Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 05:14 PM JST

PDB ID	:	5ZX5
EMDB ID	:	EMD-6975
Title	:	3.3 angstrom structure of mouse TRPM7 with EDTA
Authors	:	Zhang, J.; Li, Z.; Duan, J.; Li, J.; Hulse, R.E.; Santa-Cruz, A.; Abiria, S.A.; Krapivinsky, G.; Clapham, D.E.
Deposited on	:	2018-05-18
Resolution	:	3.28 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 (i) 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 (1)) were used in the production of this report:

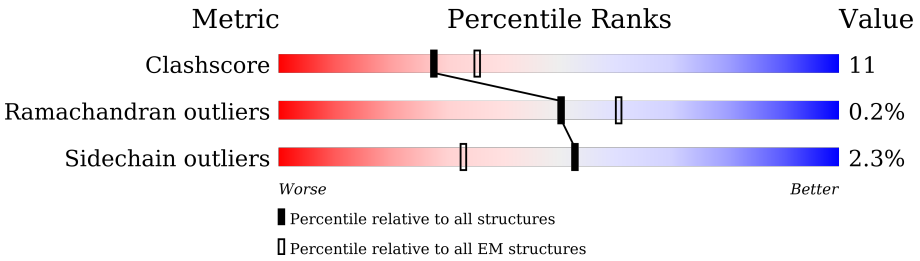
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.28 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	1229	56% 10% • 34%
1	B	1229	55% 10% • 34%
1	C	1229	56% 10% • 34%
1	D	1229	56% 9% • 34%

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
2	Y01	A	1305	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	D	1303	-	-	X	-

2 Entry composition (i)

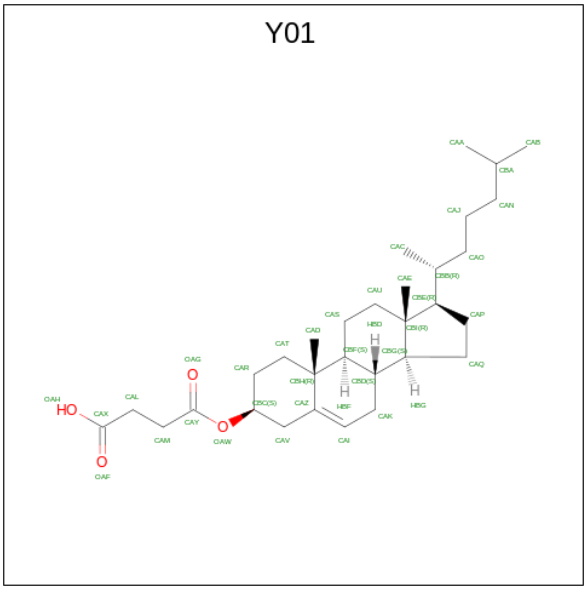
There are 2 unique types of molecules in this entry. The entry contains 25440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	814	6255	4095	1032	1087	41	0	0
1	B	814	6255	4095	1032	1087	41	0	0
1	C	814	6255	4095	1032	1087	41	0	0
1	D	814	6255	4095	1032	1087	41	0	0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	35	31	4	0
2	A	1	35	31	4	0

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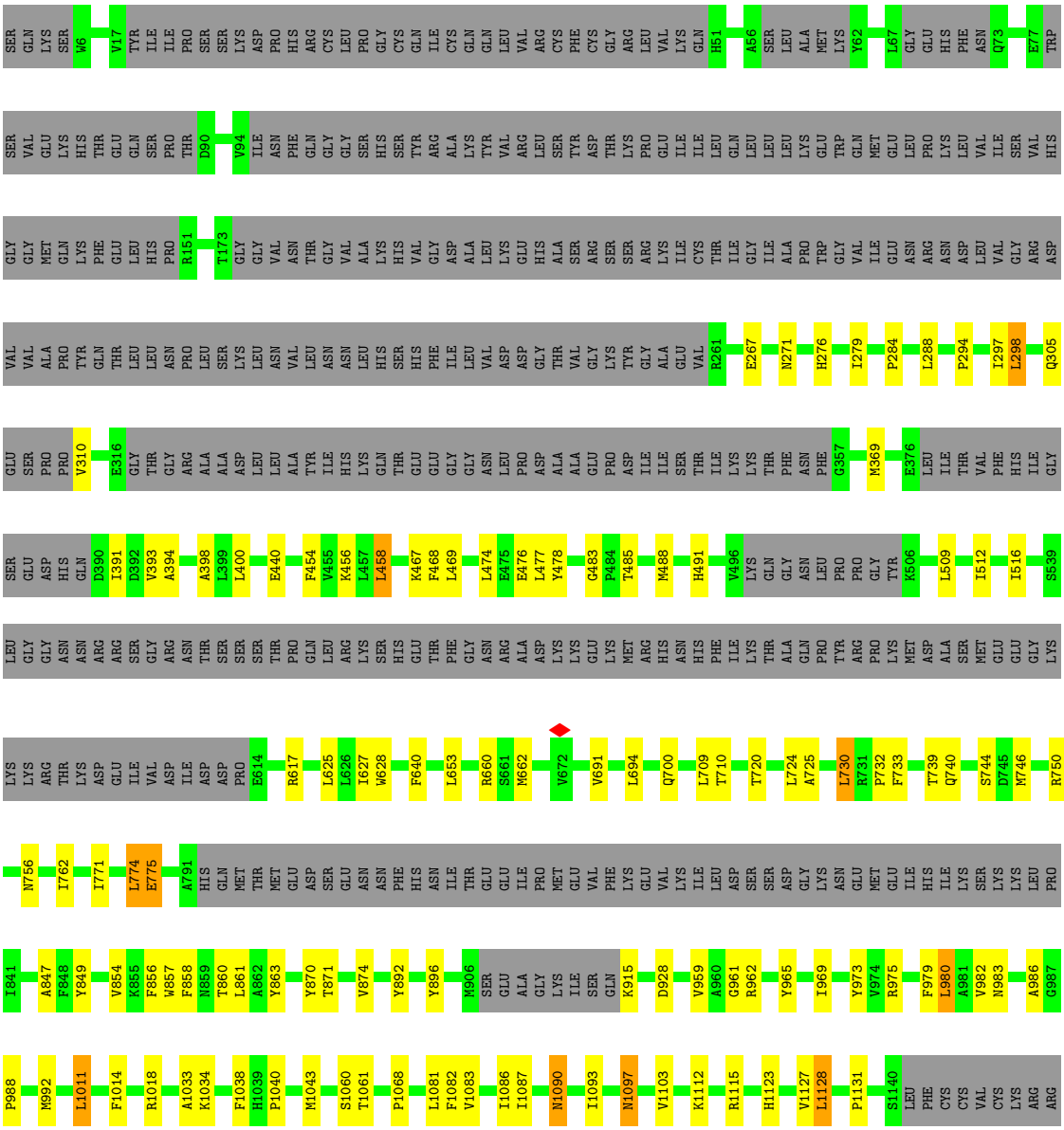
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	A	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0
			Total	C	O	
2	B	1	35	31	4	0
			Total	C	O	
2	C	1	35	31	4	0
			Total	C	O	
2	C	1	35	31	4	0
			Total	C	O	
2	D	1	35	31	4	0
			Total	C	O	
2	D	1	35	31	4	0
			Total	C	O	
2	D	1	35	31	4	0

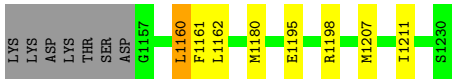
3 Residue-property plots (i)

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: Transient receptor potential cation channel subfamily M member 7

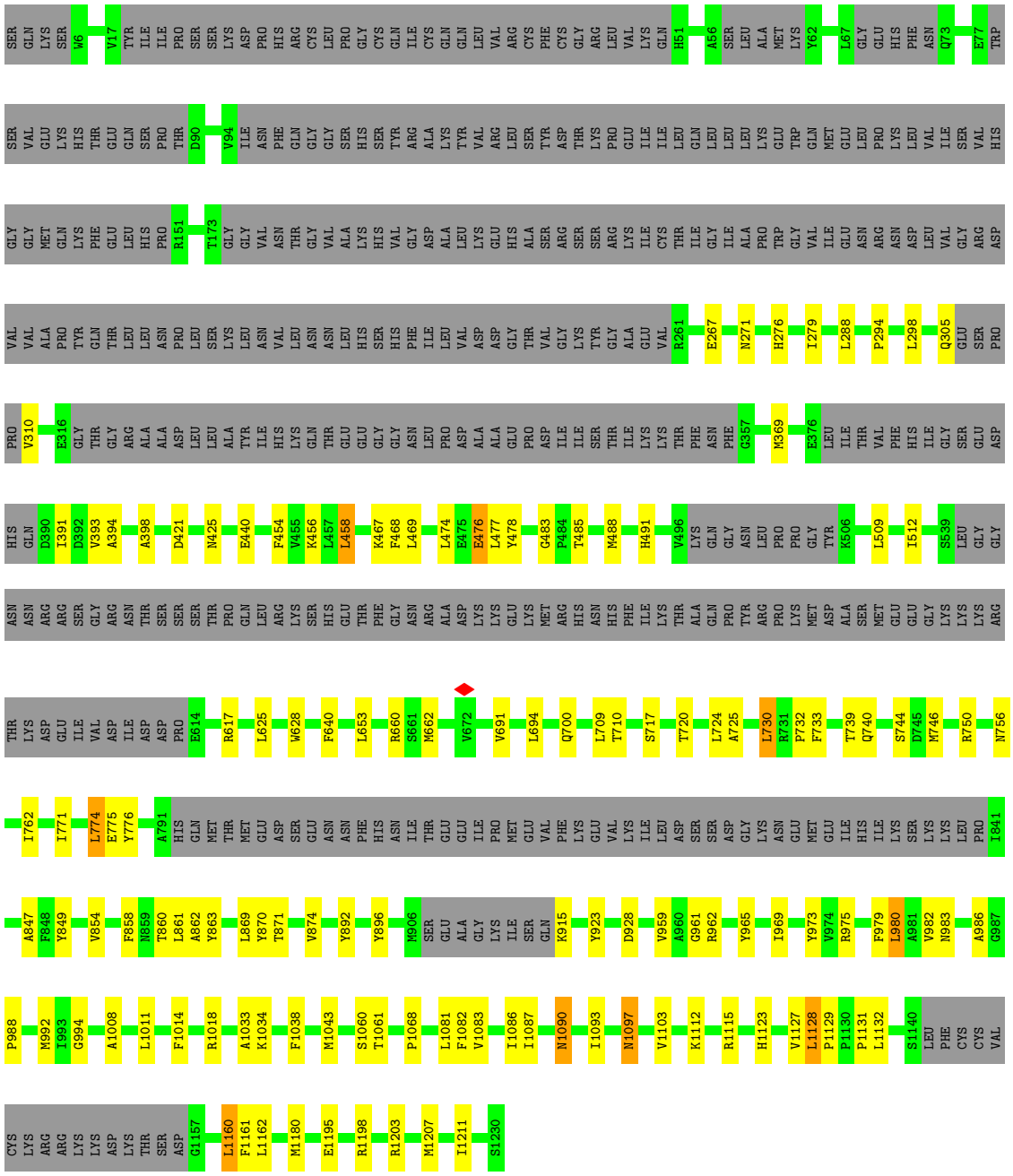
Chain A: 56% 10% • 34%





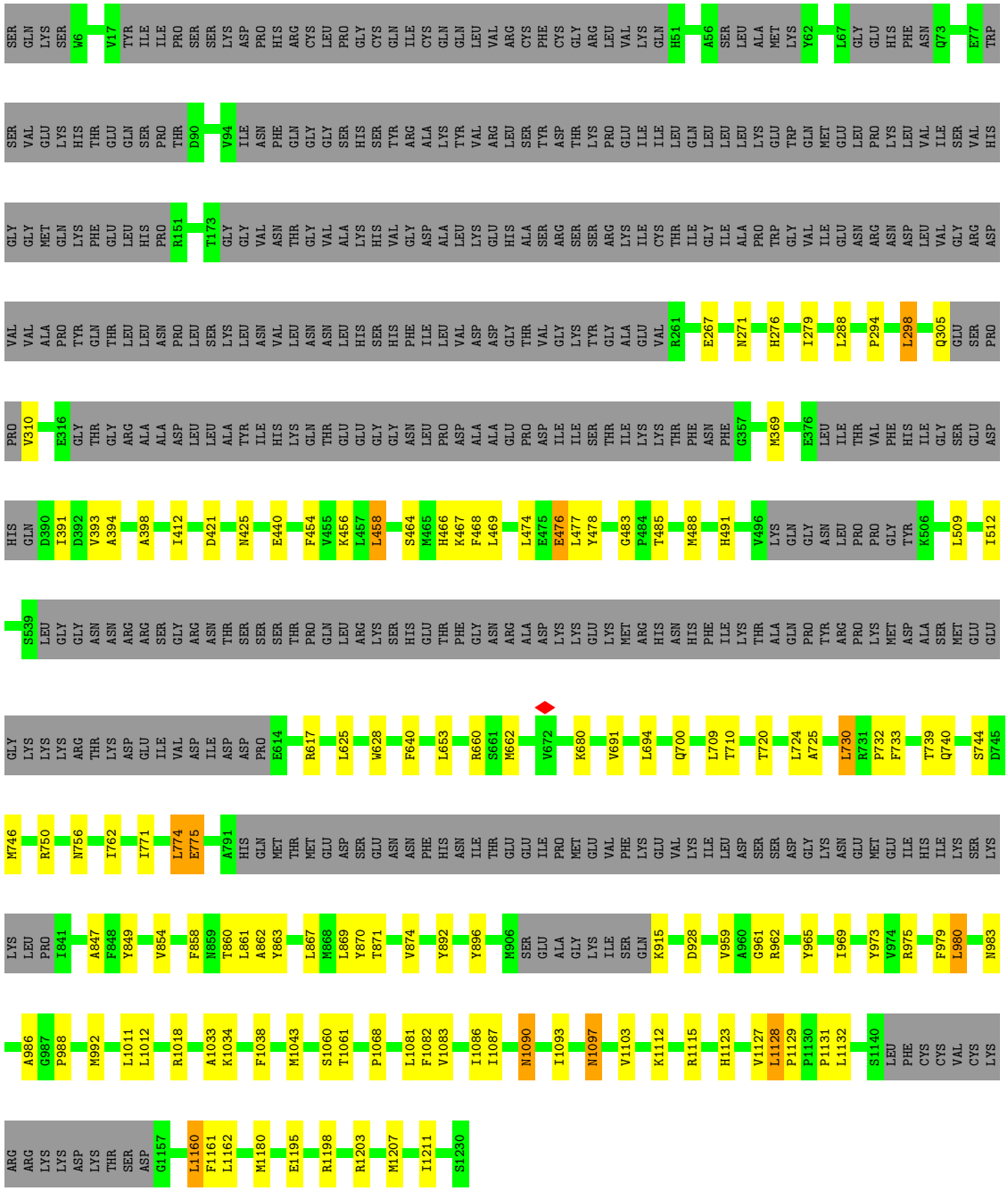
• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain B: 55% 10% • 34%



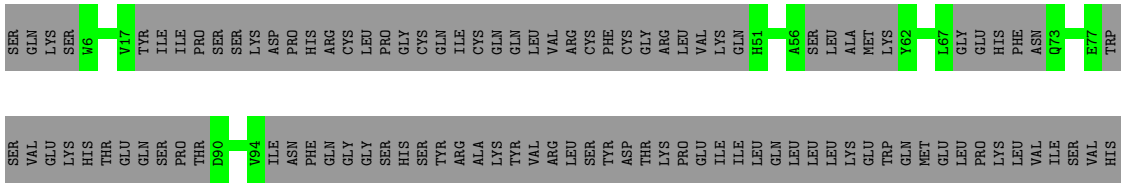
• Molecule 1: Transient receptor potential cation channel subfamily M member 7

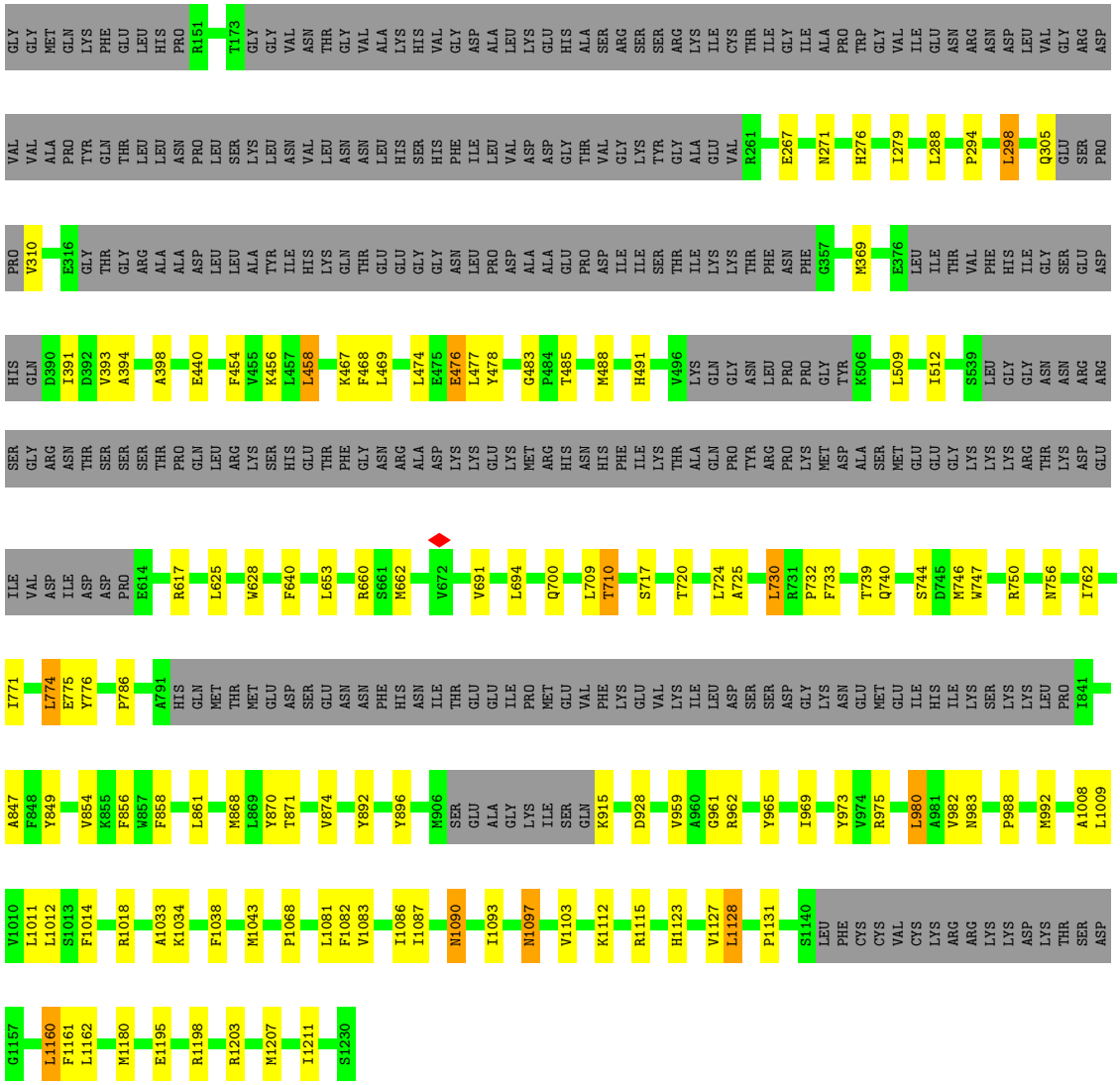
Chain C: 56% 10% • 34%



• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain D: 56% 9% • 34%




GLY GLY MET GLN LYS PHE GLU LEU HIS PRO R151 T173 GLY GLY VAL ASN THR GLY VAL ALA LYS HIS VAL GLY ASP ALA LEU LYS GLU HIS ALA SER ARG SER SER ARG LYS ILE CYS THR ILE GLY ILE ALA PRO TRP GLY VAL ILE GLU ASN ARG ASN ASP LEU VAL GLY ARG ASP
VAL VAL ALA PRO TYR GLN THR LEU LEU ASN PRO LEU SER LYS LEU ASN VAL LEU ASN ASN LEU HIS SER HIS PHE ILE LEU VAL ASP ASP GLY THR VAL GLY LYS TYR GLY ALA GLU VAL R261 E267 N271 H276 I279 L288 P294 L298 Q305 GLU SER PRO
PRO V310 E316 GLY THR GLY ARG ALA ALA ASP LEU LEU ALA TYR ILE HIS LYS GLN THR GLU GLU GLY GLY ASN LEU PRO ASP ALA ALA GLU PRO ASP ILE ILE SER THR ILE LYS LYS THR PHE ASN PHE G357 M369 E376 LEU ILE THR VAL PHE HIS ILE GLY SER GLU ASP
HIS GLN D390 I391 D392 V393 A394 A398 E440 F454 V455 K456 L457 L458 K467 F468 L469 L474 E475 E476 L477 Y478 G483 P484 T485 M488 H491 V496 LYS GLN GLY ASN LEU PRO PRO GLY TYR K506 L509 I512 S539 LEU GLY GLY ASN ASN ARG ARG
SER GLY ARG ASN THR SER SER SER THR PRO GLN LEU ARG LYS SER HIS GLU THR PHE GLY ASN ARG ALA ASP LYS LYS GLU LYS MET ARG HIS ASN HIS PHE ILE LYS THR ALA GLN PRO TYR ARG PRO LYS MET ASP ALA SER MET GLU GLU GLY LYS LYS LYS ARG THR LYS ASP GLU
ILE VAL ASP ILE ASP ASP PRO E614 R617 L625 W628 F640 L653 R660 S661 M662 V672 V691 L694 Q700 L709 T710 S717 T720 L724 A725 L730 R731 P732 F733 T739 Q740 S744 D745 M746 W747 R750 N756 I762
I771 L774 E775 Y776 P786 A791 HIS GLN MET THR MET GLU ASP SER GLU ASN ASN PHE HIS ASN ILE THR GLU GLU ILE PRO MET GLU VAL PHE LYS GLU VAL LYS ILE LEU ASP SER SER ASP GLY LYS ASN GLU MET GLU ILE HIS ILE LYS SER LYS LYS LEU PRO I841
A847 F848 Y849 V854 K855 F856 W857 F858 L861 M868 L869 Y870 T871 V874 Y892 Y896 M906 SER GLU ALA GLY LYS ILE SER GLN K915 D928 V959 A960 G961 R962 Y965 I969 Y973 V974 R975 L980 A981 V982 N983 P988 M992 A1008 L1009
V1010 L1011 L1012 S1013 F1014 R1018 A1033 K1034 F1038 M1043 P1068 L1081 F1082 V1083 I1086 I1087 N1090 I1093 N1097 V1103 K1112 R1115 H1123 V1127 L1128 P1131 S1140 LEU PHE CYS CYS VAL CYS LYS ARG ARG LYS LYS ASP LYS THR SER ASP
G1157 L1160 F1161 L1162 M1180 E1195 R1198 R1203 M1207 I1211 S1230

