



Full wwPDB EM Validation Report ⓘ

Nov 5, 2024 – 09:25 AM EST

PDB ID : 9B6G
EMDB ID : EMD-44258
Title : Cryo-EM structure of the mouse TRPM8 channel in complex with the antagonist AMTB
Authors : Yin, Y.; Park, C.-G.; Zhang, F.; Fedor, J.; Feng, S.; Suo, Y.; Im, W.; Lee, S.-Y.
Deposited on : 2024-03-25
Resolution : 2.81 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

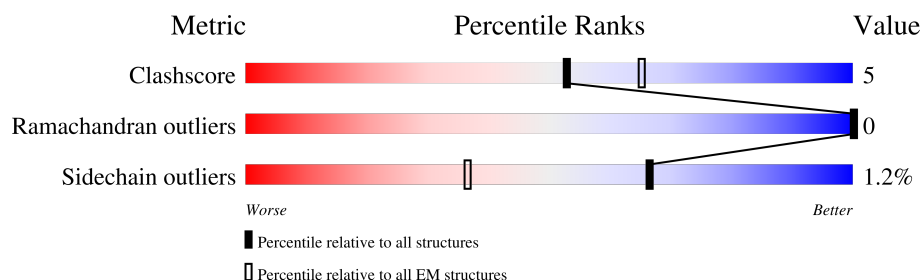
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1135	
1	B	1135	
1	C	1135	
1	D	1135	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 55292 atoms, of which 26808 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 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	915	Total	C	H	N	O	S	0	0
			13321	4524	6417	1138	1214	28		
1	B	915	Total	C	H	N	O	S	0	0
			13321	4524	6417	1138	1214	28		
1	C	915	Total	C	H	N	O	S	0	0
			13321	4524	6417	1138	1214	28		
1	D	915	Total	C	H	N	O	S	0	0
			13321	4524	6417	1138	1214	28		

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8R4D5
A	1	ALA	-	expression tag	UNP Q8R4D5
A	1105	SER	-	expression tag	UNP Q8R4D5
A	1106	ASN	-	expression tag	UNP Q8R4D5
A	1107	SER	-	expression tag	UNP Q8R4D5
A	1108	LEU	-	expression tag	UNP Q8R4D5
A	1109	GLU	-	expression tag	UNP Q8R4D5
A	1110	VAL	-	expression tag	UNP Q8R4D5
A	1111	LEU	-	expression tag	UNP Q8R4D5
A	1112	PHE	-	expression tag	UNP Q8R4D5
A	1113	GLN	-	expression tag	UNP Q8R4D5
A	1114	GLY	-	expression tag	UNP Q8R4D5
A	1115	PRO	-	expression tag	UNP Q8R4D5
A	1116	ASP	-	expression tag	UNP Q8R4D5
A	1117	TYR	-	expression tag	UNP Q8R4D5
A	1118	LYS	-	expression tag	UNP Q8R4D5
A	1119	ASP	-	expression tag	UNP Q8R4D5
A	1120	ASP	-	expression tag	UNP Q8R4D5
A	1121	ASP	-	expression tag	UNP Q8R4D5
A	1122	ASP	-	expression tag	UNP Q8R4D5
A	1123	LYS	-	expression tag	UNP Q8R4D5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1124	ALA	-	expression tag	UNP Q8R4D5
A	1125	HIS	-	expression tag	UNP Q8R4D5
A	1126	HIS	-	expression tag	UNP Q8R4D5
A	1127	HIS	-	expression tag	UNP Q8R4D5
A	1128	HIS	-	expression tag	UNP Q8R4D5
A	1129	HIS	-	expression tag	UNP Q8R4D5
A	1130	HIS	-	expression tag	UNP Q8R4D5
A	1131	HIS	-	expression tag	UNP Q8R4D5
A	1132	HIS	-	expression tag	UNP Q8R4D5
A	1133	HIS	-	expression tag	UNP Q8R4D5
A	1134	HIS	-	expression tag	UNP Q8R4D5
B	0	MET	-	initiating methionine	UNP Q8R4D5
B	1	ALA	-	expression tag	UNP Q8R4D5
B	1105	SER	-	expression tag	UNP Q8R4D5
B	1106	ASN	-	expression tag	UNP Q8R4D5
B	1107	SER	-	expression tag	UNP Q8R4D5
B	1108	LEU	-	expression tag	UNP Q8R4D5
B	1109	GLU	-	expression tag	UNP Q8R4D5
B	1110	VAL	-	expression tag	UNP Q8R4D5
B	1111	LEU	-	expression tag	UNP Q8R4D5
B	1112	PHE	-	expression tag	UNP Q8R4D5
B	1113	GLN	-	expression tag	UNP Q8R4D5
B	1114	GLY	-	expression tag	UNP Q8R4D5
B	1115	PRO	-	expression tag	UNP Q8R4D5
B	1116	ASP	-	expression tag	UNP Q8R4D5
B	1117	TYR	-	expression tag	UNP Q8R4D5
B	1118	LYS	-	expression tag	UNP Q8R4D5
B	1119	ASP	-	expression tag	UNP Q8R4D5
B	1120	ASP	-	expression tag	UNP Q8R4D5
B	1121	ASP	-	expression tag	UNP Q8R4D5
B	1122	ASP	-	expression tag	UNP Q8R4D5
B	1123	LYS	-	expression tag	UNP Q8R4D5
B	1124	ALA	-	expression tag	UNP Q8R4D5
B	1125	HIS	-	expression tag	UNP Q8R4D5
B	1126	HIS	-	expression tag	UNP Q8R4D5
B	1127	HIS	-	expression tag	UNP Q8R4D5
B	1128	HIS	-	expression tag	UNP Q8R4D5
B	1129	HIS	-	expression tag	UNP Q8R4D5
B	1130	HIS	-	expression tag	UNP Q8R4D5
B	1131	HIS	-	expression tag	UNP Q8R4D5
B	1132	HIS	-	expression tag	UNP Q8R4D5
B	1133	HIS	-	expression tag	UNP Q8R4D5

Continued on next page...

Continued from previous page...

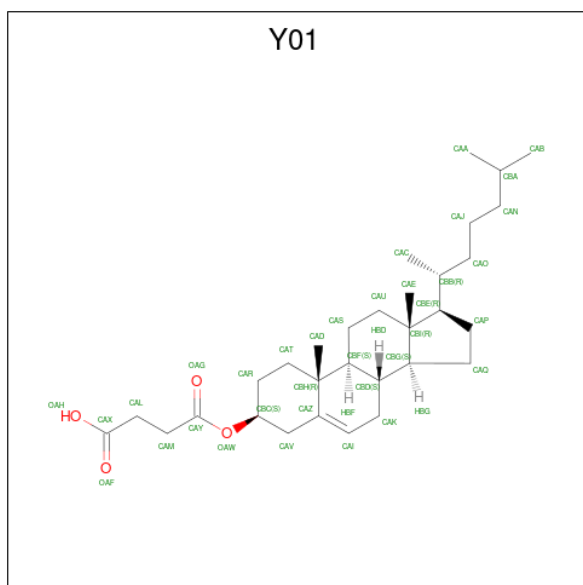
Chain	Residue	Modelled	Actual	Comment	Reference
B	1134	HIS	-	expression tag	UNP Q8R4D5
C	0	MET	-	initiating methionine	UNP Q8R4D5
C	1	ALA	-	expression tag	UNP Q8R4D5
C	1105	SER	-	expression tag	UNP Q8R4D5
C	1106	ASN	-	expression tag	UNP Q8R4D5
C	1107	SER	-	expression tag	UNP Q8R4D5
C	1108	LEU	-	expression tag	UNP Q8R4D5
C	1109	GLU	-	expression tag	UNP Q8R4D5
C	1110	VAL	-	expression tag	UNP Q8R4D5
C	1111	LEU	-	expression tag	UNP Q8R4D5
C	1112	PHE	-	expression tag	UNP Q8R4D5
C	1113	GLN	-	expression tag	UNP Q8R4D5
C	1114	GLY	-	expression tag	UNP Q8R4D5
C	1115	PRO	-	expression tag	UNP Q8R4D5
C	1116	ASP	-	expression tag	UNP Q8R4D5
C	1117	TYR	-	expression tag	UNP Q8R4D5
C	1118	LYS	-	expression tag	UNP Q8R4D5
C	1119	ASP	-	expression tag	UNP Q8R4D5
C	1120	ASP	-	expression tag	UNP Q8R4D5
C	1121	ASP	-	expression tag	UNP Q8R4D5
C	1122	ASP	-	expression tag	UNP Q8R4D5
C	1123	LYS	-	expression tag	UNP Q8R4D5
C	1124	ALA	-	expression tag	UNP Q8R4D5
C	1125	HIS	-	expression tag	UNP Q8R4D5
C	1126	HIS	-	expression tag	UNP Q8R4D5
C	1127	HIS	-	expression tag	UNP Q8R4D5
C	1128	HIS	-	expression tag	UNP Q8R4D5
C	1129	HIS	-	expression tag	UNP Q8R4D5
C	1130	HIS	-	expression tag	UNP Q8R4D5
C	1131	HIS	-	expression tag	UNP Q8R4D5
C	1132	HIS	-	expression tag	UNP Q8R4D5
C	1133	HIS	-	expression tag	UNP Q8R4D5
C	1134	HIS	-	expression tag	UNP Q8R4D5
D	0	MET	-	initiating methionine	UNP Q8R4D5
D	1	ALA	-	expression tag	UNP Q8R4D5
D	1105	SER	-	expression tag	UNP Q8R4D5
D	1106	ASN	-	expression tag	UNP Q8R4D5
D	1107	SER	-	expression tag	UNP Q8R4D5
D	1108	LEU	-	expression tag	UNP Q8R4D5
D	1109	GLU	-	expression tag	UNP Q8R4D5
D	1110	VAL	-	expression tag	UNP Q8R4D5
D	1111	LEU	-	expression tag	UNP Q8R4D5

Continued on next page...

Continued from previous page...

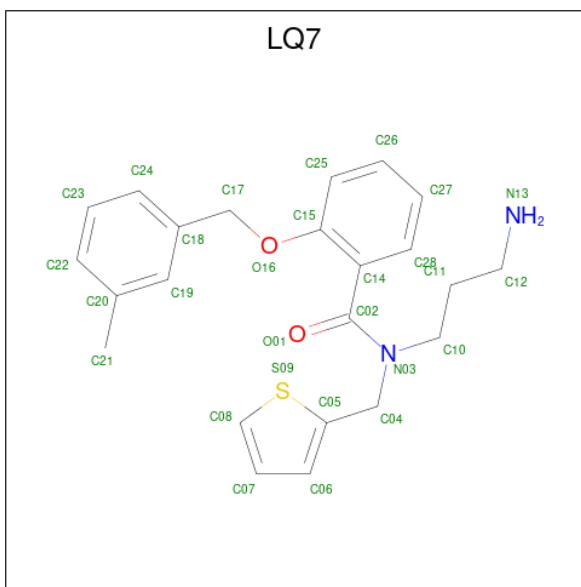
Chain	Residue	Modelled	Actual	Comment	Reference
D	1112	PHE	-	expression tag	UNP Q8R4D5
D	1113	GLN	-	expression tag	UNP Q8R4D5
D	1114	GLY	-	expression tag	UNP Q8R4D5
D	1115	PRO	-	expression tag	UNP Q8R4D5
D	1116	ASP	-	expression tag	UNP Q8R4D5
D	1117	TYR	-	expression tag	UNP Q8R4D5
D	1118	LYS	-	expression tag	UNP Q8R4D5
D	1119	ASP	-	expression tag	UNP Q8R4D5
D	1120	ASP	-	expression tag	UNP Q8R4D5
D	1121	ASP	-	expression tag	UNP Q8R4D5
D	1122	ASP	-	expression tag	UNP Q8R4D5
D	1123	LYS	-	expression tag	UNP Q8R4D5
D	1124	ALA	-	expression tag	UNP Q8R4D5
D	1125	HIS	-	expression tag	UNP Q8R4D5
D	1126	HIS	-	expression tag	UNP Q8R4D5
D	1127	HIS	-	expression tag	UNP Q8R4D5
D	1128	HIS	-	expression tag	UNP Q8R4D5
D	1129	HIS	-	expression tag	UNP Q8R4D5
D	1130	HIS	-	expression tag	UNP Q8R4D5
D	1131	HIS	-	expression tag	UNP Q8R4D5
D	1132	HIS	-	expression tag	UNP Q8R4D5
D	1133	HIS	-	expression tag	UNP Q8R4D5
D	1134	HIS	-	expression tag	UNP Q8R4D5

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



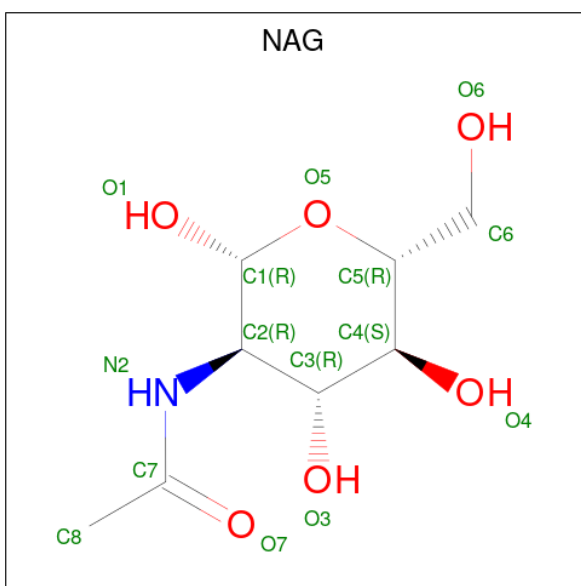
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	A	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	B	1	Total	C	H	O	0
			84	31	49	4	
2	C	1	Total	C	H	O	0
			84	31	49	4	
2	C	1	Total	C	H	O	0
			84	31	49	4	
2	C	1	Total	C	H	O	0
			84	31	49	4	
2	C	1	Total	C	H	O	0
			84	31	49	4	
2	C	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	
2	D	1	Total	C	H	O	0
			84	31	49	4	

- Molecule 3 is N-(3-aminopropyl)-2-[(3-methylphenyl)methoxy]-N-[(thiophen-2-yl)methyl]benzamide (three-letter code: LQ7) (formula: C₂₃H₂₆N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total 54	C 23	H 26	N 2	O 2	S 1	0
3	B	1	Total 54	C 23	H 26	N 2	O 2	S 1	0
3	C	1	Total 54	C 23	H 26	N 2	O 2	S 1	0
3	D	1	Total 54	C 23	H 26	N 2	O 2	S 1	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

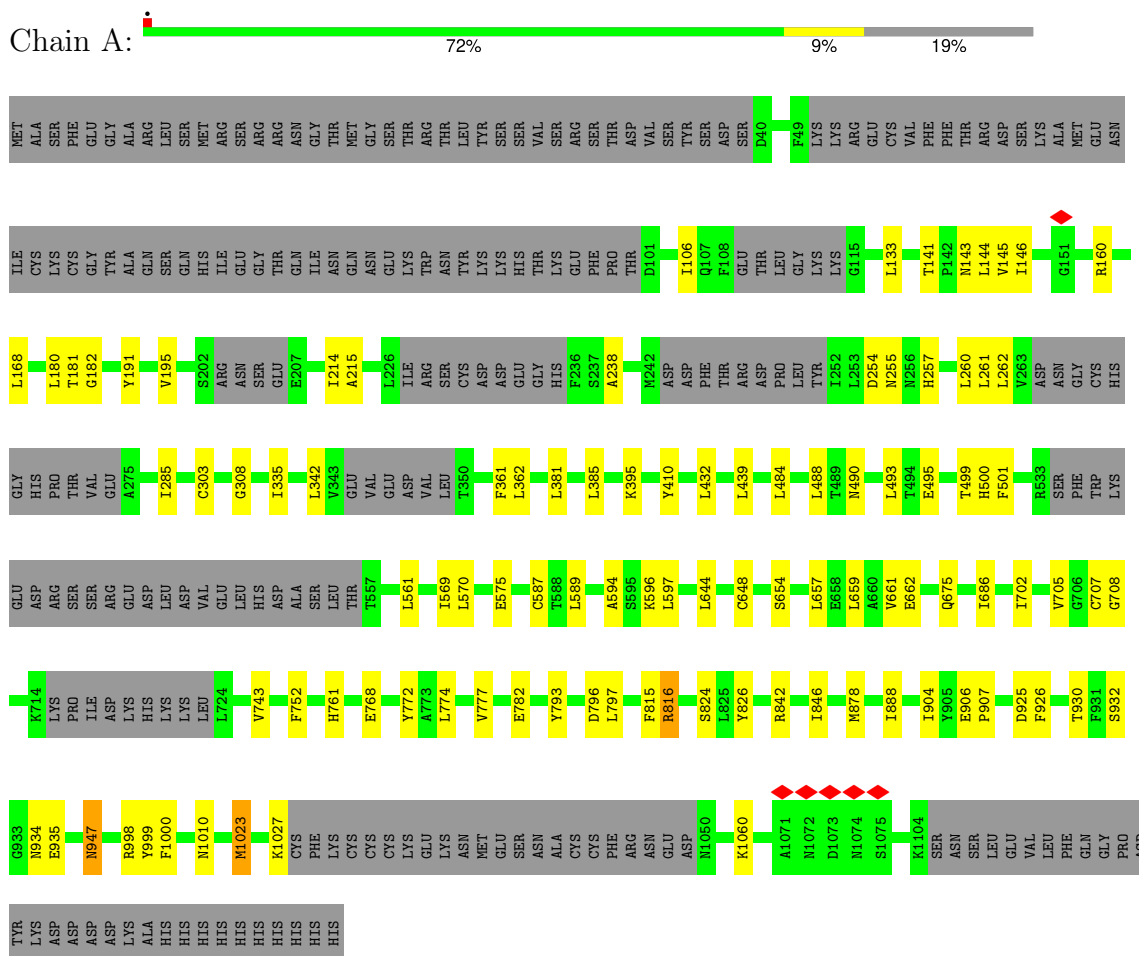


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 28	C 8	H 14	N 1	O 5	0
4	B	1	Total 28	C 8	H 14	N 1	O 5	0
4	C	1	Total 28	C 8	H 14	N 1	O 5	0
4	D	1	Total 28	C 8	H 14	N 1	O 5	0

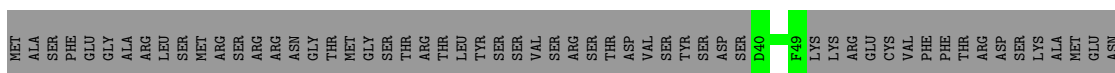
3 Residue-property plots

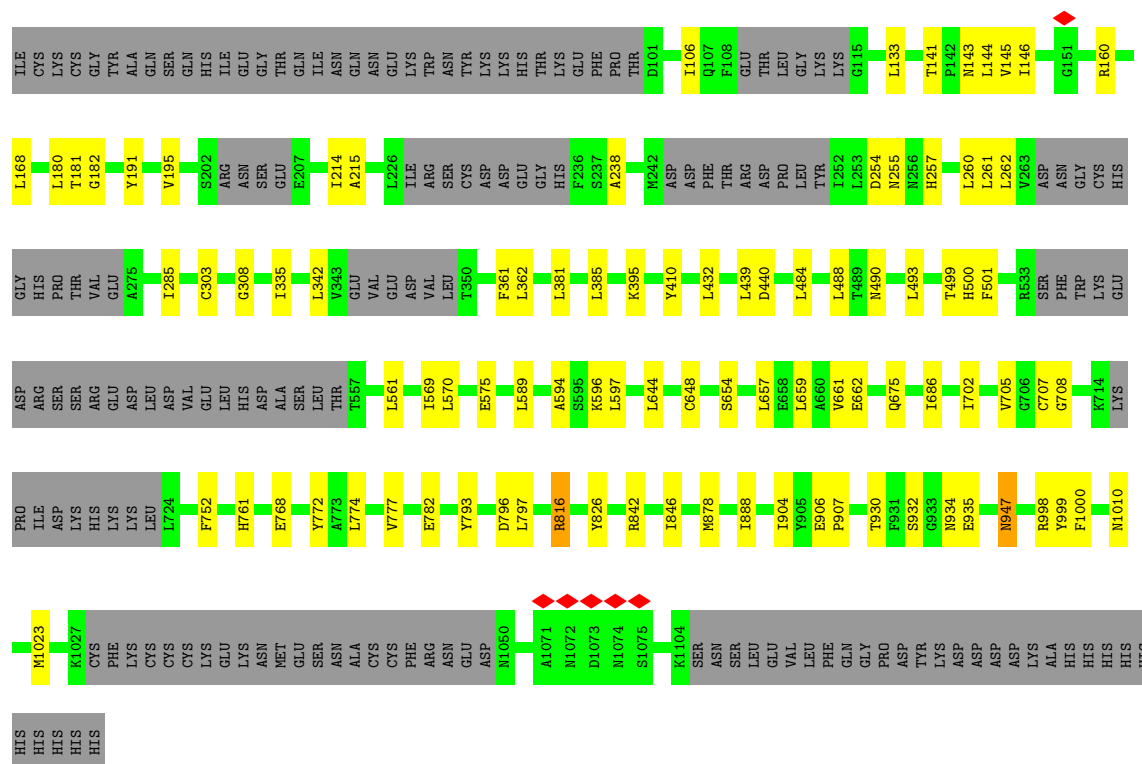
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transient receptor potential cation channel subfamily M member 8



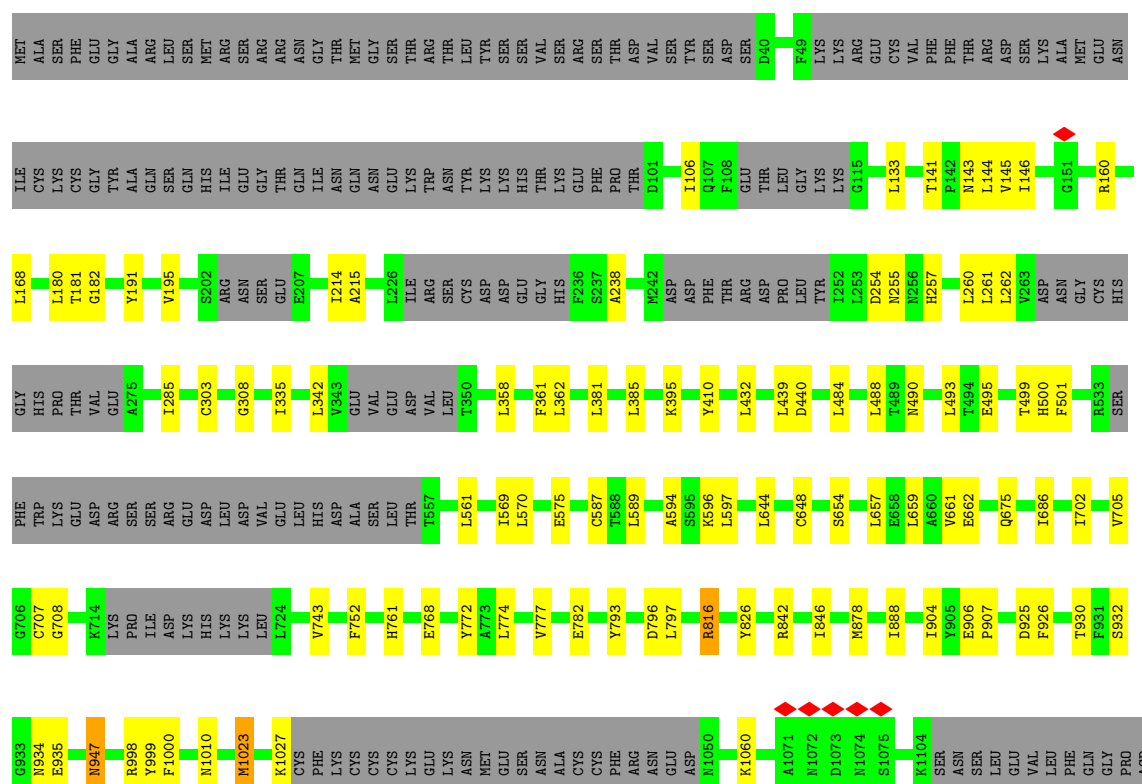
- Molecule 1: Transient receptor potential cation channel subfamily M member 8





- Molecule 1: Transient receptor potential cation channel subfamily M member 8

Chain C: 72% 9% 19%



TYR
LYS
ASP
ASP
ASP
ASP
LYS
ALA
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Transient receptor potential cation channel subfamily M member 8



MET
ALA
SER
PHE
GLY
GLY
ALA
ARG
LEU
SER
MET
MET
ARG
SER
ARG
ARG
ASN
GLY
THR
MET
GLY
SER
THR
THR
LEU
TYR
SER
SER
VAL
SER
SER
ARG
SER
THR
ASP
SER
D40
F49
LYS
LYS
ARG
GLU
CYS
VAL
PHE
THR
THR
ASP
SER
LYS
ALA
MET
GLU
ASN

ILE
CYS
LYS
CYS
GLY
TYR
ALA
GLN
SER
GLN
HIS
HIS
ILE
THR
GLY
THR
ASN
GLN
ASN
GLY
ASN
GLU
TRP
LYS
TYR
LYS
HIS
HIS
THR
VAL
SER
GLY
PHE
PRO
THR
D101
I106
Q107
F108
GLU
THR
LEU
GLY
LYS
LYS
G115
L133
T141
P142
N143
L144
V145
I146
G151
R160

L168
L180
T181
G182
Y191
V195
S202
ARG
ASN
SER
SER
E207
I214
A215
L225
ILE
ARG
SER
CYS
ASP
ASP
GLY
HIS
F236
S237
A238
M242
ASP
PHE
THR
ASP
PRO
TYR
I252
L253
D254
N255
N256
H257
L260
L261
L262
V263
ASP
ASN
GLY
CYS
HIS

GLY
HIS
PRO
THR
VAL
GLU
A275
I285
C303
G308
I335
L342
V343
GLU
VAL
ASP
VAL
LEU
T350
L358
F361
L362
L381
L385
K395
Y410
L432
L439
L484
L488
T489
N490
L493
T494
E495
T499
H500
F501
R533
PHE

TRP
LYS
GLU
ASP
ARG
SER
SER
ARG
GLU
ASP
ASP
VAL
GLU
LEU
HIS
ASP
ALA
SER
LEU
THR
T557
L561
I569
L570
E575
L589
A594
S595
K596
L597
L644
C648
S654
L657
E658
L659
A660
V661
E662
Q675
I686
F925
F926
I702
V705
G706
C707
G708

K714
LYS
PRO
ILE
ASP
LYS
HIS
LYS
LEU
L724
F752
H761
E768
Y772
A773
L774
V777
E782
Y793
D796
L797
F815
R816
S824
I825
Y826
R842
I846
M878
I888
I904
Y905
E906
P907
Q875
I686
F925
F926
I702
V705
G706
C707
G708

E935
R947
R998
Y999
F1000
M1010
M1023
K1027
CYS
PHE
LYS
CYS
CYS
CYS
LYS
GLU
LYS
ASN
MET
GLU
SER
ASN
ALA
CYS
CYS
PHE
ARG
ASN
GLU
ASP
H1050
A1071
H1072
D1073
H1074
S1075
K1104
SER
ASN
SER
LEU
VAL
LEU
PHE
GLN
GLY
PRO
ASP
TYR
LYS
ASP
ASP

ASP
LYS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	67871, 67871, 67871, 67871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.227	Depositor
Minimum map value	-1.122	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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, NAG, LQ7

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	0.27	0/7068	0.42	0/9646
1	B	0.27	0/7068	0.42	0/9646
1	C	0.27	0/7068	0.42	0/9646
1	D	0.27	0/7068	0.42	0/9646
All	All	0.27	0/28272	0.42	0/38584

There are no bond length outliers.

