



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:59 PM UTC

PDB ID : 5ZX5 / pdb_00005zx5
EMDB ID : EMD-6975
Title : 3.3 angstrom structure of mouse TRPM7 with EDTA
Authors : Zhang, J.; Li, Z.; Duan, J.; Li, J.; Hulse, R.E.; Santa-Cruz, A.; Abiria, S.A.; Krapivinsky, G.; Clapham, D.E.
Deposited on : 2018-05-18
Resolution : 3.28 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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:

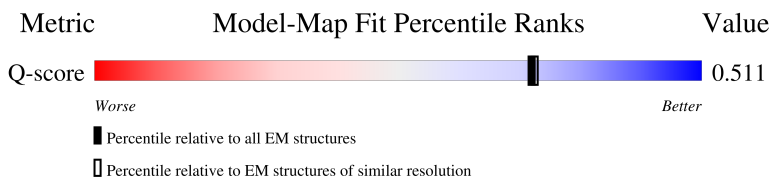
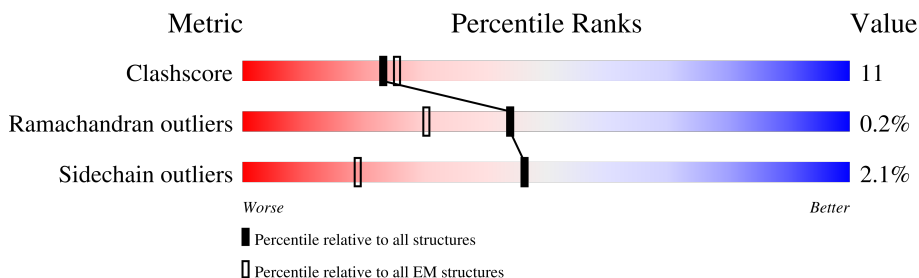
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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

Mol	Chain	Length	Quality of chain
1	A	1229	
1	B	1229	
1	C	1229	
1	D	1229	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

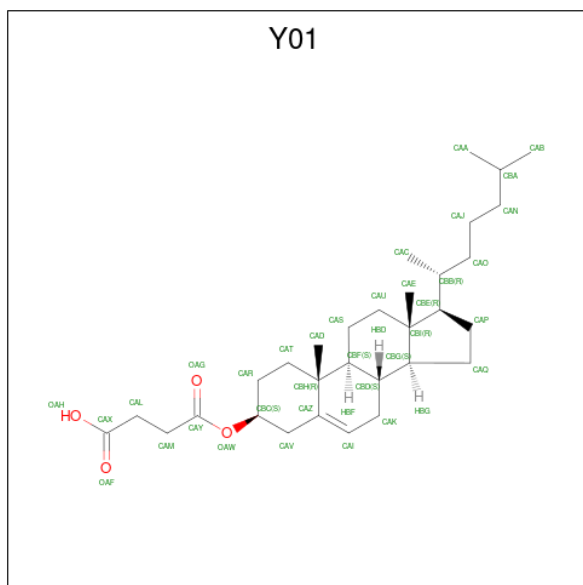
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	A	1305	-	-	X	-
2	Y01	D	1303	-	-	X	-

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	814	Total 6255	C 4095	N 1032	O 1087	S 41	0	0
1	B	814	Total 6255	C 4095	N 1032	O 1087	S 41	0	0
1	C	814	Total 6255	C 4095	N 1032	O 1087	S 41	0	0
1	D	814	Total 6255	C 4095	N 1032	O 1087	S 41	0	0

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



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

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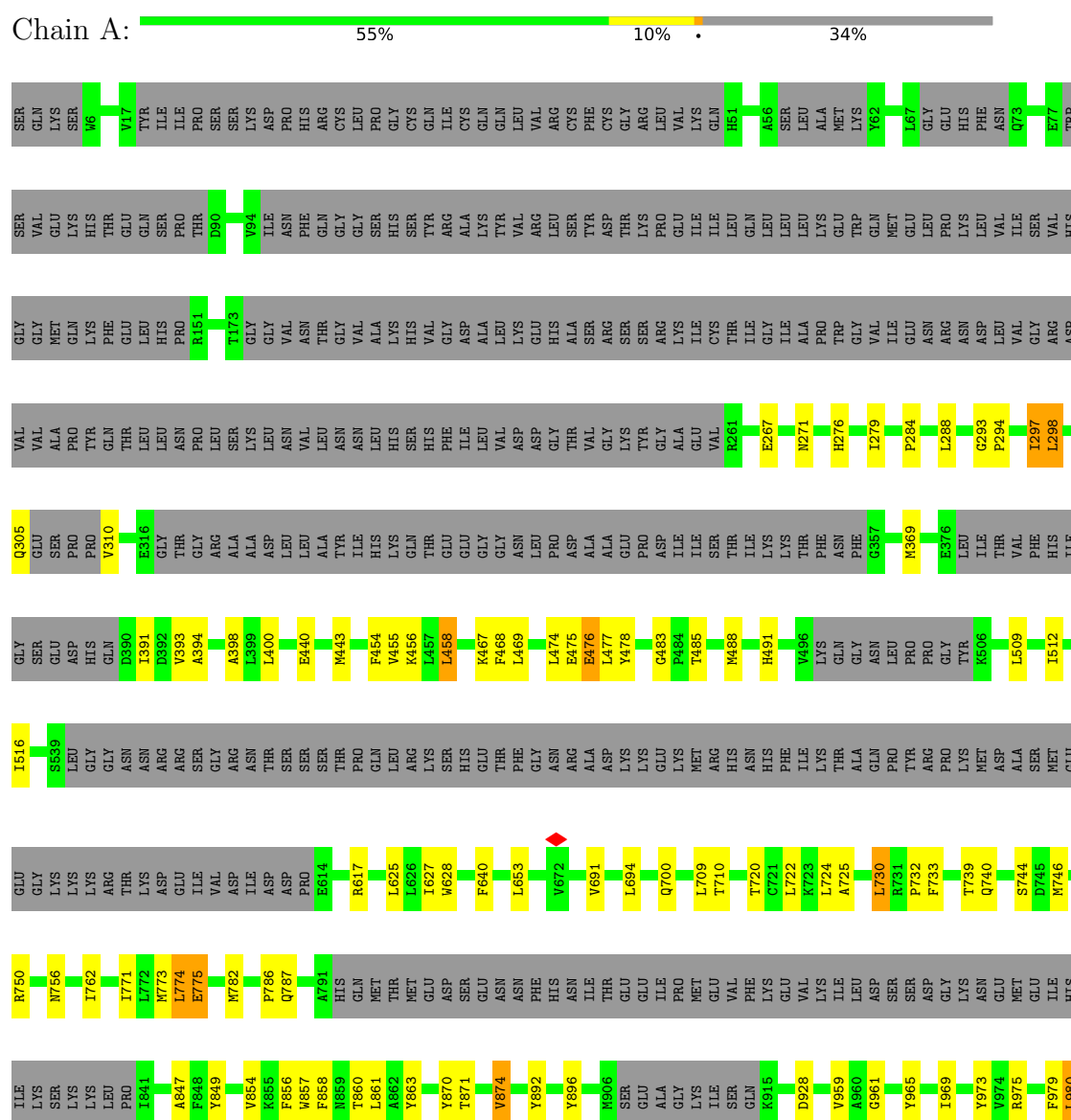
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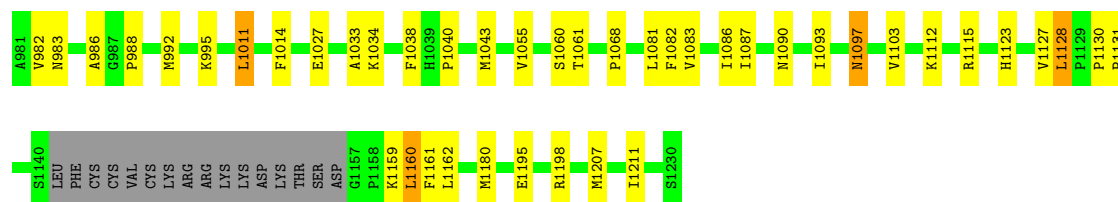
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	C	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31	4	
2	D	1	Total	C	O	0
			35	31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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