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	1039775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.377	Depositor
Minimum map value	-0.206	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01

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	0.68	0/6390	0.71	1/8683 (0.0%)
1	B	0.69	0/6390	0.71	2/8683 (0.0%)
1	C	0.68	0/6390	0.71	2/8683 (0.0%)
1	D	0.68	0/6390	0.70	2/8683 (0.0%)
All	All	0.68	0/25560	0.71	7/34732 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	476	GLU	N-CA-C	-5.47	96.24	111.00
1	D	476	GLU	N-CA-C	-5.46	96.27	111.00
1	C	476	GLU	N-CA-C	-5.45	96.30	111.00
1	B	298	LEU	CA-CB-CG	-5.37	102.94	115.30
1	C	298	LEU	CA-CB-CG	-5.37	102.94	115.30
1	D	298	LEU	CA-CB-CG	-5.37	102.94	115.30
1	A	298	LEU	N-CA-C	5.31	125.33	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6255	0	6057	142	0
1	B	6255	0	6057	132	0
1	C	6255	0	6057	116	0
1	D	6255	0	6057	125	0
2	A	175	0	245	57	0
2	B	70	0	98	17	0
2	C	70	0	98	13	0
2	D	105	0	147	32	0
All	All	25440	0	24816	536	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 11.

All (536) 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)
1:D:982:VAL:HG23	2:D:1303:Y01:CAB	1.59	1.32
1:B:982:VAL:HG23	2:B:1302:Y01:CAA	1.75	1.16
2:C:1301:Y01:HAA3	2:C:1302:Y01:HAR2	1.16	1.13
2:C:1301:Y01:HAA3	2:C:1302:Y01:CAR	1.82	1.10
1:D:982:VAL:HG23	2:D:1303:Y01:HAB1	1.31	1.08
1:A:298:LEU:HD12	1:A:400:LEU:HD11	1.32	1.08
1:A:298:LEU:CD1	1:A:400:LEU:HD11	1.85	1.06
1:A:982:VAL:CG2	2:A:1305:Y01:HAB2	1.83	1.06
2:A:1305:Y01:HAE2	2:A:1305:Y01:HAO2	1.38	1.05
1:B:982:VAL:HG23	2:B:1302:Y01:HAA2	1.42	1.01
2:D:1302:Y01:HAA3	2:D:1303:Y01:CAR	1.89	1.01
1:D:856:PHE:HE2	2:D:1303:Y01:HAC3	1.29	0.97
1:D:856:PHE:CE2	2:D:1303:Y01:HAC3	2.02	0.95
1:D:982:VAL:CG2	2:D:1303:Y01:CAB	2.45	0.94
1:A:982:VAL:CG2	2:A:1305:Y01:CAB	2.46	0.93
1:C:694:LEU:CD1	1:C:709:LEU:HD21	1.99	0.92
1:B:694:LEU:CD1	1:B:709:LEU:HD21	1.99	0.92
1:A:694:LEU:CD1	1:A:709:LEU:HD21	1.99	0.92
2:A:1305:Y01:HAN2	2:A:1305:Y01:HAC3	1.50	0.92
2:C:1302:Y01:HAE2	2:C:1302:Y01:HAC1	1.54	0.90
1:B:982:VAL:HG23	2:B:1302:Y01:HAA1	1.52	0.89
2:A:1305:Y01:HAI	1:D:1009:LEU:HD11	1.55	0.88
2:D:1302:Y01:HAA3	2:D:1303:Y01:HAR1	1.55	0.88
2:A:1305:Y01:HAC3	2:A:1305:Y01:HAB1	1.55	0.88
1:A:298:LEU:CD1	1:A:400:LEU:CD1	2.52	0.86
2:C:1301:Y01:CAA	2:C:1302:Y01:HAR2	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1302:Y01:HAC1	2:B:1302:Y01:HAU2	1.58	0.85
1:D:775:GLU:O	1:D:776:TYR:CD1	2.29	0.85
1:B:775:GLU:O	1:B:776:TYR:CD1	2.29	0.85
2:A:1305:Y01:HAE3	2:A:1305:Y01:HAC2	1.58	0.85
1:A:874:VAL:HG11	1:A:969:ILE:HD11	1.60	0.83
1:B:874:VAL:HG11	1:B:969:ILE:HD11	1.61	0.83
1:B:1034:LYS:O	1:B:1038:PHE:HB2	1.79	0.83
1:D:1034:LYS:O	1:D:1038:PHE:HB2	1.79	0.83
1:D:874:VAL:HG11	1:D:969:ILE:HD11	1.60	0.82
1:C:1034:LYS:O	1:C:1038:PHE:HB2	1.79	0.82
2:A:1305:Y01:HAB1	2:A:1305:Y01:CAC	2.10	0.82
1:A:1034:LYS:O	1:A:1038:PHE:HB2	1.79	0.82
1:B:1160:LEU:HD22	1:B:1161:PHE:N	1.94	0.82
1:A:1160:LEU:HD22	1:A:1161:PHE:N	1.94	0.82
1:C:1160:LEU:HD22	1:C:1161:PHE:N	1.94	0.82
2:A:1304:Y01:HAA3	2:A:1305:Y01:HBC	1.62	0.81
1:A:982:VAL:HG23	2:A:1305:Y01:HAB2	1.62	0.81
1:D:1160:LEU:HD22	1:D:1161:PHE:N	1.94	0.81
1:C:874:VAL:HG11	1:C:969:ILE:HD11	1.60	0.81
1:B:454:PHE:O	1:B:458:LEU:HB2	1.83	0.79
1:D:454:PHE:O	1:D:458:LEU:HB2	1.83	0.79
1:A:454:PHE:O	1:A:458:LEU:HB2	1.83	0.79
1:A:477:LEU:HD23	1:A:477:LEU:O	1.83	0.79
1:A:298:LEU:HD12	1:A:400:LEU:CD1	2.14	0.78
1:D:980:LEU:HD22	1:D:980:LEU:O	1.84	0.78
2:A:1305:Y01:HAC3	2:A:1305:Y01:CAN	2.13	0.78
1:D:694:LEU:CD1	1:D:709:LEU:HD21	2.14	0.78
1:C:454:PHE:O	1:C:458:LEU:HB2	1.83	0.77
1:D:849:TYR:HB3	1:D:1127:VAL:HG11	1.67	0.77
1:B:982:VAL:CG2	2:B:1302:Y01:HAA1	2.15	0.77
1:A:849:TYR:HB3	1:A:1127:VAL:HG11	1.67	0.77
1:A:857:TRP:CH2	2:A:1305:Y01:HAO1	2.21	0.76
1:A:857:TRP:HH2	2:A:1305:Y01:HAO1	1.50	0.76
2:A:1305:Y01:HAC2	2:A:1305:Y01:CAE	2.15	0.76
1:A:694:LEU:HD11	1:A:709:LEU:HD21	1.69	0.75
1:A:982:VAL:HG21	2:A:1305:Y01:HAB2	1.67	0.75
2:A:1303:Y01:HAA3	2:B:1302:Y01:HAV1	1.69	0.75
1:B:694:LEU:HD11	1:B:709:LEU:HD21	1.68	0.74
1:D:477:LEU:HD23	1:D:477:LEU:O	1.88	0.74
1:C:1207:MET:HG2	1:D:1207:MET:HE3	1.69	0.74
1:C:709:LEU:HD13	1:C:739:THR:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LEU:O	1:C:477:LEU:HD23	1.88	0.74
1:A:1014:PHE:HB2	2:A:1301:Y01:CAB	2.18	0.73
1:A:774:LEU:H	1:A:774:LEU:HD23	1.54	0.73
1:C:694:LEU:HD11	1:C:709:LEU:HD21	1.68	0.72
1:D:747:TRP:HE1	2:D:1303:Y01:HAA3	1.53	0.72
1:B:477:LEU:HD23	1:B:477:LEU:O	1.88	0.72
1:B:709:LEU:HD13	1:B:739:THR:HG22	1.69	0.72
1:B:1207:MET:HG2	1:C:1207:MET:HE3	1.71	0.72
1:A:709:LEU:HD13	1:A:739:THR:HG22	1.69	0.72
2:A:1305:Y01:HAN2	2:A:1305:Y01:CAC	2.19	0.72
1:D:982:VAL:HG23	2:D:1303:Y01:HAB3	1.69	0.72
1:D:694:LEU:HD11	1:D:709:LEU:HD21	1.72	0.71
1:A:476:GLU:O	1:A:477:LEU:HB3	1.89	0.71
2:D:1302:Y01:HAA3	2:D:1303:Y01:OAW	1.91	0.71
1:C:774:LEU:HD23	1:C:774:LEU:H	1.54	0.71
1:D:774:LEU:CG	1:D:775:GLU:H	2.04	0.70
1:A:1160:LEU:HD22	1:A:1161:PHE:H	1.53	0.70
1:B:774:LEU:CG	1:B:775:GLU:H	2.04	0.70
1:C:1127:VAL:O	1:C:1128:LEU:HD22	1.92	0.69
2:A:1305:Y01:HAE2	2:A:1305:Y01:CAO	2.15	0.69
1:B:774:LEU:HG	1:B:775:GLU:H	1.58	0.69
1:D:474:LEU:O	1:D:478:TYR:HB2	1.92	0.69
2:A:1305:Y01:CAB	2:A:1305:Y01:HAC3	2.22	0.69
1:B:1127:VAL:O	1:B:1128:LEU:HD13	1.92	0.69
1:A:474:LEU:O	1:A:478:TYR:HB2	1.92	0.69
1:D:774:LEU:HG	1:D:775:GLU:H	1.57	0.69
1:B:474:LEU:O	1:B:478:TYR:HB2	1.92	0.69
1:B:1011:LEU:HD23	1:B:1011:LEU:O	1.93	0.69
1:C:1011:LEU:HD23	1:C:1011:LEU:O	1.93	0.69
1:C:474:LEU:O	1:C:478:TYR:HB2	1.92	0.69
1:D:982:VAL:CG2	2:D:1303:Y01:HAB3	2.23	0.69
1:B:1127:VAL:O	1:B:1128:LEU:HD22	1.92	0.69
1:C:1127:VAL:O	1:C:1128:LEU:HD13	1.92	0.69
1:A:982:VAL:HG22	2:A:1305:Y01:HAB1	1.76	0.68
2:A:1301:Y01:HAU2	2:A:1301:Y01:HAC1	1.74	0.68
1:C:1160:LEU:HD22	1:C:1161:PHE:H	1.59	0.68
1:D:1011:LEU:O	1:D:1011:LEU:HD23	1.93	0.68
1:D:1160:LEU:HD22	1:D:1161:PHE:H	1.59	0.67
1:C:710:THR:HA	1:C:720:THR:HG23	1.77	0.67
1:B:710:THR:HA	1:B:720:THR:HG23	1.77	0.67
1:A:857:TRP:CZ2	2:A:1305:Y01:HAJ1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1303:Y01:HAA3	2:B:1302:Y01:CAV	2.24	0.66
1:B:1160:LEU:HD22	1:B:1161:PHE:H	1.59	0.66
2:C:1301:Y01:CAA	2:C:1302:Y01:CAR	2.70	0.66
1:A:710:THR:HA	1:A:720:THR:HG23	1.77	0.65
1:B:980:LEU:HA	2:B:1302:Y01:CAE	2.27	0.65
1:D:982:VAL:HG23	2:D:1303:Y01:HAB2	1.68	0.65
1:A:1207:MET:CE	1:D:1211:ILE:HD12	2.27	0.64
1:B:988:PRO:O	1:B:992:MET:HB2	1.97	0.64
1:A:988:PRO:O	1:A:992:MET:HB2	1.97	0.64
1:C:988:PRO:O	1:C:992:MET:HB2	1.97	0.64
1:A:1207:MET:HG2	1:B:1207:MET:HE3	1.80	0.64
2:D:1302:Y01:CAA	2:D:1303:Y01:HAR1	2.26	0.64
1:D:988:PRO:O	1:D:992:MET:HB2	1.97	0.63
1:A:983:ASN:HB3	2:A:1305:Y01:HBA	1.80	0.63
1:B:896:TYR:OH	1:B:975:ARG:NH1	2.32	0.63
1:C:896:TYR:OH	1:C:975:ARG:NH1	2.32	0.63
1:A:1033:ALA:HB2	2:A:1303:Y01:HAK1	1.81	0.62
1:D:896:TYR:OH	1:D:975:ARG:NH1	2.32	0.62
1:D:710:THR:HA	1:D:720:THR:HG23	1.81	0.62
1:A:979:PHE:HB3	2:A:1305:Y01:CAP	2.29	0.62
1:A:730:LEU:HD12	1:A:733:PHE:HB2	1.82	0.62
1:A:896:TYR:OH	1:A:975:ARG:NH1	2.32	0.62
1:A:857:TRP:CZ2	2:A:1305:Y01:CAJ	2.83	0.62
1:B:771:ILE:O	1:B:774:LEU:HD22	2.00	0.62
1:D:730:LEU:HD12	1:D:733:PHE:HB2	1.82	0.62
1:A:961:GLY:O	1:A:965:TYR:HB2	2.00	0.61
1:B:774:LEU:HD23	1:B:774:LEU:H	1.65	0.61
1:D:961:GLY:O	1:D:965:TYR:HB2	2.00	0.61
1:C:961:GLY:O	1:C:965:TYR:HB2	2.00	0.61
1:A:1093:ILE:O	1:A:1097:ASN:HB2	2.01	0.61
1:A:982:VAL:HG22	2:A:1305:Y01:CAB	2.26	0.61
1:D:1093:ILE:O	1:D:1097:ASN:HB2	2.01	0.61
1:B:1093:ILE:O	1:B:1097:ASN:HB2	2.01	0.61
1:C:730:LEU:HD12	1:C:733:PHE:HB2	1.82	0.61
1:B:961:GLY:O	1:B:965:TYR:HB2	2.00	0.61
1:D:771:ILE:O	1:D:774:LEU:HD22	2.00	0.60
1:D:774:LEU:HD23	1:D:774:LEU:H	1.65	0.60
1:C:1093:ILE:O	1:C:1097:ASN:HB2	2.01	0.60
1:B:730:LEU:HD12	1:B:733:PHE:HB2	1.82	0.60
2:D:1302:Y01:HAA3	2:D:1303:Y01:CBC	2.32	0.60
1:D:1195:GLU:OE2	1:D:1198:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:GLU:OE2	1:A:1198:ARG:NH1	2.35	0.59
1:A:1207:MET:HE3	1:D:1207:MET:HG2	1.85	0.59
1:B:980:LEU:CD2	1:B:986:ALA:CB	2.81	0.59
1:A:980:LEU:CD2	1:A:986:ALA:CB	2.81	0.59
1:C:980:LEU:CD2	1:C:986:ALA:CB	2.81	0.59
1:C:1195:GLU:OE2	1:C:1198:ARG:NH1	2.35	0.59
1:C:771:ILE:O	1:C:774:LEU:HD22	2.03	0.59
1:B:1034:LYS:O	1:B:1038:PHE:CB	2.51	0.58
1:B:863:TYR:CD2	1:B:979:PHE:HE2	2.21	0.58
1:B:1195:GLU:OE2	1:B:1198:ARG:NH1	2.35	0.58
1:D:1127:VAL:O	1:D:1128:LEU:HD13	2.03	0.58
1:D:1083:VAL:HA	1:D:1087:ILE:HD12	1.85	0.58
1:C:863:TYR:CD2	1:C:979:PHE:HE2	2.21	0.58
1:D:1034:LYS:O	1:D:1038:PHE:CB	2.51	0.58
1:A:709:LEU:CD1	1:A:739:THR:HG22	2.34	0.58
1:A:863:TYR:CD2	1:A:979:PHE:HE2	2.21	0.58
1:A:1207:MET:HE3	1:D:1211:ILE:HD12	1.84	0.58
1:A:771:ILE:O	1:A:774:LEU:HD22	2.03	0.58
1:A:1083:VAL:HA	1:A:1087:ILE:HD12	1.85	0.58
1:B:1008:ALA:HB1	2:C:1302:Y01:HAL2	1.85	0.57
1:D:744:SER:OG	1:D:1115:ARG:NH2	2.37	0.57
2:D:1302:Y01:HAB2	2:D:1303:Y01:HAR2	1.86	0.57
1:B:980:LEU:HA	2:B:1302:Y01:HAE3	1.85	0.57
1:A:1011:LEU:O	1:A:1011:LEU:HD23	2.03	0.57
1:A:1127:VAL:O	1:A:1128:LEU:HD13	2.04	0.57
1:B:744:SER:OG	1:B:1115:ARG:NH2	2.37	0.57
1:C:744:SER:OG	1:C:1115:ARG:NH2	2.37	0.57
1:D:488:MET:HA	1:D:491:HIS:HD2	1.70	0.57
1:D:709:LEU:HD13	1:D:739:THR:HG22	1.85	0.57
1:A:488:MET:HA	1:A:491:HIS:HD2	1.70	0.57
1:C:488:MET:HA	1:C:491:HIS:HD2	1.70	0.57
1:A:979:PHE:HB3	2:A:1305:Y01:HAP2	1.86	0.57
1:A:509:LEU:HA	1:A:512:ILE:HD12	1.87	0.57
1:B:509:LEU:HA	1:B:512:ILE:HD12	1.87	0.57
1:C:1083:VAL:HA	1:C:1087:ILE:HD12	1.85	0.57
1:A:271:ASN:HD22	1:A:297:ILE:CD1	2.18	0.56
1:C:509:LEU:HA	1:C:512:ILE:HD12	1.87	0.56
1:C:980:LEU:HD21	1:C:986:ALA:CB	2.35	0.56
1:A:982:VAL:HG23	2:A:1305:Y01:CAB	2.28	0.56
1:B:1083:VAL:HA	1:B:1087:ILE:HD12	1.85	0.56
1:D:509:LEU:HA	1:D:512:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1304:Y01:CAA	2:A:1305:Y01:HBC	2.33	0.56
1:B:980:LEU:HD21	1:B:986:ALA:CB	2.35	0.56
1:C:980:LEU:HD23	1:C:980:LEU:O	2.06	0.56
1:C:1211:ILE:CD1	1:D:1207:MET:HE2	2.35	0.56
1:D:476:GLU:O	1:D:477:LEU:HB3	2.05	0.56
1:A:744:SER:OG	1:A:1115:ARG:NH2	2.37	0.56
1:A:980:LEU:HD23	1:A:980:LEU:O	2.06	0.56
1:C:476:GLU:O	1:C:477:LEU:HB3	2.05	0.56
1:C:874:VAL:HG21	1:C:969:ILE:HD11	1.87	0.56
1:A:980:LEU:HD21	1:A:986:ALA:CB	2.35	0.56
1:B:709:LEU:CD1	1:B:739:THR:HG22	2.34	0.56
1:A:467:LYS:HA	1:A:617:ARG:HE	1.71	0.56
1:D:874:VAL:HG21	1:D:969:ILE:HD11	1.87	0.56
2:C:1302:Y01:HAN1	2:C:1302:Y01:HAP1	1.87	0.56
1:B:874:VAL:HG21	1:B:969:ILE:HD11	1.87	0.56
1:B:980:LEU:O	1:B:980:LEU:HD23	2.06	0.56
1:A:874:VAL:HG21	1:A:969:ILE:HD11	1.87	0.55
1:A:1207:MET:HE2	1:D:1211:ILE:CD1	2.36	0.55
1:B:267:GLU:O	1:B:271:ASN:HB2	2.06	0.55
1:B:488:MET:HA	1:B:491:HIS:HD2	1.70	0.55
1:C:1127:VAL:C	1:C:1128:LEU:HD22	2.26	0.55
1:D:982:VAL:CG2	2:D:1303:Y01:HAB1	2.21	0.55
1:B:467:LYS:HA	1:B:617:ARG:HE	1.71	0.55
1:D:774:LEU:CD2	1:D:775:GLU:H	2.20	0.55
1:A:476:GLU:O	1:A:477:LEU:CB	2.53	0.55
1:A:477:LEU:HD21	1:A:628:TRP:CE2	2.41	0.55
1:B:1127:VAL:C	1:B:1128:LEU:HD22	2.26	0.55
1:A:271:ASN:ND2	1:A:297:ILE:HD13	2.22	0.55
1:C:267:GLU:O	1:C:271:ASN:HB2	2.06	0.55
1:C:1034:LYS:O	1:C:1038:PHE:CB	2.51	0.55
1:A:1034:LYS:O	1:A:1038:PHE:CB	2.51	0.55
1:B:476:GLU:O	1:B:477:LEU:HB3	2.05	0.55
1:B:774:LEU:CD2	1:B:775:GLU:H	2.20	0.55
1:C:709:LEU:CD1	1:C:739:THR:HG22	2.34	0.55
1:A:267:GLU:O	1:A:271:ASN:HB2	2.06	0.54
1:C:467:LYS:HA	1:C:617:ARG:HE	1.71	0.54
1:D:267:GLU:O	1:D:271:ASN:HB2	2.06	0.54
1:A:774:LEU:H	1:A:774:LEU:CD2	2.21	0.54
1:C:762:ILE:HG23	1:C:861:LEU:HD11	1.90	0.54
1:C:849:TYR:HB3	1:C:1127:VAL:HG11	1.90	0.54
1:D:467:LYS:HA	1:D:617:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:762:ILE:HG23	1:D:861:LEU:HD11	1.90	0.54
1:B:762:ILE:HG23	1:B:861:LEU:HD11	1.90	0.54
1:B:849:TYR:HB3	1:B:1127:VAL:HG11	1.90	0.53
1:B:1211:ILE:CD1	1:C:1207:MET:HE2	2.37	0.53
1:B:1014:PHE:HB2	2:B:1301:Y01:HAA1	1.90	0.53
1:C:862:ALA:HB3	1:C:1129:PRO:HB3	1.91	0.53
1:A:284:PRO:HG2	1:A:298:LEU:HB2	1.90	0.53
1:A:857:TRP:CH2	2:A:1305:Y01:CAO	2.89	0.53
1:A:1127:VAL:O	1:A:1128:LEU:HD22	2.09	0.53
1:A:762:ILE:HG23	1:A:861:LEU:HD11	1.90	0.53
1:B:862:ALA:HB3	1:B:1129:PRO:HB3	1.91	0.53
1:C:394:ALA:O	1:C:398:ALA:CB	2.57	0.53
1:A:394:ALA:O	1:A:398:ALA:CB	2.57	0.53
1:D:1127:VAL:O	1:D:1128:LEU:HD22	2.09	0.53
1:D:394:ALA:O	1:D:398:ALA:HB3	2.09	0.53
1:A:394:ALA:O	1:A:398:ALA:HB3	2.09	0.52
2:A:1305:Y01:CAB	2:A:1305:Y01:CAC	2.85	0.52
1:B:394:ALA:O	1:B:398:ALA:CB	2.57	0.52
1:D:394:ALA:O	1:D:398:ALA:CB	2.57	0.52
1:B:394:ALA:O	1:B:398:ALA:HB3	2.09	0.52
1:A:750:ARG:HG2	1:A:847:ALA:HB1	1.92	0.52
2:A:1301:Y01:HAR1	1:B:923:TYR:CB	2.39	0.52
2:A:1305:Y01:HAL2	1:D:1008:ALA:HB1	1.91	0.52
1:D:509:LEU:HD23	1:D:512:ILE:HD12	1.92	0.52
1:A:440:GLU:HG3	1:A:468:PHE:HD1	1.75	0.52
1:B:750:ARG:HG2	1:B:847:ALA:HB1	1.92	0.52
1:D:440:GLU:HG3	1:D:468:PHE:HD1	1.75	0.52
1:B:1082:PHE:O	1:B:1086:ILE:HB	2.10	0.52
1:C:440:GLU:HG3	1:C:468:PHE:HD1	1.75	0.52
1:B:440:GLU:HG3	1:B:468:PHE:HD1	1.75	0.51
