Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 07:47 PM EST

PDB ID	:	6BWD
EMDB ID	:	EMD-7297
Title	:	3.7 angstrom cryoEM structure of truncated mouse TRPM7
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	:	2017-12-14
Resolution	:	3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

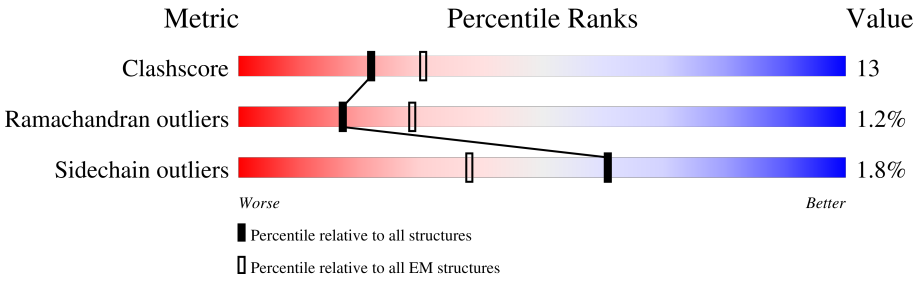
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	955	59% 19% • 19%
1	B	955	60% 19% • 19%
1	C	955	59% 20% • 19%
1	D	955	60% 19% • 19%

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
3	Y01	D	1203	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23187 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.

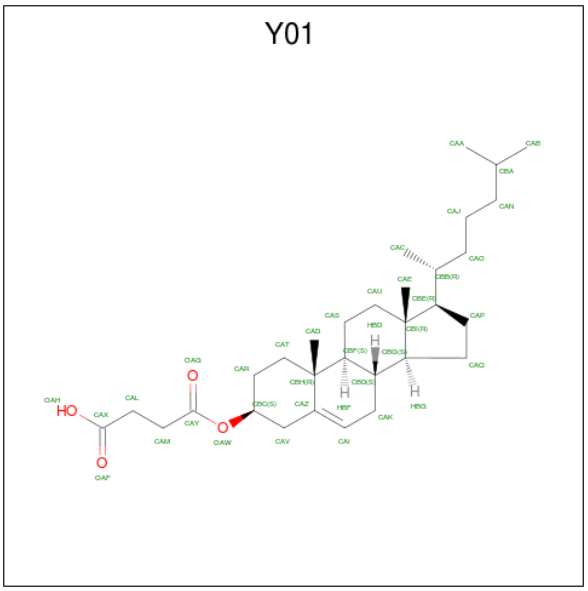
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily M member 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	771	Total 5613	C 3636	N 954	O 992	S 31	0	0
1	B	771	Total 5618	C 3636	N 957	O 995	S 30	0	0
1	C	771	Total 5628	C 3640	N 957	O 1000	S 31	0	0
1	D	771	Total 5593	C 3624	N 954	O 985	S 30	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Mg 2	0
2	B	2	Total 2	Mg 2	0
2	D	1	Total 1	Mg 1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			210	186	24	
3	A	1	Total	C	O	0
			210	186	24	
3	A	1	Total	C	O	0
			210	186	24	
3	A	1	Total	C	O	0
			210	186	24	
3	A	1	Total	C	O	0
			210	186	24	
3	A	1	Total	C	O	0
			210	186	24	
3	B	1	Total	C	O	0
			140	124	16	
3	B	1	Total	C	O	0
			140	124	16	
3	B	1	Total	C	O	0
			140	124	16	
3	B	1	Total	C	O	0
			140	124	16	
3	C	1	Total	C	O	0
			280	248	32	
3	C	1	Total	C	O	0
			280	248	32	
3	C	1	Total	C	O	0
			280	248	32	
3	C	1	Total	C	O	0
			280	248	32	

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Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C O 280 248 32	0
3	C	1	Total C O 280 248 32	0
3	C	1	Total C O 280 248 32	0
3	C	1	Total C O 280 248 32	0
3	D	1	Total C O 70 62 8	0
3	D	1	Total C O 70 62 8	0

- Molecule 4 is water.

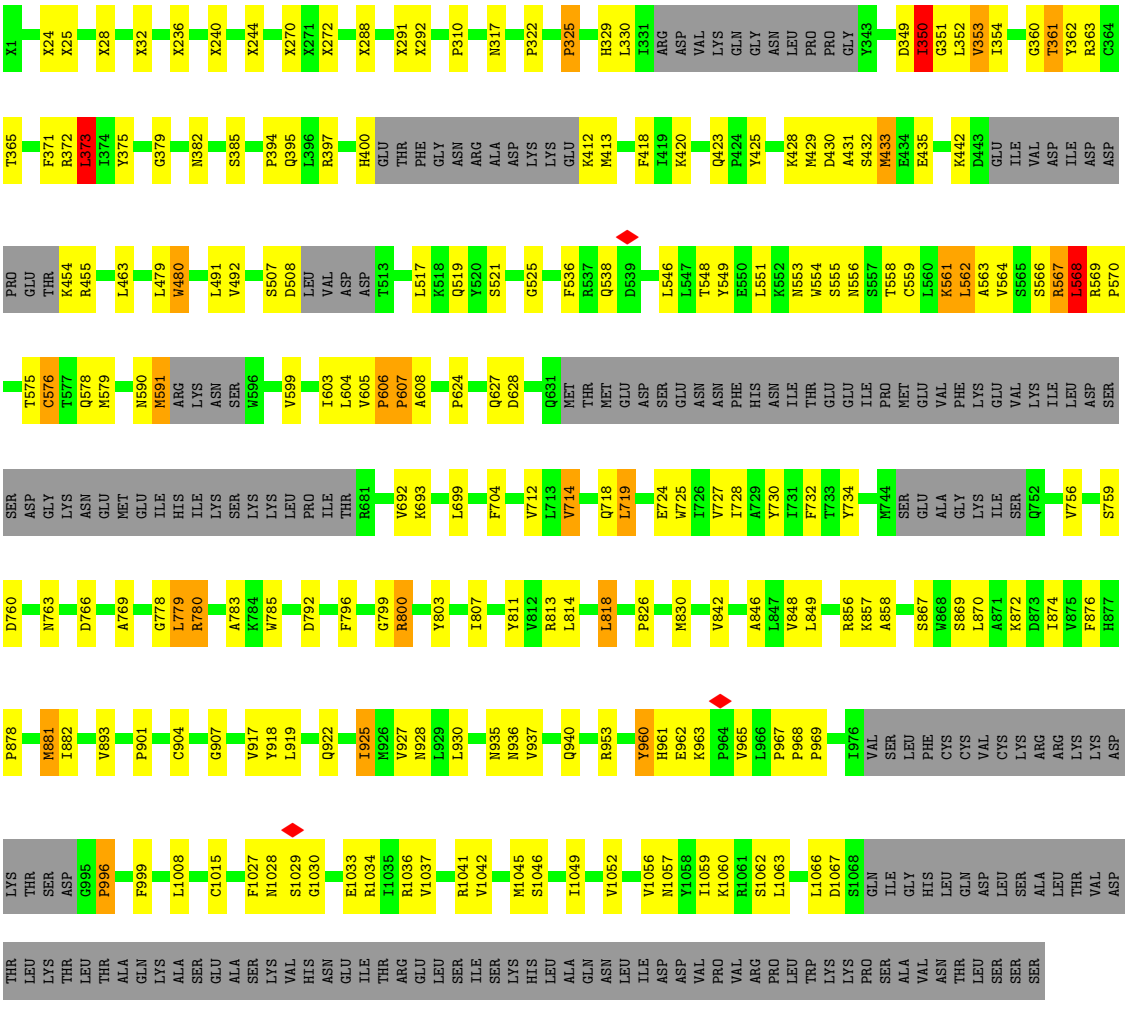
Mol	Chain	Residues	Atoms	AltConf
4	A	7	Total O 7 7	0
4	B	6	Total O 6 6	0
4	C	8	Total O 8 8	0
4	D	9	Total O 9 9	0

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.

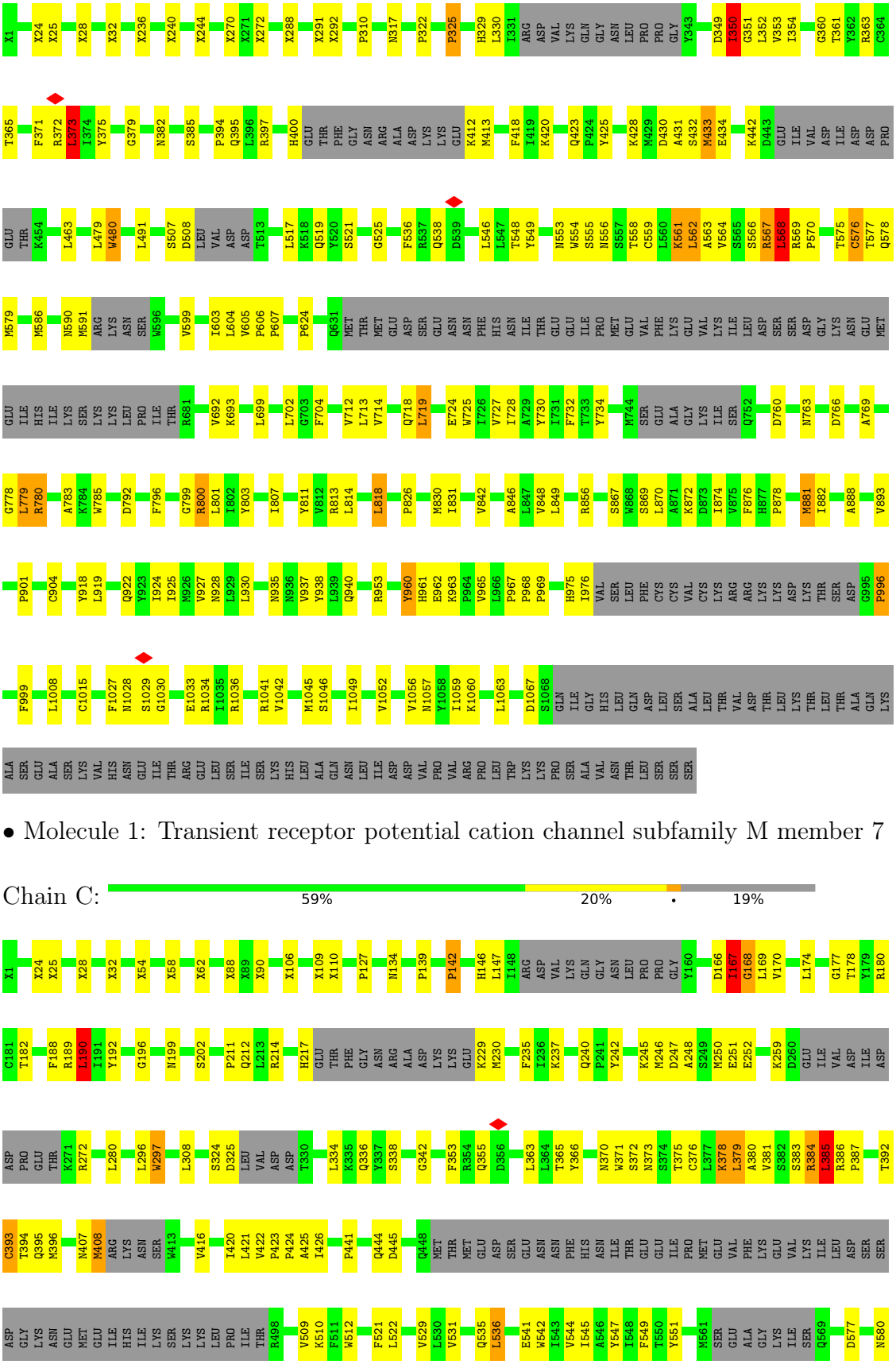
• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain A:



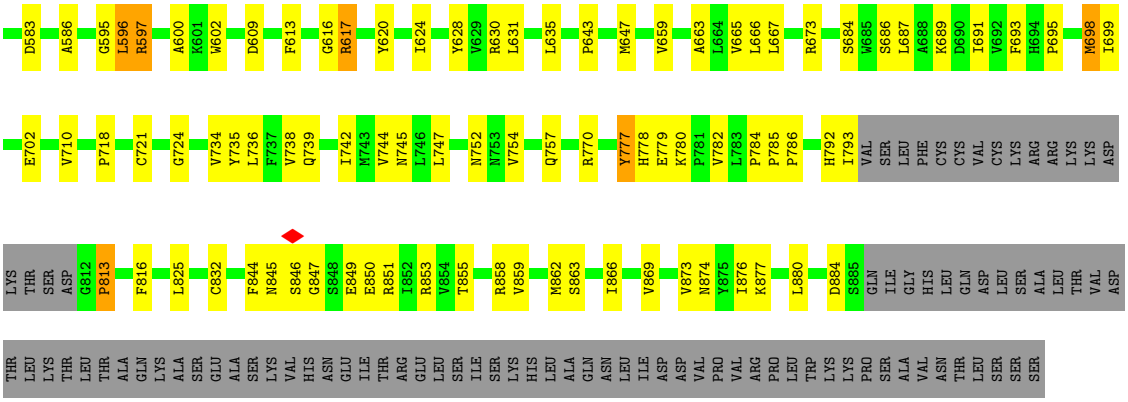
• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain B:



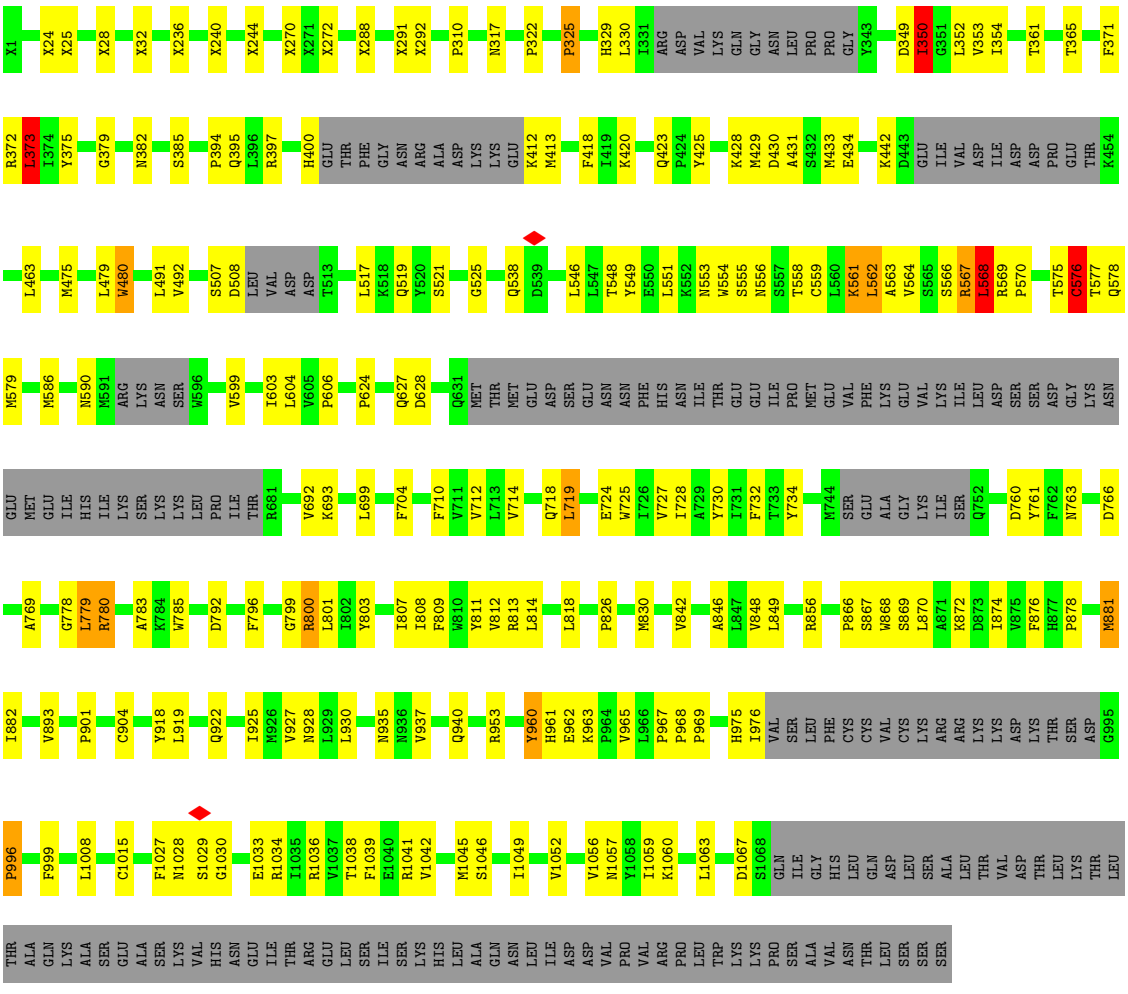
• Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain C:



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

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232930	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 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.007	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.48	0/5124	0.79	20/6947 (0.3%)
1	B	0.48	0/5129	0.79	19/6954 (0.3%)
1	C	0.49	0/5139	0.79	19/6967 (0.3%)
1	D	0.48	0/5105	0.79	20/6925 (0.3%)
All	All	0.48	0/20497	0.79	78/27793 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	26
1	B	0	26
1	C	0	27
1	D	0	26
All	All	0	105

