WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Nov 16, 2024 – 01:54 PM EST

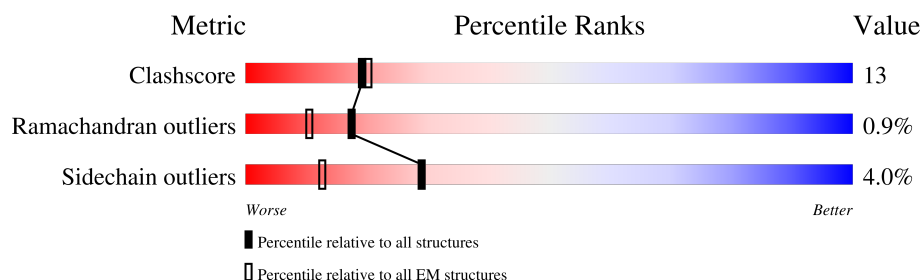|		
PDB ID	:	8TO1
EMDB ID	:	EMD-41433
Title	:	Escherichia coli RNA polymerase unwinding intermediate (I1a) at the lambda PR promoter
Authors	:	Darst, S.A.; Saecker, R.M.; Mueller, A.U.
Deposited on	:	2023-08-02
Resolution	:	2.80 Å(reported)

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 2.80 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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		0.9%
Sidechain outliers		4.0%

Worse *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 >=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	G	329	55% 15% • 29%
1	H	329	50% 15% • 34%
1	M	329	9% / 22% • 78%
2	I	1342	• / 79% 19% •
3	J	1407	• / 69% 24% • 5%
4	K	91	62% 19% 20%
5	L	613	14% / 58% 29% • 10%
6	O	105	• / 20% 7% 8% 66%

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Mol	Chain	Length	Quality of chain
7	P	105	27% 68%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 31386 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	G	232	Total 1773	C 1108	N 315	O 344	S 6	0	0
1	H	218	Total 1669	C 1044	N 293	O 326	S 6	0	0
1	M	73	Total 572	C 362	N 100	O 108	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1337	Total 10514	C 6602	N 1830	O 2039	S 43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1338	Total 10395	C 6532	N 1854	O 1961	S 48	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	73	Total 582	C 355	N 111	O 115	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	551	Total 4334	C 2711	N 775	O 823	S 25	0	0

- Molecule 6 is a DNA chain called Nontemplate strand of lamdba PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	36	Total 736	C 351	N 126	O 223	P 36	0	0

- Molecule 7 is a DNA chain called Template strand of lamdba PR promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	34	Total 701	C 331	N 140	O 196	P 34	0	0

- Molecule 8 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (three-letter code: 4QM) (formula: $C_{24}H_{42}O_3$).
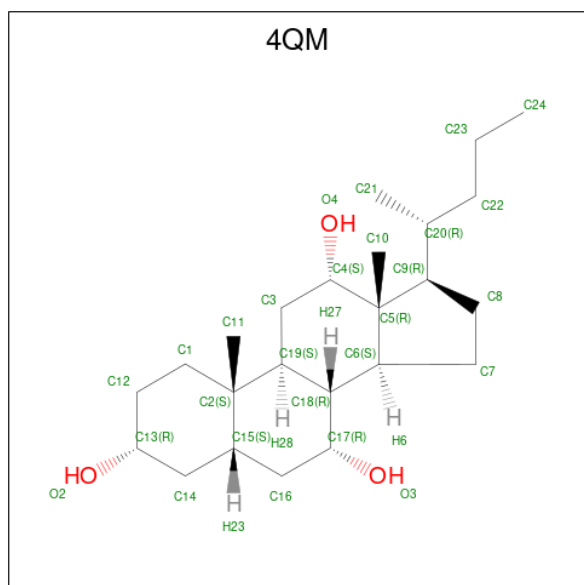
Mol	Chain	Residues	Atoms			AltConf
8	I	1	Total 27	C 24	O 3	0
8	I	1	Total 26	C 23	O 3	0
8	L	1	Total 27	C 24	O 3	0
8	L	1	Total 27	C 24	O 3	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Chain G:

- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H:

- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain M:

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

GLU ARG ILE ALA TYR ASN VAL GLU ALA ALA ARG VAL GLN ARG THR ASP LEU ASP LYS LEU VAL ILE GLU MET GLU THR ASN GLY THR ILE ASP PRO GLU GLU ALA ILE ARG ALA THR ILE LEU ALA GLU GLN GLU GLU ALA PHE VAL ASP ARG ASP VAL ARG GLN PRO

GLU VAL LYS GLU LYS PRO GLU PHE D250 P251 A272 E273 A274 G279 D280 Q283 R284 T285 E286 V287 E288 L289 L290 K291 K297 L300 T301 K304 L307 A308 S309 R310 G311 L312 S313 L314 G315 M316 R317 L318 E319 N320 W321 P322 PRO ALA SER ILE ALA ASP GLU

• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

79% 19%

MET V2 Y5 K13 K17 V21 L22 D23 V24 P25 Y26 I30 Q31 L32 F35 Q36 K37 F38 I39 E40 P43 R54 N65 S66 V70 V71 S72 Y73 R74 L75 T91 E106 R107 E111 D116 I117 K118 E119 Q120 M124 I127 T131 D132

T135 I138 I145 Q148 L149 H150 D160 K161 G162 K163 T164 H165 V170 N173 A174 R175 R180 W183 L184 D185 F186 E187 F188 D189 D192 N193 L194 F195 V196 R197 R201 L204 I209 L221 F225 E226 K227 V228 I229 F230 E231 I232 ARG ASP ASN

K236 E240 G248 GLU T250 D254 I255 G259 K260 V261 Y262 V263 E264 R267 R268 R272 H273 D280 E290 D300 D303 E304 S305 I310 N314 D320 L321 Q327 S328 G329 H330 K331 R332 I333 L336 F337 T338 N339 H343 G344 P345 Y346 I347

V353 T356 N357 D358 R359 L360 S361 E365 P372 E382 D393 V400 D427 I433 R436 I445 D446 H447 L448 G449 R452 I453 R454 S455 V456 G457 E458 E461 R465 V471 D483 Q490 I493 I498 M515 L521 I524 T525 H526

I530 T539 V550 P560 N573 S574 V577 T581 L587 Y591 R592 K593 V594 T595 D596 G597 D601 E602 I603 H604 V615 C636 R637 S638 K639 S642 D651 V655 S656 T657 V660 V661 R687 L693 R694 K697 D711 V724

V727 D728 A729 Y742 P743 G744 I748 D749 E778 R779 G780 D781 V802 P806 W807 N811 R821 I831 T893 Q894 L895 T896 P897 L902 R903 F906 G907 D912 D937 G938 V939 E940 K957 E963 L964 Q965 I966 L967 V980 A981 G982 E987

K991 L992 P993 R994 W997 L1000 D1004 E1005 E1006 N1009 Q1010 Q1013 Y1018 F1025 E1026 K1027 E1030 A1031 K1032 R1033 R1034 K1035 I1036 T1037 L1042 A1043 P1044 G1045 V1046 I1049 H1070 P1081 I1082 E1083 D1084 N1090 L1098 V1103 I1112 L1113 E1114 K1127

M1131 Q1135 Q1136 E1137 V1138 L1141 A1148 Y1149 D1154 V1159 E1167 P1181 E1192 R1211 Q1220 V1225 H1244 A1245 R1246 S1247 T1248 S1252 L1253 V1254 T1255 Q1256 Q1257 P1258 G1261 K1262 F1265 G1266 G1271 E1272 M1273 L1287 S1295 D1296 D1297 N1307 I1308

N1312 P1317 G1318 M1319 P1320 F1323 R1331 N1336 I1337 E1342

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

Chain J:

69% 24% 5%

MET LYS ASP LEU LYS PHE LEU LYS ALA GLN THR LYS THR GLU E16 F17 M29 K40 P41 E42 T48 F49 K50 P51 F57 R60 D67 Y68 E69 C70 L71 L78 K79 H80 I84 C85 E86 K87 C88 G89 V92 T93 R98 T111 S119 S122
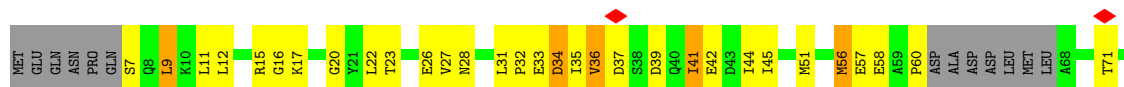
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:

62% 19% 20%

• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:

14%

58% 29% • 10%

• Molecule 6: Nontemplate strand of lamdba PR promoter DNA

Chain O: 20%   7%   8%   66%

• Molecule 7: Template strand of lamdba PR promoter DNA

Chain P: 27%   68%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230905	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 $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.072	Depositor
Minimum map value	-3.285	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	324.096, 324.096, 324.096	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84400004, 0.84400004, 0.84400004	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4QM, ZN, MG

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	G	0.43	1/1795 (0.1%)	0.61	0/2436
1	H	0.59	2/1688 (0.1%)	0.61	3/2289 (0.1%)
1	M	0.23	0/579	0.47	0/784
2	I	0.39	0/10680	0.59	1/14410 (0.0%)
3	J	0.45	2/10552 (0.0%)	0.59	1/14250 (0.0%)
4	K	0.47	0/584	0.64	0/786
5	L	0.54	1/4387 (0.0%)	0.66	5/5910 (0.1%)
6	O	0.62	0/822	1.10	8/1267 (0.6%)
7	P	0.69	2/789 (0.3%)	1.02	5/1215 (0.4%)
All	All	0.46	8/31876 (0.0%)	0.63	23/43347 (0.1%)

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
3	J	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	52	PRO	C-N	14.61	1.59	1.33
5	L	427	PHE	C-N	11.78	1.61	1.34
1	H	178	SER	C-N	10.74	1.54	1.34
3	J	1344	LEU	C-N	10.19	1.57	1.34
7	P	54	DA	P-O5'	7.70	1.67	1.59
3	J	368	LEU	C-N	6.84	1.47	1.34
7	P	55	DA	P-O5'	6.83	1.66	1.59
1	G	226	GLU	C-O	5.99	1.34	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	427	PHE	O-C-N	13.33	144.02	122.70
7	P	54	DA	P-O3'-C3'	11.74	133.79	119.70
5	L	427	PHE	CA-C-N	-8.84	97.76	117.20
7	P	42	DG	P-O3'-C3'	-8.14	109.93	119.70
6	O	74	DG	P-O3'-C3'	-7.32	110.92	119.70
6	O	63	DC	P-O3'-C3'	-7.12	111.16	119.70
5	L	425	TYR	CB-CA-C	-6.97	96.46	110.40
6	O	73	DT	P-O3'-C3'	-6.96	111.34	119.70
5	L	427	PHE	C-N-CA	-6.71	104.94	121.70
6	O	50	DG	P-O3'-C3'	-6.68	111.68	119.70
7	P	53	DC	O3'-P-O5'	6.63	116.60	104.00
7	P	54	DA	O3'-P-O5'	6.46	116.27	104.00
6	O	64	DC	P-O3'-C3'	-6.35	112.08	119.70
6	O	51	DT	P-O3'-C3'	-6.05	112.44	119.70
1	H	52	PRO	O-C-N	5.83	133.11	123.20
1	H	52	PRO	CA-C-N	-5.78	104.65	116.20
6	O	52	DT	P-O3'-C3'	-5.50	113.10	119.70
5	L	386	LEU	C-N-CA	5.47	135.39	121.70
3	J	707	ILE	C-N-CA	5.42	135.24	121.70
6	O	72	DG	P-O3'-C3'	-5.35	113.28	119.70
7	P	55	DA	OP1-P-OP2	-5.12	111.92	119.60
1	H	52	PRO	C-N-CA	-5.06	111.67	122.30
2	I	1246	ARG	CB-CA-C	-5.04	100.32	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	1309	ILE	Mainchain

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	G	1773	0	1793	30	0
1	H	1669	0	1698	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	572	0	602	1	0
2	I	10514	0	10522	175	0
3	J	10395	0	10608	330	0
4	K	582	0	593	15	0
5	L	4334	0	4338	198	0
6	O	736	0	409	24	0
7	P	701	0	379	2	0
8	I	53	0	0	5	0
8	L	54	0	0	11	0
9	J	1	0	0	0	0
10	J	2	0	0	0	0
All	All	31386	0	30942	780	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 13.

