	2.52	0.44
2:C:1018:TYR:HD1	2:C:1022:LYS:HE2	1.82	0.44
3:D:556:GLU:O	3:D:564:VAL:HG22	2.18	0.44
3:D:1040:MET:HG2	3:D:1046:ILE:HG13	1.98	0.44
3:D:1162:ILE:CD1	3:D:1203:ARG:NH2	2.80	0.44
5:F:220:LYS:HD3	5:F:223:GLU:OE2	2.17	0.44
5:F:286:LEU:HD12	5:F:287:ILE:N	2.32	0.44
5:F:324:LYS:O	5:F:328:GLU:HG2	2.18	0.44
7:Y:23:DT:C6	7:Y:23:DT:C5'	3.00	0.44
2:C:662:SER:OG	2:C:663:VAL:N	2.51	0.44
8:C:1402:1N7:H5	8:C:1402:1N7:H31	1.99	0.44
3:D:113:HIS:CE1	3:D:307:LEU:HD23	2.52	0.44
3:D:212:THR:O	3:D:216:LYS:HG3	2.18	0.44
3:D:1054:THR:O	3:D:1054:THR:HG22	2.17	0.44
3:D:1166:GLY:HA3	3:D:1174:ARG:HD3	2.00	0.44
5:F:110:LEU:HD23	5:F:111:LEU:O	2.18	0.44
5:F:146:GLU:HB3	5:F:150:ARG:NH2	2.33	0.44
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.99	0.44
1:B:91:ARG:O	1:B:91:ARG:HG3	2.18	0.44
3:D:348:ASP:O	3:D:349:TYR:C	2.60	0.44
3:D:1314:LEU:HA	3:D:1326:GLN:OE1	2.17	0.44
4:E:18:ASP:O	4:E:22:VAL:HG12	2.17	0.44
5:F:354:THR:O	5:F:358:VAL:HG23	2.18	0.44
1:B:183:ILE:HD13	1:B:205:MET:HE2	2.00	0.44
2:C:287:VAL:CG1	2:C:288:PRO:HD2	2.48	0.44
2:C:1268:GLN:OE1	3:D:352:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1289:GLU:HG3	2:C:1290:MET:N	2.33	0.44
3:D:111:THR:HG23	3:D:300:GLN:OE1	2.16	0.44
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.00	0.44
3:D:663:GLU:OE1	3:D:664:ILE:HG13	2.18	0.44
3:D:955:LYS:HA	3:D:1011:VAL:O	2.18	0.44
3:D:1161:GLY:HA2	3:D:1180:VAL:HG13	2.00	0.44
5:F:231:THR:HG21	5:F:249:ILE:HG23	2.00	0.44
5:F:333:VAL:O	5:F:337:VAL:HG12	2.17	0.44
1:B:91:ARG:O	1:B:91:ARG:CG	2.65	0.43
1:B:175:ALA:HB1	1:B:177:TYR:CE2	2.53	0.43
3:D:45:ASN:C	3:D:47:ARG:H	2.26	0.43
3:D:709:ARG:CG	3:D:710:ASP:H	2.31	0.43
5:F:253:SER:O	5:F:257:LYS:HG2	2.18	0.43
7:Y:34:DA:C2'	7:Y:35:DG:H5'	2.47	0.43
1:B:6:THR:OG1	1:B:7:GLU:N	2.47	0.43
1:B:215:GLU:OE1	1:B:218:ARG:HD2	2.18	0.43
2:C:264:GLU:HA	2:C:264:GLU:OE1	2.18	0.43
2:C:282:VAL:HG13	2:C:282:VAL:O	2.17	0.43
2:C:473:ARG:HD2	2:C:473:ARG:O	2.18	0.43
2:C:890:LYS:HD3	2:C:914:LYS:HE2	2.00	0.43
2:C:972:PHE:HE1	2:C:998:LEU:HD11	1.83	0.43
3:D:44:ILE:CD1	3:D:252:LEU:HD22	2.48	0.43
3:D:316:ILE:HG22	3:D:317:THR:H	1.83	0.43
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.99	0.43
3:D:834:PRO:HD2	3:D:837:ASP:OD1	2.18	0.43
5:F:343:LYS:HE2	5:F:343:LYS:HA	2.00	0.43
6:X:79:DA:H2''	6:X:80:DG:C8	2.53	0.43
2:C:593:LYS:HB3	2:C:600:THR:CG2	2.48	0.43
2:C:1326:LEU:HD21	3:D:338:PHE:HE1	1.82	0.43
3:D:58:CYS:SG	3:D:60:ARG:HG2	2.58	0.43
3:D:92:VAL:O	3:D:92:VAL:HG13	2.19	0.43
3:D:858:VAL:HG23	3:D:858:VAL:O	2.18	0.43
3:D:868:TRP:O	3:D:872:LEU:HG	2.17	0.43
3:D:1327:GLU:CD	3:D:1327:GLU:H	2.27	0.43
5:F:261:LEU:HB3	5:F:266:PHE:CE1	2.53	0.43
5:F:288:MET:HE3	5:F:292:VAL:HG13	2.01	0.43
5:F:425:TYR:HB3	6:X:50:DA:OP2	2.19	0.43
7:Y:23:DT:H5'	7:Y:23:DT:H6	1.79	0.43
1:B:56:VAL:HG22	1:B:146:VAL:HG12	2.00	0.43
1:B:207:THR:HG21	1:B:211:ILE:O	2.18	0.43
1:B:226:GLU:OE2	1:B:226:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:952:VAL:O	3:D:1014:GLY:N	2.28	0.43
5:F:138:PRO:O	5:F:140:ALA:N	2.49	0.43
7:Y:43:DT:C2'	7:Y:44:DT:H72	2.48	0.43
1:A:54:CYS:HB3	1:A:148:ARG:HG3	1.99	0.43
1:A:122:GLU:N	1:A:122:GLU:OE1	2.51	0.43
2:C:14:ASP:HA	2:C:1183:ALA:HB3	2.01	0.43
2:C:231:GLU:OE1	2:C:332:ARG:HG2	2.19	0.43
2:C:236:LYS:O	2:C:286:GLU:HG3	2.19	0.43
2:C:1021:LEU:O	2:C:1024:GLU:HG3	2.17	0.43
3:D:705:THR:OG1	3:D:716:GLN:HG3	2.18	0.43
3:D:823:THR:OG1	3:D:824:PRO:HD2	2.18	0.43
3:D:860:ARG:O	3:D:861:ASN:C	2.62	0.43
3:D:1062:LEU:HB2	3:D:1067:ARG:HA	2.00	0.43
3:D:1170:LYS:HD3	3:D:1189:MET:CE	2.49	0.43
5:F:283:GLN:OE1	5:F:344:LEU:HD21	2.18	0.43
5:F:283:GLN:O	5:F:286:LEU:HG	2.18	0.43
5:F:493:LYS:O	5:F:497:VAL:HG23	2.18	0.43
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.99	0.43
1:A:104:LYS:HD2	1:A:114:ASP:OD2	2.18	0.43
1:A:157:THR:HG23	1:A:158:ARG:N	2.33	0.43
1:B:15:ASP:OD2	1:B:16:ILE:N	2.51	0.43
2:C:120:GLN:OE1	2:C:120:GLN:N	2.41	0.43
2:C:253:PHE:CE2	2:C:255:ILE:HG13	2.54	0.43
2:C:696:ASP:O	2:C:790:ASP:CB	2.66	0.43
2:C:967:LEU:O	2:C:967:LEU:HD23	2.17	0.43
2:C:976:ARG:HB2	2:C:997:TRP:HZ3	1.82	0.43
3:D:291:ILE:HG12	5:F:409:ASN:HD22	1.83	0.43
3:D:475:GLU:OE1	4:E:28:ARG:NH2	2.52	0.43
3:D:567:THR:HG23	3:D:567:THR:O	2.19	0.43
3:D:872:LEU:HB3	3:D:877:VAL:CG1	2.48	0.43
3:D:1001:ALA:CB	3:D:1020:TRP:HB3	2.48	0.43
5:F:220:LYS:HB2	5:F:259:PHE:HZ	1.84	0.43
5:F:288:MET:O	5:F:292:VAL:HG22	2.19	0.43
6:X:43:DT:H2''	6:X:44:DC:C6	2.54	0.43
1:A:85:LEU:HD23	1:A:130:ILE:HD12	2.00	0.43
2:C:58:PRO:HB3	2:C:67:GLU:OE2	2.19	0.43
2:C:494:ASN:OD1	2:C:496:LYS:N	2.47	0.43
2:C:755:LYS:O	2:C:756:TYR:C	2.61	0.43
2:C:1151:LEU:CD2	2:C:1198:LEU:HD13	2.49	0.43
2:C:1298:VAL:HG23	2:C:1299:ASN:N	2.33	0.43
3:D:1006:GLY:N	3:D:1009:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1170:LYS:HG2	6:X:76:DA:H5"	2.00	0.43
5:F:230:VAL:O	5:F:234:THR:HG23	2.18	0.43
1:B:58:GLU:OE1	1:B:170:ARG:HB3	2.19	0.43
2:C:88:ARG:HG2	2:C:88:ARG:O	2.18	0.43
2:C:194:LEU:HD23	2:C:206:ALA:HB2	2.00	0.43
2:C:510:GLN:OE1	2:C:511:LEU:HD23	2.19	0.43
2:C:955:GLN:OE1	2:C:955:GLN:C	2.62	0.43
3:D:147:ILE:HG22	3:D:188:LEU:CD2	2.48	0.43
3:D:460:ASP:HB3	3:D:462:ASP:OD1	2.18	0.43
3:D:947:GLU:HG3	3:D:947:GLU:O	2.19	0.43
3:D:972:LYS:HE2	3:D:973:LEU:O	2.19	0.43
3:D:1057:SER:HB2	3:D:1107:VAL:O	2.19	0.43
3:D:1110:GLU:HG2	3:D:1111:ASP:N	2.33	0.43
4:E:7:GLN:O	4:E:11:GLU:HG3	2.19	0.43
5:F:116:GLU:OE2	5:F:427:PHE:CB	2.67	0.43
5:F:399:LEU:HD21	5:F:447:ALA:HB2	2.01	0.43
2:C:6:THR:HG23	2:C:7:GLU:OE2	2.18	0.43
2:C:211:ARG:HG3	2:C:211:ARG:HH11	1.83	0.43
2:C:262:TYR:CZ	2:C:280:ASP:OD2	2.72	0.43
2:C:297:VAL:HB	2:C:317:LEU:HD11	2.01	0.43
2:C:809:GLY:O	3:D:357:VAL:HG11	2.17	0.43
2:C:1279:GLU:O	2:C:1281:TYR:O	2.37	0.43
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	2.00	0.43
3:D:279:LEU:HD12	3:D:295:GLU:HG3	2.00	0.43
3:D:525:MET:O	3:D:548:VAL:HG13	2.18	0.43
3:D:1024:THR:HG23	3:D:1123:ARG:HA	2.00	0.43
3:D:1170:LYS:HG3	6:X:77:DC:OP1	2.19	0.43
4:E:72:GLN:O	4:E:75:GLN:NE2	2.52	0.43
5:F:235:ILE:HA	5:F:245:ALA:CB	2.49	0.43
5:F:582:VAL:HG13	5:F:582:VAL:O	2.19	0.43
5:F:586:ARG:O	5:F:589:GLN:HB2	2.18	0.43
1:A:162:GLU:HG2	1:A:163:GLU:N	2.33	0.43
1:B:75:GLN:HG2	1:B:76:GLU:N	2.34	0.43
2:C:200:ARG:C	2:C:201:ARG:HD2	2.44	0.43
2:C:1004:ASP:O	2:C:1005:GLU:HG3	2.19	0.43
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.43
2:C:1270:PHE:HB2	3:D:347:VAL:HG13	2.01	0.43
3:D:208:THR:O	3:D:214:ARG:NH1	2.48	0.43
3:D:215:LYS:HD2	3:D:215:LYS:N	2.34	0.43
3:D:470:VAL:HG13	3:D:470:VAL:O	2.19	0.43
3:D:658:GLU:O	3:D:661:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:700:ASN:O	3:D:704:GLU:HB3	2.17	0.43
3:D:925:GLU:HG3	3:D:926:PRO:CD	2.48	0.43
3:D:1062:LEU:HD12	3:D:1066:GLU:CG	2.48	0.43
3:D:1164:SER:HA	3:D:1200:GLU:OE2	2.19	0.43
3:D:1179:PRO:HG2	3:D:1183:SER:O	2.19	0.43
3:D:1203:ARG:NE	3:D:1203:ARG:CA	2.82	0.43
5:F:311:THR:HA	5:F:345:GLN:NE2	2.34	0.43
2:C:120:GLN:H	2:C:120:GLN:CD	2.24	0.42
2:C:194:LEU:H	2:C:350:THR:CG2	2.32	0.42
2:C:255:ILE:HD13	2:C:263:VAL:HB	2.01	0.42
2:C:1082:ILE:H	2:C:1082:ILE:HD12	1.83	0.42
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	2.01	0.42