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	167	ILE	C-N-CA	8.81	140.79	122.30
1	C	385	LEU	CA-CB-CG	7.84	133.33	115.30
1	B	568	LEU	CA-CB-CG	7.83	133.31	115.30
1	A	568	LEU	CA-CB-CG	7.82	133.29	115.30
1	D	568	LEU	CA-CB-CG	7.82	133.27	115.30
1	C	168	GLY	N-CA-C	7.13	130.93	113.10
1	A	996	PRO	N-CA-CB	6.86	111.53	103.30
1	B	996	PRO	N-CA-CB	6.86	111.53	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	996	PRO	N-CA-CB	6.84	111.51	103.30
1	C	813	PRO	N-CA-CB	6.81	111.47	103.30
1	A	961	HIS	N-CA-C	6.55	128.69	111.00
1	B	961	HIS	N-CA-C	6.54	128.67	111.00
1	C	778	HIS	N-CA-C	6.54	128.66	111.00
1	D	961	HIS	N-CA-C	6.54	128.65	111.00
1	D	562	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	562	LEU	CA-CB-CG	6.33	129.87	115.30
1	C	379	LEU	CA-CB-CG	6.33	129.86	115.30
1	B	562	LEU	CA-CB-CG	6.32	129.84	115.30
1	C	127	PRO	N-CA-CB	6.05	110.56	103.30
1	D	310	PRO	N-CA-CB	6.05	110.56	103.30
1	A	310	PRO	N-CA-CB	6.02	110.52	103.30
1	A	818	LEU	CA-CB-CG	6.02	129.14	115.30
1	B	818	LEU	CA-CB-CG	6.01	129.11	115.30
1	D	818	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	635	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	310	PRO	N-CA-CB	5.99	110.48	103.30
1	A	350	ILE	C-N-CA	5.86	134.62	122.30
1	A	967	PRO	N-CA-CB	5.85	110.31	103.30
1	B	967	PRO	N-CA-CB	5.84	110.31	103.30
1	C	784	PRO	N-CA-CB	5.83	110.30	103.30
1	D	967	PRO	N-CA-CB	5.82	110.29	103.30
1	A	351	GLY	N-CA-C	5.82	127.65	113.10
1	B	969	PRO	N-CA-CB	5.76	110.21	103.30
1	A	969	PRO	N-CA-CB	5.73	110.17	103.30
1	D	969	PRO	N-CA-CB	5.72	110.17	103.30
1	C	786	PRO	N-CA-CB	5.70	110.14	103.30
1	D	350	ILE	C-N-CA	5.67	134.22	122.30
1	B	350	ILE	C-N-CA	5.64	134.15	122.30
1	D	325	PRO	N-CA-CB	5.63	110.06	103.30
1	D	624	PRO	N-CA-CB	5.56	109.97	103.30
1	A	624	PRO	N-CA-CB	5.55	109.96	103.30
1	C	441	PRO	N-CA-CB	5.54	109.95	103.30
1	B	624	PRO	N-CA-CB	5.54	109.94	103.30
1	D	322	PRO	N-CA-CB	5.52	109.93	103.30
1	B	325	PRO	N-CA-CB	5.52	109.92	103.30
1	A	322	PRO	N-CA-CB	5.50	109.90	103.30
1	B	322	PRO	N-CA-CB	5.50	109.90	103.30
1	C	139	PRO	N-CA-CB	5.47	109.87	103.30
1	A	968	PRO	N-CA-CB	5.46	109.85	103.30
1	C	190	LEU	C-N-CA	5.45	135.33	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	LEU	C-N-CA	5.45	135.32	121.70
1	A	373	LEU	C-N-CA	5.44	135.31	121.70
1	B	968	PRO	N-CA-CB	5.43	109.82	103.30
1	D	373	LEU	C-N-CA	5.42	135.26	121.70
1	A	325	PRO	N-CA-CB	5.41	109.79	103.30
1	C	785	PRO	N-CA-CB	5.40	109.78	103.30
1	D	968	PRO	N-CA-CB	5.39	109.77	103.30
1	B	351	GLY	N-CA-C	5.37	126.53	113.10
1	C	142	PRO	N-CA-CB	5.35	109.72	103.30
1	B	999	PHE	N-CA-C	-5.32	96.63	111.00
1	A	999	PHE	N-CA-C	-5.32	96.63	111.00
1	D	999	PHE	N-CA-C	-5.31	96.65	111.00
1	C	816	PHE	N-CA-C	-5.31	96.66	111.00
1	A	480	TRP	C-N-CA	5.25	134.84	121.70
1	D	606	PRO	CA-N-CD	-5.25	104.14	111.50
1	B	480	TRP	C-N-CA	5.25	134.83	121.70
1	C	297	TRP	C-N-CA	5.25	134.83	121.70
1	D	480	TRP	C-N-CA	5.25	134.82	121.70
1	A	385	SER	C-N-CA	5.24	133.31	122.30
1	B	385	SER	C-N-CA	5.22	133.25	122.30
1	C	202	SER	C-N-CA	5.22	133.25	122.30
1	D	385	SER	C-N-CA	5.21	133.25	122.30
1	D	551	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	551	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	365	THR	C-N-CA	5.07	134.39	121.70
1	D	365	THR	C-N-CA	5.07	134.39	121.70
1	B	365	THR	C-N-CA	5.06	134.36	121.70
1	C	182	THR	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (105) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1028	ASN	Peptide
1	A	270	UNK	Peptide
1	A	272	UNK	Peptide
1	A	350	ILE	Peptide
1	A	353	VAL	Peptide
1	A	361	THR	Peptide
1	A	372	ARG	Peptide
1	A	418	PHE	Peptide
1	A	480	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	A	517	LEU	Peptide
1	A	519	GLN	Peptide
1	A	554	TRP	Peptide
1	A	561	LYS	Peptide
1	A	566	SER	Peptide
1	A	567	ARG	Peptide
1	A	568	LEU	Peptide
1	A	570	PRO	Peptide
1	A	714	VAL	Peptide
1	A	719	LEU	Peptide
1	A	778	GLY	Peptide
1	A	779	LEU	Peptide
1	A	792	ASP	Peptide
1	A	881	MET	Peptide
1	A	882	ILE	Peptide
1	A	925	ILE	Peptide
1	A	960	TYR	Peptide
1	B	1028	ASN	Peptide
1	B	270	UNK	Peptide
1	B	272	UNK	Peptide
1	B	350	ILE	Peptide
1	B	361	THR	Peptide
1	B	372	ARG	Peptide
1	B	412	LYS	Peptide
1	B	418	PHE	Peptide
1	B	480	TRP	Peptide
1	B	517	LEU	Peptide
1	B	519	GLN	Peptide
1	B	554	TRP	Peptide
1	B	561	LYS	Peptide
1	B	566	SER	Peptide
1	B	567	ARG	Peptide
1	B	568	LEU	Peptide
1	B	570	PRO	Peptide
1	B	714	VAL	Peptide
1	B	719	LEU	Peptide
1	B	778	GLY	Peptide
1	B	779	LEU	Peptide
1	B	792	ASP	Peptide
1	B	881	MET	Peptide
1	B	882	ILE	Peptide
1	B	925	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	960	TYR	Peptide
1	C	167	ILE	Peptide,Mainchain
1	C	178	THR	Peptide
1	C	189	ARG	Peptide
1	C	229	LYS	Peptide
1	C	235	PHE	Peptide
1	C	297	TRP	Peptide
1	C	334	LEU	Peptide
1	C	336	GLN	Peptide
1	C	371	TRP	Peptide
1	C	378	LYS	Peptide
1	C	383	SER	Peptide
1	C	384	ARG	Peptide
1	C	385	LEU	Peptide
1	C	387	PRO	Peptide
1	C	531	VAL	Peptide
1	C	536	LEU	Peptide
1	C	595	GLY	Peptide
1	C	596	LEU	Peptide
1	C	609	ASP	Peptide
1	C	698	MET	Peptide
1	C	699	ILE	Peptide
1	C	742	ILE	Peptide
1	C	777	TYR	Peptide
1	C	845	ASN	Peptide
1	C	88	UNK	Peptide
1	C	90	UNK	Peptide
1	D	1028	ASN	Peptide
1	D	270	UNK	Peptide
1	D	272	UNK	Peptide
1	D	350	ILE	Peptide
1	D	361	THR	Peptide
1	D	372	ARG	Peptide
1	D	412	LYS	Peptide
1	D	418	PHE	Peptide
1	D	480	TRP	Peptide
1	D	517	LEU	Peptide
1	D	519	GLN	Peptide
1	D	554	TRP	Peptide
1	D	561	LYS	Peptide
1	D	566	SER	Peptide
1	D	567	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	D	568	LEU	Peptide
1	D	570	PRO	Peptide
1	D	714	VAL	Peptide
1	D	719	LEU	Peptide
1	D	778	GLY	Peptide
1	D	779	LEU	Peptide
1	D	792	ASP	Peptide
1	D	881	MET	Peptide
1	D	882	ILE	Peptide
1	D	925	ILE	Peptide
1	D	960	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5613	0	4850	150	0
1	B	5618	0	4852	125	0
1	C	5628	0	4860	127	0
1	D	5593	0	4822	132	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	1	0	0	1	0
3	A	210	0	294	20	0
3	B	140	0	196	9	0
3	C	280	0	392	19	0
3	D	70	0	98	24	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
4	D	9	0	0	1	0
All	All	23187	0	20364	561	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (561) 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:428:LYS:CE	1:D:431:ALA:HB2	1.37	1.52
1:D:428:LYS:CE	1:D:431:ALA:CB	2.25	1.14
1:A:412:LYS:HD2	1:A:413:MET:CB	1.77	1.14
1:C:407:ASN:HB3	1:C:408:MET:HG2	1.28	1.12
1:B:590:ASN:HB3	1:B:591:MET:HG2	1.12	1.10
1:D:428:LYS:HE2	1:D:431:ALA:CB	1.80	1.09
1:D:428:LYS:HE3	1:D:431:ALA:HB2	1.35	1.09
1:A:429:MET:HE1	1:A:435:GLU:HG2	1.32	1.08
1:C:247:ASP:H	1:C:248:ALA:HA	1.23	1.04
1:D:812:VAL:HG11	3:D:1203:Y01:HAJ2	1.39	1.04
1:B:430:ASP:H	1:B:431:ALA:HA	1.23	1.02
1:A:429:MET:CE	1:A:435:GLU:HG2	1.89	1.00
1:B:590:ASN:HB3	1:B:591:MET:CG	1.91	1.00
1:D:428:LYS:HE3	1:D:431:ALA:CB	1.89	1.00
1:C:407:ASN:CB	1:C:408:MET:HG2	1.90	1.00
1:C:869:VAL:O	1:C:873:VAL:HB	1.66	0.96
1:B:1052:VAL:O	1:B:1056:VAL:HB	1.66	0.96
1:A:1052:VAL:O	1:A:1056:VAL:HB	1.66	0.95
1:D:1052:VAL:O	1:D:1056:VAL:HB	1.66	0.95
1:A:432:SER:O	1:A:433:MET:HG2	1.65	0.94
1:A:590:ASN:HB3	1:A:591:MET:HG2	1.47	0.93
1:A:429:MET:SD	1:A:435:GLU:OE2	2.28	0.92
1:C:246:MET:SD	1:C:252:GLU:OE2	2.28	0.91
1:A:430:ASP:H	1:A:431:ALA:HA	1.37	0.90
1:C:247:ASP:N	1:C:248:ALA:HA	1.84	0.88
1:D:428:LYS:HE2	1:D:431:ALA:HB2	0.90	0.87
3:D:1203:Y01:HAR1	3:D:1203:Y01:HAM2	1.54	0.87
1:C:246:MET:CE	1:C:252:GLU:HG2	2.04	0.86
1:A:432:SER:O	1:A:433:MET:CG	2.24	0.86
1:D:761:TYR:O	3:D:1203:Y01:HAB2	1.76	0.85
3:D:1203:Y01:HAC1	3:D:1203:Y01:HAU2	1.60	0.81
1:A:590:ASN:CG	1:A:591:MET:HB3	2.01	0.81
2:D:1201:MG:MG	4:D:1307:HOH:O	1.25	0.79
1:C:689:LYS:O	1:C:693:PHE:HB2	1.82	0.79
1:B:872:LYS:O	1:B:876:PHE:HB2	1.82	0.79
1:D:872:LYS:O	1:D:876:PHE:HB2	1.82	0.79
1:C:407:ASN:CG	1:C:408:MET:HG2	2.04	0.78
1:A:431:ALA:HB3	1:A:432:SER:CB	2.14	0.78
1:A:872:LYS:O	1:A:876:PHE:HB2	1.82	0.78
1:C:167:ILE:HA	1:C:169:LEU:H	1.47	0.77
1:B:431:ALA:HB3	1:B:432:SER:CB	2.14	0.76
1:D:846:ALA:O	1:D:849:LEU:HB3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ALA:O	1:A:849:LEU:HB3	1.85	0.76
1:C:663:ALA:O	1:C:666:LEU:HB3	1.85	0.76
1:D:809:PHE:CD1	3:D:1203:Y01:CAC	2.70	0.75
1:B:846:ALA:O	1:B:849:LEU:HB3	1.85	0.75
1:D:809:PHE:CE1	3:D:1203:Y01:HAC2	2.22	0.74
1:A:590:ASN:HB3	1:A:591:MET:CG	2.17	0.73
3:D:1203:Y01:HAR1	3:D:1203:Y01:CAM	2.17	0.73
1:C:407:ASN:HB3	1:C:408:MET:CG	2.15	0.73
3:C:1308:Y01:HAE3	3:D:1203:Y01:HAP1	1.71	0.73
1:C:246:MET:HE3	1:C:252:GLU:HG2	1.70	0.72
1:B:430:ASP:N	1:B:431:ALA:HA	1.98	0.71
1:D:1041:ARG:O	1:D:1045:MET:HB3	1.91	0.71
1:A:1041:ARG:O	1:A:1045:MET:HB3	1.91	0.71
1:B:1041:ARG:O	1:B:1045:MET:HB3	1.91	0.70
1:C:858:ARG:O	1:C:862:MET:HB3	1.91	0.70
1:A:1049:ILE:HD11	1:D:1049:ILE:HD13	1.72	0.70
1:A:429:MET:CE	1:A:435:GLU:CG	2.68	0.69
1:A:430:ASP:H	1:A:431:ALA:CA	2.06	0.69
1:C:353:PHE:CD1	1:C:393:CYS:SG	2.86	0.69
1:C:424:PRO:O	1:C:426:ILE:N	2.26	0.68
1:D:350:ILE:HA	1:D:352:LEU:H	1.59	0.68
1:C:424:PRO:C	1:C:426:ILE:H	1.97	0.68
1:A:1029:SER:HA	1:A:1034:ARG:HE	1.59	0.67
1:A:578:GLN:HE22	1:A:953:ARG:HD3	1.60	0.67
1:B:578:GLN:HE22	1:B:953:ARG:HD3	1.60	0.67
1:B:430:ASP:H	1:B:431:ALA:CA	2.03	0.67
1:C:846:SER:HA	1:C:851:ARG:HE	1.59	0.67
1:C:395:GLN:HE22	1:C:770:ARG:HD3	1.60	0.67
1:D:1029:SER:HA	1:D:1034:ARG:HE	1.59	0.66
1:D:578:GLN:HE22	1:D:953:ARG:HD3	1.60	0.66
1:A:907:GLY:HA3	1:B:801:LEU:HD11	1.76	0.66
1:A:590:ASN:CB	1:A:591:MET:HG2	2.22	0.66
1:B:867:SER:HB2	1:B:869:SER:H	1.61	0.66
1:B:1029:SER:HA	1:B:1034:ARG:HE	1.59	0.65
1:B:586:MET:HG2	1:B:590:ASN:HD22	1.61	0.65
1:B:1057:ASN:HA	1:B:1060:LYS:HD2	1.79	0.65
1:D:1057:ASN:HA	1:D:1060:LYS:HD2	1.79	0.65
1:A:1057:ASN:HA	1:A:1060:LYS:HD2	1.79	0.65
1:C:684:SER:HB2	1:C:686:SER:H	1.61	0.65
1:D:867:SER:HB2	1:D:869:SER:H	1.61	0.65
3:D:1203:Y01:HAU2	3:D:1203:Y01:CAC	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:874:ASN:HA	1:C:877:LYS:HD2	1.79	0.64
1:A:590:ASN:CB	1:A:591:MET:HB3	2.27	0.64
1:A:867:SER:HB2	1:A:869:SER:H	1.61	0.64
1:A:431:ALA:H	1:A:432:SER:CB	2.10	0.64
1:D:730:TYR:O	1:D:734:TYR:HB2	1.98	0.63
1:A:430:ASP:N	1:A:431:ALA:HA	2.05	0.63
1:A:730:TYR:O	1:A:734:TYR:HB2	1.99	0.63
1:B:350:ILE:HA	1:B:352:LEU:H	1.61	0.63
1:B:730:TYR:O	1:B:734:TYR:HB2	1.98	0.63
1:C:407:ASN:OD1	1:C:408:MET:HA	1.98	0.63
1:A:590:ASN:HA	1:A:591:MET:HB3	1.80	0.63
1:D:538:GLN:NE2	1:D:1015:CYS:SG	2.72	0.62
1:B:538:GLN:NE2	1:B:1015:CYS:SG	2.72	0.62
1:C:355:GLN:NE2	1:C:832:CYS:SG	2.72	0.62
1:D:586:MET:HG2	1:D:590:ASN:HD22	1.65	0.62
1:A:538:GLN:NE2	1:A:1015:CYS:SG	2.73	0.62
3:A:1208:Y01:HAV1	1:D:868:TRP:HB3	1.81	0.62
1:C:547:TYR:O	1:C:551:TYR:HB2	1.98	0.62
1:A:429:MET:HE1	1:A:435:GLU:CG	2.21	0.61
1:B:800:ARG:O	1:B:803:TYR:HB3	2.00	0.61
1:C:617:ARG:O	1:C:620:TYR:HB3	2.00	0.61
1:D:872:LYS:O	1:D:876:PHE:CB	2.49	0.61
1:A:800:ARG:O	1:A:803:TYR:HB3	2.00	0.61
1:C:551:TYR:OH	1:C:630:ARG:NH1	2.33	0.61
1:D:734:TYR:OH	1:D:813:ARG:NH1	2.33	0.61
1:B:872:LYS:O	1:B:876:PHE:CB	2.49	0.60
1:B:734:TYR:OH	1:B:813:ARG:NH1	2.33	0.60
1:A:590:ASN:CA	1:A:591:MET:HB3	2.31	0.60
1:A:606:PRO:O	1:A:608:ALA:N	2.34	0.60
1:D:800:ARG:O	1:D:803:TYR:HB3	2.00	0.60
1:C:689:LYS:O	1:C:693:PHE:CB	2.49	0.60
1:A:734:TYR:OH	1:A:813:ARG:NH1	2.33	0.59
1:A:872:LYS:O	1:A:876:PHE:CB	2.49	0.59
1:C:106:UNK:O	1:C:109:UNK:C	2.50	0.59
1:D:288:UNK:O	1:D:291:UNK:C	2.50	0.59
1:A:288:UNK:O	1:A:291:UNK:C	2.50	0.59
1:B:288:UNK:O	1:B:291:UNK:C	2.50	0.58
1:D:428:LYS:HE3	1:D:431:ALA:HB1	1.82	0.58
1:A:463:LEU:HB3	1:A:479:LEU:HD13	1.86	0.58
1:A:429:MET:HE2	1:A:435:GLU:HG2	1.82	0.58
1:D:809:PHE:CE1	3:D:1203:Y01:CAC	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ILE:HA	1:A:352:LEU:H	1.67	0.58
1:B:431:ALA:H	1:B:432:SER:CB	2.16	0.58
1:B:463:LEU:HB3	1:B:479:LEU:HD13	1.86	0.58
1:C:596:LEU:HD11	1:C:613:PHE:H	1.69	0.58
1:D:718:GLN:NE2	1:D:785:TRP:O	2.35	0.57
1:D:779:LEU:HD11	1:D:796:PHE:H	1.69	0.57
1:D:463:LEU:HB3	1:D:479:LEU:HD13	1.86	0.57
1:A:779:LEU:HD11	1:A:796:PHE:H	1.69	0.57
1:A:858:ALA:HB1	1:B:712:VAL:HG12	1.86	0.57
1:C:199:ASN:HA	1:C:214:ARG:HH22	1.70	0.57
1:C:280:LEU:HB3	1:C:296:LEU:HD13	1.86	0.57
1:B:779:LEU:HD11	1:B:796:PHE:H	1.69	0.57
1:C:424:PRO:C	1:C:426:ILE:N	2.57	0.57
1:A:927:VAL:HG23	1:A:930:LEU:HB3	1.87	0.57
1:B:382:ASN:HA	1:B:397:ARG:HH22	1.70	0.57
1:A:576:CYS:O	1:A:579:MET:N	2.38	0.57
1:C:393:CYS:O	1:C:396:MET:N	2.38	0.57
1:A:360:GLY:HA2	1:A:363:ARG:HB3	1.87	0.56
1:B:937:VAL:HG13	1:B:940:GLN:HE21	1.70	0.56
1:C:246:MET:HE1	1:C:252:GLU:HG2	1.85	0.56
1:D:927:VAL:HG23	1:D:930:LEU:HB3	1.87	0.56
1:D:937:VAL:HG13	1:D:940:GLN:HE21	1.70	0.56
1:C:754:VAL:HG13	1:C:757:GLN:HE21	1.70	0.56
1:B:360:GLY:HA2	1:B:363:ARG:HB3	1.87	0.56
1:C:177:GLY:HA2	1:C:180:ARG:HB3	1.87	0.56
1:C:134:ASN:HD22	1:C:170:VAL:HG13	1.71	0.56
1:A:317:ASN:HD22	1:A:353:VAL:HG13	1.71	0.56
1:A:382:ASN:HA	1:A:397:ARG:HH22	1.70	0.55
1:A:431:ALA:CA	1:A:432:SER:CB	2.84	0.55
1:A:917:VAL:HB	3:B:1205:Y01:HAA1	1.87	0.55
1:B:431:ALA:CA	1:B:432:SER:CB	2.84	0.55
1:C:744:VAL:HG23	1:C:747:LEU:HB3	1.87	0.55
1:D:317:ASN:HD22	1:D:353:VAL:HG13	1.71	0.55
1:D:382:ASN:HA	1:D:397:ARG:HH22	1.70	0.55
1:A:937:VAL:HG13	1:A:940:GLN:HE21	1.70	0.55
1:D:430:ASP:N	1:D:431:ALA:HA	2.21	0.55
1:A:431:ALA:CB	1:A:432:SER:CB	2.85	0.55
1:C:214:ARG:O	1:C:217:HIS:C	2.45	0.55
1:A:397:ARG:O	1:A:400:HIS:C	2.45	0.55
1:B:317:ASN:HD22	1:B:353:VAL:HG13	1.71	0.55
3:C:1304:Y01:HAB2	3:C:1305:Y01:HAR1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ARG:O	1:D:400:HIS:C	2.45	0.55
1:B:431:ALA:CB	1:B:432:SER:CB	2.85	0.55
1:A:605:VAL:O	1:A:607:PRO:HD2	2.07	0.55
1:A:590:ASN:CA	1:A:591:MET:CB	2.85	0.54
1:B:397:ARG:O	1:B:400:HIS:C	2.45	0.54
1:B:576:CYS:O	1:B:579:MET:N	2.40	0.54
3:B:1205:Y01:HAE3	3:B:1206:Y01:HAC2	1.90	0.54
1:B:927:VAL:HG23	1:B:930:LEU:HB3	1.87	0.54
1:D:430:ASP:N	1:D:431:ALA:CA	2.71	0.54
1:D:761:TYR:C	3:D:1203:Y01:HAB2	2.27	0.54
1:A:536:PHE:CD1	1:A:576:CYS:SG	3.00	0.54
1:D:397:ARG:NH2	1:D:413:MET:O	2.41	0.54
3:A:1206:Y01:HAE3	3:A:1207:Y01:HAC2	1.90	0.53
1:C:529:VAL:HG11	1:C:624:ILE:HD11	1.91	0.53
1:D:960:TYR:HB2	1:D:963:LYS:HG2	1.91	0.53
1:A:960:TYR:HB2	1:A:963:LYS:HG2	1.91	0.53
1:B:397:ARG:NH2	1:B:413:MET:O	2.41	0.53
1:C:214:ARG:NH2	1:C:230:MET:O	2.41	0.53
1:D:576:CYS:O	1:D:579:MET:N	2.41	0.53
1:D:761:TYR:O	3:D:1203:Y01:CAB	2.54	0.53
1:B:818:LEU:HD23	3:B:1204:Y01:HAS2	1.90	0.53
1:C:695:PRO:HA	1:C:698:MET:HG2	1.90	0.53
1:B:718:GLN:NE2	1:B:785:TRP:O	2.35	0.53
1:B:878:PRO:HA	1:B:881:MET:HG2	1.90	0.53
1:A:397:ARG:NH2	1:A:413:MET:O	2.41	0.53
1:C:777:TYR:HB2	1:C:780:LYS:HG2	1.91	0.53
1:A:712:VAL:HG11	1:A:807:ILE:HD11	1.91	0.53
1:A:818:LEU:HD23	3:A:1203:Y01:HAS2	1.89	0.53
1:B:605:VAL:O	1:B:607:PRO:HD3	2.09	0.53
1:A:430:ASP:O	1:A:433:MET:O	2.27	0.52
1:B:712:VAL:HG11	1:B:807:ILE:HD11	1.91	0.52
1:B:730:TYR:O	1:B:734:TYR:CB	2.58	0.52
1:B:960:TYR:HB2	1:B:963:LYS:HG2	1.91	0.52
1:C:421:LEU:HD21	1:C:509:VAL:HG13	1.91	0.52
1:C:547:TYR:O	1:C:551:TYR:CB	2.58	0.52
1:A:878:PRO:HA	1:A:881:MET:HG2	1.90	0.52
1:D:354:ILE:HG12	1:D:475:MET:HB2	1.91	0.52
1:D:604:LEU:HD21	1:D:692:VAL:HG13	1.92	0.52
1:D:730:TYR:O	1:D:734:TYR:CB	2.58	0.52
1:A:718:GLN:NE2	1:A:785:TRP:O	2.35	0.52
1:B:826:PRO:O	1:B:830:MET:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:643:PRO:O	1:C:647:MET:HB2	2.10	0.52
1:C:687:LEU:O	1:C:691:ILE:N	2.38	0.52
1:A:606:PRO:C	1:A:608:ALA:H	2.12	0.52
1:D:826:PRO:O	1:D:830:MET:HB2	2.10	0.52
3:D:1203:Y01:HAM2	3:D:1203:Y01:CAR	2.33	0.52
3:D:1203:Y01:CAC	3:D:1203:Y01:CAU	2.85	0.52
1:A:1037:VAL:HB	1:D:1039:PHE:HE1	1.74	0.52
1:B:604:LEU:HD21	1:B:692:VAL:HG13	1.91	0.52
1:C:876:ILE:O	1:C:880:LEU:CB	2.58	0.52
1:A:826:PRO:O	1:A:830:MET:HB2	2.10	0.51
1:B:728:ILE:O	1:B:732:PHE:HB2	2.10	0.51
1:A:604:LEU:HD21	1:A:692:VAL:HG13	1.92	0.51
1:D:712:VAL:HG11	1:D:807:ILE:HD11	1.91	0.51
1:D:842:VAL:O	1:D:846:ALA:N	2.43	0.51
1:D:878:PRO:HA	1:D:881:MET:HG2	1.90	0.51
1:D:1041:ARG:O	1:D:1045:MET:CB	2.58	0.51
1:A:893:VAL:HG12	1:A:904:CYS:HB3	1.93	0.51
1:C:545:ILE:O	1:C:549:PHE:HB2	2.10	0.51
1:A:730:TYR:O	1:A:734:TYR:CB	2.58	0.51
1:A:936:ASN:HD21	1:B:938:TYR:HD2	1.58	0.51
1:D:728:ILE:O	1:D:732:PHE:HB2	2.10	0.51
1:B:870:LEU:O	1:B:874:ILE:N	2.38	0.51
1:B:1059:ILE:O	1:B:1063:LEU:CB	2.58	0.51
1:C:422:VAL:O	1:C:424:PRO:HD3	2.11	0.51
1:C:535:GLN:NE2	1:C:602:TRP:O	2.35	0.51
1:A:1059:ILE:O	1:A:1063:LEU:CB	2.58	0.51
1:C:353:PHE:HD1	1:C:393:CYS:SG	2.32	0.51
1:C:858:ARG:O	1:C:862:MET:CB	2.58	0.51
1:D:1059:ILE:O	1:D:1063:LEU:CB	2.58	0.51
1:A:521:SER:O	1:A:525:GLY:N	2.43	0.51
1:D:893:VAL:HG12	1:D:904:CYS:HB3	1.93	0.51
1:A:1041:ARG:O	1:A:1045:MET:CB	2.58	0.51
1:A:590:ASN:CB	1:A:591:MET:CB	2.88	0.51
1:A:728:ILE:O	1:A:732:PHE:HB2	2.10	0.51
1:B:605:VAL:C	1:B:607:PRO:HD3	2.32	0.51
1:A:431:ALA:N	1:A:432:SER:CB	2.73	0.50
1:B:430:ASP:N	1:B:431:ALA:CA	2.70	0.50
1:D:808:ILE:HG21	3:D:1203:Y01:HAE1	1.93	0.50
3:A:1208:Y01:HAV2	1:D:866:PRO:HB3	1.93	0.50
1:C:698:MET:HB3	1:C:736:LEU:HD21	1.93	0.50
1:C:710:VAL:HG12	1:C:721:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:GLY:HA3	1:D:801:LEU:HD11	1.93	0.50
1:B:893:VAL:HG12	1:B:904:CYS:HB3	1.93	0.50
1:B:1041:ARG:O	1:B:1045:MET:CB	2.58	0.50
1:A:454:LYS:HG3	1:A:455:ARG:HD2	1.92	0.50
1:A:373:LEU:HD11	1:A:442:LYS:HE2	1.94	0.50
1:A:870:LEU:O	1:A:874:ILE:N	2.38	0.50
1:C:166:ASP:OD1	1:C:166:ASP:N	2.45	0.50
1:D:349:ASP:N	1:D:349:ASP:OD1	2.45	0.50
1:D:809:PHE:CD1	3:D:1203:Y01:HAC2	2.44	0.50
1:B:881:MET:HB3	1:B:919:LEU:HD21	1.93	0.50
1:C:190:LEU:HD11	1:C:259:LYS:HE2	1.94	0.49
1:A:881:MET:HB3	1:A:919:LEU:HD21	1.93	0.49
1:B:842:VAL:O	1:B:846:ALA:N	2.43	0.49
1:A:349:ASP:OD1	1:A:349:ASP:N	2.45	0.49
1:A:799:GLY:O	1:A:803:TYR:HB2	2.13	0.49
1:A:842:VAL:O	1:A:846:ALA:N	2.43	0.49
1:A:893:VAL:HG21	1:A:901:PRO:HG2	1.94	0.49
1:B:521:SER:O	1:B:525:GLY:N	2.43	0.49
1:B:893:VAL:HG21	1:B:901:PRO:HG2	1.94	0.49
1:D:799:GLY:O	1:D:803:TYR:HB2	2.13	0.49
1:D:430:ASP:H	1:D:431:ALA:C	2.16	0.49
1:D:870:LEU:O	1:D:874:ILE:N	2.38	0.49
1:D:394:PRO:O	1:D:397:ARG:HB2	2.13	0.49
1:A:394:PRO:O	1:A:397:ARG:HB2	2.13	0.49
1:C:338:SER:O	1:C:342:GLY:N	2.43	0.49
1:D:558:THR:HG22	1:D:561:LYS:H	1.78	0.49
1:D:562:LEU:HA	1:D:563:ALA:HA	1.66	0.49
1:A:558:THR:HG22	1:A:561:LYS:H	1.78	0.49
1:A:780:ARG:O	1:A:783:ALA:HB3	2.13	0.49
1:B:394:PRO:O	1:B:397:ARG:HB2	2.13	0.49
1:B:1049:ILE:HD13	1:C:866:ILE:HD11	1.94	0.49
1:C:710:VAL:HG21	1:C:718:PRO:HG2	1.94	0.49
1:A:430:ASP:N	1:A:431:ALA:CA	2.71	0.49
1:B:558:THR:HG22	1:B:561:LYS:H	1.78	0.49
1:B:799:GLY:O	1:B:803:TYR:HB2	2.13	0.49
1:C:597:ARG:O	1:C:600:ALA:HB3	2.13	0.49
1:D:780:ARG:O	1:D:783:ALA:HB3	2.13	0.49
1:D:808:ILE:CG2	3:D:1203:Y01:HAE1	2.43	0.49
1:B:1033:GLU:OE2	1:B:1036:ARG:NH1	2.46	0.48
1:C:375:THR:HG22	1:C:378:LYS:H	1.78	0.48
1:B:780:ARG:O	1:B:783:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:616:GLY:O	1:C:620:TYR:HB2	2.13	0.48
1:D:373:LEU:HD11	1:D:442:LYS:HE2	1.94	0.48
1:D:507:SER:HA	1:D:508:ASP:HA	1.65	0.48
1:B:373:LEU:HD11	1:B:442:LYS:HE2	1.94	0.48
1:C:376:CYS:O	1:C:379:LEU:O	2.32	0.48
1:D:881:MET:HB3	1:D:919:LEU:HD21	1.93	0.48
1:D:704:PHE:HE1	1:D:727:VAL:HG13	1.79	0.48
1:D:893:VAL:HG21	1:D:901:PRO:HG2	1.94	0.48
1:C:392:THR:O	1:C:396:MET:N	2.42	0.48
1:A:590:ASN:OD1	1:A:591:MET:HB3	2.13	0.48
1:A:704:PHE:HE1	1:A:727:VAL:HG13	1.79	0.48
3:C:1308:Y01:HAS2	3:C:1308:Y01:HAD2	1.65	0.48
1:B:536:PHE:CD1	1:B:576:CYS:SG	3.05	0.48
1:C:211:PRO:O	1:C:214:ARG:HB2	2.13	0.48
1:C:665:VAL:HG22	3:C:1308:Y01:HAC2	1.95	0.48
1:D:1033:GLU:OE2	1:D:1036:ARG:NH1	2.46	0.48
1:A:432:SER:C	1:A:433:MET:HG2	2.30	0.48
1:B:349:ASP:N	1:B:349:ASP:OD1	2.45	0.48
1:D:329:HIS:HA	1:D:330:LEU:HA	1.68	0.48
1:A:559:CYS:O	1:A:562:LEU:O	2.32	0.48
1:C:659:VAL:O	1:C:663:ALA:N	2.43	0.48
1:C:512:TRP:CH2	3:C:1303:Y01:HAE2	2.47	0.48
1:A:1033:GLU:OE2	1:A:1036:ARG:NH1	2.46	0.47
1:B:433:MET:HA	1:B:434:GLU:HA	1.50	0.47
1:B:704:PHE:HE1	1:B:727:VAL:HG13	1.79	0.47
1:C:521:PHE:HE1	1:C:544:VAL:HG13	1.79	0.47
1:C:850:GLU:OE2	1:C:853:ARG:NH1	2.46	0.47
1:D:433:MET:HA	1:D:434:GLU:HA	1.56	0.47
1:A:590:ASN:CB	1:A:591:MET:CG	2.86	0.47
1:B:728:ILE:O	1:B:732:PHE:CB	2.63	0.47
1:B:559:CYS:O	1:B:562:LEU:O	2.32	0.47
1:C:545:ILE:O	1:C:549:PHE:CB	2.63	0.47
1:A:724:GLU:O	1:A:727:VAL:HB	2.15	0.47
1:D:575:THR:O	1:D:579:MET:N	2.42	0.47
1:A:491:LEU:HD22	1:A:563:ALA:HB2	1.97	0.47
1:A:590:ASN:HA	1:A:591:MET:CB	2.40	0.47
1:C:324:SER:HA	1:C:325:ASP:HA	1.65	0.47
1:C:541:GLU:O	1:C:544:VAL:HB	2.15	0.47
1:D:808:ILE:HG22	3:D:1203:Y01:CAE	2.45	0.47
1:D:1030:GLY:H	1:D:1034:ARG:HG3	1.80	0.47
1:A:590:ASN:OD1	1:A:591:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ILE:O	1:A:732:PHE:CB	2.63	0.47
1:B:24:UNK:HA	1:B:25:UNK:HA	1.76	0.47
1:A:429:MET:SD	1:A:429:MET:C	2.94	0.47
1:A:1030:GLY:H	1:A:1034:ARG:HG3	1.80	0.47
1:C:847:GLY:H	1:C:851:ARG:HG3	1.80	0.47
1:B:1030:GLY:H	1:B:1034:ARG:HG3	1.80	0.47
1:D:559:CYS:O	1:D:562:LEU:O	2.32	0.47
1:B:590:ASN:HB3	1:B:591:MET:SD	2.56	0.46
1:B:724:GLU:O	1:B:727:VAL:HB	2.15	0.46
1:D:728:ILE:O	1:D:732:PHE:CB	2.63	0.46
1:A:412:LYS:HA	1:A:413:MET:CB	2.43	0.46
1:C:246:MET:SD	1:C:246:MET:C	2.94	0.46
1:D:521:SER:O	1:D:525:GLY:N	2.43	0.46
1:A:857:LYS:HD2	1:B:713:LEU:HD22	1.97	0.46
1:B:760:ASP:OD2	1:B:763:ASN:ND2	2.49	0.46
1:B:848:VAL:HG13	3:C:1306:Y01:HAJ1	1.96	0.46
1:C:512:TRP:HH2	3:C:1303:Y01:HAE2	1.80	0.46
1:C:577:ASP:OD2	1:C:580:ASN:ND2	2.49	0.46
1:A:718:GLN:HA	1:A:719:LEU:HA	1.80	0.46
1:A:760:ASP:OD2	1:A:763:ASN:ND2	2.49	0.46
1:A:1027:PHE:HA	1:A:1033:GLU:HG2	1.97	0.46
1:C:308:LEU:HD22	1:C:380:ALA:HB2	1.97	0.46
1:D:491:LEU:HD22	1:D:563:ALA:HB2	1.97	0.46
1:A:693:LYS:HG2	1:A:965:VAL:HG11	1.97	0.46
1:B:693:LYS:HG2	1:B:965:VAL:HG11	1.97	0.46
1:C:510:LYS:HG2	1:C:782:VAL:HG11	1.97	0.46
1:A:562:LEU:H	1:A:564:VAL:H	1.64	0.46
1:B:562:LEU:H	1:B:564:VAL:H	1.64	0.46
1:D:1027:PHE:HA	1:D:1033:GLU:HG2	1.97	0.46
1:D:288:UNK:O	1:D:291:UNK:O	2.34	0.46
1:C:844:PHE:HA	1:C:850:GLU:HG2	1.97	0.46
1:D:724:GLU:O	1:D:727:VAL:HB	2.15	0.46
1:D:760:ASP:OD2	1:D:763:ASN:ND2	2.48	0.46
1:B:431:ALA:N	1:B:432:SER:CB	2.78	0.46
1:B:491:LEU:HD22	1:B:563:ALA:HB2	1.97	0.46
1:B:590:ASN:CG	1:B:591:MET:SD	2.94	0.46
1:B:1027:PHE:HA	1:B:1033:GLU:HG2	1.97	0.46
1:B:288:UNK:O	1:B:291:UNK:O	2.34	0.45
1:C:24:UNK:HA	1:C:25:UNK:HA	1.76	0.45
1:C:667:LEU:HD13	3:C:1304:Y01:HAJ1	1.98	0.45
3:A:1208:Y01:HAC1	3:A:1208:Y01:HAP1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:LYS:HG2	1:D:965:VAL:HG11	1.97	0.45
1:A:288:UNK:O	1:A:291:UNK:O	2.34	0.45
1:B:605:VAL:O	1:B:607:PRO:CD	2.65	0.45
3:C:1302:Y01:HAC1	3:C:1302:Y01:HAP1	1.59	0.45
1:D:562:LEU:H	1:D:564:VAL:H	1.64	0.45
1:A:291:UNK:HA	1:A:292:UNK:HA	1.59	0.45
1:A:548:THR:HA	1:A:549:TYR:HA	1.77	0.45
1:C:106:UNK:O	1:C:109:UNK:O	2.34	0.45
1:C:146:HIS:HA	1:C:147:LEU:HA	1.68	0.45
1:C:379:LEU:H	1:C:381:VAL:H	1.64	0.45
1:D:975:HIS:HA	1:D:976:ILE:HA	1.67	0.45
1:A:562:LEU:HA	1:A:563:ALA:HA	1.66	0.45
1:C:393:CYS:O	1:C:394:THR:C	2.54	0.45
1:C:522:LEU:HB3	3:C:1302:Y01:HAB2	1.99	0.45
1:B:431:ALA:H	1:B:432:SER:C	2.20	0.45
1:C:792:HIS:HA	1:C:793:ILE:HA	1.67	0.45
1:D:291:UNK:HA	1:D:292:UNK:HA	1.59	0.45
1:B:888:ALA:HB2	1:C:702:GLU:HG2	1.99	0.45
1:B:811:TYR:O	1:B:814:LEU:HB2	2.17	0.44
1:C:109:UNK:HA	1:C:110:UNK:HA	1.59	0.44
1:D:354:ILE:HG21	1:D:475:MET:HA	1.98	0.44
3:A:1208:Y01:HAD3	3:A:1208:Y01:HBD	1.82	0.44
1:B:924:ILE:HG23	1:C:747:LEU:HD21	1.99	0.44
1:D:811:TYR:O	1:D:814:LEU:HB2	2.17	0.44
1:C:363:LEU:HB3	1:C:825:LEU:HD11	2.00	0.44
1:A:240:UNK:O	1:A:244:UNK:CB	2.66	0.44
1:A:1063:LEU:O	1:A:1067:ASP:CB	2.65	0.44
1:C:880:LEU:O	1:C:884:ASP:CB	2.65	0.44
1:B:1063:LEU:O	1:B:1067:ASP:CB	2.65	0.44
3:B:1204:Y01:HAC2	3:B:1204:Y01:HAA1	1.99	0.44
1:C:628:TYR:O	1:C:631:LEU:HB2	2.17	0.44
1:D:555:SER:HA	1:D:556:ASN:HA	1.69	0.44
3:A:1203:Y01:HAJ1	3:A:1203:Y01:HAC3	1.75	0.44
1:B:240:UNK:O	1:B:244:UNK:CB	2.65	0.44
3:C:1307:Y01:HAS2	3:C:1307:Y01:HAD2	1.77	0.44
1:B:329:HIS:HA	1:B:330:LEU:HA	1.68	0.44
1:B:975:HIS:HA	1:B:976:ILE:HA	1.67	0.44
1:C:738:VAL:HG21	3:C:1308:Y01:HAO1	1.98	0.44
1:C:859:VAL:O	1:C:863:SER:HB3	2.18	0.44
1:A:507:SER:HA	1:A:508:ASP:HA	1.65	0.44
1:D:1042:VAL:O	1:D:1046:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1063:LEU:O	1:D:1067:ASP:CB	2.65	0.44
1:B:1042:VAL:O	1:B:1046:SER:HB3	2.18	0.43
3:B:1206:Y01:HAS2	3:B:1206:Y01:HAD2	1.73	0.43
1:C:58:UNK:O	1:C:62:UNK:CB	2.66	0.43
1:D:240:UNK:O	1:D:244:UNK:CB	2.66	0.43
1:C:212:GLN:NE2	1:C:324:SER:O	2.49	0.43
1:C:541:GLU:HG2	1:C:545:ILE:HD11	2.00	0.43
1:D:546:LEU:HB3	1:D:1008:LEU:HD11	2.00	0.43
1:A:546:LEU:HB3	1:A:1008:LEU:HD11	2.00	0.43
1:A:599:VAL:HG12	1:A:603:ILE:HD11	2.00	0.43
1:A:420:LYS:O	1:A:423:GLN:HB3	2.19	0.43
1:A:811:TYR:O	1:A:814:LEU:HB2	2.18	0.43
3:A:1205:Y01:HBA	1:B:702:LEU:HD22	2.00	0.43
1:B:507:SER:HA	1:B:508:ASP:HA	1.65	0.43
1:B:562:LEU:HA	1:B:563:ALA:HA	1.66	0.43
1:C:416:VAL:HG12	1:C:420:ILE:HD11	2.00	0.43
3:D:1202:Y01:HAD2	3:D:1202:Y01:HAS2	1.76	0.43
1:B:546:LEU:HB3	1:B:1008:LEU:HD11	2.00	0.43
3:C:1308:Y01:HAP1	3:D:1203:Y01:HAQ1	2.01	0.43
1:A:1059:ILE:HD12	1:D:1060:LYS:HD3	2.00	0.43
1:B:575:THR:O	1:B:579:MET:N	2.42	0.43
1:C:734:VAL:HG21	3:D:1203:Y01:HAI	2.00	0.43
3:A:1203:Y01:HAC2	3:A:1203:Y01:HAA1	2.01	0.43
1:D:699:LEU:HD23	1:D:699:LEU:HA	1.90	0.43
3:C:1308:Y01:HAD3	3:C:1308:Y01:HBD	1.80	0.43
1:D:599:VAL:HG12	1:D:603:ILE:HD11	2.00	0.43
1:A:555:SER:HA	1:A:556:ASN:HA	1.69	0.43
1:A:1042:VAL:O	1:A:1046:SER:HB3	2.18	0.43
1:A:329:HIS:HA	1:A:330:LEU:HA	1.68	0.43
1:A:918:TYR:CZ	1:A:922:GLN:HG3	2.54	0.43
3:A:1208:Y01:HAD2	3:A:1208:Y01:HAS2	1.83	0.43
1:B:420:LYS:O	1:B:423:GLN:HB3	2.19	0.43
1:B:555:SER:HA	1:B:556:ASN:HA	1.69	0.43
3:B:1204:Y01:HAJ1	3:B:1204:Y01:HAC3	1.77	0.43
1:D:420:LYS:O	1:D:423:GLN:HB3	2.19	0.43
1:A:429:MET:HE2	1:A:435:GLU:CG	2.44	0.42
1:A:724:GLU:HG2	1:A:728:ILE:HD11	2.00	0.42
1:B:918:TYR:CZ	1:B:922:GLN:HG3	2.54	0.42
1:C:735:TYR:CZ	1:C:739:GLN:HG3	2.54	0.42
1:D:428:LYS:HE2	1:D:431:ALA:CA	2.45	0.42
1:D:430:ASP:N	1:D:431:ALA:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:710:PHE:CZ	3:D:1202:Y01:HAR2	2.53	0.42
1:A:236:UNK:O	1:A:240:UNK:CB	2.67	0.42
1:A:714:VAL:HG21	1:D:866:PRO:HG3	2.01	0.42
1:B:599:VAL:HG12	1:B:603:ILE:HD11	2.00	0.42
1:B:699:LEU:HD23	1:B:699:LEU:HA	1.90	0.42
1:D:718:GLN:HA	1:D:719:LEU:HA	1.81	0.42
1:A:575:THR:O	1:A:579:MET:N	2.42	0.42
3:A:1207:Y01:HAS2	3:A:1207:Y01:HAD2	1.73	0.42
1:C:54:UNK:O	1:C:58:UNK:CB	2.67	0.42
1:C:365:THR:HA	1:C:366:TYR:HA	1.76	0.42
1:D:918:TYR:CZ	1:D:922:GLN:HG3	2.54	0.42
3:A:1206:Y01:HAC1	3:A:1206:Y01:HAP1	1.59	0.42
1:C:542:TRP:HA	1:C:545:ILE:HD12	2.02	0.42
1:B:724:GLU:HG2	1:B:728:ILE:HD11	2.00	0.42
1:C:583:ASP:O	1:C:586:ALA:HB3	2.20	0.42
1:C:849:GLU:HG2	1:D:1030:GLY:HA3	2.01	0.42
1:D:766:ASP:O	1:D:769:ALA:HB3	2.20	0.42
1:B:236:UNK:O	1:B:240:UNK:CB	2.67	0.42
1:B:291:UNK:HA	1:B:292:UNK:HA	1.59	0.42
1:C:665:VAL:HB	1:C:739:GLN:HE21	1.85	0.42
1:D:236:UNK:O	1:D:240:UNK:CB	2.67	0.42
1:D:548:THR:HA	1:D:549:TYR:HA	1.77	0.42
1:D:724:GLU:HG2	1:D:728:ILE:HD11	2.00	0.42
1:A:766:ASP:O	1:A:769:ALA:HB3	2.20	0.42
1:B:354:ILE:H	1:B:354:ILE:HG13	1.63	0.42
1:B:371:PHE:HA	1:B:375:TYR:HB2	2.02	0.42
1:C:237:LYS:O	1:C:240:GLN:HB3	2.19	0.42
1:A:606:PRO:C	1:A:608:ALA:N	2.73	0.42
1:B:576:CYS:O	1:B:577:THR:C	2.57	0.42
1:D:725:TRP:HA	1:D:728:ILE:HD12	2.02	0.42
1:A:395:GLN:NE2	1:A:507:SER:O	2.49	0.42
1:A:725:TRP:HA	1:A:728:ILE:HD12	2.01	0.42
1:A:848:VAL:HB	1:A:922:GLN:HE21	1.85	0.42
1:B:725:TRP:HA	1:B:728:ILE:HD12	2.02	0.42
1:D:576:CYS:O	1:D:577:THR:C	2.57	0.42
1:D:848:VAL:HB	1:D:922:GLN:HE21	1.85	0.42
1:A:28:UNK:O	1:A:32:UNK:CB	2.68	0.42
1:C:379:LEU:HA	1:C:380:ALA:HA	1.66	0.42
1:C:665:VAL:HG13	3:C:1308:Y01:HAO2	2.02	0.42
3:C:1308:Y01:CAD	3:D:1203:Y01:HAN1	2.49	0.42
1:A:627:GLN:HA	1:A:628:ASP:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1205:Y01:HAJ2	3:A:1205:Y01:HAC3	1.80	0.41
1:D:28:UNK:O	1:D:32:UNK:CB	2.68	0.41
1:D:395:GLN:NE2	1:D:507:SER:O	2.49	0.41
1:D:429:MET:HA	1:D:430:ASP:HA	1.72	0.41
1:A:756:VAL:O	1:A:759:SER:OG	2.26	0.41
1:B:395:GLN:NE2	1:B:507:SER:O	2.49	0.41
1:B:766:ASP:O	1:B:769:ALA:HB3	2.20	0.41
1:C:188:PHE:HA	1:C:192:TYR:HB2	2.02	0.41
1:D:627:GLN:HA	1:D:628:ASP:HA	1.88	0.41
3:A:1205:Y01:HAD2	3:A:1205:Y01:HAS2	1.75	0.41
1:D:375:TYR:O	1:D:379:GLY:N	2.54	0.41
3:D:1203:Y01:HAA1	3:D:1203:Y01:CAO	2.50	0.41
1:A:24:UNK:HA	1:A:25:UNK:HA	1.76	0.41
1:B:590:ASN:OD1	1:B:591:MET:SD	2.79	0.41
1:C:28:UNK:O	1:C:32:UNK:CB	2.68	0.41
1:C:192:TYR:O	1:C:196:GLY:N	2.54	0.41
1:C:246:MET:SD	1:C:246:MET:O	2.78	0.41
1:C:407:ASN:OD1	1:C:408:MET:SD	2.79	0.41
1:D:1056:VAL:HG12	1:D:1060:LYS:HE3	2.02	0.41
1:B:28:UNK:O	1:B:32:UNK:CB	2.68	0.41
1:B:1056:VAL:HG12	1:B:1060:LYS:HE3	2.02	0.41
3:C:1307:Y01:HAD3	3:C:1307:Y01:HBD	1.83	0.41
1:D:24:UNK:HA	1:D:25:UNK:HA	1.76	0.41
1:D:960:TYR:HA	1:D:962:GLU:N	2.36	0.41
1:A:1056:VAL:HG12	1:A:1060:LYS:HE3	2.02	0.41
1:B:718:GLN:HA	1:B:719:LEU:HA	1.80	0.41
1:C:535:GLN:HA	1:C:536:LEU:HA	1.81	0.41
1:A:960:TYR:HA	1:A:962:GLU:N	2.36	0.41
1:B:425:TYR:CD2	1:B:428:LYS:HD2	2.56	0.41
1:C:444:GLN:HA	1:C:445:ASP:HA	1.88	0.41
1:B:693:LYS:HE2	1:B:965:VAL:HG21	2.03	0.41
3:B:1206:Y01:HAD3	3:B:1206:Y01:HBD	1.90	0.41
1:C:777:TYR:HA	1:C:779:GLU:N	2.36	0.41
1:D:425:TYR:CD2	1:D:428:LYS:HD2	2.56	0.41
1:A:371:PHE:HA	1:A:375:TYR:HB2	2.02	0.41
1:A:375:TYR:O	1:A:379:GLY:N	2.54	0.41
1:A:699:LEU:HD23	1:A:699:LEU:HA	1.90	0.41
1:A:925:ILE:HG21	1:B:831:ILE:HG23	2.03	0.41
3:A:1206:Y01:HAB1	3:A:1206:Y01:HAC3	2.01	0.41
1:B:848:VAL:HB	1:B:922:GLN:HE21	1.85	0.41
1:B:960:TYR:HA	1:B:962:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:MET:HA	1:C:251:GLU:HA	1.81	0.41
3:C:1301:Y01:HAD2	3:C:1301:Y01:HAS2	1.70	0.41
3:C:1302:Y01:HAD3	3:C:1302:Y01:HBD	1.88	0.41
1:D:371:PHE:HA	1:D:375:TYR:HB2	2.02	0.41
1:D:492:VAL:HG22	1:D:562:LEU:HD21	2.03	0.41
3:A:1208:Y01:HAI	1:D:870:LEU:HD12	2.03	0.41
1:B:375:TYR:O	1:B:379:GLY:N	2.54	0.41
1:D:693:LYS:HE2	1:D:965:VAL:HG21	2.03	0.41
1:A:361:THR:HA	1:A:362:TYR:HA	1.86	0.40
1:A:429:MET:HA	1:A:430:ASP:HA	1.90	0.40
1:C:166:ASP:OD2	1:C:174:LEU:HD21	2.21	0.40
1:A:492:VAL:HG22	1:A:562:LEU:HD21	2.03	0.40
3:A:1207:Y01:HAE2	3:A:1207:Y01:HBB	1.92	0.40
1:C:372:SER:HA	1:C:373:ASN:HA	1.69	0.40
3:A:1205:Y01:HAN1	3:B:1204:Y01:HAM1	2.03	0.40
1:B:548:THR:HA	1:B:549:TYR:HA	1.76	0.40
1:C:855:THR:O	1:C:859:VAL:HB	2.22	0.40
1:C:873:VAL:HG12	1:C:877:LYS:HE3	2.02	0.40
1:D:1038:THR:O	1:D:1042:VAL:HB	2.22	0.40
1:A:431:ALA:H	1:A:432:SER:C	2.24	0.40
3:A:1205:Y01:HAE2	3:A:1205:Y01:HBB	1.79	0.40
3:B:1203:Y01:HAD2	3:B:1203:Y01:HAS2	1.88	0.40
1:A:425:TYR:CD2	1:A:428:LYS:HD2	2.56	0.40
1:A:693:LYS:HD3	1:A:963:LYS:HB2	2.04	0.40
1:A:1062:SER:O	1:A:1066:LEU:CB	2.70	0.40
3:A:1206:Y01:HAD2	3:A:1206:Y01:HAS2	1.72	0.40
1:C:242:TYR:CD2	1:C:245:LYS:HD2	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	632/955 (66%)	544 (86%)	79 (12%)	9 (1%)	11	45
1	B	632/955 (66%)	546 (86%)	79 (12%)	7 (1%)	14	50
1	C	632/955 (66%)	544 (86%)	79 (12%)	9 (1%)	11	45
1	D	632/955 (66%)	548 (87%)	79 (12%)	5 (1%)	19	56
All	All	2528/3820 (66%)	2182 (86%)	316 (12%)	30 (1%)	17	48