All (780) 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)
8:L:702:4QM:C3	8:L:702:4QM:C19	1.82	1.56
8:I:1401:4QM:C3	8:I:1401:4QM:C19	1.82	1.54
8:L:701:4QM:C3	8:L:701:4QM:C19	1.82	1.53
3:J:965:SER:CB	3:J:973:LEU:HD11	1.52	1.38
3:J:973:LEU:O	3:J:1002:VAL:HG13	1.29	1.24
3:J:965:SER:OG	3:J:973:LEU:HD11	1.35	1.21
3:J:1034:PHE:CD2	3:J:1114:GLN:HB2	1.76	1.20
3:J:1110:GLU:HB2	3:J:1113:VAL:HG21	1.24	1.16
3:J:1089:LEU:HA	3:J:1096:PRO:HA	1.13	1.10
3:J:1034:PHE:HA	3:J:1114:GLN:HA	1.12	1.09
3:J:965:SER:CB	3:J:973:LEU:CD1	2.33	1.05
3:J:965:SER:HB2	3:J:973:LEU:CD1	1.87	1.04
3:J:1034:PHE:CZ	3:J:1114:GLN:OE1	2.09	1.03
3:J:1035:VAL:O	3:J:1112:GLY:HA2	1.60	1.02
5:L:383:ASN:HB3	5:L:412:LEU:HD11	1.38	1.02
5:L:427:PHE:C	5:L:429:THR:H	1.63	1.00
3:J:1040:MET:HG3	3:J:1046:ILE:HD13	1.44	0.99
3:J:1062:LEU:HB2	3:J:1067:ARG:HB3	1.50	0.92
3:J:965:SER:OG	3:J:973:LEU:CD1	2.17	0.92
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.52	0.91
3:J:1023:HIS:HB3	3:J:1126:GLN:HG2	1.53	0.91
3:J:1034:PHE:HA	3:J:1114:GLN:CA	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1034:PHE:CA	3:J:1114:GLN:HA	2.03	0.89
3:J:973:LEU:O	3:J:1002:VAL:CG1	2.20	0.88
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.53	0.88
3:J:1110:GLU:HB2	3:J:1113:VAL:CG2	2.03	0.87
3:J:1051:ASP:O	3:J:1055:GLY:HA2	1.74	0.86
5:L:427:PHE:O	5:L:429:THR:N	2.08	0.86
2:I:91:THR:OG1	2:I:138:ILE:O	1.93	0.85
5:L:427:PHE:C	5:L:429:THR:N	2.28	0.85
3:J:1051:ASP:HB2	3:J:1056:LEU:H	1.39	0.85
5:L:386:LEU:O	5:L:388:ILE:N	2.08	0.84
2:I:896:THR:HB	2:I:897:PRO:HD2	1.58	0.84
5:L:582:VAL:HG21	5:L:586:ARG:HB3	1.58	0.83
3:J:965:SER:HB2	3:J:973:LEU:HD11	1.44	0.82
3:J:1176:VAL:HG13	3:J:1185:PRO:HB2	1.60	0.82
3:J:876:SER:HB2	3:J:990:ARG:HD2	1.59	0.82
3:J:1167:LYS:HD2	3:J:1170:LYS:HB2	1.63	0.81
5:L:42:GLU:O	5:L:45:ILE:HG12	1.81	0.81
3:J:1037:PHE:HB3	3:J:1040:MET:HB3	1.60	0.81
3:J:1034:PHE:CG	3:J:1114:GLN:HB2	2.16	0.80
3:J:1079:LYS:HA	3:J:1098:GLN:HA	1.62	0.80
3:J:1034:PHE:CE2	3:J:1114:GLN:HB2	2.16	0.79
5:L:576:VAL:HG12	5:L:587:ILE:HD13	1.62	0.79
3:J:162:GLU:N	3:J:162:GLU:OE1	2.15	0.79
3:J:965:SER:HG	3:J:973:LEU:HD11	1.47	0.78
3:J:1089:LEU:CA	3:J:1096:PRO:HA	2.07	0.78
5:L:582:VAL:HG11	5:L:587:ILE:HG13	1.66	0.78
7:P:54:DA:H1'	7:P:55:DA:OP1	1.82	0.78
3:J:1034:PHE:CE1	3:J:1114:GLN:OE1	2.37	0.78
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.65	0.78
5:L:311:THR:HG22	5:L:348:GLU:HG3	1.66	0.78
3:J:1190:ILE:HG21	3:J:1196:LEU:HD21	1.66	0.77
2:I:749:ASP:N	2:I:749:ASP:OD1	2.17	0.77
5:L:427:PHE:O	5:L:430:TYR:N	2.17	0.76
3:J:1089:LEU:HA	3:J:1096:PRO:CA	2.05	0.76
3:J:965:SER:HB2	3:J:973:LEU:HD12	1.66	0.76
5:L:235:ILE:O	5:L:242:HIS:N	2.18	0.75
1:G:236:ASP:HA	1:H:14:VAL:HG22	1.67	0.75
3:J:1067:ARG:HH12	3:J:1076:PRO:HD3	1.52	0.75
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.52	0.74
3:J:1003:LEU:HA	3:J:1018:ALA:HB2	1.69	0.74
5:L:116:GLU:N	5:L:116:GLU:OE1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:63:DC:H2'	6:O:64:DC:C6	2.22	0.74
5:L:234:THR:OG1	5:L:248:GLU:OE1	2.05	0.73
5:L:547:VAL:HG12	5:L:598:LEU:HD22	1.68	0.73
3:J:285:LEU:HD12	5:L:410:ILE:HD11	1.70	0.73
1:H:11:PRO:HG3	1:H:31:LEU:HD21	1.70	0.73
3:J:339:ARG:CG	3:J:339:ARG:HH11	2.01	0.73
2:I:1319:MET:SD	2:I:1323:PHE:HD2	2.12	0.73
3:J:952:VAL:HG23	3:J:984:LEU:HD22	1.70	0.73
5:L:41:ILE:O	5:L:45:ILE:HG23	1.89	0.73
8:L:701:4QM:C3	8:L:701:4QM:C2	2.65	0.72
1:H:127:GLN:N	1:H:127:GLN:OE1	2.21	0.72
2:I:185:ASP:OD1	2:I:186:PHE:N	2.22	0.72
5:L:12:LEU:HD21	5:L:27:VAL:HG13	1.71	0.71
5:L:382:ALA:O	5:L:385:ARG:HB3	1.90	0.71
5:L:383:ASN:CB	5:L:412:LEU:HD21	2.20	0.71
8:L:702:4QM:C3	8:L:702:4QM:C2	2.66	0.71
5:L:15:ARG:HB3	5:L:22:LEU:HD21	1.72	0.71
1:H:12:ARG:HG2	1:H:13:LEU:HD23	1.72	0.71
5:L:554:ARG:HH12	5:L:590:ILE:HG13	1.55	0.71
3:J:1262:ARG:NH1	3:J:1281:GLU:OE2	2.24	0.71
2:I:232:ILE:HB	2:I:331:LYS:HA	1.73	0.70
4:K:3:ARG:NH1	4:K:6:VAL:HA	2.06	0.70
5:L:598:LEU:HA	5:L:603:ARG:HD2	1.73	0.70
1:G:215:GLU:O	1:G:219:ARG:HG3	1.92	0.70
3:J:910:ASN:O	3:J:913:GLU:HG3	1.91	0.70
1:H:13:LEU:HG	1:H:29:GLU:HB3	1.74	0.70
2:I:1342:GLU:N	2:I:1342:GLU:OE1	2.24	0.70
5:L:141:ILE:HD11	5:L:224:LEU:HD11	1.73	0.70
3:J:426:ALA:HB3	3:J:427:PRO:CD	2.22	0.69
2:I:1272:GLU:HB3	3:J:343:LEU:HD21	1.73	0.69
2:I:303:ASP:OD1	2:I:328:SER:OG	2.09	0.69
3:J:339:ARG:HH11	3:J:339:ARG:HG2	1.58	0.69
2:I:119:GLU:N	2:I:119:GLU:OE1	2.26	0.69
5:L:582:VAL:HG22	5:L:583:THR:H	1.57	0.69
8:I:1401:4QM:C3	8:I:1401:4QM:C2	2.67	0.69
3:J:998:PRO:HG2	3:J:1020:TRP:CE2	2.29	0.68
2:I:248:GLY:O	2:I:268:ARG:NH2	2.26	0.68
5:L:511:ILE:HD11	8:L:701:4QM:C20	2.24	0.68
2:I:225:PHE:CE2	2:I:347:ILE:HB	2.28	0.68
5:L:380:VAL:O	5:L:384:LEU:HD13	1.93	0.68
3:J:161:THR:OG1	3:J:162:GLU:OE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:211:GLU:OE1	3:J:212:THR:N	2.27	0.67
5:L:429:THR:HG22	6:O:75:DA:H2"	1.76	0.67
5:L:454:VAL:O	5:L:458:GLU:HG2	1.93	0.67
3:J:1051:ASP:O	3:J:1055:GLY:CA	2.42	0.67
3:J:1029:THR:HG21	3:J:1115:ILE:HD11	1.77	0.67
3:J:1090:ILE:HB	3:J:1093:THR:OG1	1.94	0.66
2:I:227:LYS:HD3	2:I:336:LEU:HD23	1.77	0.66
5:L:560:ARG:HD3	5:L:566:ASP:OD2	1.95	0.66
3:J:1067:ARG:NH1	3:J:1076:PRO:HD3	2.10	0.66
5:L:595:LEU:HB3	5:L:599:ARG:HH21	1.60	0.66
1:H:77:ASP:OD1	1:H:78:ILE:N	2.29	0.66
5:L:577:GLY:O	5:L:581:ASP:N	2.29	0.66
1:G:118:ASP:N	1:G:118:ASP:OD1	2.29	0.66
2:I:35:PHE:CE2	2:I:39:ILE:HD12	2.31	0.66
5:L:585:GLU:N	5:L:585:GLU:OE1	2.29	0.66
3:J:1034:PHE:CD2	3:J:1114:GLN:CB	2.69	0.65
4:K:67:ARG:O	4:K:71:GLU:HG2	1.95	0.65
1:H:93:GLN:HG2	1:H:120:ASP:O	1.96	0.65
2:I:906:PHE:CE2	5:L:608:ARG:HA	2.32	0.65
2:I:120:GLN:NE2	2:I:490:GLN:OE1	2.29	0.65
5:L:593:LYS:O	5:L:596:ARG:HG2	1.96	0.65
8:I:1401:4QM:C3	8:I:1401:4QM:C18	2.70	0.65
3:J:1063:ASP:N	3:J:1066:GLU:HB3	2.12	0.65
5:L:470:MET:HG3	5:L:486:ARG:HH11	1.61	0.65
3:J:1037:PHE:CE1	3:J:1111:ASP:HA	2.32	0.64
3:J:1048:ARG:NH2	3:J:1059:LEU:HG	2.12	0.64
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.33	0.64
3:J:967:VAL:HG13	3:J:971:GLY:HA2	1.79	0.64
2:I:1342:GLU:HB3	3:J:16:GLU:O	1.96	0.64
5:L:136:GLU:O	5:L:138:PRO:HD3	1.97	0.64
2:I:651:ASP:OD1	2:I:651:ASP:N	2.31	0.64
2:I:372:PRO:HB2	5:L:35:ILE:HB	1.79	0.64
3:J:1046:ILE:HG22	3:J:1061:VAL:HA	1.80	0.64
2:I:1336:ASN:ND2	3:J:29:MET:SD	2.71	0.63
3:J:1047:THR:HG23	3:J:1049:GLN:HG3	1.80	0.63
3:J:17:PHE:HZ	3:J:1353:VAL:HG11	1.63	0.63
3:J:712:GLN:OE1	3:J:712:GLN:N	2.32	0.63
5:L:15:ARG:O	5:L:16:GLY:C	2.37	0.63
3:J:119:SER:O	3:J:122:SER:N	2.31	0.63
3:J:1071:GLY:HA2	3:J:1074:LEU:HD12	1.81	0.63
3:J:1176:VAL:CG1	3:J:1185:PRO:HB2	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1032:LYS:O	2:I:1035:LYS:HB3	1.99	0.62
3:J:1042:ASP:OD2	3:J:1048:ARG:HB2	1.99	0.62
6:O:73:DT:H1'	6:O:74:DG:C8	2.33	0.62
3:J:1143:ASP:HB2	3:J:1148:ARG:HD2	1.81	0.62
4:K:3:ARG:HH12	4:K:6:VAL:HA	1.64	0.62
5:L:547:VAL:HG21	5:L:607:LEU:HD22	1.82	0.61
2:I:1248:THR:HG21	5:L:531:PRO:HG2	1.82	0.61
3:J:1090:ILE:HG13	3:J:1096:PRO:O	2.00	0.61
1:G:212:ASP:OD1	1:G:213:PRO:HD2	2.00	0.61
3:J:707:ILE:HA	3:J:708:ASN:HB2	1.81	0.61
1:G:5:VAL:HG23	1:H:150:ARG:HG3	1.82	0.61
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.82	0.61
5:L:293:GLU:OE1	5:L:293:GLU:N	2.34	0.61
5:L:565:ILE:HG22	5:L:566:ASP:OD1	2.00	0.61
3:J:1039:ASP:OD1	3:J:1074:LEU:HB3	2.00	0.61
5:L:452:ILE:HG22	5:L:456:MET:HB3	1.82	0.61
2:I:524:ILE:HD11	2:I:711:ASP:O	2.00	0.61
2:I:230:PHE:HB2	2:I:333:ILE:O	2.00	0.60
3:J:847:ASP:OD1	3:J:847:ASP:N	2.34	0.60
3:J:1163:VAL:HG12	3:J:1202:GLU:H	1.66	0.60
2:I:963:GLU:OE1	2:I:964:LEU:N	2.34	0.60
3:J:1035:VAL:O	3:J:1112:GLY:CA	2.45	0.60
3:J:1176:VAL:HA	3:J:1186:TYR:O	2.02	0.60
5:L:453:PRO:HG3	6:O:69:DG:H5"	1.82	0.60
3:J:930:LEU:HD11	3:J:1241:TYR:CE1	2.37	0.60
5:L:7:SER:O	5:L:11:LEU:HG	2.01	0.60
5:L:16:GLY:HA2	5:L:22:LEU:HG	1.83	0.60
5:L:407:GLU:O	5:L:410:ILE:HG22	2.02	0.60
5:L:453:PRO:CG	6:O:69:DG:H5"	2.31	0.60
2:I:728:ASP:OD1	2:I:729:ALA:N	2.34	0.60
3:J:1365:TYR:CZ	3:J:1369:ARG:HD2	2.37	0.59
5:L:386:LEU:HG	5:L:387:VAL:H	1.66	0.59
3:J:155:GLU:OE1	3:J:155:GLU:N	2.35	0.59
3:J:1023:HIS:HB3	3:J:1126:GLN:CG	2.31	0.59
5:L:9:LEU:HD13	5:L:32:PRO:HD3	1.83	0.59
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.85	0.59
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.67	0.59
3:J:495:ASN:ND2	3:J:1247:LYS:O	2.34	0.59
5:L:595:LEU:HB3	5:L:599:ARG:NH2	2.18	0.59
1:H:145:LYS:HD2	1:H:147:GLN:HE21	1.66	0.58
3:J:987:GLU:OE2	3:J:988:PHE:CZ	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1024:THR:CG2	3:J:1123:ARG:HB3	2.33	0.58
5:L:386:LEU:C	5:L:388:ILE:H	2.01	0.58
2:I:225:PHE:CZ	2:I:347:ILE:HB	2.38	0.58
5:L:401:PHE:HA	5:L:404:LEU:HD12	1.85	0.58
2:I:13:LYS:HE2	2:I:1148:ALA:O	2.04	0.58
3:J:426:ALA:CB	3:J:427:PRO:CD	2.81	0.58
5:L:499:LYS:O	5:L:501:ALA:N	2.36	0.58
2:I:36:GLN:O	2:I:40:GLU:HB2	2.03	0.58
3:J:960:LEU:HB2	3:J:963:VAL:HG11	1.86	0.58
3:J:342:LEU:HD22	3:J:1352:ILE:HG23	1.86	0.58
3:J:438:GLU:OE2	4:K:2:ALA:HB1	2.03	0.58
3:J:1036:ARG:HG3	3:J:1081:VAL:HG21	1.85	0.58
3:J:1262:ARG:NH2	3:J:1312:ALA:O	2.37	0.58
2:I:21:VAL:HG23	2:I:601:ASP:OD1	2.03	0.58
3:J:1049:GLN:O	3:J:1058:SER:HB2	2.03	0.58
5:L:56:MET:SD	5:L:60:PRO:HB3	2.43	0.58
5:L:470:MET:HG3	5:L:486:ARG:NH1	2.18	0.58
3:J:986:ASP:HB3	3:J:992:LYS:CD	2.34	0.58
3:J:1046:ILE:HA	3:J:1062:LEU:HG	1.85	0.58
5:L:502:LYS:H	5:L:502:LYS:HD3	1.68	0.58
1:H:172:LEU:HD23	1:H:172:LEU:H	1.69	0.57
3:J:1146:GLU:OE1	3:J:1310:THR:HG22	2.04	0.57
5:L:474:MET:HG2	5:L:476:ARG:HB3	1.85	0.57
2:I:254:ASP:OD1	2:I:255:ILE:N	2.37	0.57
4:K:69:ARG:O	4:K:73:GLN:HG2	2.04	0.57
5:L:452:ILE:CG2	5:L:456:MET:HB3	2.34	0.57
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.86	0.57
3:J:1047:THR:HG22	3:J:1062:LEU:HD21	1.86	0.57
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.37	0.57
3:J:70:CYS:SG	3:J:71:LEU:N	2.77	0.57
2:I:5:TYR:HB2	2:I:781:ASP:OD2	2.04	0.57
3:J:1090:ILE:HB	3:J:1093:THR:HG1	1.69	0.57
2:I:65:ASN:ND2	2:I:483:ASP:OD2	2.37	0.57
2:I:39:ILE:HD11	2:I:127:ILE:HD12	1.87	0.57
2:I:742:TYR:O	2:I:744:GLY:N	2.38	0.57
5:L:16:GLY:O	5:L:20:GLY:N	2.36	0.57
5:L:247:GLU:OE1	5:L:247:GLU:N	2.38	0.57
5:L:560:ARG:HD3	5:L:566:ASP:CG	2.25	0.57
3:J:1150:PRO:CB	3:J:1214:PRO:HB2	2.35	0.56
6:O:50:DG:H2'	6:O:51:DT:H6	1.70	0.56
2:I:39:ILE:O	2:I:39:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:951:GLN:O	3:J:952:VAL:C	2.43	0.56
3:J:1099:TYR:HD2	3:J:1121:LEU:HD12	1.70	0.56
5:L:31:LEU:HD12	5:L:32:PRO:HD2	1.87	0.56
5:L:93:ARG:O	5:L:93:ARG:HD3	2.05	0.56
5:L:401:PHE:CZ	5:L:405:ILE:HD11	2.40	0.56
5:L:453:PRO:HB3	6:O:69:DG:H3'	1.87	0.56
2:I:1319:MET:SD	2:I:1323:PHE:CD2	2.97	0.56
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.86	0.56
5:L:549:ALA:C	5:L:551:LEU:H	2.09	0.56
3:J:1165:PHE:HB2	3:J:1168:GLU:OE2	2.06	0.56
2:I:30:ILE:HG23	2:I:31:GLN:HG2	1.88	0.56
3:J:1110:GLU:CB	3:J:1113:VAL:HG21	2.16	0.56
2:I:353:VAL:HG12	2:I:353:VAL:O	2.05	0.56
2:I:1258:PRO:HD3	2:I:1295:SER:O	2.05	0.56
3:J:343:LEU:HG	3:J:343:LEU:O	2.05	0.56
3:J:786:THR:O	3:J:790:THR:HG23	2.05	0.56
3:J:797:THR:O	3:J:801:VAL:HG13	2.06	0.56
3:J:1150:PRO:HB2	3:J:1214:PRO:HB2	1.88	0.56
5:L:343:LYS:O	5:L:347:ILE:HG13	2.06	0.56
2:I:896:THR:HB	2:I:897:PRO:CD	2.34	0.56
5:L:133:SER:HA	5:L:136:GLU:CD	2.26	0.56
1:H:98:VAL:HG23	1:H:146:VAL:HG13	1.86	0.56
3:J:1024:THR:HG21	3:J:1123:ARG:HB3	1.86	0.56
1:M:307:LEU:O	1:M:312:LEU:N	2.38	0.56
1:G:207:THR:HG21	1:G:211:ILE:HG22	1.87	0.55
5:L:600:HIS:CE1	5:L:603:ARG:HE	2.25	0.55
3:J:48:THR:O	3:J:50:LYS:N	2.39	0.55
3:J:1090:ILE:HG12	3:J:1097:ALA:HA	1.89	0.55
2:I:26:TYR:HE2	2:I:32:LEU:CD1	2.19	0.55
3:J:86:GLU:CD	3:J:86:GLU:H	2.10	0.55
2:I:150:HIS:CE1	2:I:454:ARG:HG3	2.42	0.55
3:J:1069:ALA:O	3:J:1072:LYS:HB3	2.06	0.55
3:J:1163:VAL:HG11	3:J:1198:VAL:HG22	1.89	0.55
5:L:36:VAL:CG2	5:L:41:ILE:HG22	2.36	0.55
2:I:1261:GLY:O	2:I:1266:GLY:N	2.29	0.55
8:L:702:4QM:C3	8:L:702:4QM:C18	2.71	0.55
1:G:223:ILE:O	1:G:227:GLN:HG2	2.07	0.55
5:L:292:VAL:O	5:L:296:LYS:N	2.38	0.55
3:J:833:GLU:OE1	3:J:1242:ARG:NH1	2.40	0.54
1:H:202:VAL:HG12	1:H:202:VAL:O	2.08	0.54
2:I:1256:GLN:HE22	5:L:528:LEU:HD11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:39:ILE:HG23	2:I:75:LEU:HD11	1.87	0.54
2:I:116:ASP:OD1	2:I:117:ILE:N	2.40	0.54
1:G:83:LEU:HD23	2:I:694:ARG:HD3	1.88	0.54
3:J:1197:ASN:HD21	3:J:1212:ASP:HB2	1.73	0.54
3:J:1078:LEU:HD12	3:J:1101:LEU:HD11	1.89	0.54
3:J:951:GLN:HG3	3:J:1014:GLY:HA2	1.89	0.54
3:J:980:THR:HB	3:J:997:VAL:HB	1.90	0.54
5:L:134:VAL:HG21	5:L:266:PHE:CE2	2.43	0.54
5:L:502:LYS:H	5:L:502:LYS:CD	2.19	0.53
1:G:45:ARG:NH1	1:H:34:GLY:O	2.41	0.53
5:L:280:VAL:CG2	5:L:347:ILE:HG21	2.37	0.53
3:J:572:THR:HG21	3:J:589:TYR:OH	2.08	0.53
3:J:1063:ASP:H	3:J:1066:GLU:HB3	1.73	0.53
5:L:224:LEU:HD22	5:L:259:PHE:HE2	1.73	0.53
3:J:342:LEU:HD13	3:J:1352:ILE:HG23	1.90	0.53
3:J:1365:TYR:CE2	3:J:1369:ARG:HD2	2.44	0.53
1:H:181:GLU:O	3:J:535:ARG:NH1	2.42	0.53
3:J:51:PRO:HB3	3:J:57:PHE:O	2.07	0.53
3:J:1173:ARG:HH22	3:J:1200:GLU:CD	2.11	0.53
5:L:451:ARG:NH2	6:O:70:DC:OP2	2.41	0.53
2:I:1271:GLY:HA2	3:J:344:GLY:HA2	1.91	0.53
3:J:285:LEU:CD1	5:L:410:ILE:HD11	2.37	0.53
5:L:474:MET:HE3	5:L:476:ARG:O	2.09	0.53
1:G:194:GLN:O	1:G:195:ARG:C	2.47	0.53
2:I:1244:HIS:ND1	2:I:1262:LYS:CD	2.72	0.53
3:J:932:MET:O	3:J:933:ARG:C	2.47	0.53
3:J:1005:LYS:HG3	3:J:1011:VAL:HG12	1.89	0.53
2:I:1244:HIS:ND1	2:I:1262:LYS:HD2	2.24	0.53
3:J:973:LEU:HD23	3:J:1003:LEU:HD12	1.91	0.53
1:H:68:TYR:O	1:H:69:SER:OG	2.25	0.52
2:I:187:GLU:OE2	2:I:197:ARG:NH1	2.42	0.52
6:O:63:DC:H2'	6:O:64:DC:C5	2.44	0.52
2:I:445:ILE:O	2:I:445:ILE:HG22	2.10	0.52
3:J:1345:ARG:HH22	3:J:1373:ARG:HH22	1.57	0.52
5:L:582:VAL:CG2	5:L:586:ARG:HB3	2.33	0.52
3:J:515:ARG:O	3:J:545:HIS:ND1	2.42	0.52
3:J:572:THR:HG21	3:J:589:TYR:CE2	2.45	0.52
2:I:185:ASP:O	2:I:196:VAL:HG23	2.10	0.52
2:I:471:VAL:HG21	2:I:498:ILE:HD11	1.91	0.52
5:L:118:ASP:N	5:L:118:ASP:OD1	2.43	0.52
5:L:608:ARG:O	5:L:611:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1035:LYS:O	2:I:1035:LYS:HG2	2.10	0.52
5:L:554:ARG:NH1	5:L:590:ILE:HG13	2.23	0.52
3:J:291:ILE:HD12	5:L:409:ASN:HD22	1.75	0.52
3:J:538:ARG:HH22	3:J:634:ARG:NH2	2.07	0.52
5:L:108:VAL:O	5:L:385:ARG:NH2	2.40	0.52
5:L:346:GLN:O	5:L:350:GLU:HG3	2.09	0.52
5:L:425:TYR:CE2	6:O:75:DA:O4'	2.63	0.52
3:J:1081:VAL:HG12	3:J:1087:ASP:HA	1.92	0.52
5:L:316:PHE:CE1	5:L:337:VAL:HG11	2.45	0.52
2:I:160:ASP:O	2:I:161:LYS:HG2	2.10	0.51
3:J:568:SER:OG	3:J:570:LYS:NZ	2.40	0.51
3:J:1015:GLU:O	3:J:1016:THR:C	2.48	0.51
5:L:466:ILE:HD13	5:L:487:MET:HG2	1.92	0.51
8:L:701:4QM:C3	8:L:701:4QM:C1	2.88	0.51
2:I:1137:GLU:CD	2:I:1137:GLU:H	2.13	0.51
3:J:57:PHE:O	3:J:98:ARG:NH2	2.43	0.51
1:G:45:ARG:NH2	2:I:1084:ASP:OD1	2.43	0.51
1:G:150:ARG:HB2	1:H:5:VAL:HG23	1.91	0.51
3:J:1177:ILE:O	3:J:1178:THR:C	2.48	0.51
2:I:748:ILE:HD12	2:I:966:ILE:HG22	1.93	0.51
3:J:17:PHE:HZ	3:J:1353:VAL:CG1	2.24	0.51
3:J:1001:ALA:CB	3:J:1020:TRP:HB3	2.41	0.51
3:J:1050:THR:HG23	3:J:1056:LEU:C	2.31	0.51
5:L:560:ARG:HD3	5:L:566:ASP:OD1	2.10	0.51
2:I:693:LEU:CD2	2:I:831:ILE:HD11	2.40	0.51
2:I:161:LYS:HG3	2:I:163:LYS:HE3	1.92	0.51
2:I:1331:ARG:NH2	2:I:1337:ILE:O	2.44	0.51
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.92	0.51
3:J:952:VAL:HG21	3:J:1011:VAL:CG2	2.40	0.51
3:J:1005:LYS:HE3	3:J:1009:GLU:HB3	1.92	0.51
5:L:133:SER:HA	5:L:136:GLU:OE1	2.11	0.51
6:O:52:DT:OP2	6:O:52:DT:H73	2.11	0.51
3:J:1040:MET:HE3	3:J:1078:LEU:HG	1.93	0.51
3:J:1157:ALA:O	3:J:1206:ARG:HA	2.11	0.51
3:J:1158:GLU:OE1	3:J:1222:ARG:NH1	2.44	0.51
3:J:1199:PHE:HB2	3:J:1202:GLU:HG2	1.93	0.51
2:I:232:ILE:HD12	2:I:330:HIS:O	2.11	0.51
3:J:1063:ASP:O	3:J:1067:ARG:HG2	2.11	0.50
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.93	0.50
2:I:180:ARG:NH1	2:I:393:ASP:O	2.44	0.50
2:I:1005:GLU:OE1	2:I:1006:GLU:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1041:ILE:HB	3:J:1044:GLN:HB2	1.92	0.50
3:J:1158:GLU:HG2	3:J:1186:TYR:CE1	2.45	0.50
3:J:1313:SER:OG	3:J:1314:LEU:N	2.44	0.50
2:I:131:THR:HG22	2:I:132:ASP:N	2.26	0.50
3:J:1037:PHE:CD1	3:J:1111:ASP:HA	2.46	0.50
3:J:1344:LEU:H	3:J:1344:LEU:HD22	1.75	0.50
2:I:906:PHE:HD2	5:L:611:LEU:HG	1.77	0.50
3:J:208:THR:O	3:J:210:SER:N	2.44	0.50
5:L:383:ASN:CB	5:L:412:LEU:HD11	2.26	0.50
2:I:1127:LYS:O	2:I:1131:MET:HG3	2.11	0.50
3:J:1045:THR:HB	3:J:1067:ARG:CZ	2.42	0.50
3:J:1167:LYS:H	3:J:1174:ARG:HH11	1.60	0.50
5:L:466:ILE:HG22	5:L:470:MET:CE	2.42	0.50
2:I:400:VAL:HG21	2:I:452:ARG:HD2	1.94	0.50
3:J:785:ASP:O	3:J:786:THR:C	2.49	0.50
5:L:384:LEU:O	5:L:385:ARG:C	2.50	0.50
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.93	0.50
3:J:661:VAL:HG23	3:J:682:VAL:HG22	1.93	0.50
3:J:966:VAL:H	3:J:974:VAL:HG22	1.77	0.50
5:L:449:THR:CG2	5:L:504:PRO:HD2	2.41	0.50
2:I:939:VAL:HG12	2:I:940:GLU:H	1.76	0.50
2:I:1149:TYR:HB3	2:I:1159:VAL:HG22	1.93	0.50
5:L:586:ARG:NH2	5:L:590:ILE:HD11	2.27	0.50
3:J:1162:ILE:O	3:J:1177:ILE:HA	2.11	0.49
2:I:72:SER:OG	2:I:73:TYR:N	2.45	0.49
3:J:708:ASN:OD1	3:J:709:ARG:N	2.44	0.49
5:L:456:MET:O	5:L:460:ILE:HG13	2.11	0.49
2:I:39:ILE:HG23	2:I:75:LEU:CD1	2.43	0.49
3:J:1037:PHE:HA	3:J:1078:LEU:CD2	2.42	0.49
5:L:481:GLU:O	5:L:485:GLU:HG3	2.12	0.49
1:G:19:VAL:HG13	1:G:23:HIS:HB3	1.95	0.49
2:I:314:ASN:O	2:I:314:ASN:ND2	2.45	0.49
3:J:982:LEU:HG	3:J:997:VAL:CG2	2.42	0.49
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.94	0.49
6:O:51:DT:H2'	6:O:51:DT:O2	2.12	0.49
6:O:74:DG:H2''	6:O:75:DA:OP2	2.12	0.49
1:G:135:ASP:OD1	1:G:136:GLU:N	2.46	0.49
2:I:525:THR:HG21	2:I:687:ARG:CD	2.43	0.49
3:J:952:VAL:HG21	3:J:1011:VAL:HG21	1.95	0.49
3:J:1040:MET:HG3	3:J:1046:ILE:HG21	1.94	0.49
3:J:1180:VAL:HG23	3:J:1203:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.46	0.49
3:J:416:ILE:HG22	3:J:416:ILE:O	2.13	0.49
3:J:790:THR:HG22	3:J:928:THR:HG21	1.93	0.49