1:B:1207:MET:HG2	1:C:1207:MET:CE	2.39	0.51
2:C:1301:Y01:HAA3	2:C:1302:Y01:HAR1	1.85	0.51
1:D:774:LEU:H	1:D:774:LEU:CD2	2.23	0.51
1:A:477:LEU:CD2	1:A:628:TRP:CE2	2.93	0.51
1:A:509:LEU:HD23	1:A:512:ILE:HD12	1.92	0.51
2:C:1302:Y01:HAR1	2:C:1302:Y01:OAG	2.10	0.51
1:B:1211:ILE:HD12	1:C:1207:MET:CE	2.41	0.51
1:C:1082:PHE:O	1:C:1086:ILE:HB	2.10	0.51
1:D:750:ARG:HG2	1:D:847:ALA:HB1	1.92	0.51
1:C:774:LEU:N	1:C:774:LEU:CD2	2.73	0.51
1:A:1207:MET:CE	1:D:1211:ILE:CD1	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:ILE:HG22	1:D:393:VAL:H	1.76	0.51
1:A:774:LEU:CD2	1:A:774:LEU:N	2.73	0.51
1:C:394:ALA:O	1:C:398:ALA:HB3	2.09	0.51
1:C:774:LEU:H	1:C:774:LEU:CD2	2.21	0.51
1:C:1211:ILE:HD12	1:D:1207:MET:CE	2.41	0.51
1:A:1207:MET:CE	1:D:1207:MET:HG2	2.41	0.51
1:A:1211:ILE:HD12	1:B:1207:MET:CE	2.41	0.51
1:C:750:ARG:HG2	1:C:847:ALA:HB1	1.92	0.51
2:D:1303:Y01:CAB	2:D:1303:Y01:HAO2	2.41	0.51
1:A:1014:PHE:HB2	2:A:1301:Y01:HAB1	1.91	0.51
1:C:509:LEU:HD23	1:C:512:ILE:HD12	1.92	0.51
2:A:1305:Y01:HAR1	2:A:1305:Y01:OAG	2.11	0.51
1:A:1082:PHE:O	1:A:1086:ILE:HB	2.10	0.50
1:B:509:LEU:HD23	1:B:512:ILE:HD12	1.92	0.50
1:B:774:LEU:H	1:B:774:LEU:CD2	2.23	0.50
1:D:774:LEU:HD23	1:D:775:GLU:H	1.77	0.50
1:A:488:MET:HE1	1:A:662:MET:HB3	1.93	0.50
2:A:1301:Y01:HAU2	2:A:1301:Y01:CAC	2.40	0.50
1:C:1129:PRO:HB2	1:C:1131:PRO:HD2	1.93	0.50
1:C:1211:ILE:HD12	1:D:1207:MET:HE2	1.92	0.50
1:D:1082:PHE:O	1:D:1086:ILE:HB	2.10	0.50
1:B:391:ILE:HG22	1:B:393:VAL:H	1.76	0.50
1:A:774:LEU:HD23	1:A:774:LEU:N	2.23	0.50
1:B:276:HIS:HB2	1:B:279:ILE:HB	1.94	0.50
1:B:1129:PRO:HB2	1:B:1131:PRO:HD2	1.93	0.50
1:A:391:ILE:HG22	1:A:393:VAL:H	1.76	0.50
1:A:474:LEU:HB3	1:A:509:LEU:HD21	1.93	0.50
1:B:474:LEU:HB3	1:B:509:LEU:HD21	1.93	0.50
1:C:391:ILE:HG22	1:C:393:VAL:H	1.76	0.50
1:C:474:LEU:HB3	1:C:509:LEU:HD21	1.93	0.50
1:D:474:LEU:HB3	1:D:509:LEU:HD21	1.93	0.50
1:D:774:LEU:CG	1:D:775:GLU:N	2.73	0.50
1:A:305:GLN:HA	1:A:310:VAL:HG21	1.94	0.50
1:D:1043:MET:HB3	1:D:1081:LEU:HD21	1.94	0.50
1:B:982:VAL:CG2	2:B:1302:Y01:CAA	2.65	0.50
1:A:1207:MET:HG2	1:B:1207:MET:CE	2.42	0.49
1:B:1043:MET:HB3	1:B:1081:LEU:HD21	1.94	0.49
1:C:276:HIS:HB2	1:C:279:ILE:HB	1.94	0.49
1:C:1043:MET:HB3	1:C:1081:LEU:HD21	1.94	0.49
1:C:1207:MET:HG2	1:D:1207:MET:CE	2.39	0.49
1:A:857:TRP:CH2	2:A:1305:Y01:CAJ	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:MET:HB3	1:A:1081:LEU:HD21	1.94	0.49
2:A:1305:Y01:CAC	2:A:1305:Y01:CAE	2.85	0.49
1:A:276:HIS:HB2	1:A:279:ILE:HB	1.94	0.49
1:B:1129:PRO:C	1:B:1131:PRO:HD2	2.33	0.49
1:A:271:ASN:HD22	1:A:297:ILE:HD13	1.77	0.49
1:D:305:GLN:HA	1:D:310:VAL:HG21	1.94	0.49
1:B:305:GLN:HA	1:B:310:VAL:HG21	1.94	0.49
1:D:276:HIS:HB2	1:D:279:ILE:HB	1.94	0.49
1:B:774:LEU:HD23	1:B:775:GLU:H	1.76	0.49
1:C:928:ASP:OD2	1:C:975:ARG:NH1	2.46	0.49
1:D:488:MET:HE1	1:D:662:MET:HB3	1.95	0.48
1:A:298:LEU:HD13	1:A:400:LEU:CD1	2.40	0.48
1:A:856:PHE:HE2	2:A:1305:Y01:HAB3	1.78	0.48
1:B:980:LEU:CD2	1:B:986:ALA:HB1	2.43	0.48
1:C:288:LEU:O	1:C:294:PRO:HD2	2.13	0.48
1:D:288:LEU:O	1:D:294:PRO:HD2	2.13	0.48
1:B:488:MET:HE1	1:B:662:MET:HB3	1.95	0.48
1:B:928:ASP:OD2	1:B:975:ARG:NH1	2.46	0.48
1:B:774:LEU:HD23	1:B:775:GLU:N	2.29	0.48
1:C:305:GLN:HA	1:C:310:VAL:HG21	1.94	0.48
1:D:709:LEU:CD1	1:D:739:THR:HG22	2.43	0.48
2:B:1302:Y01:HAC1	2:B:1302:Y01:CAU	2.35	0.48
1:A:928:ASP:OD2	1:A:975:ARG:NH1	2.46	0.48
2:A:1301:Y01:HAV1	1:B:994:GLY:HA3	1.96	0.48
1:A:477:LEU:HD23	1:A:477:LEU:C	2.34	0.48
1:B:1033:ALA:HB2	2:C:1301:Y01:HAK1	1.95	0.47
1:C:1129:PRO:C	1:C:1131:PRO:HD2	2.33	0.47
1:A:288:LEU:O	1:A:294:PRO:HD2	2.13	0.47
1:C:488:MET:HE1	1:C:662:MET:HB3	1.96	0.47
1:A:980:LEU:CD2	1:A:986:ALA:HB1	2.43	0.47
2:A:1305:Y01:CAE	2:A:1305:Y01:CAO	2.85	0.47
1:C:980:LEU:CD2	1:C:986:ALA:HB1	2.43	0.47
1:D:928:ASP:OD2	1:D:975:ARG:NH1	2.46	0.47
2:D:1302:Y01:CAA	2:D:1303:Y01:CAR	2.79	0.47
2:A:1305:Y01:HAO2	2:A:1305:Y01:CAE	2.26	0.47
2:A:1305:Y01:HAC3	2:A:1305:Y01:CBA	2.45	0.47
1:B:774:LEU:CG	1:B:775:GLU:N	2.73	0.47
1:B:1211:ILE:HD12	1:C:1207:MET:HE2	1.95	0.47
2:D:1302:Y01:CAA	2:D:1303:Y01:OAW	2.63	0.47
1:C:980:LEU:CD2	1:C:986:ALA:HB3	2.45	0.47
1:D:1011:LEU:HD23	1:D:1011:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:O	1:B:294:PRO:HD2	2.13	0.47
1:B:980:LEU:CD2	1:B:986:ALA:HB3	2.45	0.46
1:D:856:PHE:CZ	2:D:1303:Y01:HAC3	2.49	0.46
1:C:1011:LEU:HD23	1:C:1011:LEU:C	2.35	0.46
1:A:863:TYR:CG	1:A:979:PHE:HE2	2.33	0.46
1:B:653:LEU:HD13	1:B:725:ALA:HB2	1.97	0.46
1:D:477:LEU:O	1:D:628:TRP:NE1	2.49	0.46
1:D:856:PHE:CZ	2:D:1303:Y01:CAC	2.98	0.46
1:C:477:LEU:O	1:C:628:TRP:NE1	2.49	0.46
1:C:863:TYR:CG	1:C:979:PHE:HE2	2.33	0.46
1:D:774:LEU:HD23	1:D:775:GLU:N	2.29	0.46
1:A:740:GLN:NE2	1:A:1112:LYS:O	2.49	0.46
1:B:774:LEU:CD2	1:B:774:LEU:N	2.79	0.46
1:B:863:TYR:CG	1:B:979:PHE:HE2	2.33	0.46
1:D:740:GLN:NE2	1:D:1112:LYS:O	2.49	0.46
1:A:653:LEU:HD13	1:A:725:ALA:HB2	1.97	0.46
1:C:740:GLN:NE2	1:C:1112:LYS:O	2.49	0.46
2:D:1303:Y01:HAB3	2:D:1303:Y01:HAO2	1.98	0.46
1:A:477:LEU:HD21	1:A:628:TRP:CD2	2.50	0.46
1:B:477:LEU:O	1:B:628:TRP:NE1	2.49	0.46
1:D:983:ASN:HB3	2:D:1303:Y01:HAN2	1.98	0.46
1:B:740:GLN:NE2	1:B:1112:LYS:O	2.49	0.45
1:B:854:VAL:O	1:B:858:PHE:HB2	2.16	0.45
1:B:860:THR:HG22	1:B:979:PHE:CD1	2.52	0.45
1:B:1090:ASN:HD21	1:C:1093:ILE:HA	1.81	0.45
2:B:1302:Y01:HAC3	2:B:1302:Y01:HAJ1	1.79	0.45
2:A:1305:Y01:HAB3	2:A:1305:Y01:HBB	1.98	0.45
1:C:860:THR:HG22	1:C:979:PHE:CD1	2.51	0.45
1:B:1060:SER:OG	1:B:1061:THR:O	2.34	0.45
1:D:774:LEU:CD2	1:D:774:LEU:N	2.79	0.45
1:A:298:LEU:CD1	1:A:400:LEU:HD12	2.45	0.45
1:A:980:LEU:CD2	1:A:986:ALA:HB3	2.45	0.45
2:A:1304:Y01:HAK1	1:D:1033:ALA:HB2	1.98	0.45
1:A:1090:ASN:HD21	1:B:1093:ILE:HA	1.81	0.45
1:C:1090:ASN:HD21	1:D:1093:ILE:HA	1.81	0.45
2:D:1302:Y01:HAA3	2:D:1303:Y01:HAR2	1.86	0.45
2:D:1303:Y01:HAU2	2:D:1303:Y01:HAC1	1.99	0.45
1:B:983:ASN:ND2	2:B:1302:Y01:HAC3	2.31	0.45
2:A:1302:Y01:HAB1	1:D:1014:PHE:HB2	1.98	0.45
1:B:1011:LEU:HD23	1:B:1011:LEU:C	2.35	0.45
1:C:653:LEU:HD13	1:C:725:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:MET:SD	1:B:1207:MET:HE1	2.57	0.45
2:A:1305:Y01:CAI	1:D:1009:LEU:HD11	2.37	0.45
1:C:1011:LEU:C	1:C:1011:LEU:CD2	2.86	0.45
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.71	0.45
1:D:653:LEU:HD13	1:D:725:ALA:HB2	1.97	0.45
1:D:710:THR:HG21	1:D:786:PRO:HG3	1.98	0.45
1:A:774:LEU:HG	1:A:775:GLU:H	1.83	0.44
1:A:854:VAL:O	1:A:858:PHE:HB2	2.16	0.44
1:A:860:THR:HG22	1:A:979:PHE:CD1	2.51	0.44
1:A:1060:SER:OG	1:A:1061:THR:O	2.34	0.44
1:B:1011:LEU:C	1:B:1011:LEU:CD2	2.86	0.44
1:C:854:VAL:O	1:C:858:PHE:HB2	2.16	0.44
1:A:1093:ILE:HA	1:D:1090:ASN:HD21	1.81	0.44
1:D:856:PHE:CE2	2:D:1303:Y01:CAC	2.87	0.44
1:A:1207:MET:HE1	1:D:1207:MET:CE	2.48	0.44
1:A:1011:LEU:C	1:A:1011:LEU:CD2	2.85	0.44
1:A:1033:ALA:HB2	2:A:1303:Y01:CAK	2.46	0.44
1:C:1129:PRO:HD2	1:C:1132:LEU:HD12	1.99	0.44
1:A:700:GLN:HE22	1:A:1180:MET:HG3	1.83	0.44
1:B:1129:PRO:HD2	1:B:1132:LEU:HD12	1.99	0.44
1:C:774:LEU:HG	1:C:775:GLU:H	1.83	0.44
1:C:1203:ARG:O	1:C:1207:MET:HB2	2.18	0.44
1:D:980:LEU:HD23	2:D:1303:Y01:HBG	1.99	0.44
1:B:1203:ARG:O	1:B:1207:MET:HB2	2.17	0.44
1:D:1011:LEU:C	1:D:1011:LEU:CD2	2.86	0.44
1:D:1203:ARG:O	1:D:1207:MET:HB2	2.18	0.44
1:B:746:MET:HB3	1:B:1123:HIS:HE1	1.83	0.44
1:B:870:TYR:O	1:B:874:VAL:HG23	2.17	0.44
1:A:1211:ILE:HD12	1:B:1207:MET:HE3	1.99	0.43
1:C:700:GLN:HE22	1:C:1180:MET:HG3	1.83	0.43
1:D:746:MET:HB3	1:D:1123:HIS:HE1	1.83	0.43
1:D:854:VAL:O	1:D:858:PHE:HB2	2.16	0.43
1:A:746:MET:HB3	1:A:1123:HIS:HE1	1.83	0.43
1:B:691:VAL:HG21	1:B:732:PRO:HB2	2.00	0.43
2:C:1302:Y01:CAC	2:C:1302:Y01:HAU2	2.48	0.43
1:B:1207:MET:CE	1:C:1207:MET:HE1	2.49	0.43
1:C:858:PHE:CE2	1:C:1129:PRO:HD3	2.53	0.43
1:D:298:LEU:HD23	1:D:298:LEU:HA	1.80	0.43
2:D:1303:Y01:OAG	2:D:1303:Y01:HAV2	2.17	0.43
1:A:870:TYR:O	1:A:874:VAL:HG23	2.18	0.43
1:B:858:PHE:CE2	1:B:1129:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:LYS:HE3	1:C:680:LYS:HB2	1.86	0.43
1:C:870:TYR:O	1:C:874:VAL:HG23	2.18	0.43
2:B:1301:Y01:HAJ1	2:B:1301:Y01:HAC3	1.77	0.43
1:C:1207:MET:CE	1:D:1207:MET:HE1	2.49	0.43
1:D:691:VAL:HG21	1:D:732:PRO:HB2	2.00	0.43
1:D:870:TYR:O	1:D:874:VAL:HG23	2.18	0.43
1:C:1033:ALA:HB2	2:D:1302:Y01:HAK1	2.00	0.43
1:A:469:LEU:HD11	1:A:625:LEU:HG	2.01	0.43
1:A:871:THR:HG21	1:A:973:TYR:OH	2.19	0.43
1:B:469:LEU:HD11	1:B:625:LEU:HG	2.01	0.43
1:C:871:THR:HG21	1:C:973:TYR:OH	2.19	0.43
1:D:700:GLN:HE22	1:D:1180:MET:HG3	1.83	0.43
1:D:871:THR:HG21	1:D:973:TYR:OH	2.19	0.43
1:B:871:THR:HG21	1:B:973:TYR:OH	2.19	0.43
1:C:691:VAL:HG21	1:C:732:PRO:HB2	2.00	0.43
1:D:774:LEU:HD23	1:D:774:LEU:N	2.34	0.42
1:A:477:LEU:HD23	1:A:628:TRP:NE1	2.34	0.42
2:A:1301:Y01:HAC1	2:A:1301:Y01:HAE2	2.01	0.42
1:B:892:TYR:CE2	1:B:1131:PRO:HD3	2.55	0.42
1:C:469:LEU:HD11	1:C:625:LEU:HG	2.01	0.42
1:D:868:MET:HG2	2:D:1302:Y01:HAE2	2.00	0.42
2:A:1303:Y01:HAB2	2:B:1302:Y01:HAV2	2.00	0.42
1:B:774:LEU:HG	1:B:775:GLU:N	2.30	0.42
1:C:746:MET:HB3	1:C:1123:HIS:HE1	1.83	0.42
1:D:469:LEU:HD11	1:D:625:LEU:HG	2.01	0.42
1:D:992:MET:HG3	1:D:1103:VAL:HG12	2.02	0.42
1:A:691:VAL:HG21	1:A:732:PRO:HB2	2.00	0.42
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.71	0.42
1:A:892:TYR:CE2	1:A:1131:PRO:HD3	2.55	0.42
1:A:959:VAL:HG11	1:D:1068:PRO:HB2	2.02	0.42
1:B:700:GLN:HE22	1:B:1180:MET:HG3	1.83	0.42
1:D:774:LEU:HG	1:D:775:GLU:N	2.30	0.42
1:B:717:SER:O	1:B:717:SER:OG	2.30	0.42
1:A:1068:PRO:HB2	1:B:959:VAL:HG11	2.02	0.42
1:B:288:LEU:HB3	1:B:294:PRO:HG2	2.02	0.42
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.71	0.42
1:C:983:ASN:HB3	2:C:1302:Y01:HAN2	2.02	0.42
1:A:1207:MET:CE	1:B:1207:MET:HE1	2.49	0.42
1:B:1160:LEU:HD13	1:B:1162:LEU:HG	2.02	0.42
1:D:474:LEU:HD23	1:D:474:LEU:HA	1.71	0.42
2:A:1303:Y01:HAD2	2:A:1303:Y01:HAS2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1305:Y01:HAJ1	2:A:1305:Y01:HAB3	1.82	0.42
1:B:288:LEU:O	1:B:294:PRO:CD	2.68	0.42
1:B:980:LEU:CD2	1:B:980:LEU:C	2.89	0.42
1:C:288:LEU:O	1:C:294:PRO:CD	2.68	0.42
1:D:288:LEU:HB3	1:D:294:PRO:HG2	2.02	0.41
2:A:1305:Y01:CAM	1:D:1012:LEU:HD11	2.51	0.41
1:B:980:LEU:HA	2:B:1302:Y01:HAE2	2.02	0.41
1:C:892:TYR:CE2	1:C:1131:PRO:HD3	2.55	0.41
1:C:1012:LEU:HD11	2:D:1303:Y01:HAM1	2.01	0.41
1:D:483:GLY:O	1:D:485:THR:HG23	2.20	0.41
1:D:892:TYR:CE2	1:D:1131:PRO:HD3	2.55	0.41
1:A:288:LEU:O	1:A:294:PRO:CD	2.68	0.41
1:C:1160:LEU:HD13	1:C:1162:LEU:HG	2.02	0.41
1:A:980:LEU:CD2	1:A:980:LEU:C	2.89	0.41
1:C:483:GLY:O	1:C:485:THR:HG23	2.20	0.41
1:A:288:LEU:HB3	1:A:294:PRO:HG2	2.02	0.41
1:A:483:GLY:O	1:A:485:THR:HG23	2.20	0.41
1:A:1211:ILE:CD1	1:B:1207:MET:HE2	2.50	0.41
1:B:992:MET:HG3	1:B:1103:VAL:HG12	2.02	0.41
1:A:992:MET:HG3	1:A:1103:VAL:HG12	2.02	0.41
1:B:1068:PRO:HB2	1:C:959:VAL:HG11	2.02	0.41
1:C:869:LEU:HD23	1:C:869:LEU:HA	1.90	0.41
2:D:1301:Y01:HAD2	2:D:1301:Y01:HAS2	1.84	0.41
1:C:774:LEU:CG	1:C:775:GLU:H	2.34	0.41
1:A:892:TYR:CD2	1:A:1131:PRO:HD3	2.56	0.41
1:D:717:SER:O	1:D:717:SER:OG	2.30	0.41
1:A:694:LEU:HD12	1:A:709:LEU:HD21	1.97	0.41
1:A:774:LEU:CG	1:A:775:GLU:H	2.34	0.41
1:C:1068:PRO:HB2	1:D:959:VAL:HG11	2.02	0.41
1:D:288:LEU:O	1:D:294:PRO:CD	2.68	0.41
1:A:456:LYS:HG2	1:A:640:PHE:CE1	2.56	0.41
1:B:869:LEU:HD23	1:B:869:LEU:HA	1.90	0.41
1:C:456:LYS:HG2	1:C:640:PHE:CE1	2.56	0.41
1:D:1160:LEU:HD13	1:D:1162:LEU:HG	2.02	0.41
1:A:730:LEU:HD22	1:A:730:LEU:HA	1.91	0.40
1:B:456:LYS:HG2	1:B:640:PHE:CE1	2.56	0.40
1:B:730:LEU:HD22	1:B:730:LEU:HA	1.91	0.40
1:C:288:LEU:HB3	1:C:294:PRO:HG2	2.02	0.40
1:C:298:LEU:HD23	1:C:298:LEU:HA	1.80	0.40
1:C:867:LEU:HA	1:C:867:LEU:HD23	1.89	0.40
1:C:980:LEU:CD2	1:C:980:LEU:C	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:892:TYR:CD2	1:D:1131:PRO:HD3	2.56	0.40
1:C:892:TYR:CD2	1:C:1131:PRO:HD3	2.56	0.40
1:C:992:MET:HG3	1:C:1103:VAL:HG12	2.02	0.40
1:B:421:ASP:O	1:B:425:ASN:ND2	2.55	0.40
1:B:483:GLY:O	1:B:485:THR:HG23	2.20	0.40
1:B:892:TYR:CD2	1:B:1131:PRO:HD3	2.56	0.40
1:A:298:LEU:HD13	1:A:400:LEU:HD12	2.03	0.40
1:A:516:ILE:CD1	1:A:627:ILE:HG21	2.51	0.40
1:A:1160:LEU:HD13	1:A:1162:LEU:HG	2.03	0.40
2:A:1305:Y01:HAM1	1:D:1012:LEU:HD11	2.04	0.40
1:B:874:VAL:CG1	1:B:969:ILE:HD11	2.41	0.40
1:C:421:ASP:O	1:C:425:ASN:ND2	2.55	0.40
1:A:1011:LEU:HD21	1:A:1040:PRO:HG2	2.02	0.40
1:C:412:ILE:HG21	1:C:412:ILE:HD13	1.90	0.40
1:C:464:SER:OG	1:C:466:HIS:O	2.34	0.40
1:C:1060:SER:OG	1:C:1061:THR:O	2.34	0.40
2:C:1302:Y01:HAE2	2:C:1302:Y01:CAC	2.30	0.40
1:D:456:LYS:HG2	1:D:640:PHE:CE1	2.56	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	784/1229 (64%)	750 (96%)	32 (4%)	2 (0%)	41	72
1	B	784/1229 (64%)	751 (96%)	32 (4%)	1 (0%)	51	82
1	C	784/1229 (64%)	750 (96%)	32 (4%)	2 (0%)	41	72
1	D	784/1229 (64%)	753 (96%)	30 (4%)	1 (0%)	51	82
All	All	3136/4916 (64%)	3004 (96%)	126 (4%)	6 (0%)	50	77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	MET
1	B	369	MET
1	C	369	MET
1	D	369	MET
1	A	775	GLU
1	C	775	GLU