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ILE
1	A	996	PRO
1	B	996	PRO
1	C	142	PRO
1	C	168	GLY
1	C	813	PRO
1	D	996	PRO
1	A	325	PRO
1	B	325	PRO
1	C	425	ALA
1	D	325	PRO
1	A	568	LEU
1	A	607	PRO
1	B	433	MET
1	B	568	LEU
1	B	576	CYS
1	B	606	PRO
1	C	385	LEU
1	D	568	LEU
1	D	576	CYS
1	A	569	ARG
1	A	576	CYS
1	B	569	ARG
1	C	272	ARG
1	C	386	ARG
1	C	393	CYS
1	C	423	PRO
1	D	569	ARG
1	A	433	MET
1	A	606	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	481/758 (64%)	472 (98%)	9 (2%)	57 76
1	B	482/758 (64%)	474 (98%)	8 (2%)	60 79
1	C	485/758 (64%)	476 (98%)	9 (2%)	57 76
1	D	476/758 (63%)	467 (98%)	9 (2%)	57 76
All	All	1924/3032 (64%)	1889 (98%)	35 (2%)	61 77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	553	ASN
1	A	567	ARG
1	A	591	MET
1	A	780	ARG
1	A	800	ARG
1	A	856	ARG
1	A	928	ASN
1	A	935	ASN
1	B	373	LEU
1	B	553	ASN
1	B	567	ARG
1	B	780	ARG
1	B	800	ARG
1	B	856	ARG
1	B	928	ASN
1	B	935	ASN
1	C	190	LEU
1	C	370	ASN
1	C	384	ARG
1	C	408	MET
1	C	597	ARG
1	C	617	ARG
1	C	673	ARG

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Mol	Chain	Res	Type
1	C	745	ASN
1	C	752	ASN
1	D	373	LEU
1	D	553	ASN
1	D	567	ARG
1	D	576	CYS
1	D	780	ARG
1	D	800	ARG
1	D	856	ARG
1	D	928	ASN
1	D	935	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	GLN
1	A	538	GLN
1	A	553	ASN
1	A	578	GLN
1	A	940	GLN
1	A	1005	GLN
1	B	395	GLN
1	B	538	GLN
1	B	553	ASN
1	B	578	GLN
1	B	590	ASN
1	B	940	GLN
1	C	212	GLN
1	C	355	GLN
1	C	370	ASN
1	C	395	GLN
1	C	757	GLN
1	D	395	GLN
1	D	538	GLN
1	D	553	ASN
1	D	578	GLN
1	D	590	ASN
1	D	940	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	Y01	B	1203	-	38,38,38	1.79	5 (13%)	57,57,57	1.66	13 (22%)
3	Y01	C	1304	-	38,38,38	1.84	8 (21%)	57,57,57	2.02	13 (22%)
3	Y01	B	1205	-	38,38,38	1.82	6 (15%)	57,57,57	2.01	17 (29%)
3	Y01	A	1204	-	38,38,38	1.74	4 (10%)	57,57,57	1.71	12 (21%)
3	Y01	C	1303	-	38,38,38	2.04	5 (13%)	57,57,57	1.96	15 (26%)
3	Y01	B	1206	-	38,38,38	1.77	6 (15%)	57,57,57	1.77	11 (19%)
3	Y01	C	1301	-	38,38,38	1.73	4 (10%)	57,57,57	1.91	13 (22%)
3	Y01	A	1208	-	38,38,38	1.92	7 (18%)	57,57,57	2.18	13 (22%)
3	Y01	A	1206	-	38,38,38	1.94	8 (21%)	57,57,57	2.15	18 (31%)
3	Y01	A	1207	-	38,38,38	1.75	4 (10%)	57,57,57	1.73	13 (22%)
3	Y01	C	1307	-	38,38,38	1.86	6 (15%)	57,57,57	2.28	14 (24%)
3	Y01	C	1302	-	38,38,38	2.03	9 (23%)	57,57,57	1.99	13 (22%)
3	Y01	A	1205	-	38,38,38	1.91	8 (21%)	57,57,57	1.81	12 (21%)
3	Y01	C	1306	-	38,38,38	1.97	6 (15%)	57,57,57	1.84	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	Y01	C	1308	-	38,38,38	1.74	5 (13%)	57,57,57	2.06	17 (29%)
3	Y01	D	1202	-	38,38,38	1.75	6 (15%)	57,57,57	1.75	13 (22%)
3	Y01	C	1305	-	38,38,38	1.81	4 (10%)	57,57,57	1.74	12 (21%)
3	Y01	B	1204	-	38,38,38	1.84	6 (15%)	57,57,57	1.46	9 (15%)
3	Y01	A	1203	-	38,38,38	1.88	6 (15%)	57,57,57	1.53	10 (17%)
3	Y01	D	1203	-	38,38,38	1.78	6 (15%)	57,57,57	1.64	15 (26%)