4:K:4:VAL:HG23	4:K:5:THR:HG23	1.94	0.49
5:L:449:THR:HG21	5:L:504:PRO:HG2	1.95	0.49
3:J:328:ALA:O	3:J:332:LYS:HG2	2.13	0.48
3:J:351:GLY:O	3:J:468:VAL:HG12	2.13	0.48
5:L:354:THR:HB	5:L:357:GLN:CD	2.33	0.48
2:I:320:ASP:OD1	2:I:321:LEU:N	2.45	0.48
5:L:33:GLU:O	5:L:34:ASP:C	2.50	0.48
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.46	0.48
5:L:586:ARG:O	5:L:589:GLN:HB2	2.13	0.48
2:I:811:ASN:O	2:I:811:ASN:ND2	2.37	0.48
3:J:1050:THR:OG1	3:J:1057:SER:HA	2.13	0.48
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.42	0.48
3:J:968:ASN:OD1	3:J:972:LYS:N	2.44	0.48
5:L:163:THR:O	5:L:260:ARG:NE	2.47	0.48
1:H:12:ARG:HG2	1:H:13:LEU:CD2	2.42	0.48
1:H:207:THR:HG22	1:H:208:ASN:H	1.79	0.48
2:I:521:LEU:O	2:I:525:THR:HG22	2.13	0.48
2:I:1272:GLU:HG3	2:I:1273:MET:N	2.29	0.48
3:J:1079:LYS:CA	3:J:1098:GLN:HA	2.38	0.48
2:I:148:GLN:OE1	2:I:454:ARG:NH1	2.47	0.48
3:J:84:ILE:CG2	3:J:89:GLY:HA2	2.44	0.48
3:J:111:THR:O	3:J:239:LEU:N	2.43	0.48
3:J:1134:ILE:HG22	3:J:1135:THR:O	2.13	0.48
3:J:1163:VAL:HG13	3:J:1200:GLU:O	2.13	0.48
5:L:56:MET:HB3	5:L:58:GLU:O	2.12	0.48
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.44	0.48
2:I:1255:THR:HG23	2:I:1255:THR:O	2.14	0.48
3:J:1089:LEU:O	3:J:1090:ILE:C	2.52	0.48
4:K:4:VAL:CG2	4:K:5:THR:HG23	2.44	0.48
2:I:65:ASN:OD1	2:I:66:SER:N	2.47	0.47
4:K:25:ARG:HH21	4:K:68:GLU:CD	2.16	0.47
5:L:462:LYS:HG2	5:L:466:ILE:HD11	1.97	0.47
6:O:59:DT:H4'	6:O:60:DT:OP1	2.13	0.47
3:J:800:LEU:HA	3:J:803:VAL:HG12	1.96	0.47
2:I:903:ARG:O	2:I:907:GLY:N	2.47	0.47
3:J:341:ASN:O	3:J:342:LEU:HB2	2.14	0.47
5:L:139:GLU:CD	5:L:139:GLU:H	2.17	0.47
3:J:839:VAL:HG12	3:J:839:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:975:ILE:HD12	3:J:980:THR:HG21	1.97	0.47
3:J:986:ASP:HB3	3:J:992:LYS:HD2	1.97	0.47
3:J:1041:ILE:HD12	3:J:1041:ILE:H	1.79	0.47
5:L:116:GLU:HG3	5:L:379:MET:HE1	1.96	0.47
2:I:21:VAL:HG21	2:I:592:ARG:HD3	1.97	0.47
2:I:1256:GLN:NE2	5:L:528:LEU:HD11	2.29	0.47
3:J:1162:ILE:HD12	3:J:1202:GLU:O	2.15	0.47
5:L:152:GLU:OE2	5:L:218:ARG:NH1	2.47	0.47
1:G:14:VAL:HG21	1:G:29:GLU:HB2	1.96	0.47
1:G:28:LEU:HD12	1:G:28:LEU:N	2.30	0.47
1:G:234:LEU:H	1:H:218:ARG:HD3	1.80	0.47
2:I:778:GLU:HG2	2:I:781:ASP:OD2	2.14	0.47
3:J:337:ARG:O	3:J:342:LEU:HD12	2.15	0.47
3:J:974:VAL:HG12	3:J:1002:VAL:HG22	1.97	0.47
3:J:1051:ASP:O	3:J:1055:GLY:N	2.48	0.47
5:L:401:PHE:CE2	5:L:405:ILE:HD11	2.50	0.47
3:J:972:LYS:HB2	3:J:1002:VAL:HG11	1.97	0.47
3:J:1166:GLY:HA3	3:J:1174:ARG:NH1	2.30	0.47
3:J:1171:GLY:C	3:J:1172:LYS:HD2	2.35	0.47
3:J:197:GLU:O	3:J:201:LEU:HD23	2.14	0.47
3:J:1062:LEU:O	3:J:1067:ARG:NE	2.48	0.47
3:J:982:LEU:HG	3:J:997:VAL:HG21	1.95	0.47
3:J:985:ILE:HD13	3:J:991:THR:OG1	2.15	0.47
3:J:1035:VAL:HG11	3:J:1121:LEU:HD21	1.97	0.47
5:L:502:LYS:HD3	5:L:502:LYS:N	2.30	0.47
6:O:60:DT:C6	6:O:61:DT:H72	2.50	0.47
1:H:219:ARG:O	1:H:223:ILE:HG13	2.15	0.46
3:J:1168:GLU:OE1	3:J:1173:ARG:HG2	2.15	0.46
5:L:598:LEU:O	5:L:604:SER:HB3	2.15	0.46
3:J:538:ARG:NH2	3:J:634:ARG:HH22	2.13	0.46
2:I:160:ASP:C	2:I:161:LYS:HG2	2.36	0.46
5:L:28:ASN:O	5:L:31:LEU:HB3	2.16	0.46
5:L:56:MET:C	5:L:58:GLU:N	2.69	0.46
1:H:229:GLU:HA	1:H:232:VAL:HG12	1.97	0.46
2:I:160:ASP:HB2	2:I:165:HIS:HE1	1.81	0.46
3:J:483:LEU:CD2	4:K:16:ARG:HG2	2.46	0.46
3:J:1003:LEU:HA	3:J:1018:ALA:CB	2.42	0.46
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.97	0.46
5:L:431:ALA:O	5:L:433:TRP:N	2.47	0.46
2:I:221:LEU:HD13	2:I:336:LEU:HD11	1.96	0.46
3:J:984:LEU:HG	3:J:984:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1090:ILE:CG1	3:J:1097:ALA:HA	2.44	0.46
4:K:26:ARG:HD3	4:K:64:LEU:HD21	1.97	0.46
5:L:442:SER:OG	5:L:443:ILE:N	2.49	0.46
5:L:511:ILE:HD11	8:L:701:4QM:C23	2.46	0.46
3:J:341:ASN:O	3:J:342:LEU:CB	2.63	0.46
3:J:708:ASN:ND2	3:J:712:GLN:O	2.48	0.46
3:J:902:ASP:O	3:J:903:LEU:HB2	2.14	0.46
3:J:1103:GLY:O	3:J:1104:LYS:HB2	2.16	0.46
6:O:73:DT:O2	6:O:74:DG:C5	2.69	0.46
5:L:377:LYS:O	5:L:381:GLU:HG3	2.16	0.46
2:I:1252:SER:HB3	2:I:1255:THR:O	2.15	0.46
3:J:1090:ILE:N	3:J:1095:MET:O	2.48	0.46
2:I:339:ASN:OD1	2:I:343:HIS:HB2	2.16	0.46
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.98	0.46
3:J:785:ASP:O	3:J:788:LEU:N	2.49	0.46
1:G:8:PHE:HD1	1:G:32:GLU:HG3	1.79	0.46
3:J:289:ASP:HA	3:J:292:VAL:HG22	1.98	0.46
3:J:1125:PRO:O	3:J:1126:GLN:C	2.54	0.46
5:L:23:THR:N	5:L:26:GLU:OE2	2.48	0.46
2:I:131:THR:HG22	2:I:132:ASP:H	1.81	0.45
2:I:748:ILE:HD11	2:I:967:LEU:HA	1.98	0.45
3:J:1079:LYS:HD2	3:J:1087:ASP:HB3	1.98	0.45
3:J:1289:ASN:OD1	3:J:1290:ARG:N	2.49	0.45
5:L:582:VAL:HG13	5:L:583:THR:N	2.30	0.45
2:I:779:ARG:HB2	2:I:779:ARG:CZ	2.44	0.45
2:I:1255:THR:O	2:I:1257:GLN:N	2.47	0.45
3:J:1023:HIS:O	3:J:1024:THR:O	2.34	0.45
3:J:1068:THR:O	3:J:1072:LYS:N	2.49	0.45
8:L:701:4QM:C3	8:L:701:4QM:C18	2.73	0.45
1:H:57:THR:HG21	1:H:147:GLN:NE2	2.31	0.45
2:I:22:LEU:HD13	2:I:603:ILE:HD13	1.99	0.45
3:J:357:VAL:O	3:J:449:LEU:O	2.35	0.45
3:J:1077:ALA:HB2	3:J:1100:PHE:CE2	2.51	0.45
5:L:585:GLU:O	5:L:589:GLN:HG3	2.15	0.45
1:H:11:PRO:HG3	1:H:31:LEU:CD2	2.44	0.45
2:I:358:ASP:OD1	2:I:361:SER:OG	2.31	0.45
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.97	0.45
3:J:1028:ILE:HA	3:J:1119:ASP:O	2.16	0.45
3:J:1206:ARG:HE	3:J:1206:ARG:HB2	1.49	0.45
3:J:1311:LYS:NZ	5:L:71:THR:HA	2.31	0.45
5:L:17:LYS:HB3	5:L:17:LYS:HE3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:412:LEU:CD1	5:L:435:ILE:HD11	2.46	0.45
5:L:509:THR:HG23	5:L:509:THR:O	2.17	0.45
5:L:470:MET:CE	5:L:483:LEU:HD23	2.46	0.45
6:O:50:DG:H2'	6:O:51:DT:C6	2.52	0.45
2:I:1246:ARG:HG3	2:I:1265:PHE:CE2	2.52	0.45
2:I:162:GLY:H	2:I:170:VAL:HG12	1.81	0.45
3:J:571:ASP:O	3:J:572:THR:HG23	2.16	0.45
3:J:1152:GLU:OE2	3:J:1193:TRP:HZ3	1.99	0.45
5:L:466:ILE:HG22	5:L:470:MET:HE2	1.99	0.45
5:L:554:ARG:HG3	5:L:580:PHE:CE2	2.52	0.45
5:L:576:VAL:CG1	5:L:587:ILE:HD13	2.40	0.45
8:L:702:4QM:C3	8:L:702:4QM:C1	2.94	0.45
2:I:447:HIS:C	2:I:449:GLY:H	2.21	0.45
2:I:577:VAL:HG23	2:I:661:VAL:O	2.17	0.45
3:J:413:ASP:OD1	3:J:441:LEU:HD12	2.17	0.45
3:J:1167:LYS:CD	3:J:1170:LYS:HB2	2.41	0.45
5:L:355:ILE:O	5:L:359:LYS:HG2	2.17	0.45
3:J:339:ARG:HG2	3:J:339:ARG:NH1	2.28	0.45
3:J:500:ILE:O	3:J:500:ILE:HG22	2.17	0.45
3:J:827:GLU:OE1	3:J:827:GLU:N	2.50	0.45
3:J:986:ASP:OD1	3:J:986:ASP:C	2.55	0.45
3:J:1172:LYS:HG3	3:J:1191:PRO:HA	1.98	0.45
5:L:384:LEU:C	5:L:386:LEU:N	2.70	0.45
5:L:431:ALA:C	5:L:433:TRP:N	2.69	0.45
5:L:586:ARG:CZ	5:L:590:ILE:HD11	2.46	0.45
5:L:131:GLN:O	5:L:134:VAL:HG22	2.16	0.45
3:J:1050:THR:HA	3:J:1058:SER:N	2.33	0.44
3:J:1168:GLU:C	3:J:1170:LYS:H	2.20	0.44
5:L:96:ASP:O	5:L:100:MET:HG3	2.17	0.44
2:I:24:VAL:CG1	2:I:25:PRO:HD2	2.48	0.44
3:J:362:ARG:H	3:J:365:GLN:CG	2.30	0.44
3:J:1001:ALA:HB2	3:J:1020:TRP:HB3	1.99	0.44
3:J:1150:PRO:O	3:J:1153:PRO:HD3	2.17	0.44
3:J:1365:TYR:HD2	3:J:1366:HIS:CD2	2.36	0.44
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.50	0.44
2:I:43:PRO:O	2:I:54:ARG:NH2	2.50	0.44
3:J:169:LEU:HD23	3:J:169:LEU:O	2.17	0.44
3:J:395:LYS:HE3	5:L:536:THR:HG21	1.99	0.44
5:L:337:VAL:O	5:L:341:LEU:HD13	2.16	0.44
2:I:194:LEU:HD21	2:I:433:ILE:HD11	2.00	0.44
5:L:383:ASN:OD1	5:L:427:PHE:CE2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:VAL:HG22	1:G:99:ILE:N	2.32	0.44
2:I:300:ASP:N	2:I:300:ASP:OD1	2.49	0.44
3:J:372:MET:O	3:J:376:LEU:HG	2.17	0.44
3:J:1047:THR:CG2	3:J:1062:LEU:HD21	2.47	0.44
3:J:1167:LYS:HD3	3:J:1167:LYS:C	2.38	0.44
3:J:1295:ASN:OD1	3:J:1296:GLY:N	2.42	0.44
6:O:72:DG:H2"	6:O:73:DT:O5'	2.18	0.44
2:I:660:VAL:HG21	3:J:769:VAL:HG21	1.99	0.44
5:L:394:TYR:CD2	5:L:439:ILE:HG21	2.53	0.44
5:L:416:VAL:HG22	5:L:427:PHE:CZ	2.52	0.44
5:L:574:GLU:OE1	5:L:584:ARG:NH1	2.51	0.44
1:H:13:LEU:CG	1:H:29:GLU:HB3	2.45	0.44
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.50	0.44
3:J:78:LEU:O	3:J:80:HIS:N	2.51	0.44
1:H:20:SER:OG	1:H:21:SER:N	2.51	0.44
2:I:187:GLU:CD	2:I:197:ARG:HH12	2.21	0.44
5:L:280:VAL:HG22	5:L:347:ILE:HG21	1.99	0.44
5:L:542:ALA:O	5:L:545:HIS:N	2.48	0.44
5:L:549:ALA:O	5:L:551:LEU:N	2.42	0.44
2:I:356:THR:HG22	2:I:365:GLU:OE1	2.16	0.44
2:I:1192:GLU:OE1	3:J:764:ARG:NH1	2.49	0.43
2:I:1256:GLN:HE21	2:I:1256:GLN:HB3	1.52	0.43
1:G:14:VAL:HG11	1:G:29:GLU:HB2	2.00	0.43
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.51	0.43
5:L:136:GLU:CD	5:L:364:ARG:HH21	2.22	0.43
2:I:596:ASP:OD1	2:I:597:GLY:N	2.47	0.43
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.84	0.43
3:J:975:ILE:HG12	3:J:1001:ALA:O	2.17	0.43
5:L:12:LEU:HD11	5:L:27:VAL:HA	2.01	0.43
5:L:582:VAL:HG21	5:L:586:ARG:CB	2.38	0.43
3:J:981:GLU:OE2	3:J:996:LYS:HE2	2.18	0.43
3:J:1275:LEU:N	3:J:1275:LEU:HD12	2.33	0.43
1:H:13:LEU:HD11	1:H:29:GLU:HG2	1.99	0.43
2:I:1297:ASP:OD2	2:I:1317:PRO:O	2.37	0.43
5:L:354:THR:HB	5:L:357:GLN:HG3	2.00	0.43
5:L:514:ASP:OD1	5:L:514:ASP:N	2.52	0.43
5:L:554:ARG:HH12	5:L:590:ILE:CG1	2.27	0.43
1:G:228:LEU:C	1:G:230:ALA:N	2.72	0.43
2:I:39:ILE:CD1	2:I:127:ILE:HD12	2.47	0.43
2:I:1009:ASN:OD1	2:I:1013:GLN:NE2	2.48	0.43
3:J:514:THR:HG21	3:J:596:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:961:SER:HB2	3:J:981:GLU:HB2	2.00	0.43
3:J:1165:PHE:HB3	3:J:1173:ARG:NH1	2.33	0.43
3:J:1211:SER:OG	3:J:1212:ASP:N	2.51	0.43
5:L:548:LEU:O	5:L:551:LEU:HB2	2.19	0.43
5:L:552:THR:OG1	5:L:555:GLU:OE2	2.36	0.43
5:L:581:ASP:O	5:L:582:VAL:HB	2.18	0.43
5:L:598:LEU:HD23	5:L:603:ARG:CD	2.48	0.43
2:I:124:MET:CE	2:I:498:ILE:HD13	2.49	0.43
2:I:1030:GLU:HG2	2:I:1033:ARG:NH2	2.33	0.43
3:J:1034:PHE:HE1	3:J:1083:ALA:HB2	1.84	0.43
3:J:1161:GLY:CA	3:J:1177:ILE:HG22	2.49	0.43
3:J:1162:ILE:HG22	3:J:1178:THR:O	2.19	0.43
3:J:1324:SER:OG	3:J:1352:ILE:HD11	2.19	0.43
5:L:347:ILE:O	5:L:351:THR:HG23	2.19	0.43
1:H:98:VAL:O	1:H:146:VAL:HG13	2.18	0.43
2:I:359:ARG:NH2	2:I:382:GLU:OE2	2.52	0.43
2:I:1035:LYS:C	2:I:1037:THR:H	2.21	0.43
3:J:156:ARG:NH1	3:J:157:GLN:OE1	2.52	0.43
3:J:860:ARG:O	3:J:862:THR:HG23	2.19	0.43
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.19	0.43
5:L:37:ASP:O	5:L:39:ASP:N	2.50	0.43
1:H:28:LEU:N	1:H:28:LEU:HD12	2.33	0.42
2:I:1033:ARG:C	2:I:1035:LYS:H	2.22	0.42
3:J:1093:THR:HB	3:J:1095:MET:CE	2.48	0.42
5:L:9:LEU:HD11	5:L:44:ILE:HD11	2.01	0.42
5:L:511:ILE:HD11	8:L:701:4QM:C22	2.49	0.42
2:I:17:LYS:HG3	2:I:1154:ASP:O	2.19	0.42
2:I:1083:GLU:H	2:I:1083:GLU:HG3	1.45	0.42
3:J:1042:ASP:HA	3:J:1046:ILE:HG13	2.01	0.42
5:L:433:TRP:HE3	5:L:434:TRP:CD1	2.37	0.42
6:O:59:DT:H2'	6:O:60:DT:H72	2.01	0.42
2:I:196:VAL:HG21	2:I:209:ILE:HD12	2.01	0.42
2:I:1319:MET:HG3	2:I:1320:PRO:O	2.19	0.42
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.19	0.42
6:O:62:DA:C4	6:O:63:DC:C5	3.07	0.42
2:I:493:ILE:O	5:L:472:GLN:OE1	2.37	0.42
3:J:478:LEU:CD2	4:K:47:THR:HG23	2.49	0.42
1:G:172:LEU:HD12	1:G:172:LEU:N	2.35	0.42
2:I:957:LYS:HA	2:I:1033:ARG:NH2	2.35	0.42
3:J:1082:ASP:N	3:J:1088:VAL:HG23	2.33	0.42
6:O:50:DG:C8	6:O:51:DT:H71	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:ASP:O	2:I:192:ASP:N	2.51	0.42
2:I:806:PRO:O	2:I:811:ASN:ND2	2.50	0.42
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.19	0.42
3:J:785:ASP:O	3:J:787:ALA:N	2.52	0.42
3:J:820:ILE:HG22	3:J:821:MET:N	2.35	0.42
3:J:1067:ARG:HD3	3:J:1071:GLY:O	2.19	0.42
3:J:1163:VAL:HG12	3:J:1202:GLU:N	2.31	0.42
3:J:1321:SER:HB2	3:J:1349:GLU:OE2	2.19	0.42
5:L:474:MET:SD	5:L:476:ARG:HD3	2.60	0.42
1:G:6:THR:O	1:G:7:GLU:HB2	2.20	0.42
2:I:902:LEU:HD11	5:L:610:PHE:HB2	2.01	0.42
3:J:912:GLY:O	3:J:1359:ALA:O	2.38	0.42
3:J:1033:GLY:C	3:J:1114:GLN:HG3	2.40	0.42
3:J:1063:ASP:O	3:J:1064:SER:C	2.58	0.42
3:J:1174:ARG:HE	3:J:1187:GLU:CD	2.22	0.42
5:L:470:MET:HE1	5:L:483:LEU:HD23	2.02	0.42
5:L:474:MET:HE1	5:L:478:PRO:HA	2.01	0.42
2:I:1042:LEU:HD22	2:I:1049:ILE:HD12	2.02	0.42
3:J:1163:VAL:HG12	3:J:1202:GLU:O	2.20	0.42
3:J:1199:PHE:HB2	3:J:1202:GLU:CG	2.50	0.42
5:L:36:VAL:HB	5:L:41:ILE:HG22	2.02	0.42
2:I:255:ILE:HG21	2:I:262:TYR:HB2	2.02	0.42
2:I:1042:LEU:HB3	2:I:1046:VAL:CG2	2.50	0.42
3:J:425:ARG:HD3	3:J:459:ALA:HB2	2.00	0.42
3:J:807:LEU:HD23	3:J:807:LEU:HA	1.78	0.42
3:J:975:ILE:HB	3:J:1001:ALA:H	1.85	0.42
3:J:1030:GLU:CD	3:J:1091:PRO:HB2	2.41	0.42
3:J:1095:MET:SD	3:J:1095:MET:N	2.80	0.42
5:L:23:THR:OG1	5:L:26:GLU:HG2	2.20	0.42
3:J:1036:ARG:CD	3:J:1081:VAL:HG11	2.49	0.42
5:L:465:ARG:O	5:L:467:SER:N	2.53	0.42
1:G:102:LEU:HD23	1:G:142:MET:CE	2.50	0.41
2:I:821:ARG:HG3	2:I:821:ARG:O	2.19	0.41
5:L:598:LEU:HD23	5:L:603:ARG:HD3	2.02	0.41
6:O:73:DT:H1'	6:O:74:DG:N7	2.35	0.41
5:L:354:THR:HB	5:L:357:GLN:CG	2.50	0.41
5:L:499:LYS:O	5:L:500:ILE:C	2.59	0.41
7:P:34:DC:H2"	7:P:35:DC:C6	2.55	0.41
1:H:32:GLU:HB2	1:H:35:PHE:CD2	2.55	0.41
2:I:471:VAL:HG21	2:I:498:ILE:CD1	2.50	0.41
2:I:697:LYS:HE3	2:I:1181:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1152:GLU:O	3:J:1214:PRO:HD2	2.19	0.41
5:L:80:ALA:O	5:L:83:VAL:HG22	2.19	0.41
5:L:465:ARG:O	5:L:468:ARG:N	2.54	0.41
2:I:173:ASN:OD1	2:I:173:ASN:N	2.52	0.41
2:I:821:ARG:NH2	2:I:1082:ILE:HD11	2.34	0.41
8:I:1401:4QM:C3	8:I:1401:4QM:C1	2.99	0.41
3:J:553:THR:OG1	3:J:567:THR:HG22	2.21	0.41
3:J:1040:MET:SD	3:J:1046:ILE:HG21	2.61	0.41
3:J:1110:GLU:O	3:J:1113:VAL:HG23	2.20	0.41
5:L:559:LEU:HD21	5:L:595:LEU:CD2	2.50	0.41
2:I:35:PHE:CZ	2:I:39:ILE:HD12	2.55	0.41
2:I:39:ILE:HD11	2:I:127:ILE:CD1	2.50	0.41
3:J:859:PRO:HD2	3:J:862:THR:HG21	2.03	0.41
3:J:905:ARG:HH11	4:K:16:ARG:NH2	2.18	0.41
3:J:1051:ASP:OD2	3:J:1056:LEU:HB2	2.21	0.41
3:J:1062:LEU:HB2	3:J:1067:ARG:CB	2.35	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.20	0.41
2:I:36:GLN:HE21	2:I:37:LYS:HG3	1.86	0.41
5:L:381:GLU:HA	5:L:384:LEU:HD22	2.02	0.41
5:L:547:VAL:CG1	5:L:598:LEU:HD22	2.44	0.41
2:I:75:LEU:CD2	2:I:127:ILE:HD11	2.50	0.41
2:I:980:VAL:O	2:I:980:VAL:HG12	2.20	0.41
2:I:1257:GLN:HE22	3:J:341:ASN:HB3	1.86	0.41
3:J:970:SER:HB2	3:J:972:LYS:HG2	2.02	0.41
3:J:1050:THR:O	3:J:1051:ASP:C	2.58	0.41
3:J:1140:ARG:O	3:J:1143:ASP:OD1	2.39	0.41
5:L:453:PRO:HG2	6:O:69:DG:OP2	2.20	0.41
1:H:131:CYS:SG	1:H:132:HIS:N	2.93	0.41
2:I:461:GLU:O	2:I:461:GLU:HG2	2.21	0.41
2:I:997:TRP:HE3	2:I:1000:LEU:HD11	1.86	0.41
3:J:492:SER:O	3:J:495:ASN:O	2.38	0.41
3:J:1179:PRO:HD3	3:J:1185:PRO:HA	2.02	0.41
3:J:1311:LYS:HZ3	5:L:71:THR:HA	1.85	0.41
3:J:1371:ARG:HE	3:J:1371:ARG:HB2	1.67	0.41
5:L:93:ARG:HH11	5:L:93:ARG:C	2.24	0.41
1:G:32:GLU:OE2	1:G:195:ARG:NH1	2.53	0.41
1:H:207:THR:HG22	1:H:208:ASN:N	2.36	0.41
1:H:212:ASP:OD1	1:H:212:ASP:N	2.52	0.41
2:I:175:ARG:NH2	2:I:183:TRP:HE3	2.19	0.41
2:I:453:ILE:HD12	2:I:530:ILE:HD12	2.03	0.41
2:I:471:VAL:HG21	2:I:498:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:637:ARG:HA	2:I:642:SER:HA	2.03	0.41
2:I:966:ILE:HD11	8:I:1401:4QM:C11	2.51	0.41
2:I:1262:LYS:O	2:I:1265:PHE:N	2.51	0.41
2:I:1262:LYS:C	2:I:1265:PHE:H	2.24	0.41
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	2.03	0.41
3:J:147:ILE:O	3:J:177:ASP:HB3	2.21	0.41
3:J:704:GLU:OE2	3:J:716:GLN:NE2	2.44	0.41
3:J:1031:VAL:C	3:J:1117:SER:HA	2.41	0.41
3:J:1098:GLN:HG2	3:J:1098:GLN:O	2.20	0.41
3:J:1152:GLU:O	3:J:1152:GLU:HG3	2.19	0.41
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.56	0.41
3:J:1368:ASP:OD1	3:J:1369:ARG:N	2.54	0.41
4:K:6:VAL:HG12	4:K:6:VAL:O	2.21	0.41
5:L:386:LEU:HG	5:L:387:VAL:N	2.34	0.41
1:G:14:VAL:HG11	1:G:29:GLU:CB	2.51	0.41
2:I:131:THR:HG22	2:I:132:ASP:OD1	2.21	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.03	0.41
3:J:1048:ARG:HH22	3:J:1057:SER:HB2	1.86	0.41
1:H:46:ILE:CD1	1:H:224:LEU:HB2	2.50	0.40
1:H:78:ILE:HG22	1:H:79:LEU:N	2.36	0.40
1:H:206:GLU:CD	3:J:531:LYS:HZ3	2.23	0.40
3:J:161:THR:HG23	3:J:164:GLN:H	1.85	0.40
3:J:339:ARG:CG	3:J:339:ARG:NH1	2.71	0.40
5:L:412:LEU:HD13	5:L:435:ILE:HD11	2.04	0.40
1:H:61:ILE:O	1:H:64:VAL:HG22	2.22	0.40
1:H:93:GLN:O	1:H:148:ARG:NH2	2.54	0.40
2:I:724:VAL:CG1	2:I:727:VAL:HG22	2.50	0.40
3:J:438:GLU:OE2	4:K:2:ALA:CB	2.68	0.40
3:J:801:VAL:O	3:J:805:GLN:HB2	2.21	0.40
3:J:977:SER:HB2	3:J:980:THR:OG1	2.22	0.40
3:J:1161:GLY:HA2	3:J:1203:ARG:HH12	1.86	0.40
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.55	0.40
3:J:1361:THR:HG22	4:K:21:LEU:HD21	2.03	0.40
5:L:112:THR:O	5:L:116:GLU:OE1	2.39	0.40
5:L:442:SER:O	5:L:444:ALA:N	2.54	0.40
5:L:542:ALA:O	5:L:543:ALA:C	2.60	0.40
5:L:583:THR:O	5:L:585:GLU:N	2.51	0.40
2:I:594:VAL:HG12	2:I:595:THR:O	2.22	0.40
3:J:950:ILE:O	3:J:1016:THR:HA	2.22	0.40
3:J:1067:ARG:HD3	3:J:1071:GLY:C	2.40	0.40
5:L:9:LEU:HD12	5:L:9:LEU:HA	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:474:MET:HE1	5:L:478:PRO:CA	2.51	0.40
5:L:599:ARG:HE	5:L:599:ARG:HB2	1.56	0.40
2:I:135:THR:HG21	2:I:515:MET:SD	2.62	0.40
2:I:145:ILE:HG21	2:I:456:VAL:HG13	2.04	0.40
2:I:1211:ARG:NH2	2:I:1220:GLN:OE1	2.54	0.40
3:J:78:LEU:O	3:J:78:LEU:HD23	2.21	0.40
3:J:78:LEU:C	3:J:80:HIS:H	2.24	0.40
3:J:848:VAL:HB	3:J:858:VAL:HG22	2.03	0.40
3:J:967:VAL:CG1	3:J:971:GLY:HA2	2.48	0.40
5:L:494:ILE:HG22	5:L:498:LEU:HD22	2.02	0.40
6:O:62:DA:H2"	6:O:63:DC:C6	2.56	0.40
1:G:102:LEU:HD23	1:G:142:MET:HE1	2.03	0.40
2:I:229:ILE:HD11	2:I:240:GLU:HB2	2.04	0.40
2:I:638:SER:O	2:I:639:LYS:C	2.58	0.40
2:I:1070:HIS:NE2	2:I:1114:GLU:OE1	2.51	0.40
3:J:347:VAL:HG12	3:J:348:ASP:O	2.21	0.40
3:J:388:ARG:NH2	3:J:414:GLU:OE2	2.42	0.40
3:J:984:LEU:O	3:J:985:ILE:C	2.60	0.40
5:L:383:ASN:N	5:L:383:ASN:ND2	2.69	0.40
5:L:549:ALA:C	5:L:551:LEU:N	2.72	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	G	230/329 (70%)	212 (92%)	17 (7%)	1 (0%)	30	61
1	H	214/329 (65%)	197 (92%)	15 (7%)	2 (1%)	14	42
1	M	71/329 (22%)	70 (99%)	1 (1%)	0	100	100
2	I	1331/1342 (99%)	1225 (92%)	100 (8%)	6 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1332/1407 (95%)	1224 (92%)	94 (7%)	14 (1%)	12	37
4	K	71/91 (78%)	67 (94%)	4 (6%)	0	100	100
5	L	543/613 (89%)	485 (89%)	47 (9%)	11 (2%)	6	21
All	All	3792/4440 (85%)	3480 (92%)	278 (7%)	34 (1%)	17	42