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	625/1094 (57%)	610 (98%)	15 (2%)	49	73
1	B	625/1094 (57%)	611 (98%)	14 (2%)	52	74
1	C	625/1094 (57%)	611 (98%)	14 (2%)	52	74
1	D	625/1094 (57%)	610 (98%)	15 (2%)	49	73
All	All	2500/4376 (57%)	2442 (98%)	58 (2%)	53	73

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	LEU
1	A	660	ARG
1	A	724	LEU
1	A	730	LEU
1	A	756	ASN
1	A	774	LEU
1	A	915	LYS
1	A	962	ARG
1	A	980	LEU
1	A	1011	LEU
1	A	1018	ARG
1	A	1090	ASN
1	A	1097	ASN
1	A	1128	LEU
1	A	1160	LEU
1	B	458	LEU

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Mol	Chain	Res	Type
1	B	660	ARG
1	B	724	LEU
1	B	730	LEU
1	B	756	ASN
1	B	774	LEU
1	B	915	LYS
1	B	962	ARG
1	B	980	LEU
1	B	1018	ARG
1	B	1090	ASN
1	B	1097	ASN
1	B	1128	LEU
1	B	1160	LEU
1	C	458	LEU
1	C	660	ARG
1	C	724	LEU
1	C	730	LEU
1	C	756	ASN
1	C	774	LEU
1	C	915	LYS
1	C	962	ARG
1	C	980	LEU
1	C	1018	ARG
1	C	1090	ASN
1	C	1097	ASN
1	C	1128	LEU
1	C	1160	LEU
1	D	458	LEU
1	D	660	ARG
1	D	710	THR
1	D	724	LEU
1	D	730	LEU
1	D	756	ASN
1	D	774	LEU
1	D	915	LYS
1	D	962	ARG
1	D	980	LEU
1	D	1018	ARG
1	D	1090	ASN
1	D	1097	ASN
1	D	1128	LEU
1	D	1160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	276	HIS
1	A	432	GLN
1	A	491	HIS
1	A	756	ASN
1	A	789	GLN
1	A	885	GLN
1	A	1090	ASN
1	A	1123	HIS
1	A	1137	HIS
1	B	276	HIS
1	B	425	ASN
1	B	432	GLN
1	B	491	HIS
1	B	756	ASN
1	B	789	GLN
1	B	885	GLN
1	B	1090	ASN
1	B	1123	HIS
1	B	1137	HIS
1	C	276	HIS
1	C	425	ASN
1	C	432	GLN
1	C	491	HIS
1	C	756	ASN
1	C	789	GLN
1	C	885	GLN
1	C	1090	ASN
1	C	1123	HIS
1	C	1137	HIS
1	D	276	HIS
1	D	425	ASN
1	D	432	GLN
1	D	491	HIS
1	D	756	ASN
1	D	789	GLN
1	D	885	GLN
1	D	1090	ASN
1	D	1123	HIS
1	D	1137	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	Y01	A	1302	-	38,38,38	1.70	4 (10%)	57,57,57	1.80	13 (22%)
2	Y01	A	1303	-	38,38,38	2.08	7 (18%)	57,57,57	2.42	19 (33%)
2	Y01	C	1301	-	38,38,38	2.19	6 (15%)	57,57,57	2.53	20 (35%)
2	Y01	D	1301	-	38,38,38	1.76	6 (15%)	57,57,57	1.76	12 (21%)
2	Y01	C	1302	-	38,38,38	1.89	6 (15%)	57,57,57	1.50	6 (10%)
2	Y01	B	1301	-	38,38,38	1.76	4 (10%)	57,57,57	1.63	10 (17%)
2	Y01	D	1302	-	38,38,38	2.20	6 (15%)	57,57,57	2.57	20 (35%)
2	Y01	D	1303	-	38,38,38	1.74	6 (15%)	57,57,57	1.65	13 (22%)
2	Y01	A	1304	-	38,38,38	2.27	7 (18%)	57,57,57	2.60	18 (31%)
2	Y01	A	1305	-	38,38,38	1.84	6 (15%)	57,57,57	1.55	8 (14%)
2	Y01	A	1301	-	38,38,38	1.78	5 (13%)	57,57,57	1.57	8 (14%)
2	Y01	B	1302	-	38,38,38	1.84	8 (21%)	57,57,57	2.04	16 (28%)

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
2	Y01	A	1302	-	-	6/19/77/77	0/4/4/4
2	Y01	A	1303	-	-	10/19/77/77	0/4/4/4
2	Y01	C	1301	-	-	10/19/77/77	0/4/4/4
2	Y01	D	1301	-	-	4/19/77/77	0/4/4/4
2	Y01	C	1302	-	-	10/19/77/77	0/4/4/4
2	Y01	B	1301	-	-	3/19/77/77	0/4/4/4
2	Y01	D	1302	-	-	12/19/77/77	0/4/4/4
2	Y01	D	1303	-	-	5/19/77/77	0/4/4/4
2	Y01	A	1304	-	-	10/19/77/77	0/4/4/4
2	Y01	A	1305	-	-	9/19/77/77	0/4/4/4
2	Y01	A	1301	-	-	5/19/77/77	0/4/4/4
2	Y01	B	1302	-	-	10/19/77/77	0/4/4/4

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1303	Y01	CBH-CAZ	-6.17	1.40	1.52
2	A	1304	Y01	CBH-CAZ	-6.13	1.40	1.52
2	D	1302	Y01	CAK-CAI	-6.09	1.37	1.50
2	A	1304	Y01	CAK-CAI	-6.03	1.37	1.50
2	C	1301	Y01	CBH-CAZ	-6.00	1.41	1.52
2	A	1304	Y01	CAV-CAZ	-5.97	1.38	1.51
2	D	1302	Y01	CBH-CAZ	-5.95	1.41	1.52
2	C	1302	Y01	CAV-CAZ	-5.92	1.38	1.51
2	C	1301	Y01	CAK-CAI	-5.90	1.37	1.50
2	D	1302	Y01	CAV-CAZ	-5.83	1.39	1.51
2	C	1301	Y01	CAV-CAZ	-5.74	1.39	1.51
2	A	1303	Y01	CAV-CAZ	-5.67	1.39	1.51
2	A	1303	Y01	CAK-CAI	-5.55	1.38	1.50
2	A	1305	Y01	CBH-CAZ	-5.53	1.41	1.52
2	C	1302	Y01	CBH-CAZ	-5.52	1.41	1.52
2	B	1302	Y01	CBH-CAZ	-5.51	1.41	1.52
2	A	1301	Y01	CAV-CAZ	-5.51	1.39	1.51
2	A	1305	Y01	CAV-CAZ	-5.43	1.39	1.51
2	D	1303	Y01	CAV-CAZ	-5.43	1.39	1.51
2	A	1301	Y01	CBH-CAZ	-5.41	1.42	1.52
2	B	1301	Y01	CBH-CAZ	-5.33	1.42	1.52
2	B	1301	Y01	CAV-CAZ	-5.28	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	Y01	CAK-CAI	-5.27	1.38	1.50
2	D	1301	Y01	CBH-CAZ	-5.24	1.42	1.52
2	A	1302	Y01	CBH-CAZ	-5.18	1.42	1.52
2	D	1301	Y01	CAV-CAZ	-5.17	1.40	1.51
2	D	1301	Y01	CAK-CAI	-5.12	1.39	1.50
2	D	1303	Y01	CBH-CAZ	-5.11	1.42	1.52
2	A	1304	Y01	CAK-CBD	-5.04	1.44	1.53
2	B	1302	Y01	CAV-CAZ	-5.01	1.40	1.51
2	D	1302	Y01	CAK-CBD	-4.86	1.44	1.53
2	A	1302	Y01	CAK-CAI	-4.71	1.40	1.50
2	C	1301	Y01	CAK-CBD	-4.67	1.45	1.53
2	A	1302	Y01	CAV-CAZ	-4.65	1.41	1.51
2	A	1304	Y01	CBI-CBG	-4.60	1.46	1.55
2	C	1302	Y01	CAK-CAI	-4.56	1.40	1.50
2	D	1302	Y01	CBI-CBG	-4.47	1.46	1.55
2	D	1303	Y01	CAK-CAI	-4.43	1.40	1.50
2	A	1301	Y01	CAK-CAI	-4.43	1.40	1.50
2	C	1301	Y01	CBI-CBG	-4.41	1.46	1.55
2	A	1305	Y01	CAK-CAI	-4.22	1.41	1.50
2	B	1302	Y01	CAK-CAI	-4.08	1.41	1.50
2	A	1303	Y01	CBI-CBG	-4.04	1.47	1.55
2	A	1305	Y01	CAI-CAZ	3.36	1.40	1.33
2	A	1303	Y01	CAK-CBD	-3.34	1.47	1.53
2	C	1302	Y01	CAI-CAZ	3.31	1.40	1.33
2	B	1302	Y01	CAI-CAZ	3.25	1.40	1.33
2	D	1303	Y01	CAI-CAZ	3.21	1.40	1.33
2	A	1301	Y01	CAI-CAZ	3.10	1.39	1.33
2	A	1302	Y01	CAI-CAZ	2.94	1.39	1.33
2	A	1305	Y01	CAQ-CBG	-2.89	1.48	1.54
2	D	1301	Y01	CAI-CAZ	2.82	1.39	1.33
2	B	1301	Y01	CAI-CAZ	2.67	1.38	1.33
2	C	1302	Y01	CBD-CBG	-2.67	1.48	1.53
2	A	1303	Y01	CAI-CAZ	2.66	1.38	1.33
2	C	1302	Y01	CBI-CBG	-2.56	1.50	1.55
2	B	1302	Y01	CBI-CBG	-2.55	1.50	1.55
2	B	1302	Y01	CBI-CBE	-2.54	1.50	1.55
2	C	1301	Y01	CAI-CAZ	2.44	1.38	1.33
2	D	1303	Y01	CBI-CBG	-2.40	1.50	1.55
2	D	1302	Y01	CAI-CAZ	2.35	1.38	1.33
2	A	1301	Y01	CBI-CBG	-2.33	1.50	1.55
2	A	1305	Y01	CBI-CBG	-2.27	1.50	1.55
2	D	1303	Y01	CBD-CBG	-2.26	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1304	Y01	CAI-CAZ	2.25	1.37	1.33
2	B	1302	Y01	CBD-CBG	-2.12	1.49	1.53
2	D	1301	Y01	OAW-CBC	-2.09	1.41	1.46
2	D	1301	Y01	CAQ-CBG	-2.08	1.50	1.54
2	A	1303	Y01	CBI-CBE	-2.04	1.51	1.55
2	B	1302	Y01	CAT-CBH	-2.03	1.50	1.54
2	A	1304	Y01	CBD-CBG	-2.01	1.49	1.53