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
3	Y01	B	1203	-	-	10/19/77/77	0/4/4/4
3	Y01	C	1304	-	-	13/19/77/77	0/4/4/4
3	Y01	B	1205	-	-	14/19/77/77	0/4/4/4
3	Y01	A	1204	-	-	5/19/77/77	0/4/4/4
3	Y01	C	1303	-	-	7/19/77/77	0/4/4/4
3	Y01	B	1206	-	-	6/19/77/77	0/4/4/4
3	Y01	C	1301	-	-	9/19/77/77	0/4/4/4
3	Y01	A	1208	-	-	9/19/77/77	0/4/4/4
3	Y01	A	1206	-	-	13/19/77/77	0/4/4/4
3	Y01	A	1207	-	-	9/19/77/77	0/4/4/4
3	Y01	C	1307	-	-	13/19/77/77	0/4/4/4
3	Y01	C	1302	-	-	12/19/77/77	0/4/4/4
3	Y01	A	1205	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1306	-	-	9/19/77/77	0/4/4/4
3	Y01	C	1308	-	-	11/19/77/77	0/4/4/4
3	Y01	D	1202	-	-	11/19/77/77	0/4/4/4
3	Y01	C	1305	-	-	6/19/77/77	0/4/4/4
3	Y01	B	1204	-	-	12/19/77/77	0/4/4/4
3	Y01	A	1203	-	-	11/19/77/77	0/4/4/4
3	Y01	D	1203	-	-	11/19/77/77	0/4/4/4

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	Y01	CAV-CAZ	-6.90	1.36	1.51
3	B	1204	Y01	CBH-CAZ	-6.54	1.39	1.52
3	A	1203	Y01	CBH-CAZ	-6.54	1.39	1.52
3	C	1306	Y01	CAV-CAZ	-6.17	1.38	1.51
3	C	1303	Y01	CBH-CAZ	-6.12	1.40	1.52
3	B	1205	Y01	CBH-CAZ	-6.01	1.41	1.52
3	C	1306	Y01	CBH-CAZ	-5.98	1.41	1.52
3	C	1308	Y01	CBH-CAZ	-5.90	1.41	1.52
3	C	1301	Y01	CBH-CAZ	-5.85	1.41	1.52
3	A	1207	Y01	CBH-CAZ	-5.81	1.41	1.52
3	A	1205	Y01	CBH-CAZ	-5.78	1.41	1.52
3	B	1203	Y01	CBH-CAZ	-5.70	1.41	1.52
3	B	1206	Y01	CBH-CAZ	-5.70	1.41	1.52
3	A	1204	Y01	CBH-CAZ	-5.68	1.41	1.52
3	C	1305	Y01	CBH-CAZ	-5.64	1.41	1.52
3	D	1203	Y01	CAV-CAZ	-5.63	1.39	1.51
3	C	1303	Y01	CAK-CAI	-5.62	1.38	1.50
3	A	1206	Y01	CBH-CAZ	-5.53	1.41	1.52
3	A	1208	Y01	CBH-CAZ	-5.51	1.42	1.52
3	C	1302	Y01	CBH-CAZ	-5.50	1.42	1.52
3	C	1302	Y01	CAV-CAZ	-5.49	1.39	1.51
3	A	1208	Y01	CAV-CAZ	-5.48	1.39	1.51
3	D	1203	Y01	CBH-CAZ	-5.44	1.42	1.52
3	C	1306	Y01	CAK-CAI	-5.40	1.38	1.50
3	A	1205	Y01	CAV-CAZ	-5.40	1.39	1.51
3	C	1305	Y01	CAV-CAZ	-5.38	1.39	1.51
3	B	1203	Y01	CAV-CAZ	-5.33	1.40	1.51
3	A	1208	Y01	CAK-CAI	-5.33	1.38	1.50
3	C	1302	Y01	CAK-CAI	-5.29	1.38	1.50
3	D	1202	Y01	CBH-CAZ	-5.29	1.42	1.52
3	C	1305	Y01	CAK-CAI	-5.26	1.38	1.50
3	B	1205	Y01	CAV-CAZ	-5.24	1.40	1.51
3	B	1203	Y01	CAK-CAI	-5.15	1.39	1.50
3	C	1304	Y01	CBH-CAZ	-5.11	1.42	1.52
3	A	1206	Y01	CAV-CAZ	-5.08	1.40	1.51
3	C	1307	Y01	CAK-CAI	-5.05	1.39	1.50
3	A	1204	Y01	CAV-CAZ	-5.04	1.40	1.51
3	A	1206	Y01	CAK-CAI	-5.03	1.39	1.50
3	B	1206	Y01	CAV-CAZ	-4.94	1.40	1.51
3	D	1202	Y01	CAV-CAZ	-4.93	1.40	1.51
3	A	1203	Y01	CAV-CAZ	-4.93	1.40	1.51
3	C	1304	Y01	CAV-CAZ	-4.93	1.40	1.51
3	C	1301	Y01	CAV-CAZ	-4.91	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1304	Y01	CAK-CAI	-4.89	1.39	1.50
3	C	1308	Y01	CAV-CAZ	-4.81	1.41	1.51
3	A	1204	Y01	CAK-CAI	-4.81	1.39	1.50
3	A	1207	Y01	CAV-CAZ	-4.72	1.41	1.51
3	D	1202	Y01	CAK-CAI	-4.70	1.40	1.50
3	A	1205	Y01	CAK-CAI	-4.68	1.40	1.50
3	B	1206	Y01	CAK-CAI	-4.67	1.40	1.50
3	C	1307	Y01	CBH-CAZ	-4.65	1.43	1.52
3	B	1204	Y01	CAV-CAZ	-4.57	1.41	1.51
3	B	1205	Y01	CAK-CAI	-4.55	1.40	1.50
3	D	1203	Y01	CAK-CAI	-4.52	1.40	1.50
3	C	1301	Y01	CAK-CAI	-4.35	1.40	1.50
3	A	1207	Y01	CAK-CAI	-4.34	1.40	1.50
3	C	1307	Y01	CBB-CBE	4.33	1.62	1.54
3	C	1308	Y01	CAK-CAI	-4.31	1.40	1.50
3	A	1203	Y01	CAK-CAI	-4.24	1.41	1.50
3	C	1307	Y01	CAV-CAZ	-4.15	1.42	1.51
3	B	1204	Y01	CAK-CAI	-3.99	1.41	1.50
3	C	1302	Y01	CBI-CBE	3.63	1.61	1.55
3	C	1308	Y01	CAI-CAZ	3.54	1.40	1.33
3	B	1204	Y01	CAI-CAZ	3.48	1.40	1.33
3	C	1304	Y01	CAT-CBH	-3.44	1.47	1.54
3	A	1203	Y01	CAI-CAZ	3.41	1.40	1.33
3	B	1205	Y01	CAI-CAZ	3.38	1.40	1.33
3	A	1207	Y01	CAI-CAZ	3.35	1.40	1.33
3	C	1301	Y01	CAI-CAZ	3.33	1.40	1.33
3	A	1206	Y01	CBB-CBE	3.27	1.60	1.54
3	A	1204	Y01	CAI-CAZ	3.24	1.40	1.33
3	D	1203	Y01	CAI-CAZ	3.17	1.40	1.33
3	B	1206	Y01	CAI-CAZ	3.17	1.39	1.33
3	C	1307	Y01	CAI-CAZ	3.16	1.39	1.33
3	A	1205	Y01	CAI-CAZ	3.14	1.39	1.33
3	D	1202	Y01	CAI-CAZ	3.10	1.39	1.33
3	A	1206	Y01	CAI-CAZ	3.09	1.39	1.33
3	C	1304	Y01	CAI-CAZ	3.08	1.39	1.33
3	B	1203	Y01	CAI-CAZ	2.98	1.39	1.33
3	C	1305	Y01	CAI-CAZ	2.95	1.39	1.33
3	A	1205	Y01	CBI-CBG	-2.92	1.49	1.55
3	A	1208	Y01	CAI-CAZ	2.85	1.39	1.33
3	C	1302	Y01	CAI-CAZ	2.84	1.39	1.33
3	C	1303	Y01	CAI-CAZ	2.75	1.39	1.33
3	C	1306	Y01	CAI-CAZ	2.70	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	Y01	CBI-CBG	-2.67	1.49	1.55
3	A	1206	Y01	CBI-CBE	2.62	1.60	1.55
3	C	1302	Y01	CBB-CBE	2.56	1.58	1.54
3	C	1306	Y01	CBH-CBF	-2.54	1.51	1.56
3	C	1304	Y01	CAQ-CBG	-2.53	1.49	1.54
3	C	1306	Y01	OAW-CBC	-2.48	1.40	1.46
3	B	1205	Y01	CBB-CBE	2.48	1.58	1.54
3	A	1208	Y01	CBB-CBE	2.48	1.58	1.54
3	C	1304	Y01	CBH-CBF	-2.47	1.51	1.56
3	C	1302	Y01	CAQ-CBG	-2.38	1.49	1.54
3	B	1206	Y01	CAQ-CBG	-2.35	1.49	1.54
3	A	1205	Y01	CAU-CAS	-2.33	1.48	1.53
3	B	1204	Y01	CBH-CBF	-2.31	1.52	1.56
3	B	1205	Y01	CBI-CBG	-2.26	1.50	1.55
3	A	1203	Y01	CBH-CBF	-2.25	1.52	1.56
3	C	1302	Y01	CAU-CAS	2.25	1.58	1.53
3	C	1307	Y01	CAQ-CBG	-2.23	1.49	1.54
3	A	1205	Y01	CBH-CBF	-2.23	1.52	1.56
3	A	1208	Y01	CAQ-CBG	-2.22	1.49	1.54
3	A	1206	Y01	CAQ-CBG	-2.21	1.49	1.54
3	C	1304	Y01	CBD-CBG	-2.20	1.49	1.53
3	D	1202	Y01	CBH-CBF	-2.20	1.52	1.56
3	B	1206	Y01	CBI-CBG	-2.19	1.50	1.55
3	D	1203	Y01	CBI-CBG	-2.15	1.50	1.55
3	C	1308	Y01	CBB-CBE	2.14	1.58	1.54
3	A	1203	Y01	CBB-CBE	2.14	1.58	1.54
3	B	1204	Y01	CBB-CBE	2.14	1.58	1.54
3	A	1206	Y01	CAU-CAS	2.13	1.57	1.53
3	A	1205	Y01	CAU-CBI	-2.12	1.50	1.54
3	A	1208	Y01	CBI-CBG	-2.05	1.51	1.55
3	D	1203	Y01	CBD-CBG	-2.05	1.49	1.53
3	D	1202	Y01	CAQ-CBG	-2.04	1.50	1.54
3	C	1302	Y01	CBI-CBG	-2.03	1.51	1.55
3	B	1203	Y01	CAQ-CBG	-2.03	1.50	1.54

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1307	Y01	CAV-CAZ-CBH	6.80	125.45	116.42
3	A	1206	Y01	CBH-CBF-CBD	-5.90	103.88	112.73
3	A	1206	Y01	CAQ-CBG-CBD	-5.78	109.56	119.08
3	A	1208	Y01	CAV-CAZ-CBH	5.66	123.94	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1208	Y01	CAQ-CBG-CBD	-5.63	109.81	119.08
3	A	1208	Y01	CBG-CBI-CBE	-5.34	93.74	100.07
3	C	1308	Y01	CBH-CBF-CBD	-5.22	104.91	112.73
3	C	1302	Y01	CAQ-CBG-CBD	-5.21	110.49	119.08
3	A	1206	Y01	CAV-CAZ-CBH	5.21	123.34	116.42
3	C	1307	Y01	CAD-CBH-CBF	-5.17	105.52	111.68
3	C	1307	Y01	CAQ-CBG-CBD	-5.16	110.58	119.08
3	C	1307	Y01	CAV-CAZ-CAI	-5.15	113.19	120.61
3	A	1208	Y01	CBH-CBF-CBD	-5.12	105.05	112.73
3	C	1304	Y01	CAQ-CBG-CBD	-5.10	110.68	119.08
3	C	1304	Y01	CAV-CAZ-CBH	5.08	123.17	116.42
3	A	1205	Y01	CBI-CBE-CBB	-5.07	111.55	119.49
3	A	1208	Y01	CAV-CAZ-CAI	-4.87	113.59	120.61
3	B	1205	Y01	CBH-CBF-CBD	-4.87	105.44	112.73
3	C	1305	Y01	CAQ-CBG-CBD	-4.85	111.10	119.08
3	C	1307	Y01	CAO-CBB-CBE	4.84	120.29	110.28
3	C	1302	Y01	CBG-CBI-CBE	-4.84	94.34	100.07
3	C	1302	Y01	CBH-CBF-CBD	-4.84	105.48	112.73
3	C	1303	Y01	CBI-CBG-CBD	-4.83	107.23	114.38
3	C	1308	Y01	CAC-CBB-CAO	-4.80	102.84	110.36
3	B	1205	Y01	CBI-CBG-CBD	-4.69	107.43	114.38
3	C	1302	Y01	CAV-CAZ-CBH	4.66	122.61	116.42
3	C	1304	Y01	CBG-CBI-CBE	-4.54	94.70	100.07
3	B	1205	Y01	CBI-CBE-CBB	-4.48	112.47	119.49
3	C	1306	Y01	CAV-CAZ-CAI	-4.45	114.20	120.61
3	C	1301	Y01	CAC-CBB-CBE	4.40	119.65	112.92
3	D	1202	Y01	CAQ-CBG-CBD	-4.38	111.87	119.08
3	C	1306	Y01	CAV-CAZ-CBH	4.37	122.22	116.42
3	B	1206	Y01	CAQ-CBG-CBD	-4.36	111.90	119.08
3	C	1304	Y01	CBH-CBF-CBD	-4.35	106.21	112.73
3	A	1204	Y01	CAQ-CBG-CBD	-4.33	111.95	119.08
3	C	1303	Y01	CAP-CBE-CBB	-4.28	105.52	112.15
3	A	1205	Y01	CBC-OAW-CAY	-4.26	107.30	117.79
3	D	1202	Y01	CBH-CBF-CBD	-4.24	106.38	112.73
3	B	1205	Y01	CAP-CBE-CBI	-4.24	98.74	103.84
3	B	1203	Y01	CAQ-CBG-CBD	-4.21	112.15	119.08
3	C	1303	Y01	CAR-CBC-CAV	-4.20	104.73	110.99
3	A	1204	Y01	CBG-CBI-CBE	-4.19	95.11	100.07
3	A	1206	Y01	CAV-CAZ-CAI	-4.19	114.57	120.61
3	C	1303	Y01	CAQ-CBG-CBD	-4.18	112.19	119.08
3	C	1301	Y01	CBH-CBF-CBD	-4.17	106.48	112.73
3	B	1206	Y01	CBH-CBF-CBD	-4.17	106.49	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1307	Y01	CBH-CBF-CBD	-4.15	106.51	112.73
3	B	1203	Y01	CAV-CAZ-CBH	4.08	121.84	116.42
3	C	1305	Y01	CAP-CBE-CBB	-4.06	105.86	112.15
3	C	1307	Y01	CBG-CBI-CBE	-4.05	95.27	100.07
3	C	1308	Y01	CAV-CAZ-CBH	4.04	121.79	116.42
3	C	1307	Y01	CAP-CBE-CBI	-4.03	98.98	103.84
3	C	1308	Y01	CAQ-CBG-CBD	-4.03	112.45	119.08
3	A	1207	Y01	CBH-CBF-CBD	-4.02	106.70	112.73
3	C	1306	Y01	CBG-CBI-CBE	-4.02	95.32	100.07
3	C	1301	Y01	CAQ-CBG-CBD	-3.98	112.53	119.08
3	C	1308	Y01	CBI-CBG-CBD	-3.96	108.51	114.38
3	C	1302	Y01	CAV-CAZ-CAI	-3.96	114.90	120.61
3	C	1305	Y01	CAV-CAZ-CBH	3.96	121.68	116.42
3	C	1305	Y01	CBH-CBF-CBD	-3.94	106.82	112.73
3	A	1204	Y01	CAV-CAZ-CBH	3.93	121.65	116.42
3	C	1301	Y01	CAP-CBE-CBB	-3.92	106.08	112.15
3	B	1206	Y01	CAV-CAZ-CBH	3.91	121.62	116.42
3	C	1308	Y01	CAS-CBF-CBH	-3.90	107.95	113.08
3	C	1301	Y01	CBI-CBG-CBD	-3.89	108.62	114.38
3	C	1306	Y01	CBC-OAW-CAY	-3.89	108.22	117.79
3	A	1206	Y01	CBG-CBI-CBE	-3.87	95.49	100.07
3	C	1303	Y01	CAV-CAZ-CAI	-3.87	115.03	120.61
3	C	1302	Y01	CAP-CBE-CBB	-3.86	106.17	112.15
3	A	1207	Y01	CAQ-CBG-CBD	-3.84	112.76	119.08
3	B	1206	Y01	CBI-CBG-CBD	-3.83	108.71	114.38
3	C	1307	Y01	CBI-CBE-CBB	3.82	125.46	119.49
3	C	1308	Y01	CAC-CBB-CBE	3.81	118.76	112.92
3	A	1205	Y01	CAS-CBF-CBH	-3.80	108.08	113.08
3	C	1303	Y01	CBH-CBF-CBD	-3.75	107.11	112.73
3	D	1203	Y01	CBI-CBE-CBB	-3.71	113.67	119.49
3	B	1205	Y01	CAQ-CBG-CBD	-3.71	112.98	119.08
3	D	1202	Y01	CAV-CAZ-CBH	3.70	121.34	116.42
3	C	1301	Y01	CAV-CAZ-CBH	3.69	121.32	116.42
3	A	1205	Y01	CBH-CBF-CBD	-3.68	107.22	112.73
3	D	1202	Y01	CAP-CBE-CBB	-3.66	106.47	112.15
3	A	1207	Y01	CAV-CAZ-CBH	3.66	121.28	116.42
3	D	1202	Y01	CBI-CBG-CBD	-3.65	108.97	114.38
3	C	1307	Y01	CAT-CAR-CBC	3.63	116.51	110.33
3	D	1202	Y01	CAT-CAR-CBC	-3.60	104.18	110.33
3	C	1304	Y01	CAV-CAZ-CAI	-3.60	115.43	120.61
3	A	1207	Y01	CAS-CBF-CBH	-3.58	108.36	113.08
3	C	1304	Y01	CAC-CBB-CAO	-3.56	104.79	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1205	Y01	CAV-CAZ-CBH	3.55	121.13	116.42
3	A	1207	Y01	CBI-CBG-CBD	-3.50	109.19	114.38
3	C	1302	Y01	CBI-CBE-CBB	3.49	124.96	119.49
3	B	1205	Y01	CAV-CAZ-CBH	3.49	121.05	116.42
3	B	1203	Y01	CAV-CAZ-CAI	-3.48	115.60	120.61
3	C	1305	Y01	CAV-CAZ-CAI	-3.47	115.61	120.61
3	D	1203	Y01	CAQ-CBG-CBD	-3.47	113.37	119.08
3	C	1308	Y01	CAP-CBE-CBI	-3.47	99.66	103.84
3	B	1205	Y01	CAS-CBF-CBH	-3.44	108.54	113.08
3	C	1301	Y01	CAS-CBF-CBH	-3.44	108.55	113.08
3	A	1206	Y01	CAD-CBH-CBF	-3.42	107.60	111.68
3	A	1205	Y01	CBI-CBG-CBD	-3.42	109.31	114.38
3	A	1206	Y01	CBC-CAV-CAZ	3.42	116.83	111.52
3	C	1304	Y01	CAP-CBE-CBI	-3.40	99.75	103.84
3	B	1204	Y01	CAP-CBE-CBB	-3.38	106.91	112.15
3	A	1204	Y01	CBH-CBF-CBD	-3.37	107.68	112.73
3	C	1306	Y01	CAQ-CBG-CBD	-3.35	113.56	119.08
3	C	1304	Y01	CAR-CBC-CAV	-3.34	106.00	110.99
3	A	1203	Y01	CAP-CBE-CBB	-3.34	106.97	112.15
3	A	1208	Y01	CAO-CBB-CBE	3.33	117.17	110.28
3	A	1208	Y01	CAD-CBH-CBF	-3.33	107.71	111.68
3	A	1208	Y01	CBI-CBE-CBB	3.32	124.68	119.49
3	C	1307	Y01	CBC-CAV-CAZ	3.22	116.51	111.52
3	C	1307	Y01	CAD-CBH-CAZ	3.21	113.54	108.34
3	A	1204	Y01	CAV-CAZ-CAI	-3.21	115.98	120.61
3	C	1308	Y01	CBC-CAV-CAZ	3.21	116.50	111.52
3	D	1202	Y01	CAS-CBF-CBH	-3.20	108.86	113.08
3	B	1204	Y01	CAV-CAZ-CBH	3.19	120.66	116.42
3	A	1207	Y01	CAP-CBE-CBB	-3.18	107.22	112.15
3	C	1305	Y01	CBG-CBI-CBE	-3.18	96.31	100.07
3	A	1204	Y01	CAP-CBE-CBI	-3.17	100.02	103.84
3	A	1208	Y01	CAP-CBE-CBB	-3.16	107.26	112.15
3	B	1203	Y01	CAC-CBB-CAO	-3.15	105.42	110.36
3	C	1306	Y01	CAK-CBD-CBG	-3.15	106.34	110.91
3	B	1206	Y01	CAS-CBF-CBH	-3.13	108.95	113.08
3	B	1206	Y01	CBI-CBE-CBB	-3.13	114.58	119.49
3	B	1203	Y01	CBG-CBI-CBE	-3.13	96.37	100.07
3	A	1203	Y01	CAV-CAZ-CBH	3.10	120.54	116.42
3	C	1306	Y01	CAP-CBE-CBB	-3.09	107.37	112.15
3	B	1205	Y01	CAO-CBB-CBE	3.08	116.66	110.28
3	A	1203	Y01	CBG-CBI-CBE	-3.07	96.43	100.07
3	C	1303	Y01	CAC-CBB-CAO	-3.07	105.55	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1306	Y01	CAC-CBB-CAO	-3.07	105.56	110.36
3	A	1205	Y01	CAP-CBE-CBI	-3.05	100.17	103.84
3	A	1206	Y01	CBF-CBD-CBG	3.04	113.16	109.09
3	B	1206	Y01	CAP-CBE-CBB	-3.03	107.46	112.15
3	C	1303	Y01	CAE-CBI-CAU	3.02	115.35	110.59
3	B	1203	Y01	CBH-CBF-CBD	-3.01	108.22	112.73
3	C	1304	Y01	CAT-CAR-CBC	-2.99	105.23	110.33
3	C	1301	Y01	CAC-CBB-CAO	-2.95	105.73	110.36
3	C	1304	Y01	CBC-OAW-CAY	-2.95	110.54	117.79
3	A	1207	Y01	CAP-CBE-CBI	-2.94	100.30	103.84
3	B	1204	Y01	CAP-CBE-CBI	-2.93	100.31	103.84
3	B	1205	Y01	CAV-CAZ-CAI	-2.93	116.38	120.61
3	A	1203	Y01	CBC-OAW-CAY	-2.92	110.61	117.79
3	A	1206	Y01	CBI-CBE-CBB	2.91	124.05	119.49
3	B	1206	Y01	CAV-CAZ-CAI	-2.90	116.43	120.61
3	B	1205	Y01	CAD-CBH-CBF	-2.89	108.24	111.68
3	A	1206	Y01	CBI-CBG-CBD	-2.88	110.11	114.38
3	A	1203	Y01	CAP-CBE-CBI	-2.87	100.38	103.84
3	B	1203	Y01	CAP-CBE-CBI	-2.87	100.39	103.84
3	C	1308	Y01	CAV-CAZ-CAI	-2.86	116.49	120.61
3	A	1208	Y01	CAJ-CAO-CBB	-2.84	106.86	115.03
3	C	1307	Y01	CBC-OAW-CAY	-2.84	110.81	117.79
3	A	1205	Y01	CAV-CAZ-CAI	-2.81	116.56	120.61
3	C	1308	Y01	CAP-CBE-CBB	-2.80	107.80	112.15
3	A	1208	Y01	CBC-CAV-CAZ	2.80	115.86	111.52
3	D	1202	Y01	CAV-CAZ-CAI	-2.79	116.58	120.61
3	C	1305	Y01	CAC-CBB-CAO	-2.79	105.99	110.36
3	C	1308	Y01	CAE-CBI-CAU	2.78	114.99	110.59
3	B	1205	Y01	CAE-CBI-CBE	-2.78	106.53	111.71
3	C	1302	Y01	CAD-CBH-CBF	-2.77	108.38	111.68
3	D	1203	Y01	CBF-CBD-CBG	-2.77	105.39	109.09
3	B	1204	Y01	CAS-CBF-CBH	-2.76	109.44	113.08
3	C	1301	Y01	CAV-CAZ-CAI	-2.75	116.65	120.61
3	C	1304	Y01	CAK-CBD-CBG	-2.73	106.95	110.91
3	C	1303	Y01	CAP-CBE-CBI	-2.73	100.56	103.84
3	B	1206	Y01	CAP-CBE-CBI	-2.73	100.56	103.84
3	D	1203	Y01	CBI-CBG-CBD	-2.72	110.35	114.38
3	C	1306	Y01	CAU-CAS-CBF	-2.70	108.44	113.11
3	A	1204	Y01	CAP-CBE-CBB	-2.70	107.97	112.15
3	D	1203	Y01	CBG-CBI-CBE	-2.68	96.89	100.07
3	A	1204	Y01	CAD-CBH-CBF	-2.68	108.49	111.68
3	A	1206	Y01	OAW-CBC-CAV	-2.68	102.64	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1308	Y01	CAD-CBH-CBF	-2.66	108.51	111.68
3	C	1305	Y01	CBI-CBG-CBD	-2.65	110.46	114.38
3	C	1301	Y01	CAE-CBI-CAU	2.65	114.77	110.59
3	B	1205	Y01	CBF-CBD-CBG	2.64	112.62	109.09
3	A	1206	Y01	CAO-CBB-CBE	2.63	115.71	110.28
3	A	1203	Y01	CAS-CBF-CBH	-2.62	109.62	113.08
3	D	1203	Y01	CAS-CAU-CBI	-2.62	108.28	112.78
3	C	1305	Y01	CAR-CBC-CAV	-2.61	107.10	110.99
3	C	1303	Y01	CBD-CAK-CAI	-2.57	109.05	112.73
3	B	1205	Y01	CBD-CAK-CAI	-2.56	109.06	112.73
3	A	1204	Y01	CAC-CBB-CAO	-2.55	106.36	110.36
3	B	1203	Y01	CBC-OAW-CAY	-2.50	111.62	117.79
3	A	1203	Y01	CAQ-CBG-CBD	-2.50	114.96	119.08
3	B	1205	Y01	CAE-CBI-CAU	2.49	114.52	110.59
3	D	1203	Y01	CAP-CBE-CBI	-2.49	100.85	103.84
3	C	1302	Y01	CAP-CAQ-CBG	-2.49	100.21	105.13
3	D	1202	Y01	CAC-CBB-CAO	-2.48	106.48	110.36
3	A	1205	Y01	CAR-CBC-CAV	-2.46	107.32	110.99
3	A	1206	Y01	CBC-OAW-CAY	2.45	123.82	117.79
3	C	1302	Y01	CAE-CBI-CBE	2.44	116.27	111.71
3	D	1203	Y01	CBF-CBH-CAZ	2.43	113.46	109.65
3	D	1203	Y01	CAC-CBB-CBE	-2.42	109.21	112.92
3	A	1207	Y01	CAV-CAZ-CAI	-2.42	117.12	120.61
3	C	1306	Y01	CBF-CBD-CBG	-2.42	105.86	109.09
3	D	1203	Y01	CAU-CAS-CBF	-2.40	108.96	113.11
3	A	1206	Y01	CAJ-CAN-CBA	-2.40	104.68	115.98
3	B	1204	Y01	CBG-CBI-CBE	-2.39	97.24	100.07
3	A	1207	Y01	OAW-CBC-CAV	2.39	113.01	108.12
3	B	1203	Y01	CBI-CBG-CBD	-2.38	110.86	114.38
3	C	1301	Y01	CAD-CBH-CBF	-2.37	108.85	111.68
3	C	1306	Y01	CAD-CBH-CBF	-2.37	108.86	111.68
3	C	1308	Y01	CBF-CBD-CBG	2.36	112.25	109.09
3	B	1204	Y01	CAQ-CBG-CBD	-2.36	115.20	119.08
3	C	1306	Y01	CBI-CBG-CBD	-2.35	110.89	114.38
3	C	1306	Y01	CAP-CAQ-CBG	-2.35	100.47	105.13
3	A	1205	Y01	CAC-CBB-CBE	-2.35	109.33	112.92
3	A	1204	Y01	CBC-OAW-CAY	-2.33	112.05	117.79
3	D	1203	Y01	CBC-OAW-CAY	-2.30	112.12	117.79
3	A	1203	Y01	CAU-CAS-CBF	-2.30	109.12	113.11
3	C	1306	Y01	CAS-CBF-CBD	-2.30	108.44	111.75
3	A	1205	Y01	CAQ-CBG-CBD	-2.30	115.30	119.08
3	B	1204	Y01	CBC-CAV-CAZ	2.28	115.07	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1307	Y01	CBI-CBG-CBD	-2.27	111.02	114.38
3	C	1304	Y01	CAP-CAQ-CBG	-2.27	100.64	105.13
3	C	1301	Y01	CAP-CBE-CBI	-2.26	101.12	103.84
3	B	1204	Y01	CAU-CAS-CBF	-2.26	109.20	113.11
3	A	1208	Y01	CBF-CBD-CBG	2.24	112.09	109.09
3	C	1304	Y01	CAD-CBH-CAT	-2.24	105.89	109.43
3	A	1207	Y01	CAD-CBH-CBF	-2.24	109.01	111.68
3	B	1206	Y01	CAD-CBH-CBF	-2.24	109.01	111.68
3	A	1206	Y01	CAP-CBE-CBB	-2.22	108.71	112.15
3	D	1202	Y01	CAC-CBB-CBE	2.22	116.32	112.92
3	C	1303	Y01	CBC-CAV-CAZ	-2.22	108.08	111.52
3	C	1302	Y01	CAM-CAL-CAX	-2.20	108.86	113.60
3	D	1203	Y01	CAK-CBD-CBG	-2.20	107.72	110.91
3	A	1207	Y01	CAC-CBB-CAO	-2.20	106.92	110.36
3	B	1204	Y01	CAC-CBB-CBE	2.19	116.28	112.92
3	A	1207	Y01	OAW-CAY-CAM	2.19	116.21	111.50
3	C	1306	Y01	CAM-CAL-CAX	-2.18	108.90	113.60
3	B	1203	Y01	CBI-CBE-CBB	-2.18	116.07	119.49
3	A	1206	Y01	CBD-CAK-CAI	-2.18	109.60	112.73
3	D	1203	Y01	CAD-CBH-CBF	-2.18	109.08	111.68
3	B	1205	Y01	CBG-CBI-CBE	2.17	102.64	100.07
3	C	1306	Y01	OAW-CBC-CAV	-2.17	103.68	108.12
3	C	1306	Y01	OAF-CAX-CAL	-2.16	116.13	123.08
3	A	1206	Y01	CAR-CAT-CBH	-2.16	108.06	112.74
3	A	1204	Y01	CAS-CBF-CBH	-2.14	110.26	113.08
3	C	1303	Y01	CAV-CAZ-CBH	2.14	119.26	116.42
3	C	1302	Y01	CBI-CBG-CBD	-2.13	111.22	114.38
3	C	1305	Y01	CAK-CBD-CBG	-2.13	107.82	110.91
3	B	1206	Y01	CAJ-CAO-CBB	-2.13	108.92	115.03
3	D	1202	Y01	CAT-CBH-CAZ	2.12	112.64	108.75
3	C	1305	Y01	CAD-CBH-CBF	-2.11	109.16	111.68
3	C	1305	Y01	CAP-CAQ-CBG	-2.11	100.95	105.13
3	B	1203	Y01	CAD-CBH-CBF	-2.10	109.17	111.68
3	D	1203	Y01	CAV-CAZ-CAI	-2.10	117.58	120.61
3	A	1207	Y01	CBI-CBE-CBB	-2.10	116.19	119.49
3	D	1203	Y01	CBD-CAK-CAI	2.10	115.75	112.73
3	C	1301	Y01	CAO-CBB-CBE	-2.10	105.95	110.28
3	B	1205	Y01	CAR-CBC-CAV	-2.09	107.86	110.99
3	C	1303	Y01	CAS-CBF-CBH	-2.09	110.33	113.08
3	A	1208	Y01	CAK-CBD-CBG	-2.08	107.89	110.91
3	A	1206	Y01	CAU-CBI-CBG	-2.08	104.05	107.27
3	C	1308	Y01	CBD-CAK-CAI	-2.08	109.75	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1202	Y01	CAP-CAQ-CBG	-2.07	101.02	105.13
3	A	1203	Y01	CAV-CAZ-CAI	-2.07	117.63	120.61
3	C	1303	Y01	OAF-CAX-CAL	-2.07	116.44	123.08
3	D	1202	Y01	CAE-CBI-CAU	2.07	113.85	110.59
3	B	1205	Y01	CAU-CBI-CBG	-2.05	104.08	107.27
3	C	1308	Y01	CAR-CAT-CBH	-2.05	108.30	112.74
3	C	1303	Y01	CAC-CBB-CBE	2.04	116.05	112.92
3	C	1306	Y01	CAP-CBE-CBI	-2.04	101.39	103.84
3	C	1308	Y01	CAM-CAL-CAX	-2.03	109.23	113.60
3	C	1306	Y01	CAS-CBF-CBH	-2.03	110.41	113.08
3	C	1302	Y01	CAS-CBF-CBD	-2.03	108.83	111.75
3	A	1205	Y01	CAT-CAR-CBC	-2.02	106.88	110.33
3	B	1203	Y01	CAS-CBF-CBH	-2.02	110.42	113.08
3	A	1204	Y01	CAM-CAL-CAX	-2.02	109.26	113.60
3	A	1203	Y01	CAC-CBB-CBE	2.01	116.00	112.92
3	B	1203	Y01	CAK-CBD-CBG	-2.00	108.01	110.91