There are no bond angle outliers.

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	6904	6417	6420	69	0
1	B	6904	6417	6420	64	0
1	C	6904	6417	6420	71	0
1	D	6904	6417	6420	69	0
2	A	175	245	245	3	0
2	B	175	245	245	2	0
2	C	175	245	245	4	0
2	D	175	245	245	3	0
3	A	28	26	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	26	0	0	0
3	C	28	26	0	0	0
3	D	28	26	0	0	0
4	A	14	14	13	1	0
4	B	14	14	13	1	0
4	C	14	14	13	1	0
4	D	14	14	13	1	0
All	All	28484	26808	26712	279	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 5.

All (279) 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:761:HIS:O	1:D:816:ARG:NH2	2.15	0.80
1:B:761:HIS:O	1:B:816:ARG:NH2	2.15	0.80
1:A:761:HIS:O	1:A:816:ARG:NH2	2.15	0.80
1:C:761:HIS:O	1:C:816:ARG:NH2	2.15	0.79
1:B:596:LYS:NZ	1:B:662:GLU:OE1	2.18	0.77
1:B:342:LEU:HD21	1:B:381:LEU:HD21	1.67	0.77
1:A:596:LYS:NZ	1:A:662:GLU:OE1	2.18	0.76
1:C:596:LYS:NZ	1:C:662:GLU:OE1	2.18	0.76
1:A:342:LEU:HD21	1:A:381:LEU:HD21	1.67	0.75
1:D:596:LYS:NZ	1:D:662:GLU:OE1	2.18	0.75
1:C:342:LEU:HD21	1:C:381:LEU:HD21	1.67	0.75
1:D:342:LEU:HD21	1:D:381:LEU:HD21	1.67	0.74
1:C:146:ILE:HG22	1:C:180:LEU:HB2	1.71	0.72
1:B:146:ILE:HG22	1:B:180:LEU:HB2	1.71	0.72
1:A:342:LEU:CD2	1:A:381:LEU:HD21	2.19	0.72
1:B:342:LEU:CD2	1:B:381:LEU:HD21	2.19	0.72
1:D:342:LEU:CD2	1:D:381:LEU:HD21	2.19	0.71
1:A:146:ILE:HG22	1:A:180:LEU:HB2	1.71	0.71
1:C:342:LEU:CD2	1:C:381:LEU:HD21	2.19	0.71
1:D:146:ILE:HG22	1:D:180:LEU:HB2	1.71	0.71
1:A:702:ILE:O	1:A:705:VAL:HG12	1.92	0.70
1:D:702:ILE:O	1:D:705:VAL:HG12	1.92	0.69
1:B:702:ILE:O	1:B:705:VAL:HG12	1.92	0.69
1:D:932:SER:OG	1:D:934:ASN:OD1	2.11	0.69
1:C:702:ILE:O	1:C:705:VAL:HG12	1.92	0.69
1:C:934:ASN:ND2	4:C:1207:NAG:O6	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:934:ASN:ND2	4:B:1207:NAG:O6	2.26	0.68
1:A:934:ASN:ND2	4:A:1207:NAG:O6	2.26	0.67
1:D:934:ASN:ND2	4:D:1207:NAG:O6	2.26	0.67
1:A:932:SER:OG	1:A:934:ASN:OD1	2.11	0.67
1:C:932:SER:OG	1:C:934:ASN:OD1	2.11	0.66
1:B:932:SER:OG	1:B:934:ASN:OD1	2.11	0.65
1:B:768:GLU:OE2	1:B:772:TYR:OH	2.13	0.65
1:A:145:VAL:HG11	1:A:168:LEU:HD11	1.80	0.64
1:B:145:VAL:HG11	1:B:168:LEU:HD11	1.80	0.63
1:C:768:GLU:OE2	1:C:772:TYR:OH	2.13	0.62
1:D:145:VAL:HG11	1:D:168:LEU:HD11	1.80	0.62
1:D:768:GLU:OE2	1:D:772:TYR:OH	2.13	0.62
1:C:145:VAL:HG11	1:C:168:LEU:HD11	1.80	0.62
1:D:661:VAL:HG21	1:D:999:TYR:CE2	2.38	0.59
1:B:661:VAL:HG21	1:B:999:TYR:CE2	2.38	0.59
1:A:661:VAL:HG21	1:A:999:TYR:CE2	2.38	0.58
1:A:260:LEU:HD12	1:A:260:LEU:H	1.69	0.58
1:B:260:LEU:HD12	1:B:260:LEU:H	1.69	0.58
1:C:661:VAL:HG21	1:C:999:TYR:CE2	2.38	0.58
1:B:254:ASP:OD1	1:B:255:ASN:N	2.37	0.58
1:D:260:LEU:HD12	1:D:260:LEU:H	1.69	0.58
1:C:254:ASP:OD1	1:C:255:ASN:N	2.37	0.57
1:A:254:ASP:OD1	1:A:255:ASN:N	2.37	0.57
1:A:644:LEU:HD22	1:A:657:LEU:HG	1.87	0.57
1:B:644:LEU:HD22	1:B:657:LEU:HG	1.87	0.56
1:B:106:ILE:HG22	1:B:238:ALA:O	2.05	0.56
1:C:260:LEU:HD12	1:C:260:LEU:H	1.69	0.56
1:C:644:LEU:HD22	1:C:657:LEU:HG	1.87	0.56
1:D:254:ASP:OD1	1:D:255:ASN:N	2.37	0.56
1:D:106:ILE:HG22	1:D:238:ALA:O	2.05	0.56
1:D:644:LEU:HD22	1:D:657:LEU:HG	1.87	0.56
1:A:782:GLU:OE2	1:A:793:TYR:OH	2.24	0.56
1:A:106:ILE:HG22	1:A:238:ALA:O	2.05	0.56
1:C:106:ILE:HG22	1:C:238:ALA:O	2.06	0.55
1:A:768:GLU:OE2	1:A:772:TYR:OH	2.13	0.55
1:B:342:LEU:HD23	1:B:385:LEU:HD11	1.88	0.55
1:C:782:GLU:OE2	1:C:793:TYR:OH	2.24	0.55
1:D:768:GLU:OE1	1:D:816:ARG:NH1	2.40	0.55
1:D:782:GLU:OE2	1:D:793:TYR:OH	2.24	0.55
1:C:768:GLU:OE1	1:C:816:ARG:NH1	2.40	0.55
1:B:768:GLU:OE1	1:B:816:ARG:NH1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HD23	1:A:385:LEU:HD11	1.88	0.55
1:C:342:LEU:HD23	1:C:385:LEU:HD11	1.88	0.55
1:A:768:GLU:OE1	1:A:816:ARG:NH1	2.40	0.54
1:D:342:LEU:HD23	1:D:385:LEU:HD11	1.88	0.54
1:A:826:TYR:OH	1:B:888:ILE:O	2.20	0.54
1:B:842:ARG:O	1:B:846:ILE:HG23	2.08	0.54
1:A:842:ARG:O	1:A:846:ILE:HG23	2.08	0.54
1:C:842:ARG:O	1:C:846:ILE:HG23	2.08	0.54
1:C:575:GLU:OE1	1:C:575:GLU:N	2.41	0.54
1:B:782:GLU:OE2	1:B:793:TYR:OH	2.24	0.53
1:A:648:CYS:SG	1:A:654:SER:N	2.82	0.53
1:D:648:CYS:SG	1:D:654:SER:N	2.82	0.53
1:A:575:GLU:OE1	1:A:575:GLU:N	2.41	0.53
1:D:146:ILE:HG22	1:D:180:LEU:CB	2.38	0.53
1:B:146:ILE:HG22	1:B:180:LEU:CG	2.39	0.53
1:B:575:GLU:N	1:B:575:GLU:OE1	2.41	0.53
1:B:648:CYS:SG	1:B:654:SER:N	2.82	0.53
1:D:575:GLU:N	1:D:575:GLU:OE1	2.41	0.52
1:B:146:ILE:HG22	1:B:180:LEU:CB	2.38	0.52
1:C:648:CYS:SG	1:C:654:SER:N	2.82	0.52
1:D:842:ARG:O	1:D:846:ILE:HG23	2.08	0.52
2:A:1205:Y01:HAU2	2:A:1205:Y01:HAC1	1.92	0.52
2:D:1205:Y01:HAC1	2:D:1205:Y01:HAU2	1.92	0.52
1:A:146:ILE:HG22	1:A:180:LEU:CB	2.38	0.52
1:C:146:ILE:HG22	1:C:180:LEU:CB	2.38	0.52
2:C:1205:Y01:HAC1	2:C:1205:Y01:HAU2	1.92	0.52
1:C:146:ILE:HG22	1:C:180:LEU:CG	2.39	0.52
2:B:1205:Y01:HAC1	2:B:1205:Y01:HAU2	1.92	0.52
1:D:146:ILE:HG22	1:D:180:LEU:CG	2.39	0.52
1:A:146:ILE:HG22	1:A:180:LEU:CG	2.39	0.51
1:A:146:ILE:CG2	1:A:180:LEU:HD12	2.41	0.51
1:B:146:ILE:CG2	1:B:180:LEU:HD12	2.41	0.51
1:C:361:PHE:C	1:C:362:LEU:HD12	2.31	0.51
1:C:657:LEU:O	1:C:661:VAL:HG23	2.11	0.51
1:A:361:PHE:C	1:A:362:LEU:HD12	2.31	0.51
1:B:361:PHE:C	1:B:362:LEU:HD12	2.31	0.51
1:B:657:LEU:O	1:B:661:VAL:HG23	2.11	0.51
1:B:878:MET:SD	1:B:904:ILE:HG23	2.51	0.51
1:B:342:LEU:HD23	1:B:385:LEU:CD1	2.41	0.51
1:C:146:ILE:CG2	1:C:180:LEU:HD12	2.41	0.51
1:A:308:GLY:HA2	1:A:335:ILE:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:LEU:O	1:A:661:VAL:HG23	2.11	0.51
1:D:308:GLY:HA2	1:D:335:ILE:HG22	1.93	0.51
1:D:361:PHE:C	1:D:362:LEU:HD12	2.31	0.51
1:B:1010:ASN:O	1:B:1010:ASN:ND2	2.44	0.50
1:C:930:THR:HG21	1:C:935:GLU:HB2	1.93	0.50
1:A:878:MET:SD	1:A:904:ILE:HG23	2.51	0.50
1:D:878:MET:SD	1:D:904:ILE:HG23	2.51	0.50
1:D:930:THR:HG21	1:D:935:GLU:HB2	1.93	0.50
1:D:1010:ASN:O	1:D:1010:ASN:ND2	2.44	0.50
1:B:930:THR:HG21	1:B:935:GLU:HB2	1.93	0.50
1:D:657:LEU:O	1:D:661:VAL:HG23	2.11	0.50
1:A:1010:ASN:O	1:A:1010:ASN:ND2	2.44	0.50
1:C:342:LEU:HD23	1:C:385:LEU:CD1	2.41	0.50
1:D:146:ILE:CG2	1:D:180:LEU:HD12	2.41	0.50
1:A:342:LEU:HD23	1:A:385:LEU:CD1	2.41	0.50
1:C:878:MET:SD	1:C:904:ILE:HG23	2.51	0.50
1:D:342:LEU:HD23	1:D:385:LEU:CD1	2.41	0.50
1:A:888:ILE:O	1:D:826:TYR:OH	2.21	0.49
1:C:308:GLY:HA2	1:C:335:ILE:HG22	1.93	0.49
1:B:308:GLY:HA2	1:B:335:ILE:HG22	1.93	0.49
1:C:1010:ASN:O	1:C:1010:ASN:ND2	2.44	0.49
1:B:143:ASN:OD1	1:B:144:LEU:N	2.46	0.49
1:A:143:ASN:OD1	1:A:144:LEU:N	2.46	0.49
1:A:930:THR:HG21	1:A:935:GLU:HB2	1.93	0.49
1:C:143:ASN:OD1	1:C:144:LEU:N	2.46	0.49
1:D:143:ASN:OD1	1:D:144:LEU:N	2.46	0.49
1:C:488:LEU:HD12	1:C:493:LEU:HD21	1.95	0.48
1:A:488:LEU:HD12	1:A:493:LEU:HD21	1.95	0.48
1:B:257:HIS:HB2	1:B:260:LEU:HD11	1.95	0.48
1:B:589:LEU:HD12	1:B:659:LEU:HD12	1.96	0.48
1:D:488:LEU:HD12	1:D:493:LEU:HD21	1.95	0.48
1:C:589:LEU:HD12	1:C:659:LEU:HD12	1.96	0.48
1:D:257:HIS:HB2	1:D:260:LEU:HD11	1.95	0.48
1:A:589:LEU:HD12	1:A:659:LEU:HD12	1.96	0.47
1:C:257:HIS:HB2	1:C:260:LEU:HD11	1.95	0.47
1:A:257:HIS:HB2	1:A:260:LEU:HD11	1.95	0.47
1:B:488:LEU:HD12	1:B:493:LEU:HD21	1.96	0.47
1:D:214:ILE:HG13	1:D:261:LEU:HD21	1.97	0.47
1:D:589:LEU:HD12	1:D:659:LEU:HD12	1.96	0.47
1:D:686:ILE:HD12	1:D:686:ILE:H	1.80	0.47
1:A:214:ILE:HG13	1:A:261:LEU:HD21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:ILE:H	1:C:686:ILE:HD12	1.80	0.47
1:B:589:LEU:CD1	1:B:659:LEU:HD12	2.46	0.46
1:D:146:ILE:HG13	1:D:303:CYS:HA	1.98	0.46
1:A:589:LEU:CD1	1:A:659:LEU:HD12	2.46	0.46
1:A:686:ILE:HD12	1:A:686:ILE:H	1.80	0.46
1:C:214:ILE:HG13	1:C:261:LEU:HD21	1.97	0.46
1:B:686:ILE:HD12	1:B:686:ILE:H	1.80	0.46
1:C:796:ASP:OD1	1:C:797:LEU:N	2.49	0.46
1:D:589:LEU:CD1	1:D:659:LEU:HD12	2.46	0.46
1:D:796:ASP:OD1	1:D:797:LEU:N	2.49	0.46
1:A:146:ILE:HG13	1:A:303:CYS:HA	1.98	0.46
1:B:214:ILE:HG13	1:B:261:LEU:HD21	1.97	0.46
1:B:796:ASP:OD1	1:B:797:LEU:N	2.49	0.45
1:C:589:LEU:CD1	1:C:659:LEU:HD12	2.46	0.45
1:B:146:ILE:HG13	1:B:303:CYS:HA	1.98	0.45
1:C:146:ILE:HG13	1:C:303:CYS:HA	1.98	0.45
1:A:796:ASP:OD1	1:A:797:LEU:N	2.49	0.45
1:D:499:THR:HG23	1:D:500:HIS:N	2.32	0.45
1:B:160:ARG:NH2	1:B:395:LYS:O	2.50	0.45
1:B:214:ILE:HD12	1:B:214:ILE:N	2.32	0.45
1:A:261:LEU:N	1:A:261:LEU:HD23	2.32	0.44
1:A:499:THR:HG23	1:A:500:HIS:N	2.32	0.44
1:C:160:ARG:NH2	1:C:395:LYS:O	2.50	0.44
1:C:261:LEU:N	1:C:261:LEU:HD23	2.32	0.44
1:C:499:THR:HG23	1:C:500:HIS:N	2.32	0.44
1:B:499:THR:HG23	1:B:500:HIS:N	2.32	0.44
1:C:214:ILE:N	1:C:214:ILE:HD12	2.32	0.44
1:D:261:LEU:HD23	1:D:261:LEU:N	2.32	0.44
1:C:826:TYR:OH	1:D:888:ILE:O	2.21	0.44
1:B:215:ALA:HB3	1:B:262:LEU:HD13	2.00	0.44
1:A:484:LEU:HD23	1:A:561:LEU:HD21	2.00	0.44
1:B:261:LEU:N	1:B:261:LEU:HD23	2.32	0.44
1:C:133:LEU:HD23	1:C:133:LEU:O	2.18	0.44
1:D:133:LEU:O	1:D:133:LEU:HD23	2.18	0.44
1:C:146:ILE:HG22	1:C:180:LEU:HD12	2.00	0.44
1:A:214:ILE:N	1:A:214:ILE:HD12	2.32	0.44
1:A:215:ALA:HB3	1:A:262:LEU:HD13	2.00	0.44
1:D:146:ILE:HG22	1:D:180:LEU:HD12	2.00	0.43
1:D:214:ILE:HD12	1:D:214:ILE:N	2.32	0.43
1:D:484:LEU:HD23	1:D:561:LEU:HD21	2.00	0.43
1:C:432:LEU:HD13	1:C:432:LEU:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:THR:O	1:C:141:THR:HG23	2.19	0.43
1:A:160:ARG:NH2	1:A:395:LYS:O	2.50	0.43
1:C:439:LEU:HD13	1:C:439:LEU:C	2.39	0.43
1:A:439:LEU:HD13	1:A:439:LEU:C	2.39	0.43
1:A:1023:MET:O	1:A:1027:LYS:N	2.49	0.43
1:B:826:TYR:OH	1:C:888:ILE:O	2.21	0.43
1:C:215:ALA:HB3	1:C:262:LEU:HD13	2.00	0.43
1:D:215:ALA:HB3	1:D:262:LEU:HD13	2.00	0.43
1:B:146:ILE:HG22	1:B:180:LEU:HD12	2.00	0.43
1:B:432:LEU:C	1:B:432:LEU:HD13	2.39	0.43
1:D:675:GLN:OE1	1:D:998:ARG:NH1	2.52	0.43
1:A:432:LEU:HD13	1:A:432:LEU:C	2.39	0.43
1:A:774:LEU:O	1:A:777:VAL:HG22	2.19	0.43
1:D:439:LEU:HD13	1:D:439:LEU:C	2.39	0.43
1:A:675:GLN:OE1	1:A:998:ARG:NH1	2.52	0.43
1:A:947:ASN:N	1:A:947:ASN:HD22	2.16	0.43
1:B:906:GLU:HB2	1:B:907:PRO:HD3	2.01	0.43
1:D:432:LEU:HD13	1:D:432:LEU:C	2.39	0.43
1:C:947:ASN:N	1:C:947:ASN:HD22	2.16	0.42
1:B:675:GLN:OE1	1:B:998:ARG:NH1	2.52	0.42
1:B:774:LEU:O	1:B:777:VAL:HG22	2.19	0.42
1:C:675:GLN:OE1	1:C:998:ARG:NH1	2.52	0.42
1:C:906:GLU:HB2	1:C:907:PRO:HD3	2.01	0.42
1:D:141:THR:HG23	1:D:141:THR:O	2.19	0.42
1:D:160:ARG:NH2	1:D:395:LYS:O	2.50	0.42
1:A:133:LEU:O	1:A:133:LEU:HD23	2.18	0.42
1:A:141:THR:O	1:A:141:THR:HG23	2.19	0.42
1:A:144:LEU:HD21	1:A:285:ILE:HD13	2.02	0.42
1:B:133:LEU:HD23	1:B:133:LEU:O	2.18	0.42
1:B:141:THR:HG23	1:B:141:THR:O	2.19	0.42
1:B:947:ASN:N	1:B:947:ASN:HD22	2.16	0.42
2:B:1203:Y01:HAC1	2:B:1203:Y01:HAU2	2.01	0.42
1:D:774:LEU:O	1:D:777:VAL:HG22	2.19	0.42
1:B:144:LEU:HD21	1:B:285:ILE:HD13	2.02	0.42
1:B:439:LEU:C	1:B:439:LEU:HD13	2.39	0.42
1:C:484:LEU:HD23	1:C:561:LEU:HD21	2.00	0.42
1:A:146:ILE:HG22	1:A:180:LEU:HD12	2.00	0.42
1:C:144:LEU:HD21	1:C:285:ILE:HD13	2.02	0.42
1:C:707:CYS:SG	1:C:708:GLY:N	2.93	0.42
2:C:1203:Y01:HAU2	2:C:1203:Y01:HAC1	2.02	0.42
1:D:181:THR:HG22	1:D:182:GLY:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:ASN:N	1:D:947:ASN:HD22	2.16	0.42
2:A:1203:Y01:HAU2	2:A:1203:Y01:HAC1	2.02	0.42
1:D:569:ILE:CD1	1:D:594:ALA:HB1	2.50	0.42
1:D:707:CYS:SG	1:D:708:GLY:N	2.93	0.42
1:D:815:PHE:O	1:D:824:SER:OG	2.31	0.42
1:A:707:CYS:SG	1:A:708:GLY:N	2.93	0.42
1:D:570:LEU:HD21	1:D:597:LEU:HD21	2.02	0.42
1:D:1023:MET:O	1:D:1027:LYS:N	2.49	0.42
1:B:181:THR:HG22	1:B:182:GLY:N	2.35	0.41
1:B:707:CYS:SG	1:B:708:GLY:N	2.93	0.41
1:A:815:PHE:O	1:A:824:SER:OG	2.31	0.41
1:A:906:GLU:HB2	1:A:907:PRO:HD3	2.01	0.41
1:B:484:LEU:HD23	1:B:561:LEU:HD21	2.00	0.41
1:C:569:ILE:CD1	1:C:594:ALA:HB1	2.50	0.41
1:C:774:LEU:O	1:C:777:VAL:HG22	2.19	0.41
1:B:569:ILE:CD1	1:B:594:ALA:HB1	2.50	0.41
1:B:570:LEU:HD21	1:B:597:LEU:HD21	2.02	0.41
1:A:191:TYR:O	1:A:195:VAL:HG23	2.20	0.41
1:A:570:LEU:HD21	1:A:597:LEU:HD21	2.02	0.41
1:B:191:TYR:O	1:B:195:VAL:HG23	2.20	0.41
1:C:1023:MET:O	1:C:1027:LYS:N	2.49	0.41
1:D:144:LEU:HD21	1:D:285:ILE:HD13	2.02	0.41
1:C:570:LEU:HD21	1:C:597:LEU:HD21	2.02	0.41
1:D:191:TYR:O	1:D:195:VAL:HG23	2.20	0.41
1:D:488:LEU:HD12	1:D:493:LEU:CD2	2.51	0.41
2:D:1203:Y01:HAC1	2:D:1203:Y01:HAU2	2.01	0.41
1:A:569:ILE:CD1	1:A:594:ALA:HB1	2.50	0.41
1:C:181:THR:HG22	1:C:182:GLY:N	2.35	0.41
1:C:191:TYR:O	1:C:195:VAL:HG23	2.20	0.41
1:C:440:ASP:OD1	1:C:440:ASP:N	2.54	0.41
1:A:743:VAL:HG22	2:A:1203:Y01:HAQ2	2.03	0.41
1:B:440:ASP:N	1:B:440:ASP:OD1	2.54	0.41
1:C:488:LEU:HD12	1:C:493:LEU:CD2	2.51	0.41
2:C:1202:Y01:HAD2	2:C:1202:Y01:HAS2	1.94	0.41
1:D:358:LEU:O	1:D:362:LEU:N	2.48	0.41
1:D:906:GLU:HB2	1:D:907:PRO:HD3	2.01	0.41
1:A:181:THR:HG22	1:A:182:GLY:N	2.35	0.40
1:A:925:ASP:OD1	1:A:926:PHE:N	2.55	0.40
1:C:587:CYS:SG	1:C:1060:LYS:HD3	2.62	0.40
1:D:925:ASP:OD1	1:D:926:PHE:N	2.55	0.40
1:C:495:GLU:O	1:C:499:THR:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:CYS:SG	1:A:1060:LYS:HD3	2.62	0.40
1:C:743:VAL:HG22	2:C:1203:Y01:HAQ2	2.03	0.40
1:C:925:ASP:OD1	1:C:926:PHE:N	2.55	0.40
1:D:495:GLU:O	1:D:499:THR:HG22	2.21	0.40
2:D:1202:Y01:HAD2	2:D:1202:Y01:HAS2	1.95	0.40
1:A:495:GLU:O	1:A:499:THR:HG22	2.21	0.40
1:C:358:LEU:O	1:C:362:LEU:N	2.48	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	893/1135 (79%)	870 (97%)	23 (3%)	0	100	100
1	B	893/1135 (79%)	870 (97%)	23 (3%)	0	100	100
1	C	893/1135 (79%)	870 (97%)	23 (3%)	0	100	100
1	D	893/1135 (79%)	870 (97%)	23 (3%)	0	100	100
All	All	3572/4540 (79%)	3480 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	660/1022 (65%)	652 (99%)	8 (1%)	67	89
1	B	660/1022 (65%)	652 (99%)	8 (1%)	67	89
1	C	660/1022 (65%)	652 (99%)	8 (1%)	67	89
1	D	660/1022 (65%)	652 (99%)	8 (1%)	67	89
All	All	2640/4088 (65%)	2608 (99%)	32 (1%)	66	89

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	410	TYR
1	A	490	ASN
1	A	501	PHE
1	A	752	PHE
1	A	816	ARG
1	A	947	ASN
1	A	1000	PHE
1	A	1023	MET
1	B	410	TYR
1	B	490	ASN
1	B	501	PHE
1	B	752	PHE
1	B	816	ARG
1	B	947	ASN
1	B	1000	PHE
1	B	1023	MET
1	C	410	TYR
1	C	490	ASN
1	C	501	PHE
1	C	752	PHE
1	C	816	ARG
1	C	947	ASN
1	C	1000	PHE
1	C	1023	MET
1	D	410	TYR
1	D	490	ASN
1	D	501	PHE
1	D	752	PHE
1	D	816	ARG
1	D	947	ASN
1	D	1000	PHE
1	D	1023	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	947	ASN
1	A	968	ASN
1	B	199	ASN
1	B	947	ASN
1	B	968	ASN
1	C	199	ASN
1	C	947	ASN
1	C	968	ASN
1	D	199	ASN
1	D	947	ASN
1	D	968	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	1201	-	38,38,38	1.14	3 (7%)	57,57,57	2.72	17 (29%)
3	LQ7	A	1204	-	30,30,30	1.91	5 (16%)	33,39,39	1.21	3 (9%)
2	Y01	D	1205	-	38,38,38	1.10	3 (7%)	57,57,57	2.39	13 (22%)
2	Y01	A	1202	-	38,38,38	1.13	2 (5%)	57,57,57	2.42	17 (29%)
2	Y01	D	1202	-	38,38,38	1.13	2 (5%)	57,57,57	2.43	17 (29%)
2	Y01	A	1206	-	38,38,38	1.11	2 (5%)	57,57,57	2.43	16 (28%)
3	LQ7	B	1204	-	30,30,30	1.92	5 (16%)	33,39,39	1.21	3 (9%)
4	NAG	A	1207	-	14,14,15	2.67	7 (50%)	17,19,21	1.19	1 (5%)
2	Y01	B	1202	-	38,38,38	1.13	2 (5%)	57,57,57	2.42	17 (29%)
3	LQ7	C	1204	-	30,30,30	1.92	5 (16%)	33,39,39	1.21	3 (9%)
2	Y01	C	1201	-	38,38,38	1.14	3 (7%)	57,57,57	2.72	17 (29%)
4	NAG	D	1207	-	14,14,15	2.65	7 (50%)	17,19,21	1.18	1 (5%)
2	Y01	D	1203	-	38,38,38	1.12	3 (7%)	57,57,57	2.32	16 (28%)
2	Y01	D	1201	-	38,38,38	1.14	3 (7%)	57,57,57	2.72	17 (29%)
2	Y01	A	1203	-	38,38,38	1.12	3 (7%)	57,57,57	2.32	16 (28%)
4	NAG	C	1207	-	14,14,15	2.66	7 (50%)	17,19,21	1.18	1 (5%)
4	NAG	B	1207	-	14,14,15	2.66	7 (50%)	17,19,21	1.18	1 (5%)
2	Y01	D	1206	-	38,38,38	1.11	2 (5%)	57,57,57	2.43	16 (28%)
2	Y01	C	1205	-	38,38,38	1.10	3 (7%)	57,57,57	2.39	13 (22%)
2	Y01	C	1203	-	38,38,38	1.12	3 (7%)	57,57,57	2.32	16 (28%)
2	Y01	B	1205	-	38,38,38	1.10	3 (7%)	57,57,57	2.39	13 (22%)
2	Y01	C	1202	-	38,38,38	1.13	2 (5%)	57,57,57	2.42	17 (29%)
2	Y01	C	1206	-	38,38,38	1.11	2 (5%)	57,57,57	2.43	16 (28%)
2	Y01	B	1203	-	38,38,38	1.12	3 (7%)	57,57,57	2.32	16 (28%)
2	Y01	B	1206	-	38,38,38	1.11	2 (5%)	57,57,57	2.43	16 (28%)
3	LQ7	D	1204	-	30,30,30	1.91	5 (16%)	33,39,39	1.22	3 (9%)
2	Y01	A	1205	-	38,38,38	1.10	3 (7%)	57,57,57	2.39	13 (22%)
2	Y01	B	1201	-	38,38,38	1.14	3 (7%)	57,57,57	2.72	17 (29%)