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	49	PHE
3	J	340	GLN
3	J	342	LEU
3	J	426	ALA
3	J	952	VAL
5	L	387	VAL
5	L	428	SER
5	L	500	ILE
5	L	582	VAL
3	J	1024	THR
5	L	386	LEU
1	H	93	GLN
3	J	1016	THR
3	J	1030	GLU
5	L	34	ASP
5	L	56	MET
5	L	581	ASP
2	I	338	THR
2	I	345	PRO
3	J	786	THR
3	J	1164	SER
1	G	7	GLU
2	I	893	THR
2	I	1036	ILE
3	J	79	LYS
3	J	343	LEU
3	J	1186	TYR
3	J	1211	SER
5	L	57	GLU
1	H	98	VAL
2	I	1135	GLN
5	L	550	GLY
5	L	480	PRO

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Mol	Chain	Res	Type
2	I	1081	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	G	193/286 (68%)	180 (93%)	13 (7%)	13	38
1	H	184/286 (64%)	178 (97%)	6 (3%)	33	67
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1145/1157 (99%)	1091 (95%)	54 (5%)	22	54
3	J	1118/1168 (96%)	1080 (97%)	38 (3%)	32	66
4	K	63/75 (84%)	62 (98%)	1 (2%)	58	85
5	L	457/540 (85%)	440 (96%)	17 (4%)	29	63
All	All	3225/3798 (85%)	3096 (96%)	129 (4%)	29	60

