Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 05:36 PM EST

PDB ID	:	7KHB
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*
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:

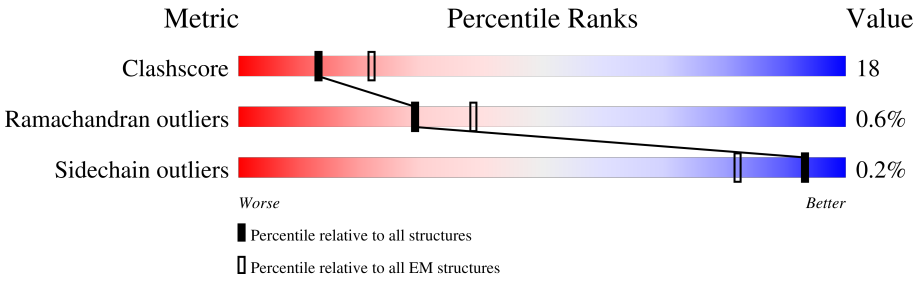
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	47% 23% 30%
1	B	329	42% 27% 30%
2	C	1342	66% 34%
3	D	1407	60% 35% 5%
4	E	91	13% 51% 33% 16%
5	F	613	40% 36% 23%
6	X	64	11% 31% 61% 6%
7	Y	64	8% 42% 58%

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		

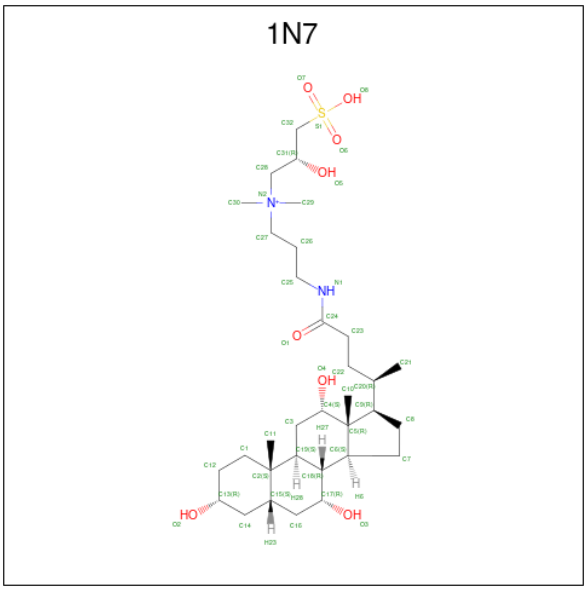
- Molecule 6 is a DNA chain called DNA (60-MER).

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 (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	S	0
			86	64	4	16	2	
8	C	1	Total	C	N	O	S	0
			86	64	4	16	2	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

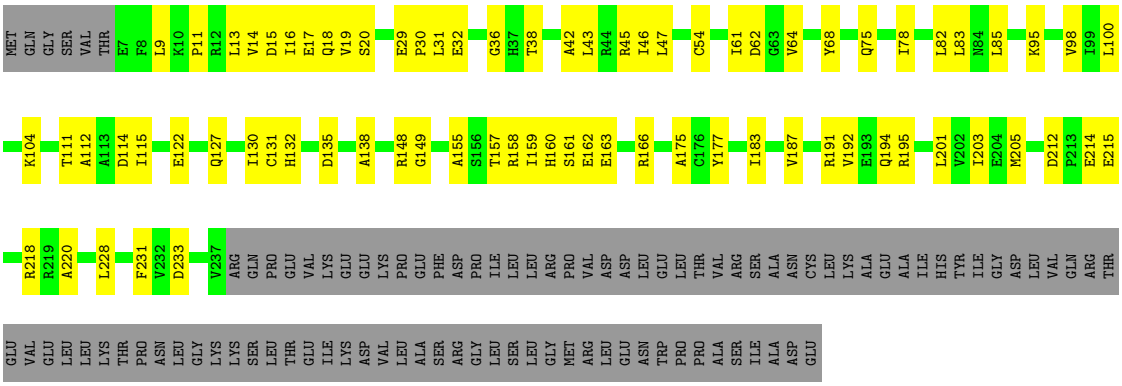
Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

3 Residue-property plots (i)

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.

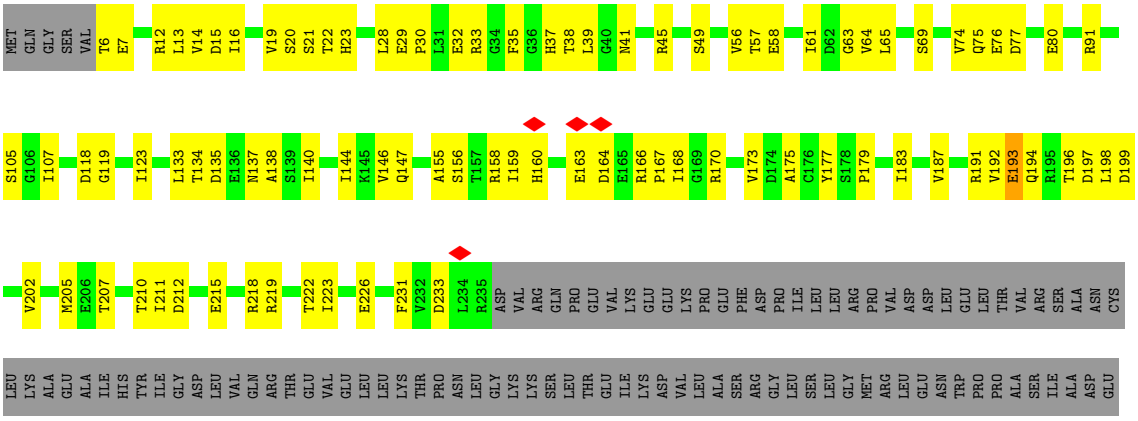
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



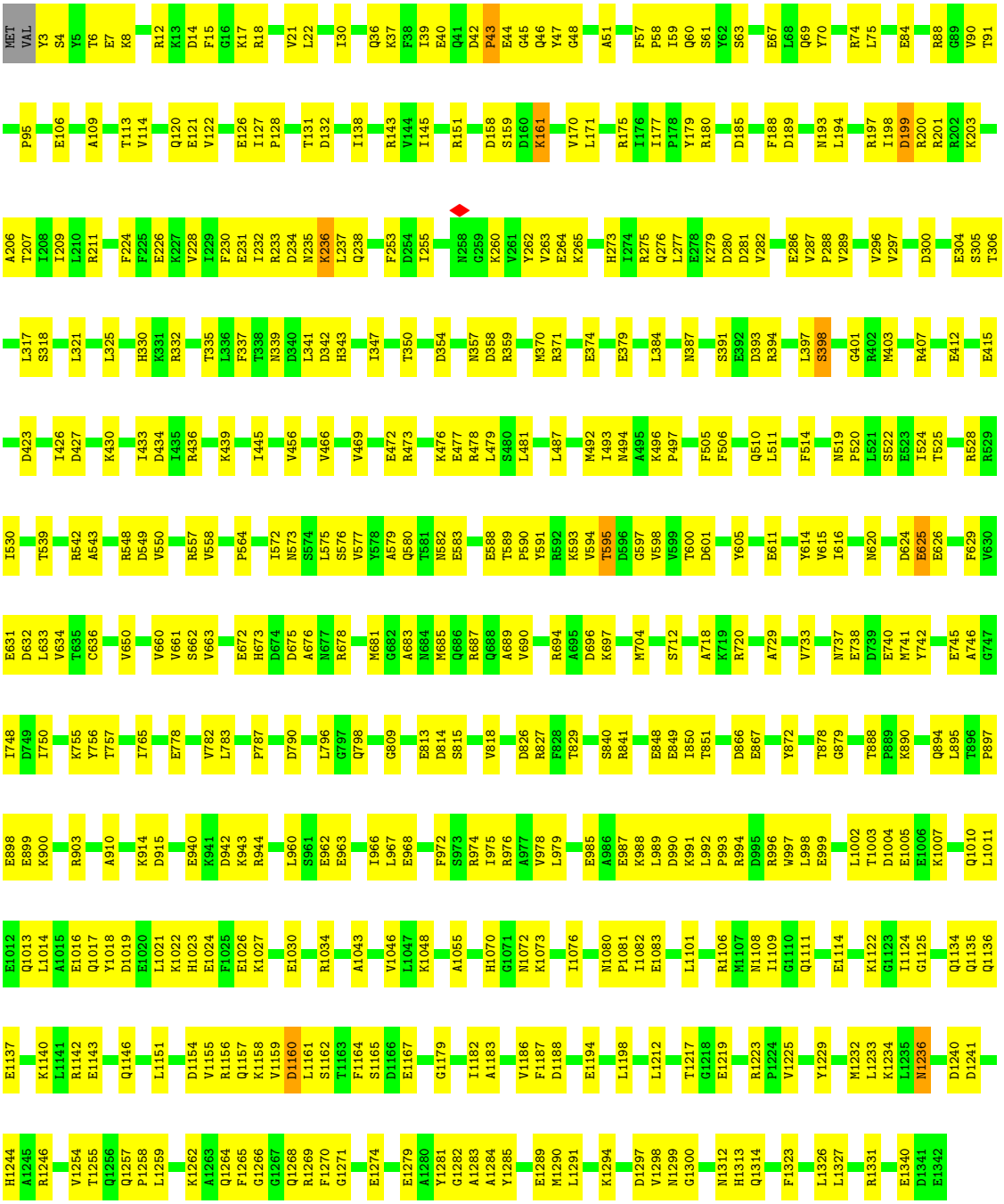
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