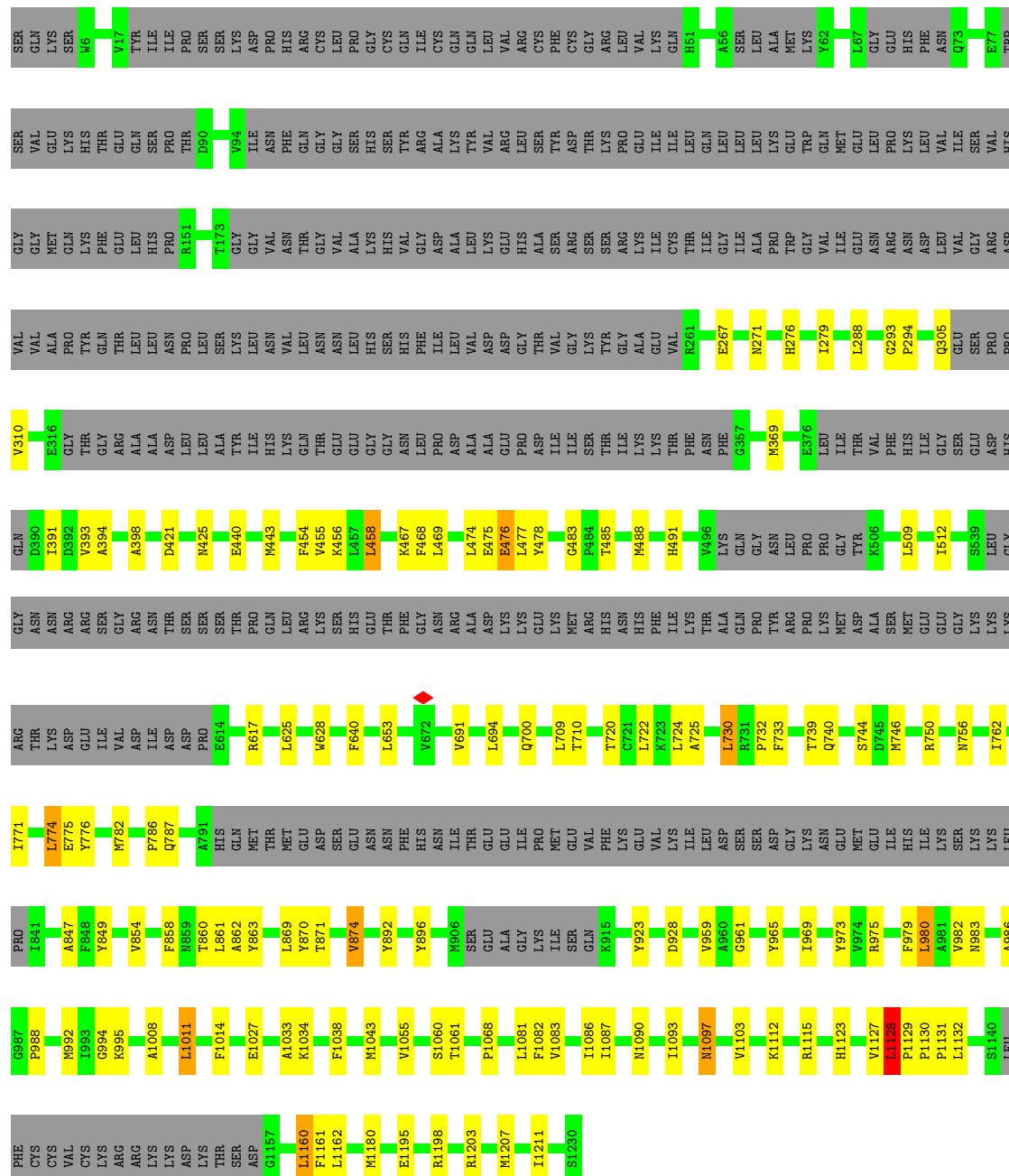
- Molecule 1: Transient receptor potential cation channel subfamily M member 7





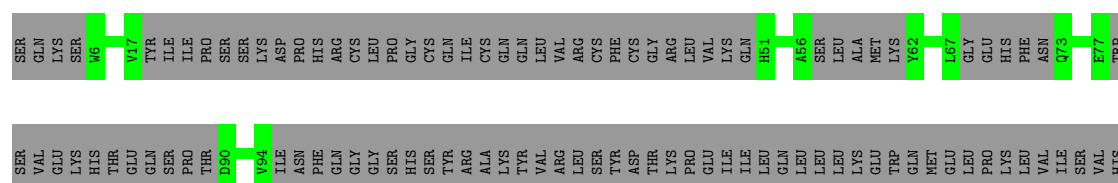
- Molecule 1: Transient receptor potential cation channel subfamily M member 7