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	1201	-	-	4/19/77/77	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LQ7	A	1204	-	-	2/20/21/21	0/3/3/3
2	Y01	D	1205	-	-	5/19/77/77	0/4/4/4
2	Y01	A	1202	-	-	8/19/77/77	0/4/4/4
2	Y01	D	1202	-	-	8/19/77/77	0/4/4/4
2	Y01	A	1206	-	-	11/19/77/77	0/4/4/4
3	LQ7	B	1204	-	-	2/20/21/21	0/3/3/3
4	NAG	A	1207	-	-	2/6/23/26	0/1/1/1
2	Y01	B	1202	-	-	8/19/77/77	0/4/4/4
3	LQ7	C	1204	-	-	2/20/21/21	0/3/3/3
2	Y01	C	1201	-	-	4/19/77/77	0/4/4/4
4	NAG	D	1207	-	-	2/6/23/26	0/1/1/1
2	Y01	D	1203	-	-	9/19/77/77	0/4/4/4
2	Y01	D	1201	-	-	4/19/77/77	0/4/4/4
2	Y01	A	1203	-	-	9/19/77/77	0/4/4/4
4	NAG	C	1207	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1207	-	-	2/6/23/26	0/1/1/1
2	Y01	D	1206	-	-	11/19/77/77	0/4/4/4
2	Y01	C	1205	-	-	5/19/77/77	0/4/4/4
2	Y01	C	1203	-	-	9/19/77/77	0/4/4/4
2	Y01	B	1205	-	-	5/19/77/77	0/4/4/4
2	Y01	C	1202	-	-	8/19/77/77	0/4/4/4
2	Y01	C	1206	-	-	11/19/77/77	0/4/4/4
2	Y01	B	1203	-	-	9/19/77/77	0/4/4/4
2	Y01	B	1206	-	-	11/19/77/77	0/4/4/4
3	LQ7	D	1204	-	-	2/20/21/21	0/3/3/3
2	Y01	A	1205	-	-	5/19/77/77	0/4/4/4
2	Y01	B	1201	-	-	4/19/77/77	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1204	LQ7	C05-S09	-5.58	1.62	1.73
3	B	1204	LQ7	C05-S09	-5.58	1.62	1.73
3	C	1204	LQ7	C05-S09	-5.58	1.62	1.73
3	D	1204	LQ7	C05-S09	-5.58	1.62	1.73
3	B	1204	LQ7	C02-N03	5.42	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1204	LQ7	C02-N03	5.42	1.46	1.34
3	A	1204	LQ7	C02-N03	5.38	1.46	1.34
3	D	1204	LQ7	C02-N03	5.38	1.46	1.34
4	A	1207	NAG	O5-C5	5.14	1.53	1.43
4	D	1207	NAG	O5-C5	5.14	1.53	1.43
4	B	1207	NAG	O5-C5	5.13	1.53	1.43
4	C	1207	NAG	O5-C5	5.13	1.53	1.43
4	A	1207	NAG	C2-N2	4.28	1.53	1.46
4	B	1207	NAG	C2-N2	4.28	1.53	1.46
4	C	1207	NAG	C2-N2	4.28	1.53	1.46
4	D	1207	NAG	C2-N2	4.28	1.53	1.46
3	A	1204	LQ7	C07-C06	4.15	1.53	1.39
3	B	1204	LQ7	C07-C06	4.15	1.53	1.39
3	C	1204	LQ7	C07-C06	4.15	1.53	1.39
3	D	1204	LQ7	C07-C06	4.15	1.53	1.39
4	A	1207	NAG	C7-N2	3.52	1.45	1.34
4	B	1207	NAG	C7-N2	3.51	1.45	1.34
4	C	1207	NAG	C7-N2	3.51	1.45	1.34
4	D	1207	NAG	C7-N2	3.51	1.45	1.34
2	B	1203	Y01	OAW-CAY	3.31	1.43	1.34
2	C	1203	Y01	OAW-CAY	3.31	1.43	1.34
2	D	1203	Y01	OAW-CAY	3.31	1.43	1.34
2	A	1203	Y01	OAW-CAY	3.30	1.43	1.34
2	A	1201	Y01	OAW-CAY	3.27	1.43	1.34
2	B	1201	Y01	OAW-CAY	3.27	1.43	1.34
2	C	1201	Y01	OAW-CAY	3.27	1.43	1.34
2	D	1201	Y01	OAW-CAY	3.27	1.43	1.34
2	A	1202	Y01	OAW-CAY	3.24	1.43	1.34
2	B	1202	Y01	OAW-CAY	3.24	1.43	1.34
2	C	1202	Y01	OAW-CAY	3.24	1.43	1.34
2	D	1202	Y01	OAW-CAY	3.24	1.43	1.34
2	A	1206	Y01	OAW-CAY	3.24	1.43	1.34
2	B	1206	Y01	OAW-CAY	3.24	1.43	1.34
2	C	1206	Y01	OAW-CAY	3.24	1.43	1.34
2	D	1206	Y01	OAW-CAY	3.24	1.43	1.34
2	A	1205	Y01	OAW-CAY	3.22	1.43	1.34
2	B	1205	Y01	OAW-CAY	3.22	1.43	1.34
2	C	1205	Y01	OAW-CAY	3.22	1.43	1.34
2	D	1205	Y01	OAW-CAY	3.22	1.43	1.34
4	A	1207	NAG	C3-C2	-3.21	1.45	1.52
4	B	1207	NAG	C3-C2	-3.18	1.45	1.52
4	C	1207	NAG	C3-C2	-3.18	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1207	NAG	C3-C2	-3.18	1.45	1.52
4	A	1207	NAG	C6-C5	-3.04	1.41	1.51
4	B	1207	NAG	C6-C5	-3.04	1.41	1.51
4	C	1207	NAG	C6-C5	-3.04	1.41	1.51
4	D	1207	NAG	C6-C5	-3.04	1.41	1.51
3	A	1204	LQ7	C07-C08	3.02	1.43	1.34
3	B	1204	LQ7	C07-C08	3.02	1.43	1.34
3	C	1204	LQ7	C07-C08	3.02	1.43	1.34
3	D	1204	LQ7	C07-C08	3.02	1.43	1.34
2	A	1205	Y01	OAH-CAX	-2.89	1.21	1.30
2	B	1205	Y01	OAH-CAX	-2.89	1.21	1.30
2	C	1205	Y01	OAH-CAX	-2.89	1.21	1.30
2	D	1205	Y01	OAH-CAX	-2.89	1.21	1.30
2	B	1201	Y01	OAH-CAX	-2.85	1.21	1.30
2	D	1201	Y01	OAH-CAX	-2.85	1.21	1.30
2	A	1201	Y01	OAH-CAX	-2.84	1.21	1.30
2	B	1202	Y01	OAH-CAX	-2.84	1.21	1.30
2	C	1201	Y01	OAH-CAX	-2.84	1.21	1.30
2	C	1202	Y01	OAH-CAX	-2.84	1.21	1.30
2	D	1202	Y01	OAH-CAX	-2.84	1.21	1.30
2	A	1203	Y01	OAH-CAX	-2.84	1.21	1.30
2	A	1206	Y01	OAH-CAX	-2.83	1.21	1.30
2	B	1206	Y01	OAH-CAX	-2.83	1.21	1.30
2	C	1206	Y01	OAH-CAX	-2.83	1.21	1.30
2	D	1206	Y01	OAH-CAX	-2.83	1.21	1.30
2	B	1203	Y01	OAH-CAX	-2.83	1.21	1.30
2	C	1203	Y01	OAH-CAX	-2.83	1.21	1.30
2	D	1203	Y01	OAH-CAX	-2.83	1.21	1.30
2	A	1202	Y01	OAH-CAX	-2.83	1.21	1.30
4	A	1207	NAG	O3-C3	2.30	1.48	1.43
4	A	1207	NAG	O5-C1	2.27	1.47	1.43
4	B	1207	NAG	O5-C1	2.27	1.47	1.43
4	C	1207	NAG	O5-C1	2.27	1.47	1.43
4	B	1207	NAG	O3-C3	2.26	1.48	1.43
4	C	1207	NAG	O3-C3	2.26	1.48	1.43
4	D	1207	NAG	O3-C3	2.26	1.48	1.43
4	D	1207	NAG	O5-C1	2.21	1.47	1.43
3	A	1204	LQ7	C06-C05	2.14	1.43	1.37
3	B	1204	LQ7	C06-C05	2.14	1.43	1.37
3	C	1204	LQ7	C06-C05	2.14	1.43	1.37
3	D	1204	LQ7	C06-C05	2.14	1.43	1.37
2	C	1205	Y01	CAK-CAI	2.12	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1205	Y01	CAK-CAI	2.11	1.54	1.50
2	B	1205	Y01	CAK-CAI	2.11	1.54	1.50
2	D	1205	Y01	CAK-CAI	2.11	1.54	1.50
2	A	1203	Y01	CAS-CBF	2.11	1.57	1.53
2	B	1203	Y01	CAS-CBF	2.11	1.57	1.53
2	C	1203	Y01	CAS-CBF	2.11	1.57	1.53
2	D	1203	Y01	CAS-CBF	2.11	1.57	1.53
2	A	1201	Y01	CAK-CAI	2.09	1.54	1.50
2	B	1201	Y01	CAK-CAI	2.09	1.54	1.50
2	C	1201	Y01	CAK-CAI	2.09	1.54	1.50
2	D	1201	Y01	CAK-CAI	2.09	1.54	1.50

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1203	Y01	CAT-CBH-CBF	-10.24	95.18	108.74
2	B	1203	Y01	CAT-CBH-CBF	-10.24	95.18	108.74
2	C	1203	Y01	CAT-CBH-CBF	-10.24	95.18	108.74
2	D	1203	Y01	CAT-CBH-CBF	-10.24	95.18	108.74
2	A	1205	Y01	CAT-CBH-CBF	-9.95	95.57	108.74
2	C	1205	Y01	CAT-CBH-CBF	-9.93	95.60	108.74
2	B	1205	Y01	CAT-CBH-CBF	-9.93	95.60	108.74
2	D	1205	Y01	CAT-CBH-CBF	-9.93	95.60	108.74
2	C	1206	Y01	CAT-CBH-CBF	-9.76	95.82	108.74
2	D	1202	Y01	CAT-CBH-CBF	-9.74	95.84	108.74
2	A	1206	Y01	CAT-CBH-CBF	-9.74	95.84	108.74
2	B	1206	Y01	CAT-CBH-CBF	-9.74	95.84	108.74
2	D	1206	Y01	CAT-CBH-CBF	-9.74	95.84	108.74
2	A	1202	Y01	CAT-CBH-CBF	-9.72	95.87	108.74
2	B	1202	Y01	CAT-CBH-CBF	-9.72	95.87	108.74
2	C	1202	Y01	CAT-CBH-CBF	-9.72	95.87	108.74
2	C	1201	Y01	CAT-CBH-CBF	-9.36	96.35	108.74
2	A	1201	Y01	CAT-CBH-CBF	-9.35	96.37	108.74
2	B	1201	Y01	CAT-CBH-CBF	-9.35	96.37	108.74
2	D	1201	Y01	CAT-CBH-CBF	-9.35	96.37	108.74
2	A	1201	Y01	CAV-CAZ-CAI	7.07	130.16	120.57
2	B	1201	Y01	CAV-CAZ-CAI	7.07	130.16	120.57
2	C	1201	Y01	CAV-CAZ-CAI	7.07	130.16	120.57
2	D	1201	Y01	CAV-CAZ-CAI	7.07	130.16	120.57
2	B	1205	Y01	CAV-CAZ-CAI	6.94	129.97	120.57
2	D	1205	Y01	CAV-CAZ-CAI	6.94	129.97	120.57
2	A	1205	Y01	CAV-CAZ-CAI	6.93	129.97	120.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1205	Y01	CAV-CAZ-CAI	6.93	129.97	120.57
2	B	1202	Y01	CAV-CAZ-CAI	6.91	129.94	120.57
2	C	1202	Y01	CAV-CAZ-CAI	6.91	129.94	120.57
2	D	1202	Y01	CAV-CAZ-CAI	6.91	129.94	120.57
2	A	1206	Y01	CAV-CAZ-CAI	6.90	129.92	120.57
2	B	1206	Y01	CAV-CAZ-CAI	6.90	129.92	120.57
2	C	1206	Y01	CAV-CAZ-CAI	6.90	129.92	120.57
2	A	1202	Y01	CAV-CAZ-CAI	6.89	129.91	120.57
2	D	1206	Y01	CAV-CAZ-CAI	6.87	129.88	120.57
2	A	1203	Y01	CAV-CAZ-CAI	6.39	129.23	120.57
2	B	1203	Y01	CAV-CAZ-CAI	6.39	129.23	120.57
2	C	1203	Y01	CAV-CAZ-CAI	6.39	129.23	120.57
2	D	1203	Y01	CAV-CAZ-CAI	6.39	129.23	120.57
2	C	1201	Y01	CBH-CBF-CBD	-5.73	104.33	112.71
2	A	1201	Y01	CBH-CBF-CBD	-5.73	104.34	112.71
2	B	1201	Y01	CBH-CBF-CBD	-5.73	104.34	112.71
2	D	1201	Y01	CBH-CBF-CBD	-5.73	104.34	112.71
2	C	1201	Y01	CBD-CAK-CAI	-5.73	104.83	112.76
2	B	1201	Y01	CBD-CAK-CAI	-5.71	104.85	112.76
2	D	1201	Y01	CBD-CAK-CAI	-5.71	104.85	112.76
2	A	1201	Y01	CBD-CAK-CAI	-5.71	104.85	112.76
2	D	1201	Y01	CAK-CBD-CBG	5.58	118.83	110.93
2	A	1201	Y01	CAK-CBD-CBG	5.58	118.83	110.93
2	B	1201	Y01	CAK-CBD-CBG	5.58	118.83	110.93
2	C	1201	Y01	CAK-CBD-CBG	5.54	118.77	110.93
2	C	1205	Y01	CAD-CBH-CBF	5.27	117.58	111.66
2	A	1205	Y01	CAD-CBH-CBF	5.25	117.56	111.66
2	B	1205	Y01	CAD-CBH-CBF	5.25	117.56	111.66
2	D	1205	Y01	CAD-CBH-CBF	5.25	117.56	111.66
2	A	1205	Y01	CBH-CBF-CBD	-5.15	105.19	112.71
2	B	1205	Y01	CBH-CBF-CBD	-5.15	105.19	112.71
2	D	1205	Y01	CBH-CBF-CBD	-5.15	105.19	112.71
2	C	1205	Y01	CBH-CBF-CBD	-5.13	105.22	112.71
2	A	1202	Y01	CBH-CBF-CBD	-4.97	105.46	112.71
2	B	1202	Y01	CBH-CBF-CBD	-4.97	105.46	112.71
2	C	1202	Y01	CBH-CBF-CBD	-4.97	105.46	112.71
2	D	1202	Y01	CBH-CBF-CBD	-4.97	105.46	112.71
2	C	1201	Y01	CAD-CBH-CAZ	4.92	115.89	108.38
2	B	1201	Y01	CAD-CBH-CAZ	4.90	115.87	108.38
2	A	1201	Y01	CAD-CBH-CAZ	4.90	115.87	108.38
2	D	1201	Y01	CAD-CBH-CAZ	4.90	115.86	108.38
2	C	1206	Y01	CBH-CBF-CBD	-4.66	105.90	112.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1206	Y01	CBH-CBF-CBD	-4.64	105.93	112.71
2	B	1206	Y01	CBH-CBF-CBD	-4.62	105.96	112.71
2	D	1206	Y01	CBH-CBF-CBD	-4.62	105.96	112.71
2	D	1206	Y01	CAU-CBI-CBE	-4.44	110.06	116.60
2	A	1206	Y01	CAU-CBI-CBE	-4.42	110.08	116.60
2	B	1206	Y01	CAU-CBI-CBE	-4.41	110.11	116.60
2	C	1206	Y01	CAU-CBI-CBE	-4.41	110.11	116.60
2	A	1201	Y01	CAK-CBD-CBF	-4.24	104.81	109.72
2	C	1201	Y01	CAK-CBD-CBF	-4.24	104.82	109.72
2	B	1201	Y01	CAK-CBD-CBF	-4.22	104.85	109.72
2	D	1201	Y01	CAK-CBD-CBF	-4.22	104.85	109.72
2	A	1201	Y01	OAW-CAY-CAM	4.03	120.21	111.48
2	B	1201	Y01	OAW-CAY-CAM	4.03	120.21	111.48
2	C	1201	Y01	OAW-CAY-CAM	4.03	120.21	111.48
2	D	1201	Y01	OAW-CAY-CAM	4.03	120.21	111.48
3	A	1204	LQ7	C07-C08-S09	-4.03	109.71	112.98
3	B	1204	LQ7	C07-C08-S09	-4.03	109.71	112.98
3	C	1204	LQ7	C07-C08-S09	-4.03	109.71	112.98
3	D	1204	LQ7	C07-C08-S09	-4.03	109.71	112.98
2	A	1206	Y01	OAW-CAY-CAM	4.01	120.17	111.48
2	B	1206	Y01	OAW-CAY-CAM	4.01	120.15	111.48
2	C	1206	Y01	OAW-CAY-CAM	4.01	120.15	111.48
2	D	1206	Y01	OAW-CAY-CAM	4.01	120.15	111.48
2	C	1201	Y01	CAV-CAZ-CBH	-3.94	111.38	116.42
2	C	1205	Y01	CBH-CAZ-CAI	-3.93	117.18	122.93
2	A	1205	Y01	CBH-CAZ-CAI	-3.93	117.19	122.93
2	B	1205	Y01	CBH-CAZ-CAI	-3.93	117.19	122.93
2	D	1205	Y01	CBH-CAZ-CAI	-3.93	117.19	122.93
2	A	1203	Y01	OAW-CAY-CAM	3.93	119.98	111.48
2	B	1201	Y01	CAV-CAZ-CBH	-3.92	111.40	116.42
2	D	1201	Y01	CAV-CAZ-CBH	-3.92	111.40	116.42
2	A	1201	Y01	CAV-CAZ-CBH	-3.92	111.40	116.42
2	B	1203	Y01	OAW-CAY-CAM	3.92	119.95	111.48
2	C	1203	Y01	OAW-CAY-CAM	3.92	119.95	111.48
2	D	1203	Y01	OAW-CAY-CAM	3.92	119.95	111.48
2	A	1202	Y01	CAU-CBI-CBE	-3.87	110.90	116.60
2	B	1202	Y01	CAU-CBI-CBE	-3.87	110.90	116.60
2	C	1202	Y01	CAU-CBI-CBE	-3.87	110.90	116.60
2	D	1202	Y01	CAU-CBI-CBE	-3.87	110.90	116.60
2	C	1205	Y01	CAU-CBI-CBE	-3.83	110.96	116.60
2	A	1202	Y01	CAD-CBH-CBF	3.82	115.94	111.66
2	B	1202	Y01	CAD-CBH-CBF	3.82	115.94	111.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1202	Y01	CAD-CBH-CBF	3.82	115.94	111.66
2	D	1202	Y01	CAD-CBH-CBF	3.82	115.94	111.66
2	A	1205	Y01	CAU-CBI-CBE	-3.81	110.98	116.60
2	B	1205	Y01	CAU-CBI-CBE	-3.81	110.99	116.60
2	D	1205	Y01	CAU-CBI-CBE	-3.81	110.99	116.60
2	C	1206	Y01	CAD-CBH-CBF	3.73	115.85	111.66
2	B	1206	Y01	CAD-CBH-CBF	3.72	115.83	111.66
2	D	1206	Y01	CAD-CBH-CBF	3.72	115.83	111.66
2	A	1206	Y01	CAD-CBH-CBF	3.70	115.82	111.66
2	A	1202	Y01	OAW-CAY-CAM	3.70	119.49	111.48
2	B	1202	Y01	OAW-CAY-CAM	3.70	119.49	111.48
2	C	1202	Y01	OAW-CAY-CAM	3.70	119.49	111.48
2	D	1202	Y01	OAW-CAY-CAM	3.70	119.49	111.48
2	A	1203	Y01	CAD-CBH-CAZ	3.69	114.03	108.38
2	B	1203	Y01	CAD-CBH-CAZ	3.67	113.99	108.38
2	C	1203	Y01	CAD-CBH-CAZ	3.67	113.99	108.38
2	D	1203	Y01	CAD-CBH-CAZ	3.67	113.99	108.38
2	A	1201	Y01	CAU-CBI-CBE	-3.58	111.32	116.60
2	B	1201	Y01	CAU-CBI-CBE	-3.58	111.32	116.60
2	C	1201	Y01	CAU-CBI-CBE	-3.58	111.32	116.60
2	D	1201	Y01	CAU-CBI-CBE	-3.58	111.32	116.60
2	A	1206	Y01	CBH-CAZ-CAI	-3.52	117.79	122.93
2	B	1206	Y01	CBH-CAZ-CAI	-3.52	117.79	122.93
2	C	1206	Y01	CBH-CAZ-CAI	-3.52	117.79	122.93
2	D	1206	Y01	CBH-CAZ-CAI	-3.50	117.83	122.93
2	B	1202	Y01	CAC-CBB-CBE	-3.49	107.64	112.88
2	D	1202	Y01	CAC-CBB-CBE	-3.49	107.64	112.88
2	A	1205	Y01	OAW-CAY-CAM	3.49	119.02	111.48
2	A	1202	Y01	CAC-CBB-CBE	-3.49	107.65	112.88
2	C	1202	Y01	CAC-CBB-CBE	-3.49	107.65	112.88
2	A	1202	Y01	CAK-CBD-CBF	-3.48	105.69	109.72
2	B	1205	Y01	OAW-CAY-CAM	3.48	119.00	111.48
2	C	1205	Y01	OAW-CAY-CAM	3.48	119.00	111.48
2	D	1205	Y01	OAW-CAY-CAM	3.48	119.00	111.48
2	B	1202	Y01	CAK-CBD-CBF	-3.46	105.72	109.72
2	C	1202	Y01	CAK-CBD-CBF	-3.46	105.72	109.72
2	D	1202	Y01	CAK-CBD-CBF	-3.46	105.72	109.72
2	A	1202	Y01	CAV-CAZ-CBH	-3.42	112.05	116.42
2	B	1202	Y01	CAV-CAZ-CBH	-3.42	112.05	116.42
2	C	1202	Y01	CAV-CAZ-CBH	-3.42	112.05	116.42
2	D	1202	Y01	CAV-CAZ-CBH	-3.42	112.05	116.42
2	A	1203	Y01	CAU-CBI-CBE	-3.38	111.62	116.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1203	Y01	CAU-CBI-CBE	-3.38	111.62	116.60
2	C	1203	Y01	CAU-CBI-CBE	-3.38	111.62	116.60
2	D	1203	Y01	CAU-CBI-CBE	-3.38	111.62	116.60
2	A	1201	Y01	CAU-CAS-CBF	3.38	118.88	113.14
2	B	1201	Y01	CAU-CAS-CBF	3.37	118.87	113.14
2	C	1201	Y01	CAU-CAS-CBF	3.37	118.87	113.14
2	D	1201	Y01	CAU-CAS-CBF	3.37	118.87	113.14
2	B	1202	Y01	CBH-CAZ-CAI	-3.37	118.01	122.93
2	C	1202	Y01	CBH-CAZ-CAI	-3.37	118.01	122.93
2	D	1202	Y01	CBH-CAZ-CAI	-3.37	118.01	122.93
2	A	1202	Y01	CBH-CAZ-CAI	-3.35	118.04	122.93
2	A	1203	Y01	CBH-CBF-CBD	-3.33	107.84	112.71
2	B	1203	Y01	CBH-CBF-CBD	-3.33	107.84	112.71
2	C	1203	Y01	CBH-CBF-CBD	-3.33	107.84	112.71
2	D	1203	Y01	CBH-CBF-CBD	-3.33	107.84	112.71
2	B	1203	Y01	CBH-CAZ-CAI	-3.31	118.09	122.93
2	C	1203	Y01	CBH-CAZ-CAI	-3.31	118.09	122.93
2	D	1203	Y01	CBH-CAZ-CAI	-3.31	118.09	122.93
2	A	1203	Y01	CBH-CAZ-CAI	-3.31	118.09	122.93
2	D	1202	Y01	CAU-CAS-CBF	3.24	118.64	113.14
2	B	1206	Y01	CAV-CAZ-CBH	-3.24	112.28	116.42
2	C	1206	Y01	CAV-CAZ-CBH	-3.24	112.28	116.42
2	A	1202	Y01	CAU-CAS-CBF	3.24	118.64	113.14
2	B	1202	Y01	CAU-CAS-CBF	3.24	118.64	113.14
2	C	1202	Y01	CAU-CAS-CBF	3.24	118.64	113.14
2	A	1206	Y01	CAV-CAZ-CBH	-3.23	112.28	116.42
2	D	1206	Y01	CAV-CAZ-CBH	-3.23	112.29	116.42
2	B	1206	Y01	CAD-CBH-CAZ	3.14	113.18	108.38
2	C	1206	Y01	CAD-CBH-CAZ	3.14	113.18	108.38
2	D	1206	Y01	CAD-CBH-CAZ	3.14	113.18	108.38
2	A	1206	Y01	CAD-CBH-CAZ	3.13	113.17	108.38
2	B	1203	Y01	CBF-CBH-CAZ	3.13	114.24	109.65
2	C	1203	Y01	CBF-CBH-CAZ	3.13	114.24	109.65
2	D	1203	Y01	CBF-CBH-CAZ	3.13	114.24	109.65
2	A	1203	Y01	CBF-CBH-CAZ	3.12	114.23	109.65
2	A	1202	Y01	CAD-CBH-CAZ	3.12	113.14	108.38
2	B	1202	Y01	CAD-CBH-CAZ	3.12	113.14	108.38
2	C	1202	Y01	CAD-CBH-CAZ	3.12	113.14	108.38
2	D	1202	Y01	CAD-CBH-CAZ	3.12	113.14	108.38
2	A	1201	Y01	CBH-CAZ-CAI	-3.08	118.43	122.93
2	B	1201	Y01	CBH-CAZ-CAI	-3.08	118.43	122.93
2	D	1201	Y01	CBH-CAZ-CAI	-3.08	118.43	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	Y01	CBH-CAZ-CAI	-3.06	118.45	122.93
2	A	1205	Y01	CAU-CAS-CBF	3.00	118.24	113.14
2	C	1205	Y01	CAU-CAS-CBF	3.00	118.24	113.14
2	A	1206	Y01	CAU-CAS-CBF	3.00	118.23	113.14
2	B	1206	Y01	CAU-CAS-CBF	3.00	118.23	113.14
2	D	1206	Y01	CAU-CAS-CBF	3.00	118.23	113.14
2	C	1206	Y01	CAU-CAS-CBF	3.00	118.23	113.14
2	B	1205	Y01	CAU-CAS-CBF	2.99	118.22	113.14
2	D	1205	Y01	CAU-CAS-CBF	2.99	118.22	113.14
2	A	1203	Y01	CAV-CAZ-CBH	-2.92	112.68	116.42
2	B	1203	Y01	CAV-CAZ-CBH	-2.92	112.68	116.42
2	C	1203	Y01	CAV-CAZ-CBH	-2.92	112.68	116.42
2	D	1203	Y01	CAV-CAZ-CBH	-2.92	112.68	116.42
2	D	1206	Y01	CAP-CBE-CBI	-2.89	100.45	103.84
2	C	1206	Y01	CAS-CBF-CBH	-2.87	109.55	113.08
2	B	1206	Y01	CAP-CBE-CBI	-2.86	100.47	103.84
2	A	1201	Y01	CAS-CAU-CBI	2.86	117.57	112.74
2	B	1201	Y01	CAS-CAU-CBI	2.86	117.57	112.74
2	C	1201	Y01	CAS-CAU-CBI	2.86	117.57	112.74
2	D	1201	Y01	CAS-CAU-CBI	2.86	117.57	112.74
2	A	1206	Y01	CAP-CBE-CBI	-2.86	100.47	103.84
2	C	1206	Y01	CAP-CBE-CBI	-2.86	100.47	103.84
2	A	1206	Y01	CAS-CBF-CBH	-2.86	109.56	113.08
2	B	1206	Y01	CAS-CBF-CBH	-2.86	109.56	113.08
2	D	1206	Y01	CAS-CBF-CBH	-2.86	109.56	113.08
2	A	1203	Y01	CAT-CBH-CAZ	-2.83	103.87	108.74
2	D	1206	Y01	CBI-CBE-CBB	-2.82	115.15	119.50
2	B	1205	Y01	CAV-CAZ-CBH	-2.82	112.81	116.42
2	D	1205	Y01	CAV-CAZ-CBH	-2.82	112.81	116.42
2	B	1206	Y01	CBI-CBE-CBB	-2.82	115.15	119.50
2	A	1205	Y01	CAV-CAZ-CBH	-2.81	112.82	116.42
2	C	1205	Y01	CAV-CAZ-CBH	-2.81	112.82	116.42
2	B	1203	Y01	CAT-CBH-CAZ	-2.81	103.90	108.74
2	C	1203	Y01	CAT-CBH-CAZ	-2.81	103.90	108.74
2	D	1203	Y01	CAT-CBH-CAZ	-2.81	103.90	108.74
2	A	1205	Y01	CBI-CBE-CBB	-2.81	115.16	119.50
2	C	1205	Y01	CBI-CBE-CBB	-2.81	115.16	119.50
2	A	1206	Y01	CBI-CBE-CBB	-2.80	115.17	119.50
2	C	1206	Y01	CBI-CBE-CBB	-2.80	115.17	119.50
2	C	1205	Y01	CAK-CBD-CBF	-2.80	106.49	109.72
2	B	1205	Y01	CBI-CBE-CBB	-2.79	115.18	119.50
2	D	1205	Y01	CBI-CBE-CBB	-2.79	115.18	119.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1205	Y01	CAK-CBD-CBF	-2.77	106.52	109.72
2	B	1205	Y01	CAK-CBD-CBF	-2.77	106.52	109.72
2	D	1205	Y01	CAK-CBD-CBF	-2.77	106.52	109.72
2	A	1203	Y01	CAD-CBH-CBF	2.74	114.74	111.66
2	B	1203	Y01	CAD-CBH-CBF	2.74	114.74	111.66
2	C	1203	Y01	CAD-CBH-CBF	2.74	114.74	111.66
2	D	1203	Y01	CAD-CBH-CBF	2.74	114.74	111.66
3	D	1204	LQ7	C14-C02-N03	2.73	122.47	118.24
2	C	1201	Y01	CAD-CBH-CAT	2.72	113.57	109.43
3	A	1204	LQ7	C14-C02-N03	2.71	122.45	118.24
2	A	1201	Y01	CAD-CBH-CAT	2.71	113.55	109.43
3	B	1204	LQ7	C14-C02-N03	2.70	122.44	118.24
3	C	1204	LQ7	C14-C02-N03	2.70	122.44	118.24
2	D	1201	Y01	CAD-CBH-CAT	2.70	113.53	109.43
2	B	1201	Y01	CAD-CBH-CAT	2.69	113.52	109.43
2	B	1202	Y01	CBD-CAK-CAI	-2.64	109.11	112.76
2	C	1202	Y01	CBD-CAK-CAI	-2.64	109.11	112.76
2	D	1202	Y01	CBD-CAK-CAI	-2.64	109.11	112.76
2	A	1206	Y01	CAK-CBD-CBF	-2.63	106.68	109.72
2	C	1206	Y01	CAK-CBD-CBF	-2.63	106.68	109.72
2	B	1206	Y01	CAK-CBD-CBF	-2.63	106.68	109.72
2	D	1206	Y01	CAK-CBD-CBF	-2.63	106.69	109.72
2	A	1202	Y01	CBD-CAK-CAI	-2.61	109.14	112.76
2	A	1203	Y01	CAP-CBE-CBB	-2.56	108.31	112.18
2	B	1203	Y01	CAP-CBE-CBB	-2.53	108.34	112.18
2	C	1203	Y01	CAP-CBE-CBB	-2.53	108.34	112.18
2	D	1203	Y01	CAP-CBE-CBB	-2.53	108.34	112.18
2	B	1206	Y01	CAC-CBB-CBE	-2.48	109.16	112.88
2	D	1206	Y01	CAC-CBB-CBE	-2.48	109.16	112.88
2	A	1202	Y01	CBI-CBE-CBB	-2.46	115.69	119.50
2	B	1202	Y01	CBI-CBE-CBB	-2.46	115.69	119.50
2	C	1202	Y01	CBI-CBE-CBB	-2.46	115.69	119.50
2	D	1202	Y01	CBI-CBE-CBB	-2.46	115.69	119.50
2	A	1206	Y01	CAC-CBB-CBE	-2.46	109.19	112.88
2	C	1206	Y01	CAC-CBB-CBE	-2.46	109.20	112.88
2	D	1202	Y01	CAS-CBF-CBD	2.44	115.19	111.78
2	A	1202	Y01	CAS-CBF-CBD	2.44	115.18	111.78
2	B	1202	Y01	CAS-CBF-CBD	2.44	115.18	111.78
2	C	1202	Y01	CAS-CBF-CBD	2.44	115.18	111.78
2	A	1202	Y01	CAP-CBE-CBI	-2.40	101.01	103.84
2	B	1202	Y01	CAP-CBE-CBI	-2.40	101.01	103.84
2	C	1202	Y01	CAP-CBE-CBI	-2.40	101.01	103.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1202	Y01	CAP-CBE-CBI	-2.40	101.01	103.84
2	A	1201	Y01	CBI-CBE-CBB	-2.35	115.87	119.50
2	B	1201	Y01	CBI-CBE-CBB	-2.35	115.87	119.50
2	C	1201	Y01	CBI-CBE-CBB	-2.35	115.87	119.50
2	D	1201	Y01	CBI-CBE-CBB	-2.35	115.87	119.50
4	A	1207	NAG	C8-C7-N2	2.28	119.90	116.12
4	B	1207	NAG	C8-C7-N2	2.26	119.86	116.12
4	C	1207	NAG	C8-C7-N2	2.26	119.86	116.12
4	D	1207	NAG	C8-C7-N2	2.26	119.86	116.12
2	A	1202	Y01	CAS-CBF-CBH	-2.21	110.35	113.08
2	B	1202	Y01	CAS-CBF-CBH	-2.21	110.35	113.08
2	C	1202	Y01	CAS-CBF-CBH	-2.21	110.35	113.08
2	A	1206	Y01	CAS-CBF-CBD	2.21	114.86	111.78
2	B	1203	Y01	CBI-CBE-CBB	-2.21	116.09	119.50
2	C	1203	Y01	CBI-CBE-CBB	-2.21	116.09	119.50
2	D	1203	Y01	CBI-CBE-CBB	-2.21	116.09	119.50
2	B	1206	Y01	CAS-CBF-CBD	2.20	114.85	111.78
2	D	1206	Y01	CAS-CBF-CBD	2.20	114.85	111.78
2	A	1203	Y01	CBI-CBE-CBB	-2.20	116.10	119.50
2	C	1206	Y01	CAS-CBF-CBD	2.20	114.84	111.78
2	D	1202	Y01	CAS-CBF-CBH	-2.19	110.38	113.08
2	D	1203	Y01	CBC-CAV-CAZ	2.18	114.67	111.45
2	A	1203	Y01	CBC-CAV-CAZ	2.17	114.66	111.45
2	B	1203	Y01	CBC-CAV-CAZ	2.17	114.66	111.45
2	C	1203	Y01	CBC-CAV-CAZ	2.17	114.66	111.45
2	A	1201	Y01	CAT-CBH-CAZ	-2.17	105.00	108.74
2	C	1201	Y01	CAT-CBH-CAZ	-2.16	105.01	108.74
2	B	1205	Y01	CAS-CBF-CBD	2.16	114.80	111.78
2	D	1205	Y01	CAS-CBF-CBD	2.16	114.80	111.78
2	A	1205	Y01	CAS-CBF-CBD	2.15	114.77	111.78
2	B	1201	Y01	CAT-CBH-CAZ	-2.14	105.05	108.74
2	D	1201	Y01	CAT-CBH-CAZ	-2.14	105.05	108.74
2	A	1203	Y01	CAD-CBH-CAT	2.14	112.69	109.43
2	B	1203	Y01	CAD-CBH-CAT	2.14	112.69	109.43
2	C	1203	Y01	CAD-CBH-CAT	2.14	112.69	109.43
2	D	1203	Y01	CAD-CBH-CAT	2.14	112.69	109.43
2	C	1205	Y01	CAS-CBF-CBD	2.12	114.74	111.78
2	C	1201	Y01	CBI-CBG-CBD	-2.11	111.42	114.41
2	A	1201	Y01	CBI-CBG-CBD	-2.10	111.43	114.41
2	D	1201	Y01	CBI-CBG-CBD	-2.10	111.43	114.41
2	A	1205	Y01	CAD-CBH-CAZ	2.08	111.56	108.38
2	B	1205	Y01	CAD-CBH-CAZ	2.08	111.56	108.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1205	Y01	CAD-CBH-CAZ	2.08	111.56	108.38
2	B	1203	Y01	CAR-CBC-CAV	2.08	113.87	110.97
2	C	1203	Y01	CAR-CBC-CAV	2.08	113.87	110.97
3	B	1204	LQ7	O01-C02-N03	-2.08	119.08	122.35
3	C	1204	LQ7	O01-C02-N03	-2.08	119.08	122.35
2	B	1201	Y01	CBI-CBG-CBD	-2.08	111.46	114.41
2	D	1203	Y01	CAR-CBC-CAV	2.08	113.86	110.97
3	A	1204	LQ7	O01-C02-N03	-2.06	119.10	122.35
3	D	1204	LQ7	O01-C02-N03	-2.06	119.10	122.35
2	A	1203	Y01	CAR-CBC-CAV	2.06	113.84	110.97
2	C	1205	Y01	CAD-CBH-CAZ	2.06	111.53	108.38