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1204	Y01	CAM-CAY-OAW-CBC
3	A	1206	Y01	CAO-CBB-CBE-CBI
3	A	1207	Y01	CAV-CBC-OAW-CAY
3	A	1207	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAO-CBB-CBE-CBI
3	B	1204	Y01	CAR-CBC-OAW-CAY
3	B	1204	Y01	CAM-CAY-OAW-CBC
3	B	1206	Y01	CAR-CBC-OAW-CAY
3	C	1301	Y01	CAM-CAY-OAW-CBC
3	C	1302	Y01	CAV-CBC-OAW-CAY
3	C	1303	Y01	CAM-CAY-OAW-CBC
3	C	1307	Y01	CAO-CBB-CBE-CAP
3	C	1307	Y01	CAO-CBB-CBE-CBI
3	C	1307	Y01	CAC-CBB-CBE-CAP
3	C	1307	Y01	CAC-CBB-CBE-CBI
3	C	1307	Y01	CAM-CAY-OAW-CBC
3	C	1308	Y01	CAM-CAY-OAW-CBC
3	D	1202	Y01	OAG-CAY-OAW-CBC
3	D	1203	Y01	OAG-CAY-OAW-CBC
3	A	1205	Y01	CAC-CBB-CBE-CBI
3	A	1204	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	B	1204	Y01	OAG-CAY-OAW-CBC
3	B	1205	Y01	OAG-CAY-OAW-CBC
3	B	1206	Y01	OAG-CAY-OAW-CBC
3	C	1301	Y01	OAG-CAY-OAW-CBC
3	C	1303	Y01	OAG-CAY-OAW-CBC
3	C	1307	Y01	OAG-CAY-OAW-CBC
3	B	1206	Y01	CAM-CAY-OAW-CBC
3	D	1202	Y01	CAM-CAY-OAW-CBC
3	D	1203	Y01	CAM-CAY-OAW-CBC
3	C	1307	Y01	CAJ-CAO-CBB-CAC
3	A	1205	Y01	CAC-CBB-CBE-CAP
3	A	1208	Y01	CAO-CBB-CBE-CAP
3	A	1205	Y01	CAO-CBB-CBE-CBI
3	B	1205	Y01	CAO-CBB-CBE-CBI
3	A	1207	Y01	OAG-CAY-OAW-CBC
3	C	1304	Y01	OAG-CAY-OAW-CBC
3	C	1308	Y01	OAG-CAY-OAW-CBC
3	A	1206	Y01	CAC-CBB-CBE-CAP
3	A	1208	Y01	CAC-CBB-CBE-CAP
3	C	1304	Y01	CAJ-CAO-CBB-CBE
3	B	1205	Y01	CAM-CAY-OAW-CBC
3	C	1304	Y01	CAM-CAY-OAW-CBC
3	D	1202	Y01	CAX-CAL-CAM-CAY
3	A	1207	Y01	CAJ-CAO-CBB-CBE
3	B	1203	Y01	CAJ-CAO-CBB-CBE
3	C	1301	Y01	CAJ-CAO-CBB-CBE
3	C	1306	Y01	CAJ-CAO-CBB-CBE
3	C	1302	Y01	OAG-CAY-OAW-CBC
3	B	1203	Y01	CAJ-CAO-CBB-CAC
3	C	1304	Y01	CAJ-CAO-CBB-CAC
3	C	1306	Y01	CAJ-CAO-CBB-CAC
3	A	1206	Y01	CAO-CBB-CBE-CAP
3	C	1302	Y01	CAO-CBB-CBE-CBI
3	C	1308	Y01	CAJ-CAO-CBB-CBE
3	A	1206	Y01	CAJ-CAO-CBB-CAC
3	A	1207	Y01	CAJ-CAO-CBB-CAC
3	B	1204	Y01	CAJ-CAO-CBB-CAC
3	C	1301	Y01	CAJ-CAO-CBB-CAC
3	C	1308	Y01	CAJ-CAO-CBB-CAC
3	C	1302	Y01	CAC-CBB-CBE-CAP
3	C	1302	Y01	CAM-CAY-OAW-CBC
3	B	1204	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
3	B	1204	Y01	CAN-CAJ-CAO-CBB
3	C	1307	Y01	CAJ-CAO-CBB-CBE
3	A	1203	Y01	CAO-CAJ-CAN-CBA
3	A	1203	Y01	CAN-CAJ-CAO-CBB
3	B	1206	Y01	CAN-CAJ-CAO-CBB
3	C	1304	Y01	CAN-CAJ-CAO-CBB
3	A	1205	Y01	CAO-CBB-CBE-CAP
3	A	1205	Y01	CAN-CAJ-CAO-CBB
3	C	1308	Y01	CAO-CAJ-CAN-CBA
3	C	1308	Y01	CAN-CAJ-CAO-CBB
3	C	1303	Y01	CAN-CAJ-CAO-CBB
3	D	1202	Y01	CAN-CAJ-CAO-CBB
3	C	1302	Y01	CAO-CBB-CBE-CAP
3	A	1203	Y01	CAX-CAL-CAM-CAY
3	B	1205	Y01	CAX-CAL-CAM-CAY
3	C	1307	Y01	CAX-CAL-CAM-CAY
3	C	1306	Y01	CAM-CAY-OAW-CBC
3	B	1203	Y01	CAO-CAJ-CAN-CBA
3	B	1205	Y01	CAN-CAJ-CAO-CBB
3	C	1303	Y01	CAO-CAJ-CAN-CBA
3	C	1304	Y01	CAC-CBB-CBE-CBI
3	C	1306	Y01	OAG-CAY-OAW-CBC
3	A	1203	Y01	CAJ-CAO-CBB-CAC
3	A	1203	Y01	CAJ-CAN-CBA-CAB
3	B	1204	Y01	CAJ-CAN-CBA-CAB
3	A	1203	Y01	CAM-CAY-OAW-CBC
3	C	1305	Y01	CAJ-CAO-CBB-CBE
3	B	1203	Y01	CAJ-CAN-CBA-CAA
3	A	1203	Y01	OAG-CAY-OAW-CBC
3	C	1303	Y01	CAJ-CAO-CBB-CBE
3	A	1208	Y01	CAX-CAL-CAM-CAY
3	C	1305	Y01	CAX-CAL-CAM-CAY
3	A	1206	Y01	CAJ-CAN-CBA-CAA
3	A	1206	Y01	CAJ-CAN-CBA-CAB
3	B	1203	Y01	CAJ-CAN-CBA-CAB
3	C	1307	Y01	CAN-CAJ-CAO-CBB
3	D	1203	Y01	CAJ-CAO-CBB-CAC
3	B	1205	Y01	CAJ-CAN-CBA-CAB
3	A	1206	Y01	CAC-CBB-CBE-CBI
3	C	1301	Y01	CAX-CAL-CAM-CAY
3	A	1206	Y01	OAG-CAY-OAW-CBC
3	C	1305	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	B	1204	Y01	CAJ-CAN-CBA-CAA
3	B	1205	Y01	CAC-CBB-CBE-CBI
3	A	1203	Y01	CAJ-CAN-CBA-CAA
3	A	1208	Y01	CAC-CBB-CBE-CBI
3	C	1308	Y01	CAO-CBB-CBE-CAP
3	D	1203	Y01	CAO-CBB-CBE-CAP
3	A	1205	Y01	CAM-CAY-OAW-CBC
3	A	1206	Y01	CAM-CAY-OAW-CBC
3	A	1205	Y01	OAG-CAY-OAW-CBC
3	A	1205	Y01	CAJ-CAN-CBA-CAA
3	C	1307	Y01	CAJ-CAN-CBA-CAA
3	D	1202	Y01	CAJ-CAN-CBA-CAA
3	B	1203	Y01	CAC-CBB-CBE-CBI
3	A	1206	Y01	CAO-CAJ-CAN-CBA
3	B	1203	Y01	CAM-CAY-OAW-CBC
3	A	1205	Y01	CAO-CAJ-CAN-CBA
3	C	1307	Y01	CAJ-CAN-CBA-CAB
3	D	1202	Y01	CAO-CAJ-CAN-CBA
3	C	1303	Y01	CAJ-CAO-CBB-CAC
3	C	1302	Y01	CAJ-CAN-CBA-CAB
3	C	1302	Y01	CAO-CAJ-CAN-CBA
3	C	1302	Y01	CAJ-CAN-CBA-CAA
3	C	1304	Y01	CAO-CBB-CBE-CBI
3	B	1203	Y01	OAG-CAY-OAW-CBC
3	D	1202	Y01	CAJ-CAN-CBA-CAB
3	A	1205	Y01	CAJ-CAN-CBA-CAB
3	B	1205	Y01	CAJ-CAN-CBA-CAA
3	C	1306	Y01	CAJ-CAN-CBA-CAB
3	C	1301	Y01	CAO-CBB-CBE-CAP
3	B	1203	Y01	CAO-CBB-CBE-CBI
3	A	1208	Y01	CAO-CAJ-CAN-CBA
3	C	1306	Y01	CAO-CAJ-CAN-CBA
3	C	1306	Y01	CAJ-CAN-CBA-CAA
3	C	1302	Y01	CAC-CBB-CBE-CBI
3	B	1205	Y01	CAO-CAJ-CAN-CBA
3	C	1305	Y01	OAG-CAY-OAW-CBC
3	C	1305	Y01	CAR-CBC-OAW-CAY
3	B	1205	Y01	CAO-CBB-CBE-CAP
3	B	1203	Y01	CAN-CAJ-CAO-CBB
3	A	1207	Y01	CAO-CAJ-CAN-CBA
3	C	1304	Y01	CAJ-CAN-CBA-CAB
3	B	1206	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	C	1303	Y01	CAX-CAL-CAM-CAY
3	C	1304	Y01	CAJ-CAN-CBA-CAA
3	C	1304	Y01	CAC-CBB-CBE-CAP
3	B	1204	Y01	CAX-CAL-CAM-CAY
3	D	1203	Y01	CAJ-CAN-CBA-CAA
3	D	1203	Y01	CAJ-CAN-CBA-CAB
3	A	1204	Y01	CAM-CAL-CAX-OAF
3	D	1202	Y01	CAM-CAL-CAX-OAH
3	D	1203	Y01	CAJ-CAO-CBB-CBE
3	A	1203	Y01	CAV-CBC-OAW-CAY
3	B	1204	Y01	CAV-CBC-OAW-CAY
3	B	1206	Y01	CAO-CBB-CBE-CBI
3	B	1205	Y01	CAM-CAL-CAX-OAF
3	D	1203	Y01	CAM-CAL-CAX-OAH
3	A	1204	Y01	CAM-CAL-CAX-OAH
3	C	1308	Y01	CAM-CAL-CAX-OAF
3	D	1203	Y01	CAM-CAL-CAX-OAF
3	A	1205	Y01	CAX-CAL-CAM-CAY
3	B	1204	Y01	CAM-CAL-CAX-OAH
3	C	1301	Y01	CAN-CAJ-CAO-CBB
3	D	1203	Y01	CAN-CAJ-CAO-CBB
3	C	1302	Y01	CAM-CAL-CAX-OAH
3	B	1204	Y01	CAM-CAL-CAX-OAF
3	D	1202	Y01	CAM-CAL-CAX-OAF
3	C	1308	Y01	CAM-CAL-CAX-OAH
3	C	1302	Y01	CAM-CAL-CAX-OAF
3	C	1301	Y01	CAM-CAL-CAX-OAH
3	A	1203	Y01	CAM-CAL-CAX-OAH
3	A	1207	Y01	CAN-CAJ-CAO-CBB
3	B	1205	Y01	CAM-CAL-CAX-OAH
3	A	1203	Y01	CAM-CAL-CAX-OAF
3	C	1301	Y01	CAM-CAL-CAX-OAF
3	A	1204	Y01	CAN-CAJ-CAO-CBB
3	A	1206	Y01	CAL-CAM-CAY-OAW
3	B	1205	Y01	CAL-CAM-CAY-OAW
3	C	1308	Y01	CAL-CAM-CAY-OAW
3	A	1207	Y01	CAM-CAL-CAX-OAH
3	A	1207	Y01	CAM-CAL-CAX-OAF
3	C	1304	Y01	CAL-CAM-CAY-OAW
3	C	1305	Y01	CAM-CAY-OAW-CBC
3	A	1208	Y01	CAM-CAL-CAX-OAF
3	D	1203	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
3	B	1205	Y01	CAL-CAM-CAY-OAG
3	A	1206	Y01	CAL-CAM-CAY-OAG
3	A	1206	Y01	CAN-CAJ-CAO-CBB
3	C	1308	Y01	CAL-CAM-CAY-OAG
3	D	1202	Y01	CAL-CAM-CAY-OAG
3	C	1304	Y01	CAO-CAJ-CAN-CBA
3	C	1304	Y01	CAL-CAM-CAY-OAG
3	A	1208	Y01	CAN-CAJ-CAO-CBB
3	C	1306	Y01	CAL-CAM-CAY-OAW
3	D	1202	Y01	CAL-CAM-CAY-OAW
3	A	1208	Y01	CAM-CAL-CAX-OAH
3	C	1306	Y01	CAL-CAM-CAY-OAG
3	C	1307	Y01	CAM-CAL-CAX-OAH

There are no ring outliers.

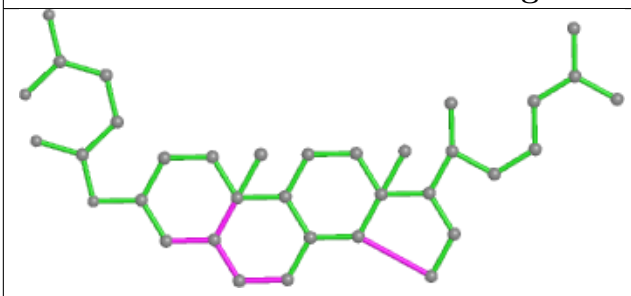
19 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1203	Y01	1	0
3	C	1304	Y01	2	0
3	B	1205	Y01	2	0
3	C	1303	Y01	2	0
3	B	1206	Y01	3	0
3	C	1301	Y01	1	0
3	A	1208	Y01	6	0
3	A	1206	Y01	4	0
3	A	1207	Y01	3	0
3	C	1307	Y01	2	0
3	C	1302	Y01	3	0
3	A	1205	Y01	5	0
3	C	1306	Y01	1	0
3	C	1308	Y01	8	0
3	D	1202	Y01	2	0
3	C	1305	Y01	1	0
3	B	1204	Y01	4	0
3	A	1203	Y01	3	0
3	D	1203	Y01	22	0

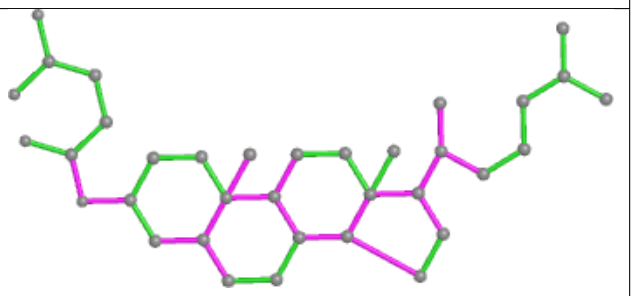
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