Chain B: 55% 10% 34%



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

PHE	F979	ILE	R750	GLY	LEU	ASP	PRO	VAL	GLY	SER																																																																													
CYS	L980	LYS	N756	LYS	LYS	HIS	PRO	ALA	VAL	GLN																																																																													
VAL	N983	LYS	L762	LYS	ARG	D390	GLY	PRO	GLM	LYS																																																																													
CYS	A986	LEU	I771	THR	ASN	B392	ASN	TYR	LYS	PHE																																																																													
ARG	G987	PRO	L772	LYS	ASN	V393	THR	GLM	GLU	THR																																																																													
ARG	P988	ILE	L773	ASP	ARG	A394	GLY	THR	GLU	GLN																																																																													
LYS	M773	GLU	M774	GLU	ARG	A398	THR	LEU	LEU	HIS																																																																													
LYS	M992	ILE	L774	ILE	SER	A398	ALA	ASN	PRO	ILE																																																																													
ASP	E775	VAL	E775	VAL	GLY	I412	ALA	PRO	THR	PRO																																																																													
THR	M782	ASP	M782	ASP	ARG	I412	ASP	LEU	D90	SER																																																																													
SER	V854	ILE	P786	ILE	ASN	D421	LEU	SER	T173	SER																																																																													
ASP	L1011	ASP	P786	ASP	THR	M425	ALA	LYS	GLY	LYS																																																																													
ASP	L1012	ASP	Q787	ASP	SER	E440	TYR	ASN	GLY	ASP																																																																													
G1157	M858	PRO	E514	PRO	SER	M443	ILE	VAL	ASN	ASN																																																																													
L1160	A1033	M859	E514	THR	THR	F454	HIS	LEU	VAL	PHE																																																																													
F1161	K1034	T860	R617	PRO	PRO	V455	LYS	ASN	ASN	HIS																																																																													
L1162	L861	L861	L625	GLN	GLN	K456	GLY	GLY	GLY	ARG																																																																													
M1180	F1038	Y863	L625	LEU	THR	L457	GLY	LEU	GLY	CYS																																																																													
E1195	M1043	THR	M628	ARG	ARG	L458	GLY	LEU	ALA	PRO																																																																													
R1198	V1055	M867	F640	LYS	SER	K467	GLY	VAL	GLY	LYS																																																																													
R1203	S1060	L869	Y870	GLU	HIS	F468	ASN	ASP	LEU	GLN																																																																													
M1207	T1061	T871	L653	THR	THR	L489	PRO	ASP	TYR	GLN																																																																													
I1211	P1068	V874	V672	PHE	GLY	L474	ALA	ASP	VAL	LEU																																																																													
S1230	L1081	Y892	K680	ASN	ASN	E475	ALA	ASP	GLY	ARG																																																																													
	F1082	ASN	V691	ALA	ALA	E476	GLU	THR	ALA	CYS																																																																													
	V1083	ILE	L694	ASP	ASP	L477	PRO	GLY	VAL	PHE																																																																													
	I1086	THR	L694	LYS	LYS	Y478	ASP	GLY	GLY	CYS																																																																													
	I1087	GLU	Q700	LYS	GLU	G483	ILE	TYR	LEU	GLY																																																																													
	N1090	ILE	L709	MET	MET	P484	THR	ARG	PRO	LEU																																																																													
	I1093	GLY	T710	ARG	HIS	T485	ILE	ALA	LYS	VAL																																																																													
	N1097	LYS	T720	ASN	ASN	M488	LYS	VAL	CYS	GLN																																																																													
	V1103	ILE	C721	HIS	HIS	H491	THR	R261	THR	H51																																																																													
	K1112	GLN	L722	PHE	PHE	V496	ILE	E267	ILE	A56																																																																													
	R1115	VAL	L724	LYS	LYS	LYS	ASN	N271	ILE	SER																																																																													
	H1123	VAL	L724	THR	THR	LYS	PHE	H276	GLY	ALA																																																																													
	V1127	ILE	A725	ALA	ALA	LYS	GLN	I279	TRP	LEU																																																																													
	P1129	ASP	L730	GLN	PRO	GLY	LEU	L288	VAL	GLY																																																																													
	P1130	LEU	R731	PRO	TYR	ASN	ILE	G253	GLU	L67																																																																													
	L1132	SER	P732	ARG	ARG	LEU	LEU	P294	GLY	ASN </tr <tr><td></td><td>L1132</td><td>ASP</td><td>F733</td><td>THR</td><td>PRO</td><td>PRO</td><td>ILE</td><td>L298</td><td>ASN</td><td>GLY</td></tr> <tr><td></td><td>L1132</td><td>GLY</td><td>T739</td><td>LYS</td><td>PRO</td><td>GLY</td><td>THR</td><td>Q305</td><td>VAL</td><td>THR</td></tr> <tr><td></td><td>P1129</td><td>MET</td><td>Q740</td><td>MET</td><td>TYR</td><td>R506</td><td>VAL</td><td>L298</td><td>GLY</td><td>GLY</td></tr> <tr><td></td><td>P1131</td><td>GLU</td><td>S744</td><td>SER</td><td>ASP</td><td>L509</td><td>HIS</td><td>Q305</td><td>GLY</td><td>SER</td></tr> <tr><td></td><td>L1132</td><td>GLU</td><td>D745</td><td>MET</td><td>THR</td><td>L509</td><td>ILE</td><td>E267</td><td>VAL</td><td>VAL</td></tr> <tr><td></td><td>L1140</td><td>ILE</td><td>M746</td><td>GLU</td><td>GLU</td><td>T512</td><td>SER</td><td>R261</td><td>GLY</td><td>THR</td></tr> <tr><td></td><td>L1140</td><td>THR</td><td>M746</td><td>GLU</td><td>GLU</td><td>T512</td><td>GLN</td><td>E267</td><td>GLY</td><td>THR</td></tr>		L1132	ASP	F733	THR	PRO	PRO	ILE	L298	ASN	GLY		L1132	GLY	T739	LYS	PRO	GLY	THR	Q305	VAL	THR		P1129	MET	Q740	MET	TYR	R506	VAL	L298	GLY	GLY		P1131	GLU	S744	SER	ASP	L509	HIS	Q305	GLY	SER		L1132	GLU	D745	MET	THR	L509	ILE	E267	VAL	VAL		L1140	ILE	M746	GLU	GLU	T512	SER	R261	GLY	THR		L1140	THR	M746	GLU	GLU	T512	GLN	E267	GLY	THR
	L1132	ASP	F733	THR	PRO	PRO	ILE	L298	ASN	GLY																																																																													
	L1132	GLY	T739	LYS	PRO	GLY	THR	Q305	VAL	THR																																																																													
	P1129	MET	Q740	MET	TYR	R506	VAL	L298	GLY	GLY																																																																													
	P1131	GLU	S744	SER	ASP	L509	HIS	Q305	GLY	SER																																																																													
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	L1140	ILE	M746	GLU	GLU	T512	SER	R261	GLY	THR																																																																													
	L1140	THR	M746	GLU	GLU	T512	GLN	E267	GLY	THR																																																																													