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	12	ARG
1	G	13	LEU
1	G	50	SER
1	G	100	LEU
1	G	118	ASP
1	G	173	VAL
1	G	174	ASP
1	G	177	TYR
1	G	181	GLU
1	G	187	VAL
1	G	188	GLU
1	G	211	ILE
1	G	233	ASP
1	H	13	LEU
1	H	23	HIS
1	H	27	THR

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Mol	Chain	Res	Type
1	H	38	THR
1	H	98	VAL
1	H	146	VAL
2	I	2	VAL
2	I	21	VAL
2	I	30	ILE
2	I	36	GLN
2	I	70	TYR
2	I	106	GLU
2	I	107	ARG
2	I	111	GLU
2	I	161	LYS
2	I	173	ASN
2	I	201	ARG
2	I	204	LEU
2	I	272	ARG
2	I	360	LEU
2	I	427	ASP
2	I	456	VAL
2	I	465	ARG
2	I	521	LEU
2	I	526	HIS
2	I	539	THR
2	I	550	VAL
2	I	573	ASN
2	I	574	SER
2	I	581	THR
2	I	587	LEU
2	I	604	HIS
2	I	615	VAL
2	I	636	CYS
2	I	651	ASP
2	I	655	VAL
2	I	657	THR
2	I	697	LYS
2	I	749	ASP
2	I	779	ARG
2	I	807	TRP
2	I	811	ASN
2	I	894	GLN
2	I	912	ASP
2	I	937	ASP

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Mol	Chain	Res	Type
2	I	992	LEU
2	I	1005	GLU
2	I	1010	GLN
2	I	1018	TYR
2	I	1027	LYS
2	I	1081	PRO
2	I	1082	ILE
2	I	1083	GLU
2	I	1138	VAL
2	I	1141	LEU
2	I	1167	GLU
2	I	1225	VAL
2	I	1262	LYS
2	I	1287	LEU
2	I	1319	MET
3	J	40	LYS
3	J	42	GLU
3	J	60	ARG
3	J	67	ASP
3	J	85	CYS
3	J	86	GLU
3	J	88	CYS
3	J	93	THR
3	J	282	LEU
3	J	299	LEU
3	J	304	ASP
3	J	338	PHE
3	J	339	ARG
3	J	343	LEU
3	J	371	LYS
3	J	430	HIS
3	J	470	VAL
3	J	473	THR
3	J	527	LEU
3	J	744	ARG
3	J	751	ASP
3	J	800	LEU
3	J	807	LEU
3	J	847	ASP
3	J	858	VAL
3	J	925	GLU
3	J	928	THR

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Mol	Chain	Res	Type
3	J	960	LEU
3	J	1086	ASN
3	J	1093	THR
3	J	1095	MET
3	J	1121	LEU
3	J	1244	GLN
3	J	1250	ASP
3	J	1261	LEU
3	J	1341	ARG
3	J	1367	GLN
3	J	1368	ASP
4	K	43	ASN
5	L	9	LEU
5	L	36	VAL
5	L	41	ILE
5	L	51	MET
5	L	93	ARG
5	L	102	MET
5	L	124	GLU
5	L	132	CYS
5	L	289	LYS
5	L	384	LEU
5	L	389	SER
5	L	443	ILE
5	L	498	LEU
5	L	502	LYS
5	L	504	PRO
5	L	507	MET
5	L	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	147	GLN
1	H	227	GLN
2	I	36	GLN
2	I	150	HIS
2	I	450	ASN
2	I	1256	GLN
2	I	1257	GLN
2	I	1336	ASN
3	J	910	ASN

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Mol	Chain	Res	Type
3	J	954	ASN
3	J	979	ASN
3	J	1108	GLN
3	J	1126	GLN
3	J	1350	ASN
4	K	43	ASN
5	L	28	ASN
5	L	82	GLN
5	L	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	4QM	I	1402	-	29,29,30	0.33	0	47,47,48	0.54	0
8	4QM	L	702	-	30,30,30	5.26	15 (50%)	47,48,48	2.51	17 (36%)
8	4QM	I	1401	-	30,30,30	5.27	15 (50%)	47,48,48	2.49	14 (29%)
8	4QM	L	701	-	30,30,30	5.28	15 (50%)	47,48,48	2.67	18 (38%)

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	4QM	I	1402	-	-	0/6/71/72	0/4/4/4
8	4QM	L	702	-	-	7/7/72/72	0/4/4/4
8	4QM	I	1401	-	-	4/7/72/72	0/4/4/4
8	4QM	L	701	-	-	2/7/72/72	0/4/4/4

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	701	4QM	C3-C19	18.04	1.82	1.53
8	I	1401	4QM	C3-C19	17.95	1.82	1.53
8	L	702	4QM	C3-C19	17.91	1.82	1.53
8	I	1401	4QM	C3-C4	12.38	1.73	1.53
8	L	702	4QM	C3-C4	12.34	1.73	1.53
8	L	701	4QM	C3-C4	12.27	1.73	1.53
8	I	1401	4QM	C5-C4	-9.71	1.39	1.54
8	L	702	4QM	C5-C4	-9.61	1.39	1.54
8	L	701	4QM	C2-C19	-9.48	1.39	1.56
8	L	701	4QM	C5-C4	-9.47	1.40	1.54
8	I	1401	4QM	C2-C19	-9.42	1.39	1.56
8	L	702	4QM	C2-C19	-9.29	1.39	1.56
8	I	1401	4QM	C8-C7	6.23	1.71	1.54
8	L	701	4QM	C8-C7	6.20	1.70	1.54
8	L	702	4QM	C8-C7	6.17	1.70	1.54
8	L	701	4QM	C5-C6	-5.05	1.47	1.55
8	L	702	4QM	C5-C6	-4.90	1.47	1.55
8	L	701	4QM	C18-C6	-4.84	1.44	1.53
8	I	1401	4QM	C5-C6	-4.83	1.47	1.55
8	L	702	4QM	C18-C6	-4.73	1.44	1.53
8	I	1401	4QM	C18-C6	-4.61	1.45	1.53
8	L	702	4QM	O4-C4	-4.23	1.36	1.43
8	L	701	4QM	O4-C4	-4.21	1.36	1.43
8	I	1401	4QM	O4-C4	-4.16	1.36	1.43
8	I	1401	4QM	C7-C6	3.39	1.61	1.54
8	L	702	4QM	C14-C15	-3.35	1.48	1.53
8	L	702	4QM	C7-C6	3.29	1.61	1.54
8	I	1401	4QM	C14-C15	-3.29	1.48	1.53
8	L	701	4QM	C14-C15	-3.26	1.48	1.53
8	L	701	4QM	C7-C6	3.22	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1401	4QM	C20-C9	-3.08	1.49	1.54
8	L	702	4QM	C20-C9	-2.94	1.49	1.54
8	L	701	4QM	C20-C9	-2.92	1.49	1.54
8	L	701	4QM	C2-C15	2.81	1.59	1.55
8	L	701	4QM	C5-C9	2.61	1.59	1.55
8	L	702	4QM	C2-C15	2.59	1.59	1.55
8	I	1401	4QM	C5-C9	2.50	1.59	1.55
8	L	702	4QM	C14-C13	2.44	1.56	1.52
8	I	1401	4QM	C14-C13	2.42	1.56	1.52
8	L	701	4QM	C14-C13	2.38	1.56	1.52
8	L	702	4QM	C5-C9	2.37	1.59	1.55
8	L	701	4QM	O2-C13	-2.32	1.36	1.43
8	L	702	4QM	O2-C13	-2.27	1.36	1.43
8	I	1401	4QM	C2-C15	2.27	1.58	1.55
8	I	1401	4QM	O2-C13	-2.21	1.36	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	702	4QM	C9-C5-C4	-8.59	109.94	117.67
8	L	701	4QM	C9-C5-C4	-8.12	110.36	117.67
8	I	1401	4QM	C9-C5-C4	-7.94	110.52	117.67
8	L	701	4QM	C7-C6-C18	-6.32	109.69	118.36
8	L	702	4QM	C7-C6-C18	-5.76	110.45	118.36
8	L	702	4QM	C5-C9-C20	-5.63	112.66	119.48
8	I	1401	4QM	C7-C6-C18	-5.49	110.83	118.36
8	L	701	4QM	C5-C9-C20	-5.17	113.22	119.48
8	I	1401	4QM	C19-C3-C4	-5.06	107.67	114.29
8	I	1401	4QM	C5-C9-C20	-4.99	113.44	119.48
8	L	702	4QM	C6-C5-C4	4.74	111.75	107.42
8	L	701	4QM	C9-C5-C6	4.64	104.77	100.11
8	I	1401	4QM	C6-C5-C4	4.37	111.41	107.42
8	L	701	4QM	C19-C18-C17	-4.26	106.49	111.86
8	L	701	4QM	C2-C19-C18	-4.20	107.16	111.84
8	L	702	4QM	C19-C3-C4	-4.18	108.83	114.29
8	I	1401	4QM	C14-C15-C2	-4.09	108.31	112.66
8	L	701	4QM	C6-C5-C4	3.89	110.97	107.42
8	L	701	4QM	C19-C3-C4	-3.69	109.46	114.29
8	I	1401	4QM	C16-C15-C2	-3.62	108.81	112.66
8	I	1401	4QM	C7-C6-C5	3.53	106.96	103.54
8	L	701	4QM	C7-C6-C5	3.51	106.94	103.54
8	L	702	4QM	C9-C5-C6	3.46	103.58	100.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	702	4QM	C14-C15-C2	-3.41	109.03	112.66
8	L	701	4QM	C8-C9-C5	3.38	106.82	103.54
8	L	701	4QM	C16-C15-C2	-3.20	109.26	112.66
8	L	701	4QM	C3-C19-C2	-3.15	110.50	113.70
8	I	1401	4QM	C6-C18-C17	-3.04	107.81	111.85
8	I	1401	4QM	C8-C9-C5	2.90	106.36	103.54
8	L	702	4QM	C8-C9-C5	2.86	106.32	103.54
8	L	702	4QM	C16-C15-C2	-2.81	109.67	112.66
8	L	702	4QM	C2-C19-C18	-2.75	108.77	111.84
8	L	701	4QM	C5-C6-C18	-2.70	111.29	114.72
8	L	702	4QM	C21-C20-C9	-2.66	108.89	112.88
8	L	702	4QM	C3-C19-C2	-2.66	111.01	113.70
8	L	701	4QM	C14-C15-C2	-2.60	109.89	112.66
8	I	1401	4QM	C9-C5-C6	2.58	102.70	100.11
8	I	1401	4QM	C15-C16-C17	-2.57	111.34	114.40
8	I	1401	4QM	C21-C20-C9	-2.57	109.03	112.88
8	L	702	4QM	C6-C18-C17	-2.56	108.45	111.85
8	L	702	4QM	C7-C6-C5	2.50	105.96	103.54
8	L	701	4QM	C15-C16-C17	-2.42	111.52	114.40
8	L	701	4QM	C6-C18-C17	-2.42	108.64	111.85
8	L	701	4QM	C12-C1-C2	-2.27	108.90	112.74
8	I	1401	4QM	C3-C19-C18	-2.22	107.62	110.89
8	L	702	4QM	C19-C18-C17	-2.16	109.14	111.86
8	L	701	4QM	C1-C2-C15	2.13	110.80	107.75
8	L	702	4QM	C15-C16-C17	-2.05	111.96	114.40
8	L	702	4QM	C15-C14-C13	-2.01	109.67	112.71