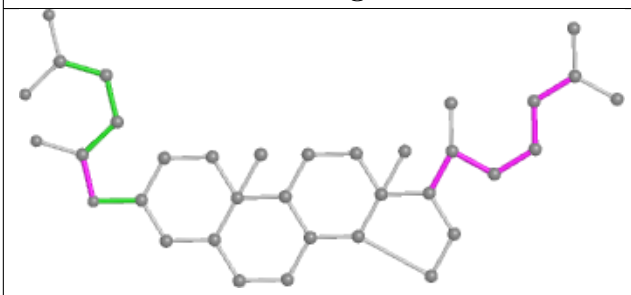
Ligand Y01 B 1203



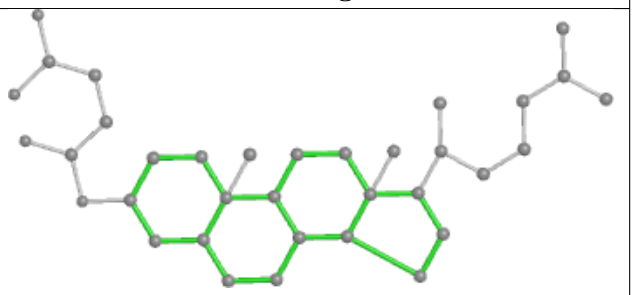
Bond lengths



Bond angles

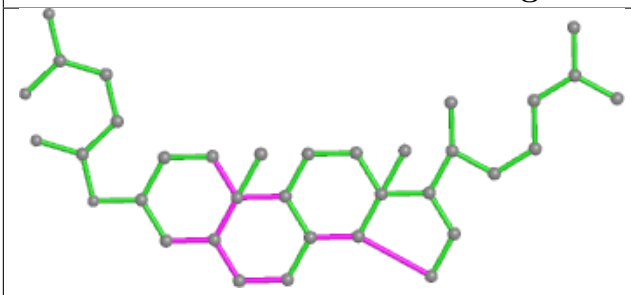


Torsions

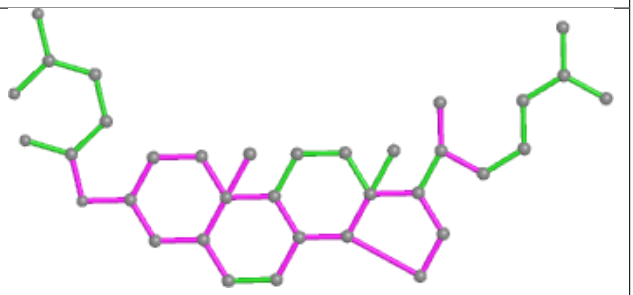


Rings

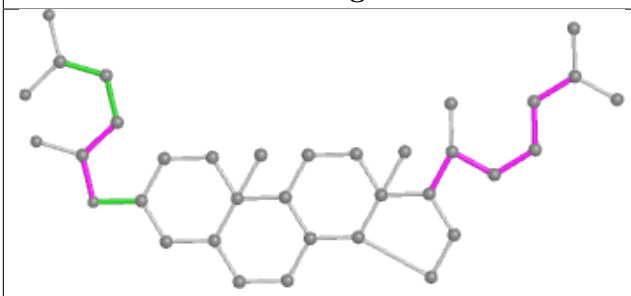
Ligand Y01 C 1304



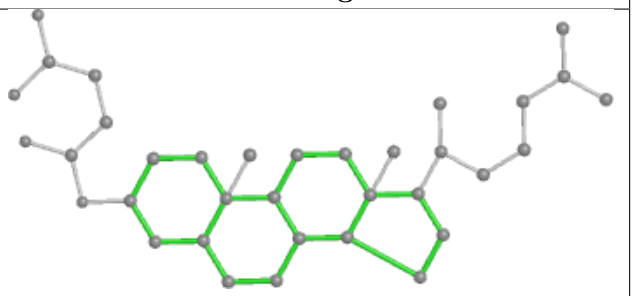
Bond lengths



Bond angles

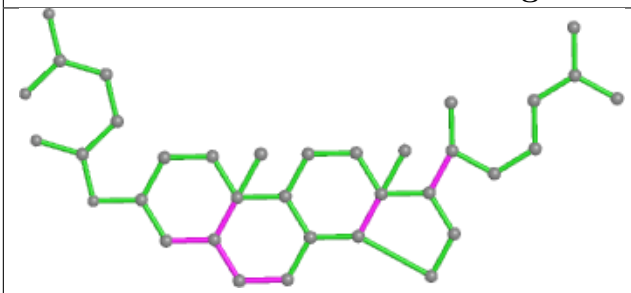


Torsions

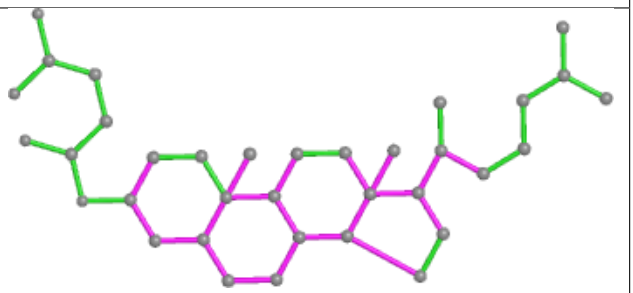


Rings

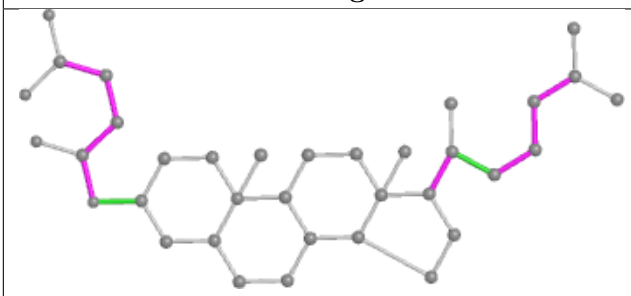
Ligand Y01 B 1205



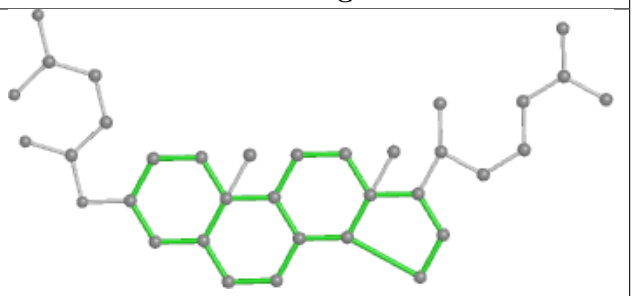
Bond lengths



Bond angles

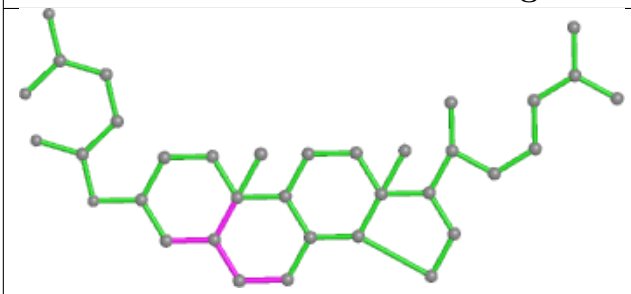


Torsions

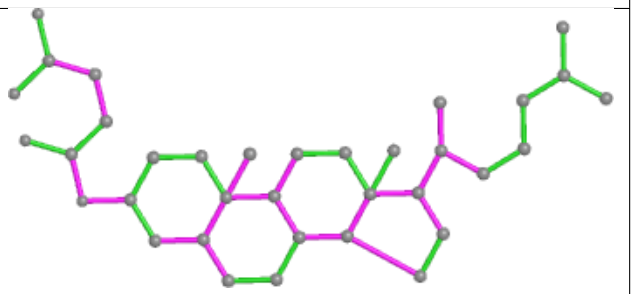


Rings

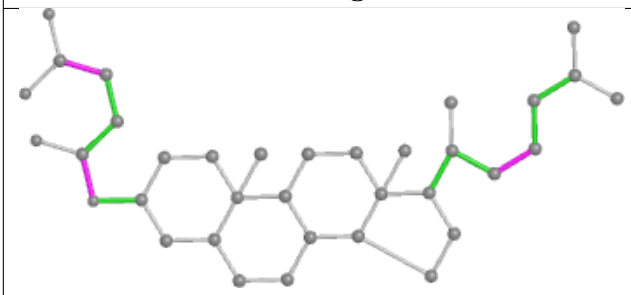
Ligand Y01 A 1204



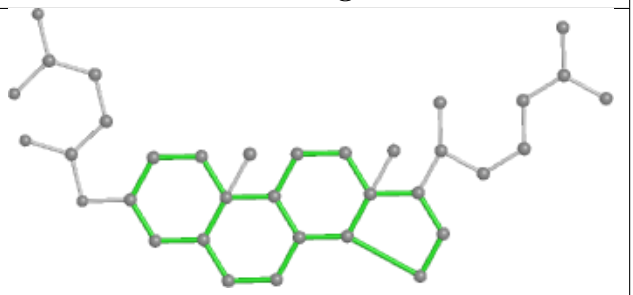
Bond lengths



Bond angles

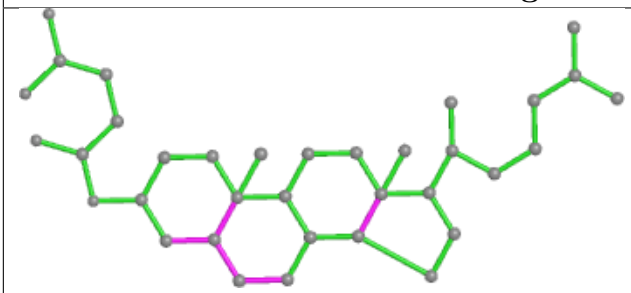


Torsions

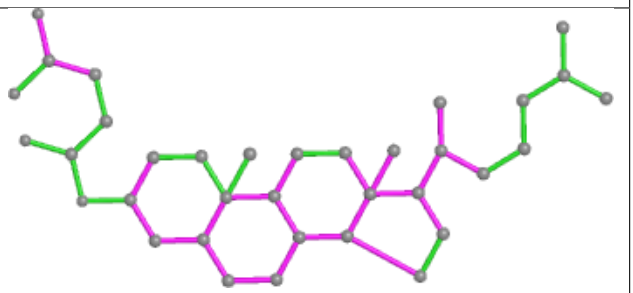


Rings

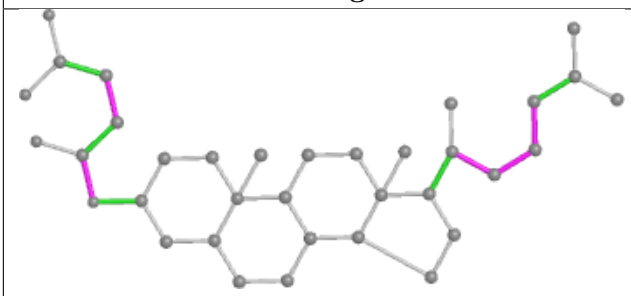
Ligand Y01 C 1303



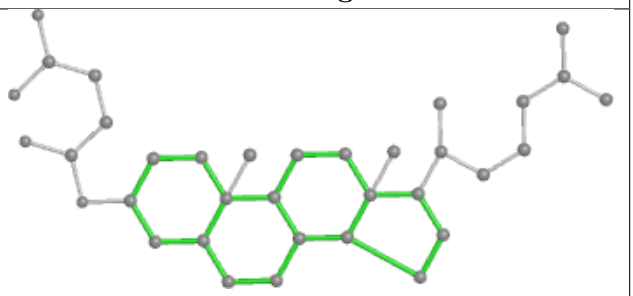
Bond lengths



Bond angles

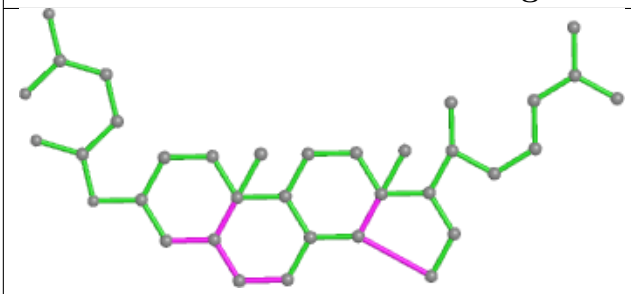


Torsions

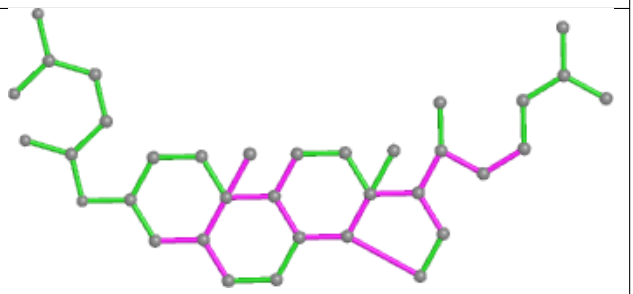


Rings

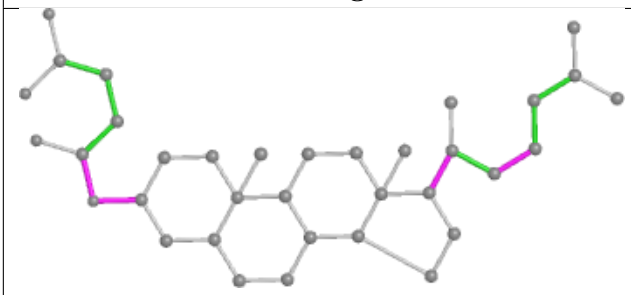
Ligand Y01 B 1206



Bond lengths



Bond angles



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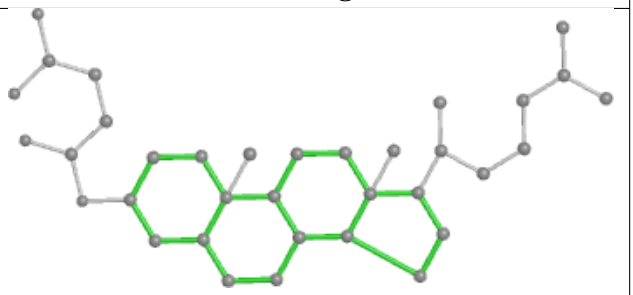
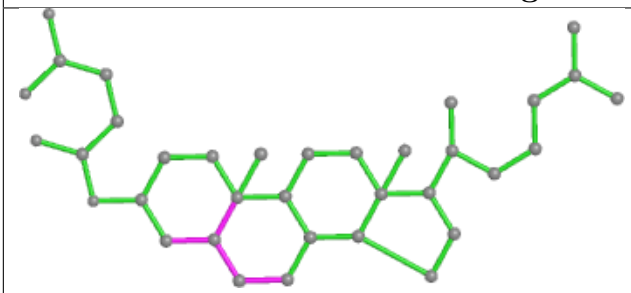


Rings

Ligand Y01 C 1301



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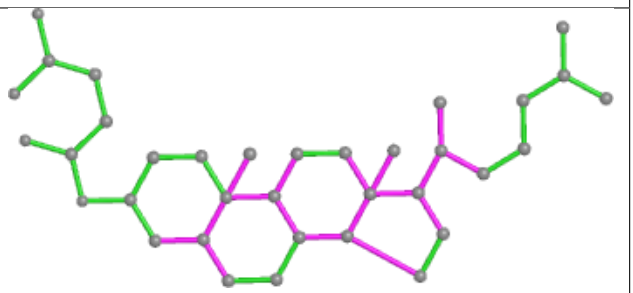
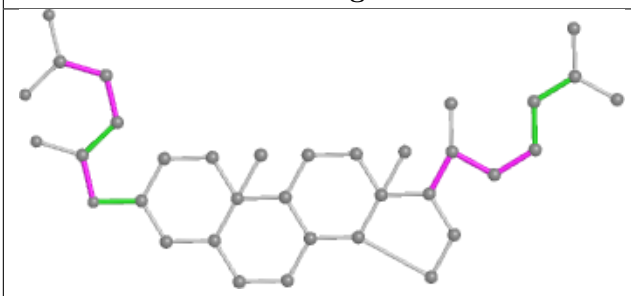
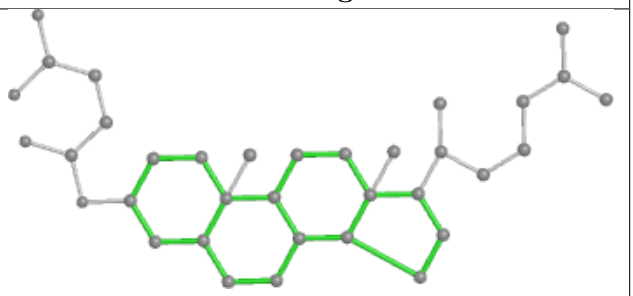


Bond angles

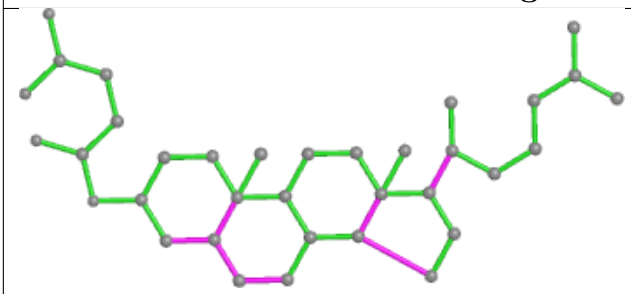


Torsions

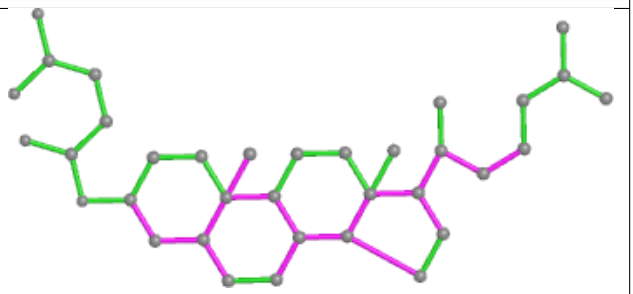


Rings

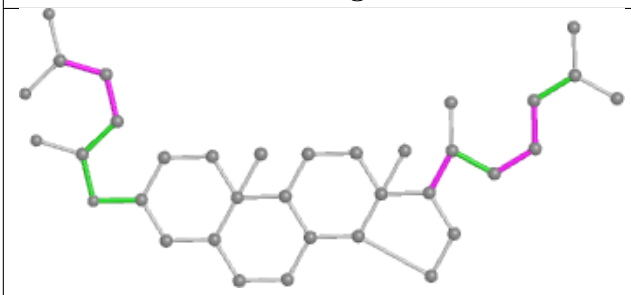
Ligand Y01 A 1208



Bond lengths



Bond angles



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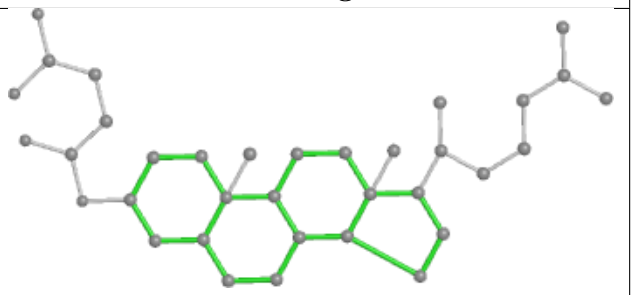
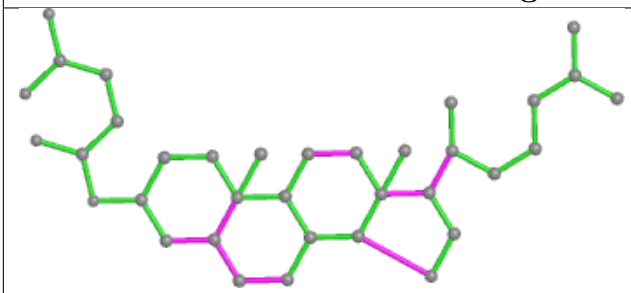


Rings

Ligand Y01 A 1206



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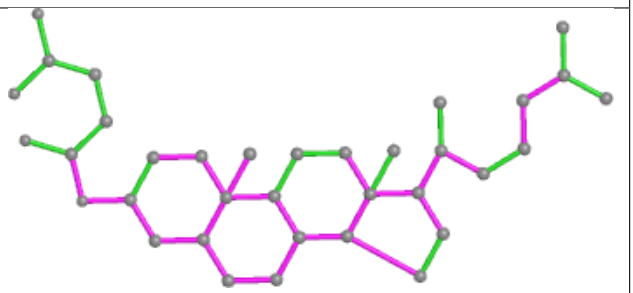
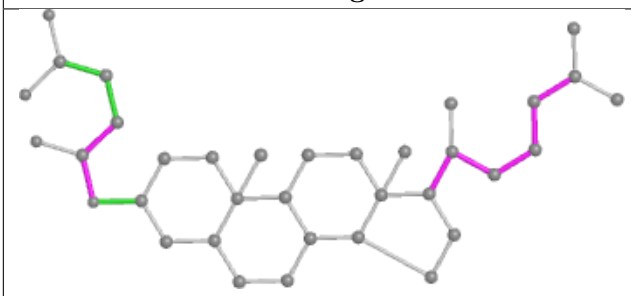


Bond angles



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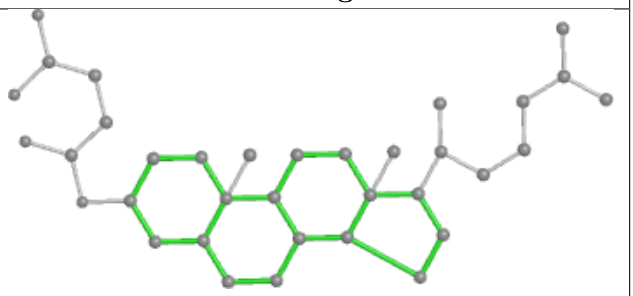
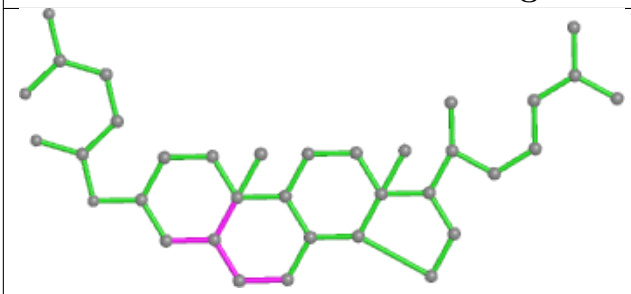
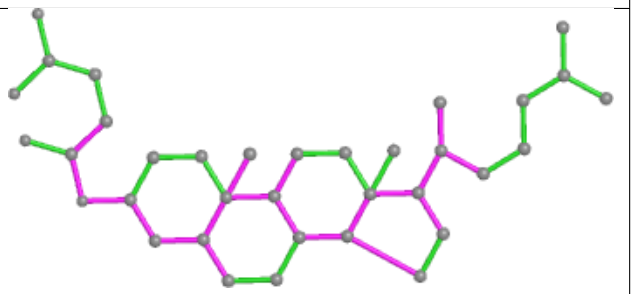


Rings

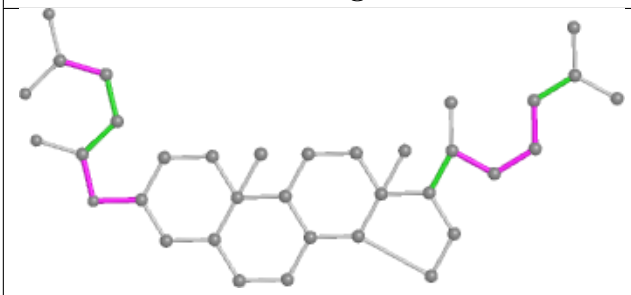
Ligand Y01 A 1207



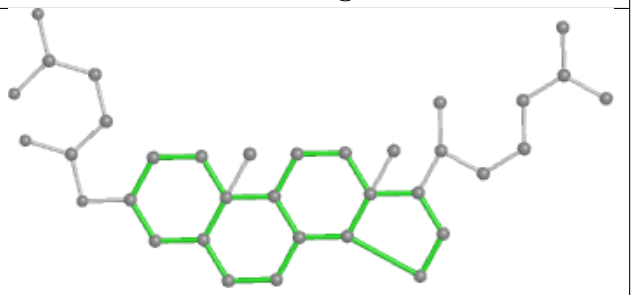
Bond lengths



Bond angles

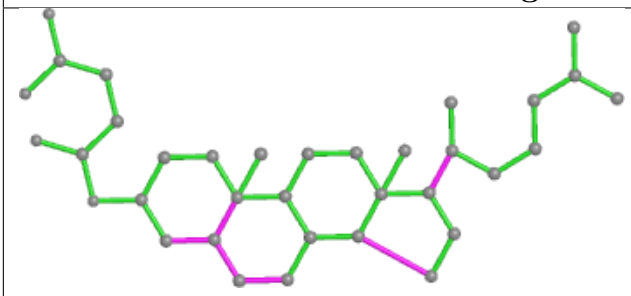


Torsions

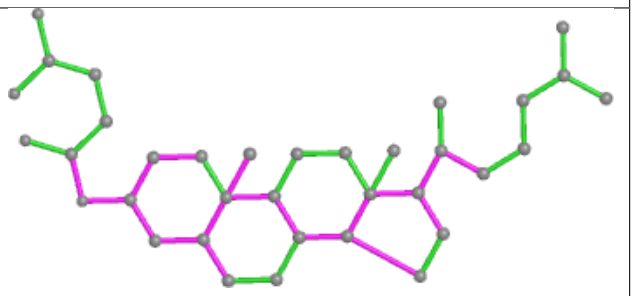


Rings

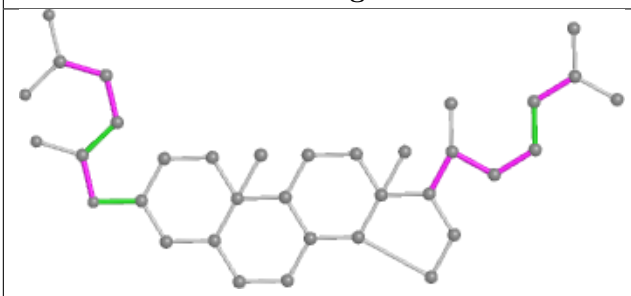
Ligand Y01 C 1307



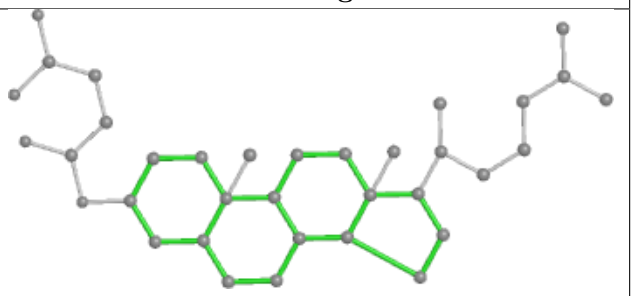
Bond lengths



Bond angles

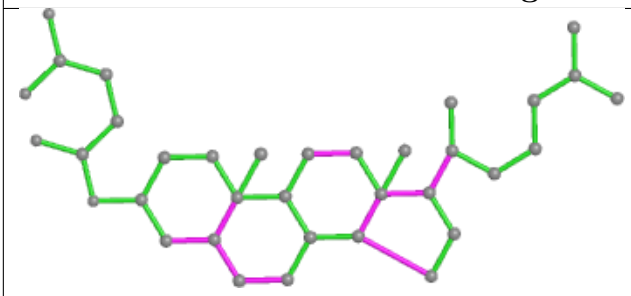


Torsions

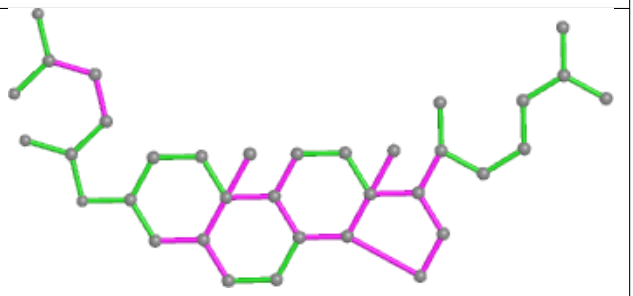


Rings

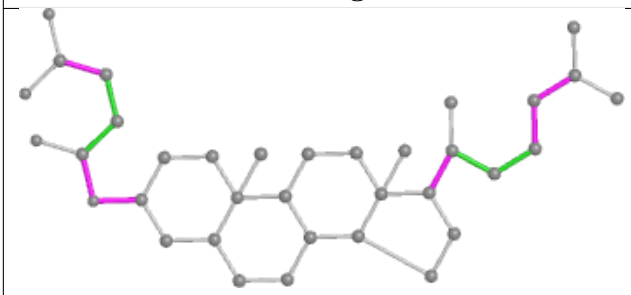
Ligand Y01 C 1302



Bond lengths



Bond angles



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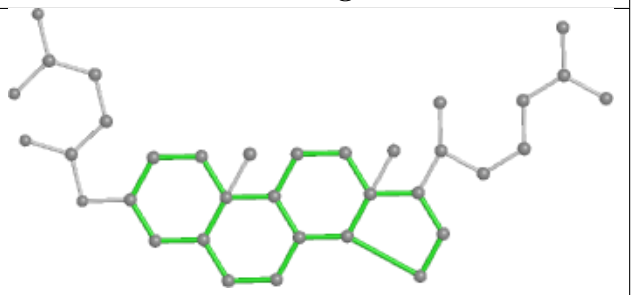
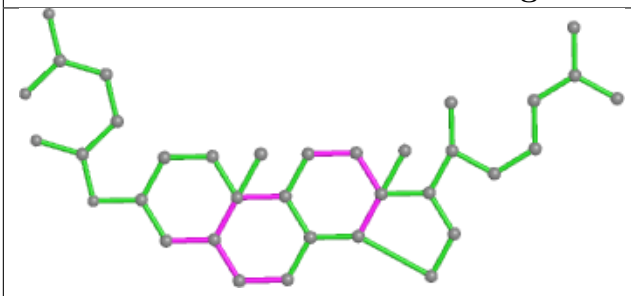
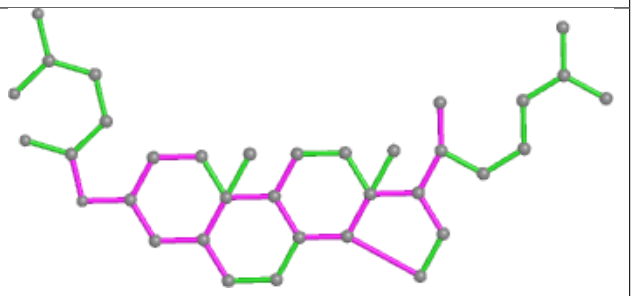