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	1039775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.377	Depositor
Minimum map value	-0.206	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	314.88, 314.88, 314.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: 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	0.63	0/6390	0.79	13/8683 (0.1%)
1	B	0.63	1/6390 (0.0%)	0.78	12/8683 (0.1%)
1	C	0.62	1/6390 (0.0%)	0.77	10/8683 (0.1%)
1	D	0.62	0/6390	0.76	8/8683 (0.1%)
All	All	0.63	2/25560 (0.0%)	0.77	43/34732 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1128	LEU	C-N	5.11	1.39	1.33
1	B	1128	LEU	C-N	5.05	1.39	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	LEU	N-CA-C	12.89	125.33	111.28
1	B	476	GLU	N-CA-C	-9.65	96.24	110.52
1	D	476	GLU	N-CA-C	-9.63	96.27	110.52
1	C	476	GLU	N-CA-C	-9.61	96.30	110.52
1	A	476	GLU	N-CA-C	-8.67	98.84	110.55
1	B	475	GLU	N-CA-C	-7.65	102.94	111.28
1	C	475	GLU	N-CA-C	-7.65	102.94	111.28
1	D	475	GLU	N-CA-C	-7.65	102.94	111.28
1	A	1159	LYS	N-CA-C	7.57	120.92	110.24
1	D	710	THR	N-CA-C	7.14	122.09	112.88
1	A	874	VAL	N-CA-C	7.12	117.91	110.72
1	D	874	VAL	N-CA-C	7.12	117.91	110.72
1	C	874	VAL	N-CA-C	7.11	117.90	110.72
1	B	874	VAL	N-CA-C	7.11	117.90	110.72
1	A	773	MET	N-CA-C	6.66	119.48	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	773	MET	N-CA-C	6.66	119.48	108.49
1	A	475	GLU	N-CA-C	-6.63	104.05	111.28
1	A	293	GLY	N-CA-C	5.91	124.39	112.34
1	B	293	GLY	N-CA-C	5.91	124.39	112.34
1	C	293	GLY	N-CA-C	5.91	124.39	112.34
1	D	293	GLY	N-CA-C	5.91	124.39	112.34
1	B	1027	GLU	CA-C-N	-5.89	113.69	119.76
1	B	1027	GLU	C-N-CA	-5.89	113.69	119.76
1	A	1130	PRO	N-CA-C	5.80	117.77	110.70
1	B	1130	PRO	N-CA-C	5.80	117.77	110.70
1	C	1130	PRO	N-CA-C	5.80	117.77	110.70
1	D	1130	PRO	N-CA-C	5.80	117.77	110.70
1	B	1128	LEU	CA-C-N	-5.75	114.46	120.38
1	B	1128	LEU	C-N-CA	-5.75	114.46	120.38
1	C	1128	LEU	CA-C-N	-5.74	114.47	120.38
1	C	1128	LEU	C-N-CA	-5.74	114.47	120.38
1	A	293	GLY	CA-C-N	-5.60	114.02	119.78
1	A	293	GLY	C-N-CA	-5.60	114.02	119.78
1	B	293	GLY	CA-C-N	-5.60	114.02	119.78
1	B	293	GLY	C-N-CA	-5.60	114.02	119.78
1	C	293	GLY	CA-C-N	-5.60	114.02	119.78
1	C	293	GLY	C-N-CA	-5.60	114.02	119.78
1	D	293	GLY	CA-C-N	-5.60	114.02	119.78
1	D	293	GLY	C-N-CA	-5.60	114.02	119.78
1	A	1027	GLU	CA-C-N	-5.59	113.79	119.83
1	A	1027	GLU	C-N-CA	-5.59	113.79	119.83
1	B	1027	GLU	N-CA-C	-5.43	101.95	110.14
1	A	297	ILE	N-CA-C	-5.36	100.17	107.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6255	0	6057	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6255	0	6057	137	0
1	C	6255	0	6057	122	0
1	D	6255	0	6057	133	0
2	A	175	0	245	57	0
2	B	70	0	98	17	0
2	C	70	0	98	13	0
2	D	105	0	147	32	0
All	All	25440	0	24816	557	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:982:VAL:HG23	2:D:1303:Y01:CAB	1.59	1.32
1:B:982:VAL:HG23	2:B:1302:Y01:CAA	1.75	1.16
2:C:1301:Y01:HAA3	2:C:1302:Y01:HAR2	1.16	1.13
2:C:1301:Y01:HAA3	2:C:1302:Y01:CAR	1.82	1.10
1:D:982:VAL:HG23	2:D:1303:Y01:HAB1	1.31	1.08
1:A:298:LEU:HD12	1:A:400:LEU:HD11	1.32	1.08
1:A:298:LEU:CD1	1:A:400:LEU:HD11	1.85	1.06
1:A:982:VAL:CG2	2:A:1305:Y01:HAB2	1.83	1.06
2:A:1305:Y01:HAE2	2:A:1305:Y01:HAO2	1.38	1.05
1:A:1207:MET:HE3	1:D:1211:ILE:HD12	1.41	1.01
1:B:982:VAL:HG23	2:B:1302:Y01:HAA2	1.42	1.01
2:D:1302:Y01:HAA3	2:D:1303:Y01:CAR	1.89	1.01
1:D:856:PHE:HE2	2:D:1303:Y01:HAC3	1.29	0.97
1:D:856:PHE:CE2	2:D:1303:Y01:HAC3	2.02	0.95
1:D:982:VAL:CG2	2:D:1303:Y01:CAB	2.45	0.94
1:A:982:VAL:CG2	2:A:1305:Y01:CAB	2.46	0.93
1:C:694:LEU:CD1	1:C:709:LEU:HD21	1.99	0.92
1:B:694:LEU:CD1	1:B:709:LEU:HD21	1.99	0.92
1:A:694:LEU:CD1	1:A:709:LEU:HD21	1.99	0.92
2:A:1305:Y01:HAN2	2:A:1305:Y01:HAC3	1.50	0.92
2:C:1302:Y01:HAE2	2:C:1302:Y01:HAC1	1.54	0.90
1:B:982:VAL:HG23	2:B:1302:Y01:HAA1	1.52	0.89
2:A:1305:Y01:HAI	1:D:1009:LEU:HD11	1.55	0.88
2:D:1302:Y01:HAA3	2:D:1303:Y01:HAR1	1.55	0.88
2:A:1305:Y01:HAC3	2:A:1305:Y01:HAB1	1.55	0.88