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1304	Y01	CBG-CBI-CBE	-9.30	89.06	100.07
2	A	1303	Y01	CAC-CBB-CBE	-8.67	99.65	112.92
2	C	1301	Y01	CAC-CBB-CBE	-8.20	100.36	112.92
2	D	1302	Y01	CAC-CBB-CBE	-8.06	100.58	112.92
2	C	1301	Y01	CBG-CBI-CBE	-7.81	90.83	100.07
2	A	1304	Y01	CAC-CBB-CBE	-7.60	101.29	112.92
2	D	1302	Y01	CBG-CBI-CBE	-7.45	91.25	100.07
2	A	1303	Y01	CBG-CBI-CBE	-7.42	91.28	100.07
2	D	1302	Y01	CAV-CAZ-CBH	5.84	124.17	116.42
2	A	1304	Y01	CAK-CBD-CBG	-5.11	103.50	110.91
2	B	1302	Y01	CBI-CBE-CBB	-5.11	111.49	119.49
2	C	1301	Y01	CAV-CAZ-CBH	5.09	123.18	116.42
2	A	1304	Y01	CAV-CAZ-CBH	5.00	123.07	116.42
2	D	1302	Y01	CAV-CAZ-CAI	-4.94	113.49	120.61
2	D	1302	Y01	CAK-CBD-CBG	-4.86	103.87	110.91
2	B	1302	Y01	CAV-CAZ-CBH	4.84	122.86	116.42
2	A	1303	Y01	CAV-CAZ-CBH	4.66	122.61	116.42
2	B	1301	Y01	CAV-CAZ-CBH	4.65	122.60	116.42
2	C	1301	Y01	CAK-CBD-CBG	-4.61	104.22	110.91
2	D	1303	Y01	CAQ-CBG-CBD	-4.59	111.52	119.08
2	C	1302	Y01	CAQ-CBG-CBD	-4.53	111.62	119.08
2	D	1301	Y01	CAV-CAZ-CBH	4.51	122.41	116.42
2	A	1304	Y01	CAK-CBD-CBF	-4.51	104.25	109.71
2	A	1301	Y01	CBI-CBE-CBB	-4.38	112.62	119.49
2	A	1303	Y01	CBH-CBF-CBD	-4.34	106.22	112.73
2	A	1302	Y01	CAV-CAZ-CBH	4.34	122.18	116.42
2	C	1301	Y01	CBH-CBF-CBD	-4.24	106.38	112.73
2	C	1301	Y01	CAV-CAZ-CAI	-4.21	114.54	120.61
2	A	1304	Y01	CAV-CAZ-CAI	-4.09	114.71	120.61
2	D	1302	Y01	CBH-CBF-CBD	-4.09	106.60	112.73
2	A	1302	Y01	CBH-CBF-CBD	-4.05	106.66	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1304	Y01	CBH-CBF-CBD	-4.01	106.72	112.73
2	D	1303	Y01	CBI-CBE-CBB	-4.00	113.22	119.49
2	B	1301	Y01	CAQ-CBG-CBD	-3.97	112.54	119.08
2	D	1301	Y01	CAQ-CBG-CBD	-3.95	112.58	119.08
2	B	1302	Y01	CAQ-CBG-CBD	-3.94	112.58	119.08
2	A	1302	Y01	CAQ-CBG-CBD	-3.93	112.61	119.08
2	A	1305	Y01	CBI-CBG-CBD	-3.90	108.60	114.38
2	C	1302	Y01	CBI-CBG-CBD	-3.88	108.63	114.38
2	A	1303	Y01	CAV-CAZ-CAI	-3.88	115.02	120.61
2	C	1302	Y01	CBI-CBE-CBB	-3.82	113.50	119.49
2	A	1301	Y01	CAQ-CBG-CBD	-3.77	112.87	119.08
2	A	1302	Y01	CAP-CBE-CBB	-3.77	106.32	112.15
2	A	1305	Y01	CAQ-CBG-CBD	-3.75	112.90	119.08
2	B	1302	Y01	CBI-CBG-CBD	-3.74	108.84	114.38
2	B	1301	Y01	CAV-CAZ-CAI	-3.73	115.24	120.61
2	A	1303	Y01	CBI-CBG-CBD	-3.71	108.89	114.38
2	D	1301	Y01	CAP-CBE-CBB	-3.67	106.46	112.15
2	B	1302	Y01	CBC-CAV-CAZ	3.66	117.20	111.52
2	C	1301	Y01	CBI-CBG-CBD	-3.58	109.08	114.38
2	D	1302	Y01	CBI-CBG-CBD	-3.53	109.16	114.38
2	A	1303	Y01	CAK-CBD-CBG	-3.52	105.81	110.91
2	A	1304	Y01	CAJ-CAO-CBB	-3.51	104.94	115.03
2	D	1301	Y01	CBH-CBF-CBD	-3.51	107.47	112.73
2	A	1305	Y01	CAP-CAQ-CBG	-3.49	98.21	105.13
2	A	1302	Y01	CAD-CBH-CBF	-3.47	107.54	111.68
2	C	1301	Y01	CAK-CBD-CBF	-3.47	105.51	109.71
2	D	1301	Y01	CBG-CBI-CBE	-3.47	95.97	100.07
2	D	1302	Y01	CAD-CBH-CBF	-3.47	107.55	111.68
2	A	1305	Y01	CBF-CBH-CAZ	3.46	115.08	109.65
2	A	1302	Y01	CBG-CBI-CBE	-3.46	95.98	100.07
2	A	1304	Y01	CAE-CBI-CBE	3.44	118.12	111.71
2	A	1303	Y01	CAO-CBB-CBE	3.39	117.30	110.28
2	D	1301	Y01	CAV-CAZ-CAI	-3.38	115.73	120.61
2	B	1302	Y01	CAD-CBH-CBF	-3.38	107.65	111.68
2	B	1302	Y01	CBC-OAW-CAY	-3.37	109.48	117.79
2	C	1301	Y01	CAJ-CAO-CBB	-3.36	105.36	115.03
2	A	1304	Y01	CBI-CBG-CBD	-3.35	109.42	114.38
2	D	1302	Y01	CAJ-CAO-CBB	-3.32	105.49	115.03
2	C	1301	Y01	CAD-CBH-CBF	-3.32	107.73	111.68
2	C	1301	Y01	CAO-CBB-CBE	3.31	117.12	110.28
2	A	1304	Y01	CAD-CBH-CBF	-3.30	107.75	111.68
2	C	1302	Y01	CAP-CBE-CBB	-3.29	107.05	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1302	Y01	CBH-CBF-CBD	-3.29	107.80	112.73
2	D	1303	Y01	CBI-CBG-CBD	-3.25	109.56	114.38
2	B	1302	Y01	CBF-CBH-CAZ	3.25	114.75	109.65
2	D	1302	Y01	CAO-CBB-CBE	3.25	117.00	110.28
2	B	1302	Y01	CAV-CAZ-CAI	-3.21	115.98	120.61
2	D	1302	Y01	CAK-CBD-CBF	-3.18	105.86	109.71
2	D	1301	Y01	CAC-CBB-CAO	-3.16	105.41	110.36
2	B	1302	Y01	CAC-CBB-CBE	-3.13	108.14	112.92
2	A	1303	Y01	CAD-CBH-CBF	-3.11	107.98	111.68
2	A	1301	Y01	CBF-CBH-CAZ	3.09	114.50	109.65
2	A	1304	Y01	CAQ-CAP-CBE	-3.08	99.02	105.13
2	A	1301	Y01	CBI-CBG-CBD	-3.07	109.83	114.38
2	C	1301	Y01	CAQ-CBG-CBD	-3.04	114.07	119.08
2	A	1304	Y01	CAO-CBB-CBE	3.02	116.52	110.28
2	A	1303	Y01	CAJ-CAO-CBB	-3.01	106.39	115.03
2	A	1302	Y01	CAC-CBB-CAO	-3.01	105.65	110.36
2	C	1301	Y01	CAC-CBB-CAO	-3.00	105.65	110.36
2	D	1302	Y01	CAQ-CBG-CBD	-2.97	114.18	119.08
2	A	1304	Y01	CAQ-CBG-CBD	-2.97	114.18	119.08
2	A	1305	Y01	CBC-OAW-CAY	-2.97	110.49	117.79
2	D	1302	Y01	CBC-CAV-CAZ	2.97	116.12	111.52
2	D	1303	Y01	CAD-CBH-CBF	-2.96	108.15	111.68
2	D	1302	Y01	CBC-OAW-CAY	-2.95	110.53	117.79
2	C	1302	Y01	CBF-CBH-CAZ	2.93	114.25	109.65
2	B	1301	Y01	CBH-CBF-CBD	-2.91	108.36	112.73
2	D	1302	Y01	CAC-CBB-CAO	-2.90	105.82	110.36
2	B	1302	Y01	CAS-CAU-CBI	-2.89	107.83	112.78
2	A	1301	Y01	CAS-CAU-CBI	-2.86	107.88	112.78
2	A	1303	Y01	CAQ-CBG-CBD	-2.86	114.37	119.08
2	A	1305	Y01	CBI-CBE-CBB	-2.83	115.05	119.49
2	B	1301	Y01	CBG-CBI-CBE	-2.80	96.75	100.07
2	D	1301	Y01	CAD-CBH-CBF	-2.80	108.34	111.68
2	A	1303	Y01	CBC-CAV-CAZ	2.75	115.80	111.52
2	C	1301	Y01	CBC-OAW-CAY	-2.75	111.02	117.79
2	A	1302	Y01	CAV-CAZ-CAI	-2.74	116.66	120.61
2	A	1302	Y01	CAC-CBB-CBE	2.70	117.06	112.92
2	A	1305	Y01	CAQ-CBG-CBI	-2.69	100.61	103.84
2	A	1304	Y01	CAK-CAI-CAZ	-2.68	120.12	125.06
2	B	1301	Y01	CAP-CBE-CBB	-2.66	108.02	112.15
2	B	1302	Y01	CAR-CBC-CAV	2.66	114.95	110.99
2	A	1303	Y01	CBC-OAW-CAY	-2.65	111.28	117.79
2	D	1303	Y01	CAC-CBB-CBE	-2.64	108.89	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1302	Y01	CAS-CBF-CBD	-2.64	107.96	111.75
2	C	1301	Y01	CBC-CAV-CAZ	2.63	115.61	111.52
2	A	1303	Y01	CAQ-CAP-CBE	-2.63	99.92	105.13
2	C	1301	Y01	CAQ-CAP-CBE	-2.62	99.94	105.13
2	D	1303	Y01	CBF-CBH-CAZ	2.60	113.73	109.65
2	D	1303	Y01	CAP-CBE-CBB	-2.59	108.13	112.15
2	A	1304	Y01	CBC-OAW-CAY	-2.58	111.44	117.79
2	A	1301	Y01	CAC-CBB-CBE	-2.56	109.00	112.92
2	C	1302	Y01	CAC-CBB-CBE	-2.51	109.07	112.92
2	C	1301	Y01	CAS-CBF-CBD	-2.51	108.14	111.75
2	A	1304	Y01	CBC-CAV-CAZ	2.50	115.41	111.52
2	D	1302	Y01	CAQ-CAP-CBE	-2.49	100.19	105.13
2	B	1301	Y01	CAD-CBH-CBF	-2.46	108.75	111.68
2	D	1301	Y01	CAM-CAL-CAX	-2.45	108.33	113.60
2	B	1301	Y01	CAM-CAL-CAX	-2.45	108.33	113.60
2	A	1303	Y01	CAS-CBF-CBD	-2.44	108.24	111.75
2	C	1301	Y01	CAE-CBI-CBE	2.43	116.25	111.71
2	A	1303	Y01	CAE-CBI-CBE	2.40	116.19	111.71
2	D	1303	Y01	CAS-CAU-CBI	-2.37	108.71	112.78
2	B	1301	Y01	CAK-CBD-CBG	-2.33	107.54	110.91
2	A	1302	Y01	CAK-CBD-CBF	-2.32	106.90	109.71
2	D	1303	Y01	CAT-CAR-CBC	-2.32	106.37	110.33
2	A	1301	Y01	CAP-CBE-CBB	-2.30	108.58	112.15
2	A	1302	Y01	CAP-CBE-CBI	-2.29	101.08	103.84
2	A	1302	Y01	CAS-CBF-CBH	-2.27	110.08	113.08
2	D	1302	Y01	CBI-CBE-CBB	-2.27	115.93	119.49
2	A	1305	Y01	CAJ-CAO-CBB	-2.26	108.53	115.03
2	D	1303	Y01	CAV-CAZ-CBH	2.25	119.41	116.42
2	C	1301	Y01	CBI-CBE-CBB	-2.25	115.96	119.49
2	B	1302	Y01	CBD-CAK-CAI	2.23	115.94	112.73
2	D	1302	Y01	CAE-CBI-CBE	2.22	115.86	111.71
2	A	1301	Y01	CAV-CAZ-CBH	2.20	119.34	116.42
2	A	1304	Y01	CAS-CBF-CBD	-2.19	108.60	111.75
2	D	1303	Y01	CAP-CAQ-CBG	-2.19	100.80	105.13
2	A	1303	Y01	CAC-CBB-CAO	-2.19	106.93	110.36
2	A	1303	Y01	CAK-CBD-CBF	-2.18	107.07	109.71
2	D	1303	Y01	CBH-CBF-CBD	-2.17	109.48	112.73
2	D	1301	Y01	CAP-CBE-CBI	-2.17	101.23	103.84
2	C	1301	Y01	CAK-CAI-CAZ	-2.15	121.09	125.06
2	D	1303	Y01	CAR-CBC-CAV	-2.15	107.78	110.99
2	D	1302	Y01	CAK-CAI-CAZ	-2.13	121.13	125.06
2	D	1301	Y01	CAC-CBB-CBE	2.12	116.17	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1303	Y01	CBI-CBE-CBB	-2.12	116.17	119.49
2	A	1302	Y01	CAR-CAT-CBH	-2.08	108.23	112.74
2	D	1301	Y01	CAS-CBF-CBH	-2.06	110.36	113.08
2	B	1302	Y01	CBF-CBD-CBG	-2.05	106.34	109.09
2	B	1301	Y01	CAP-CAQ-CBG	-2.04	101.08	105.13
2	B	1302	Y01	OAW-CAY-CAM	2.02	115.85	111.50

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	Y01	CAX-CAL-CAM-CAY
2	D	1303	Y01	CAV-CBC-OAW-CAY
2	A	1305	Y01	CAO-CBB-CBE-CAP
2	A	1305	Y01	CAO-CBB-CBE-CBI
2	B	1302	Y01	CAM-CAY-OAW-CBC
2	B	1302	Y01	OAG-CAY-OAW-CBC
2	C	1302	Y01	CAJ-CAO-CBB-CBE
2	C	1302	Y01	CAJ-CAO-CBB-CAC
2	D	1302	Y01	CAO-CBB-CBE-CAP
2	A	1303	Y01	CAO-CBB-CBE-CBI
2	A	1304	Y01	CAO-CBB-CBE-CBI
2	C	1301	Y01	CAO-CBB-CBE-CBI
2	D	1302	Y01	CAO-CBB-CBE-CBI
2	D	1302	Y01	CAJ-CAO-CBB-CAC
2	A	1305	Y01	CAO-CAJ-CAN-CBA
2	A	1303	Y01	CAC-CBB-CBE-CAP
2	C	1301	Y01	CAC-CBB-CBE-CAP
2	D	1302	Y01	CAC-CBB-CBE-CAP
2	D	1301	Y01	CAX-CAL-CAM-CAY
2	D	1302	Y01	CAX-CAL-CAM-CAY
2	A	1303	Y01	CAC-CBB-CBE-CBI
2	C	1301	Y01	CAC-CBB-CBE-CBI
2	D	1302	Y01	CAC-CBB-CBE-CBI
2	C	1301	Y01	CAO-CBB-CBE-CAP
2	A	1304	Y01	CAJ-CAO-CBB-CAC
2	C	1301	Y01	CAJ-CAO-CBB-CAC
2	A	1304	Y01	CAC-CBB-CBE-CAP
2	A	1305	Y01	CAC-CBB-CBE-CAP
2	A	1304	Y01	CAC-CBB-CBE-CBI
2	A	1301	Y01	CAX-CAL-CAM-CAY
2	A	1302	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
2	A	1305	Y01	CAX-CAL-CAM-CAY
2	C	1301	Y01	CAX-CAL-CAM-CAY
2	A	1303	Y01	CAN-CAJ-CAO-CBB
2	C	1301	Y01	CAN-CAJ-CAO-CBB
2	D	1302	Y01	CAN-CAJ-CAO-CBB
2	A	1304	Y01	CAN-CAJ-CAO-CBB
2	A	1303	Y01	CAO-CBB-CBE-CAP
2	A	1301	Y01	CAJ-CAN-CBA-CAB
2	C	1302	Y01	CAO-CBB-CBE-CAP
2	B	1301	Y01	CAN-CAJ-CAO-CBB
2	B	1302	Y01	CAO-CAJ-CAN-CBA
2	A	1301	Y01	CAJ-CAN-CBA-CAA
2	A	1303	Y01	CAJ-CAO-CBB-CAC
2	A	1303	Y01	CAX-CAL-CAM-CAY
2	A	1304	Y01	CAX-CAL-CAM-CAY
2	D	1303	Y01	CAJ-CAO-CBB-CAC
2	A	1305	Y01	CAM-CAY-OAW-CBC
2	A	1305	Y01	OAG-CAY-OAW-CBC
2	B	1302	Y01	CAJ-CAO-CBB-CAC
2	C	1301	Y01	CAJ-CAN-CBA-CAA
2	A	1302	Y01	CAN-CAJ-CAO-CBB
2	A	1303	Y01	CAJ-CAN-CBA-CAA
2	A	1304	Y01	CAJ-CAN-CBA-CAA
2	B	1302	Y01	CAX-CAL-CAM-CAY
2	D	1302	Y01	CAM-CAY-OAW-CBC
2	D	1302	Y01	CAJ-CAN-CBA-CAA
2	A	1302	Y01	CAM-CAY-OAW-CBC
2	A	1304	Y01	CAO-CAJ-CAN-CBA
2	D	1302	Y01	CAO-CAJ-CAN-CBA
2	A	1302	Y01	OAG-CAY-OAW-CBC
2	D	1301	Y01	CAN-CAJ-CAO-CBB
2	C	1301	Y01	CAO-CAJ-CAN-CBA
2	D	1303	Y01	CAO-CAJ-CAN-CBA
2	A	1303	Y01	CAO-CAJ-CAN-CBA
2	A	1303	Y01	CAJ-CAN-CBA-CAB
2	C	1301	Y01	CAJ-CAN-CBA-CAB
2	D	1302	Y01	CAJ-CAN-CBA-CAB
2	D	1302	Y01	OAG-CAY-OAW-CBC
2	A	1304	Y01	CAJ-CAN-CBA-CAB
2	C	1302	Y01	CAN-CAJ-CAO-CBB
2	D	1303	Y01	CAJ-CAO-CBB-CBE
2	A	1304	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	C	1302	Y01	CAV-CBC-OAW-CAY
2	B	1302	Y01	CAJ-CAN-CBA-CAA
2	D	1303	Y01	CAR-CBC-OAW-CAY
2	A	1302	Y01	CAJ-CAN-CBA-CAA
2	C	1302	Y01	CAR-CBC-OAW-CAY
2	C	1302	Y01	OAG-CAY-OAW-CBC
2	B	1302	Y01	CAM-CAL-CAX-OAF
2	A	1301	Y01	CAL-CAM-CAY-OAW
2	A	1305	Y01	CAM-CAL-CAX-OAF
2	B	1302	Y01	CAM-CAL-CAX-OAH
2	A	1305	Y01	CAM-CAL-CAX-OAH
2	D	1301	Y01	CAL-CAM-CAY-OAW
2	B	1302	Y01	CAN-CAJ-CAO-CBB
2	B	1301	Y01	CAL-CAM-CAY-OAW
2	C	1302	Y01	CAM-CAY-OAW-CBC
2	D	1301	Y01	CAM-CAL-CAX-OAH
2	A	1301	Y01	OAG-CAY-OAW-CBC
2	C	1302	Y01	CAL-CAM-CAY-OAW
2	C	1302	Y01	CAL-CAM-CAY-OAG
2	A	1302	Y01	CAM-CAL-CAX-OAF
2	B	1302	Y01	CAJ-CAN-CBA-CAB

There are no ring outliers.

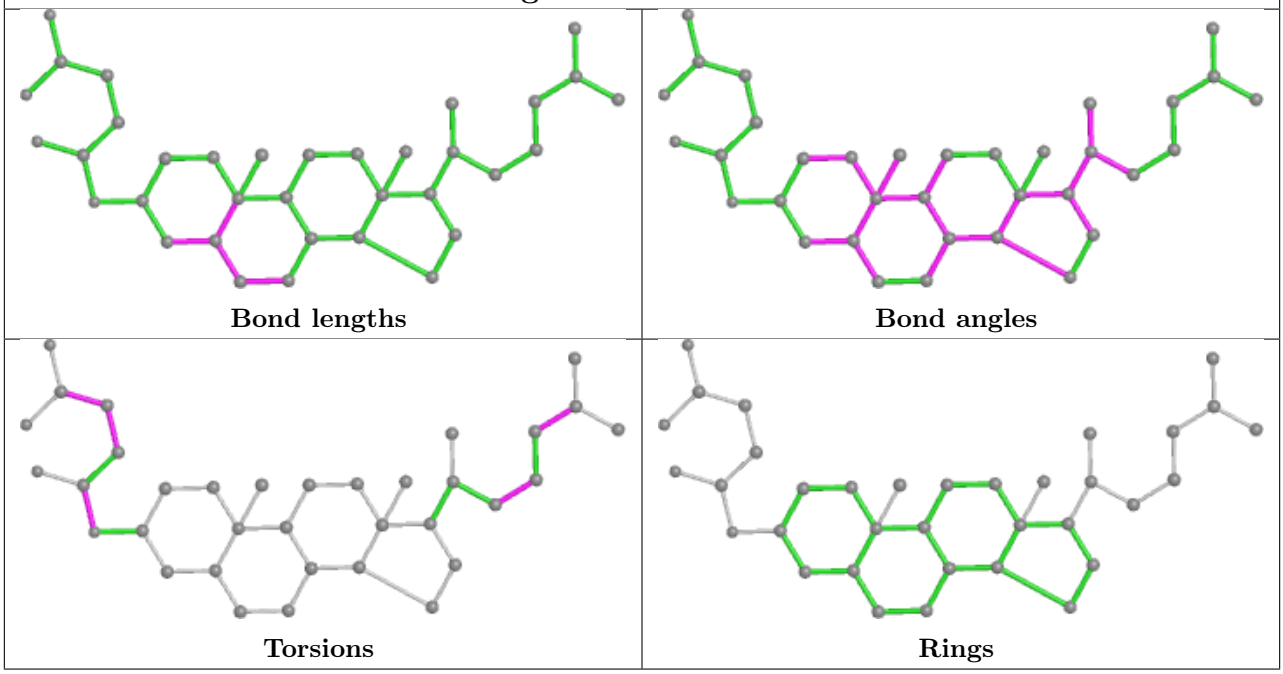
12 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	Y01	1	0
2	A	1303	Y01	6	0
2	C	1301	Y01	6	0
2	D	1301	Y01	1	0
2	C	1302	Y01	12	0
2	B	1301	Y01	2	0
2	D	1302	Y01	11	0
2	D	1303	Y01	29	0
2	A	1304	Y01	3	0
2	A	1305	Y01	42	0
2	A	1301	Y01	7	0
2	B	1302	Y01	15	0