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1206	Y01	CAM-CAY-OAW-CBC
2	B	1206	Y01	CAM-CAY-OAW-CBC
2	C	1206	Y01	CAM-CAY-OAW-CBC
2	D	1206	Y01	CAM-CAY-OAW-CBC
3	A	1204	LQ7	N03-C04-C05-C06
3	B	1204	LQ7	N03-C04-C05-C06
3	C	1204	LQ7	N03-C04-C05-C06
3	D	1204	LQ7	N03-C04-C05-C06
4	A	1207	NAG	C3-C2-N2-C7
4	B	1207	NAG	C3-C2-N2-C7
4	C	1207	NAG	C3-C2-N2-C7
4	D	1207	NAG	C3-C2-N2-C7
2	A	1202	Y01	CAC-CBB-CBE-CBI
2	B	1202	Y01	CAC-CBB-CBE-CBI
2	C	1202	Y01	CAC-CBB-CBE-CBI
2	D	1202	Y01	CAC-CBB-CBE-CBI
2	A	1202	Y01	CAO-CBB-CBE-CBI
2	B	1202	Y01	CAO-CBB-CBE-CBI
2	C	1202	Y01	CAO-CBB-CBE-CBI
2	D	1202	Y01	CAO-CBB-CBE-CBI
2	A	1206	Y01	OAG-CAY-OAW-CBC
2	B	1206	Y01	OAG-CAY-OAW-CBC
2	C	1206	Y01	OAG-CAY-OAW-CBC
2	D	1206	Y01	OAG-CAY-OAW-CBC
2	A	1203	Y01	CAJ-CAO-CBB-CBE
2	B	1203	Y01	CAJ-CAO-CBB-CBE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1203	Y01	CAJ-CAO-CBB-CBE
2	D	1203	Y01	CAJ-CAO-CBB-CBE
2	A	1203	Y01	CAJ-CAO-CBB-CAC
2	B	1203	Y01	CAJ-CAO-CBB-CAC
2	C	1203	Y01	CAJ-CAO-CBB-CAC
2	D	1203	Y01	CAJ-CAO-CBB-CAC
2	A	1206	Y01	CAO-CAJ-CAN-CBA
2	B	1206	Y01	CAO-CAJ-CAN-CBA
2	C	1206	Y01	CAO-CAJ-CAN-CBA
2	D	1206	Y01	CAO-CAJ-CAN-CBA
2	A	1202	Y01	CAO-CAJ-CAN-CBA
2	B	1202	Y01	CAO-CAJ-CAN-CBA
2	C	1202	Y01	CAO-CAJ-CAN-CBA
2	D	1202	Y01	CAO-CAJ-CAN-CBA
2	A	1203	Y01	CAN-CAJ-CAO-CBB
2	B	1203	Y01	CAN-CAJ-CAO-CBB
2	C	1203	Y01	CAN-CAJ-CAO-CBB
2	D	1203	Y01	CAN-CAJ-CAO-CBB
2	A	1206	Y01	CAC-CBB-CBE-CBI
2	B	1206	Y01	CAC-CBB-CBE-CBI
2	C	1206	Y01	CAC-CBB-CBE-CBI
2	D	1206	Y01	CAC-CBB-CBE-CBI
2	A	1202	Y01	CAC-CBB-CBE-CAP
2	B	1202	Y01	CAC-CBB-CBE-CAP
2	C	1202	Y01	CAC-CBB-CBE-CAP
2	D	1202	Y01	CAC-CBB-CBE-CAP
2	A	1206	Y01	CAJ-CAN-CBA-CAB
2	B	1206	Y01	CAJ-CAN-CBA-CAB
2	C	1206	Y01	CAJ-CAN-CBA-CAB
2	D	1206	Y01	CAJ-CAN-CBA-CAB
2	A	1203	Y01	CAJ-CAN-CBA-CAB
2	B	1203	Y01	CAJ-CAN-CBA-CAB
2	C	1203	Y01	CAJ-CAN-CBA-CAB
2	D	1203	Y01	CAJ-CAN-CBA-CAB
2	A	1206	Y01	CAJ-CAN-CBA-CAA
2	B	1206	Y01	CAJ-CAN-CBA-CAA
2	C	1206	Y01	CAJ-CAN-CBA-CAA
2	D	1206	Y01	CAJ-CAN-CBA-CAA
2	A	1201	Y01	CAJ-CAN-CBA-CAB
2	B	1201	Y01	CAJ-CAN-CBA-CAB
2	C	1201	Y01	CAJ-CAN-CBA-CAB
2	D	1201	Y01	CAJ-CAN-CBA-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1203	Y01	CAJ-CAN-CBA-CAA
2	B	1203	Y01	CAJ-CAN-CBA-CAA
2	C	1203	Y01	CAJ-CAN-CBA-CAA
2	D	1203	Y01	CAJ-CAN-CBA-CAA
2	A	1206	Y01	CAO-CBB-CBE-CBI
2	B	1206	Y01	CAO-CBB-CBE-CBI
2	C	1206	Y01	CAO-CBB-CBE-CBI
2	D	1206	Y01	CAO-CBB-CBE-CBI
2	A	1205	Y01	CAM-CAY-OAW-CBC
2	B	1205	Y01	CAM-CAY-OAW-CBC
2	C	1205	Y01	CAM-CAY-OAW-CBC
2	D	1205	Y01	CAM-CAY-OAW-CBC
2	A	1206	Y01	CAC-CBB-CBE-CAP
2	B	1206	Y01	CAC-CBB-CBE-CAP
2	C	1206	Y01	CAC-CBB-CBE-CAP
2	D	1206	Y01	CAC-CBB-CBE-CAP
2	A	1202	Y01	CAO-CBB-CBE-CAP
2	B	1202	Y01	CAO-CBB-CBE-CAP
2	C	1202	Y01	CAO-CBB-CBE-CAP
2	D	1202	Y01	CAO-CBB-CBE-CAP
4	A	1207	NAG	C1-C2-N2-C7
4	B	1207	NAG	C1-C2-N2-C7
4	C	1207	NAG	C1-C2-N2-C7
4	D	1207	NAG	C1-C2-N2-C7
2	A	1201	Y01	CAJ-CAN-CBA-CAA
2	B	1201	Y01	CAJ-CAN-CBA-CAA
2	C	1201	Y01	CAJ-CAN-CBA-CAA
2	D	1201	Y01	CAJ-CAN-CBA-CAA
2	A	1203	Y01	CAM-CAY-OAW-CBC
2	B	1203	Y01	CAM-CAY-OAW-CBC
2	C	1203	Y01	CAM-CAY-OAW-CBC
2	D	1203	Y01	CAM-CAY-OAW-CBC
2	A	1205	Y01	OAG-CAY-OAW-CBC
2	B	1205	Y01	OAG-CAY-OAW-CBC
2	C	1205	Y01	OAG-CAY-OAW-CBC
2	D	1205	Y01	OAG-CAY-OAW-CBC
2	A	1202	Y01	CAX-CAL-CAM-CAY
2	B	1202	Y01	CAX-CAL-CAM-CAY
2	C	1202	Y01	CAX-CAL-CAM-CAY
2	D	1202	Y01	CAX-CAL-CAM-CAY
2	A	1203	Y01	OAG-CAY-OAW-CBC
2	B	1203	Y01	OAG-CAY-OAW-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	1203	Y01	OAG-CAY-OAW-CBC
2	D	1203	Y01	OAG-CAY-OAW-CBC
2	A	1202	Y01	OAG-CAY-OAW-CBC
2	B	1202	Y01	OAG-CAY-OAW-CBC
2	C	1202	Y01	OAG-CAY-OAW-CBC
2	D	1202	Y01	OAG-CAY-OAW-CBC
2	A	1202	Y01	CAM-CAY-OAW-CBC
2	B	1202	Y01	CAM-CAY-OAW-CBC
2	C	1202	Y01	CAM-CAY-OAW-CBC
2	D	1202	Y01	CAM-CAY-OAW-CBC
2	A	1205	Y01	CAJ-CAO-CBB-CBE
2	B	1205	Y01	CAJ-CAO-CBB-CBE
2	C	1205	Y01	CAJ-CAO-CBB-CBE
2	D	1205	Y01	CAJ-CAO-CBB-CBE
2	A	1206	Y01	CAO-CBB-CBE-CAP
2	B	1206	Y01	CAO-CBB-CBE-CAP
2	C	1206	Y01	CAO-CBB-CBE-CAP
2	D	1206	Y01	CAO-CBB-CBE-CAP
2	A	1203	Y01	CAM-CAL-CAX-OAF
2	B	1203	Y01	CAM-CAL-CAX-OAF
2	C	1203	Y01	CAM-CAL-CAX-OAF
2	D	1203	Y01	CAM-CAL-CAX-OAF
2	A	1203	Y01	CAM-CAL-CAX-OAH
2	B	1203	Y01	CAM-CAL-CAX-OAH
2	C	1203	Y01	CAM-CAL-CAX-OAH
2	D	1203	Y01	CAM-CAL-CAX-OAH
2	A	1206	Y01	CAM-CAL-CAX-OAF
2	B	1206	Y01	CAM-CAL-CAX-OAF
2	C	1206	Y01	CAM-CAL-CAX-OAF
2	D	1206	Y01	CAM-CAL-CAX-OAF
2	A	1206	Y01	CAM-CAL-CAX-OAH
2	B	1206	Y01	CAM-CAL-CAX-OAH
2	C	1206	Y01	CAM-CAL-CAX-OAH
2	D	1206	Y01	CAM-CAL-CAX-OAH
3	A	1204	LQ7	C25-C15-O16-C17
3	B	1204	LQ7	C25-C15-O16-C17
3	C	1204	LQ7	C25-C15-O16-C17
3	D	1204	LQ7	C25-C15-O16-C17
2	A	1201	Y01	CAM-CAL-CAX-OAF
2	B	1201	Y01	CAM-CAL-CAX-OAF
2	C	1201	Y01	CAM-CAL-CAX-OAF
2	D	1201	Y01	CAM-CAL-CAX-OAF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1201	Y01	CAM-CAL-CAX-OAH
2	D	1201	Y01	CAM-CAL-CAX-OAH
2	A	1201	Y01	CAM-CAL-CAX-OAH
2	C	1201	Y01	CAM-CAL-CAX-OAH
2	A	1205	Y01	CAM-CAL-CAX-OAH
2	B	1205	Y01	CAM-CAL-CAX-OAH
2	C	1205	Y01	CAM-CAL-CAX-OAH
2	D	1205	Y01	CAM-CAL-CAX-OAH
2	A	1205	Y01	CAL-CAM-CAY-OAW
2	B	1205	Y01	CAL-CAM-CAY-OAW
2	C	1205	Y01	CAL-CAM-CAY-OAW
2	D	1205	Y01	CAL-CAM-CAY-OAW

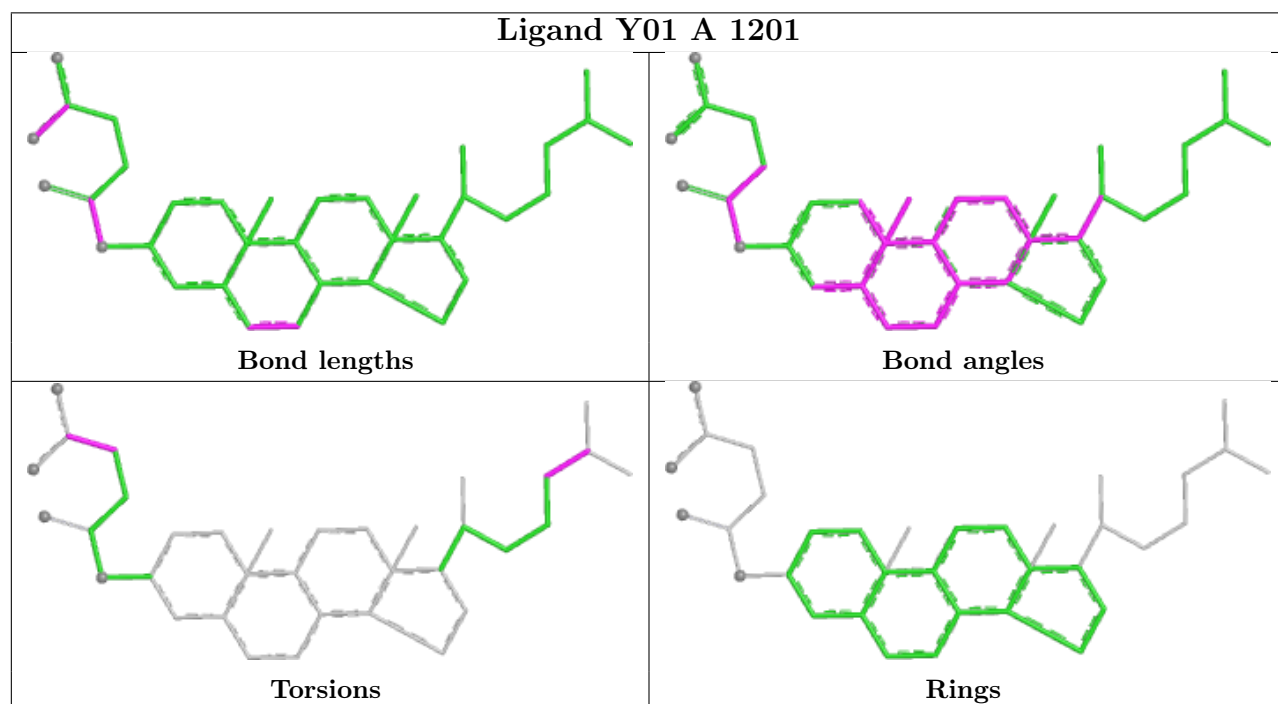
There are no ring outliers.