1:A:1211:ILE:HD12	1:B:1207:MET:HE3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LEU:CD1	1:A:400:LEU:CD1	2.52	0.86
1:B:1211:ILE:HD12	1:C:1207:MET:HE3	1.56	0.86
2:C:1301:Y01:CAA	2:C:1302:Y01:HAR2	2.04	0.86
1:C:1211:ILE:HD12	1:D:1207:MET:HE3	1.56	0.86
2:B:1302:Y01:HAC1	2:B:1302:Y01:HAU2	1.58	0.85
1:D:775:GLU:O	1:D:776:TYR:CD1	2.29	0.85
1:B:775:GLU:O	1:B:776:TYR:CD1	2.29	0.85
2:A:1305:Y01:HAE3	2:A:1305:Y01:HAC2	1.58	0.85
1:A:874:VAL:HG11	1:A:969:ILE:HD11	1.60	0.83
1:B:874:VAL:HG11	1:B:969:ILE:HD11	1.61	0.83
1:B:1034:LYS:O	1:B:1038:PHE:HB2	1.79	0.83
1:D:1034:LYS:O	1:D:1038:PHE:HB2	1.79	0.83
1:D:874:VAL:HG11	1:D:969:ILE:HD11	1.60	0.82
1:C:1034:LYS:O	1:C:1038:PHE:HB2	1.79	0.82
2:A:1305:Y01:HAB1	2:A:1305:Y01:CAC	2.10	0.82
1:A:1034:LYS:O	1:A:1038:PHE:HB2	1.79	0.82
1:B:1160:LEU:HD22	1:B:1161:PHE:N	1.94	0.82
1:A:1160:LEU:HD22	1:A:1161:PHE:N	1.94	0.82
1:C:1160:LEU:HD22	1:C:1161:PHE:N	1.94	0.82
2:A:1304:Y01:HAA3	2:A:1305:Y01:HBC	1.62	0.81
1:A:982:VAL:HG23	2:A:1305:Y01:HAB2	1.62	0.81
1:D:1160:LEU:HD22	1:D:1161:PHE:N	1.94	0.81
1:C:874:VAL:HG11	1:C:969:ILE:HD11	1.60	0.81
1:B:454:PHE:O	1:B:458:LEU:HB2	1.83	0.79
1:D:454:PHE:O	1:D:458:LEU:HB2	1.83	0.79
1:A:1207:MET:HE3	1:D:1211:ILE:CD1	2.13	0.79
1:A:454:PHE:O	1:A:458:LEU:HB2	1.83	0.79
1:A:477:LEU:HD23	1:A:477:LEU:O	1.83	0.79
1:A:298:LEU:HD12	1:A:400:LEU:CD1	2.14	0.78
1:D:980:LEU:HD22	1:D:980:LEU:O	1.84	0.78
2:A:1305:Y01:HAC3	2:A:1305:Y01:CAN	2.13	0.78
1:D:694:LEU:CD1	1:D:709:LEU:HD21	2.14	0.78
1:C:454:PHE:O	1:C:458:LEU:HB2	1.83	0.77
1:D:849:TYR:HB3	1:D:1127:VAL:HG11	1.67	0.77
1:B:982:VAL:CG2	2:B:1302:Y01:HAA1	2.15	0.77
1:A:849:TYR:HB3	1:A:1127:VAL:HG11	1.67	0.77
1:A:857:TRP:CH2	2:A:1305:Y01:HAO1	2.21	0.76
1:A:857:TRP:HH2	2:A:1305:Y01:HAO1	1.50	0.76
2:A:1305:Y01:HAC2	2:A:1305:Y01:CAE	2.15	0.76
1:A:694:LEU:HD11	1:A:709:LEU:HD21	1.69	0.75
1:A:982:VAL:HG21	2:A:1305:Y01:HAB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1303:Y01:HAA3	2:B:1302:Y01:HAV1	1.69	0.75
1:B:694:LEU:HD11	1:B:709:LEU:HD21	1.68	0.74
1:D:477:LEU:HD23	1:D:477:LEU:O	1.88	0.74
1:C:709:LEU:HD13	1:C:739:THR:HG22	1.69	0.74
1:C:477:LEU:O	1:C:477:LEU:HD23	1.88	0.74
1:A:1014:PHE:HB2	2:A:1301:Y01:CAB	2.18	0.73
1:A:774:LEU:H	1:A:774:LEU:HD23	1.54	0.73
1:C:694:LEU:HD11	1:C:709:LEU:HD21	1.68	0.72
1:D:747:TRP:HE1	2:D:1303:Y01:HAA3	1.53	0.72
1:B:477:LEU:HD23	1:B:477:LEU:O	1.88	0.72
1:B:709:LEU:HD13	1:B:739:THR:HG22	1.69	0.72
1:A:709:LEU:HD13	1:A:739:THR:HG22	1.69	0.72
2:A:1305:Y01:HAN2	2:A:1305:Y01:CAC	2.19	0.72
1:D:982:VAL:HG23	2:D:1303:Y01:HAB3	1.69	0.72
1:D:694:LEU:HD11	1:D:709:LEU:HD21	1.72	0.71
1:A:476:GLU:O	1:A:477:LEU:HB3	1.89	0.71
2:D:1302:Y01:HAA3	2:D:1303:Y01:OAW	1.91	0.71
1:C:774:LEU:HD23	1:C:774:LEU:H	1.54	0.71
1:D:774:LEU:CG	1:D:775:GLU:H	2.04	0.70
1:A:1160:LEU:HD22	1:A:1161:PHE:H	1.53	0.70
1:B:774:LEU:CG	1:B:775:GLU:H	2.04	0.70
1:A:443:MET:HE1	1:A:455:VAL:HG13	1.74	0.70
1:B:443:MET:HE1	1:B:455:VAL:HG13	1.74	0.70
1:C:1127:VAL:O	1:C:1128:LEU:HD22	1.92	0.69
2:A:1305:Y01:HAE2	2:A:1305:Y01:CAO	2.15	0.69
1:B:774:LEU:HG	1:B:775:GLU:H	1.58	0.69
1:D:474:LEU:O	1:D:478:TYR:HB2	1.92	0.69
1:D:443:MET:HE1	1:D:455:VAL:HG13	1.74	0.69
2:A:1305:Y01:CAB	2:A:1305:Y01:HAC3	2.22	0.69
1:B:1127:VAL:O	1:B:1128:LEU:HD13	1.92	0.69
1:A:474:LEU:O	1:A:478:TYR:HB2	1.92	0.69
1:D:774:LEU:HG	1:D:775:GLU:H	1.57	0.69
1:B:474:LEU:O	1:B:478:TYR:HB2	1.92	0.69
1:B:1011:LEU:HD23	1:B:1011:LEU:O	1.93	0.69
1:C:443:MET:HE1	1:C:455:VAL:HG13	1.74	0.69
1:C:1011:LEU:HD23	1:C:1011:LEU:O	1.93	0.69
1:C:474:LEU:O	1:C:478:TYR:HB2	1.92	0.69
1:D:982:VAL:CG2	2:D:1303:Y01:HAB3	2.23	0.69
1:B:1127:VAL:O	1:B:1128:LEU:HD22	1.92	0.69
1:C:1127:VAL:O	1:C:1128:LEU:HD13	1.92	0.69
1:A:982:VAL:HG22	2:A:1305:Y01:HAB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1301:Y01:HAU2	2:A:1301:Y01:HAC1	1.74	0.68
1:C:1160:LEU:HD22	1:C:1161:PHE:H	1.59	0.68
1:D:1011:LEU:O	1:D:1011:LEU:HD23	1.93	0.68
1:D:1160:LEU:HD22	1:D:1161:PHE:H	1.59	0.67
1:C:710:THR:HA	1:C:720:THR:HG23	1.77	0.67
1:B:710:THR:HA	1:B:720:THR:HG23	1.77	0.67