3:D:78:LEU:C	3:D:78:LEU:HD23	2.44	0.42
3:D:1267:VAL:CG1	3:D:1301:THR:HG23	2.49	0.42
4:E:46:THR:HA	4:E:49:ILE:HD12	2.01	0.42
5:F:94:THR:HG23	5:F:94:THR:O	2.19	0.42
5:F:464:ASN:O	5:F:467:SER:OG	2.29	0.42
6:X:77:DC:H2''	6:X:78:DG:C8	2.53	0.42
7:Y:19:DG:N9	7:Y:20:DT:H72	2.34	0.42
1:B:191:ARG:HD2	1:B:191:ARG:O	2.20	0.42
2:C:1080:ASN:OD1	2:C:1081:PRO:CD	2.67	0.42
2:C:1186:VAL:HG23	2:C:1187:PHE:N	2.33	0.42
3:D:555:TYR:CD2	3:D:585:LYS:HE2	2.54	0.42
3:D:646:ILE:CD1	3:D:762:ASN:HD21	2.32	0.42
3:D:972:LYS:NZ	3:D:1001:ALA:O	2.49	0.42
3:D:981:GLU:OE2	3:D:994:SER:OG	2.27	0.42
3:D:1001:ALA:HA	3:D:1020:TRP:HB3	2.00	0.42
3:D:1005:LYS:CE	3:D:1015:GLU:OE2	2.67	0.42
3:D:1059:LEU:HB2	3:D:1107:VAL:HB	2.00	0.42
3:D:1316:THR:HG22	3:D:1317:GLU:N	2.34	0.42
5:F:267:ASP:O	5:F:271:ASN:CG	2.62	0.42
2:C:15:PHE:HE2	2:C:1194:GLU:HB3	1.84	0.42
2:C:1164:PHE:CE2	2:C:1167:GLU:N	2.84	0.42
2:C:1254:VAL:HG13	2:C:1255:THR:N	2.34	0.42
5:F:435:ILE:O	5:F:439:ILE:HG12	2.19	0.42
7:Y:27:DG:H4'	7:Y:28:DC:H5	1.83	0.42
1:A:233:ASP:OD1	1:A:233:ASP:N	2.51	0.42
1:B:14:VAL:HG22	1:B:28:LEU:CD1	2.49	0.42
1:B:19:VAL:O	1:B:23:HIS:O	2.37	0.42
1:B:156:SER:HA	1:B:159:ILE:HG22	2.00	0.42
2:C:564:PRO:HD2	2:C:572:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:690:VAL:HG12	2:C:1234:LYS:O	2.20	0.42
2:C:1186:VAL:HG23	2:C:1187:PHE:H	1.84	0.42
2:C:1244:HIS:NE2	2:C:1265:PHE:O	2.53	0.42
3:D:200:GLN:OE1	3:D:201:LEU:HD12	2.19	0.42
3:D:1078:LEU:HB3	3:D:1101:LEU:HD21	2.02	0.42
4:E:21:LEU:O	4:E:25:ARG:HG2	2.19	0.42
5:F:470:MET:SD	5:F:486:ARG:HG3	2.59	0.42
7:Y:41:DT:H2''	7:Y:42:DA:OP2	2.19	0.42
1:A:11:PRO:HA	1:A:30:PRO:HG2	2.00	0.42
1:A:218:ARG:HD3	1:B:233:ASP:OD1	2.20	0.42
1:B:202:VAL:HG23	1:B:202:VAL:O	2.19	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.02	0.42
3:D:44:ILE:HG22	3:D:45:ASN:H	1.84	0.42
3:D:104:HIS:NE2	3:D:106:GLU:OE2	2.44	0.42
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.00	0.42
3:D:1186:TYR:CZ	3:D:1188:GLU:HG2	2.54	0.42
5:F:244:THR:HA	5:F:247:GLU:OE1	2.19	0.42
5:F:303:ILE:O	5:F:307:THR:HB	2.18	0.42
5:F:400:GLN:HA	5:F:400:GLN:OE1	2.19	0.42
5:F:568:ASN:O	5:F:569:THR:C	2.62	0.42
7:Y:31:DT:H5''	7:Y:31:DT:C6	2.55	0.42
1:B:179:PRO:HG2	1:B:211:ILE:HD11	2.02	0.42
1:B:197:ASP:O	1:B:198:LEU:HD12	2.20	0.42
2:C:741:MET:HG3	2:C:746:ALA:CB	2.49	0.42
2:C:765:ILE:HG13	2:C:787:PRO:HG3	2.01	0.42
2:C:1142:ARG:HD2	2:C:1161:LEU:CD1	2.49	0.42
3:D:129:ASP:HB2	3:D:220:ARG:NH1	2.34	0.42
3:D:222:LYS:HA	3:D:225:GLU:OE1	2.20	0.42
3:D:268:LEU:HD21	3:D:324:LEU:HD11	2.01	0.42
3:D:849:LEU:HD12	3:D:855:ASP:N	2.33	0.42
3:D:1179:PRO:CD	3:D:1184:ASP:HA	2.49	0.42
3:D:1186:TYR:CE2	3:D:1188:GLU:HG2	2.55	0.42
3:D:1279:GLN:HG2	3:D:1281:GLU:H	1.84	0.42
5:F:584:ARG:HH22	5:F:586:ARG:HE	1.66	0.42
7:Y:11:DC:H2''	7:Y:12:DC:C6	2.55	0.42
2:C:233:ARG:C	2:C:235:ASN:H	2.27	0.42
2:C:481:LEU:HB3	7:Y:33:DT:O4	2.18	0.42
3:D:77:ARG:HG3	3:D:79:LYS:H	1.84	0.42
3:D:663:GLU:C	3:D:663:GLU:CD	2.88	0.42
5:F:412:LEU:HD23	5:F:412:LEU:C	2.44	0.42
2:C:128:PRO:HG2	2:C:506:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:PHE:HA	2:C:265:LYS:HD2	2.02	0.42
2:C:595:THR:O	2:C:598:VAL:N	2.52	0.42
2:C:615:VAL:HG13	2:C:615:VAL:O	2.19	0.42
3:D:141:PHE:HA	3:D:180:MET:HE2	2.00	0.42
3:D:709:ARG:O	3:D:710:ASP:C	2.63	0.42
3:D:749:LYS:HE3	3:D:755:ILE:HD13	2.02	0.42
5:F:119:ILE:HA	5:F:122:ARG:HG3	2.02	0.42
5:F:295:CYS:SG	5:F:326:TRP:CD1	3.12	0.42
5:F:362:ASN:HA	5:F:365:MET:HG3	2.00	0.42
2:C:813:GLU:C	2:C:815:SER:N	2.77	0.42
2:C:1273:MET:HE2	7:Y:20:DT:O4'	2.20	0.42
3:D:377:PHE:O	3:D:378:LYS:C	2.60	0.42
3:D:1105:ALA:HA	3:D:1122:ALA:HB2	2.02	0.42
3:D:1287:ILE:CD1	3:D:1300:ALA:H	2.33	0.42
5:F:279:ARG:NH1	5:F:280:VAL:HA	2.35	0.42
5:F:334:SER:HA	5:F:337:VAL:HG12	2.02	0.42
5:F:481:GLU:N	5:F:481:GLU:OE2	2.51	0.42
2:C:95:PRO:HA	2:C:126:GLU:OE1	2.19	0.42
2:C:580:GLN:NE2	2:C:605:TYR:CZ	2.88	0.42
2:C:588:GLU:OE1	2:C:605:TYR:HB3	2.20	0.42
3:D:1046:ILE:HD12	3:D:1060:VAL:O	2.20	0.42
5:F:288:MET:HE3	5:F:292:VAL:CG1	2.49	0.42
2:C:48:GLY:O	2:C:49:LEU:C	2.62	0.41
2:C:321:LEU:O	2:C:325:LEU:HD23	2.20	0.41
2:C:704:MET:O	2:C:704:MET:HG3	2.20	0.41
2:C:888:THR:OG1	2:C:914:LYS:HB3	2.20	0.41
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.50	0.41
3:D:205:LEU:O	3:D:214:ARG:NH1	2.40	0.41
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.50	0.41
3:D:1078:LEU:CB	3:D:1101:LEU:HD21	2.50	0.41
4:E:45:LYS:O	4:E:49:ILE:HG13	2.20	0.41
5:F:437:GLN:OE1	6:X:46:DC:N4	2.52	0.41
5:F:598:LEU:O	5:F:604:SER:HB3	2.20	0.41
7:Y:16:DT:H2''	7:Y:17:DC:C6	2.55	0.41
1:A:31:LEU:HD13	1:A:36:GLY:HA2	2.01	0.41
1:A:75:GLN:O	2:C:729:ALA:HB2	2.20	0.41
1:B:16:ILE:HG23	1:B:16:ILE:O	2.20	0.41
1:B:137:ASN:O	1:B:138:ALA:C	2.63	0.41
2:C:18:ARG:NE	2:C:620:ASN:HA	2.35	0.41
2:C:631:GLU:OE2	2:C:633:LEU:HD23	2.20	0.41
2:C:895:LEU:CD1	2:C:899:GLU:OE1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:ILE:O	2:C:1076:ILE:HG23	2.19	0.41
3:D:156:ARG:NH2	3:D:157:GLN:OE1	2.43	0.41
3:D:326:SER:OG	3:D:327:LEU:N	2.52	0.41
3:D:811:GLU:O	3:D:895:CYS:HA	2.20	0.41
3:D:1035:VAL:HG23	3:D:1078:LEU:HD21	2.03	0.41
3:D:1162:ILE:HD12	3:D:1203:ARG:HH22	1.85	0.41
5:F:423:ARG:HG3	6:X:48:DA:C2	2.56	0.41
6:X:72:DC:C6	6:X:73:DT:H72	2.55	0.41
1:B:166:ARG:NE	1:B:167:PRO:HD2	2.35	0.41
2:C:42:ASP:OD1	2:C:42:ASP:O	2.38	0.41
2:C:145:ILE:HB	2:C:456:VAL:HG22	2.01	0.41
2:C:300:ASP:O	2:C:300:ASP:OD2	2.38	0.41
2:C:430:LYS:O	2:C:433:ILE:HG13	2.20	0.41
2:C:805:MET:HE1	2:C:1221:PHE:CE2	2.55	0.41
2:C:972:PHE:CD2	2:C:994:ARG:HD3	2.55	0.41
2:C:1019:ASP:HA	2:C:1022:LYS:CE	2.51	0.41
2:C:1109:ILE:O	2:C:1109:ILE:HG22	2.21	0.41
2:C:1217:THR:HG23	2:C:1219:GLU:H	1.85	0.41
3:D:42:GLU:O	3:D:55:GLY:HA3	2.20	0.41
3:D:373:ALA:O	3:D:377:PHE:HD1	2.04	0.41
3:D:666:GLU:HA	3:D:669:GLN:NE2	2.34	0.41
3:D:1170:LYS:HE2	6:X:76:DA:H4'	2.02	0.41
3:D:1174:ARG:CZ	3:D:1187:GLU:HG3	2.50	0.41
3:D:1273:ASP:H	3:D:1276:GLU:CD	2.28	0.41
5:F:392:LYS:HE2	6:X:54:DC:C3'	2.51	0.41
1:A:187:VAL:O	1:A:187:VAL:HG13	2.20	0.41
2:C:113:THR:HG23	2:C:113:THR:O	2.21	0.41
2:C:594:VAL:HG11	2:C:650:VAL:HG23	2.02	0.41
2:C:895:LEU:HB2	2:C:899:GLU:OE1	2.20	0.41
2:C:899:GLU:OE2	2:C:903:ARG:NH2	2.53	0.41
2:C:996:ARG:HA	2:C:999:GLU:OE1	2.21	0.41
3:D:195:GLU:H	3:D:195:GLU:CD	2.24	0.41
3:D:531:LYS:HA	3:D:581:MET:HE1	2.02	0.41
3:D:534:GLU:HA	3:D:578:ILE:CD1	2.51	0.41
3:D:1027:VAL:HG13	3:D:1199:PHE:CZ	2.56	0.41
3:D:1035:VAL:O	3:D:1111:ASP:OD2	2.38	0.41
1:A:149:GLY:O	1:A:177:TYR:HB3	2.20	0.41
1:B:33:ARG:NH1	2:C:1081:PRO:HG3	2.35	0.41
1:B:61:ILE:CG2	1:B:64:VAL:HG12	2.51	0.41
2:C:530:ILE:HD11	2:C:575:LEU:HD12	2.03	0.41
2:C:992:LEU:HD13	2:C:996:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:ARG:HB3	3:D:79:LYS:HG2	2.02	0.41
3:D:894:VAL:HG12	3:D:895:CYS:N	2.35	0.41
3:D:1040:MET:O	3:D:1040:MET:SD	2.78	0.41
3:D:1078:LEU:HB2	3:D:1101:LEU:HD11	2.03	0.41
5:F:484:ALA:O	5:F:487:MET:O	2.38	0.41
1:A:16:ILE:N	1:A:16:ILE:HD12	2.36	0.41
1:B:215:GLU:OE1	1:B:215:GLU:HA	2.20	0.41
2:C:224:PHE:CD1	2:C:347:ILE:HG13	2.55	0.41
2:C:487:LEU:HD12	2:C:492:MET:HG2	2.01	0.41