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	702	4QM	C21-C20-C22-C23
8	L	702	4QM	C21-C20-C9-C5
8	L	702	4QM	C9-C20-C22-C23
8	L	702	4QM	C20-C22-C23-C24
8	L	701	4QM	C20-C22-C23-C24
8	L	702	4QM	C21-C20-C9-C8
8	L	702	4QM	C22-C20-C9-C5
8	I	1401	4QM	C21-C20-C9-C5
8	I	1401	4QM	C21-C20-C9-C8
8	L	702	4QM	C22-C20-C9-C8
8	I	1401	4QM	C22-C20-C9-C5

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Mol	Chain	Res	Type	Atoms
8	I	1401	4QM	C22-C20-C9-C8
8	L	701	4QM	C21-C20-C9-C5

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	702	4QM	4	0
8	I	1401	4QM	5	0
8	L	701	4QM	7	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 4QM L 702

Bond lengths

Bond angles

Torsions

Rings

Ligand 4QM I 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand 4QM L 701

Bond lengths

Bond angles

Torsions

Rings
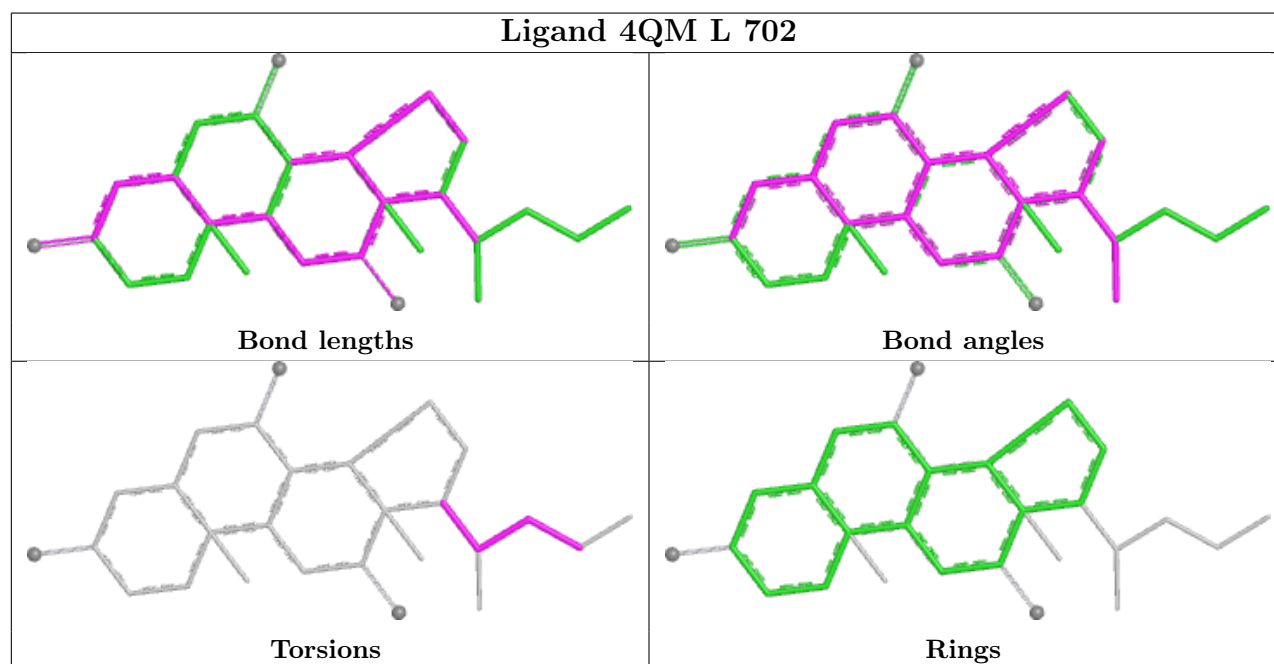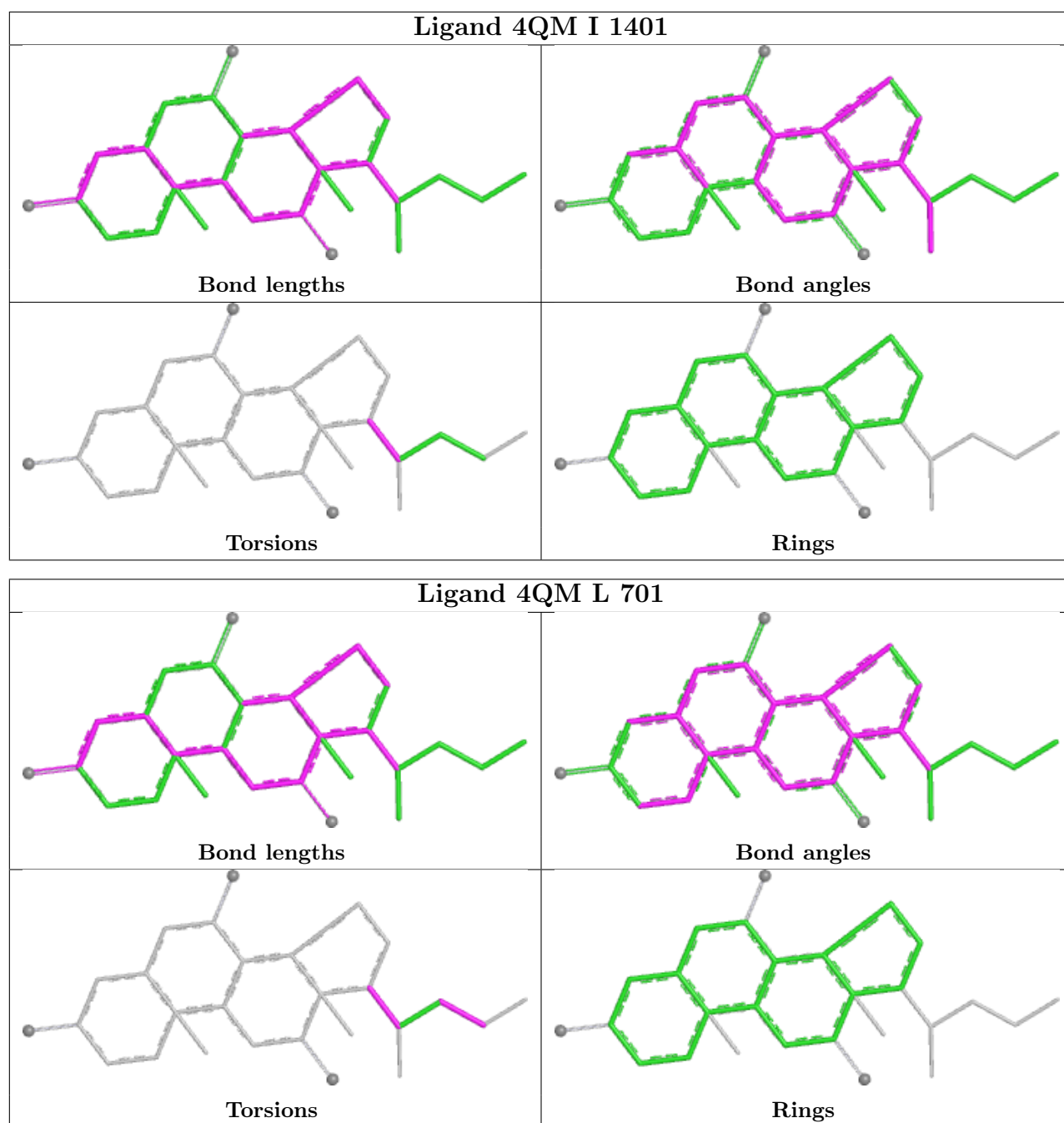
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	427:PHE	C	428:SER	N	1.61

6　Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-41433. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1　Orthogonal projections ⓘ
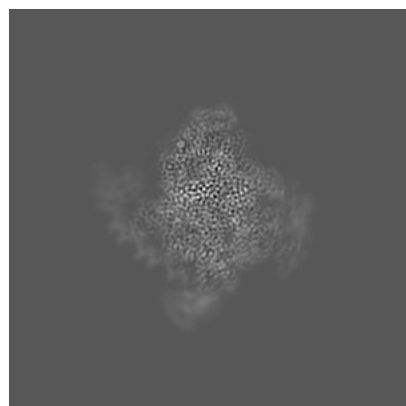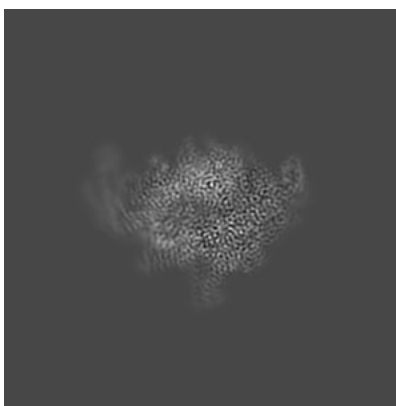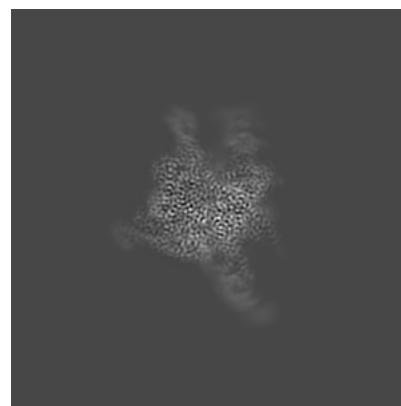
6.1.1　Primary map

| X | Y | Z |

6.1.2　Raw map

| X | Y | Z |
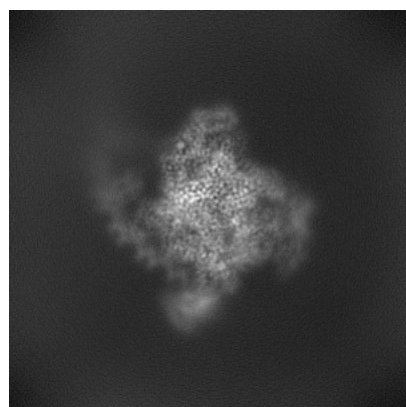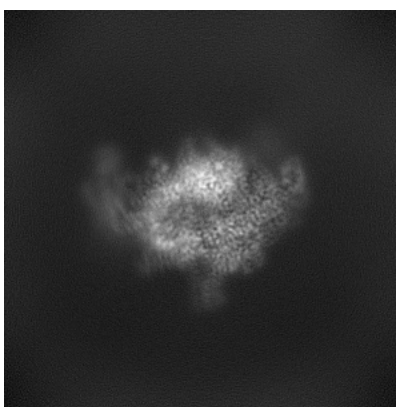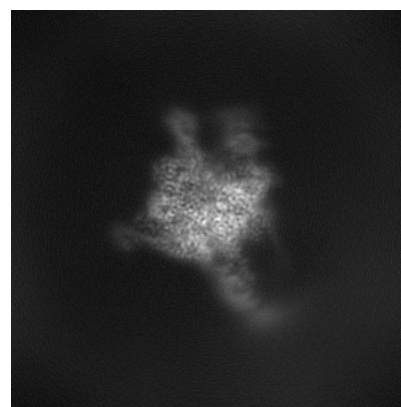
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
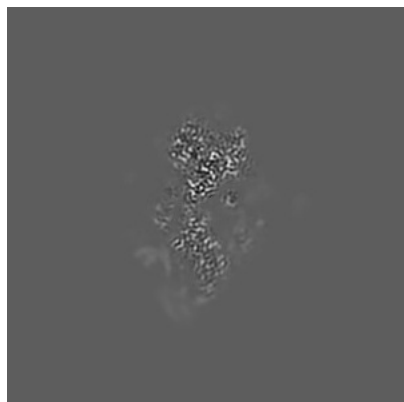
6.2.1 Primary map
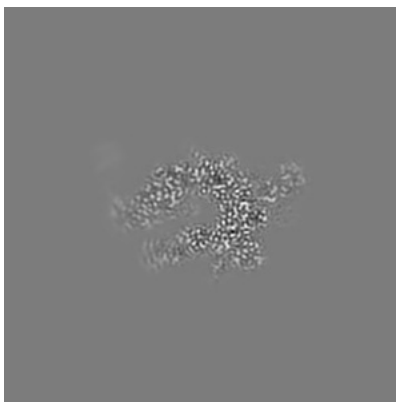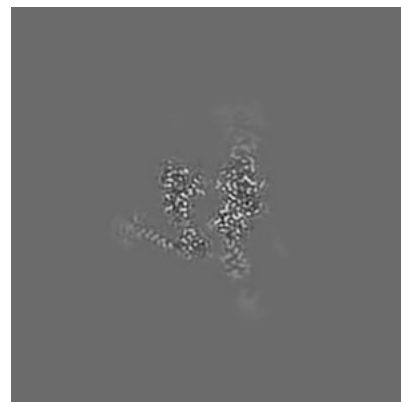
X Index: 192	Y Index: 192	Z Index: 192

6.2.2 Raw map
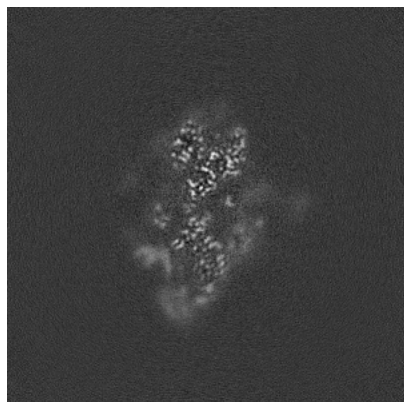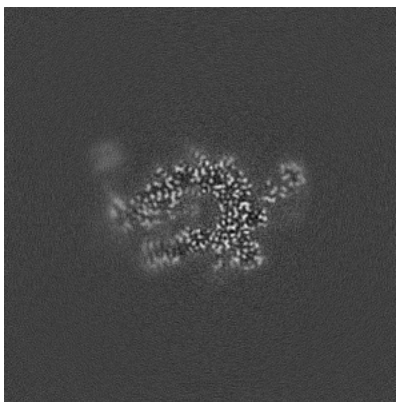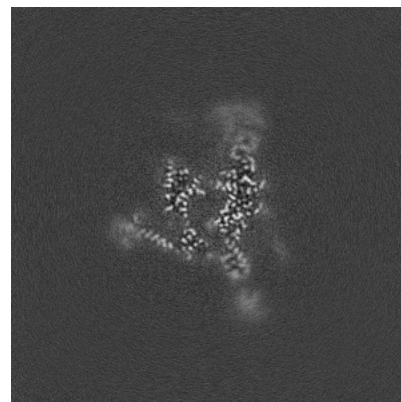
X Index: 192	Y Index: 192	Z Index: 192