1:A:857:TRP:CZ2	2:A:1305:Y01:HAJ1	2.30	0.66
2:A:1303:Y01:HAA3	2:B:1302:Y01:CAV	2.24	0.66
1:B:1160:LEU:HD22	1:B:1161:PHE:H	1.59	0.66
2:C:1301:Y01:CAA	2:C:1302:Y01:CAR	2.70	0.66
1:A:710:THR:HA	1:A:720:THR:HG23	1.77	0.65
1:B:980:LEU:HA	2:B:1302:Y01:CAE	2.27	0.65
1:D:982:VAL:HG23	2:D:1303:Y01:HAB2	1.68	0.65
1:A:1207:MET:HE1	1:D:1207:MET:HG2	1.78	0.64
1:B:988:PRO:O	1:B:992:MET:HB2	1.97	0.64
1:A:988:PRO:O	1:A:992:MET:HB2	1.97	0.64
1:C:988:PRO:O	1:C:992:MET:HB2	1.97	0.64
2:D:1302:Y01:CAA	2:D:1303:Y01:HAR1	2.26	0.64
1:D:988:PRO:O	1:D:992:MET:HB2	1.97	0.63
1:A:983:ASN:HB3	2:A:1305:Y01:HBA	1.80	0.63
1:B:896:TYR:OH	1:B:975:ARG:NH1	2.32	0.63
1:C:896:TYR:OH	1:C:975:ARG:NH1	2.32	0.63
1:A:1033:ALA:HB2	2:A:1303:Y01:HAK1	1.81	0.62
1:D:896:TYR:OH	1:D:975:ARG:NH1	2.32	0.62
1:D:710:THR:HA	1:D:720:THR:HG23	1.81	0.62
1:A:979:PHE:HB3	2:A:1305:Y01:CAP	2.29	0.62
1:A:730:LEU:HD12	1:A:733:PHE:HB2	1.82	0.62
1:A:896:TYR:OH	1:A:975:ARG:NH1	2.32	0.62
1:C:1207:MET:HG2	1:D:1207:MET:HE1	1.82	0.62
1:A:857:TRP:CZ2	2:A:1305:Y01:CAJ	2.83	0.62
1:B:771:ILE:O	1:B:774:LEU:HD22	2.00	0.62
1:D:730:LEU:HD12	1:D:733:PHE:HB2	1.82	0.62
1:A:961:GLY:O	1:A:965:TYR:HB2	2.00	0.61
1:B:774:LEU:HD23	1:B:774:LEU:H	1.65	0.61
1:D:961:GLY:O	1:D:965:TYR:HB2	2.00	0.61
1:B:1207:MET:HG2	1:C:1207:MET:HE1	1.82	0.61
1:C:961:GLY:O	1:C:965:TYR:HB2	2.00	0.61
1:A:1093:ILE:O	1:A:1097:ASN:HB2	2.01	0.61
1:A:982:VAL:HG22	2:A:1305:Y01:CAB	2.26	0.61
1:D:1093:ILE:O	1:D:1097:ASN:HB2	2.01	0.61
1:B:1093:ILE:O	1:B:1097:ASN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1211:ILE:CD1	1:C:1207:MET:HE3	2.30	0.61
1:C:730:LEU:HD12	1:C:733:PHE:HB2	1.82	0.61
1:B:961:GLY:O	1:B:965:TYR:HB2	2.00	0.61
1:D:771:ILE:O	1:D:774:LEU:HD22	2.00	0.60
1:A:1211:ILE:CD1	1:B:1207:MET:HE3	2.29	0.60
1:D:774:LEU:HD23	1:D:774:LEU:H	1.65	0.60
1:C:1093:ILE:O	1:C:1097:ASN:HB2	2.01	0.60
1:B:730:LEU:HD12	1:B:733:PHE:HB2	1.82	0.60
2:D:1302:Y01:HAA3	2:D:1303:Y01:CBC	2.32	0.60
1:D:1195:GLU:OE2	1:D:1198:ARG:NH1	2.35	0.60
1:C:1127:VAL:C	1:C:1128:LEU:HD22	2.26	0.60
1:B:1127:VAL:C	1:B:1128:LEU:HD22	2.26	0.59
1:C:1211:ILE:CD1	1:D:1207:MET:HE3	2.29	0.59
1:A:1195:GLU:OE2	1:A:1198:ARG:NH1	2.35	0.59
1:B:980:LEU:CD2	1:B:986:ALA:CB	2.81	0.59
1:A:980:LEU:CD2	1:A:986:ALA:CB	2.81	0.59
1:C:980:LEU:CD2	1:C:986:ALA:CB	2.81	0.59
1:C:1195:GLU:OE2	1:C:1198:ARG:NH1	2.35	0.59
1:C:771:ILE:O	1:C:774:LEU:HD22	2.03	0.59
1:B:1034:LYS:O	1:B:1038:PHE:CB	2.51	0.58
1:B:863:TYR:CD2	1:B:979:PHE:HE2	2.21	0.58
1:B:1195:GLU:OE2	1:B:1198:ARG:NH1	2.35	0.58
1:D:1127:VAL:O	1:D:1128:LEU:HD13	2.03	0.58
1:D:1083:VAL:HA	1:D:1087:ILE:HD12	1.85	0.58
1:C:863:TYR:CD2	1:C:979:PHE:HE2	2.21	0.58
1:D:1034:LYS:O	1:D:1038:PHE:CB	2.51	0.58
1:A:709:LEU:CD1	1:A:739:THR:HG22	2.34	0.58
1:A:863:TYR:CD2	1:A:979:PHE:HE2	2.21	0.58
1:A:771:ILE:O	1:A:774:LEU:HD22	2.03	0.58
1:A:1083:VAL:HA	1:A:1087:ILE:HD12	1.85	0.58
1:B:1008:ALA:HB1	2:C:1302:Y01:HAL2	1.85	0.57
1:D:744:SER:OG	1:D:1115:ARG:NH2	2.37	0.57
2:D:1302:Y01:HAB2	2:D:1303:Y01:HAR2	1.86	0.57
1:B:980:LEU:HA	2:B:1302:Y01:HAE3	1.85	0.57
1:A:1011:LEU:O	1:A:1011:LEU:HD23	2.03	0.57
1:A:1127:VAL:O	1:A:1128:LEU:HD13	2.04	0.57
1:B:744:SER:OG	1:B:1115:ARG:NH2	2.37	0.57
1:C:744:SER:OG	1:C:1115:ARG:NH2	2.37	0.57
1:D:488:MET:HA	1:D:491:HIS:HD2	1.70	0.57
1:D:709:LEU:HD13	1:D:739:THR:HG22	1.85	0.57
1:A:488:MET:HA	1:A:491:HIS:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:MET:HA	1:C:491:HIS:HD2	1.70	0.57
1:A:979:PHE:HB3	2:A:1305:Y01:HAP2	1.86	0.57
1:A:509:LEU:HA	1:A:512:ILE:HD12	1.87	0.57
1:B:509:LEU:HA	1:B:512:ILE:HD12	1.87	0.57
1:C:1083:VAL:HA	1:C:1087:ILE:HD12	1.85	0.57
1:A:271:ASN:HD22	1:A:297:ILE:CD1	2.18	0.56
1:C:509:LEU:HA	1:C:512:ILE:HD12	1.87	0.56
1:C:980:LEU:HD21	1:C:986:ALA:CB	2.35	0.56
1:A:982:VAL:HG23	2:A:1305:Y01:CAB	2.28	0.56
1:B:1083:VAL:HA	1:B:1087:ILE:HD12	1.85	0.56
1:D:509:LEU:HA	1:D:512:ILE:HD12	1.87	0.56
2:A:1304:Y01:CAA	2:A:1305:Y01:HBC	2.33	0.56
1:B:980:LEU:HD21	1:B:986:ALA:CB	2.35	0.56
1:C:980:LEU:HD23	1:C:980:LEU:O	2.06	0.56