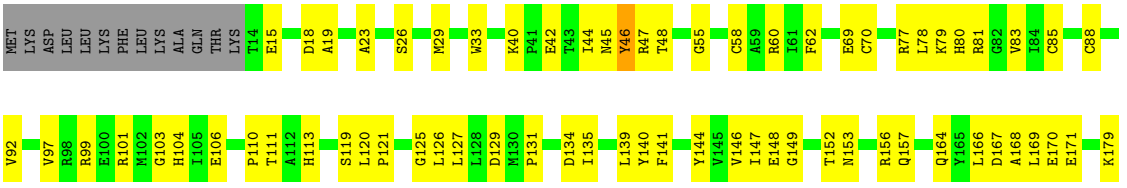
• Molecule 2: DNA-directed RNA polymerase subunit beta

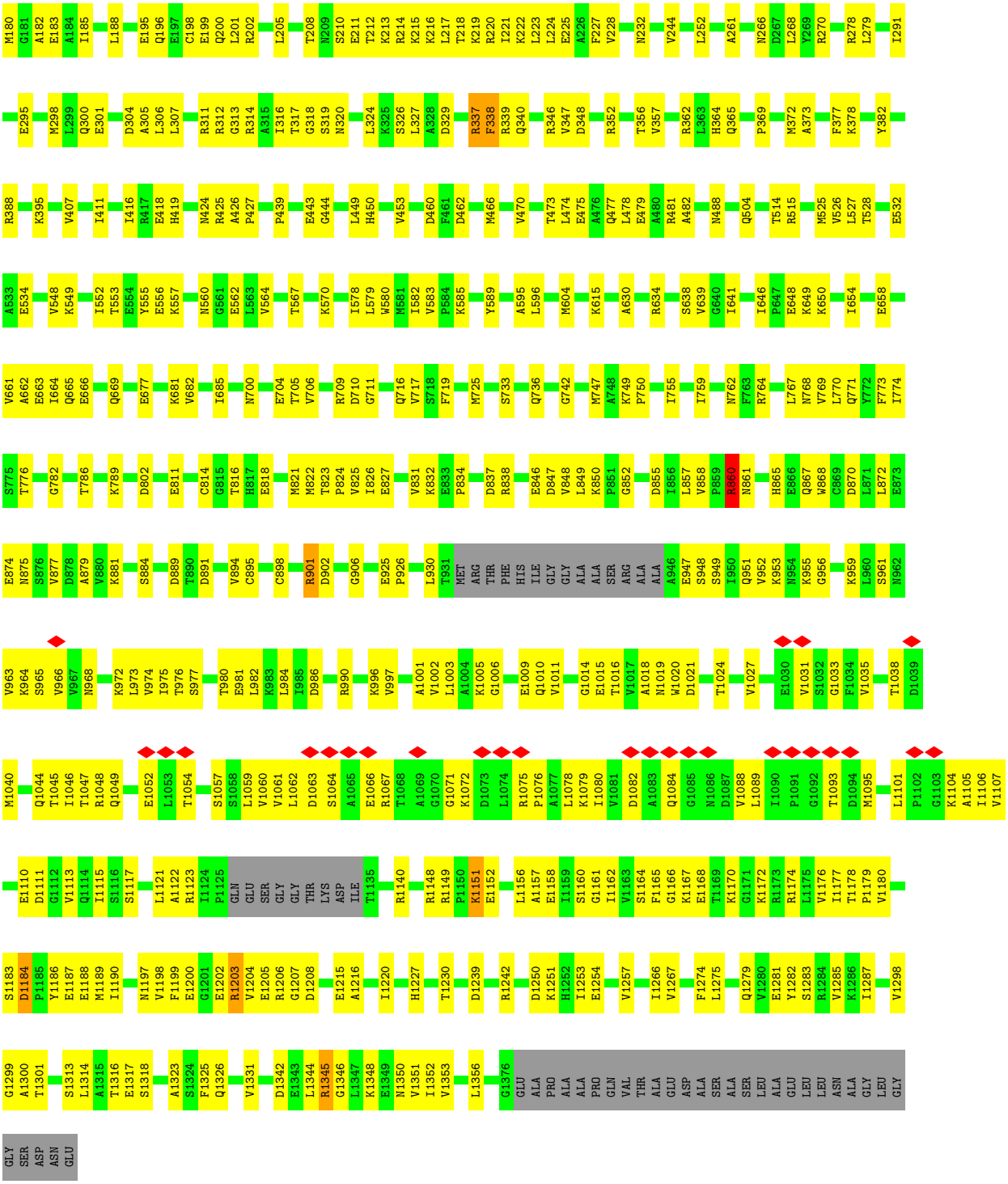
Chain C:



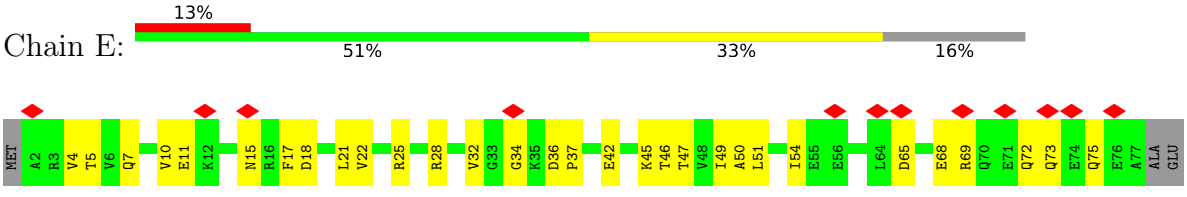
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:



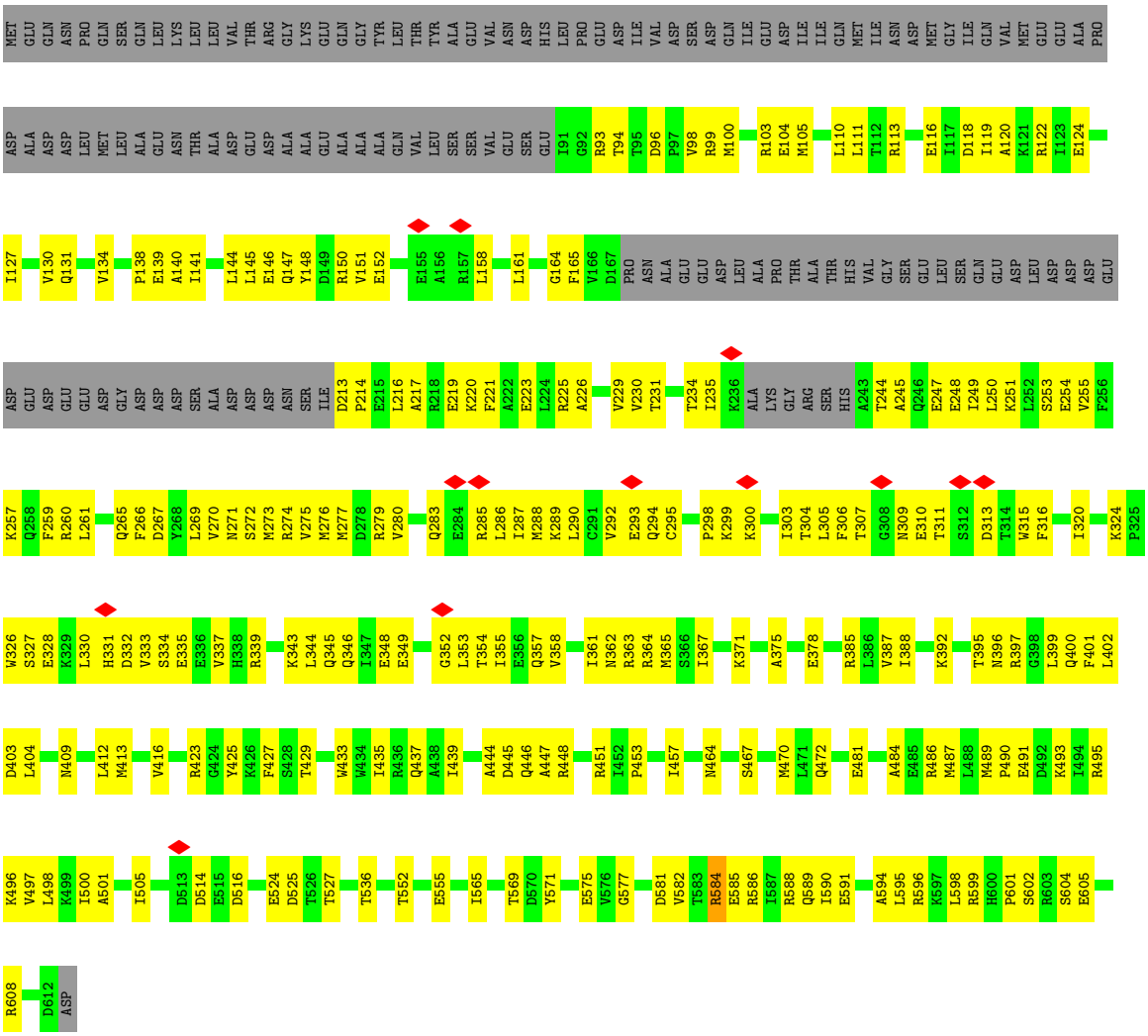


• Molecule 4: DNA-directed RNA polymerase subunit omega



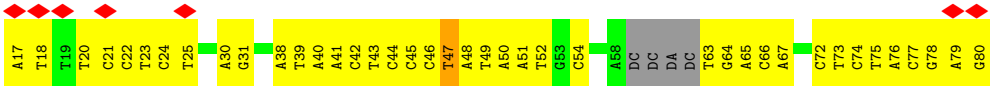
• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 6: DNA (60-MER)

Chain X:



• Molecule 7: DNA (64-MER)

Chain Y:


C1
T2
G7
A8
G9
T10
C11
C12
G13
T14
G15
T16
C17
A18
G19
T20
G21
G22
T23
G24
G25
C26
G27
C28
A29
T30
T31
A32
T33
A34
G35
G36
G37
T41
A42
T43
T44
C49
C50
A56
G57
A58
G59
A62
A63
T64

4 Experimental information (i)

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 ($e^-/Å^2$)	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: ZN, MG, 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	0.33	0/1816	0.60	0/2461
1	B	0.31	0/1808	0.63	0/2450
2	C	0.36	0/10739	0.60	0/14489
3	D	0.33	0/10539	0.62	1/14234 (0.0%)
4	E	0.27	0/607	0.60	0/817
5	F	0.29	0/3887	0.65	0/5224
6	X	0.76	0/1366	1.06	2/2101 (0.1%)
7	Y	0.74	0/1488	1.04	0/2298
All	All	0.39	0/32250	0.67	3/44074 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	23	DT	O4'-C1'-N1	6.83	112.78	108.00
3	D	1203	ARG	CG-CD-NE	-6.07	99.04	111.80
6	X	47	DT	O4'-C1'-N1	5.87	112.11	108.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1819	60	0
1	B	1786	0	1813	71	0
2	C	10570	0	10582	367	0
3	D	10382	0	10571	422	0
4	E	605	0	612	24	0
5	F	3836	0	3907	189	0
6	X	1221	0	677	40	0
7	Y	1325	0	721	37	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	1139	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 18.

All (1139) 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
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
3:D:1318:SER:OG	3:D:1342:ASP:OD1	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:288:MET:HE1	5:F:299:LYS:HG3	1.75	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
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
3:D:925:GLU:HG3	3:D:926:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:479:LEU:HD21	2:C:492:MET:HE1	1.81	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
3:D:215:LYS:HB3	3:D:219:LYS:HZ1	1.70	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: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:141:PHE:HA	3:D:180:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:987:GLU:O	2:C:991:LYS:NZ	2.32	0.56
3:D:895:CYS:HG	10:D:2003:ZN:ZN	1.19	0.56
3:D:1162:ILE:CD1	3:D:1203:ARG:HH22	2.19	0.56
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
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: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:848:VAL:HG12	3:D:858:VAL:HG22	1.88	0.55
3:D:1172:LYS:HB2	3:D:1189:MET:HE3	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
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:26:SER:H	3:D:29:MET:HE3	1.73	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
2:C:850:ILE:HG22	2:C:850:ILE:O	2.08	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: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
1:B:183:ILE:HD13	1:B:205:MET:HE2	1.91	0.53
2:C:12:ARG:NH1	2:C:1182:ILE:O	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
2:C:765:ILE:HG23	2:C:765:ILE:O	2.10	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: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
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
3:D:337:ARG:O	3:D:338:PHE:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:THR:OG1	2:C:354:ASP:OD1	2.26	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
3:D:1170:LYS:HD3	3:D:1189:MET:HE1	1.93	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: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
5:F:601:PRO:O	5:F:602:SER:OG	2.29	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
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:604:SER:OG	5:F:608:ARG:NH1	2.22	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:138:PRO:C	5:F:140:ALA:H	2.17	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: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:982:LEU:HD23	3:D:997:VAL:HB	1.95	0.48
3:D:449:LEU:HD13	3:D:466:MET:HE1	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:128:PRO:HG2	2:C:506:PHE:HD2	1.79	0.47
3:D:560:ASN:OD1	3:D:562:GLU:OE2	2.33	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
2:C:778:GLU:OE2	2:C:778:GLU:HA	2.15	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:HB3	1:B:80:GLU:OE2	2.14	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
1:B:6:THR:OG1	1:B:7:GLU:N	2.47	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
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
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:1165:PHE:HB3	3:D:1168:GLU:OE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:318:GLY:O	3:D:319:SER:OG	2.27	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
5:F:392:LYS:HE2	6:X:54:DC:H3'	1.98	0.46
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
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:424:ASN:OD1	3:D:424:ASN:C	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1259:LEU:HD11	5:F:524:GLU:HB3	1.99	0.45
3:D:141:PHE:CA	3:D:180:MET:HE2	2.47	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:275:ARG:C	2:C:275:ARG:HD2	2.37	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:103:GLY:C	3:D:244:VAL:HG22	2.38	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
2:C:228:VAL:HB	2:C:335:THR:CG2	2.47	0.44
2:C:234:ASP:O	2:C:235:ASN:HB3	2.17	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:821:MET:HE3	3:D:879:ALA:HB1	1.98	0.44
3:D:1045:THR:OG1	3:D:1071:GLY:HA3	2.17	0.44
3:D:1054:THR:HG22	3:D:1054:THR:O	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:369:PRO:HD2	3:D:372:MET:HE2	2.00	0.44
3:D:677:GLU:O	3:D:681:LYS:HG3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:166:ARG:HD3	1:A:166:ARG:N	2.32	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: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: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
3:D:1166:GLY:O	3:D:1167:LYS:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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: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: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:96:ASP:OD1	5:F:96:ASP:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:261:LEU:HB3	5:F:266:PHE:CE1	2.53	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
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:1062:LEU:HB2	3:D:1067:ARG:HA	2.00	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:528:THR:HG22	3:D:532:GLU:CD	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:233:ASP:OD1	1:A:233:ASP:N	2.51	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:813:GLU:C	2:C:815:SER:H	2.21	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
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:615:VAL:HG13	2:C:615:VAL:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:996:ARG:C	2:C:997:TRP:HD1	2.21	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
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: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:745:GLU:CD	2:C:1017:GLN:OE1	2.58	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: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: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:1170:LYS:HD3	3:D:1189:MET:CE	2.49	0.42
3:D:1316:THR:HG22	3:D:1317:GLU:N	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:C:1264:GLN:O	2:C:1265:PHE:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:11:DC:H2"	7:Y:12:DC:C6	2.55	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
2:C:128:PRO:HG2	2:C:506:PHE:CD2	2.54	0.42
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
3:D:119:SER:O	3:D:120:LEU:C	2.58	0.42
3:D:749:LYS:HE3	3:D:755:ILE:HD13	2.02	0.42
3:D:1250:ASP:OD2	3:D:1250:ASP:C	2.57	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:434:ASP:OD1	2:C:434:ASP:C	2.58	0.42
3:D:822:MET:HE3	3:D:838:ARG:HE	1.84	0.42
3:D:972:LYS:HZ3	3:D:974:VAL:HA	1.85	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
1:B:212:ASP:N	1:B:212:ASP:OD1	2.53	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
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
3:D:1170:LYS:HG2	3:D:1170:LYS:O	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:895:LEU:CD1	2:C:899:GLU:OE1	2.67	0.41
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: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:1275:LEU:HD12	3:D:1275:LEU:C	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1156:LEU:HD12	3:D:1207:GLY:C	2.41	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: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
3:D:596:LEU:HD21	3:D:604:MET:HE3	2.02	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
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:1323:PHE:CZ	2:C:1327:LEU:HD11	2.56	0.41
3:D:304:ASP:OD1	3:D:304:ASP:C	2.59	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
1:A:15:ASP:OD2	1:A:15:ASP:C	2.58	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1075:ARG:HE	3:D:1168:GLU:CD	2.23	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: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
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: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:198:ILE:O	2:C:199:ASP:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:914:LYS:HG2	2:C:915:ASP:N	2.36	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: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:1290:MET:SD	2:C:1294:LYS:NZ	2.95	0.40
3:D:638:SER:OG	3:D:639:VAL:N	2.53	0.40
3:D:902:ASP:HB3	3:D:1251:LYS:HZ1	1.86	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
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
2:C:1232:MET:C	2:C:1233:LEU:HD12	2.41	0.40
3:D:139:LEU:HD21	3:D:185:ILE:HG13	2.03	0.40
3:D:767:LEU:N	3:D:767:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:889:ASP:O	3:D:889:ASP:OD2	2.38	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:134:VAL:N	5:F:365:MET:HE2	2.36	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:614:TYR:N	2:C:614:TYR:CD1	2.89	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:948:SER:OG	3:D:949:SER:N	2.54	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 (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	229/329 (70%)	211 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	228/329 (69%)	207 (91%)	19 (8%)	2 (1%)	17	58
2	C	1338/1342 (100%)	1228 (92%)	100 (8%)	10 (1%)	22	62
3	D	1334/1407 (95%)	1211 (91%)	117 (9%)	6 (0%)	34	71
4	E	74/91 (81%)	68 (92%)	6 (8%)	0	100	100
5	F	465/613 (76%)	430 (92%)	32 (7%)	3 (1%)	25	65
All	All	3668/4111 (89%)	3355 (92%)	292 (8%)	21 (1%)	29	65