2:C:575:LEU:HD23	2:C:576:SER:N	2.35	0.41
2:C:631:GLU:CD	2:C:632:ASP:N	2.77	0.41
2:C:866:ASP:OD1	2:C:944:ARG:NH1	2.53	0.41
2:C:895:LEU:N	2:C:895:LEU:HD23	2.35	0.41
3:D:131:PRO:HG2	3:D:134:ASP:OD2	2.21	0.41
3:D:301:GLU:O	3:D:304:ASP:OD1	2.38	0.41
3:D:377:PHE:HE2	3:D:419:HIS:ND1	2.19	0.41
5:F:272:SER:O	5:F:275:VAL:HG12	2.21	0.41
5:F:285:ARG:HG2	5:F:285:ARG:HH11	1.85	0.41
5:F:355:ILE:O	5:F:358:VAL:N	2.53	0.41
5:F:577:GLY:C	5:F:583:THR:HG22	2.45	0.41
1:B:45:ARG:O	1:B:49:SER:OG	2.37	0.41
1:B:156:SER:O	1:B:160:HIS:CD2	2.74	0.41
2:C:524:ILE:HD11	2:C:712:SER:CA	2.50	0.41
2:C:733:VAL:HG22	2:C:750:ILE:HG13	2.02	0.41
2:C:1331:ARG:HG2	3:D:33:TRP:CZ3	2.56	0.41
3:D:44:ILE:HD12	3:D:252:LEU:HD22	2.02	0.41
3:D:77:ARG:HG2	3:D:77:ARG:HH11	1.85	0.41
3:D:167:ASP:O	3:D:170:GLU:HG2	2.21	0.41
3:D:450:HIS:O	3:D:453:VAL:HG22	2.20	0.41
3:D:473:THR:O	3:D:477:GLN:HG3	2.20	0.41
3:D:1282:TYR:HA	3:D:1285:VAL:HG12	2.03	0.41
5:F:320:ILE:HD13	5:F:331:HIS:NE2	2.35	0.41
5:F:429:THR:HG22	6:X:50:DA:H2'	2.03	0.41
6:X:17:DA:H4'	6:X:18:DT:OP1	2.19	0.41
1:A:68:TYR:HE1	2:C:1055:ALA:CB	2.34	0.41
2:C:979:LEU:C	2:C:979:LEU:HD23	2.45	0.41
2:C:1323:PHE:CZ	2:C:1327:LEU:HD11	2.56	0.41
3:D:43:THR:C	3:D:44:ILE:HG13	2.45	0.41
3:D:802:ASP:OD1	3:D:1325:PHE:CD1	2.74	0.41
3:D:1199:PHE:N	3:D:1199:PHE:CD1	2.89	0.41
3:D:1348:LYS:O	3:D:1352:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TYR:CD2	1:A:68:TYR:N	2.87	0.41
2:C:12:ARG:HD3	2:C:1183:ALA:HB2	2.02	0.41
2:C:21:VAL:HG23	2:C:22:LEU:N	2.36	0.41
2:C:280:ASP:O	2:C:281:ASP:HB3	2.21	0.41
2:C:519:ASN:HB3	2:C:522:SER:OG	2.21	0.41
2:C:629:PHE:CD1	2:C:634:VAL:HG11	2.56	0.41
2:C:737:ASN:HB2	2:C:740:GLU:OE2	2.21	0.41
2:C:940:GLU:HA	2:C:940:GLU:OE1	2.21	0.41
2:C:1109:ILE:HD12	3:D:644:MET:HE1	2.02	0.41
2:C:1255:THR:O	2:C:1257:GLN:N	2.49	0.41
2:C:1262:LYS:HB2	7:Y:23:DT:OP2	2.20	0.41
3:D:416:ILE:O	3:D:417:ARG:C	2.63	0.41
3:D:884:SER:HB2	3:D:1254:GLU:OE1	2.21	0.41
3:D:1005:LYS:HB3	3:D:1009:GLU:OE1	2.21	0.41
3:D:1064:SER:HA	3:D:1067:ARG:HH11	1.86	0.41
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.85	0.41
5:F:127:ILE:HA	5:F:130:VAL:HG12	2.03	0.41
5:F:145:LEU:HD23	5:F:221:PHE:CD2	2.55	0.41
5:F:147:GLN:OE1	5:F:161:LEU:HD21	2.21	0.41
5:F:166:VAL:O	5:F:167:ASP:C	2.64	0.41
5:F:226:ALA:O	5:F:230:VAL:HG13	2.21	0.41
5:F:444:ALA:HA	5:F:457:ILE:HD13	2.02	0.41
6:X:51:DA:H2'	6:X:51:DA:P	2.61	0.41
7:Y:7:DG:H2''	7:Y:8:DA:C8	2.56	0.41
7:Y:62:DA:H2''	7:Y:63:DA:C8	2.56	0.41
1:A:229:GLU:C	1:A:229:GLU:CD	2.88	0.41
2:C:57:PHE:CD1	2:C:70:TYR:HB2	2.56	0.41
2:C:224:PHE:HD1	2:C:347:ILE:HG21	1.86	0.41
2:C:230:PHE:CE2	2:C:335:THR:HG21	2.55	0.41
2:C:387:ASN:HA	2:C:391:SER:HB3	2.03	0.41
2:C:660:VAL:HG21	3:D:769:VAL:HG11	2.02	0.41
3:D:80:HIS:HB3	3:D:83:VAL:HG22	2.03	0.41
3:D:369:PRO:HB3	3:D:444:GLY:O	2.21	0.41
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.55	0.41
3:D:802:ASP:OD1	3:D:1325:PHE:CG	2.73	0.41
3:D:872:LEU:HB3	3:D:877:VAL:HG11	2.03	0.41
5:F:273:MET:O	5:F:277:MET:HG2	2.21	0.41
6:X:73:DT:H2''	6:X:74:DC:C6	2.56	0.41
1:A:47:LEU:HD12	1:A:220:ALA:HB2	2.03	0.40
1:A:194:GLN:O	1:A:195:ARG:HG2	2.21	0.40
1:B:15:ASP:OD2	1:B:15:ASP:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LEU:HB3	1:B:168:ILE:CG2	2.52	0.40
1:B:107:ILE:HD12	1:B:135:ASP:HB3	2.02	0.40
2:C:426:ILE:HG13	2:C:427:ASP:N	2.36	0.40
2:C:519:ASN:OD1	2:C:520:PRO:N	2.54	0.40
2:C:757:THR:OG1	2:C:765:ILE:CG2	2.69	0.40
2:C:842:ASP:OD2	2:C:842:ASP:C	2.63	0.40
2:C:976:ARG:HG3	2:C:989:LEU:HD21	2.03	0.40
3:D:23:ALA:HB1	3:D:232:ASN:HD21	1.86	0.40
3:D:110:PRO:O	3:D:182:ALA:HB3	2.22	0.40
3:D:362:ARG:H	3:D:365:GLN:HE21	1.68	0.40
3:D:630:ALA:O	3:D:634:ARG:HG2	2.21	0.40
3:D:952:VAL:HG13	3:D:984:LEU:CD2	2.51	0.40
3:D:977:SER:HB2	3:D:980:THR:HG23	2.03	0.40
3:D:1253:ILE:O	3:D:1257:VAL:HG23	2.21	0.40
4:E:47:THR:O	4:E:51:LEU:HD13	2.21	0.40
1:B:210:THR:OG1	1:B:211:ILE:N	2.55	0.40
2:C:151:ARG:HD2	2:C:445:ILE:CG2	2.52	0.40
2:C:589:THR:HG23	2:C:591:TYR:CE1	2.56	0.40
2:C:1101:LEU:CD2	3:D:725:MET:HG2	2.51	0.40
2:C:1136:GLN:O	2:C:1137:GLU:HB3	2.21	0.40
3:D:313:GLY:HA2	3:D:314:ARG:HH21	1.86	0.40
3:D:553:THR:HG22	3:D:567:THR:OG1	2.21	0.40
5:F:305:LEU:O	5:F:315:TRP:HB3	2.21	0.40
1:A:212:ASP:OD2	1:A:215:GLU:HB3	2.22	0.40
1:B:144:ILE:HG13	1:B:144:ILE:O	2.22	0.40
2:C:159:SER:O	2:C:171:LEU:O	2.40	0.40
2:C:276:GLN:HA	2:C:279:LYS:HE2	2.03	0.40
2:C:354:ASP:OD2	2:C:354:ASP:C	2.65	0.40
2:C:894:GLN:HG2	2:C:894:GLN:O	2.21	0.40
2:C:1124:ILE:HD11	2:C:1198:LEU:HD12	2.02	0.40
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.03	0.40
2:C:1246:ARG:HD2	2:C:1266:GLY:C	2.47	0.40
2:C:1290:MET:SD	2:C:1294:LYS:NZ	2.95	0.40
3:D:147:ILE:C	3:D:148:GLU:OE2	2.65	0.40
3:D:369:PRO:HD2	3:D:372:MET:HE2	2.04	0.40
3:D:589:TYR:O	3:D:590:SER:C	2.63	0.40
3:D:638:SER:OG	3:D:639:VAL:N	2.53	0.40
3:D:956:GLY:CA	3:D:984:LEU:HD11	2.50	0.40
3:D:1048:ARG:HG2	3:D:1059:LEU:HD21	2.04	0.40
5:F:433:TRP:CE3	6:X:47:DT:C2	3.10	0.40
7:Y:24:DG:OP1	7:Y:24:DG:H4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH1	1:B:231:PHE:O	2.54	0.40
1:A:228:LEU:HA	1:A:231:PHE:HD2	1.86	0.40
2:C:17:LYS:HG3	2:C:1154:ASP:O	2.22	0.40
2:C:423:ASP:O	2:C:426:ILE:HG12	2.21	0.40
2:C:493:ILE:O	5:F:472:GLN:NE2	2.54	0.40
2:C:898:GLU:OE1	2:C:898:GLU:N	2.40	0.40
3:D:139:LEU:HD21	3:D:185:ILE:HG13	2.03	0.40
3:D:141:PHE:HB3	3:D:180:MET:HE2	2.03	0.40
3:D:767:LEU:N	3:D:767:LEU:HD12	2.36	0.40
3:D:821:MET:HE3	3:D:879:ALA:HB1	2.02	0.40
3:D:889:ASP:O	3:D:889:ASP:OD2	2.38	0.40
3:D:902:ASP:H	3:D:1251:LYS:HZ3	1.70	0.40
3:D:1038:THR:HG21	3:D:1079:LYS:HD3	2.04	0.40
3:D:1176:VAL:HG23	3:D:1176:VAL:O	2.21	0.40
3:D:1202:GLU:OE1	3:D:1204:VAL:CG1	2.69	0.40
3:D:1353:VAL:O	3:D:1353:VAL:HG12	2.20	0.40
5:F:165:PHE:CE1	5:F:259:PHE:CD1	3.09	0.40
5:F:363:ARG:HD2	5:F:367:ILE:HG12	2.04	0.40
5:F:433:TRP:CE3	6:X:47:DT:O2	2.74	0.40
6:X:49:DT:O5'	6:X:49:DT:H6	2.04	0.40
7:Y:41:DT:H1'	7:Y:42:DA:H5'	2.03	0.40
1:B:29:GLU:HB2	1:B:30:PRO:HA	2.04	0.40
2:C:67:GLU:CD	2:C:69:GLN:HG3	2.46	0.40
2:C:256:GLU:HG2	2:C:260:LYS:C	2.47	0.40
2:C:614:TYR:N	2:C:614:TYR:CD1	2.89	0.40
2:C:914:LYS:HG2	2:C:915:ASP:N	2.36	0.40
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	2.02	0.40
3:D:79:LYS:HB3	5:F:569:THR:HB	2.03	0.40
3:D:224:LEU:O	3:D:228:VAL:HG12	2.22	0.40
3:D:364:HIS:CG	4:E:4:VAL:HG23	2.56	0.40
3:D:772:TYR:O	3:D:773:PHE:C	2.63	0.40
3:D:948:SER:OG	3:D:949:SER:N	2.54	0.40
3:D:1053:LEU:C	3:D:1055:GLY:N	2.80	0.40
5:F:346:GLN:O	5:F:349:GLU:HG3	2.20	0.40
5:F:353:LEU:HB3	5:F:357:GLN:NE2	2.37	0.40
5:F:357:GLN:O	5:F:361:ILE:HG23	2.20	0.40
5:F:385:ARG:HB3	6:X:52:DT:H1'	2.04	0.40
5:F:387:VAL:HG23	5:F:412:LEU:HD12	2.04	0.40
6:X:40:DA:H2''	6:X:41:DA:C8	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	229/329 (70%)	211 (92%)	18 (8%)	0	100	100
1	B	228/329 (69%)	207 (91%)	19 (8%)	2 (1%)	14	49
2	C	1338/1342 (100%)	1228 (92%)	100 (8%)	10 (1%)	19	54
3	D	1334/1407 (95%)	1211 (91%)	117 (9%)	6 (0%)	30	63
4	E	74/91 (81%)	68 (92%)	6 (8%)	0	100	100
5	F	465/613 (76%)	430 (92%)	32 (7%)	3 (1%)	22	56
All	All	3668/4111 (89%)	3355 (92%)	292 (8%)	21 (1%)	24	56