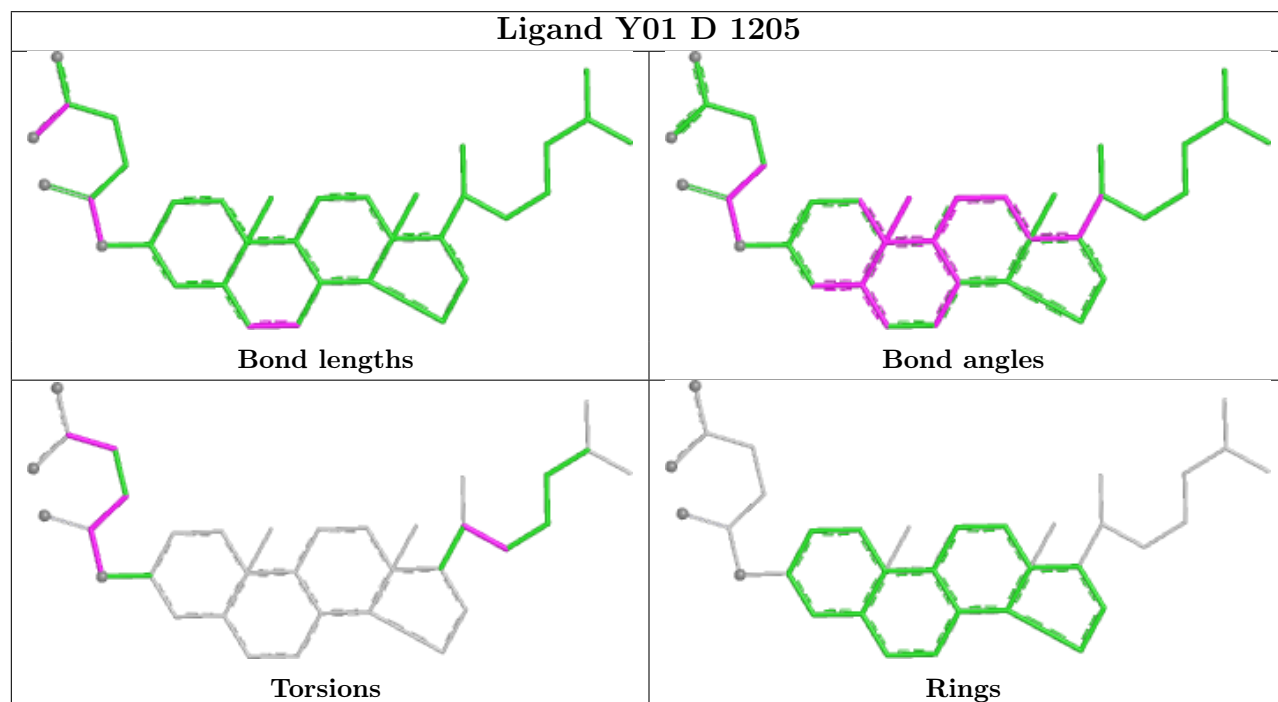
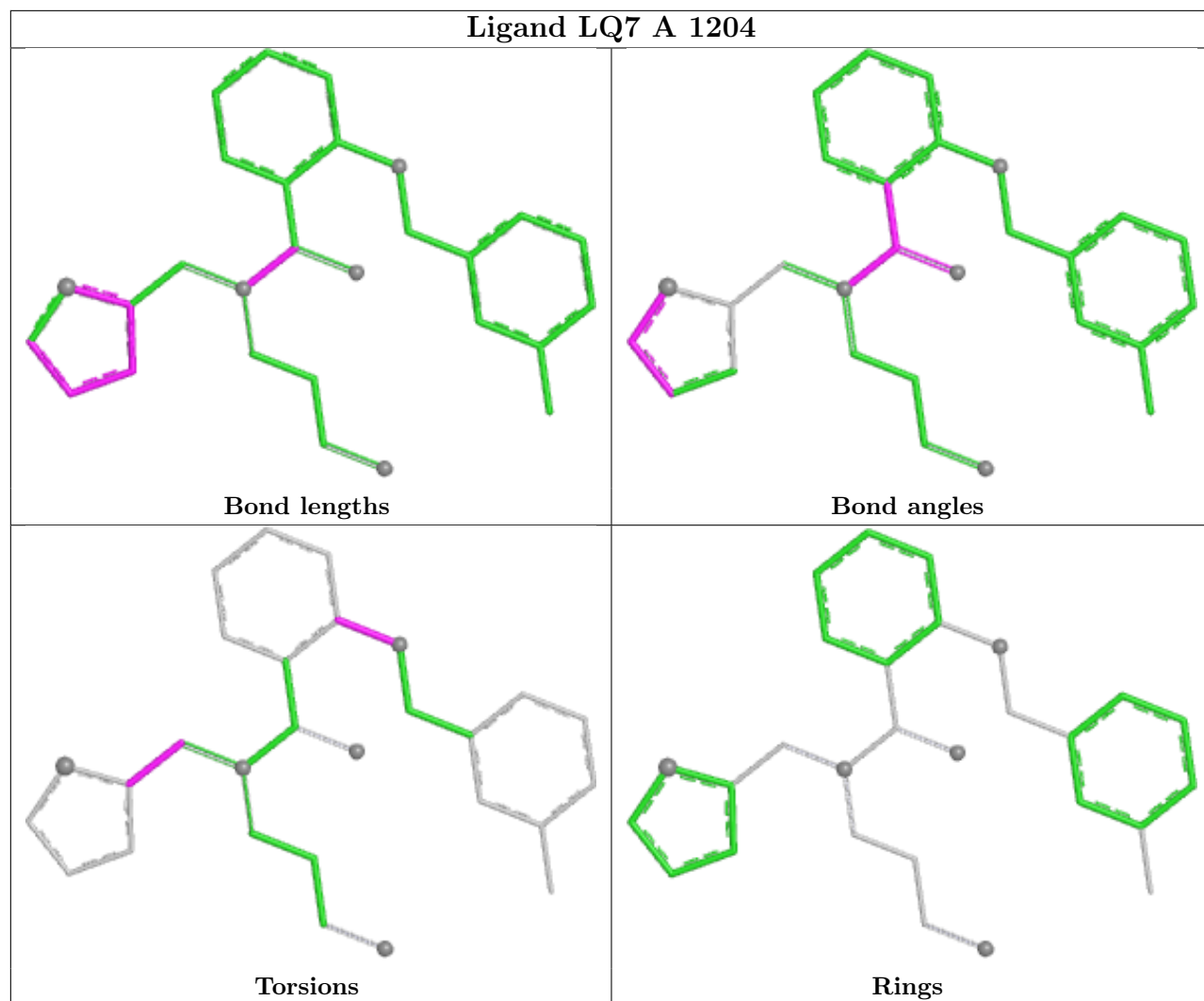
14 monomers are involved in 16 short contacts:

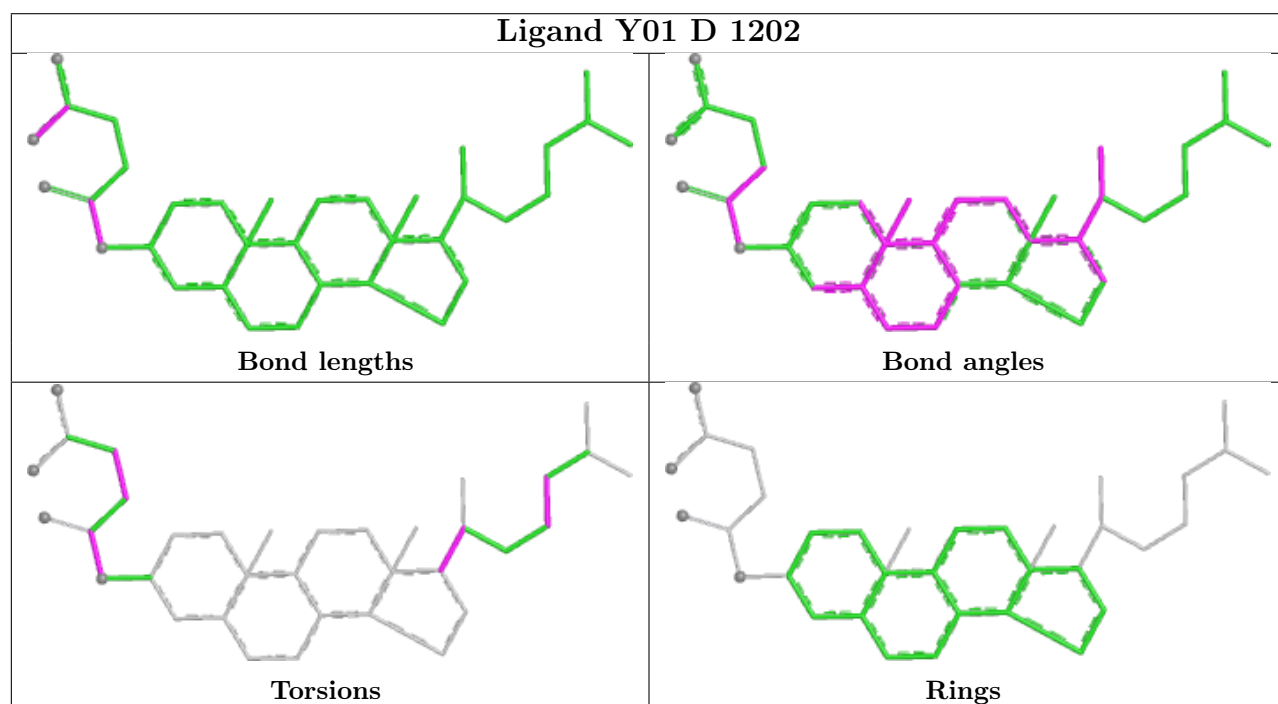
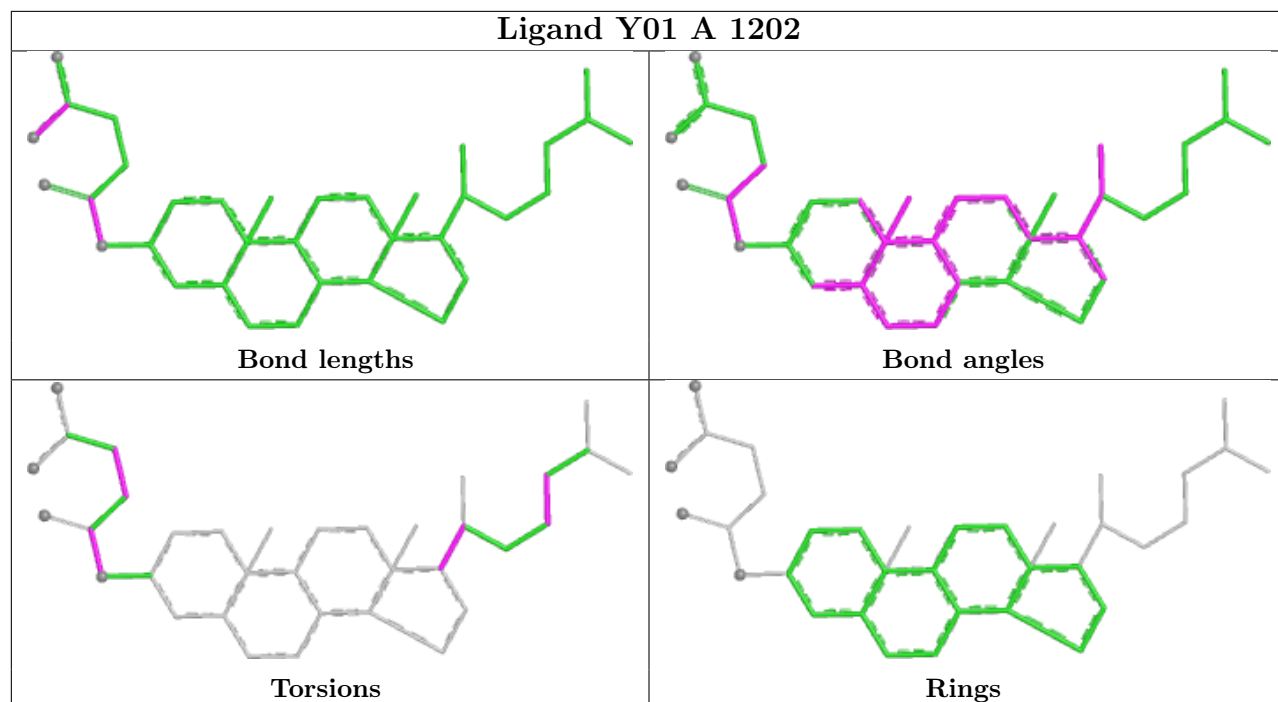
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1205	Y01	1	0
2	D	1202	Y01	1	0
4	A	1207	NAG	1	0
4	D	1207	NAG	1	0
2	D	1203	Y01	1	0
2	A	1203	Y01	2	0
4	C	1207	NAG	1	0
4	B	1207	NAG	1	0
2	C	1205	Y01	1	0
2	C	1203	Y01	2	0
2	B	1205	Y01	1	0
2	C	1202	Y01	1	0
2	B	1203	Y01	1	0
2	A	1205	Y01	1	0

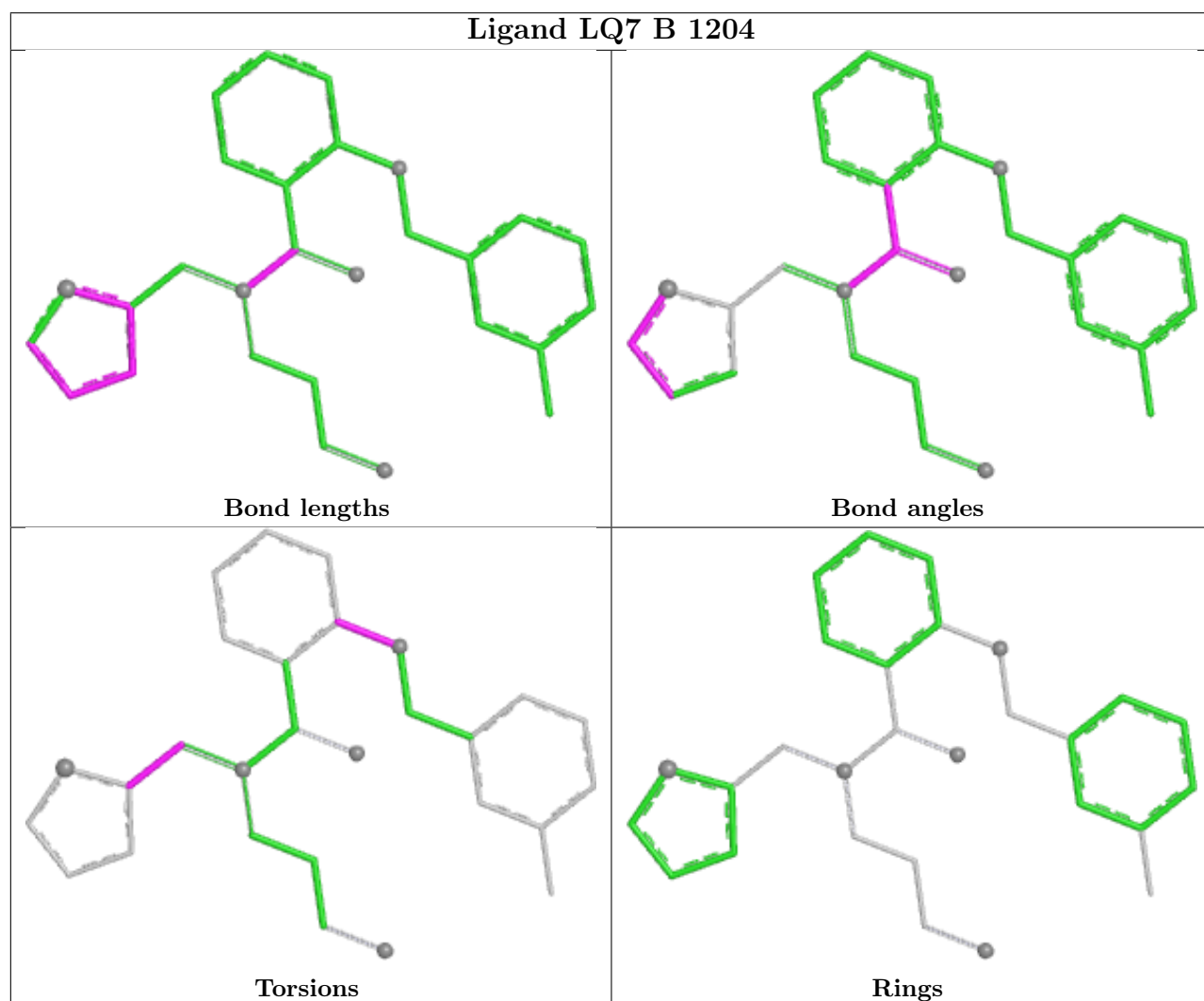
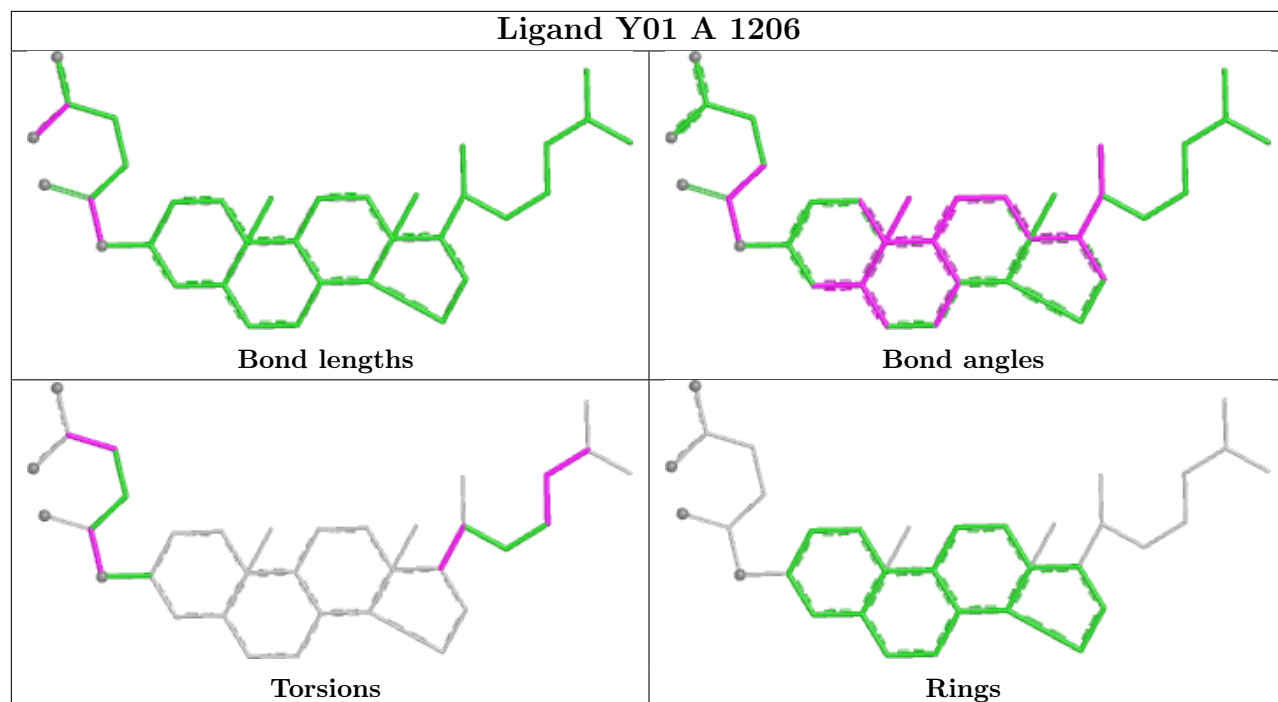
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

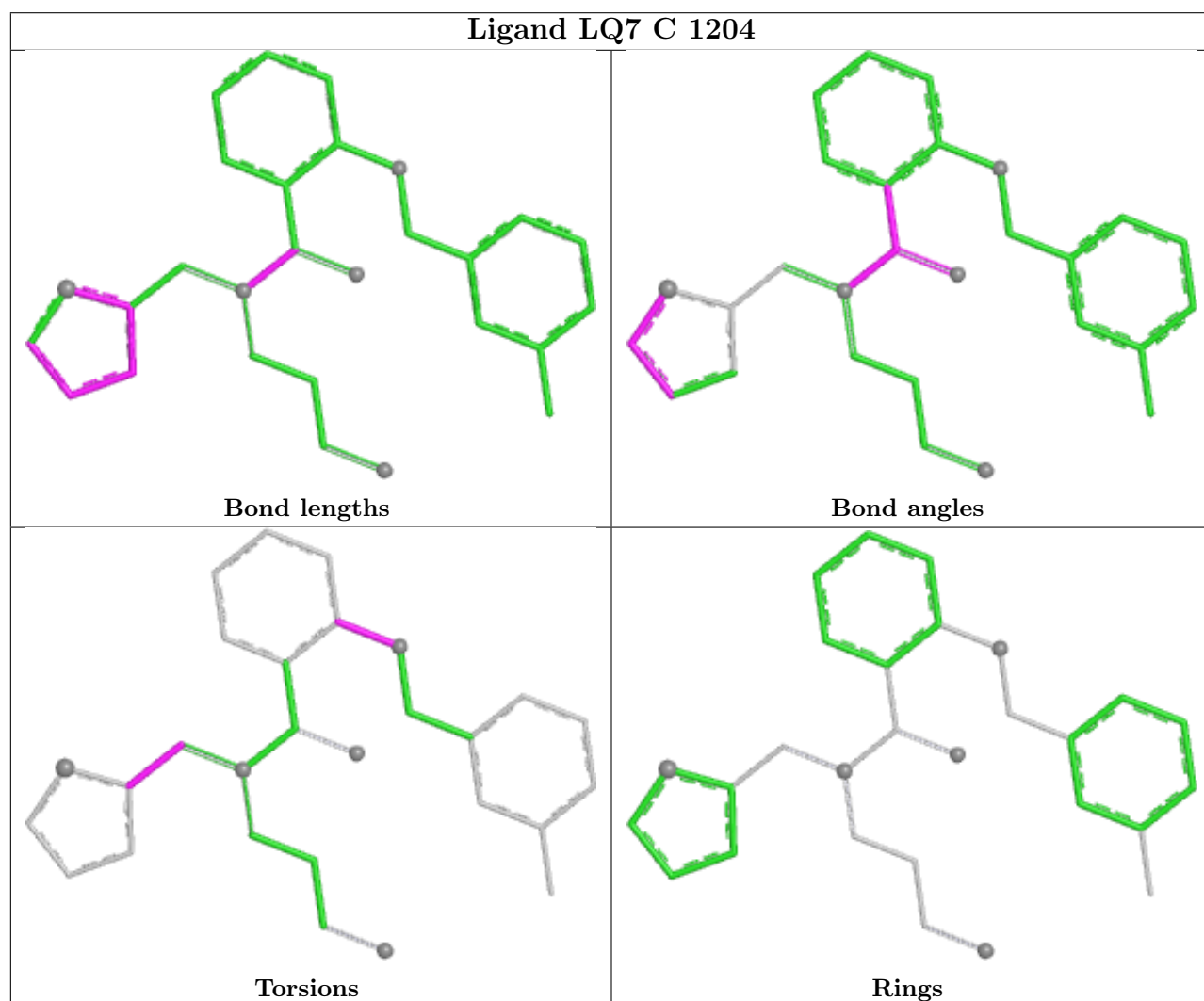
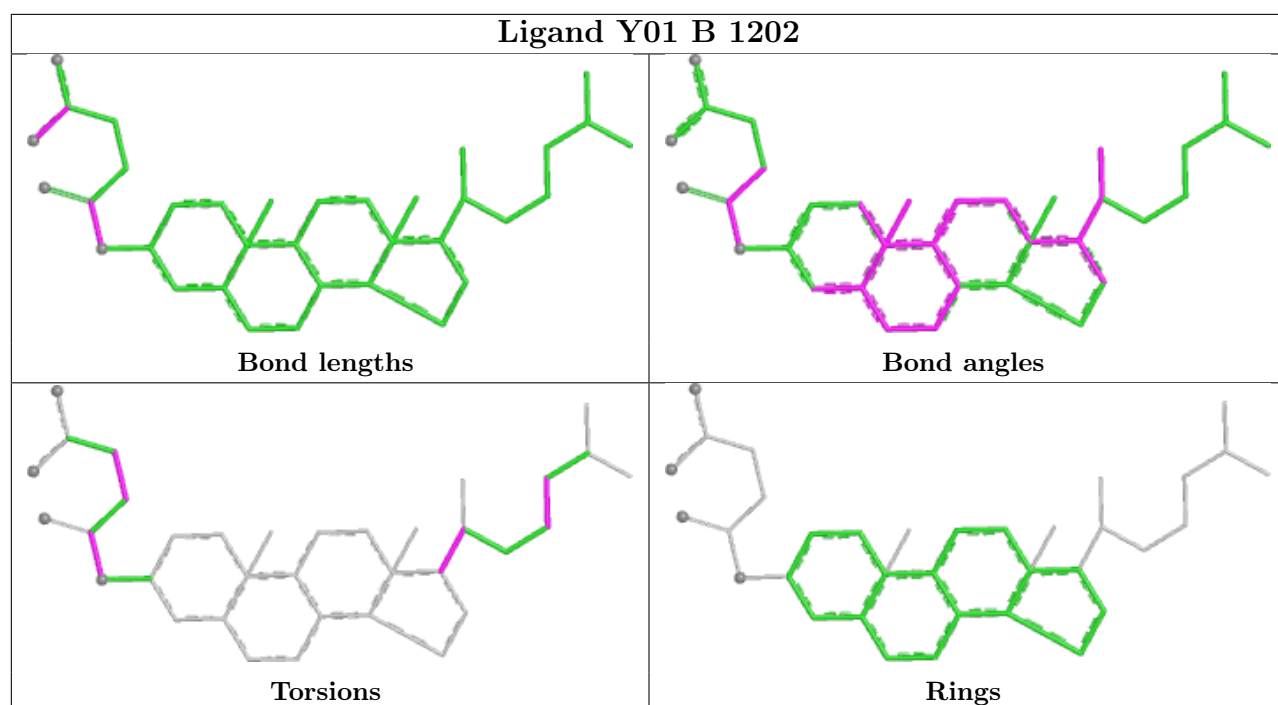
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

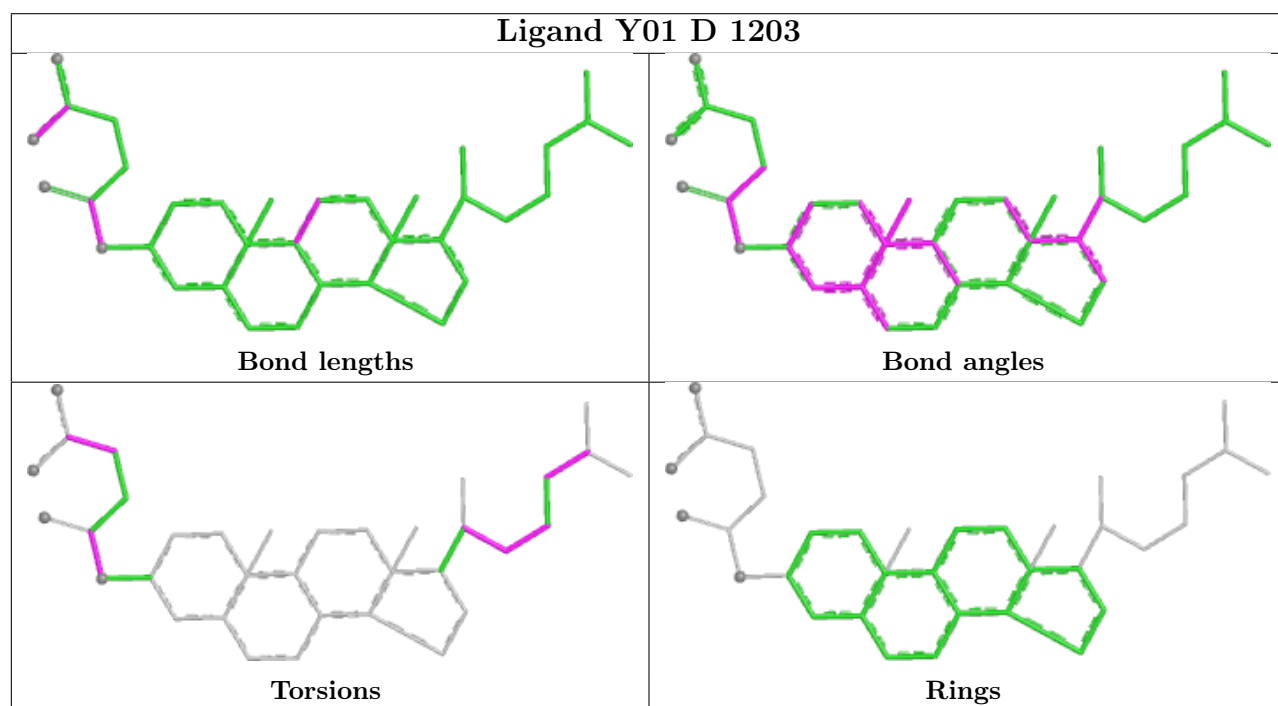
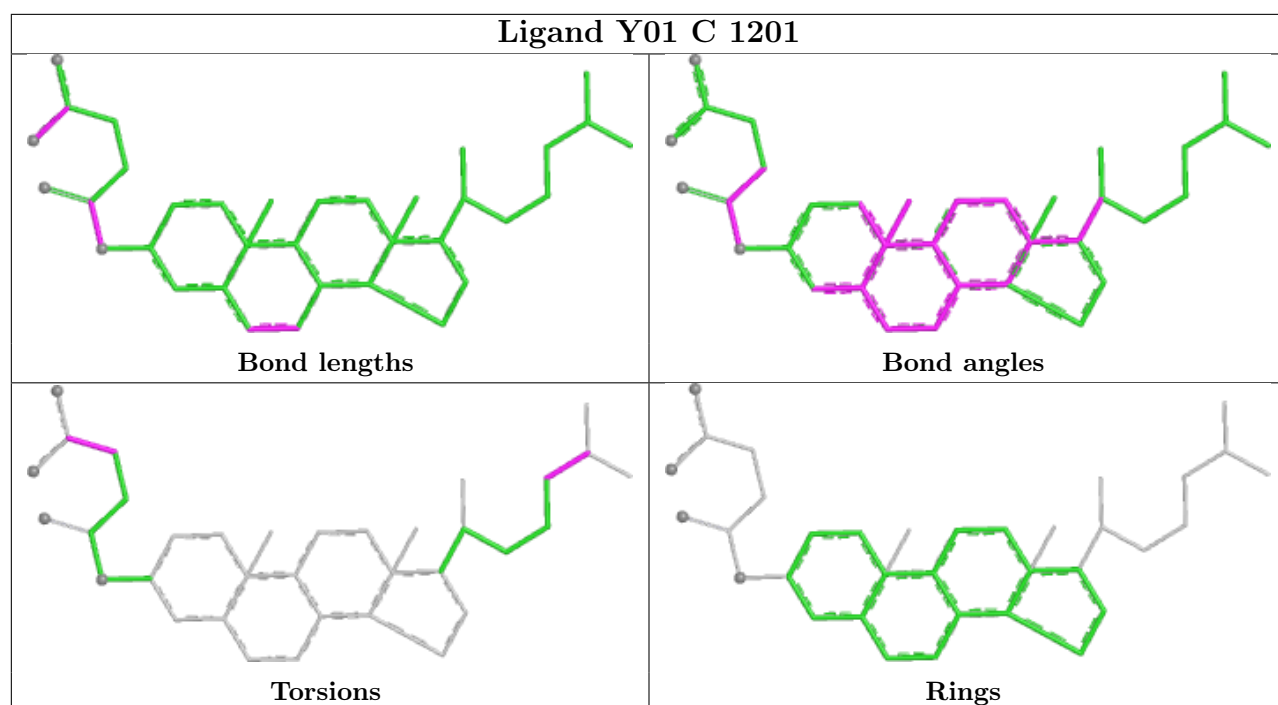