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
5	F	298	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	199/286 (70%)	199 (100%)	0	100 100
1	B	198/286 (69%)	198 (100%)	0	100 100
2	C	1155/1157 (100%)	1152 (100%)	3 (0%)	92 98
3	D	1113/1168 (95%)	1112 (100%)	1 (0%)	93 98
4	E	65/75 (87%)	65 (100%)	0	100 100
5	F	419/540 (78%)	416 (99%)	3 (1%)	84 93
All	All	3149/3512 (90%)	3142 (100%)	7 (0%)	93 98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	161	LYS
2	C	720	ARG
2	C	1236	ASN
3	D	1140	ARG
5	F	93	ARG
5	F	113	ARG
5	F	584	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	618	GLN
2	C	1146	GLN
2	C	1288	GLN
3	D	667	GLN
3	D	762	ASN
3	D	962	ASN
5	F	345	GLN
5	F	357	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	1401	-	45,46,46	4.05	20 (44%)	69,72,72	2.18	22 (31%)
8	1N7	C	1402	-	45,46,46	4.07	20 (44%)	69,72,72	1.84	16 (23%)

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	1401	-	-	4/27/92/92	1/4/4/4
8	1N7	C	1402	-	-	6/27/92/92	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	-12.47	1.32	1.53
8	C	1401	1N7	C3-C4	-12.38	1.32	1.53
8	C	1402	1N7	C5-C9	-11.03	1.36	1.55
8	C	1401	1N7	C5-C9	-10.51	1.37	1.55
8	C	1402	1N7	C3-C19	-9.22	1.38	1.53
8	C	1401	1N7	C3-C19	-8.92	1.38	1.53
8	C	1401	1N7	C2-C19	7.19	1.69	1.56
8	C	1401	1N7	C5-C4	7.00	1.65	1.54
8	C	1402	1N7	C5-C4	6.71	1.65	1.54
8	C	1401	1N7	C24-N1	6.54	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1402	1N7	C24-N1	6.54	1.48	1.33
8	C	1402	1N7	C2-C19	6.38	1.67	1.56
8	C	1401	1N7	C7-C6	-6.11	1.41	1.54
8	C	1402	1N7	C7-C6	-6.10	1.41	1.54
8	C	1401	1N7	C18-C19	-5.74	1.42	1.53
8	C	1402	1N7	C18-C19	-5.55	1.43	1.53
8	C	1401	1N7	C8-C7	5.25	1.68	1.54
8	C	1402	1N7	C8-C7	5.19	1.68	1.54
8	C	1401	1N7	C5-C6	5.07	1.64	1.55
8	C	1402	1N7	C5-C6	5.05	1.64	1.55
8	C	1402	1N7	C18-C6	4.59	1.62	1.53
8	C	1402	1N7	C2-C15	-4.47	1.48	1.55
8	C	1401	1N7	C18-C6	4.42	1.62	1.53
8	C	1401	1N7	C20-C9	3.96	1.61	1.54
8	C	1402	1N7	C20-C9	3.52	1.60	1.54
8	C	1402	1N7	O3-C17	-3.27	1.36	1.43
8	C	1401	1N7	C2-C15	-3.18	1.50	1.55
8	C	1401	1N7	O3-C17	-3.17	1.36	1.43
8	C	1402	1N7	C23-C24	3.05	1.57	1.51
8	C	1401	1N7	C23-C24	2.91	1.56	1.51
8	C	1402	1N7	O1-C24	-2.57	1.18	1.23
8	C	1401	1N7	O1-C24	-2.54	1.18	1.23
8	C	1401	1N7	C8-C9	2.49	1.59	1.54
8	C	1401	1N7	O7-S1	2.44	1.52	1.45
8	C	1402	1N7	O7-S1	2.44	1.52	1.45
8	C	1402	1N7	C8-C9	2.41	1.59	1.54
8	C	1401	1N7	O6-S1	2.05	1.51	1.45
8	C	1401	1N7	O4-C4	2.04	1.47	1.43
8	C	1402	1N7	O4-C4	2.03	1.47	1.43
8	C	1402	1N7	O6-S1	2.02	1.51	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1401	1N7	C5-C6-C18	-7.23	105.50	114.74
8	C	1402	1N7	C5-C6-C18	-5.37	107.89	114.74
8	C	1401	1N7	C5-C9-C20	-4.85	113.70	119.50
8	C	1401	1N7	C6-C5-C4	-4.77	102.96	107.40
8	C	1401	1N7	C23-C22-C20	-4.44	106.40	114.52
8	C	1402	1N7	C6-C5-C4	-4.44	103.27	107.40
8	C	1401	1N7	C16-C17-C18	-4.01	107.20	111.48
8	C	1402	1N7	C8-C7-C6	-4.01	97.19	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1402	1N7	O7-S1-C32	3.92	111.60	106.94
8	C	1402	1N7	C5-C9-C20	-3.89	114.86	119.50
8	C	1402	1N7	O6-S1-C32	3.89	111.56	106.94
8	C	1401	1N7	C8-C7-C6	-3.84	97.51	105.13
8	C	1401	1N7	O7-S1-C32	3.83	111.49	106.94
8	C	1402	1N7	O6-S1-O7	-3.80	100.81	113.95
8	C	1401	1N7	O6-S1-O7	-3.67	101.23	113.95
8	C	1401	1N7	C16-C15-C2	3.65	116.53	112.66
8	C	1402	1N7	C23-C22-C20	-3.49	108.15	114.52
8	C	1401	1N7	C2-C19-C18	-3.42	108.15	111.82
8	C	1401	1N7	C19-C2-C15	3.28	113.18	108.58
8	C	1401	1N7	O6-S1-C32	3.27	110.82	106.94
8	C	1402	1N7	C6-C18-C17	-3.25	107.50	111.81
8	C	1401	1N7	C16-C15-C14	-3.20	107.51	111.19
8	C	1402	1N7	C2-C19-C18	-3.12	108.47	111.82
8	C	1402	1N7	C3-C19-C2	-2.95	110.69	113.73
8	C	1401	1N7	O8-S1-C32	2.80	110.20	105.74
8	C	1401	1N7	C1-C2-C15	2.69	111.74	107.77
8	C	1402	1N7	O8-S1-C32	2.61	109.91	105.74
8	C	1402	1N7	C31-C28-N2	-2.52	112.78	116.81
8	C	1401	1N7	C11-C2-C15	-2.51	106.11	110.36
8	C	1401	1N7	C21-C20-C9	-2.50	109.10	112.92
8	C	1402	1N7	C26-C25-N1	-2.41	105.32	112.21
8	C	1401	1N7	C19-C3-C4	2.41	117.48	114.30
8	C	1401	1N7	C31-C28-N2	-2.28	113.17	116.81
8	C	1401	1N7	C6-C18-C17	-2.13	108.98	111.81
8	C	1402	1N7	C26-C27-N2	-2.12	110.88	115.38
8	C	1401	1N7	C3-C19-C2	-2.08	111.58	113.73
8	C	1402	1N7	C15-C14-C13	-2.07	109.72	112.76
8	C	1401	1N7	C15-C16-C17	-2.06	112.19	114.46