Rings

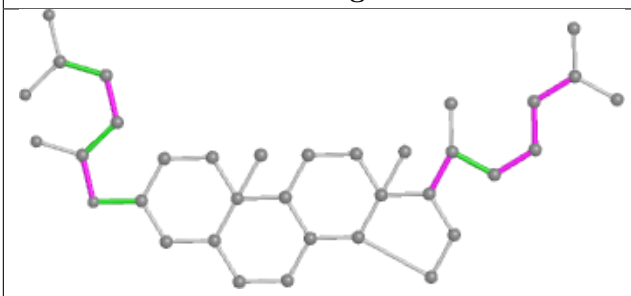
Ligand Y01 A 1205



Bond lengths



Bond angles



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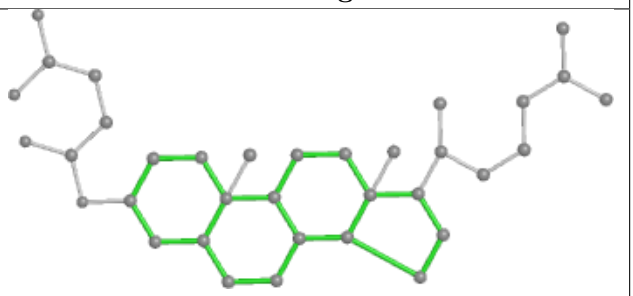
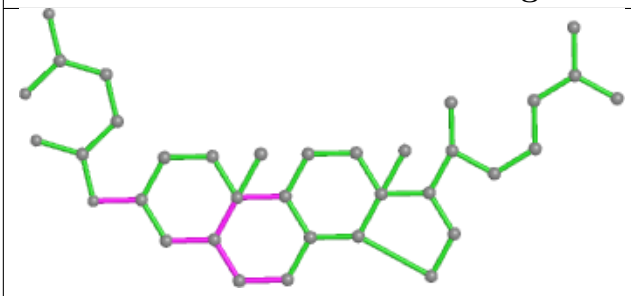
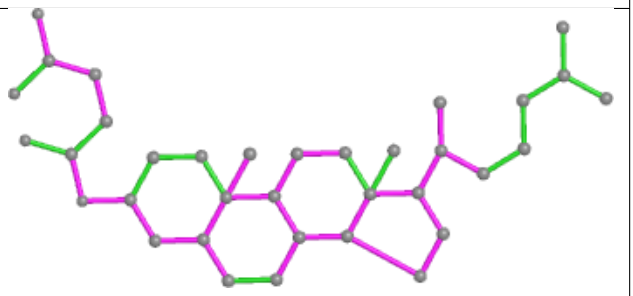


Rings

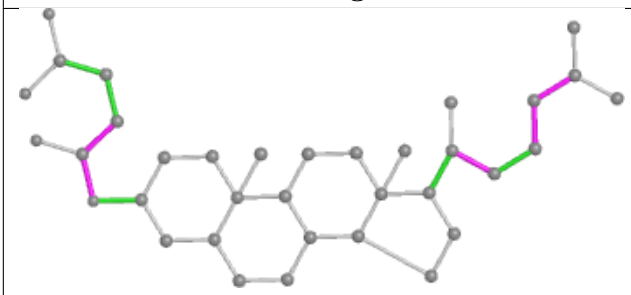
Ligand Y01 C 1306



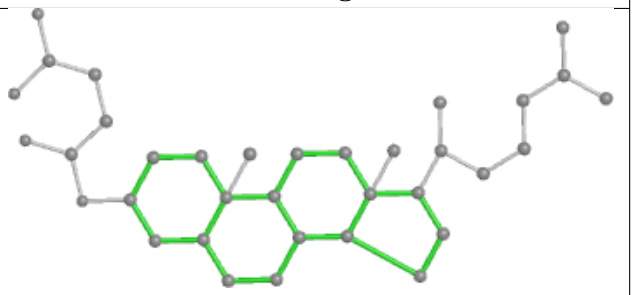
Bond lengths



Bond angles

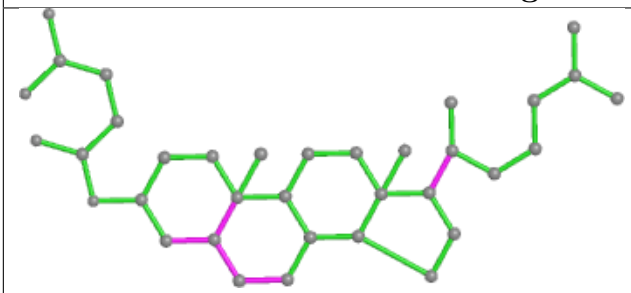


Torsions

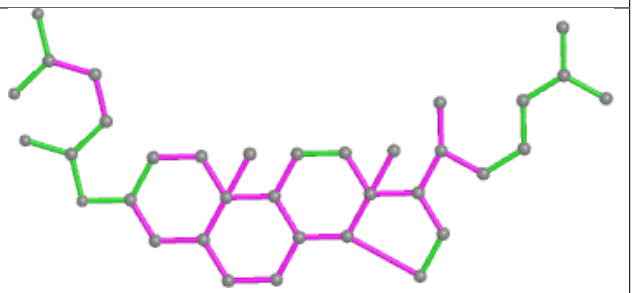


Rings

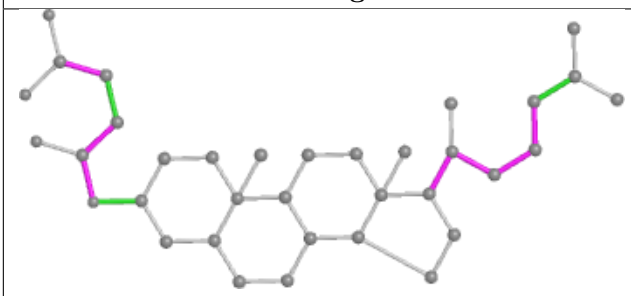
Ligand Y01 C 1308



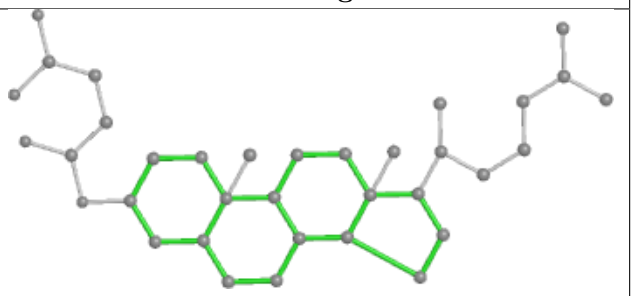
Bond lengths



Bond angles

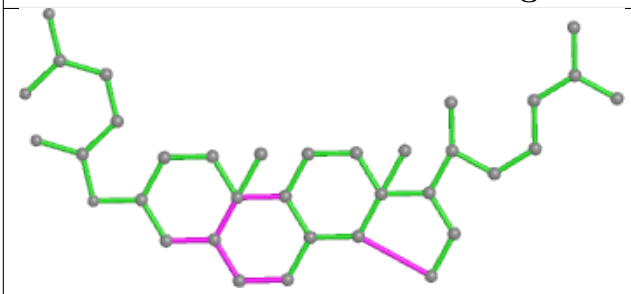


Torsions

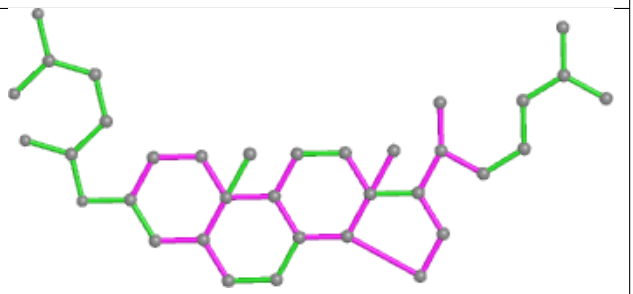


Rings

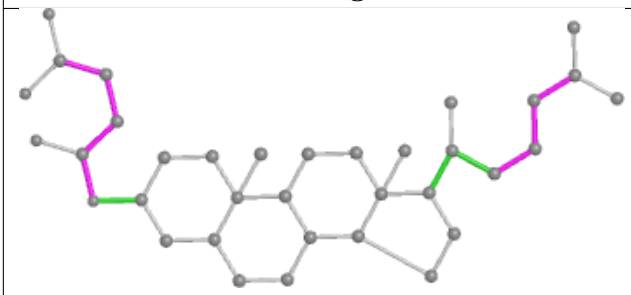
Ligand Y01 D 1202



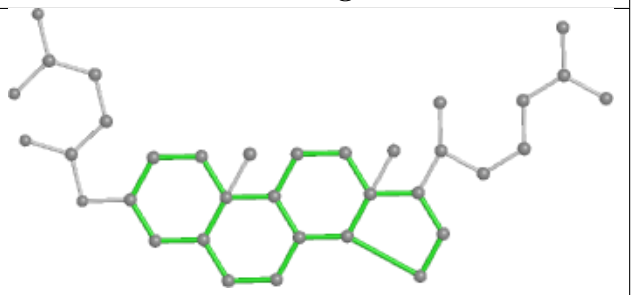
Bond lengths



Bond angles

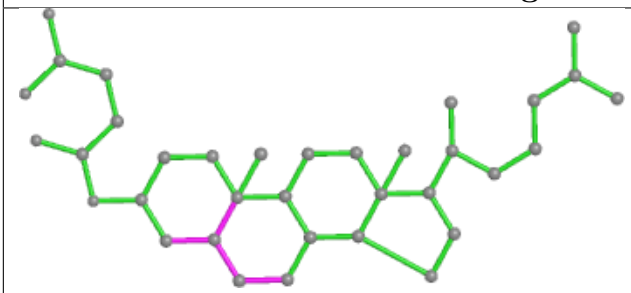


Torsions

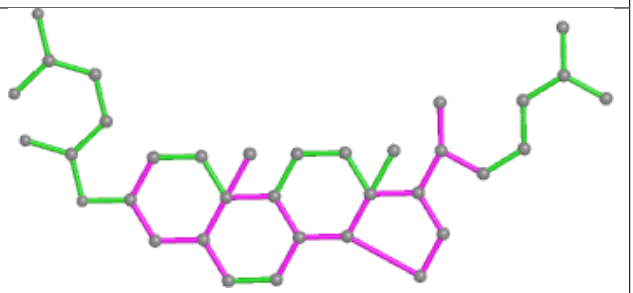


Rings

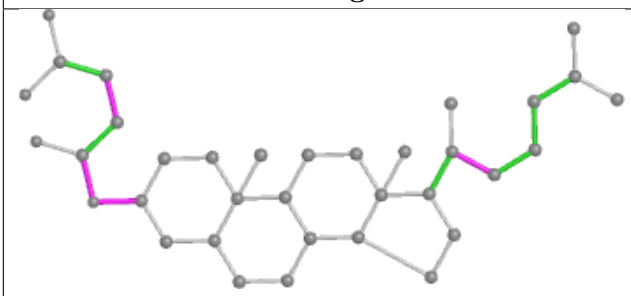
Ligand Y01 C 1305



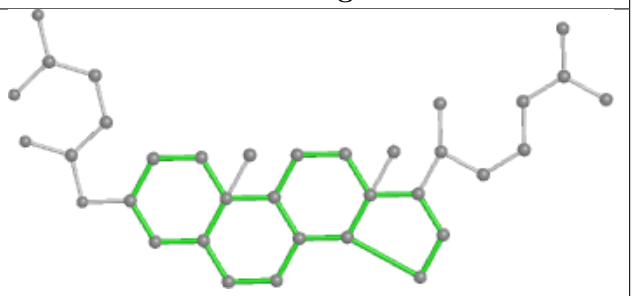
Bond lengths



Bond angles

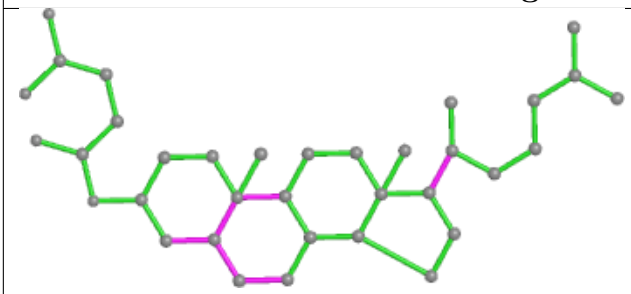


Torsions

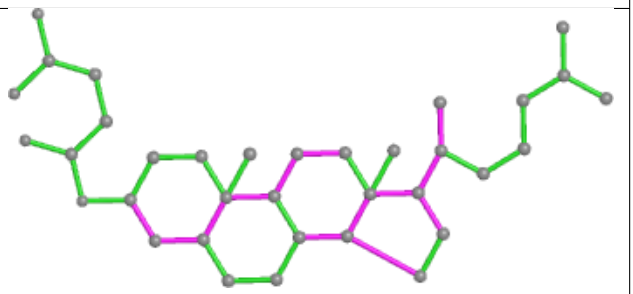


Rings

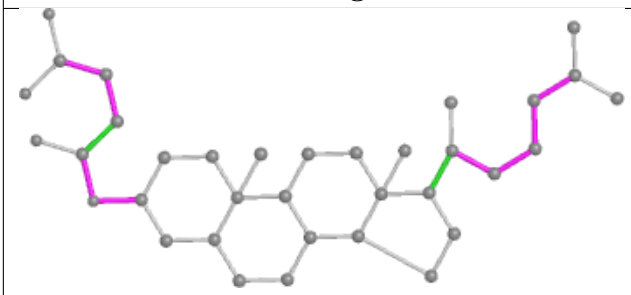
Ligand Y01 B 1204



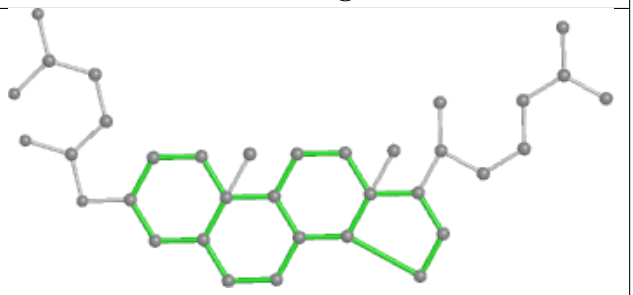
Bond lengths



Bond angles

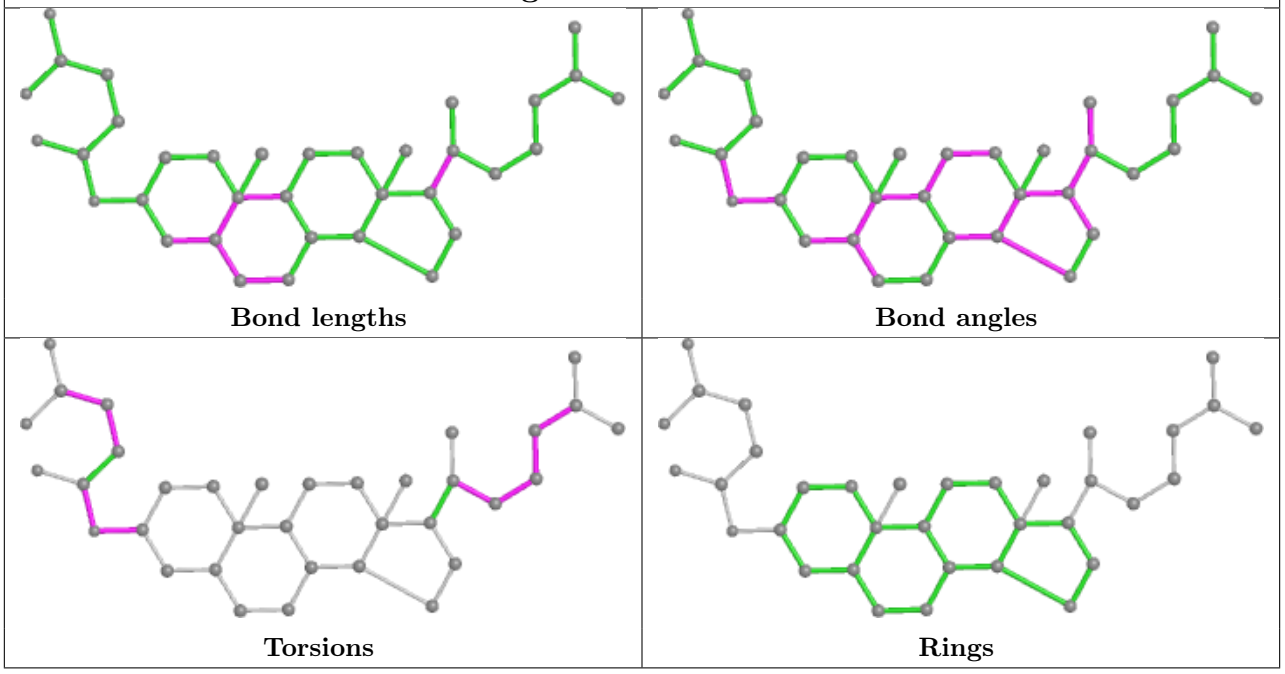


Torsions

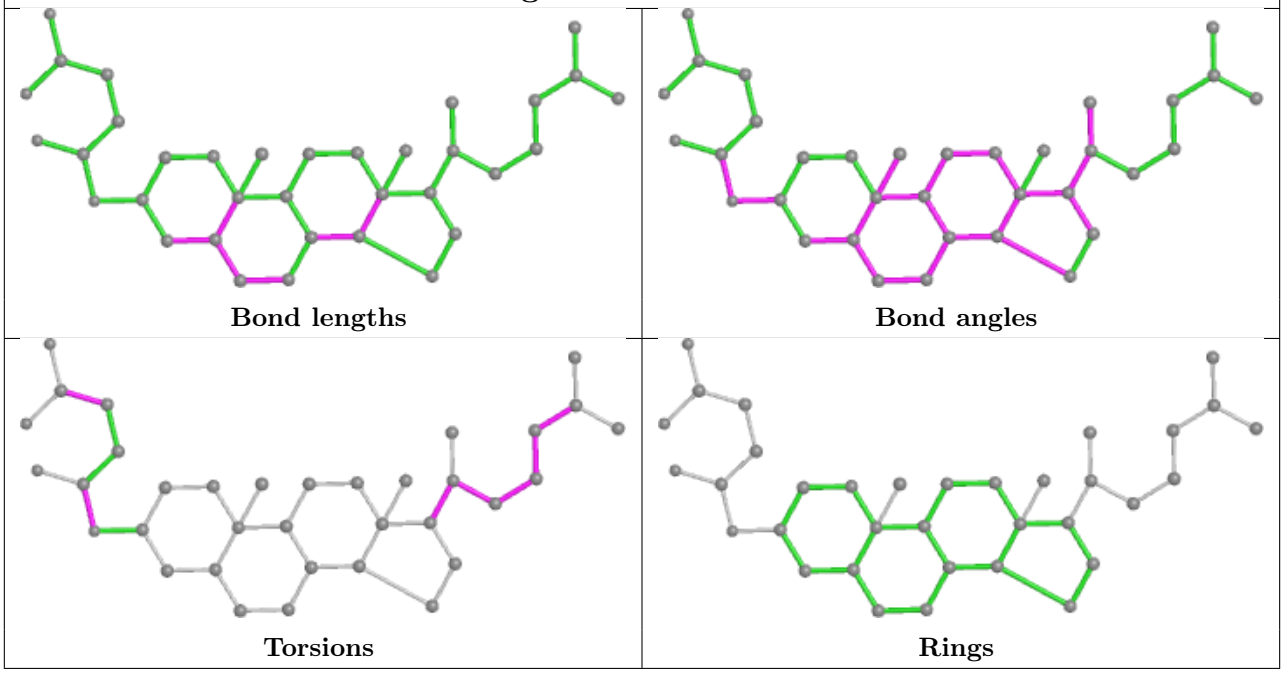


Rings

Ligand Y01 A 1203



Ligand Y01 D 1203



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
1	B	7
1	C	7
1	D	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:UNK	C	159:UNK	N	27.67
1	B	36:UNK	C	159:UNK	N	27.67
1	C	36:UNK	C	37:UNK	N	27.67
1	D	36:UNK	C	159:UNK	N	27.67
1	A	303:UNK	C	305:LYS	N	27.63
1	B	303:UNK	C	305:LYS	N	27.63
1	C	121:UNK	C	122:LYS	N	27.63
1	D	303:UNK	C	305:LYS	N	27.63
1	A	285:UNK	C	286:UNK	N	24.70
1	B	285:UNK	C	286:UNK	N	24.70
1	C	103:UNK	C	104:UNK	N	24.70
1	D	285:UNK	C	286:UNK	N	24.70
1	A	164:UNK	C	225:UNK	N	21.86
1	B	164:UNK	C	225:UNK	N	21.86
1	C	42:UNK	C	43:UNK	N	21.86
1	D	164:UNK	C	225:UNK	N	21.86
1	A	16:UNK	C	17:UNK	N	17.94
1	B	16:UNK	C	17:UNK	N	17.94
1	C	16:UNK	C	17:UNK	N	17.94
1	D	16:UNK	C	17:UNK	N	17.94
1	A	234:UNK	C	235:UNK	N	15.66
1	B	234:UNK	C	235:UNK	N	15.66
1	C	52:UNK	C	53:UNK	N	15.66
1	D	234:UNK	C	235:UNK	N	15.66
1	A	295:UNK	C	296:UNK	N	10.48
1	B	295:UNK	C	296:UNK	N	10.48
1	C	113:UNK	C	114:UNK	N	10.48
1	D	295:UNK	C	296:UNK	N	10.48

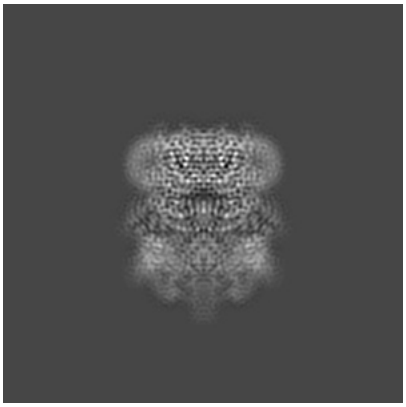
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7297. These allow visual inspection of the internal detail of the map and identification of artifacts.