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

X Index: 209   Y Index: 197   Z Index: 206
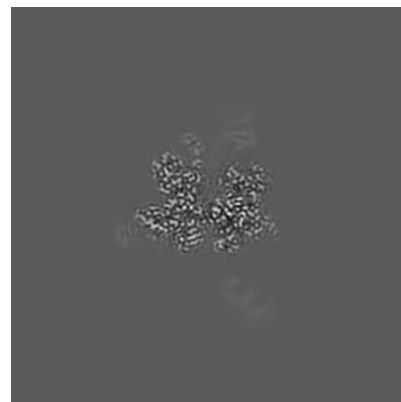
6.3.2 Raw map
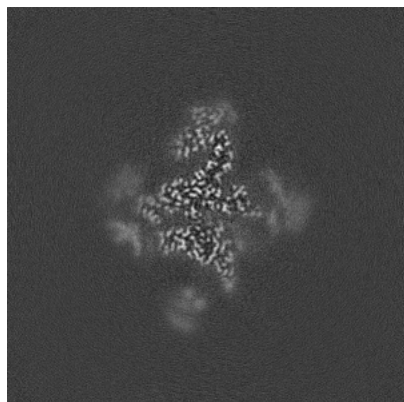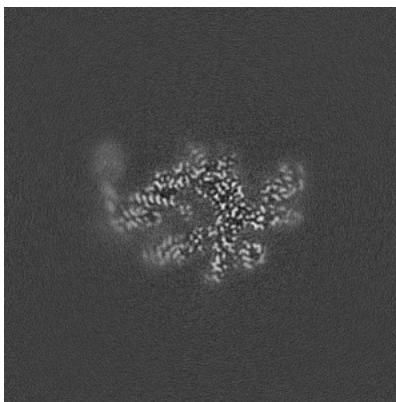
X Index: 210   Y Index: 186   Z Index: 206
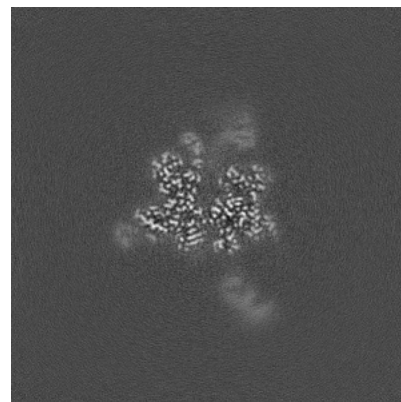
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
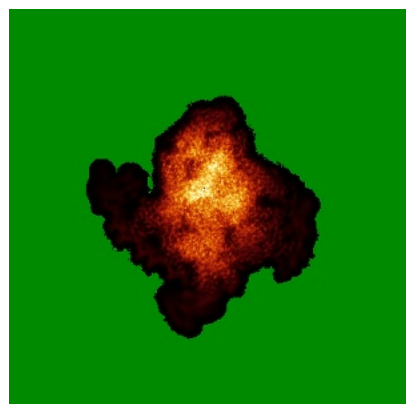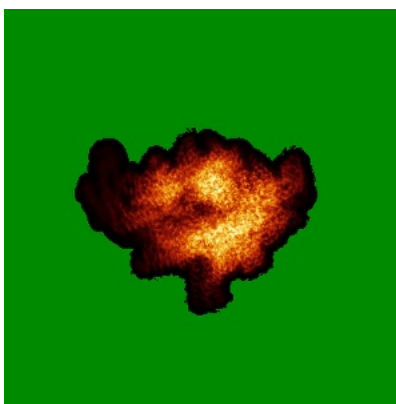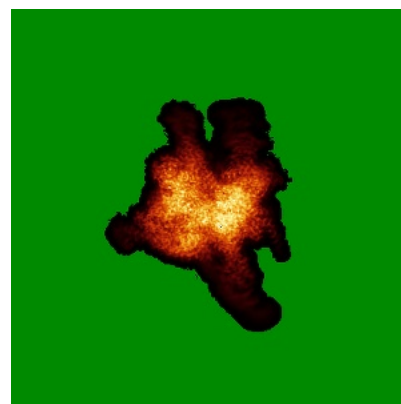
| X | Y | Z |

6.4.2 Raw map

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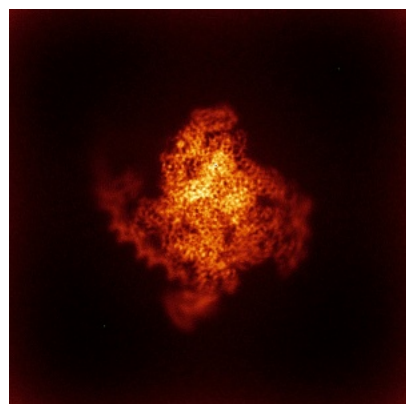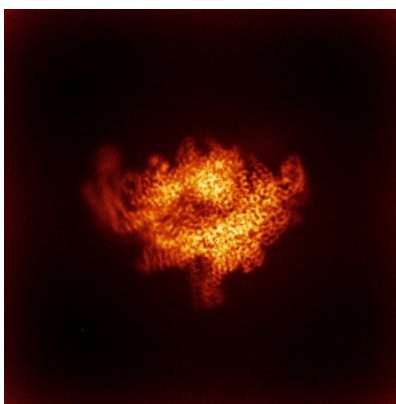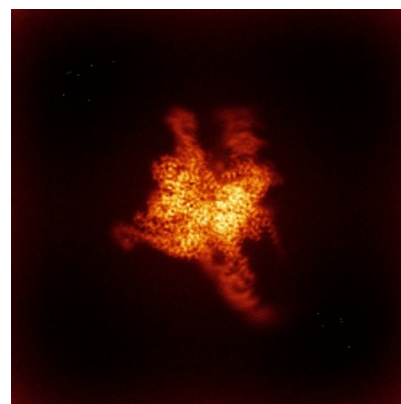
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
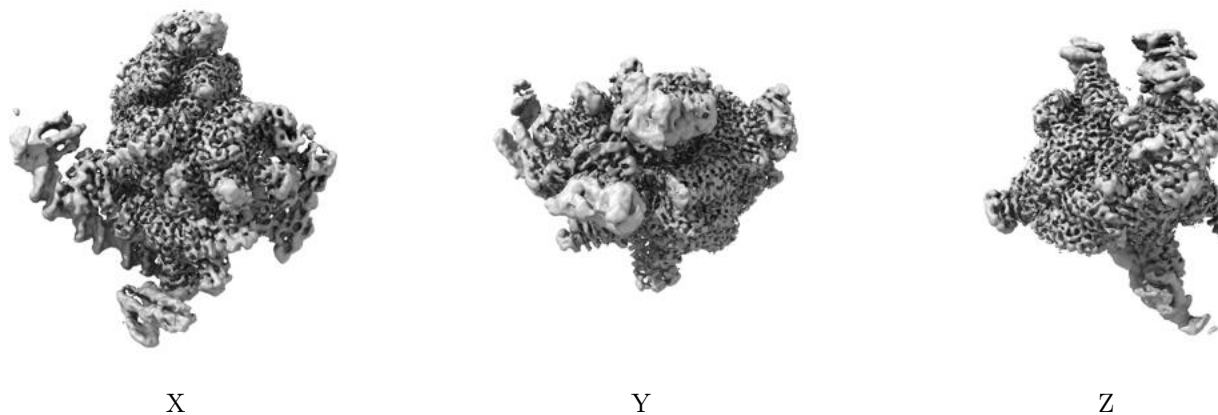
The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X   Y   Z
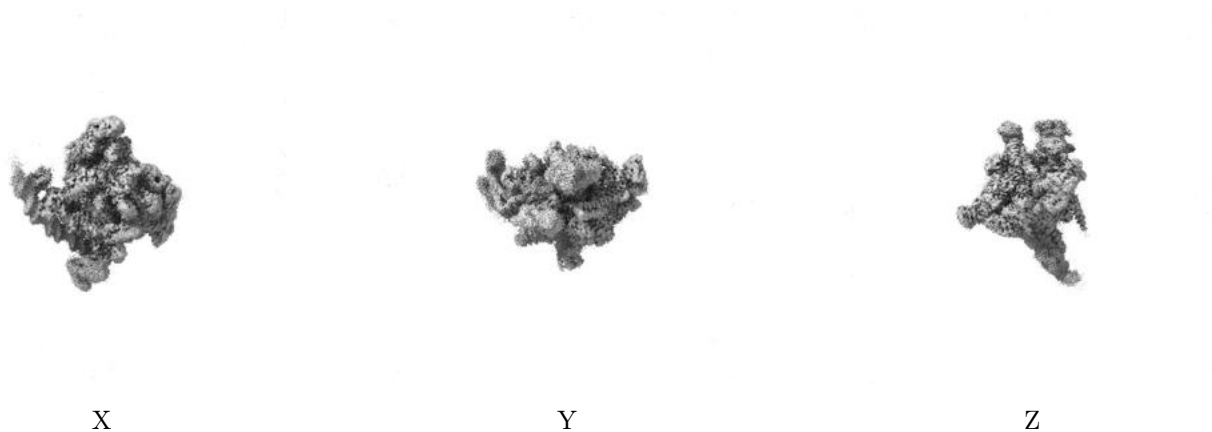
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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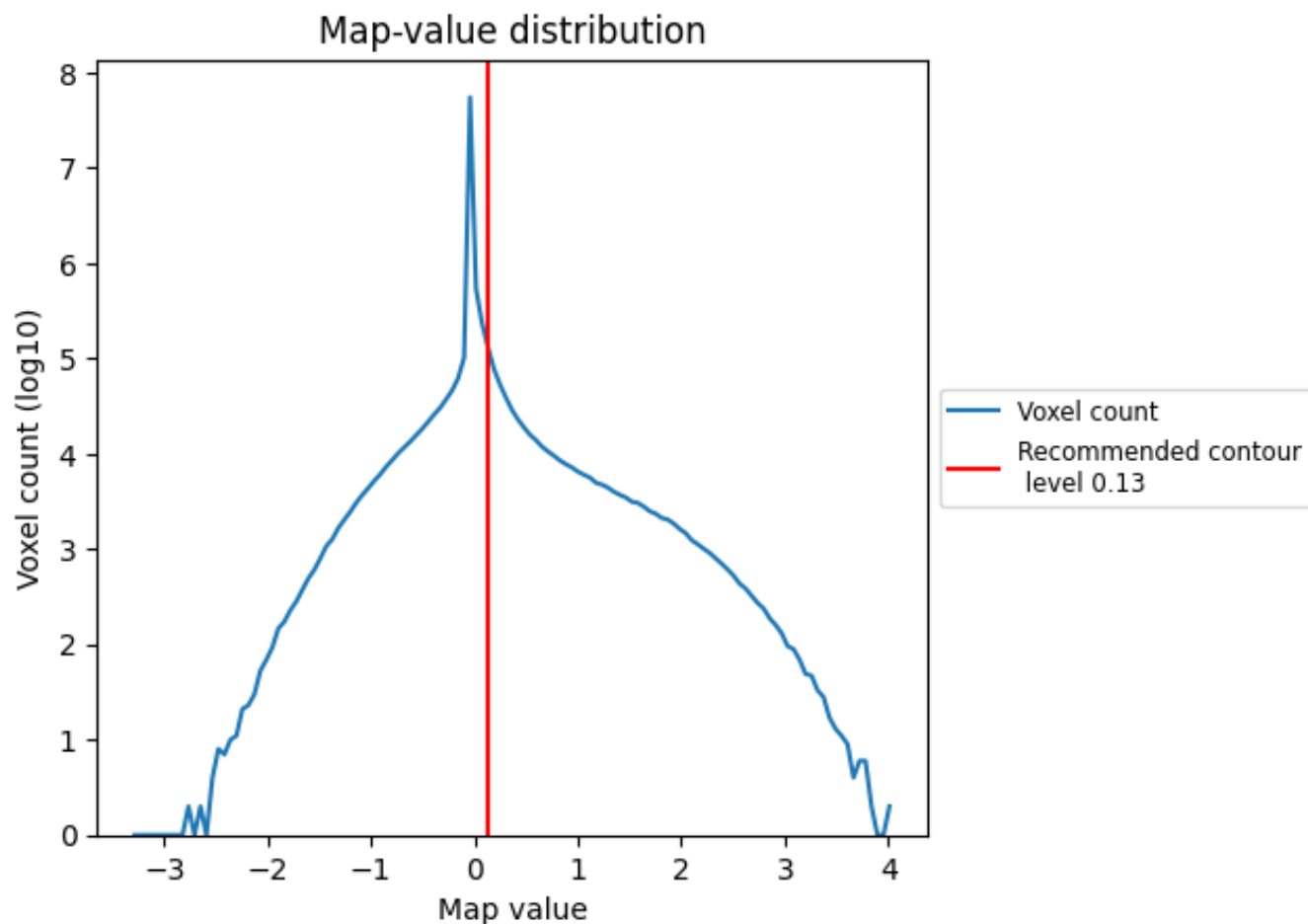
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
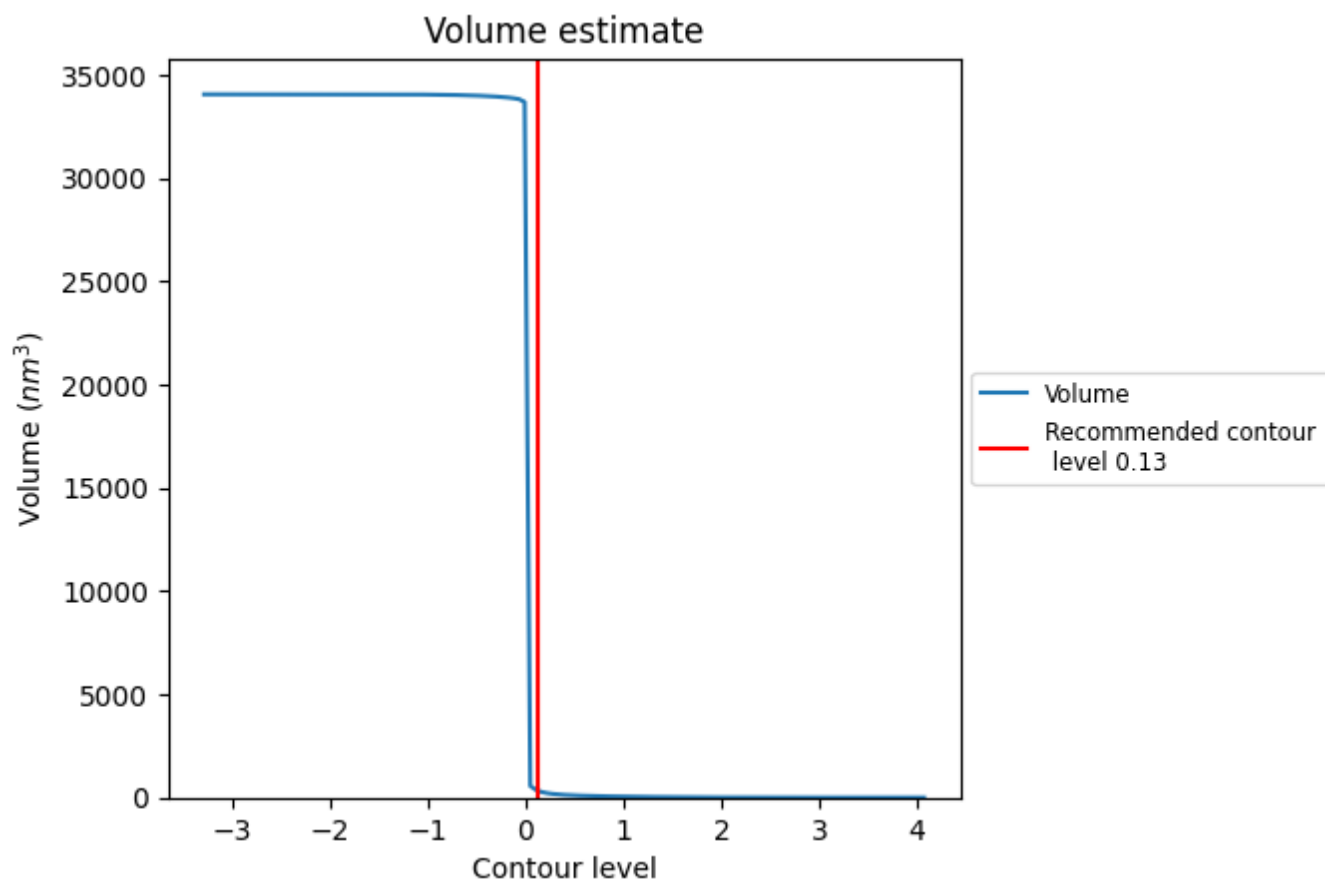
The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 298 kDa.