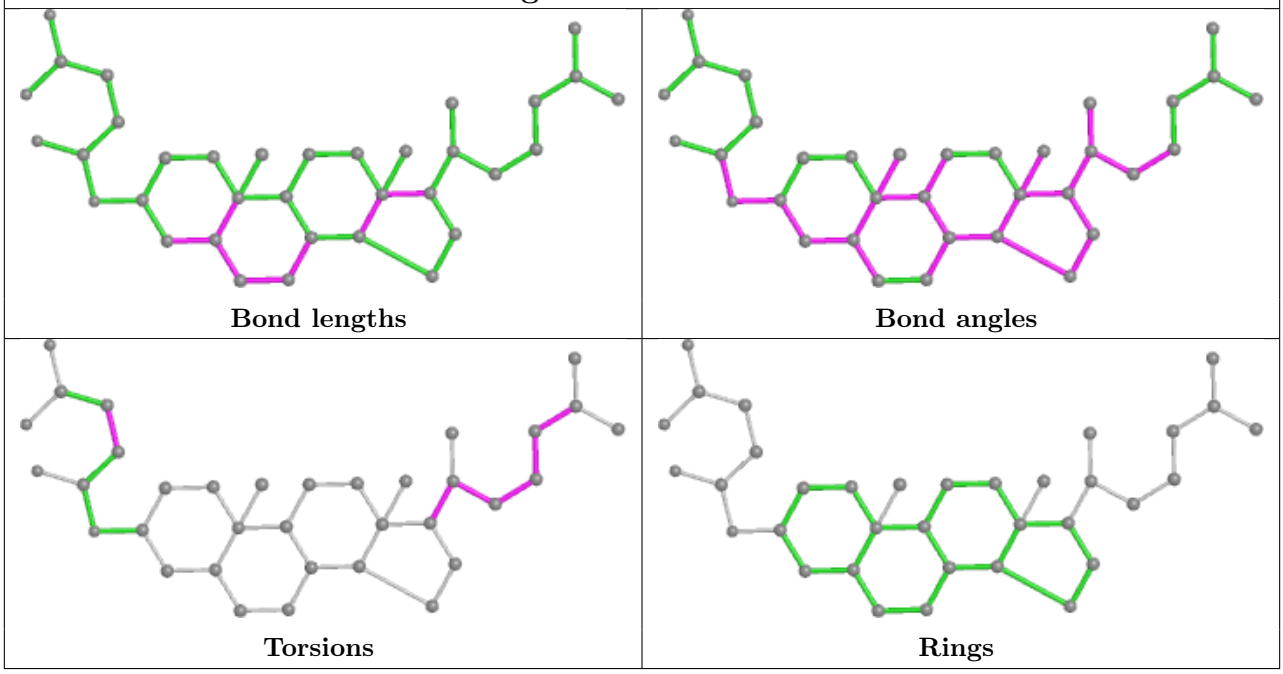
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