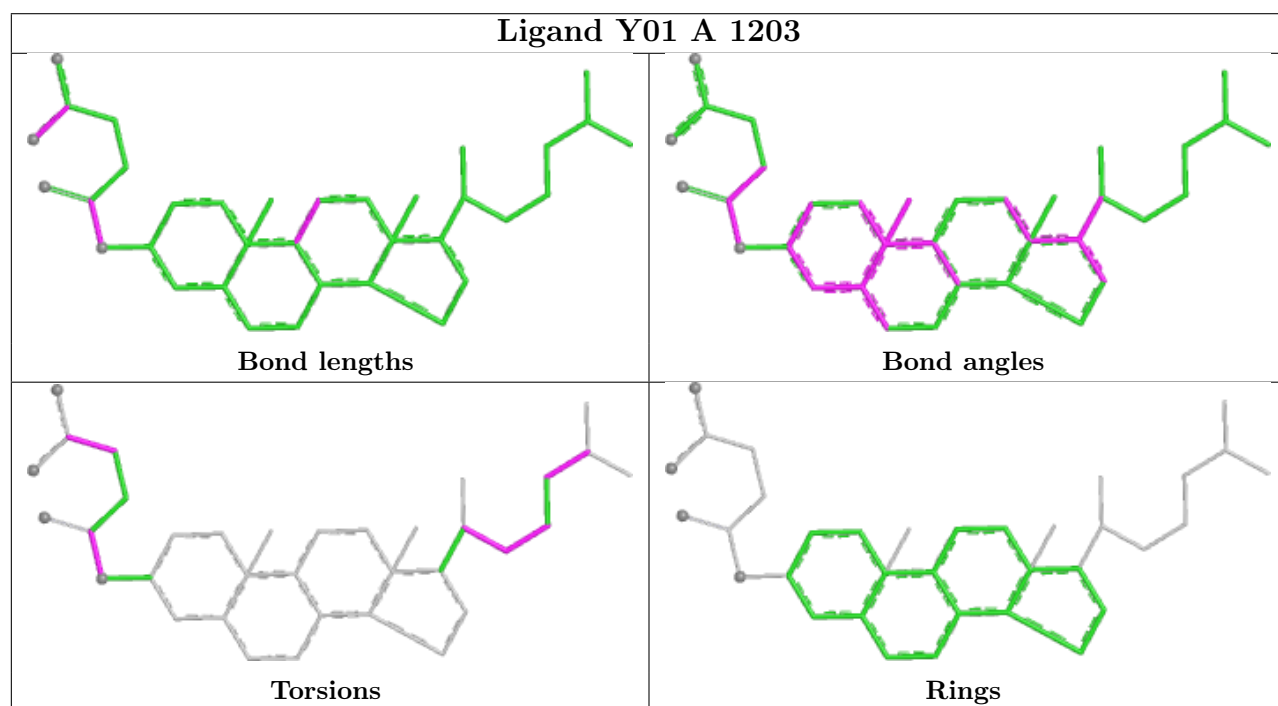
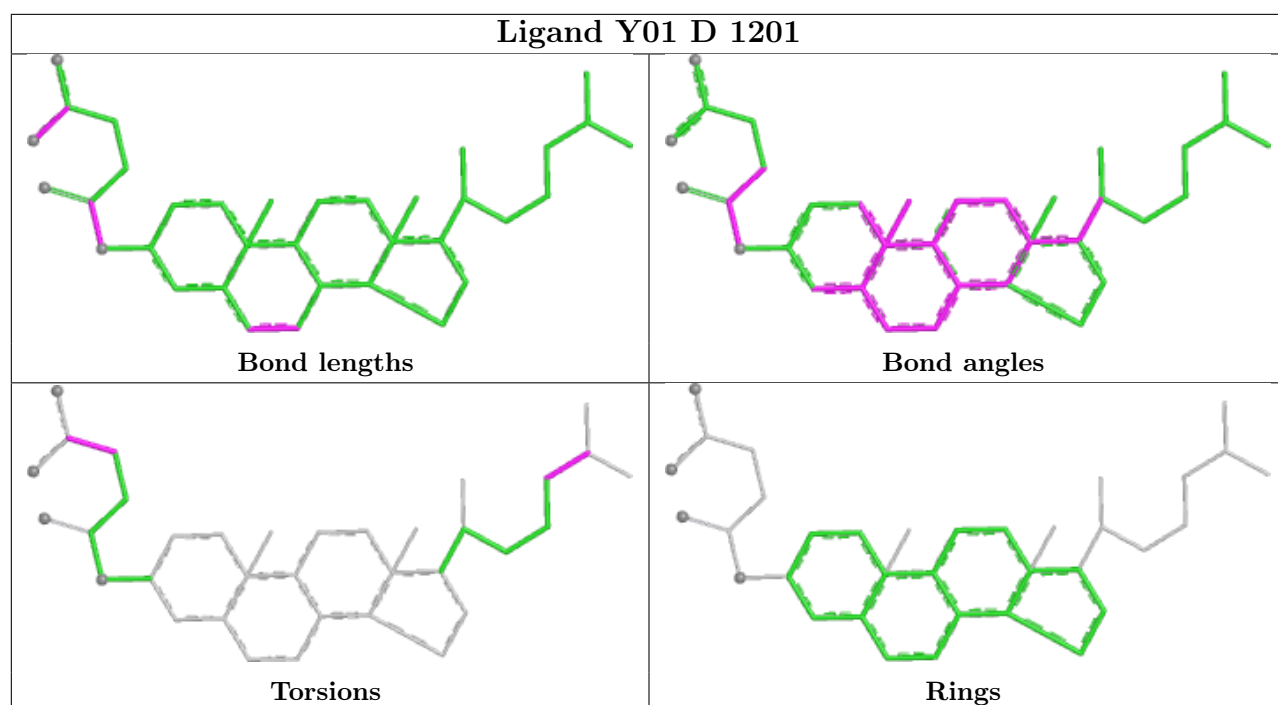


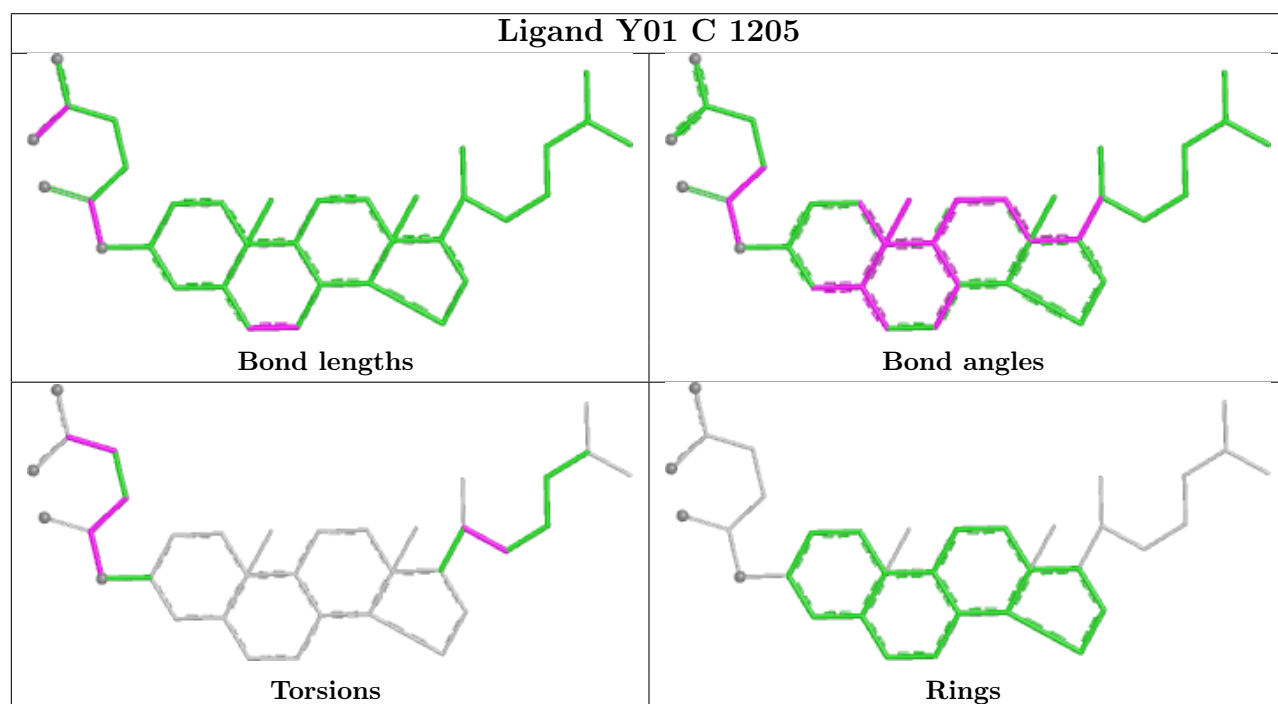
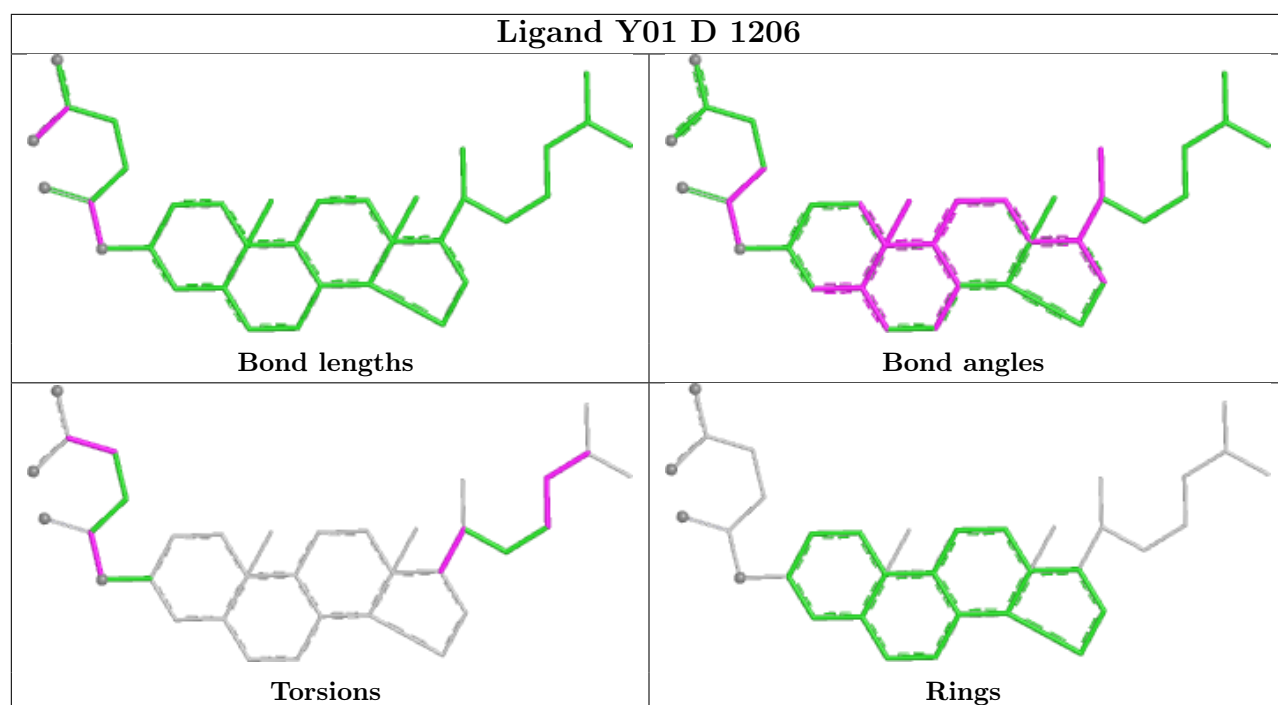


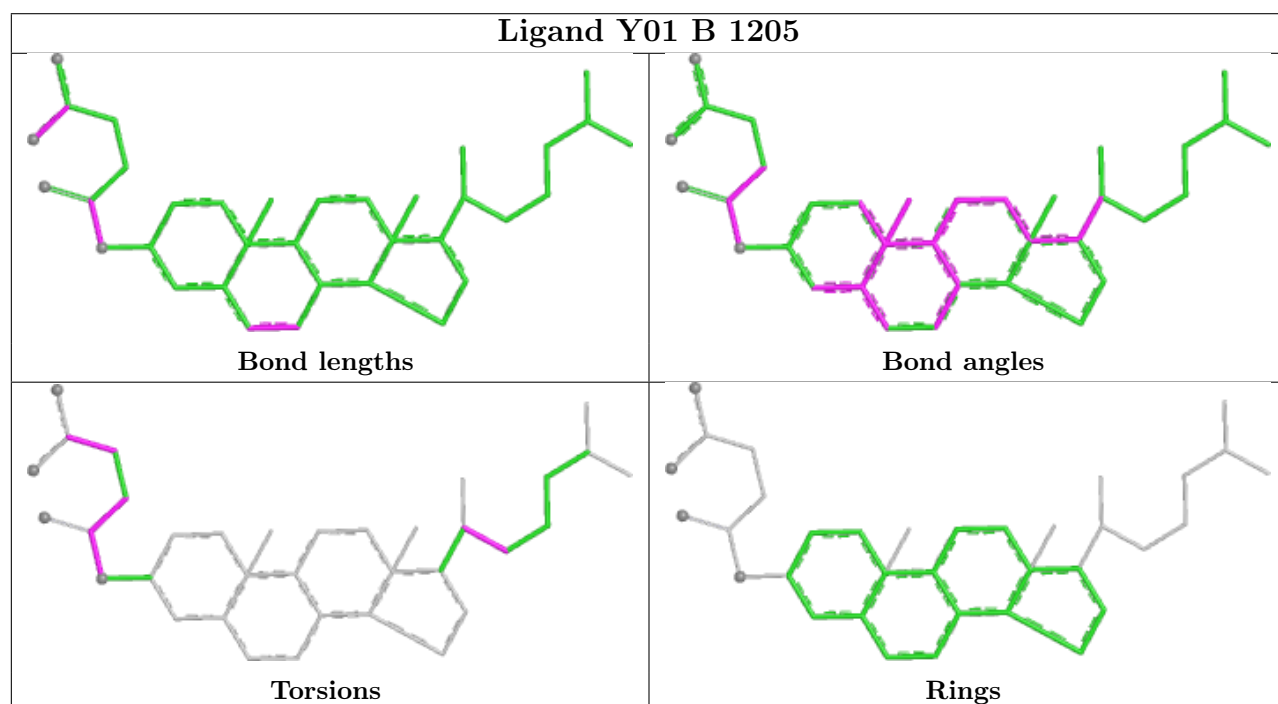
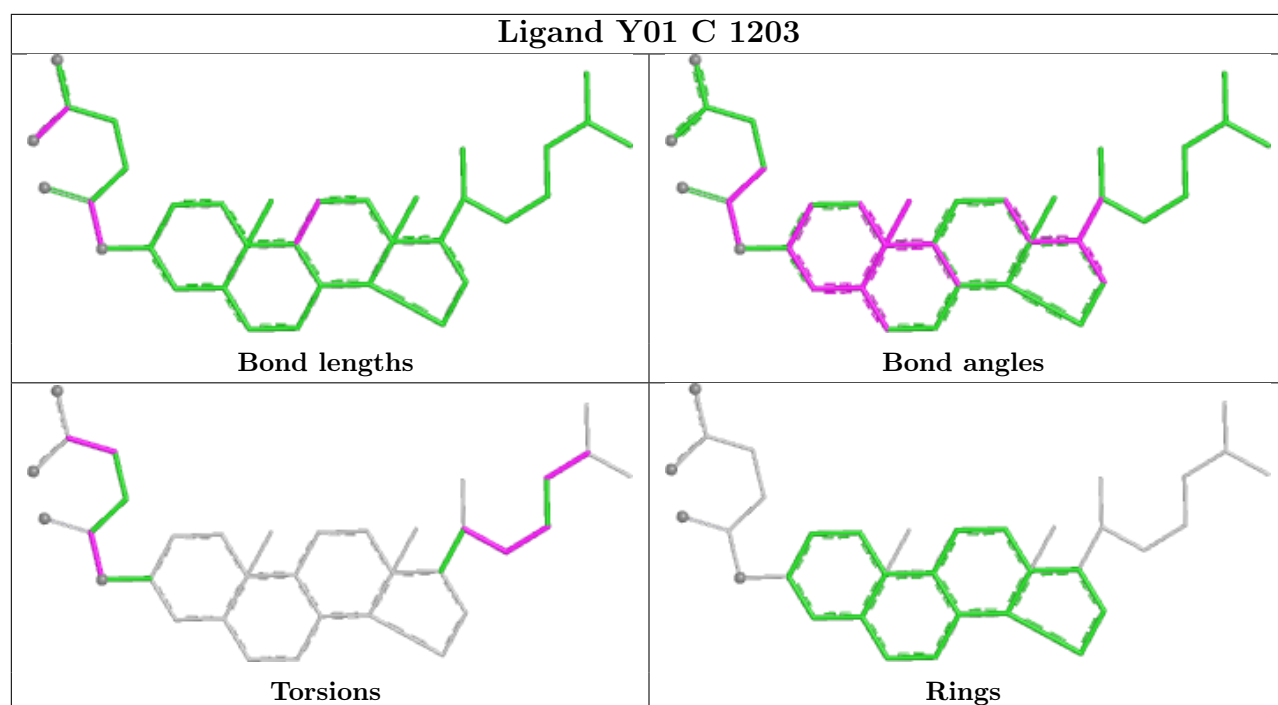


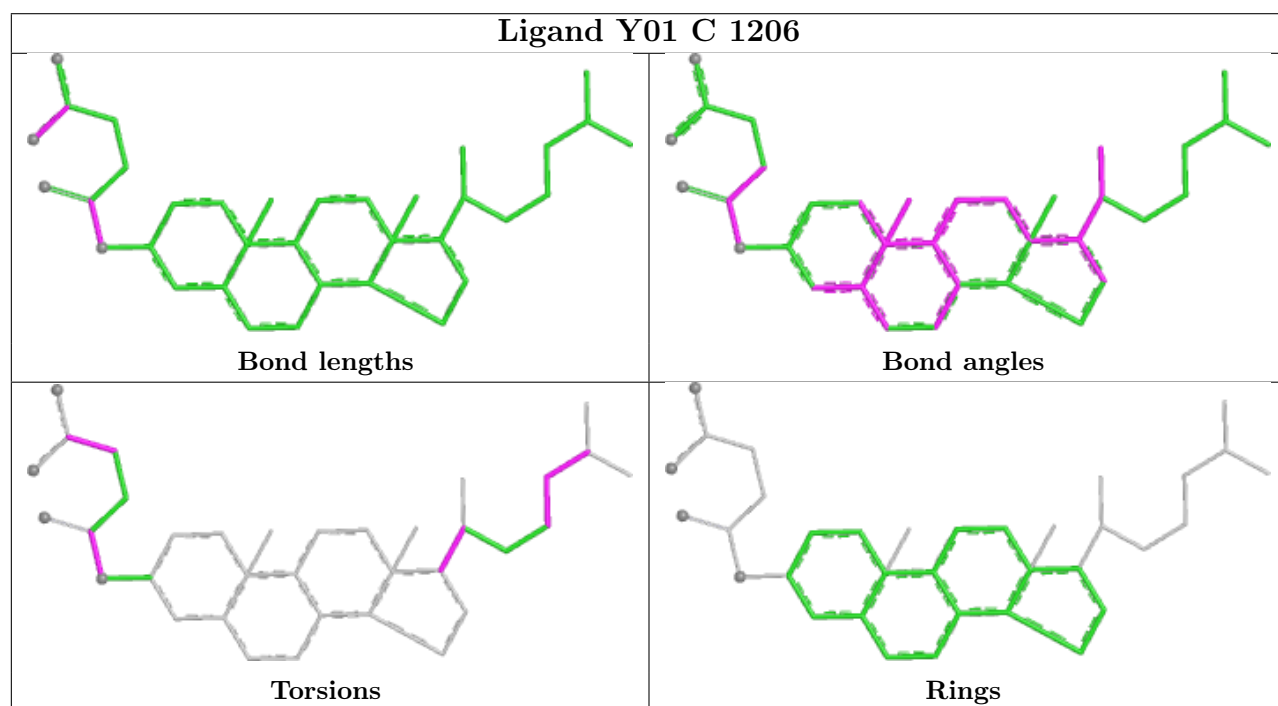
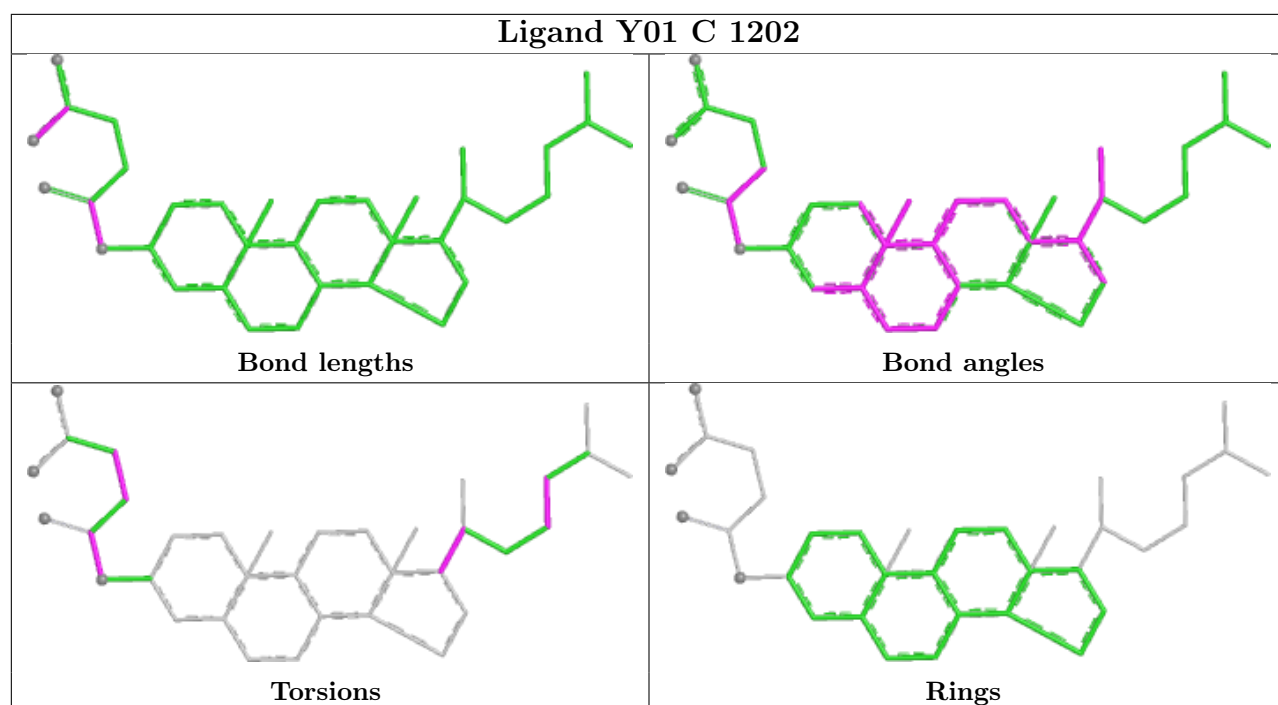