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

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Mol	Chain	Res	Type	Atoms
8	C	1402	1N7	C21-C20-C22-C23
8	C	1401	1N7	C21-C20-C22-C23
8	C	1401	1N7	C9-C20-C22-C23

All (1) ring outliers are listed below:

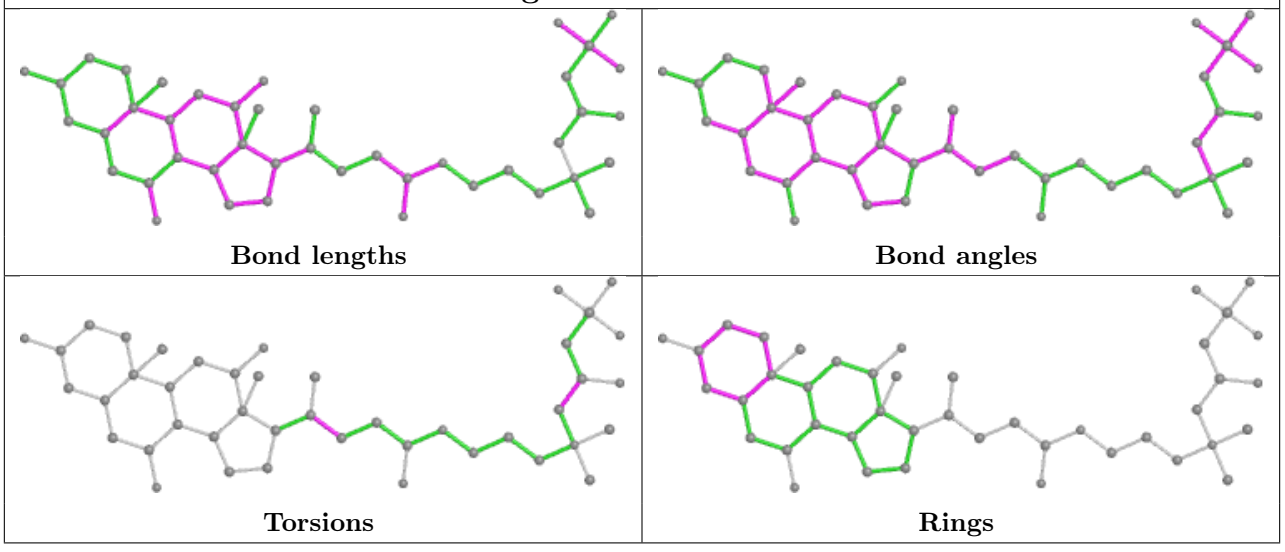
Mol	Chain	Res	Type	Atoms
8	C	1401	1N7	C1-C12-C13-C14-C15-C2

2 monomers are involved in 2 short contacts:

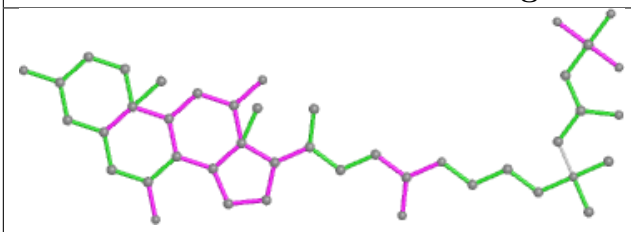
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1401	1N7	1	0
8	C	1402	1N7	1	0

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 then 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.

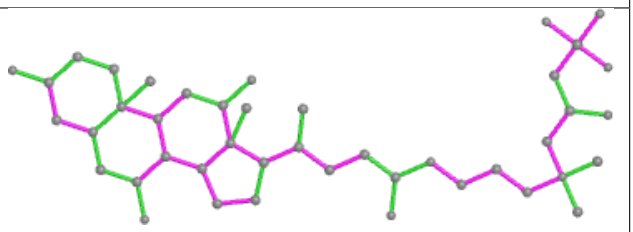
Ligand 1N7 C 1401



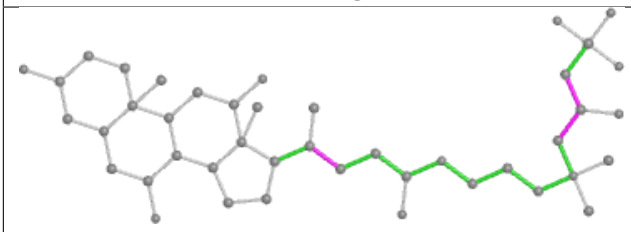
Ligand 1N7 C 1402



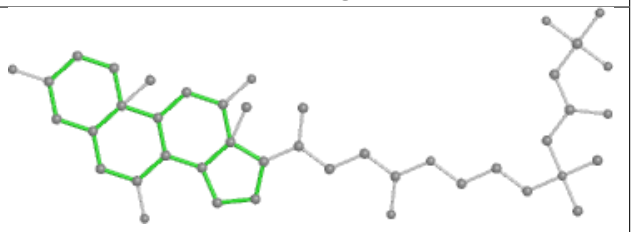
Bond lengths



Bond angles



Torsions



Rings

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.

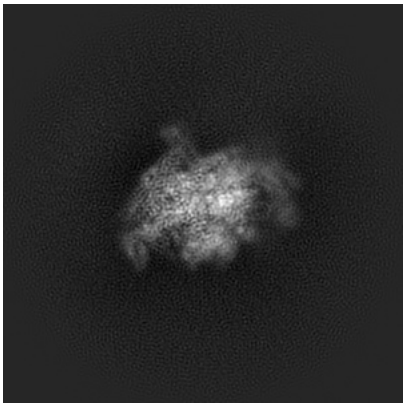
6 Map visualisation

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.

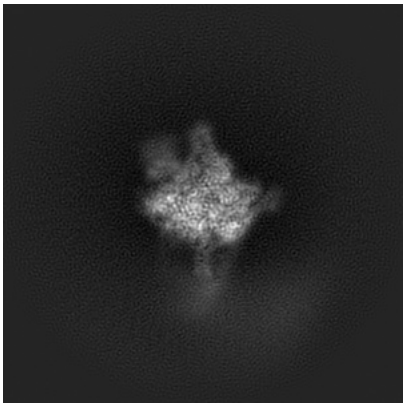
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

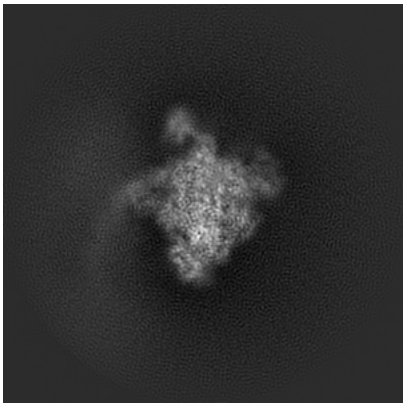
6.1.1 Primary map



X



Y

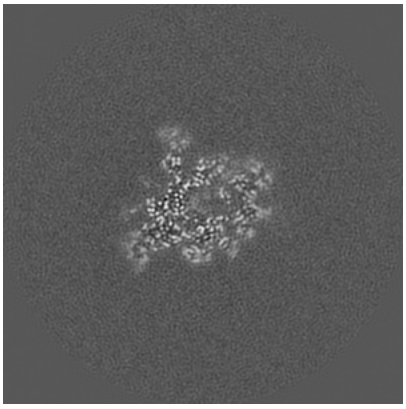


Z

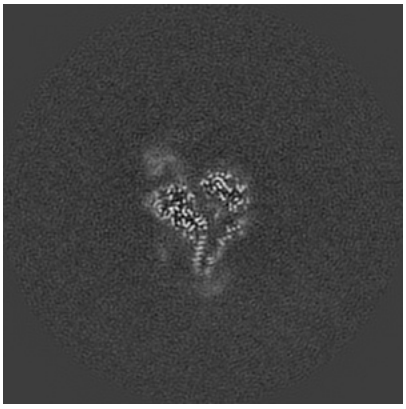
The images above show the map projected in three orthogonal directions.