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
2	C	199	ASP
2	C	1160	ASP
3	D	338	PHE
3	D	1345	ARG
2	C	398	SER
3	D	860	ARG
5	F	396	ASN
1	B	193	GLU
2	C	625	GLU
5	F	139	GLU
2	C	43	PRO
3	D	46	TYR
2	C	756	TYR
2	C	814	ASP
2	C	1223	ARG
3	D	337	ARG
3	D	1151	LYS
2	C	45	GLY
2	C	39	ILE

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Mol	Chain	Res	Type
5	F	298	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/286 (70%)	199 (100%)	0	100	100
1	B	198/286 (69%)	198 (100%)	0	100	100
2	C	1155/1157 (100%)	1153 (100%)	2 (0%)	92	97
3	D	1113/1168 (95%)	1113 (100%)	0	100	100
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	419/540 (78%)	419 (100%)	0	100	100
All	All	3149/3512 (90%)	3147 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1154	ASP
2	C	1236	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	132	HIS
1	B	103	ASN
2	C	580	GLN
2	C	604	HIS
2	C	618	GLN
2	C	620	ASN
2	C	677	ASN
2	C	688	GLN
2	C	760	ASN

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Mol	Chain	Res	Type
2	C	1023	HIS
2	C	1072	ASN
2	C	1111	GLN
2	C	1237	HIS
3	D	158	GLN
3	D	186	GLN
3	D	232	ASN
3	D	667	GLN
3	D	762	ASN
3	D	910	ASN
3	D	962	ASN
3	D	1218	HIS
3	D	1227	HIS
3	D	1367	GLN
5	F	131	GLN
5	F	317	ASN
5	F	357	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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z  > 2$
8	1N7	C	1402	-	44,46,46	4.20	20 (45%)	69,72,72	1.80	15 (21%)
8	1N7	C	1401	-	44,46,46	4.18	20 (45%)	69,72,72	2.14	21 (30%)