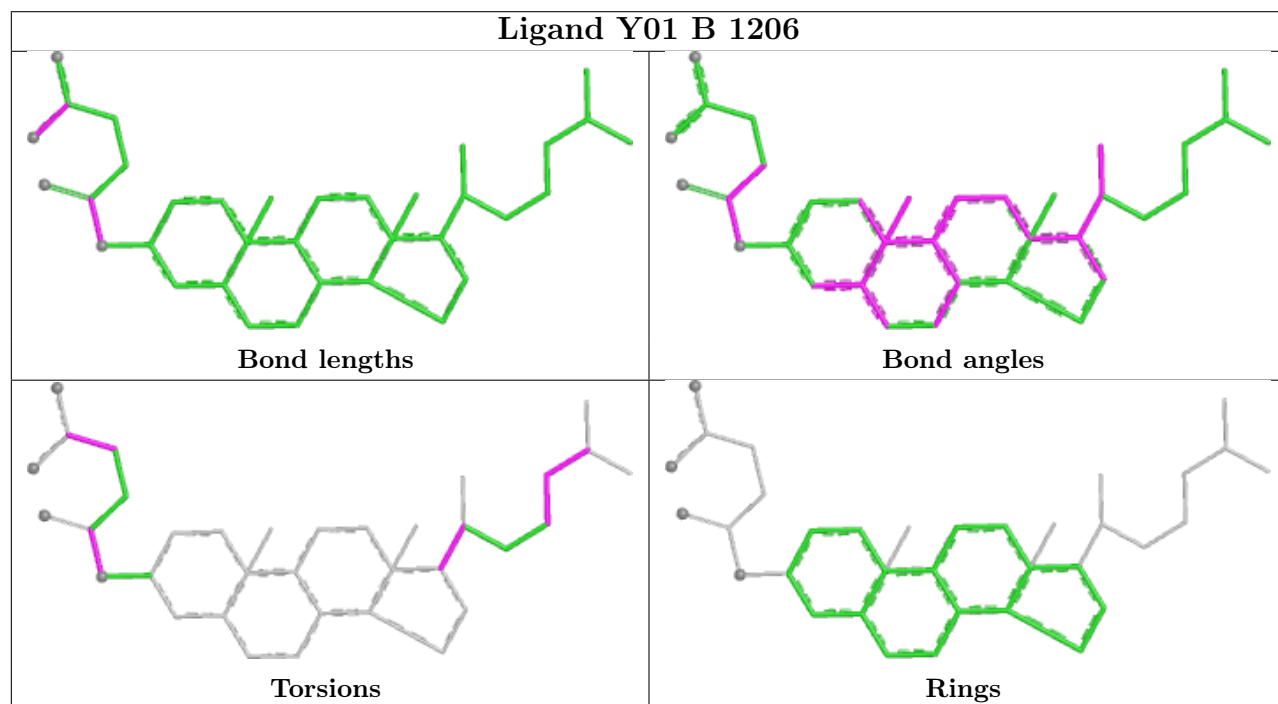
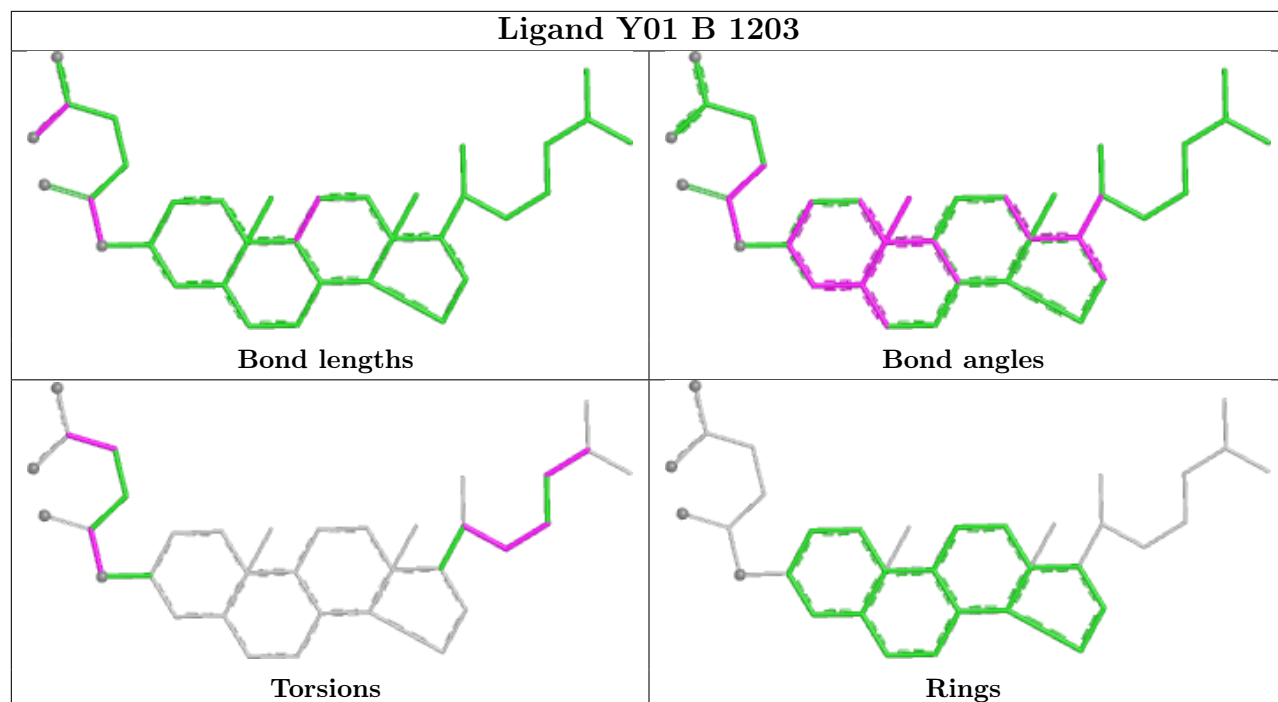


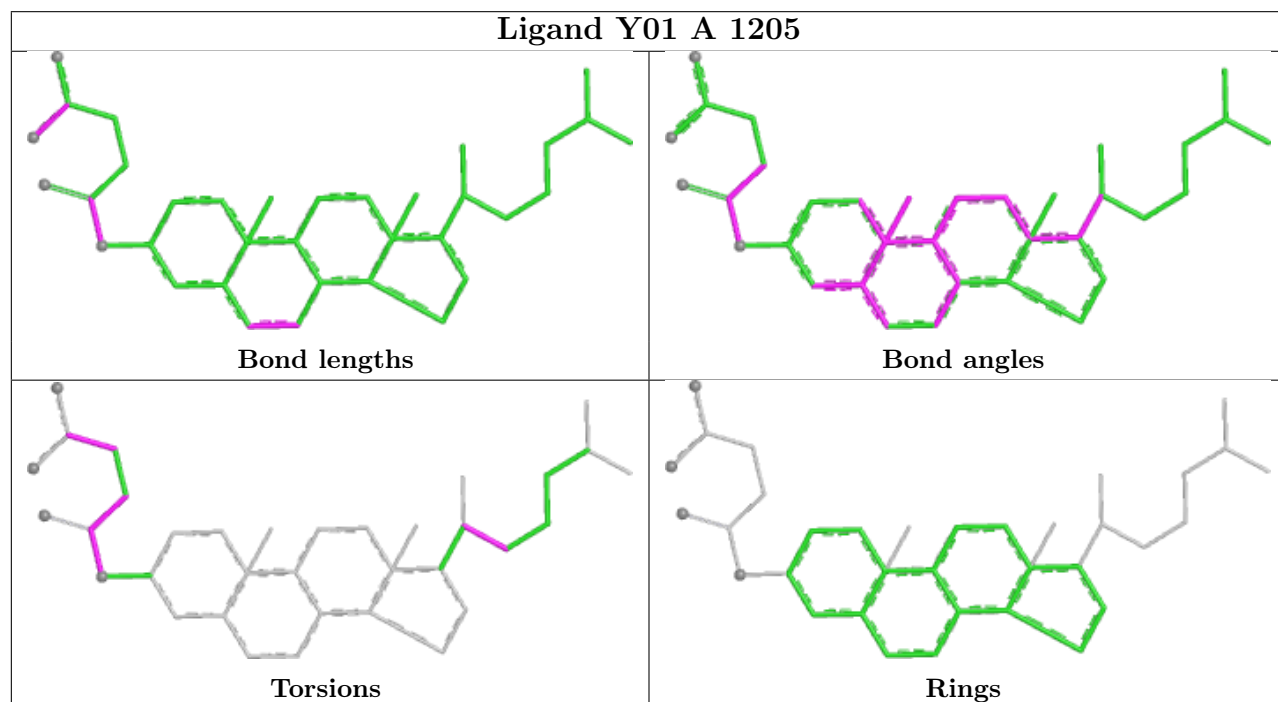
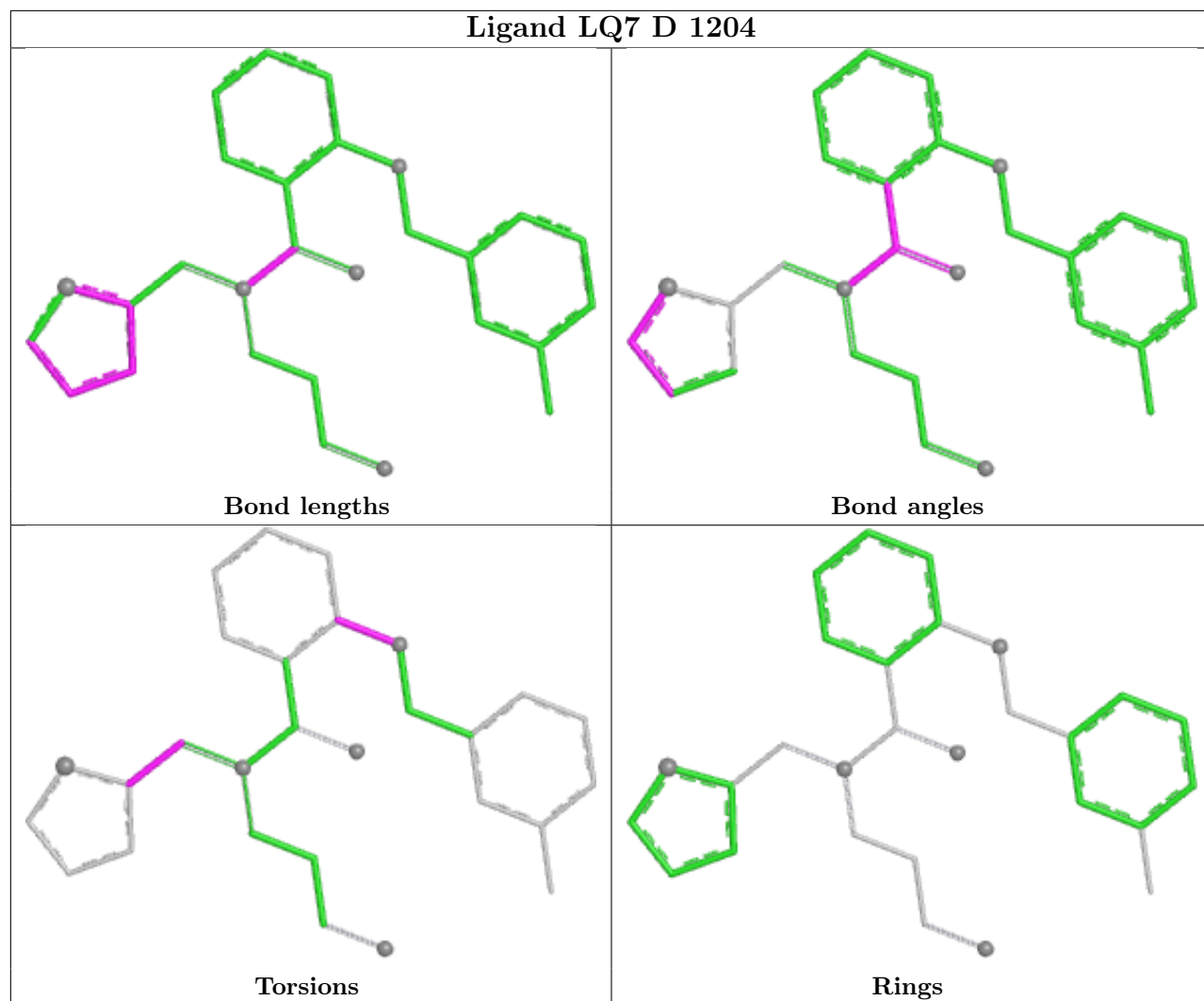


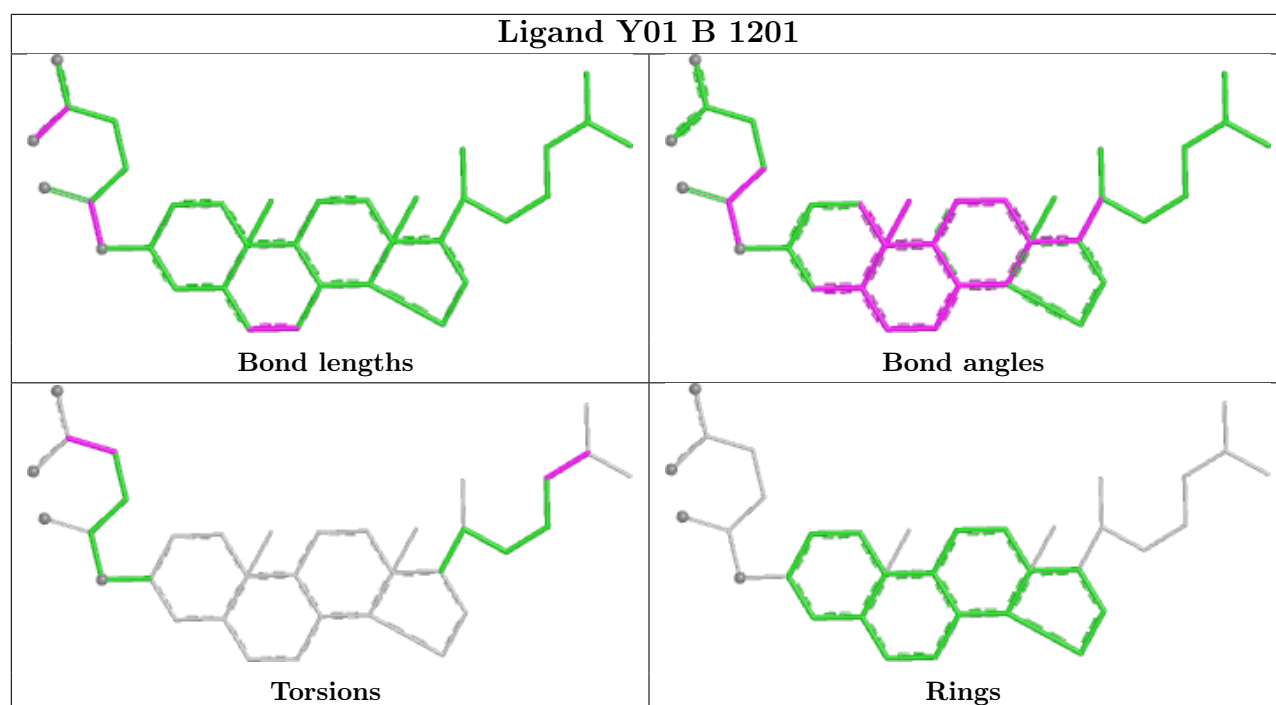












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

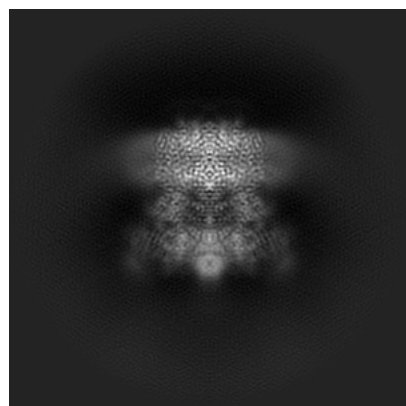
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44258. These allow visual inspection of the internal detail of the map and identification of artifacts.

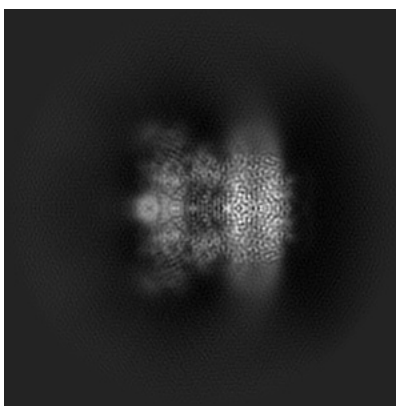
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

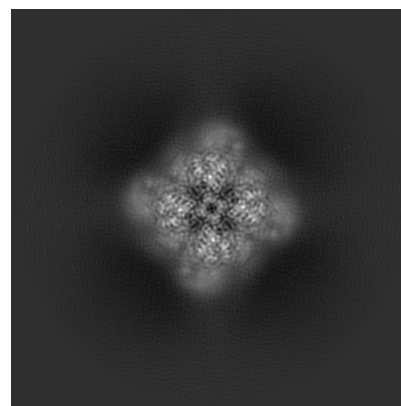
6.1.1 Primary map



X

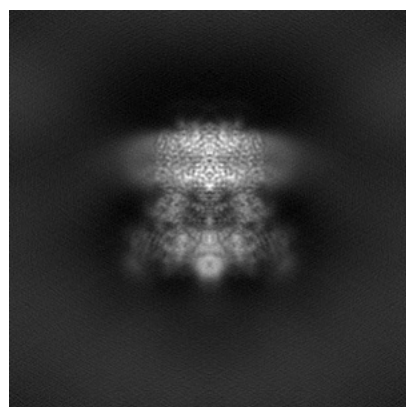


Y

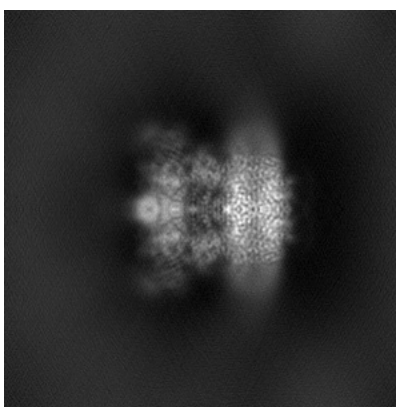


Z

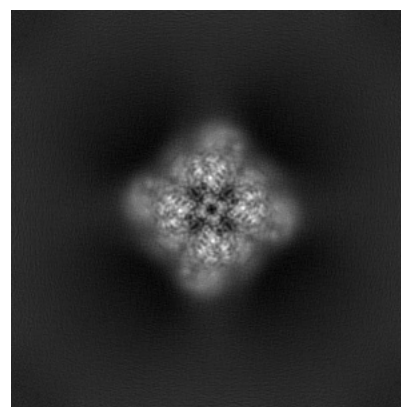
6.1.2 Raw map



X



Y

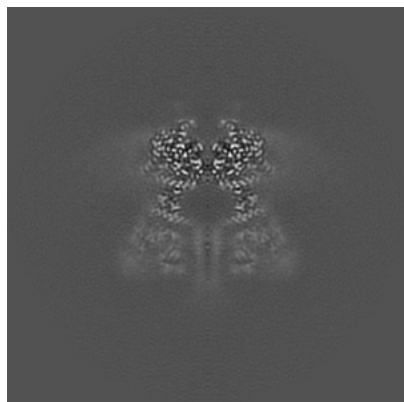


Z

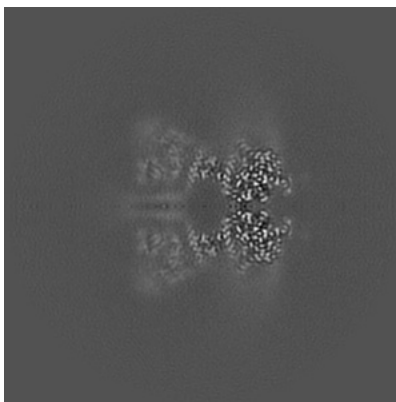
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

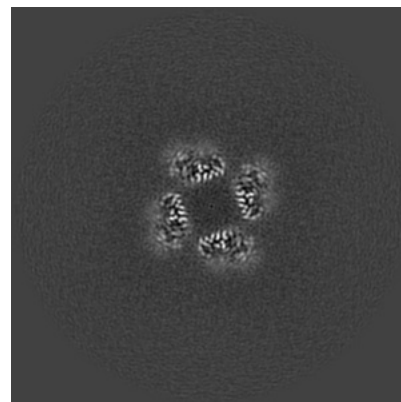
6.2.1 Primary map



X Index: 160

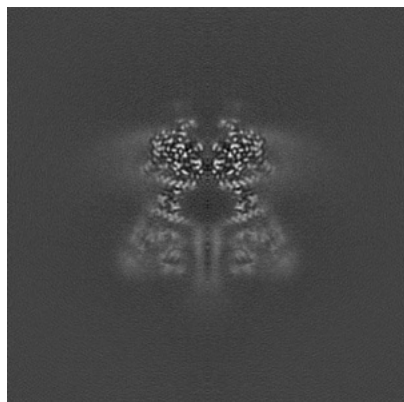


Y Index: 160

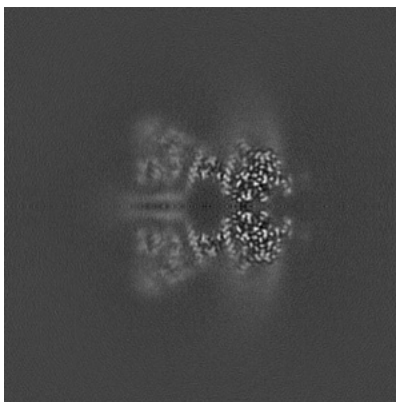


Z Index: 160

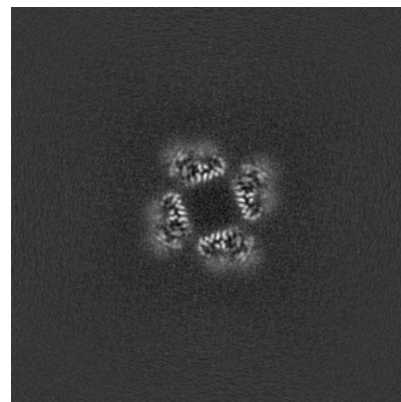
6.2.2 Raw map



X Index: 160



Y Index: 160

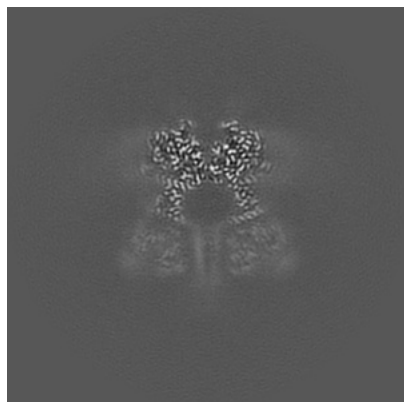


Z Index: 160

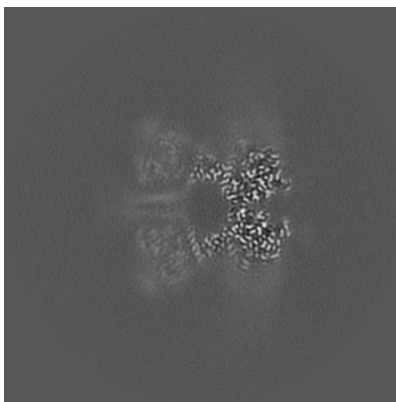
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

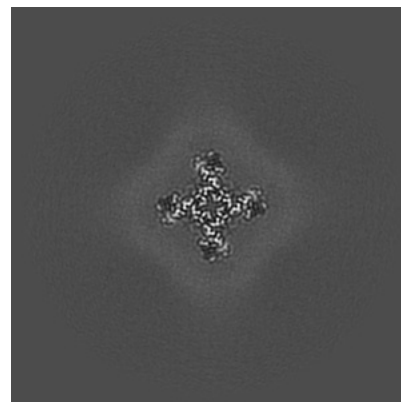
6.3.1 Primary map



X Index: 162

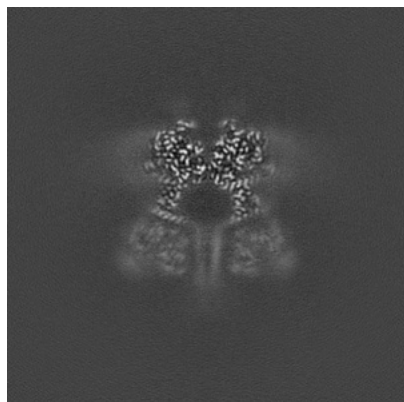


Y Index: 162

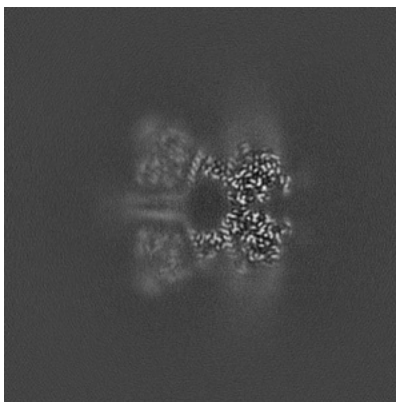


Z Index: 204

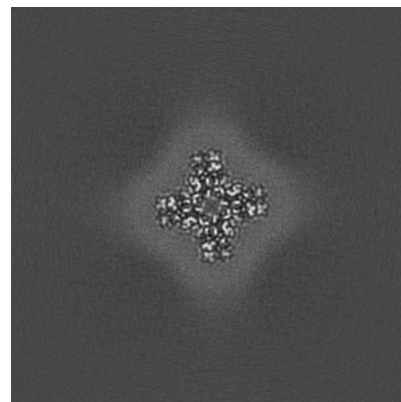
6.3.2 Raw map



X Index: 158



Y Index: 158

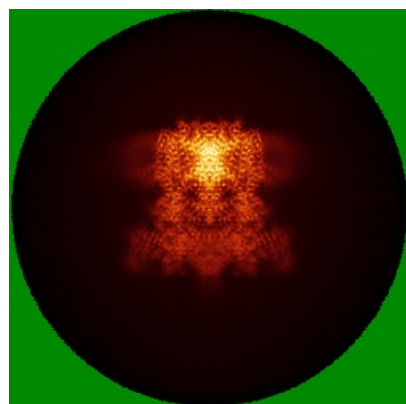


Z Index: 211

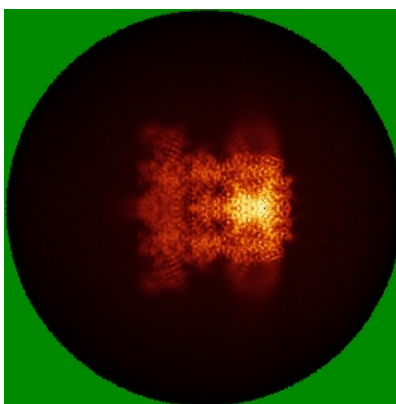
The images above show the largest variance slices of the map in three orthogonal directions.

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

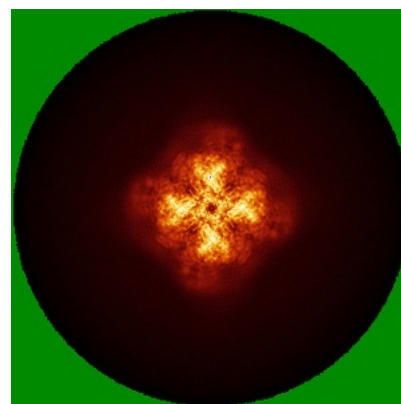
6.4.1 Primary map



X

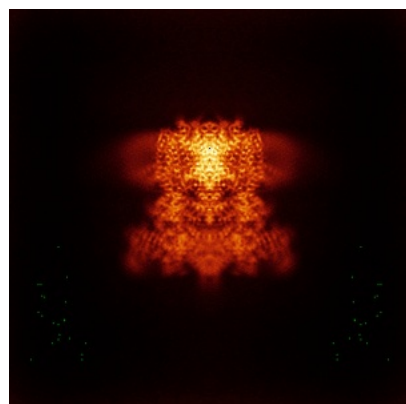


Y

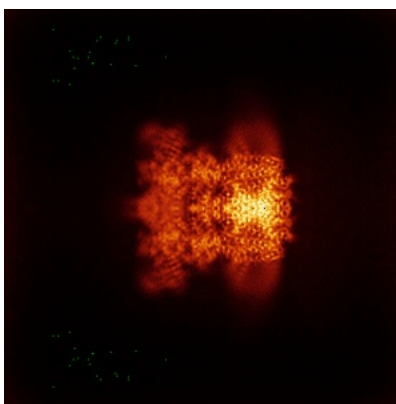


Z

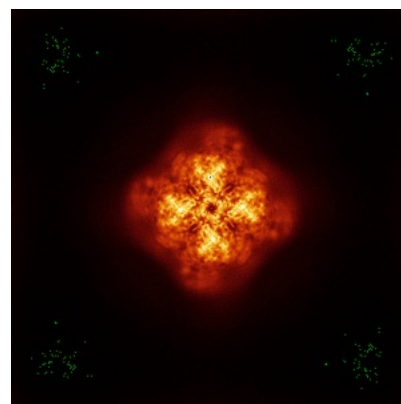
6.4.2 Raw map



X



Y

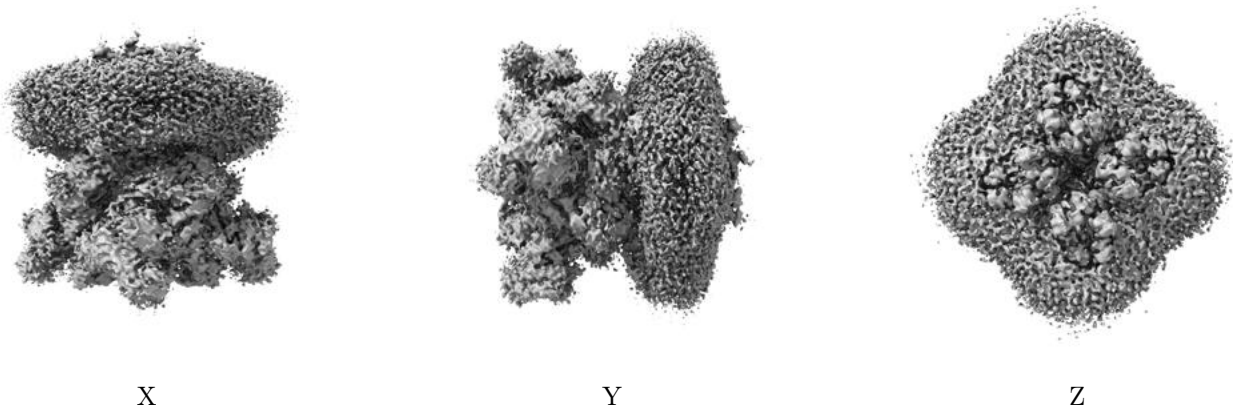


Z

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.