6.2 Central slices

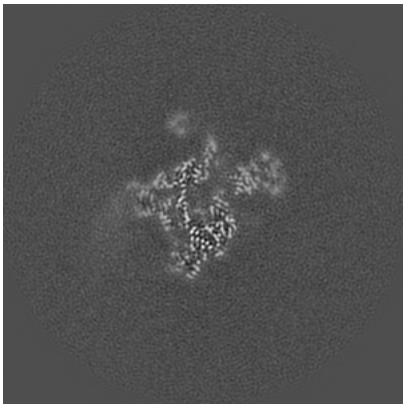
6.2.1 Primary map



X Index: 180



Y Index: 180

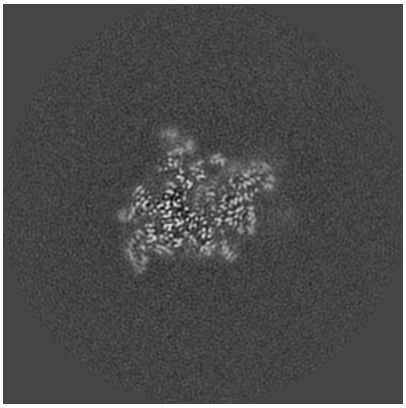


Z Index: 180

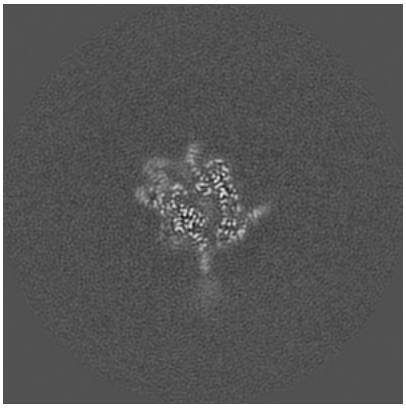
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

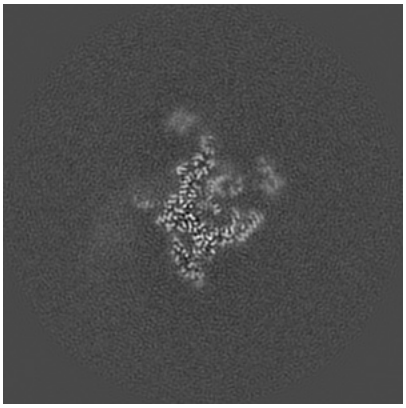
6.3.1 Primary map



X Index: 175



Y Index: 170

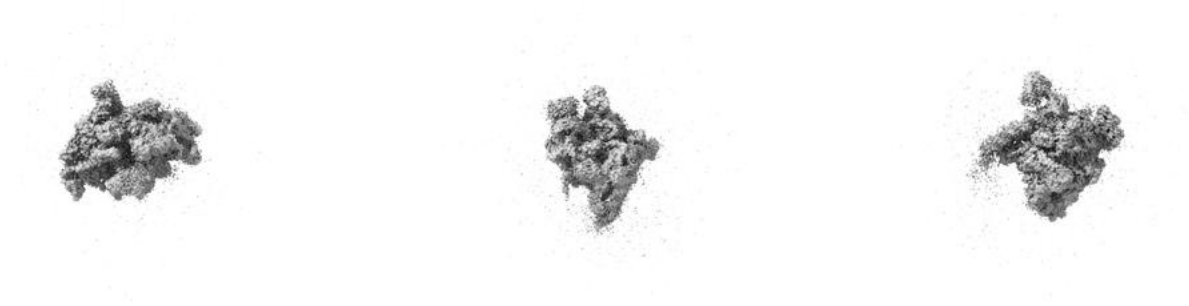


Z Index: 172

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

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.

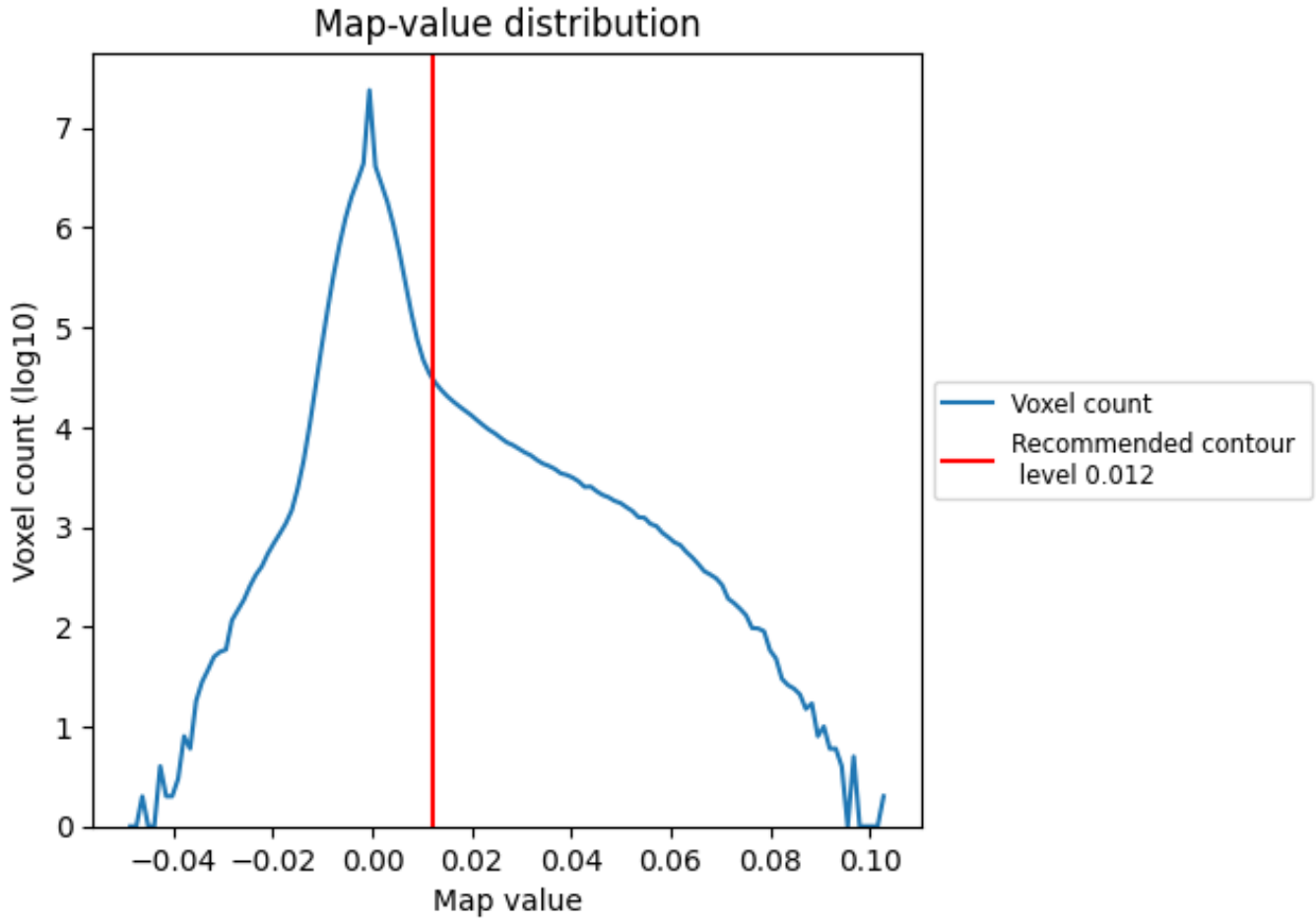
6.5 Mask visualisation (i)