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
8	1N7	C	1402	-	-	6/27/92/92	0/4/4/4
8	1N7	C	1401	-	-	4/27/92/92	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1402	1N7	C3-C4	-12.87	1.32	1.53
8	C	1401	1N7	C3-C4	-12.78	1.32	1.53
8	C	1402	1N7	C5-C9	-11.25	1.36	1.55
8	C	1401	1N7	C5-C9	-10.72	1.37	1.55
8	C	1402	1N7	C3-C19	-9.49	1.38	1.53
8	C	1401	1N7	C3-C19	-9.18	1.38	1.53
8	C	1401	1N7	C2-C19	7.59	1.69	1.56
8	C	1401	1N7	C5-C4	7.14	1.65	1.54
8	C	1402	1N7	C5-C4	6.84	1.65	1.54
8	C	1402	1N7	C2-C19	6.73	1.67	1.56
8	C	1401	1N7	C24-N1	6.27	1.48	1.33
8	C	1402	1N7	C24-N1	6.27	1.48	1.33
8	C	1401	1N7	C7-C6	-6.22	1.41	1.54
8	C	1402	1N7	C7-C6	-6.21	1.41	1.54
8	C	1401	1N7	C18-C19	-5.85	1.42	1.53
8	C	1402	1N7	C18-C19	-5.65	1.43	1.53
8	C	1401	1N7	C8-C7	5.27	1.68	1.54
8	C	1402	1N7	C8-C7	5.21	1.68	1.54
8	C	1401	1N7	C5-C6	5.18	1.64	1.55
8	C	1402	1N7	C5-C6	5.16	1.64	1.55
8	C	1402	1N7	C18-C6	4.67	1.62	1.53
8	C	1402	1N7	C2-C15	-4.66	1.48	1.55
8	C	1401	1N7	C18-C6	4.50	1.62	1.53
8	C	1401	1N7	C20-C9	4.06	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1402	1N7	C20-C9	3.61	1.60	1.54
8	C	1401	1N7	C2-C15	-3.32	1.50	1.55
8	C	1402	1N7	O3-C17	-3.30	1.36	1.43
8	C	1401	1N7	O3-C17	-3.20	1.36	1.43
8	C	1402	1N7	C23-C24	2.90	1.57	1.51
8	C	1401	1N7	C23-C24	2.77	1.56	1.51
8	C	1402	1N7	O1-C24	-2.63	1.18	1.23
8	C	1401	1N7	O1-C24	-2.60	1.18	1.23
8	C	1401	1N7	O7-S1	2.53	1.52	1.45
8	C	1401	1N7	C8-C9	2.53	1.59	1.54
8	C	1402	1N7	O7-S1	2.52	1.52	1.45
8	C	1402	1N7	C8-C9	2.45	1.59	1.54
8	C	1401	1N7	O6-S1	2.11	1.51	1.45
8	C	1401	1N7	O4-C4	2.09	1.47	1.43
8	C	1402	1N7	O6-S1	2.09	1.51	1.45
8	C	1402	1N7	O4-C4	2.08	1.47	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1401	1N7	C5-C6-C18	-7.27	105.50	114.72
8	C	1402	1N7	C5-C6-C18	-5.39	107.89	114.72
8	C	1401	1N7	C6-C5-C4	-4.87	102.96	107.42
8	C	1401	1N7	C5-C9-C20	-4.77	113.70	119.48
8	C	1402	1N7	C6-C5-C4	-4.53	103.27	107.42
8	C	1401	1N7	C23-C22-C20	-4.31	106.40	114.46
8	C	1402	1N7	C8-C7-C6	-4.06	97.19	105.14
8	C	1402	1N7	O6-S1-O7	-4.00	100.81	113.82
8	C	1401	1N7	C16-C17-C18	-3.94	107.20	111.50
8	C	1401	1N7	C8-C7-C6	-3.90	97.51	105.14
8	C	1401	1N7	O6-S1-O7	-3.87	101.23	113.82
8	C	1402	1N7	C5-C9-C20	-3.82	114.86	119.48
8	C	1401	1N7	C16-C15-C2	3.64	116.53	112.66
8	C	1402	1N7	C23-C22-C20	-3.38	108.15	114.46
8	C	1401	1N7	C19-C2-C15	3.36	113.18	108.51
8	C	1401	1N7	C2-C19-C18	-3.31	108.15	111.84
8	C	1402	1N7	C6-C18-C17	-3.28	107.50	111.85
8	C	1401	1N7	C16-C15-C14	-3.25	107.51	111.23
8	C	1402	1N7	O7-S1-C32	3.24	111.60	106.76
8	C	1402	1N7	O6-S1-C32	3.22	111.56	106.76
8	C	1401	1N7	O7-S1-C32	3.17	111.49	106.76
8	C	1402	1N7	C2-C19-C18	-3.02	108.47	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1402	1N7	C3-C19-C2	-2.97	110.69	113.70
8	C	1401	1N7	C1-C2-C15	2.78	111.74	107.75
8	C	1401	1N7	O6-S1-C32	2.72	110.82	106.76
8	C	1401	1N7	C11-C2-C15	-2.59	106.11	110.44
8	C	1401	1N7	C21-C20-C9	-2.52	109.10	112.88
8	C	1402	1N7	C26-C25-N1	-2.45	105.32	112.20
8	C	1401	1N7	C19-C3-C4	2.43	117.48	114.29
8	C	1402	1N7	C31-C28-N2	-2.25	112.78	116.69
8	C	1402	1N7	C26-C27-N2	-2.20	110.88	115.35
8	C	1401	1N7	O8-S1-C32	2.19	110.20	105.97
8	C	1401	1N7	C6-C18-C17	-2.17	108.98	111.85
8	C	1401	1N7	C3-C19-C2	-2.09	111.58	113.70
8	C	1402	1N7	O8-S1-C32	2.04	109.91	105.97
8	C	1401	1N7	C31-C28-N2	-2.03	113.17	116.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1401	1N7	N2-C28-C31-C32
8	C	1401	1N7	N2-C28-C31-O5
8	C	1402	1N7	N2-C28-C31-C32
8	C	1402	1N7	N2-C28-C31-O5
8	C	1402	1N7	C28-C31-C32-S1
8	C	1402	1N7	O5-C31-C32-S1
8	C	1402	1N7	C9-C20-C22-C23
8	C	1402	1N7	C21-C20-C22-C23
8	C	1401	1N7	C21-C20-C22-C23
8	C	1401	1N7	C9-C20-C22-C23

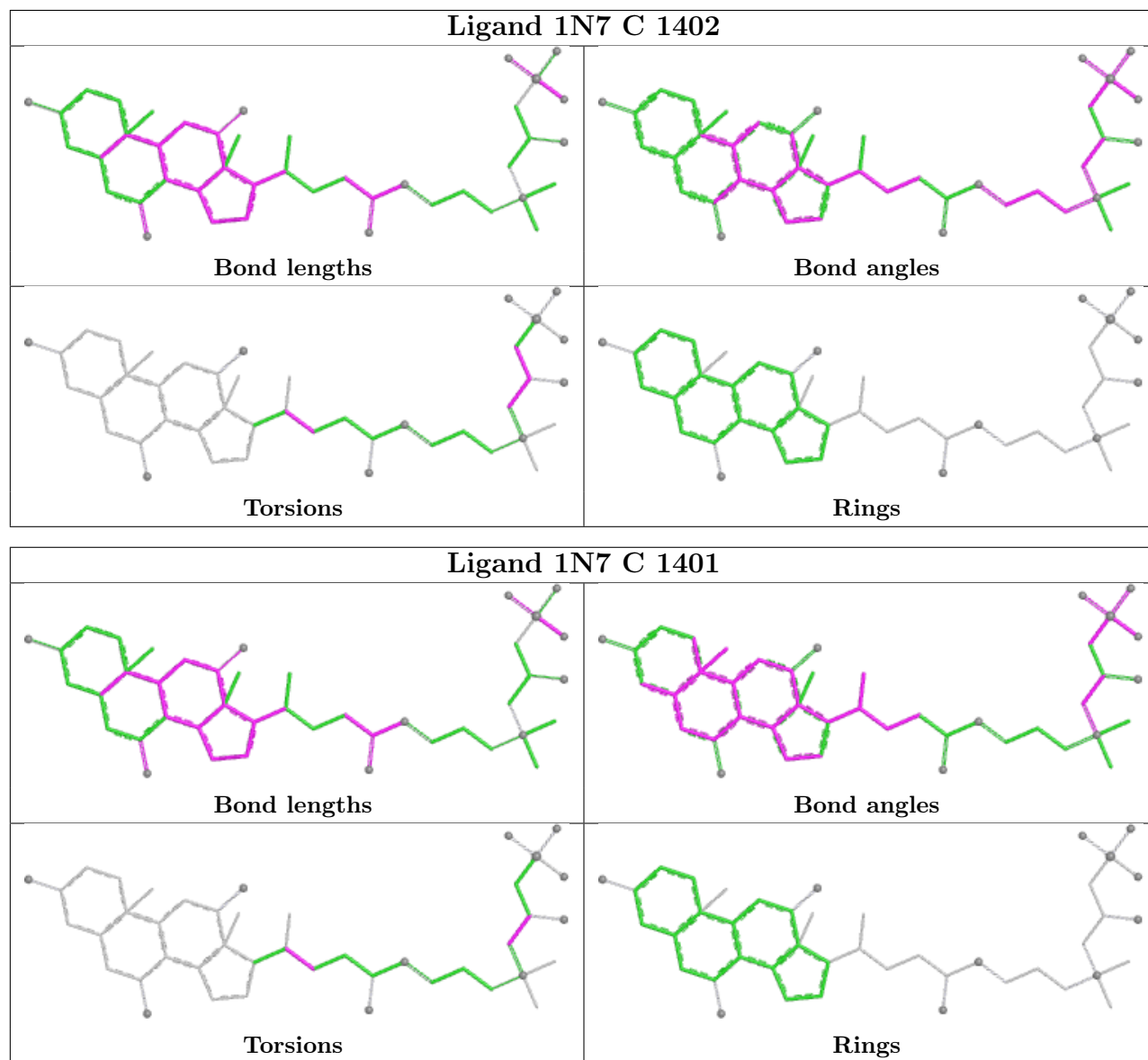
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1402	1N7	1	0
8	C	1401	1N7	1	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

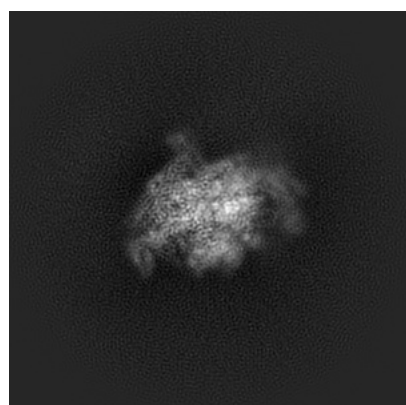
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21880. These allow visual inspection of the internal detail of the map and identification of artifacts.