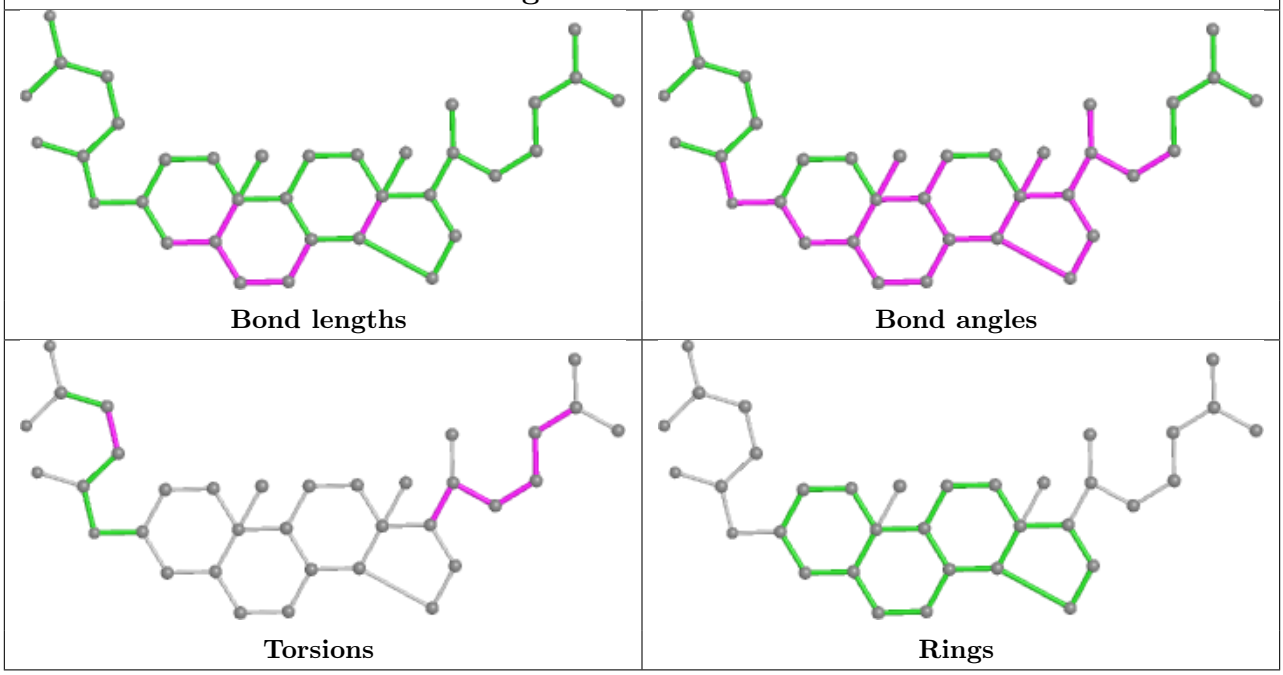
Ligand Y01 A 1302



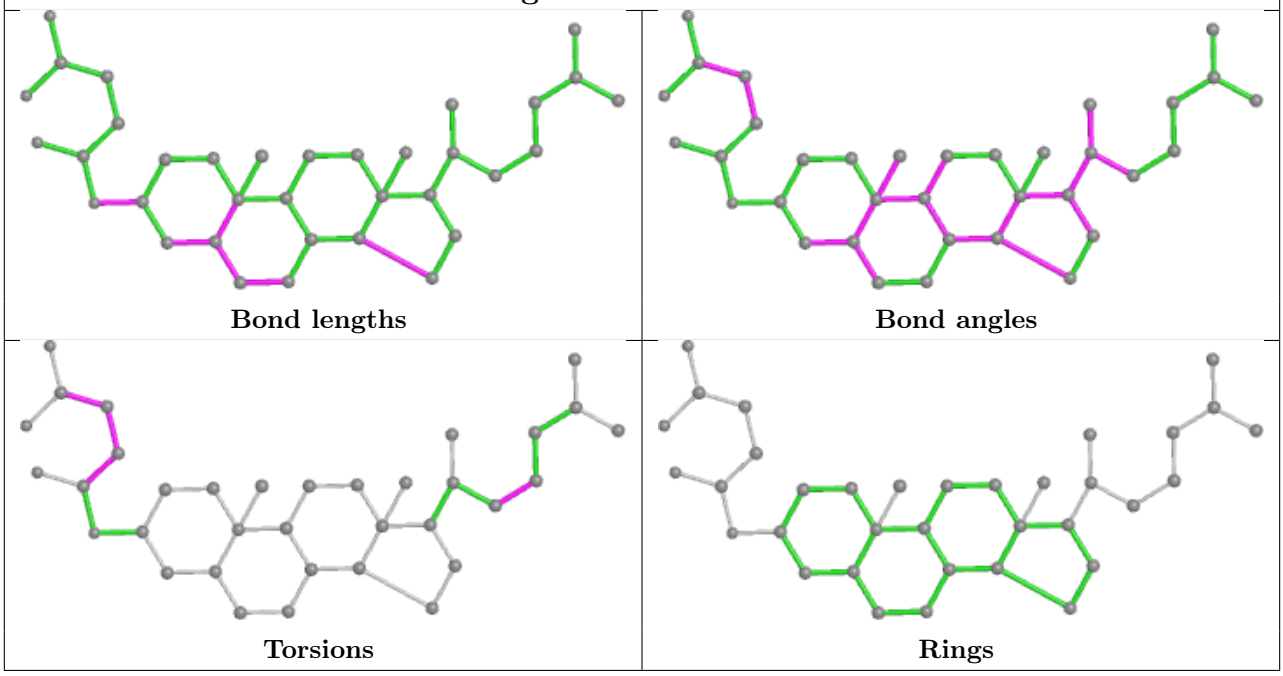
Ligand Y01 A 1303



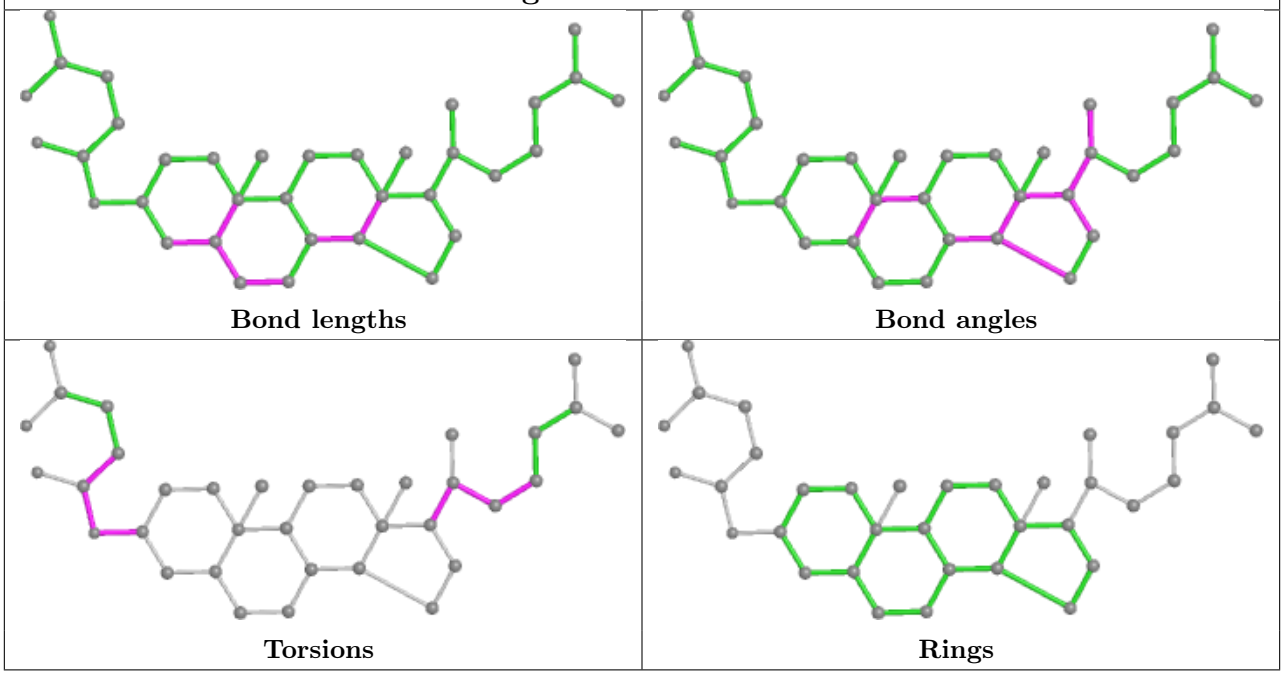
Ligand Y01 C 1301



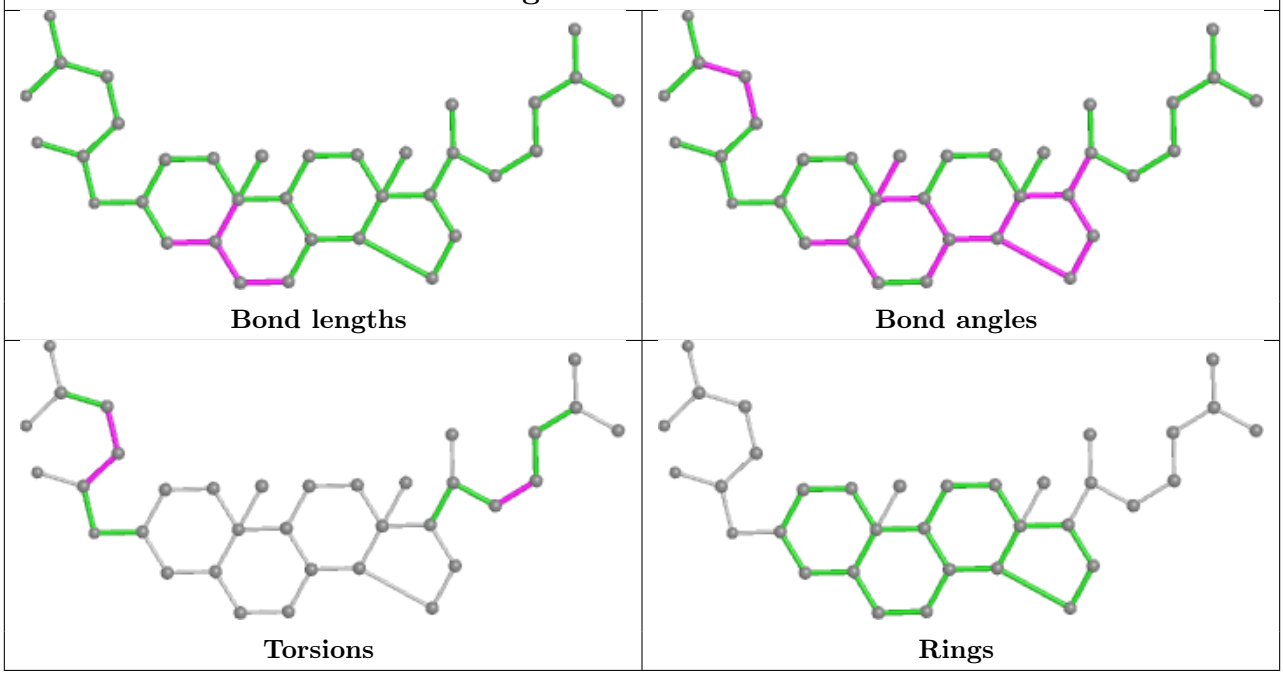
Ligand Y01 D 1301



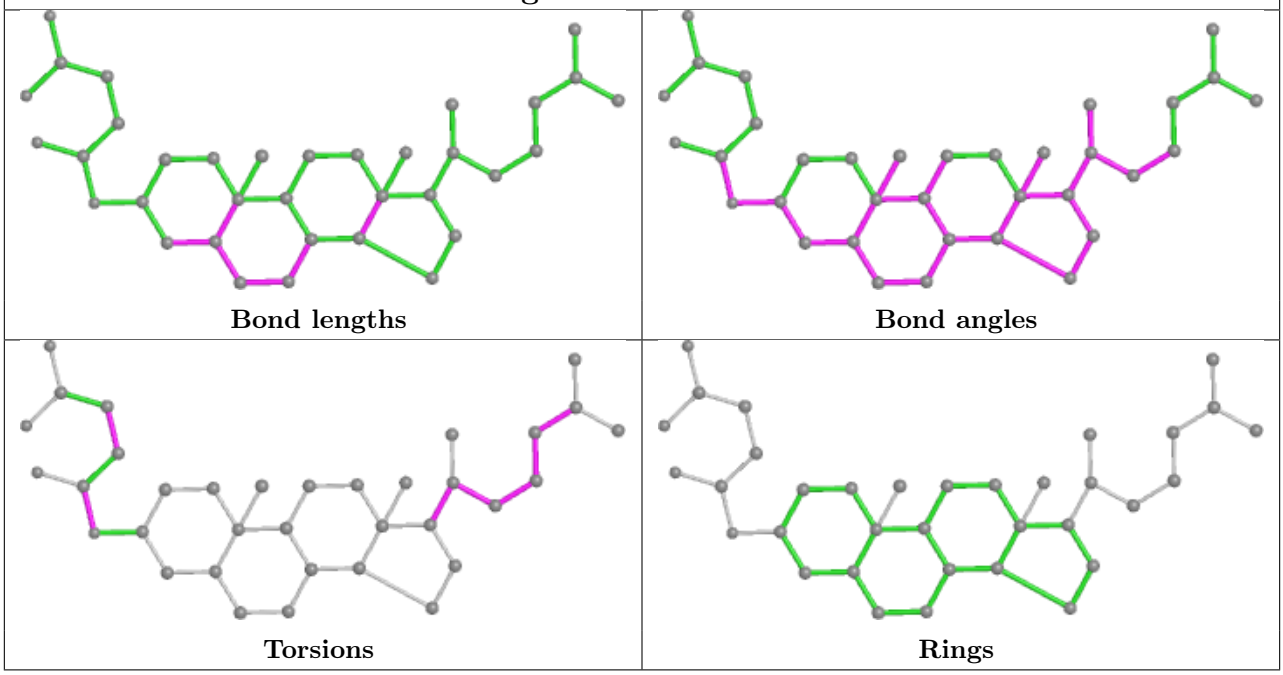
Ligand Y01 C 1302



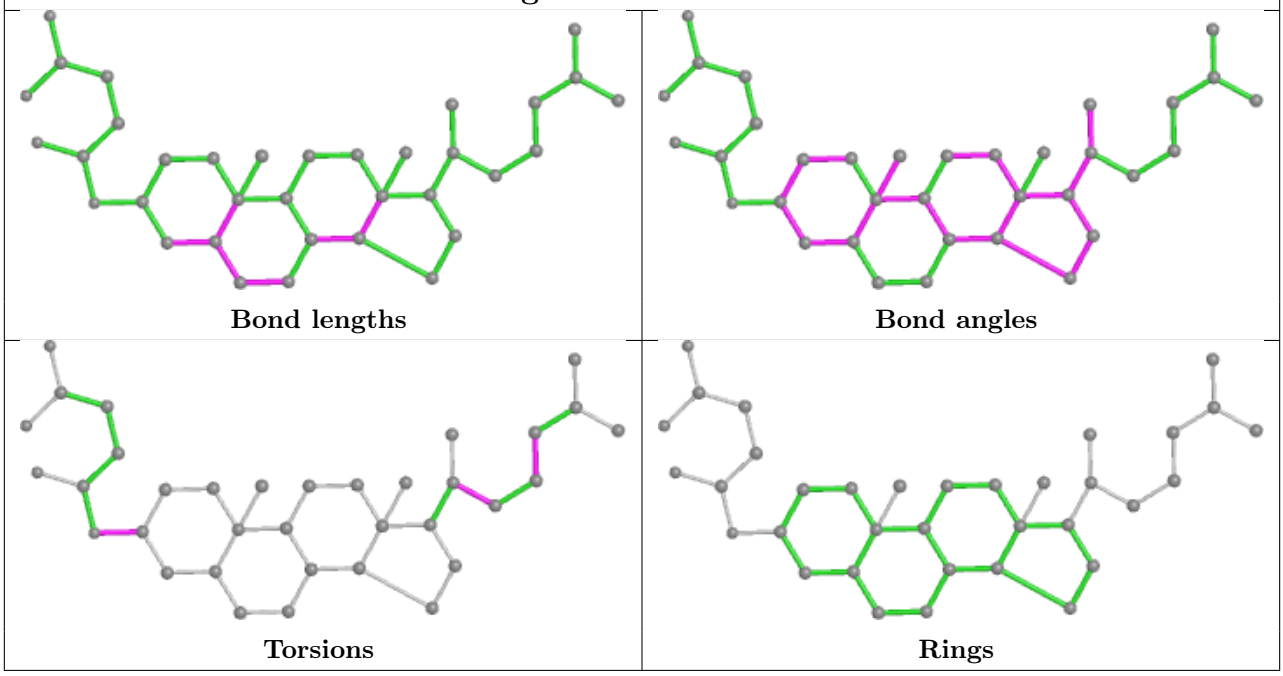
Ligand Y01 B 1301



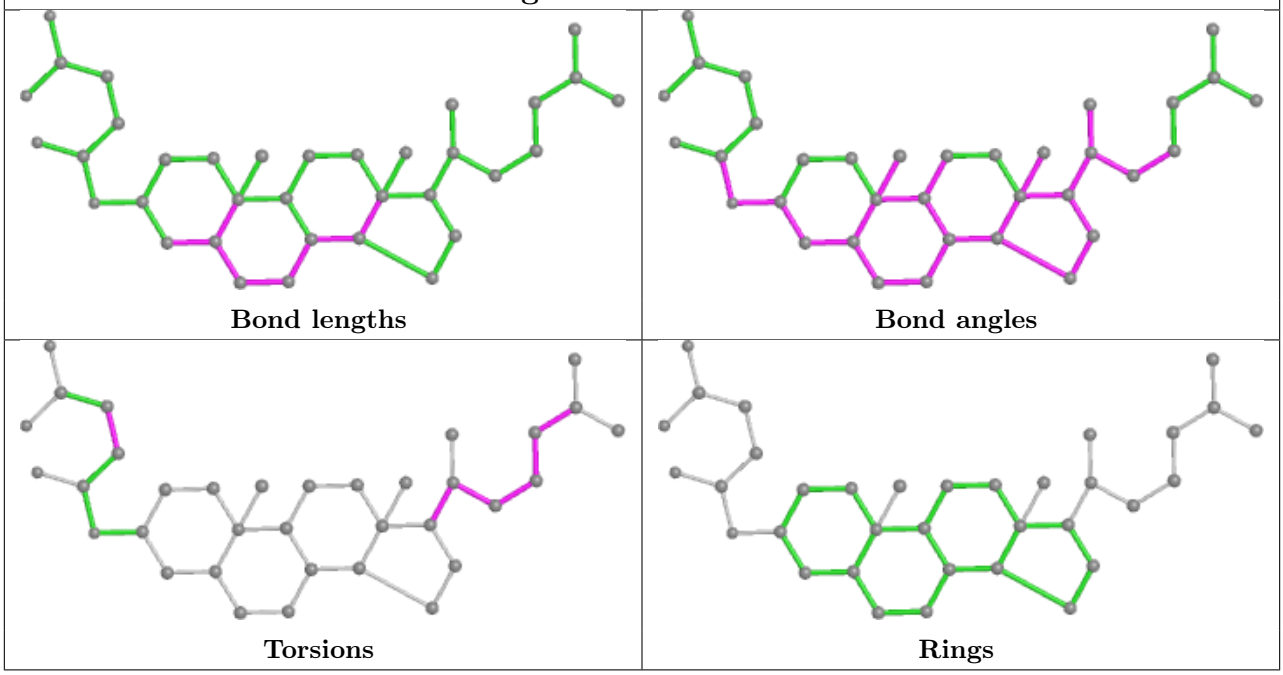
Ligand Y01 D 1302



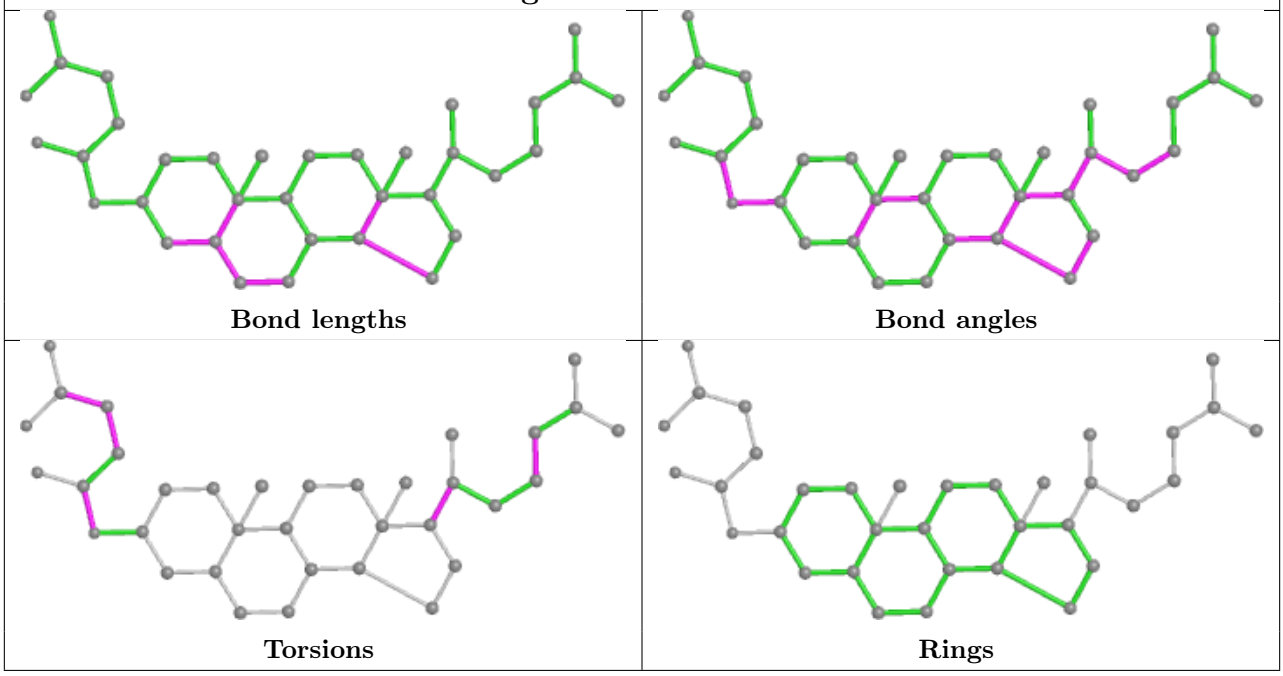
Ligand Y01 D 1303



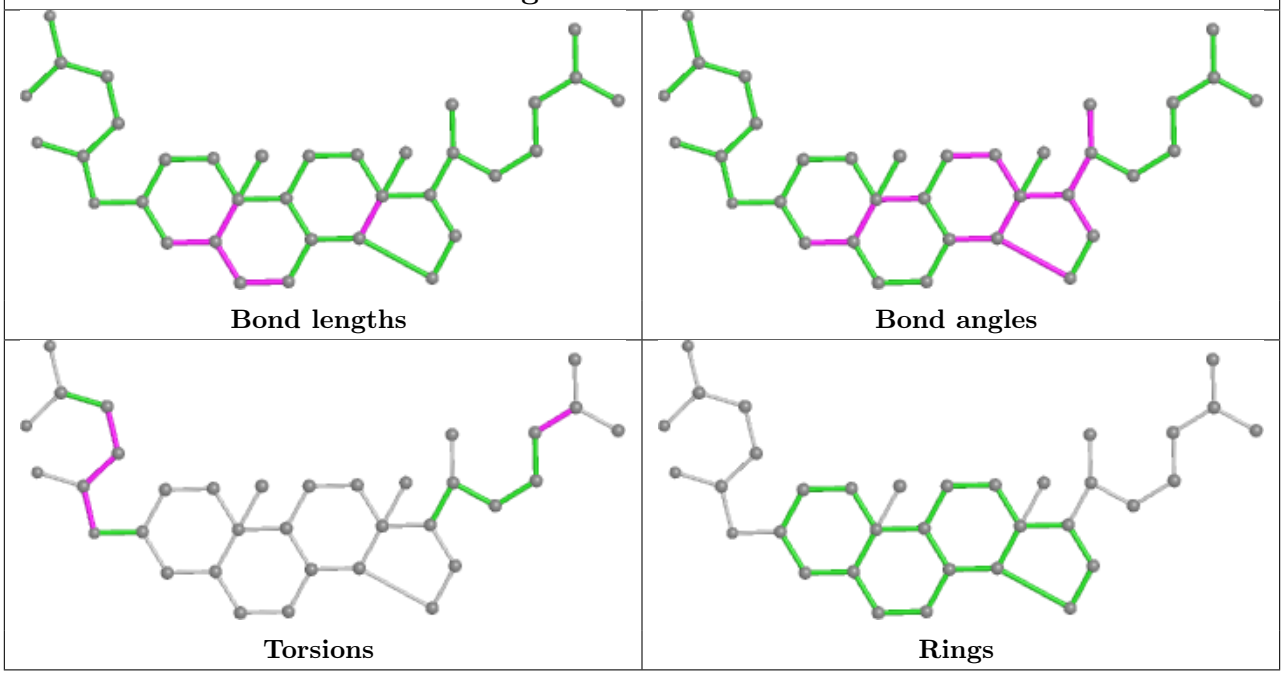
Ligand Y01 A 1304



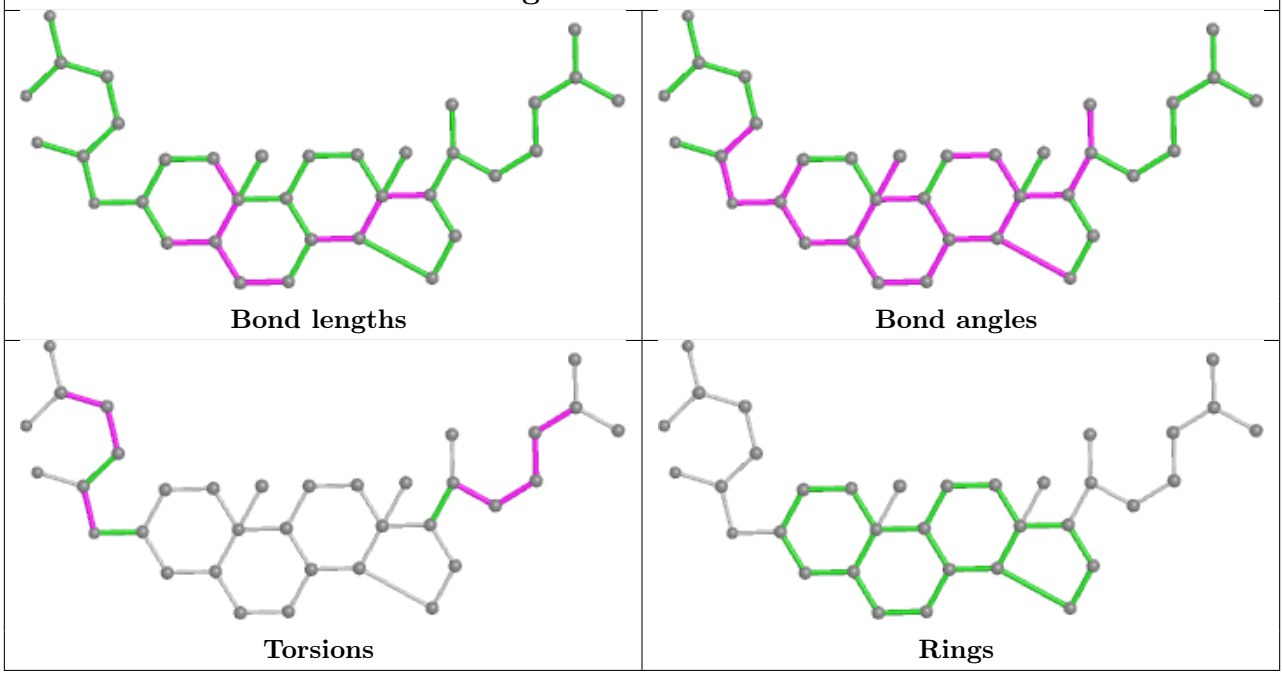
Ligand Y01 A 1305



Ligand Y01 A 1301



Ligand Y01 B 1302



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

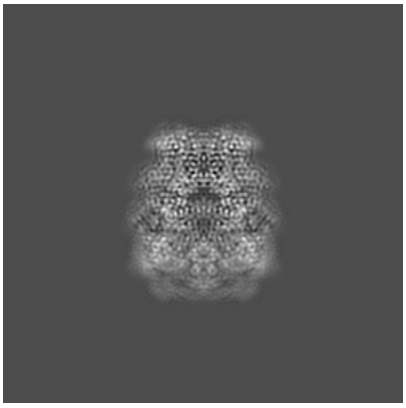
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6975. These allow visual inspection of the internal detail of the map and identification of artifacts.

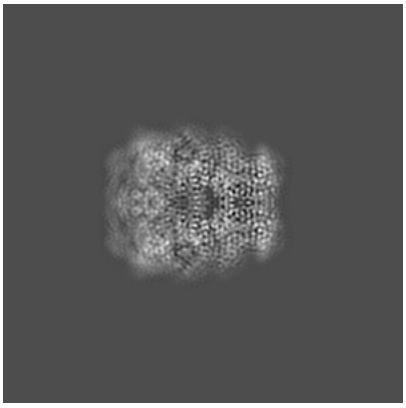
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

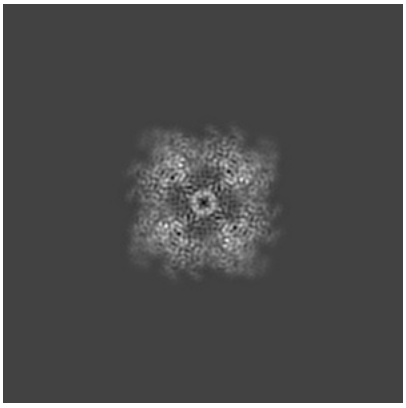
6.1.1 Primary map



X



Y

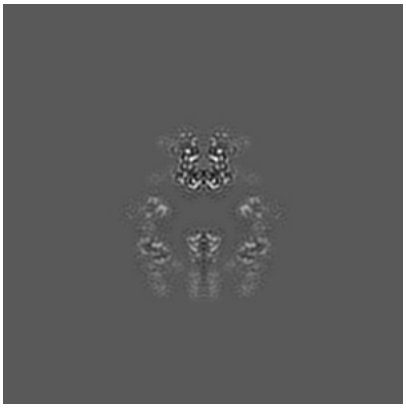


Z

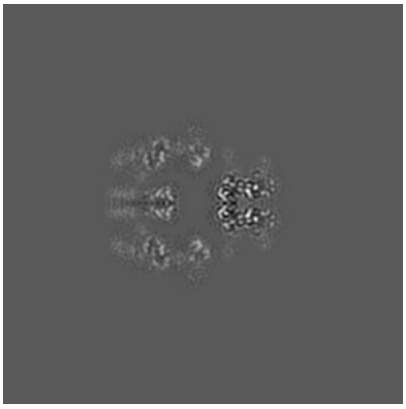
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

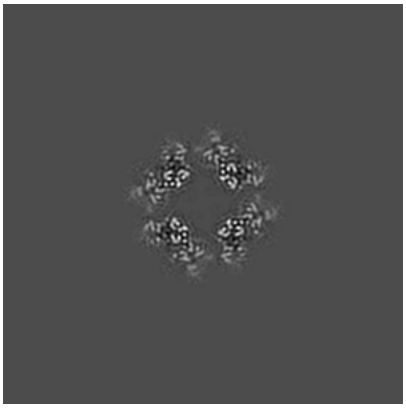
6.2.1 Primary map



X Index: 128



Y Index: 128



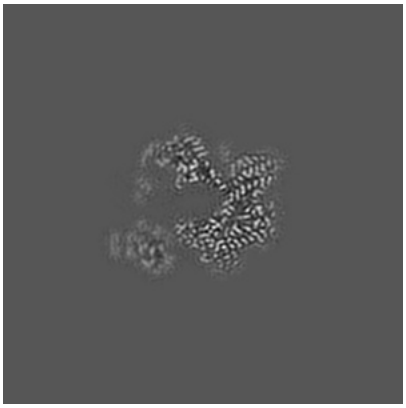
Z Index: 128

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

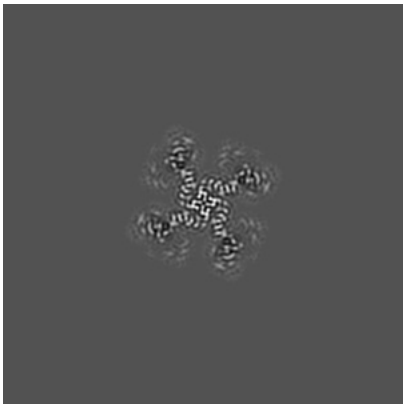
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 142



Y Index: 114

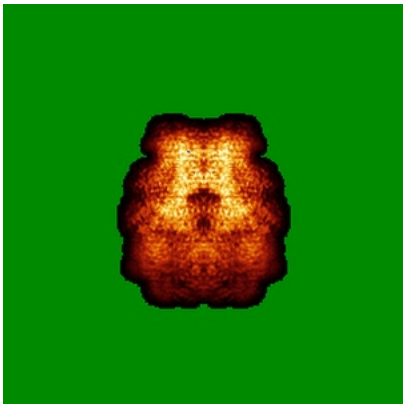


Z Index: 142

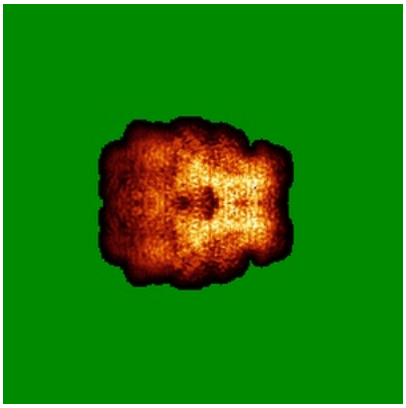
The images above show the largest variance slices of the map in three orthogonal directions.

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

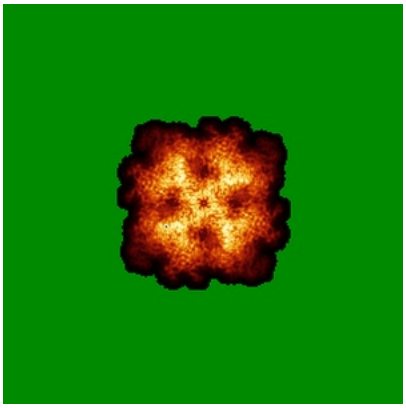
6.4.1 Primary map



X



Y

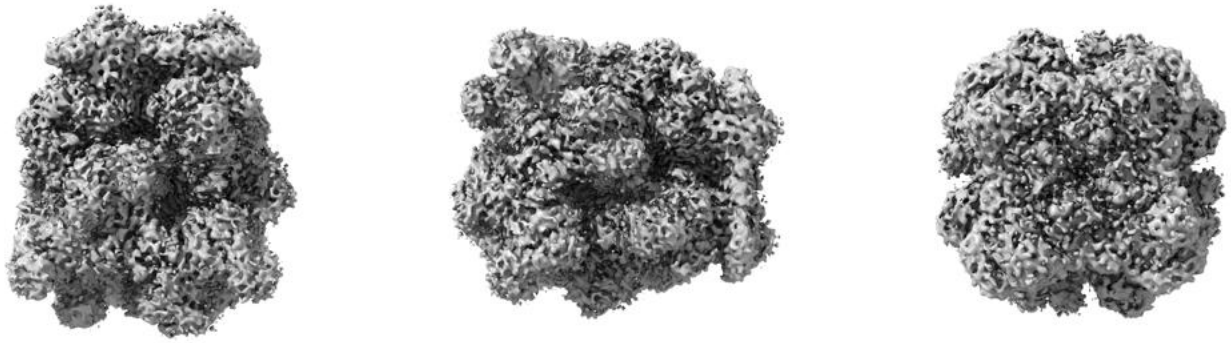


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

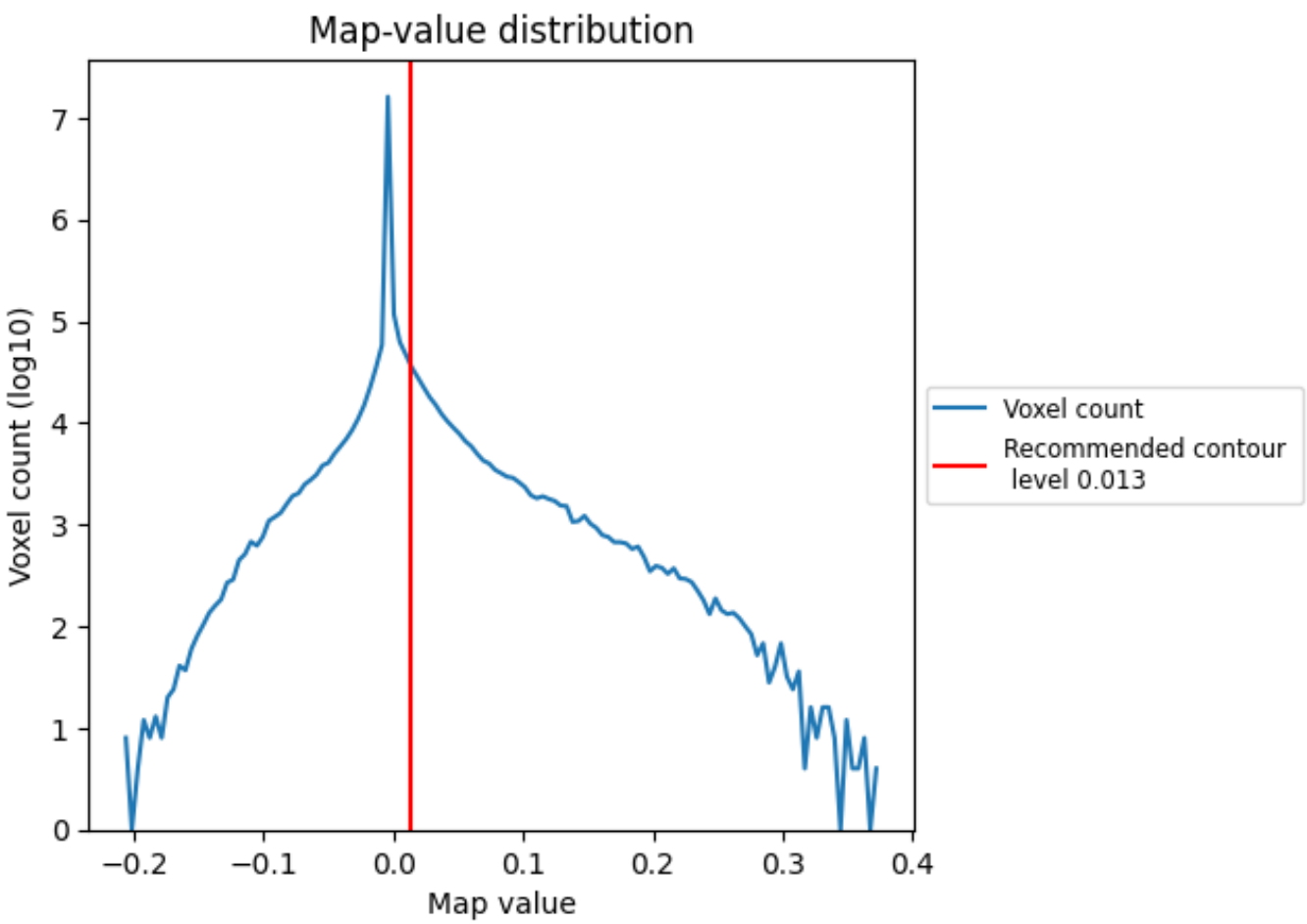
6.6 Mask visualisation (i)