1:D:476:GLU:O	1:D:477:LEU:HB3	2.05	0.56
1:A:744:SER:OG	1:A:1115:ARG:NH2	2.37	0.56
1:A:980:LEU:HD23	1:A:980:LEU:O	2.06	0.56
1:C:476:GLU:O	1:C:477:LEU:HB3	2.05	0.56
1:C:874:VAL:HG21	1:C:969:ILE:HD11	1.87	0.56
1:A:980:LEU:HD21	1:A:986:ALA:CB	2.35	0.56
1:B:709:LEU:CD1	1:B:739:THR:HG22	2.34	0.56
1:A:467:LYS:HA	1:A:617:ARG:HE	1.71	0.56
1:D:874:VAL:HG21	1:D:969:ILE:HD11	1.87	0.56
2:C:1302:Y01:HAN1	2:C:1302:Y01:HAP1	1.87	0.56
1:B:874:VAL:HG21	1:B:969:ILE:HD11	1.87	0.56
1:B:980:LEU:O	1:B:980:LEU:HD23	2.06	0.56
1:A:874:VAL:HG21	1:A:969:ILE:HD11	1.87	0.55
1:A:1207:MET:CE	1:D:1211:ILE:HD12	2.27	0.55
1:B:267:GLU:O	1:B:271:ASN:HB2	2.06	0.55
1:B:488:MET:HA	1:B:491:HIS:HD2	1.70	0.55
1:D:982:VAL:CG2	2:D:1303:Y01:HAB1	2.21	0.55
1:B:467:LYS:HA	1:B:617:ARG:HE	1.71	0.55
1:D:774:LEU:CD2	1:D:775:GLU:H	2.20	0.55
1:A:476:GLU:O	1:A:477:LEU:CB	2.53	0.55
1:A:477:LEU:HD21	1:A:628:TRP:CE2	2.41	0.55
1:A:271:ASN:ND2	1:A:297:ILE:HD13	2.22	0.55
1:C:267:GLU:O	1:C:271:ASN:HB2	2.06	0.55
1:C:1034:LYS:O	1:C:1038:PHE:CB	2.51	0.55
1:A:1034:LYS:O	1:A:1038:PHE:CB	2.51	0.55
1:B:476:GLU:O	1:B:477:LEU:HB3	2.05	0.55
1:B:774:LEU:CD2	1:B:775:GLU:H	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:LEU:CD1	1:C:739:THR:HG22	2.34	0.55
1:A:267:GLU:O	1:A:271:ASN:HB2	2.06	0.54
1:C:467:LYS:HA	1:C:617:ARG:HE	1.71	0.54
1:D:267:GLU:O	1:D:271:ASN:HB2	2.06	0.54
1:A:774:LEU:H	1:A:774:LEU:CD2	2.21	0.54
1:B:1129:PRO:C	1:B:1131:PRO:HD2	2.33	0.54
1:C:762:ILE:HG23	1:C:861:LEU:HD11	1.90	0.54
1:C:849:TYR:HB3	1:C:1127:VAL:HG11	1.90	0.54
1:A:1207:MET:HG2	1:B:1207:MET:HE1	1.89	0.54
1:D:467:LYS:HA	1:D:617:ARG:HE	1.71	0.54
1:D:762:ILE:HG23	1:D:861:LEU:HD11	1.90	0.54
1:B:762:ILE:HG23	1:B:861:LEU:HD11	1.90	0.54
1:B:849:TYR:HB3	1:B:1127:VAL:HG11	1.90	0.53
1:B:1014:PHE:HB2	2:B:1301:Y01:HAA1	1.90	0.53
1:C:862:ALA:HB3	1:C:1129:PRO:HB3	1.91	0.53
1:A:284:PRO:HG2	1:A:298:LEU:HB2	1.90	0.53
1:A:857:TRP:CH2	2:A:1305:Y01:CAO	2.89	0.53
1:A:1127:VAL:O	1:A:1128:LEU:HD22	2.09	0.53
1:A:762:ILE:HG23	1:A:861:LEU:HD11	1.90	0.53
1:B:862:ALA:HB3	1:B:1129:PRO:HB3	1.91	0.53
1:B:1207:MET:HG2	1:C:1207:MET:CE	2.39	0.53
1:C:394:ALA:O	1:C:398:ALA:CB	2.57	0.53
1:A:394:ALA:O	1:A:398:ALA:CB	2.57	0.53
1:D:1127:VAL:O	1:D:1128:LEU:HD22	2.09	0.53
1:C:1207:MET:HG2	1:D:1207:MET:CE	2.39	0.53
1:D:394:ALA:O	1:D:398:ALA:HB3	2.09	0.53
1:A:394:ALA:O	1:A:398:ALA:HB3	2.09	0.52
1:A:477:LEU:HD23	1:A:477:LEU:C	2.34	0.52
2:A:1305:Y01:CAB	2:A:1305:Y01:CAC	2.85	0.52
1:A:1207:MET:SD	1:B:1207:MET:HE1	2.49	0.52
1:B:394:ALA:O	1:B:398:ALA:CB	2.57	0.52
1:D:394:ALA:O	1:D:398:ALA:CB	2.57	0.52
1:B:394:ALA:O	1:B:398:ALA:HB3	2.09	0.52
1:C:1129:PRO:C	1:C:1131:PRO:HD2	2.33	0.52
1:A:750:ARG:HG2	1:A:847:ALA:HB1	1.92	0.52
2:A:1301:Y01:HAR1	1:B:923:TYR:CB	2.39	0.52
2:A:1305:Y01:HAL2	1:D:1008:ALA:HB1	1.91	0.52
1:D:509:LEU:HD23	1:D:512:ILE:HD12	1.92	0.52
1:D:1011:LEU:HD23	1:D:1011:LEU:C	2.35	0.52
1:A:440:GLU:HG3	1:A:468:PHE:HD1	1.75	0.52
1:B:750:ARG:HG2	1:B:847:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:GLU:HG3	1:D:468:PHE:HD1	1.75	0.52
1:B:1082:PHE:O	1:B:1086:ILE:HB	2.10	0.52
1:C:440:GLU:HG3	1:C:468:PHE:HD1	1.75	0.52
1:B:440:GLU:HG3	1:B:468:PHE:HD1	1.75	0.51
2:C:1301:Y01:HAA3	2:C:1302:Y01:HAR1	1.85	0.51
1:D:774:LEU:H	1:D:774:LEU:CD2	2.23	0.51
1:A:477:LEU:CD2	1:A:628:TRP:CE2	2.93	0.51
1:A:509:LEU:HD23	1:A:512:ILE:HD12	1.92	0.51
2:C:1302:Y01:HAR1	2:C:1302:Y01:OAG	2.10	0.51
1:C:1082:PHE:O	1:C:1086:ILE:HB	2.10	0.51
1:D:750:ARG:HG2	1:D:847:ALA:HB1	1.92	0.51
1:C:774:LEU:N	1:C:774:LEU:CD2	2.73	0.51
1:D:391:ILE:HG22	1:D:393:VAL:H	1.76	0.51
1:A:774:LEU:CD2	1:A:774:LEU:N	2.73	0.51
1:C:394:ALA:O	1:C:398:ALA:HB3	2.09	0.51
1:C:774:LEU:H	1:C:774:LEU:CD2	2.21	0.51
1:C:1011:LEU:HD23	1:C:1011:LEU:C	2.35	0.51
1:A:1207:MET:CE	1:D:1207:MET:HG2	2.41	0.51
1:C:750:ARG:HG2	1:C:847:ALA:HB1	1.92	0.51
2:D:1303:Y01:CAB	2:D:1303:Y01:HAO2	2.41	0.51
1:A:1014:PHE:HB2	2:A:1301:Y01:HAB1	1.91	0.51
1:C:509:LEU:HD23	1:C:512:ILE:HD12	1.92	0.51
2:A:1305:Y01:HAR1	2:A:1305:Y01:OAG	2.11	0.51