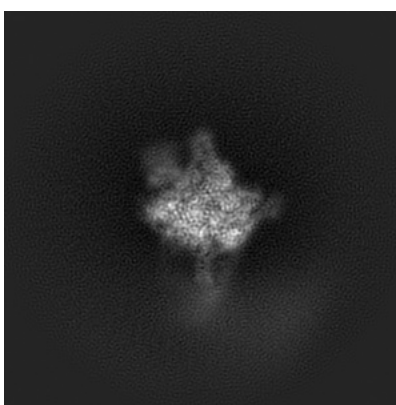
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

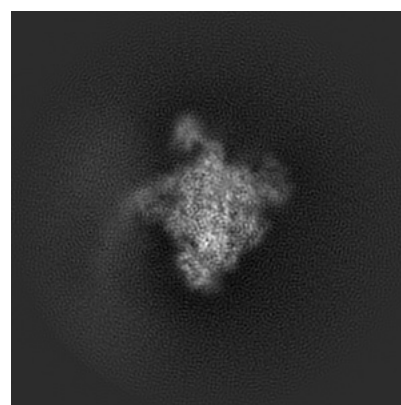
#### 6.1.1 Primary map



X



Y

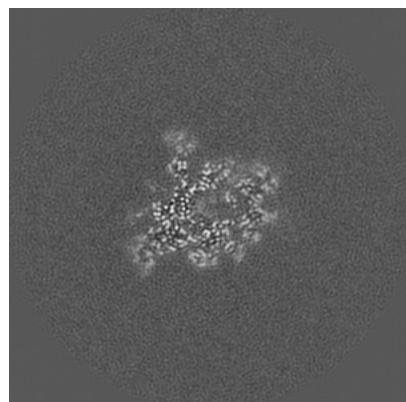


Z

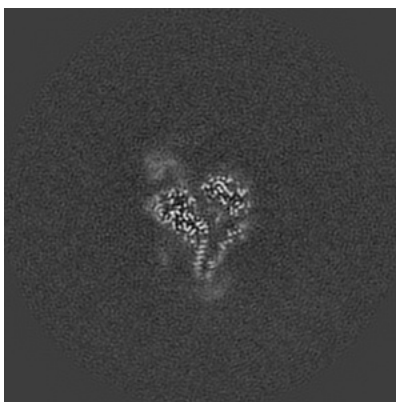
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

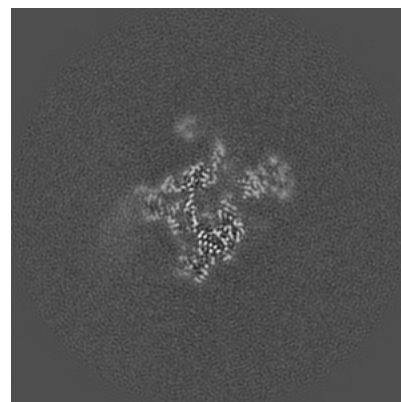
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

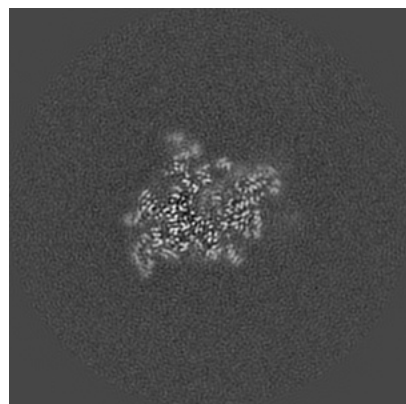


Z Index: 180

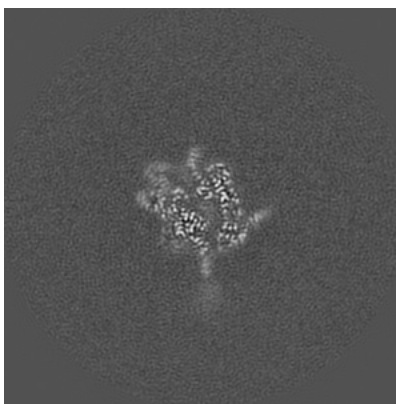
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

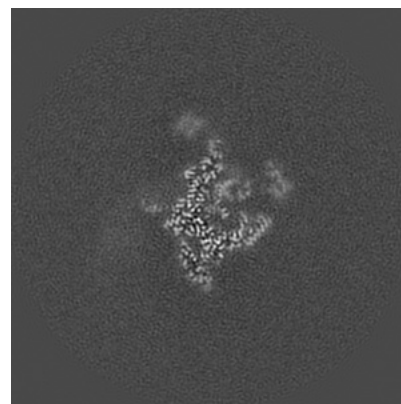
### 6.3.1 Primary map



X Index: 175



Y Index: 170

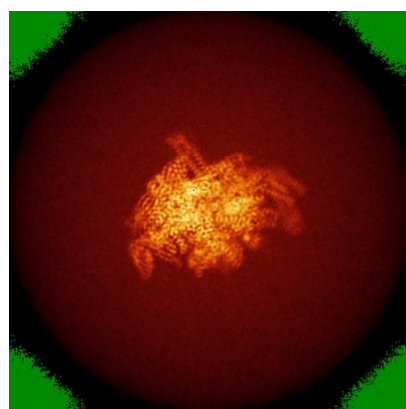


Z Index: 172

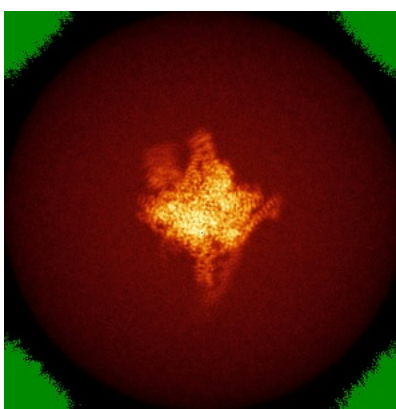
The images above show the largest variance slices of the map in three orthogonal directions.