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

7 Map analysis (i)

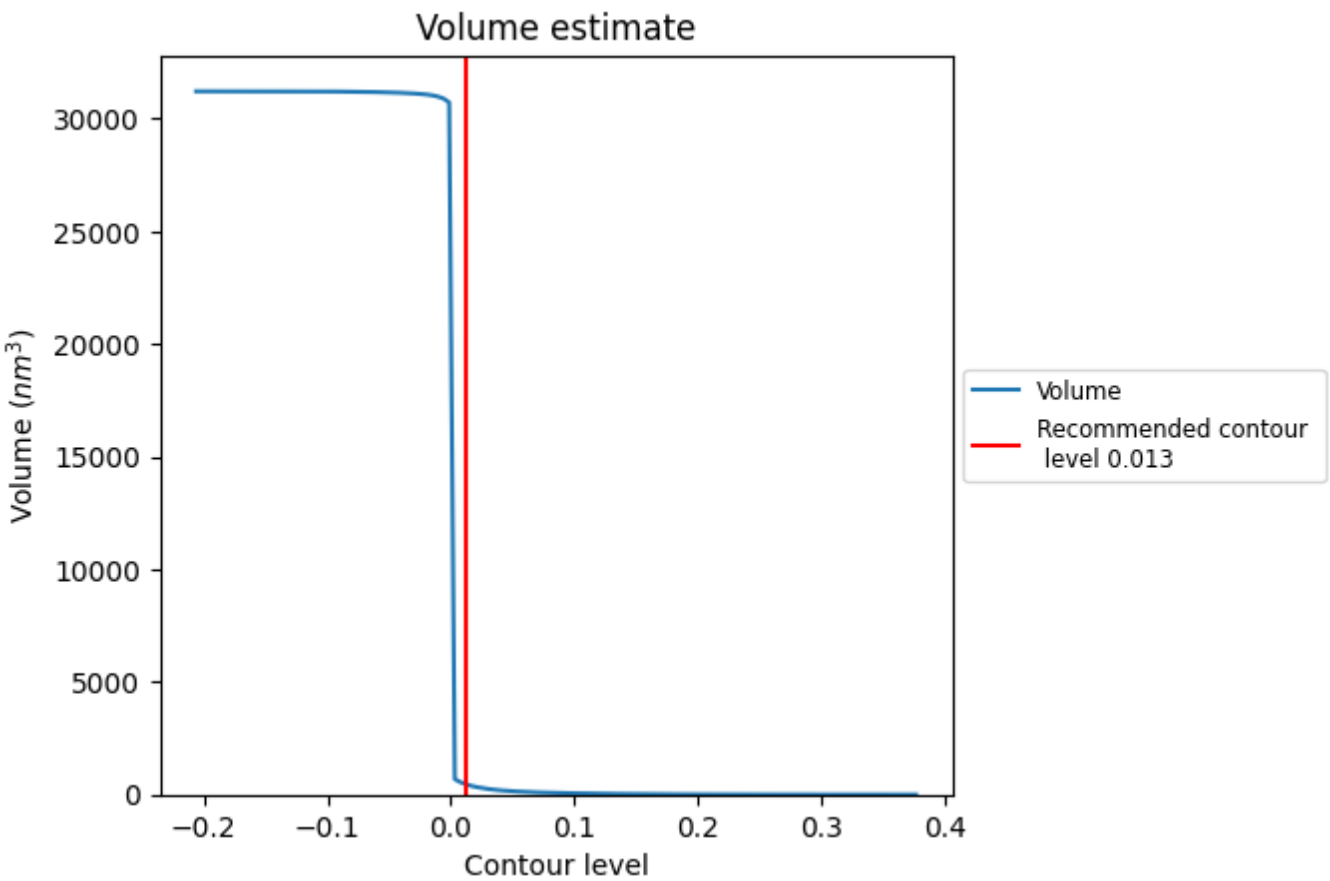
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

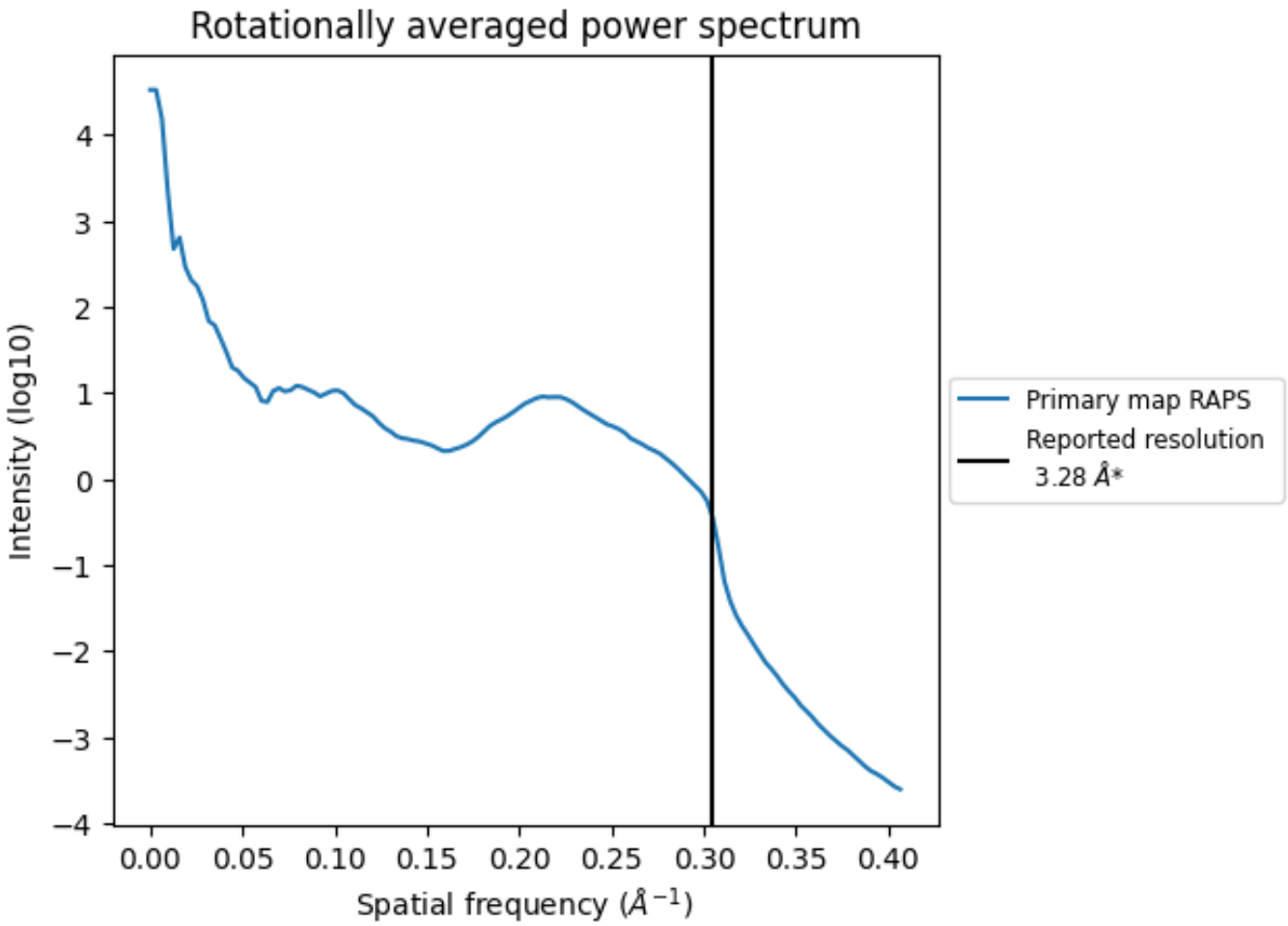
7.2 Volume estimate (i)



The volume at the recommended contour level is 445 nm^3; this corresponds to an approximate mass of 402 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)

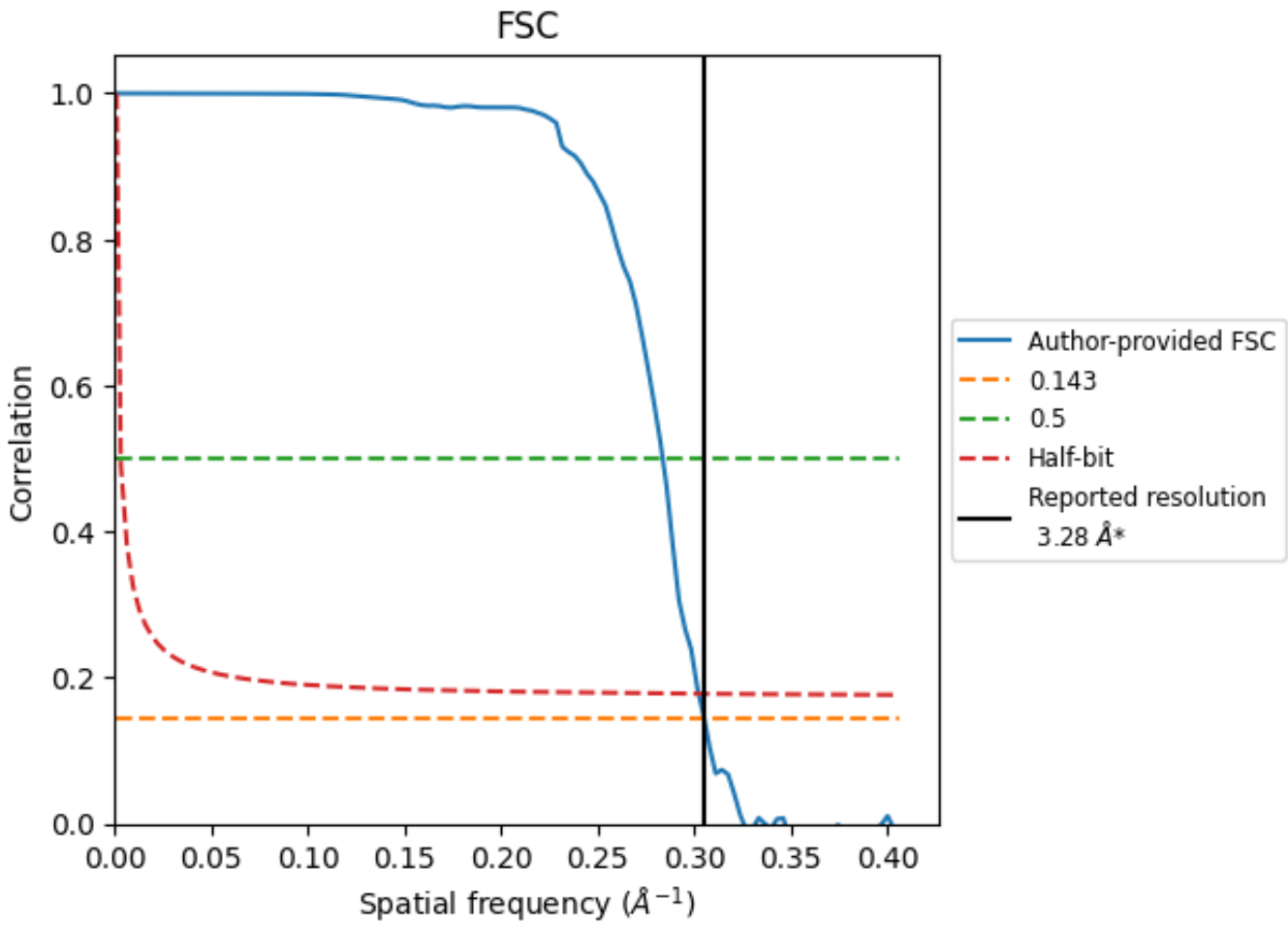


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

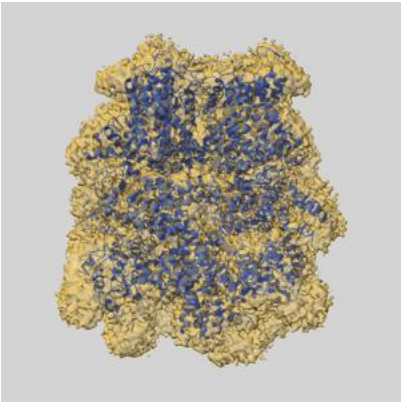
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.52	3.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

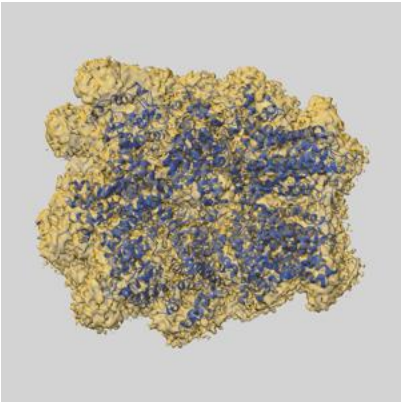
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6975 and PDB model 5ZX5. Per-residue inclusion information can be found in section 3 on page 6.

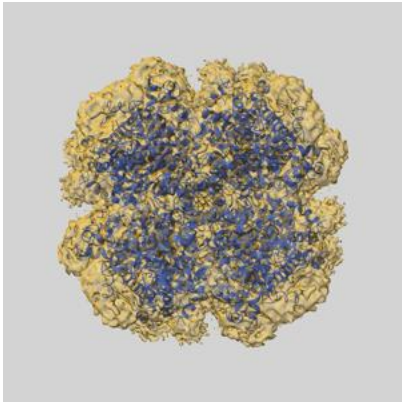
9.1 Map-model overlay (i)



X



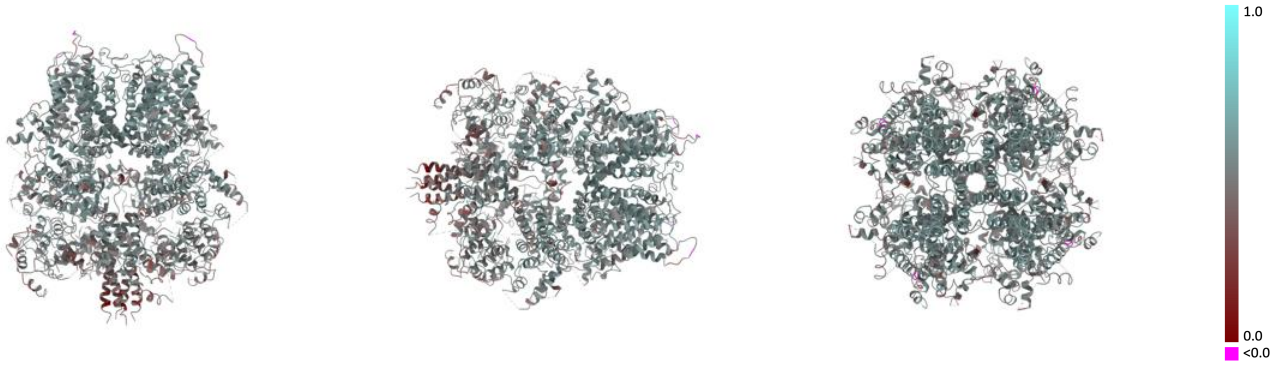
Y



Z

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

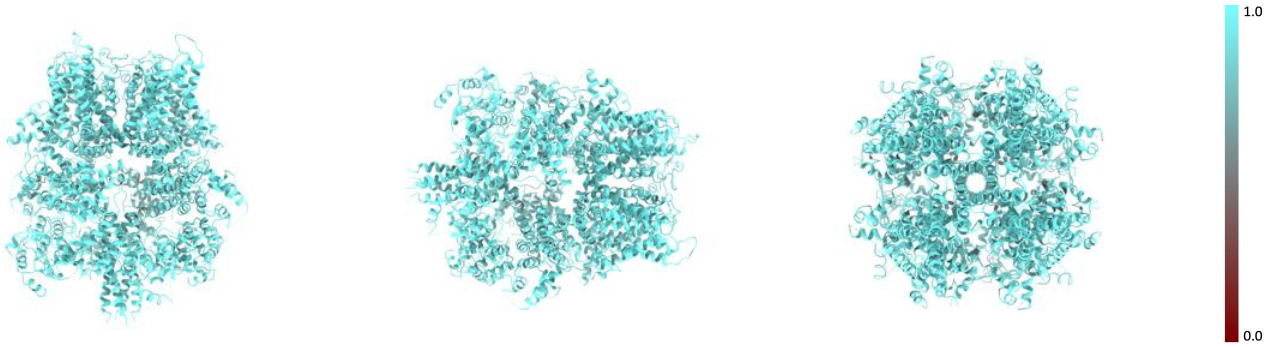
9.2 Q-score mapped to coordinate model (i)



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.

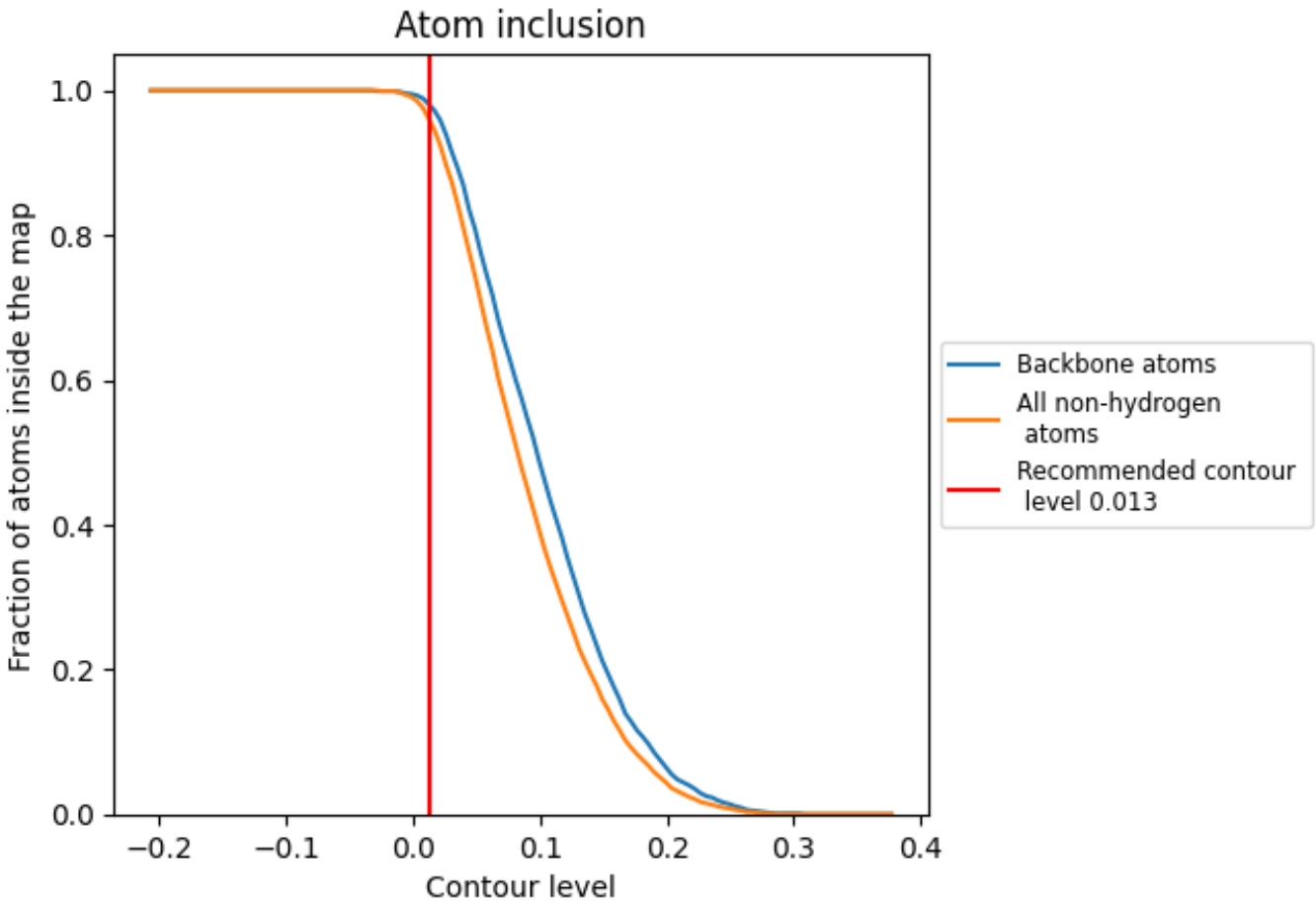
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.9590	0.5110
A	0.9590	0.5110
B	0.9600	0.5110
C	0.9590	0.5110
D	0.9590	0.5110