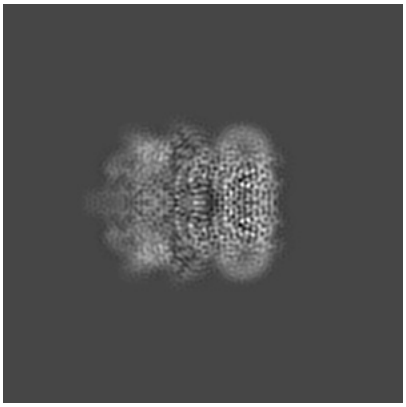
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

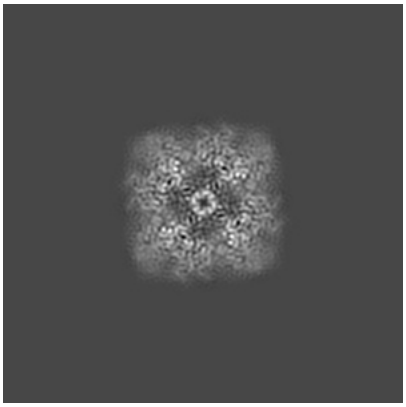
6.1.1 Primary map



X



Y



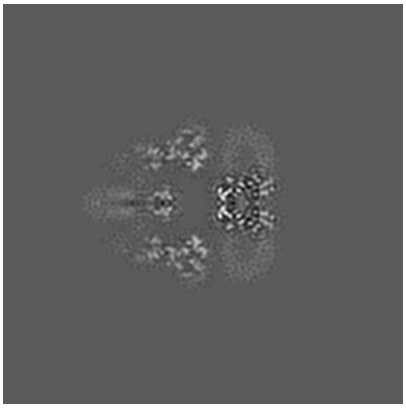
Z

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

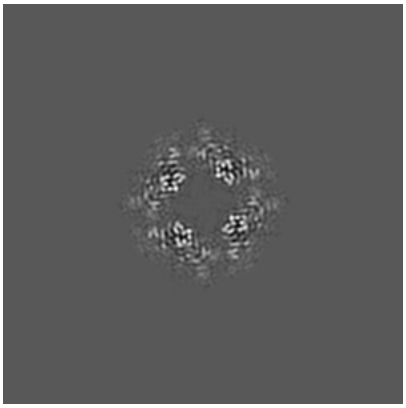
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

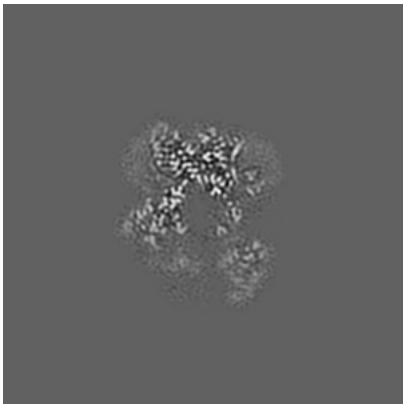


Z Index: 128

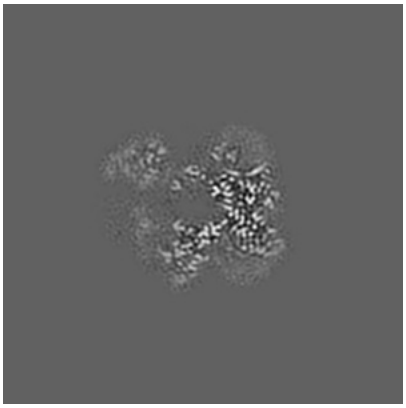
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

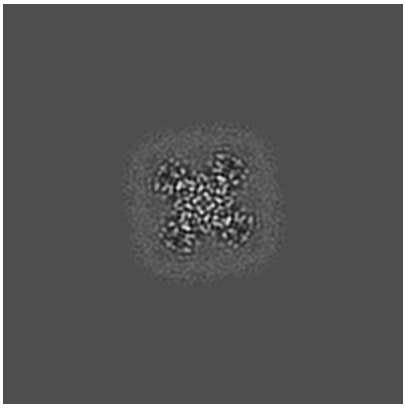
6.3.1 Primary map



X Index: 115



Y Index: 141



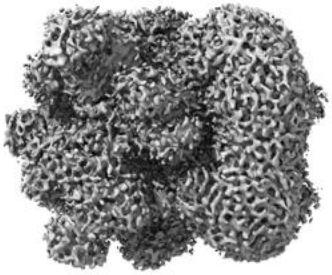
Z Index: 161

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

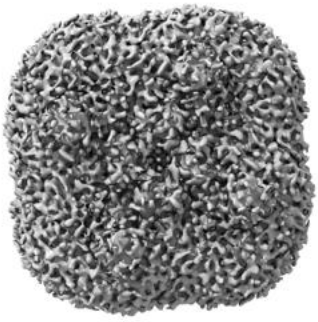
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

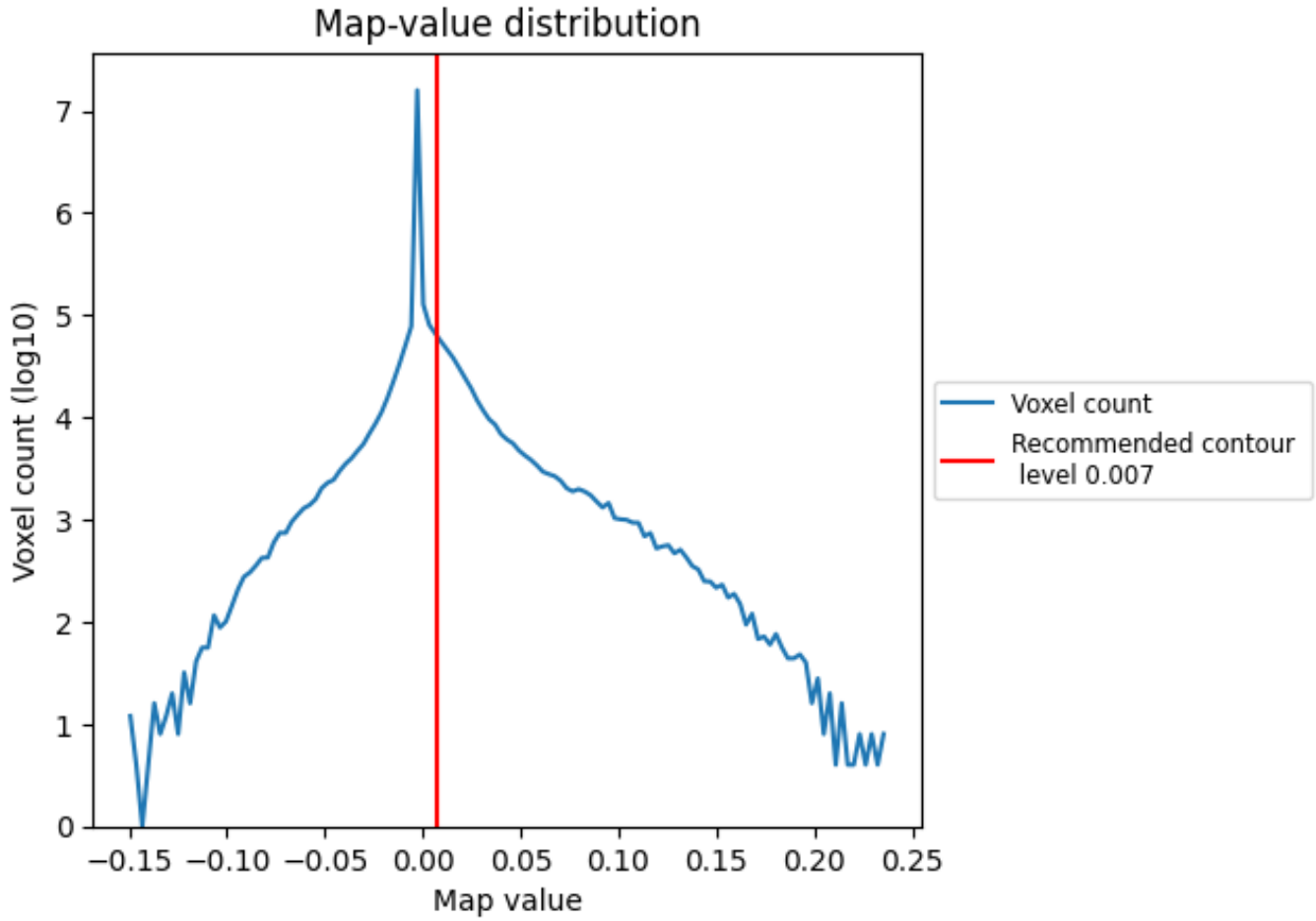
6.5 Mask visualisation (i)

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

7 Map analysis

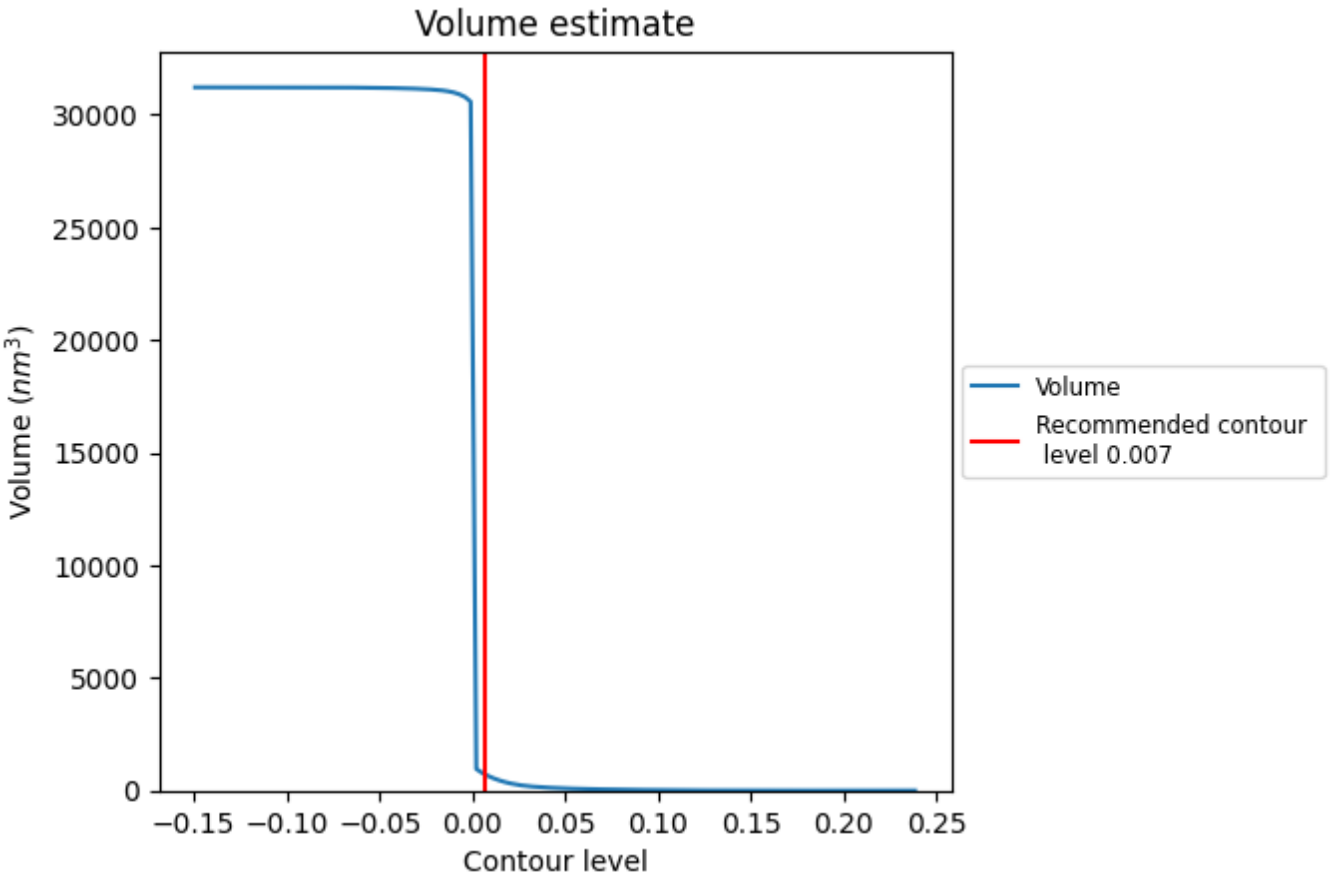
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

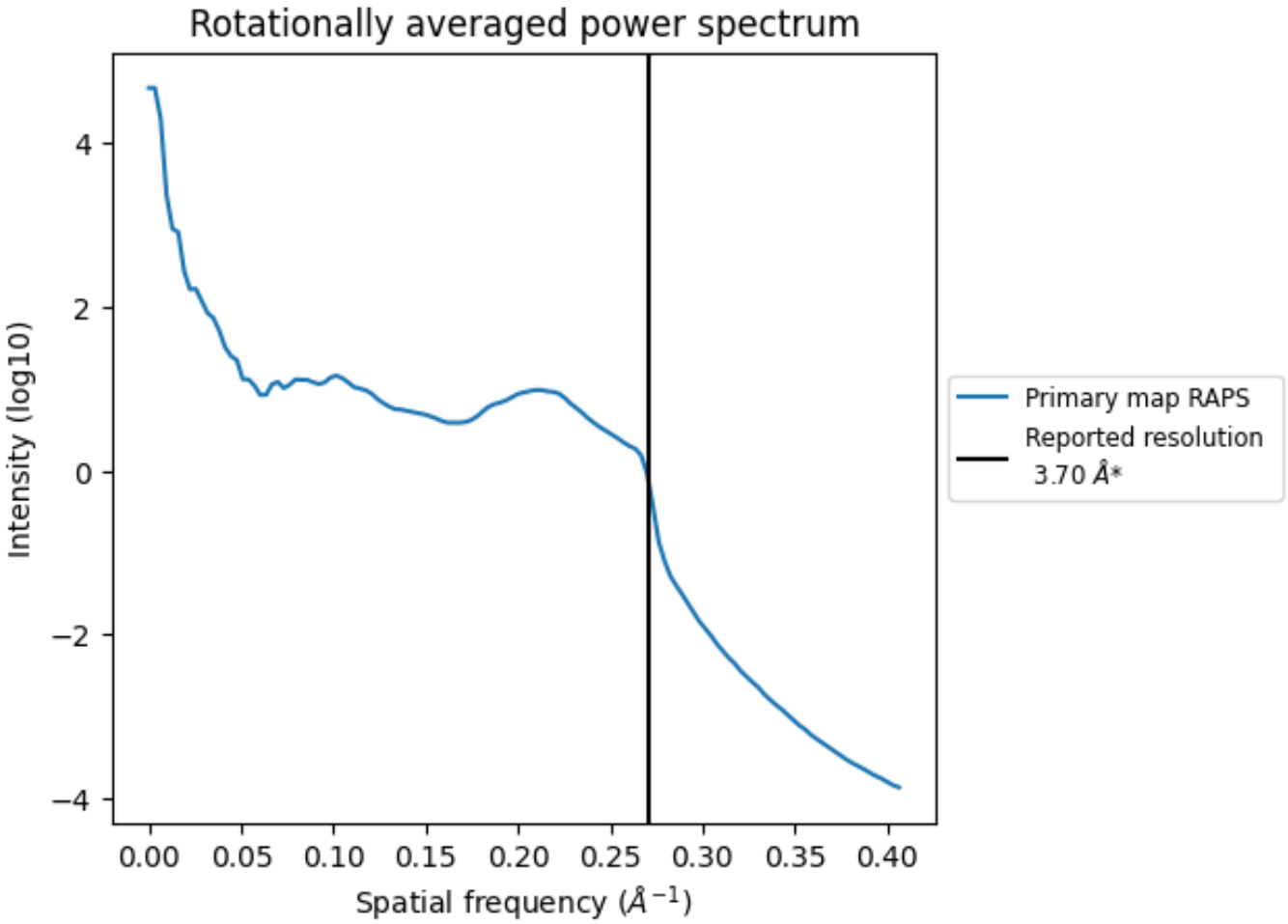
7.2 Volume estimate



The volume at the recommended contour level is 713 nm^3; this corresponds to an approximate mass of 644 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)

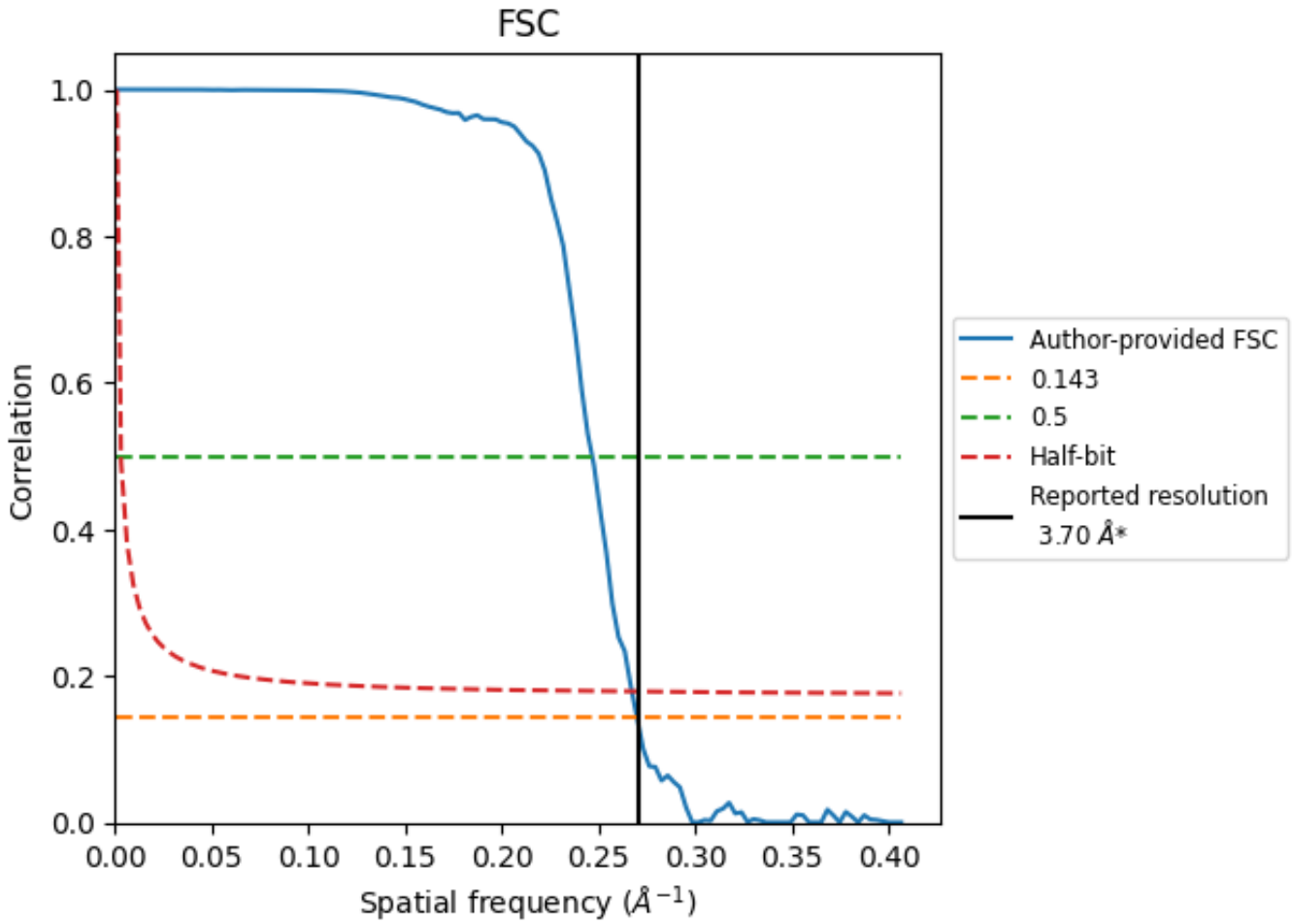


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

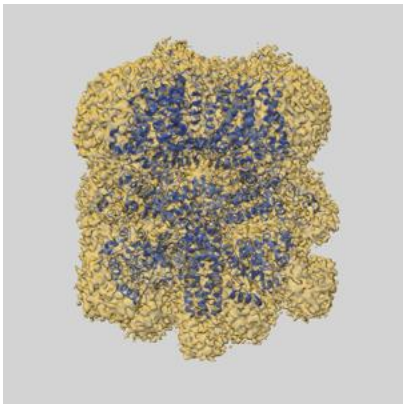
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.06	3.75
Unmasked-calculated*	-	-	-

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

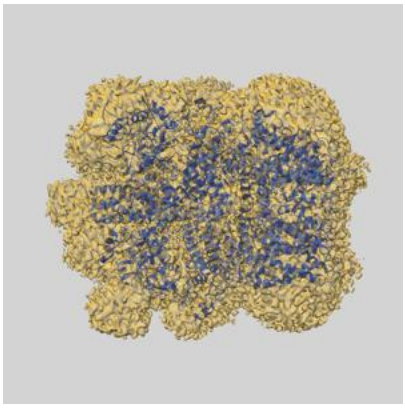
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7297 and PDB model 6BWD. Per-residue inclusion information can be found in section 3 on page 6.

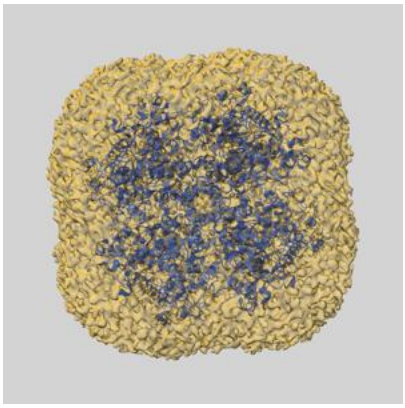
9.1 Map-model overlay



X



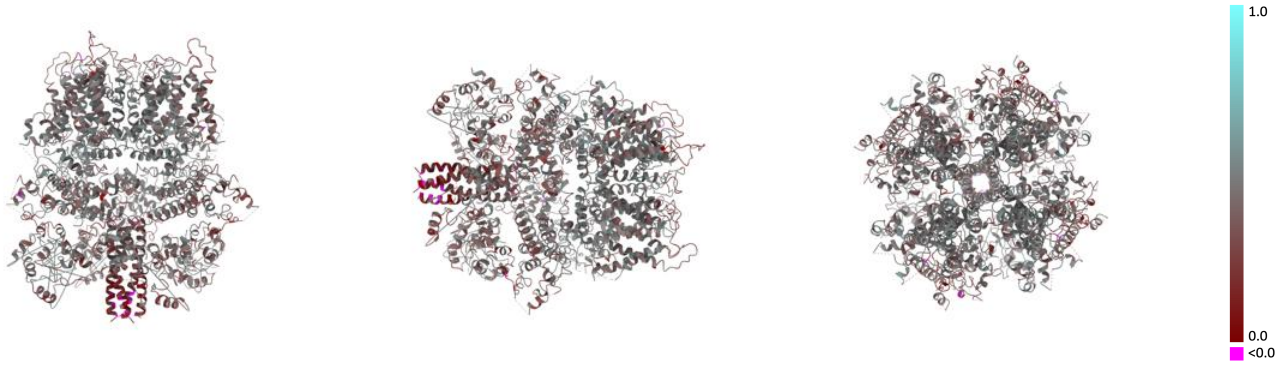
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

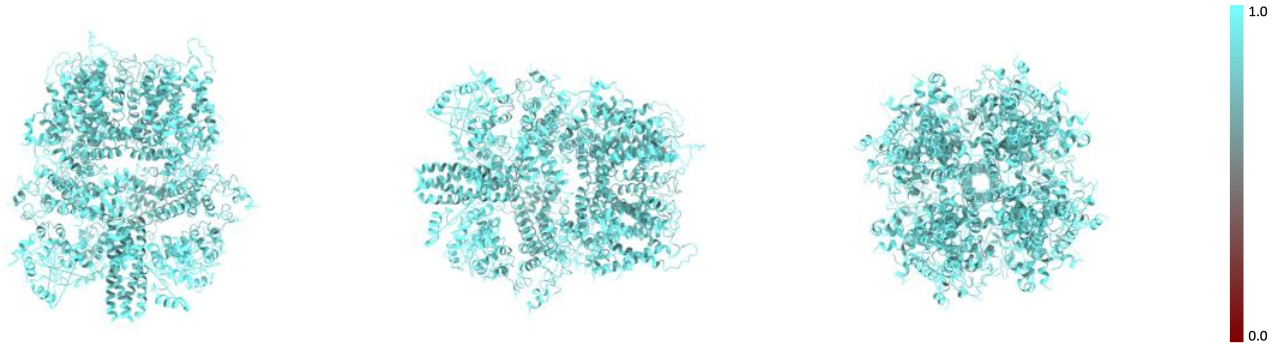
9.2 Q-score mapped to coordinate model (i)



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.

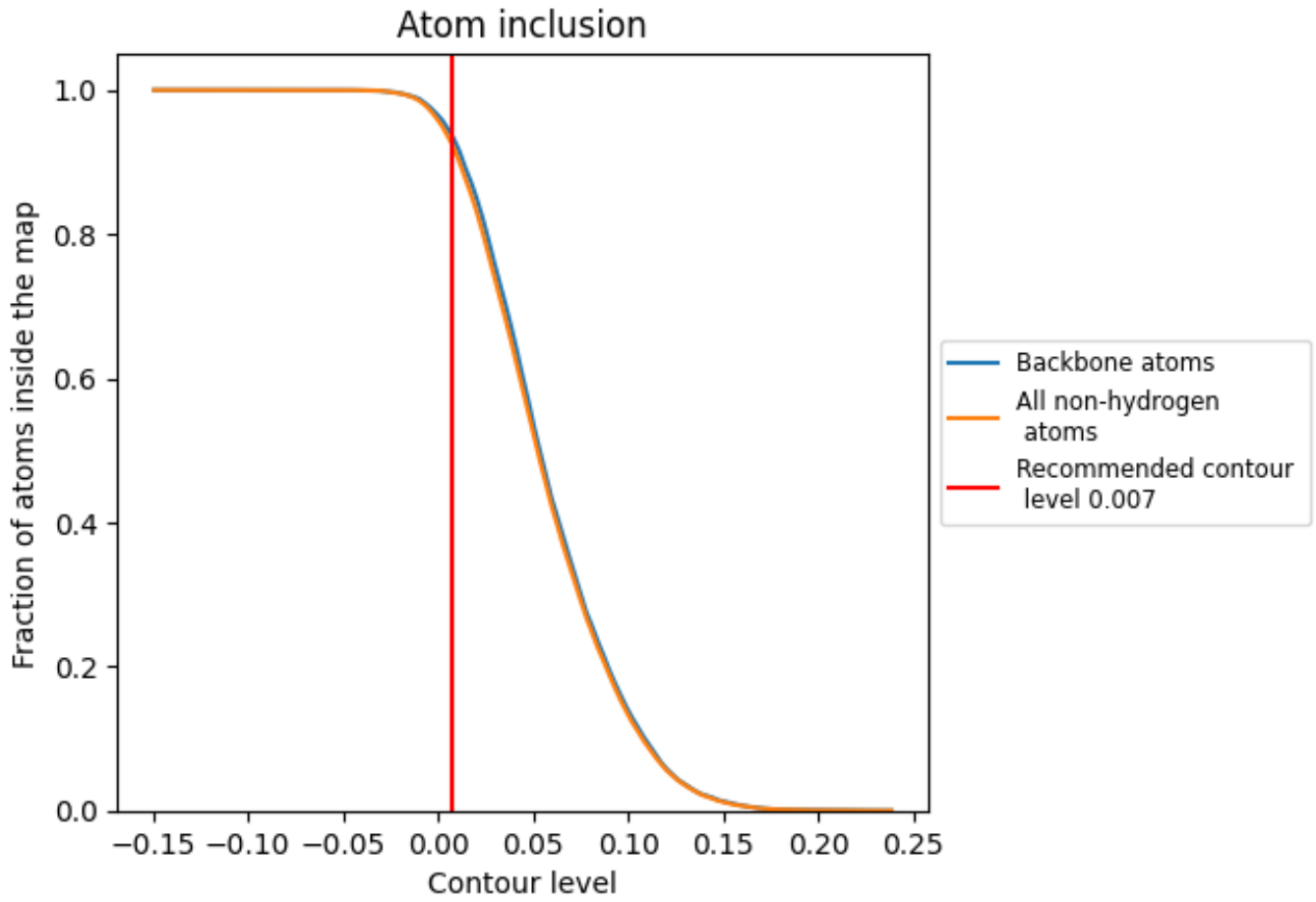
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 94% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9266	0.4180
A	0.9207	0.4030
B	0.9272	0.4230
C	0.9334	0.4270
D	0.9318	0.4200