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

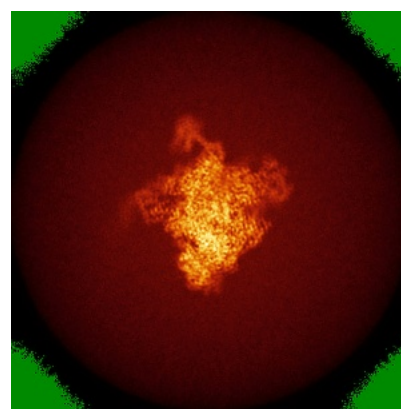
### 6.4.1 Primary map



X



Y

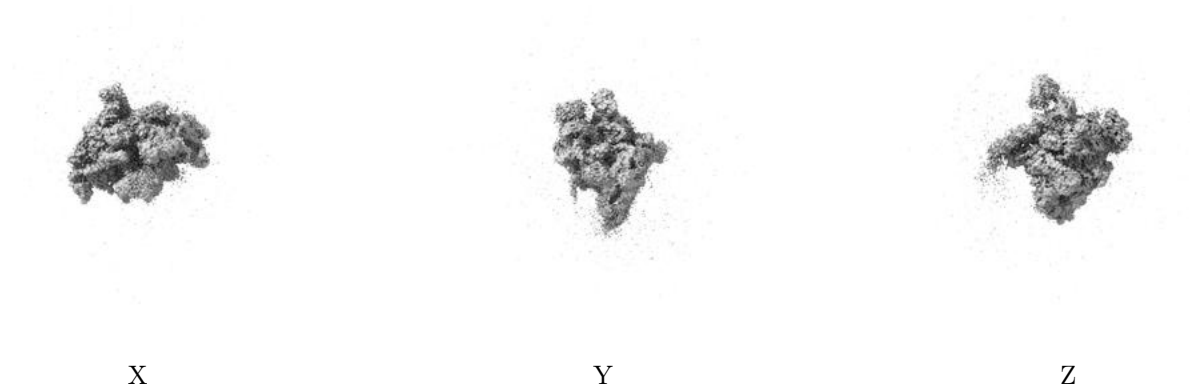


Z

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

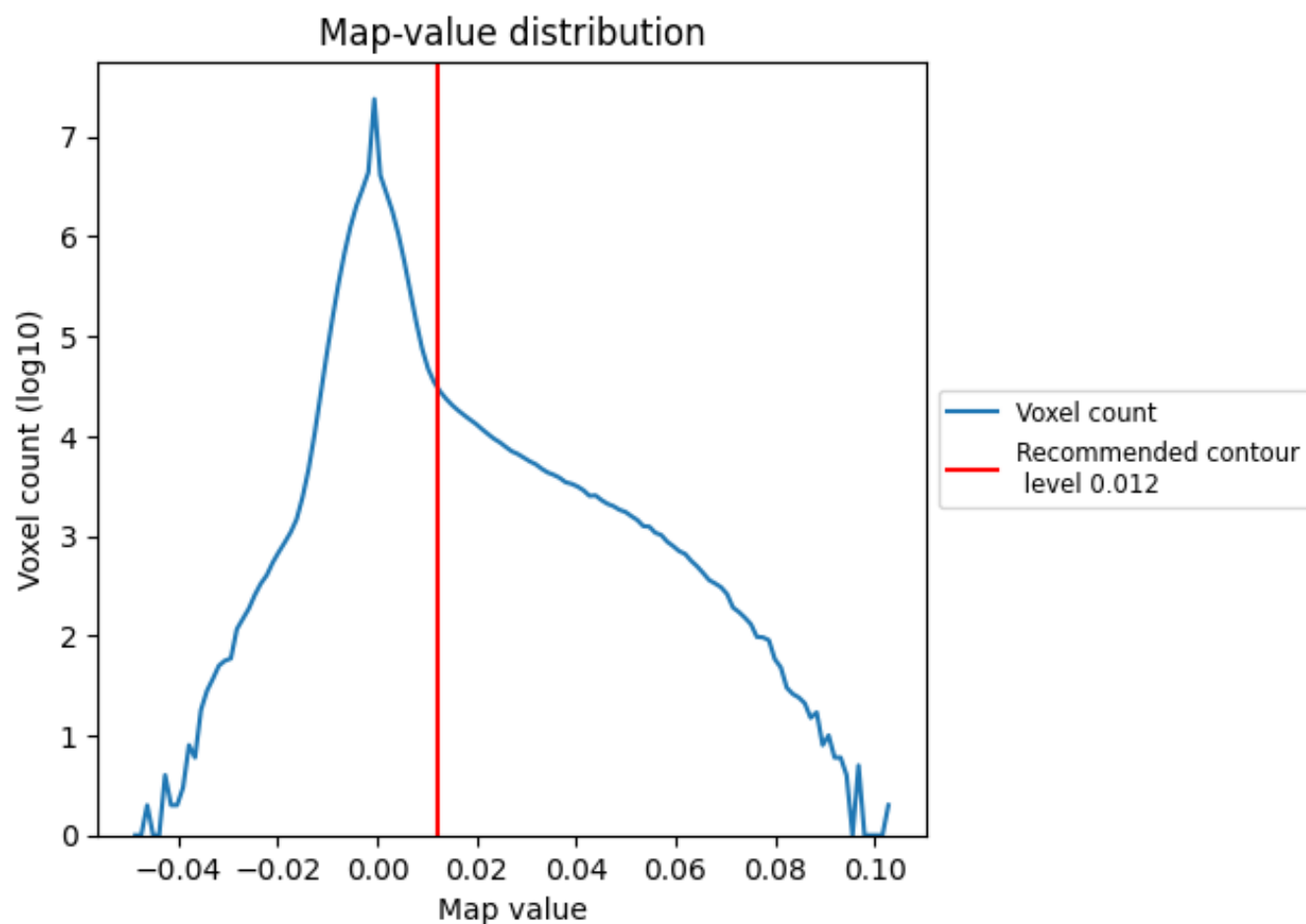
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

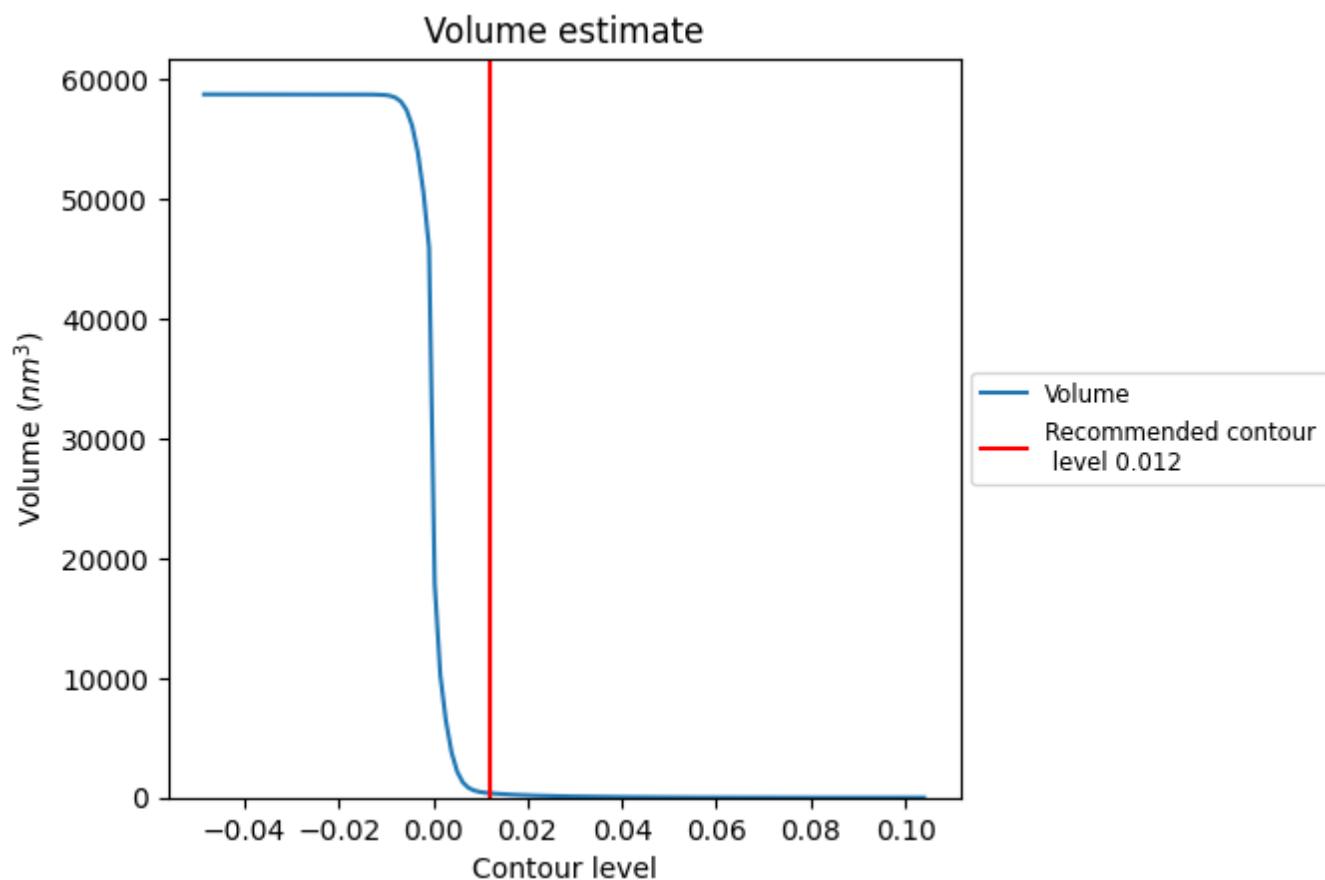
This section contains the results of statistical analysis of the map.

### 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](#)

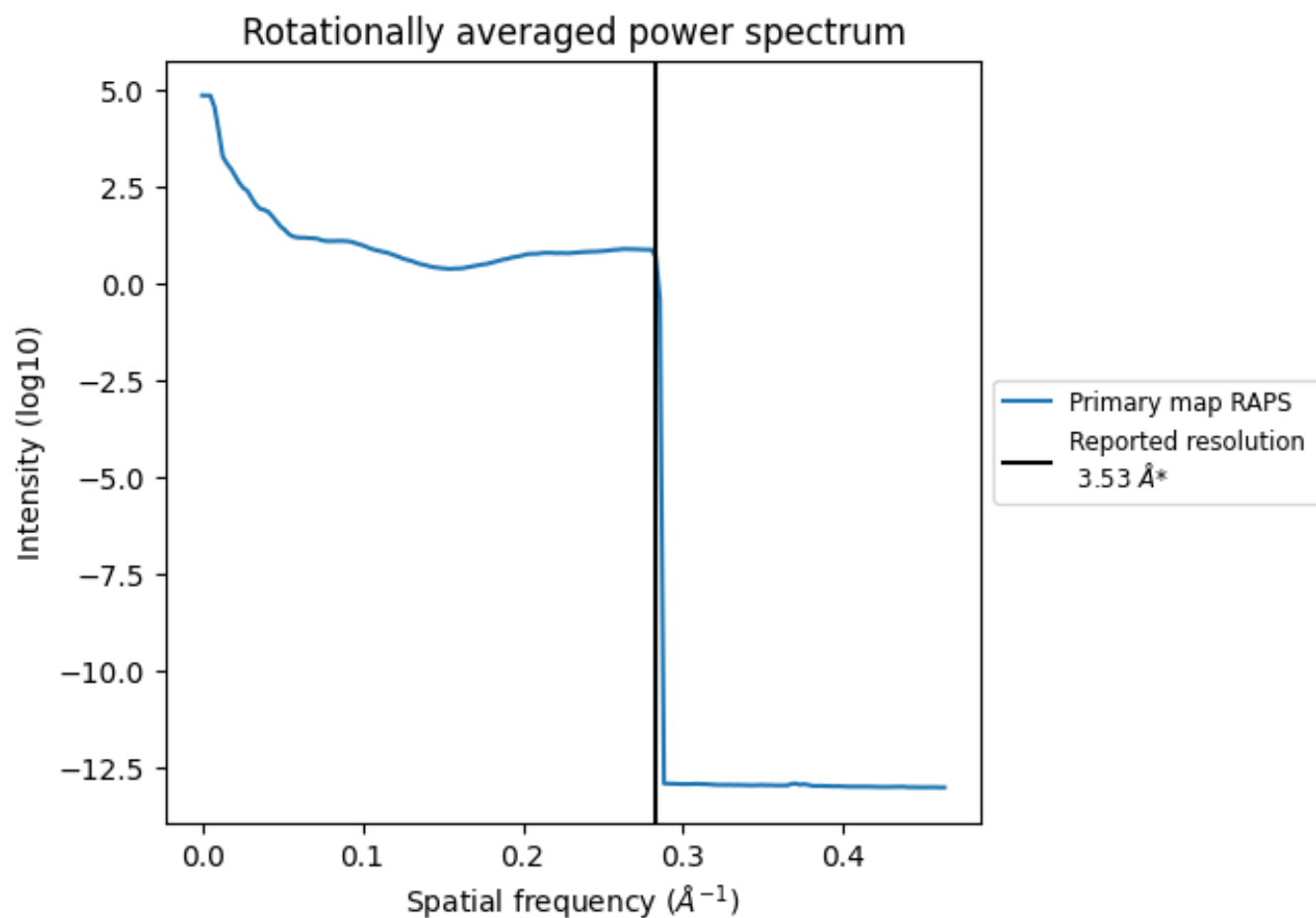


The volume at the recommended contour level is 366 nm<sup>3</sup>; this corresponds to an approximate mass of 331 kDa.