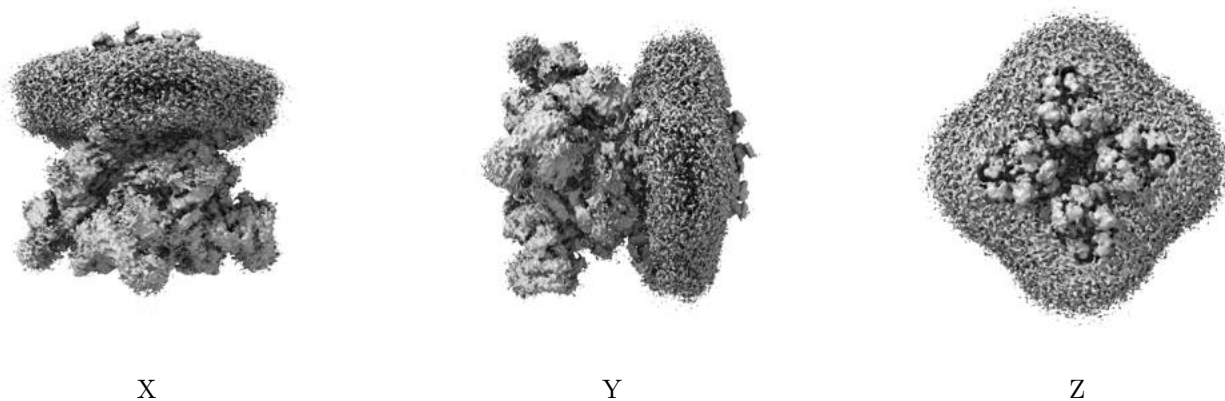
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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



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.

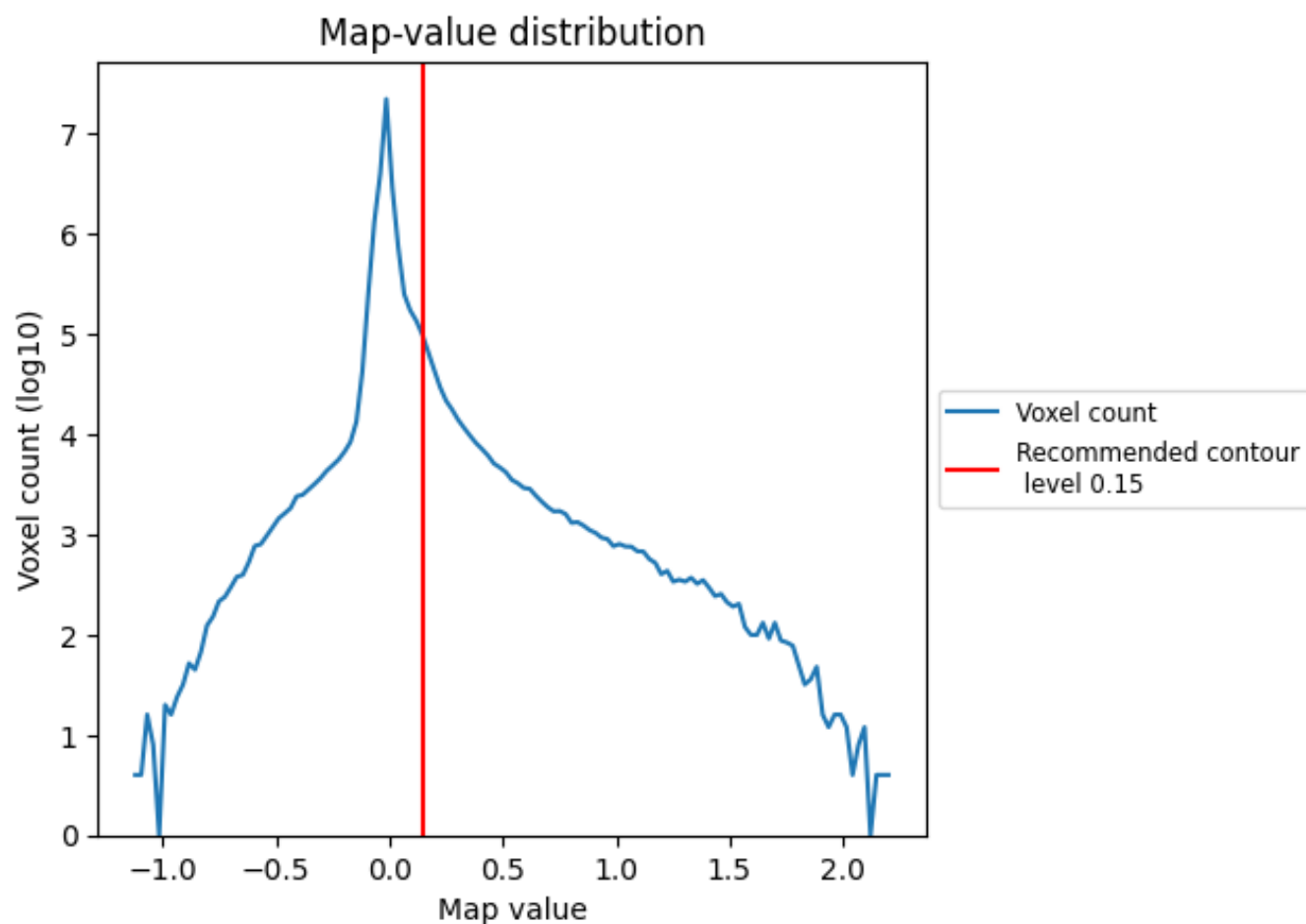
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

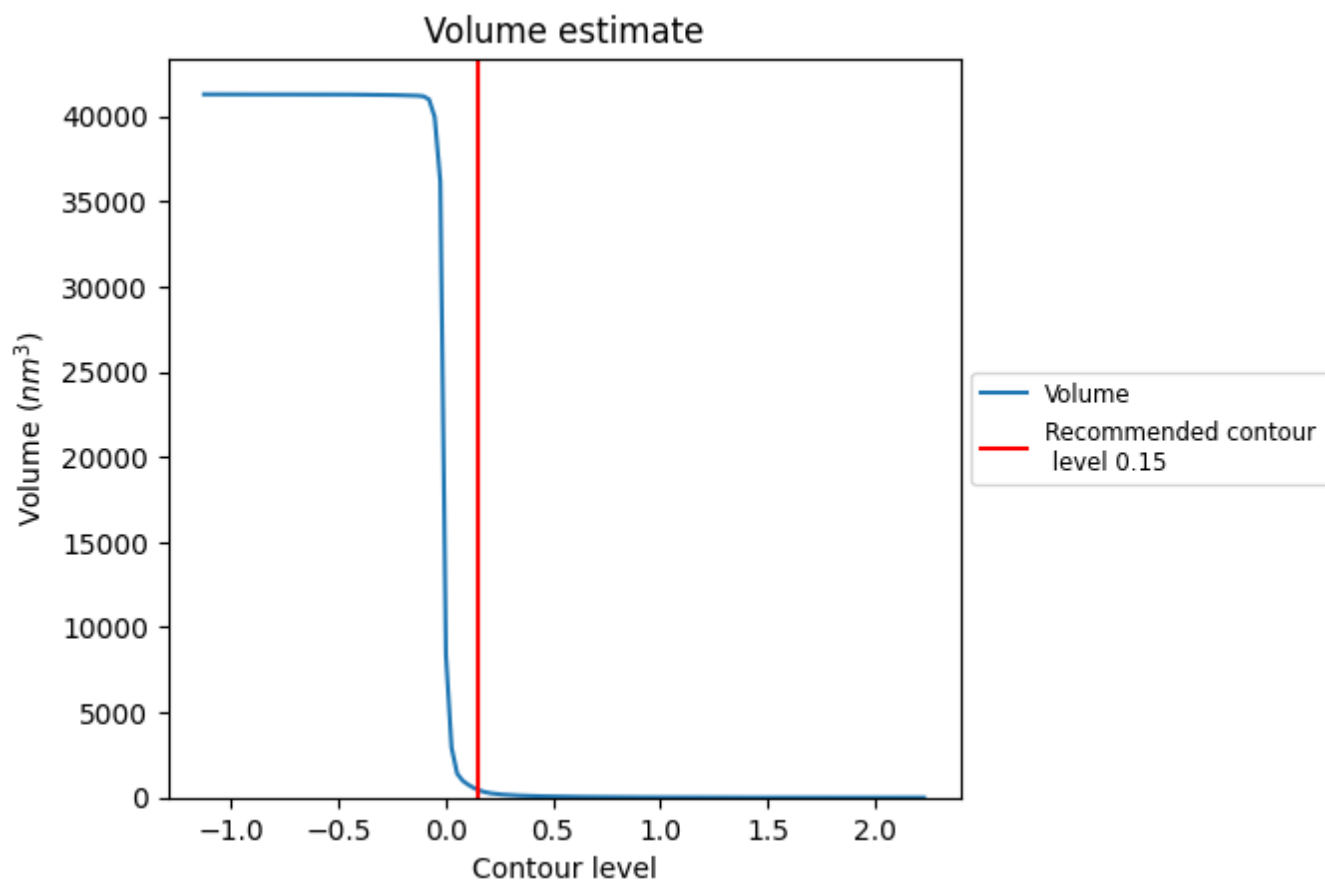
This section contains the results of statistical analysis of the map.

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.

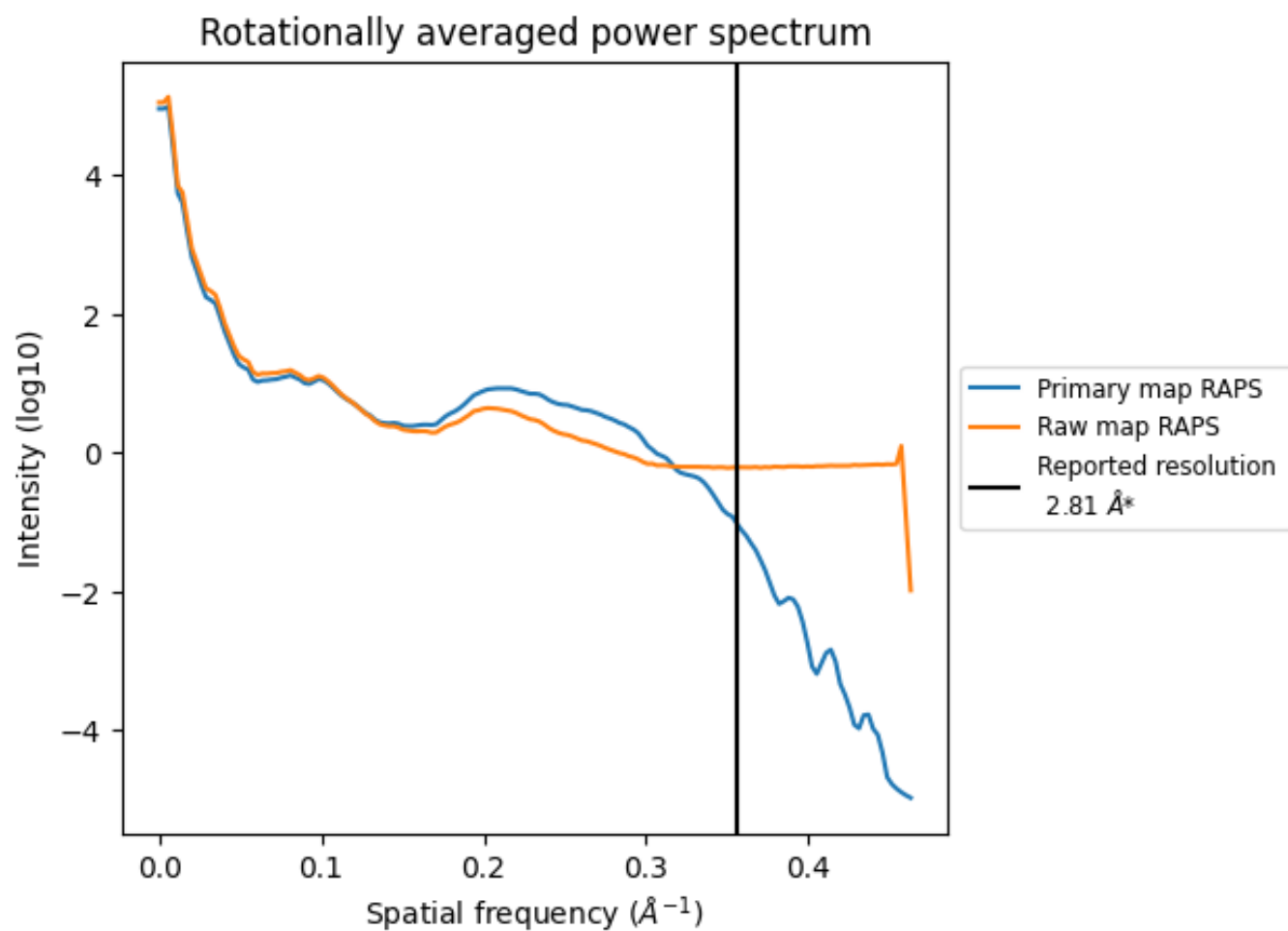
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm^3 ; this corresponds to an approximate mass of 424 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 ⓘ

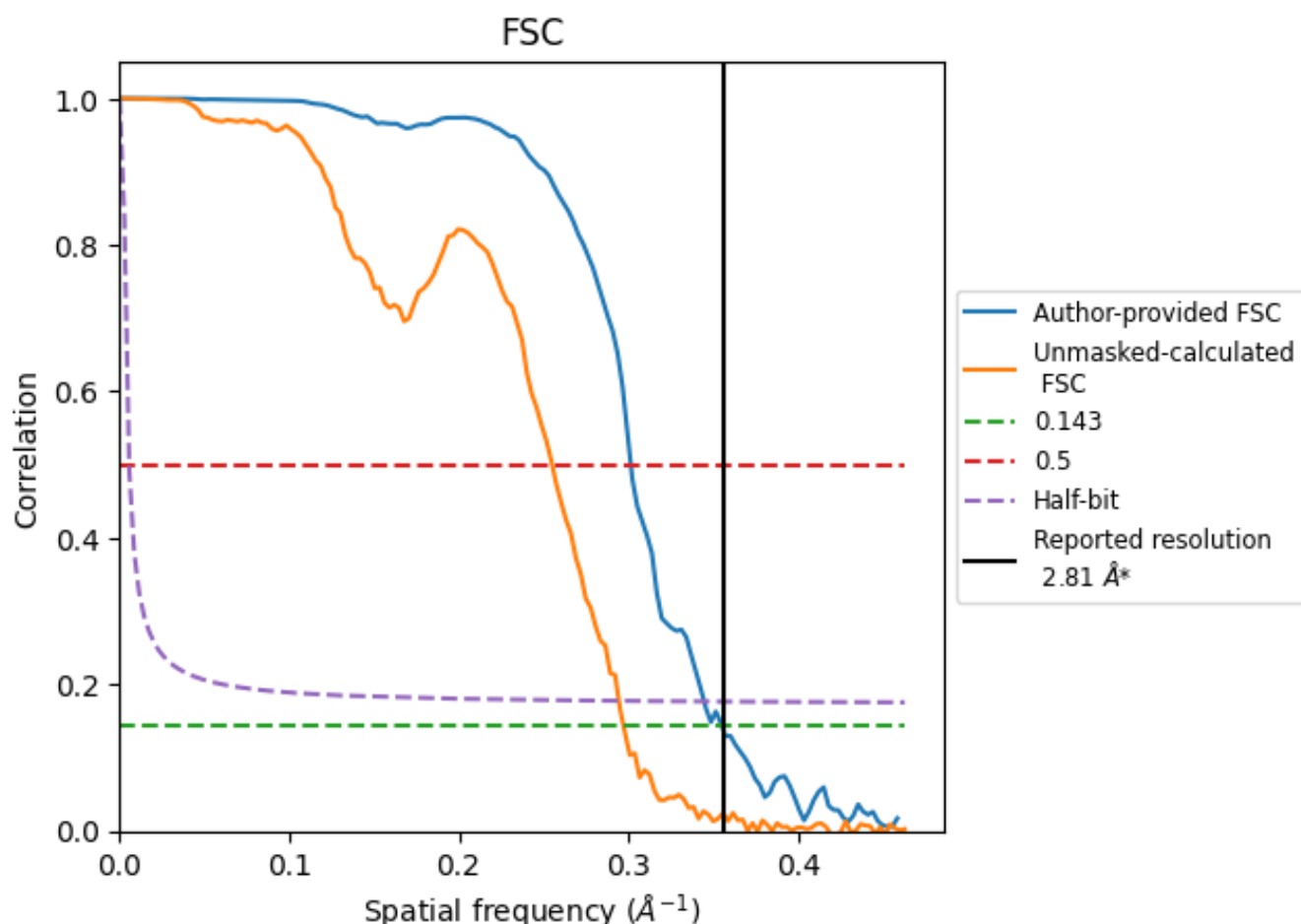


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 0.356 \AA^{-1}

8.2 Resolution estimates [i](#)

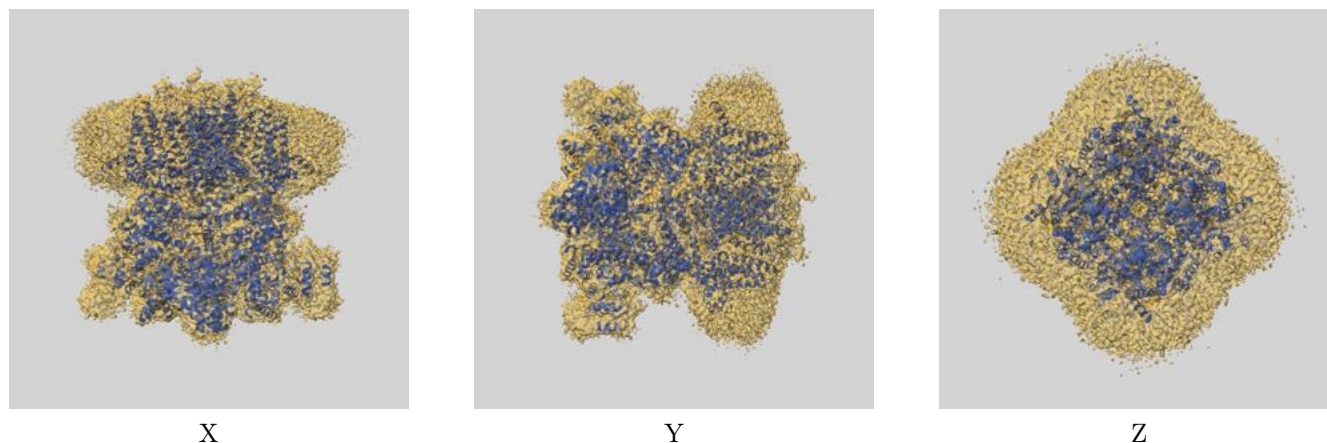
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	2.82	3.32	2.90
Unmasked-calculated*	3.36	3.92	3.40

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

9 Map-model fit [i](#)

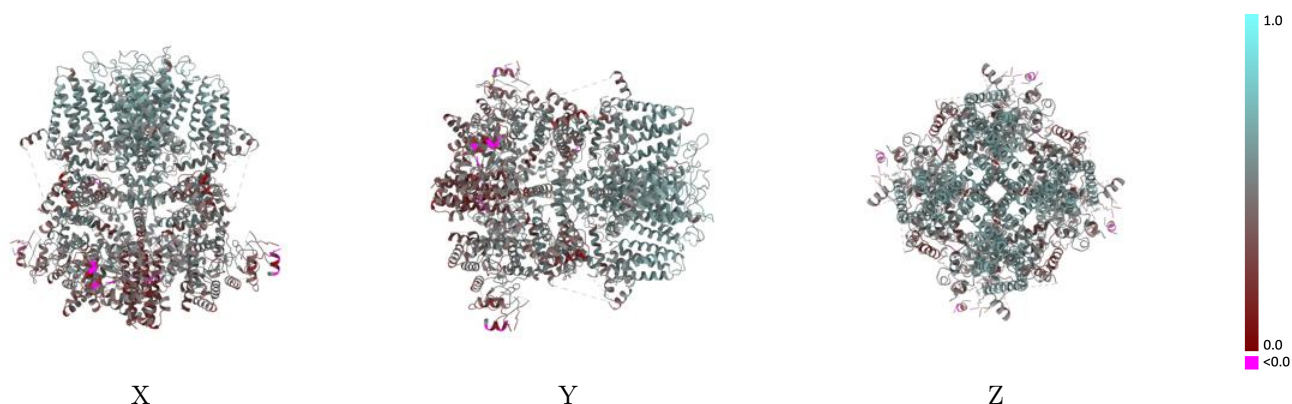
This section contains information regarding the fit between EMDB map EMD-44258 and PDB model 9B6G. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



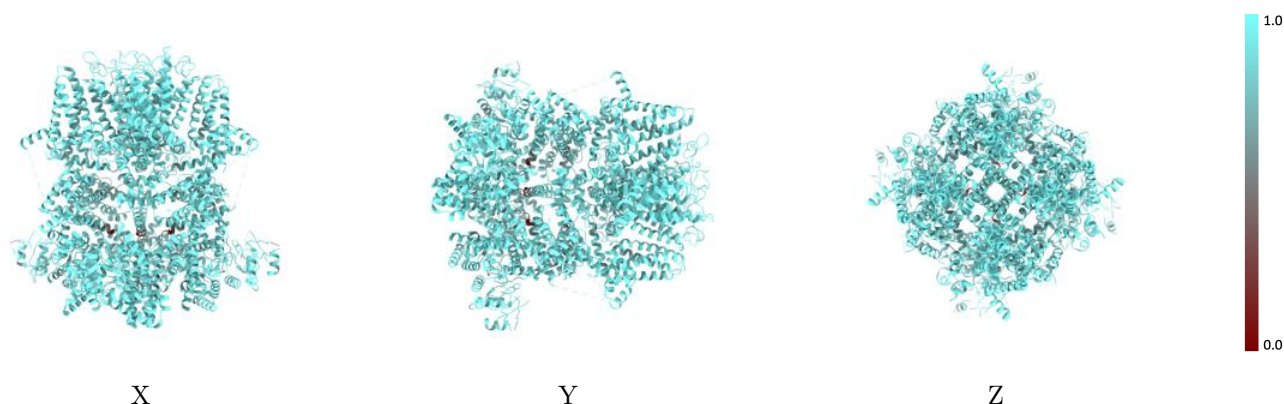
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



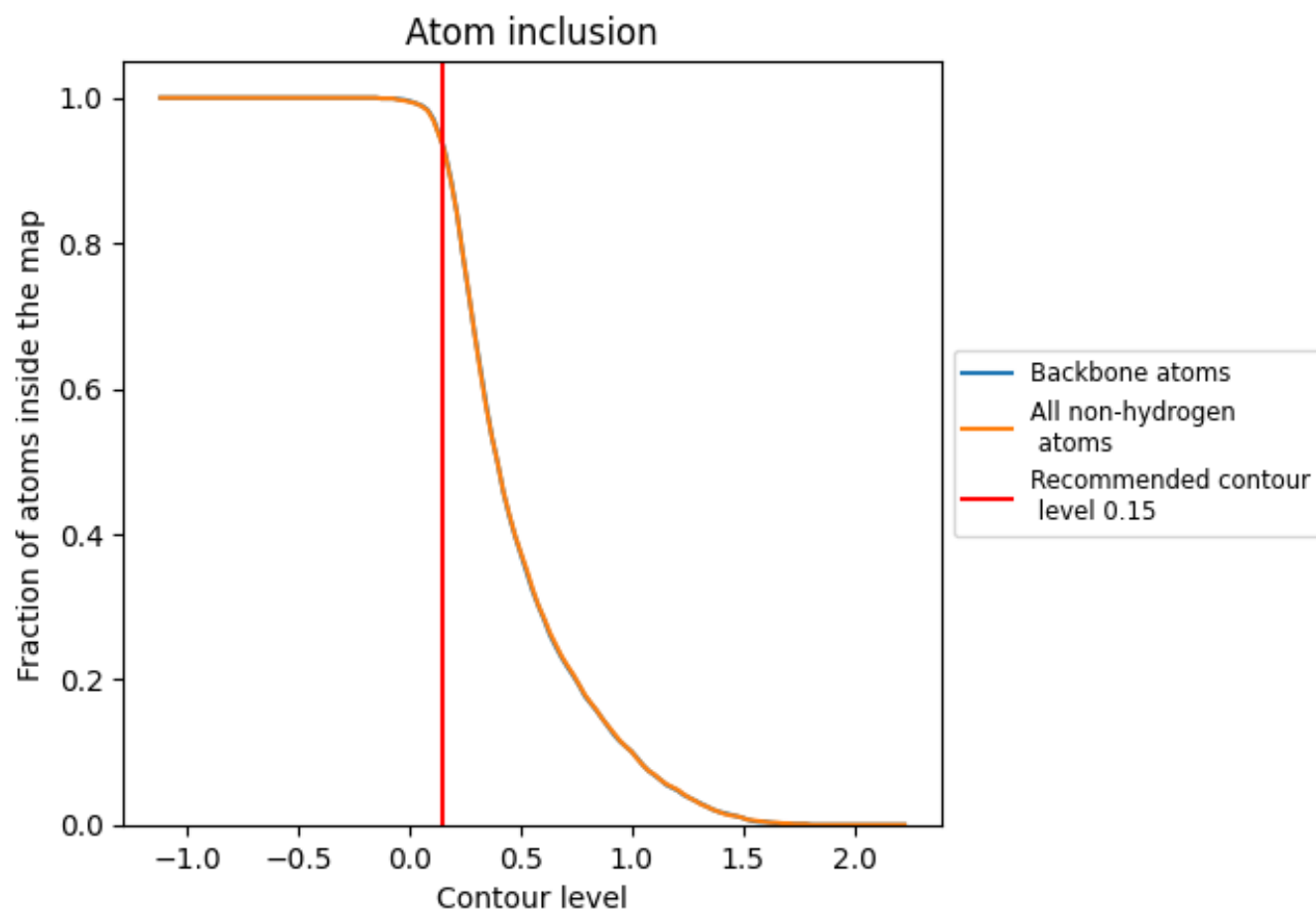
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9330	<div></div> 0.4810
A	<div></div> 0.9350	<div></div> 0.4810
B	<div></div> 0.9350	<div></div> 0.4810
C	<div></div> 0.9350	<div></div> 0.4820
D	<div></div> 0.9350	<div></div> 0.4810