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

7 Map analysis

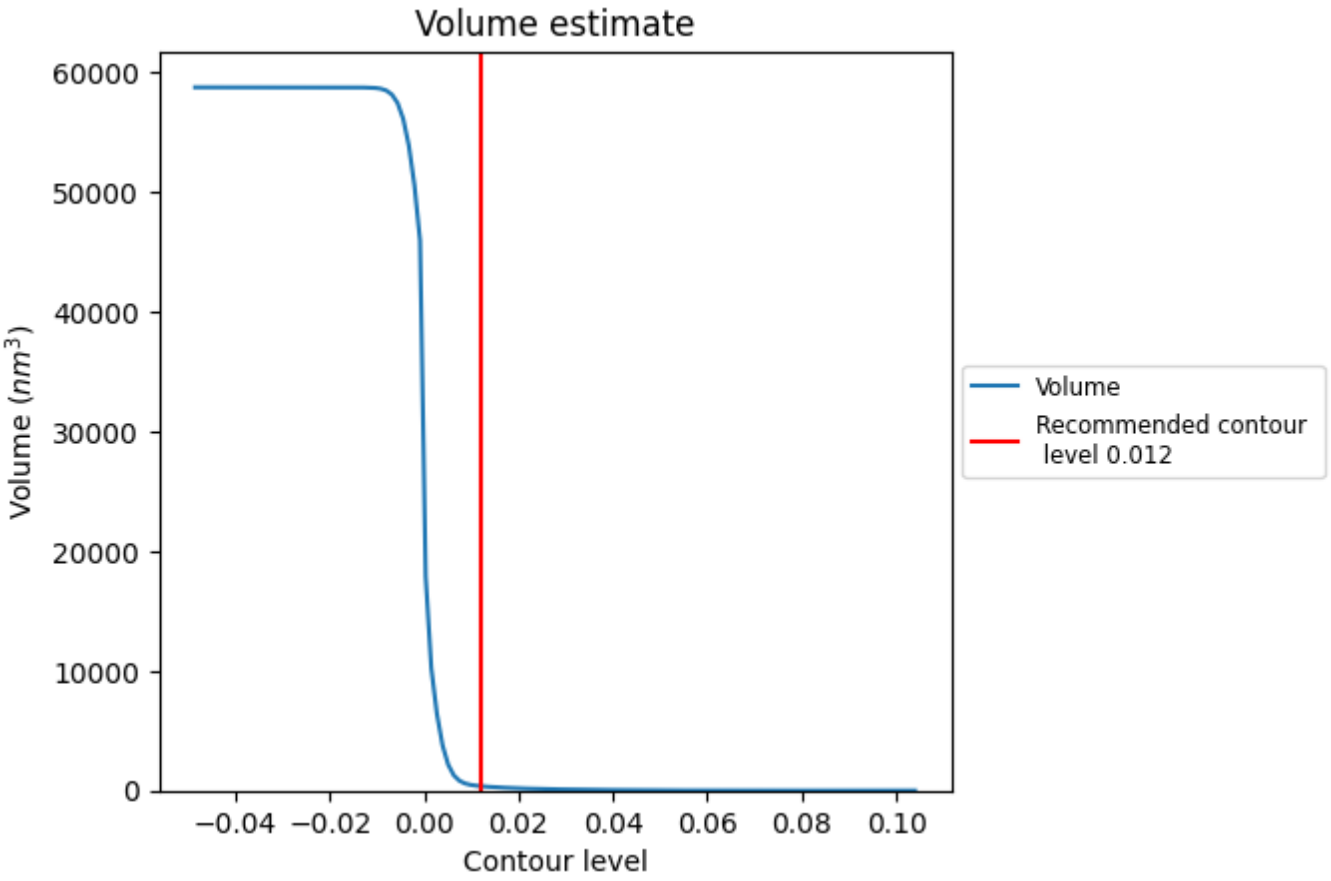
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

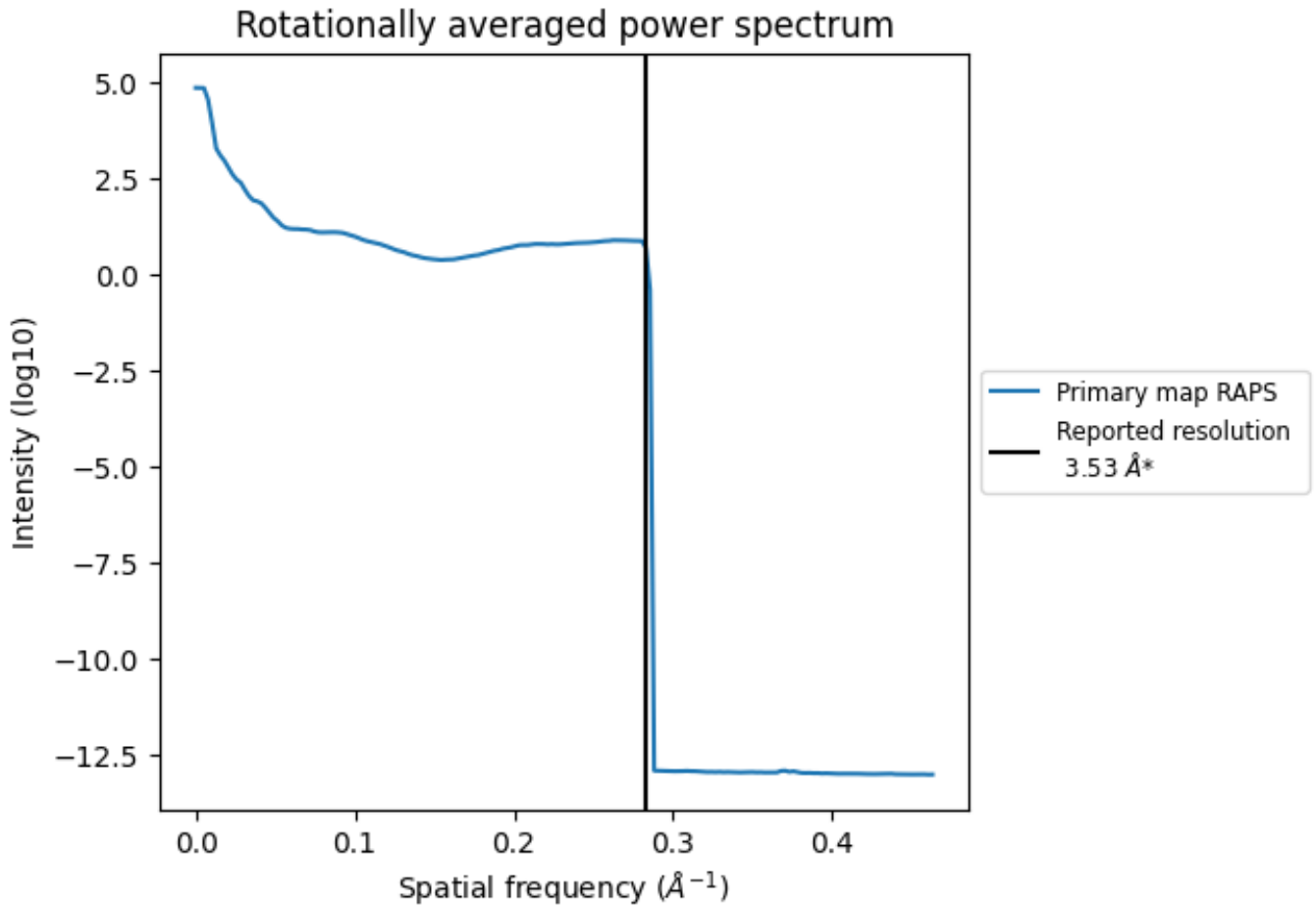
7.2 Volume estimate



The volume at the recommended contour level is 366 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.283 $Å^{-1}$

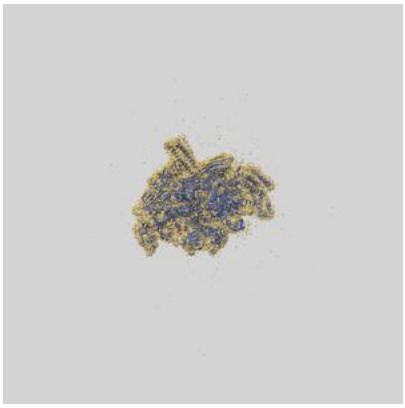
8 Fourier-Shell correlation (i)

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

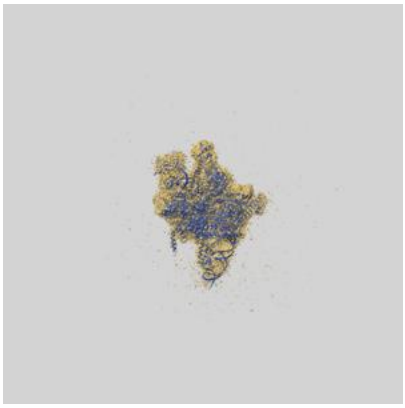
9 Map-model fit

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.