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 0.283 Å<sup>-1</sup>

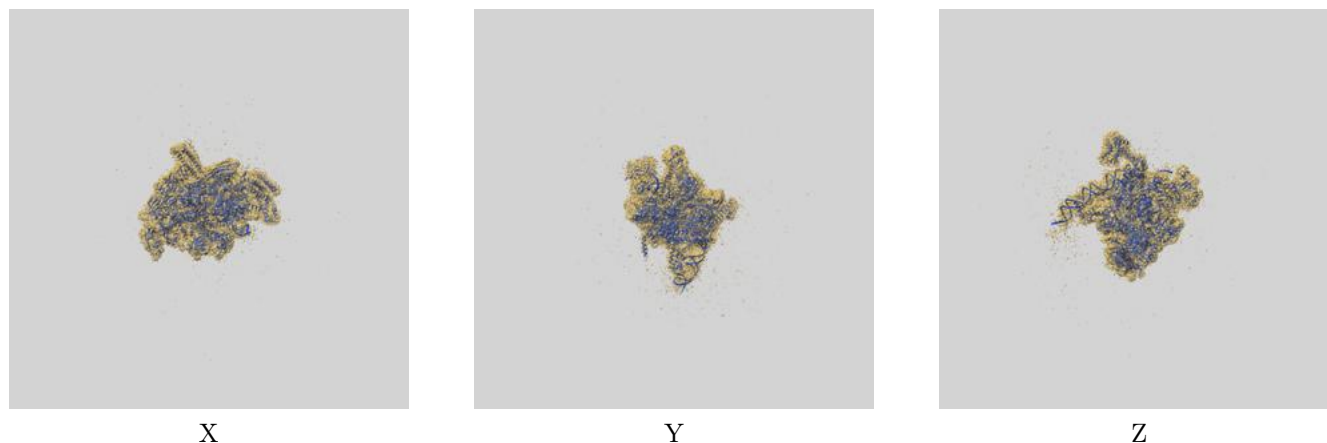
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

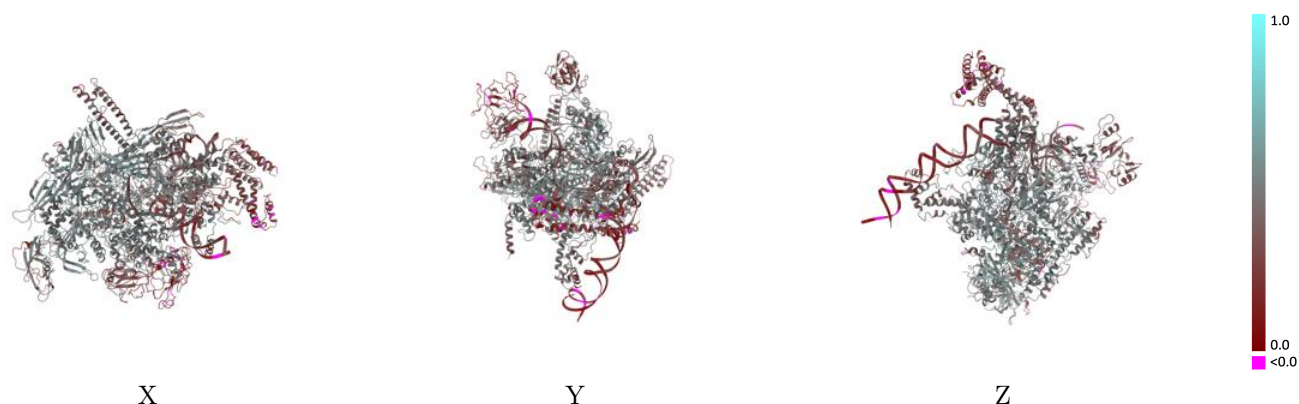
This section contains information regarding the fit between EMDB map EMD-21880 and PDB model 7KHB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

### 9.1 Map-model overlay [i](#)



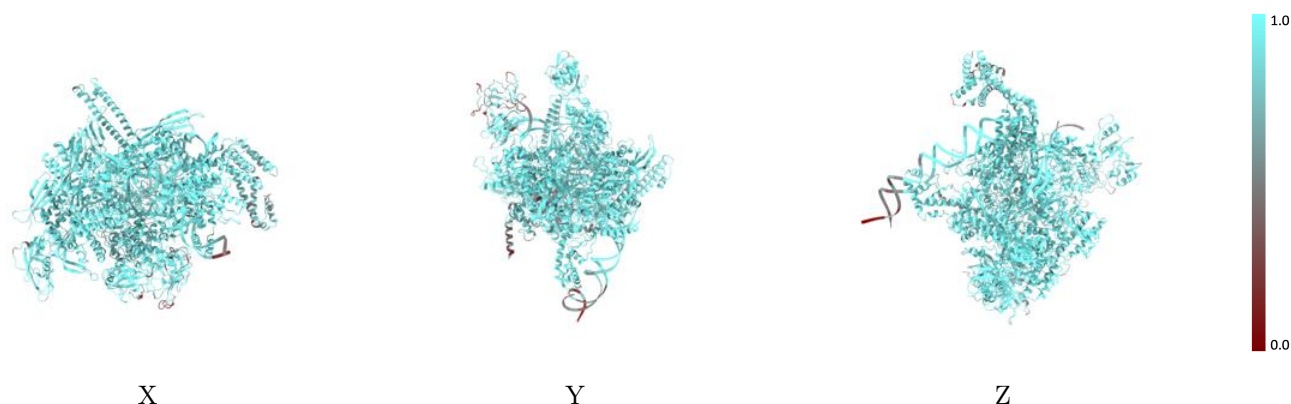
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



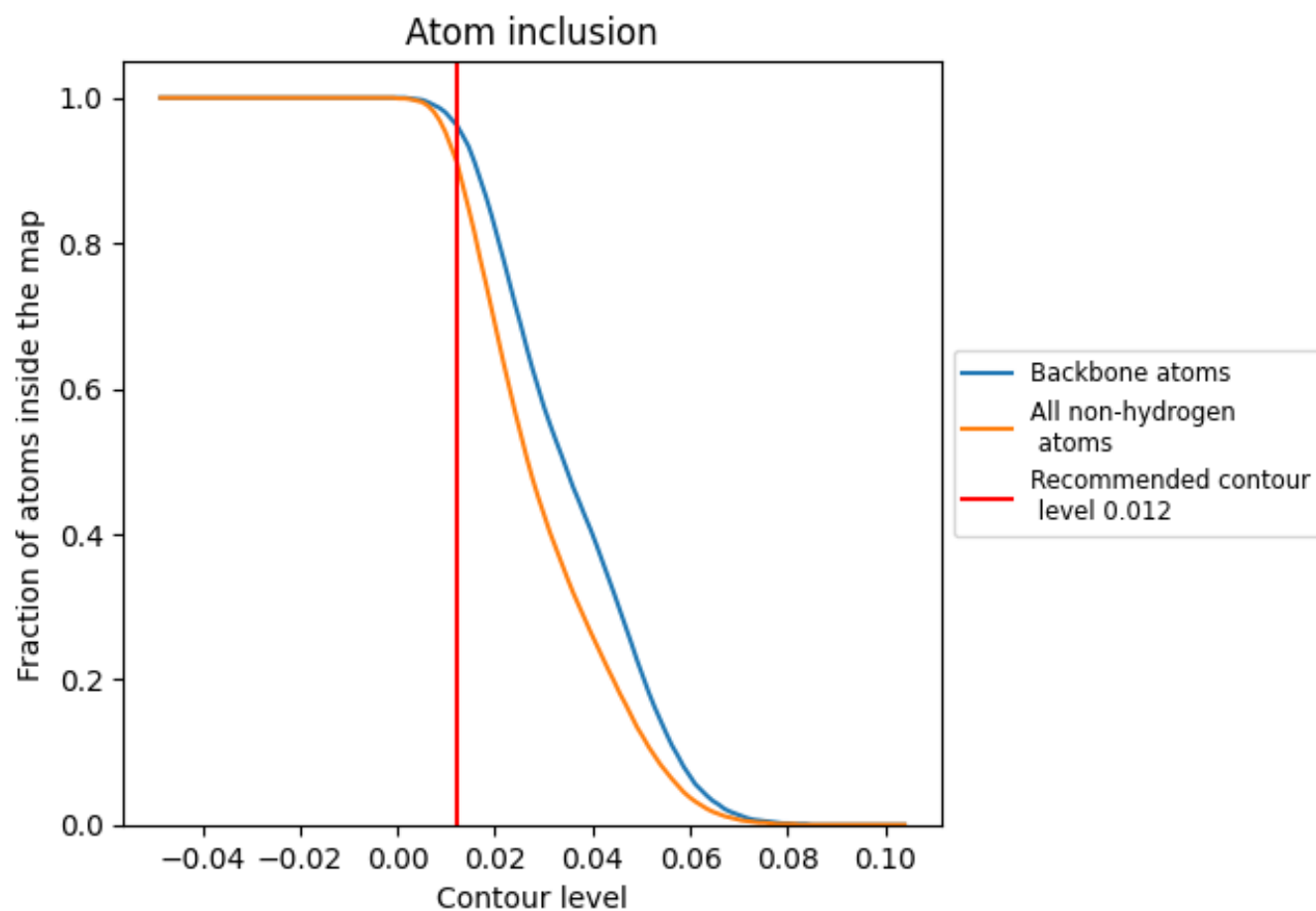
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9140</div>	<div><div></div>0.4300</div>
A	<div><div></div>0.9480</div>	<div><div></div>0.4870</div>
B	<div><div></div>0.9260</div>	<div><div></div>0.4500</div>
C	<div><div></div>0.9510</div>	<div><div></div>0.4760</div>
D	<div><div></div>0.9290</div>	<div><div></div>0.4500</div>
E	<div><div></div>0.6620</div>	<div><div></div>0.4320</div>
F	<div><div></div>0.8710</div>	<div><div></div>0.3410</div>
X	<div><div></div>0.7990</div>	<div><div></div>0.2310</div>
Y	<div><div></div>0.7970</div>	<div><div></div>0.2400</div>

1.0

0.0

<0.0