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 ⓘ
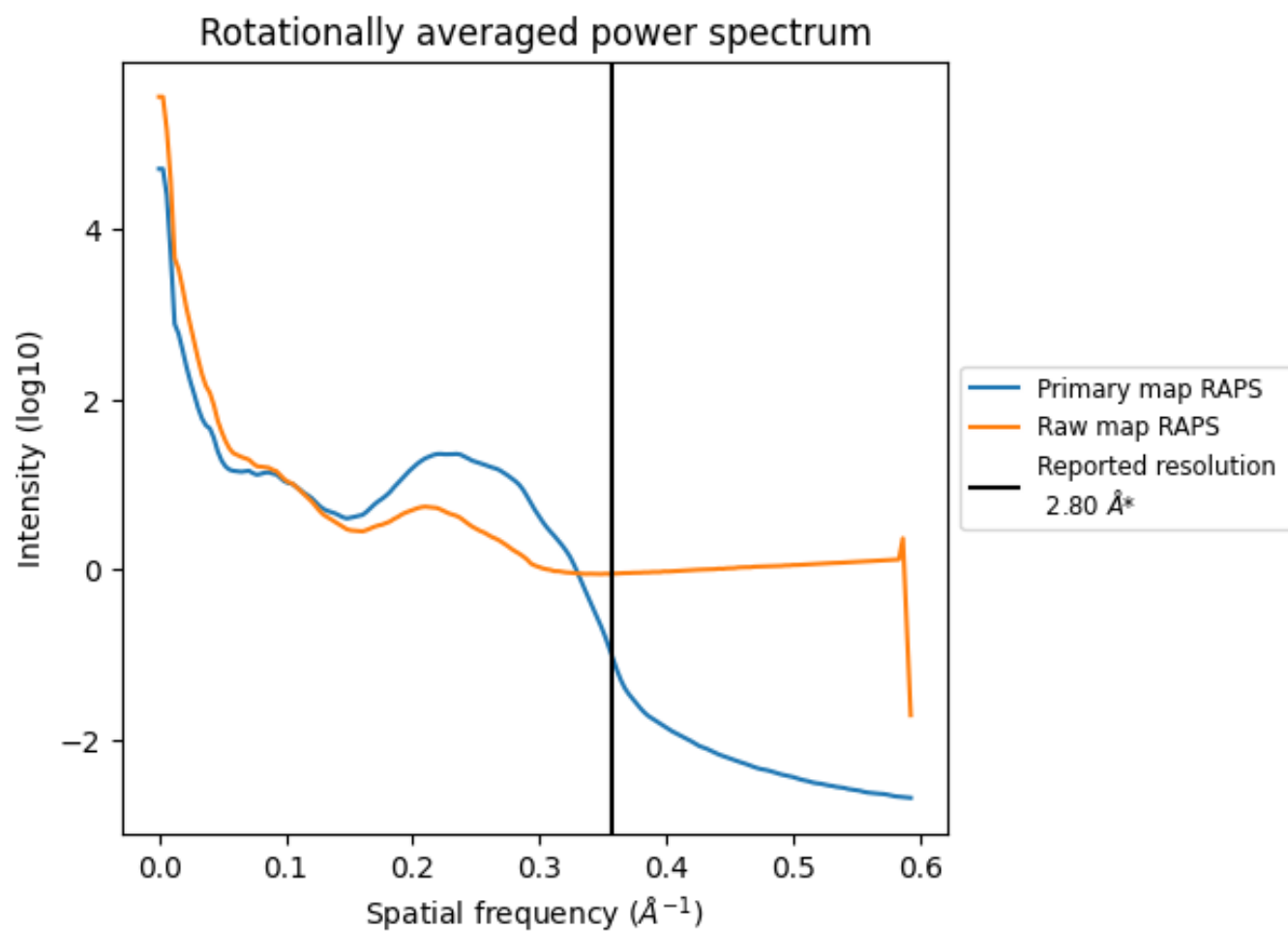
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ
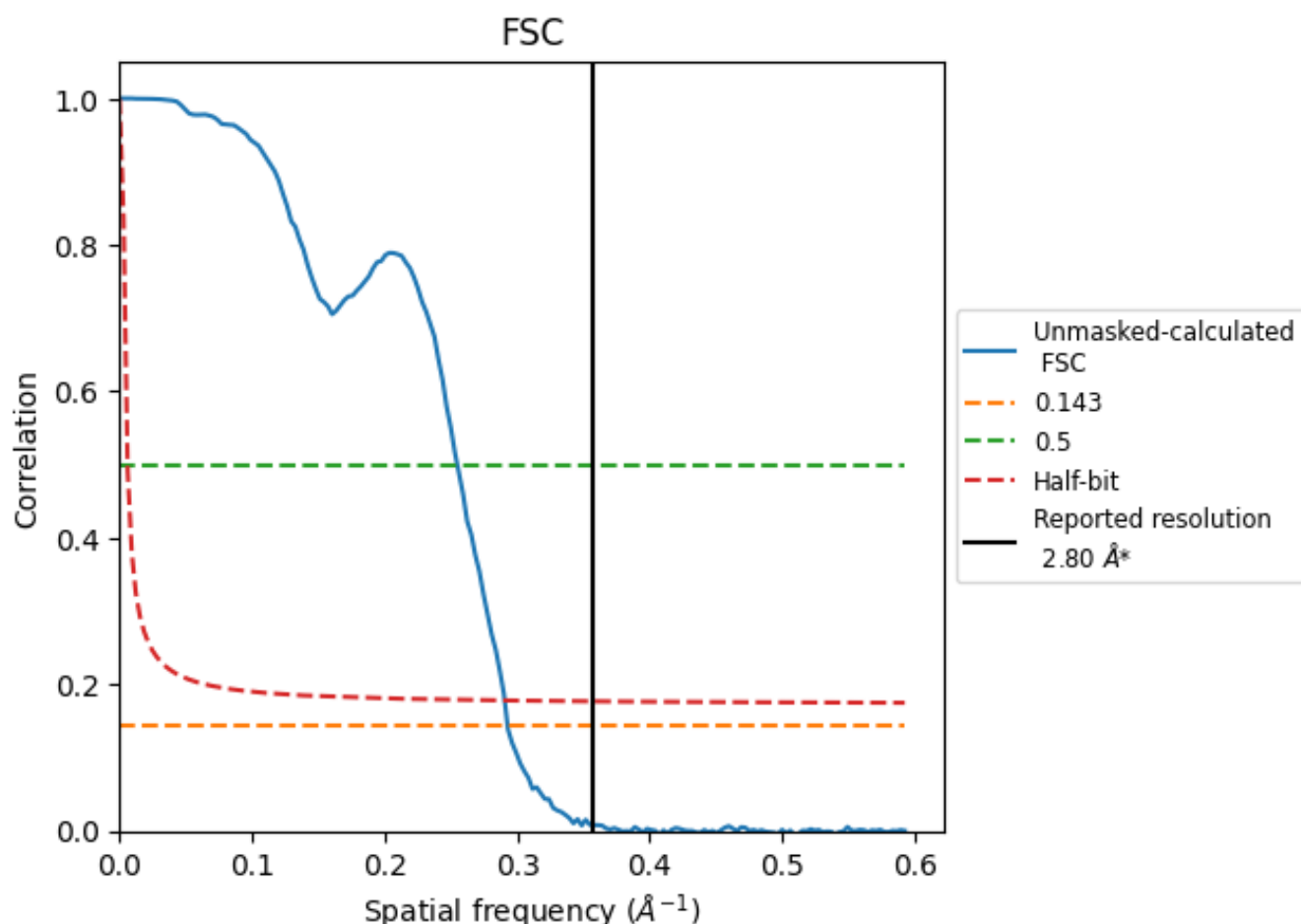
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2　Resolution estimates　ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	3.92	3.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.8 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-41433 and PDB model 8TO1. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

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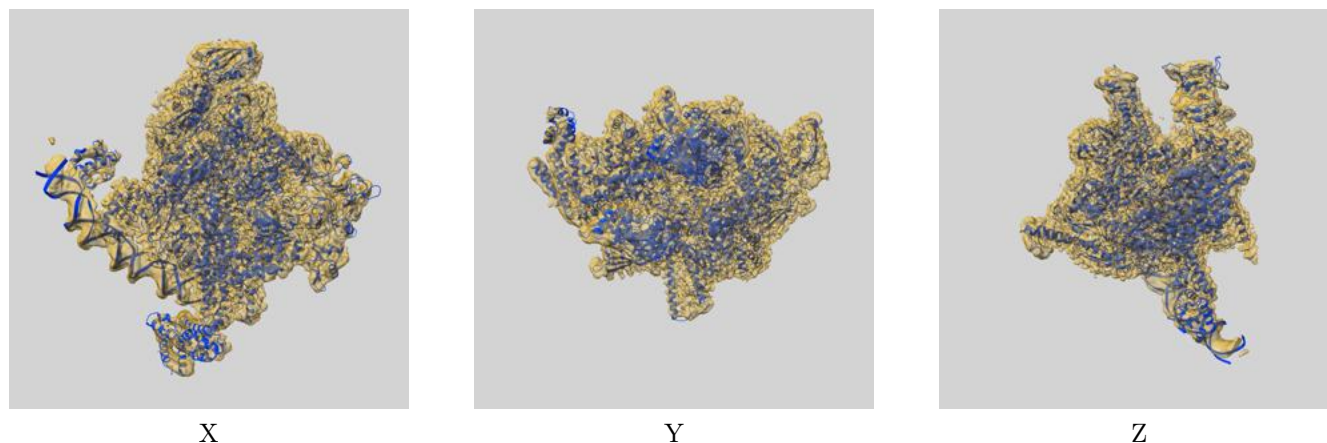
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　　　Y　　　　　　　　　　　　Z
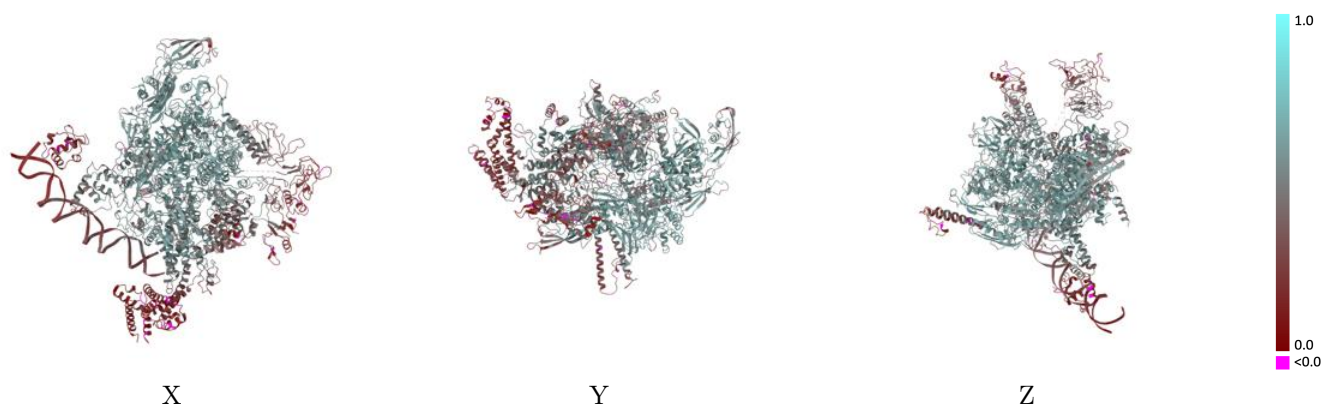
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
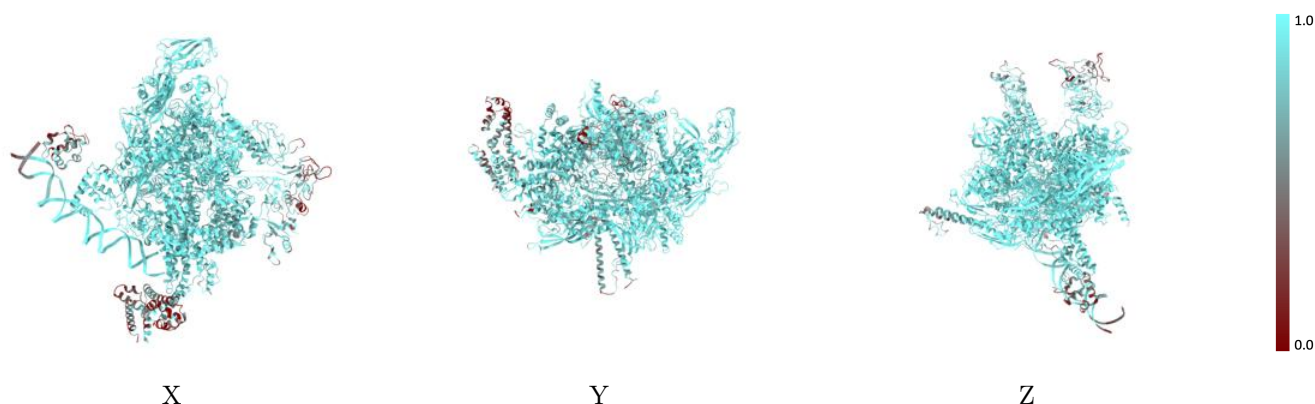
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion ⓘ
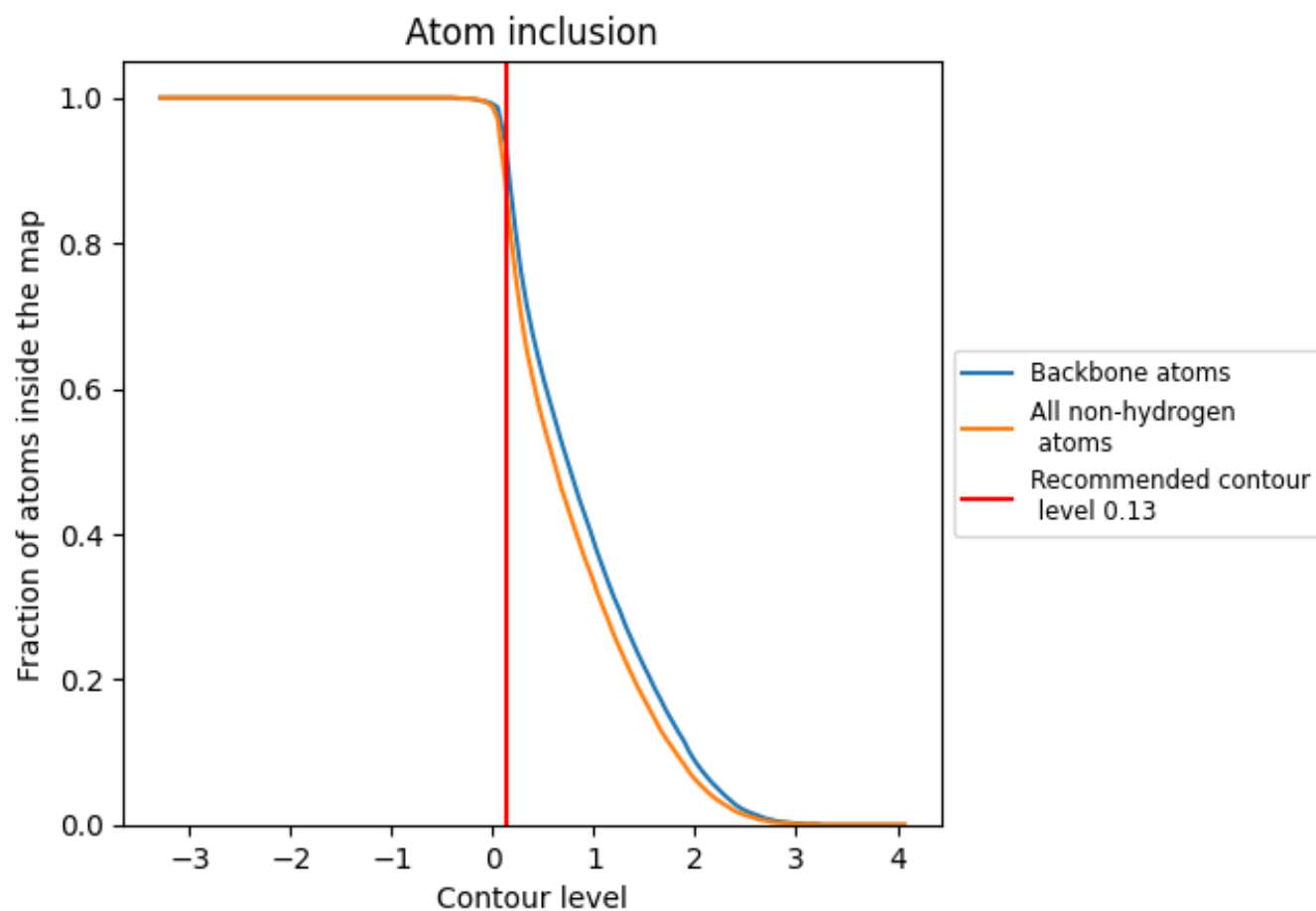
At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.4770
G	0.9590	0.5720
H	0.9380	0.5330
I	0.9160	0.5140
J	0.8990	0.5160
K	0.9330	0.5520
L	0.7360	0.3350
M	0.4860	0.1810
O	0.8570	0.2780
P	0.8660	0.2500

1.0

0.0
<0.0