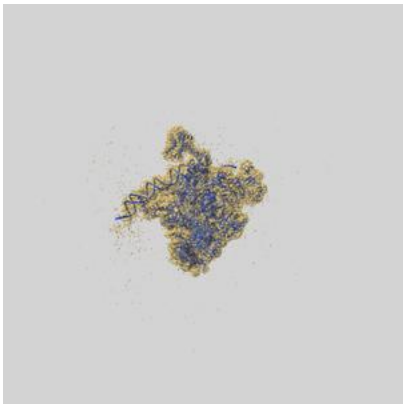
9.1 Map-model overlay



X



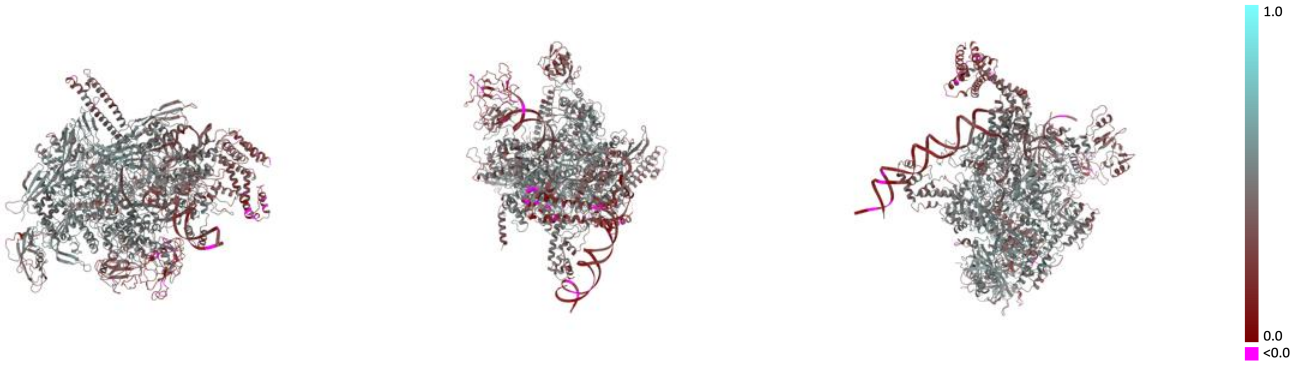
Y



Z

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.

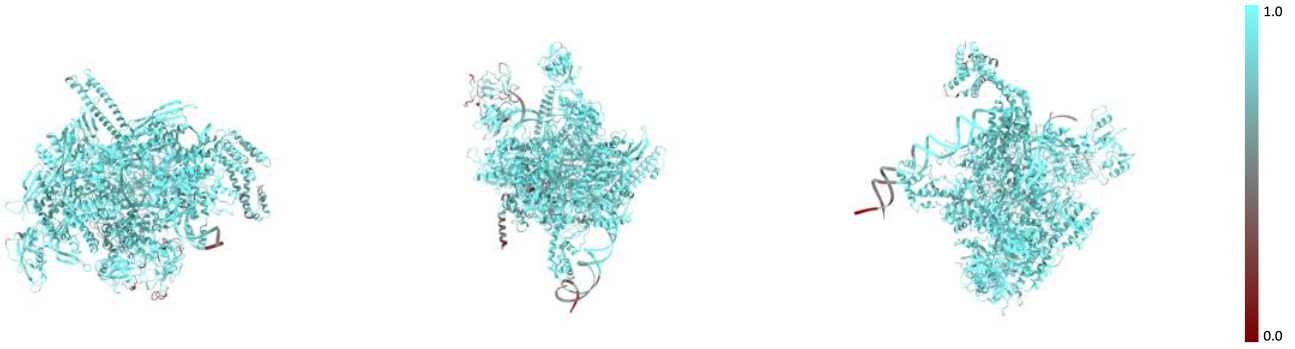
9.2 Q-score mapped to coordinate model



X Y Z

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.

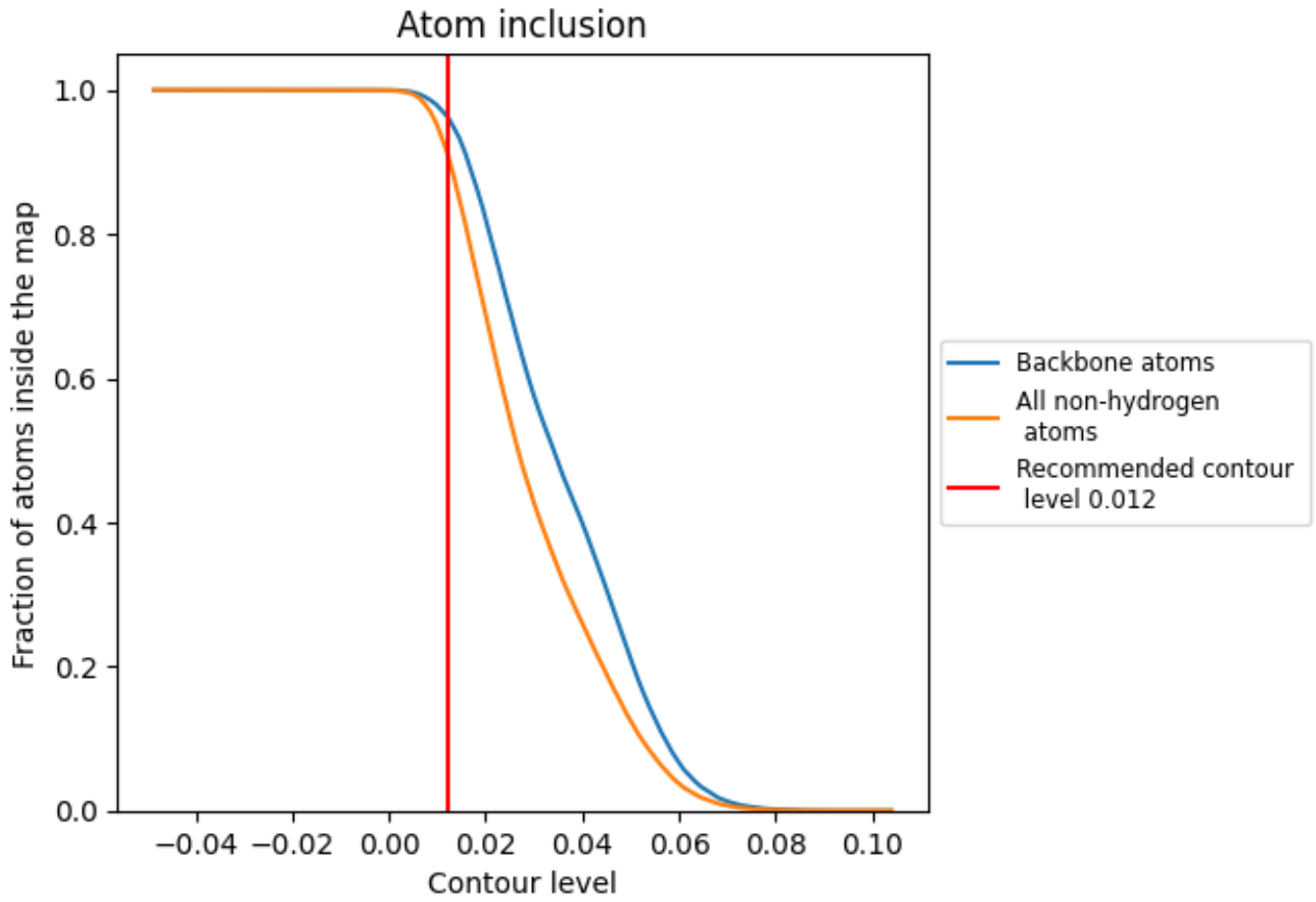
9.3 Atom inclusion mapped to coordinate model



X Y Z

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	0.9144	0.4300
A	0.9476	0.4870
B	0.9256	0.4500
C	0.9510	0.4760
D	0.9292	0.4500
E	0.6621	0.4320
F	0.8706	0.3410
X	0.7993	0.2310
Y	0.7970	0.2400