1:A:1082:PHE:O	1:A:1086:ILE:HB	2.10	0.50
1:B:509:LEU:HD23	1:B:512:ILE:HD12	1.92	0.50
1:B:774:LEU:H	1:B:774:LEU:CD2	2.23	0.50
1:D:774:LEU:HD23	1:D:775:GLU:H	1.77	0.50
2:A:1301:Y01:HAU2	2:A:1301:Y01:CAC	2.40	0.50
1:C:1129:PRO:HB2	1:C:1131:PRO:HD2	1.93	0.50
1:D:1082:PHE:O	1:D:1086:ILE:HB	2.10	0.50
1:B:391:ILE:HG22	1:B:393:VAL:H	1.76	0.50
1:A:774:LEU:HD23	1:A:774:LEU:N	2.23	0.50
1:B:276:HIS:HB2	1:B:279:ILE:HB	1.94	0.50
1:B:1129:PRO:HB2	1:B:1131:PRO:HD2	1.93	0.50
1:A:391:ILE:HG22	1:A:393:VAL:H	1.76	0.50
1:A:474:LEU:HB3	1:A:509:LEU:HD21	1.93	0.50
1:B:474:LEU:HB3	1:B:509:LEU:HD21	1.93	0.50
1:C:391:ILE:HG22	1:C:393:VAL:H	1.76	0.50
1:C:474:LEU:HB3	1:C:509:LEU:HD21	1.93	0.50
1:D:474:LEU:HB3	1:D:509:LEU:HD21	1.93	0.50
1:A:305:GLN:HA	1:A:310:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1043:MET:HB3	1:D:1081:LEU:HD21	1.94	0.50
1:A:1207:MET:HE2	1:B:1207:MET:CE	2.42	0.50
1:B:982:VAL:CG2	2:B:1302:Y01:CAA	2.65	0.50
1:C:1207:MET:CG	1:D:1207:MET:HE1	2.41	0.50
1:A:1207:MET:HG2	1:B:1207:MET:CE	2.42	0.49
1:B:1011:LEU:HD23	1:B:1011:LEU:C	2.35	0.49
1:B:1043:MET:HB3	1:B:1081:LEU:HD21	1.94	0.49
1:C:276:HIS:HB2	1:C:279:ILE:HB	1.94	0.49
1:C:1043:MET:HB3	1:C:1081:LEU:HD21	1.94	0.49
1:A:1207:MET:CE	1:D:1211:ILE:CD1	2.88	0.49
1:A:857:TRP:CH2	2:A:1305:Y01:CAJ	2.95	0.49
1:A:1043:MET:HB3	1:A:1081:LEU:HD21	1.94	0.49
2:A:1305:Y01:CAC	2:A:1305:Y01:CAE	2.85	0.49
1:A:276:HIS:HB2	1:A:279:ILE:HB	1.94	0.49
1:A:271:ASN:HD22	1:A:297:ILE:HD13	1.77	0.49
1:A:1207:MET:HE1	1:D:1207:MET:CG	2.42	0.49
1:D:305:GLN:HA	1:D:310:VAL:HG21	1.94	0.49
1:B:305:GLN:HA	1:B:310:VAL:HG21	1.94	0.49
1:C:1011:LEU:C	1:C:1011:LEU:CD2	2.86	0.49
1:D:276:HIS:HB2	1:D:279:ILE:HB	1.94	0.49
1:A:1011:LEU:C	1:A:1011:LEU:CD2	2.85	0.49
1:B:774:LEU:HD23	1:B:775:GLU:H	1.76	0.49
1:C:928:ASP:OD2	1:C:975:ARG:NH1	2.46	0.49
1:B:1207:MET:CG	1:C:1207:MET:HE1	2.41	0.49
1:C:1207:MET:SD	1:D:1207:MET:HE1	2.53	0.48
1:D:1011:LEU:C	1:D:1011:LEU:CD2	2.86	0.48
1:A:298:LEU:HD13	1:A:400:LEU:CD1	2.40	0.48
1:A:856:PHE:HE2	2:A:1305:Y01:HAB3	1.78	0.48
1:B:980:LEU:CD2	1:B:986:ALA:HB1	2.43	0.48
1:C:288:LEU:O	1:C:294:PRO:HD2	2.13	0.48
1:D:288:LEU:O	1:D:294:PRO:HD2	2.13	0.48
1:B:928:ASP:OD2	1:B:975:ARG:NH1	2.46	0.48
1:B:1011:LEU:C	1:B:1011:LEU:CD2	2.86	0.48
1:B:774:LEU:HD23	1:B:775:GLU:N	2.29	0.48
1:C:305:GLN:HA	1:C:310:VAL:HG21	1.94	0.48
1:D:709:LEU:CD1	1:D:739:THR:HG22	2.43	0.48
2:B:1302:Y01:HAC1	2:B:1302:Y01:CAU	2.35	0.48
1:A:928:ASP:OD2	1:A:975:ARG:NH1	2.46	0.48
2:A:1301:Y01:HAV1	1:B:994:GLY:HA3	1.96	0.48
1:B:1033:ALA:HB2	2:C:1301:Y01:HAK1	1.95	0.47
1:B:1207:MET:SD	1:C:1207:MET:HE1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LEU:O	1:A:294:PRO:HD2	2.13	0.47
1:D:774:LEU:CG	1:D:775:GLU:N	2.73	0.47
1:A:980:LEU:CD2	1:A:986:ALA:HB1	2.43	0.47
2:A:1305:Y01:CAE	2:A:1305:Y01:CAO	2.85	0.47
1:C:980:LEU:CD2	1:C:986:ALA:HB1	2.43	0.47
1:D:928:ASP:OD2	1:D:975:ARG:NH1	2.46	0.47
2:D:1302:Y01:CAA	2:D:1303:Y01:CAR	2.79	0.47
1:A:1207:MET:CG	1:B:1207:MET:HE1	2.45	0.47
2:A:1305:Y01:HAO2	2:A:1305:Y01:CAE	2.26	0.47
2:A:1305:Y01:HAC3	2:A:1305:Y01:CBA	2.45	0.47
1:B:774:LEU:CG	1:B:775:GLU:N	2.73	0.47
2:D:1302:Y01:CAA	2:D:1303:Y01:OAW	2.63	0.47
1:C:980:LEU:CD2	1:C:986:ALA:HB3	2.45	0.47
1:C:1207:MET:HE2	1:D:1207:MET:CE	2.45	0.47
1:B:288:LEU:O	1:B:294:PRO:HD2	2.13	0.47
1:C:782:MET:HE3	1:C:787:GLN:HE21	1.80	0.47
1:A:1207:MET:CE	1:D:1207:MET:HE2	2.44	0.46
1:B:980:LEU:CD2	1:B:986:ALA:HB3	2.45	0.46
1:D:856:PHE:CZ	2:D:1303:Y01:HAC3	2.49	0.46
1:B:980:LEU:CD2	1:B:980:LEU:C	2.89	0.46
1:D:782:MET:HE3	1:D:787:GLN:HE21	1.80	0.46
1:A:863:TYR:CG	1:A:979:PHE:HE2	2.33	0.46
1:B:653:LEU:HD13	1:B:725:ALA:HB2	1.97	0.46
1:B:782:MET:HE3	1:B:787:GLN:HE21	1.80	0.46
1:D:477:LEU:O	1:D:628:TRP:NE1	2.49	0.46
1:D:856:PHE:CZ	2:D:1303:Y01:CAC	2.98	0.46
1:C:477:LEU:O	1:C:628:TRP:NE1	2.49	0.46
1:C:863:TYR:CG	1:C:979:PHE:HE2	2.33	0.46
1:D:774:LEU:HD23	1:D:775:GLU:N	2.29	0.46
1:A:980:LEU:CD2	1:A:980:LEU:C	2.89	0.46
1:A:740:GLN:NE2	1:A:1112:LYS:O	2.49	0.46
1:B:774:LEU:CD2	1:B:774:LEU:N	2.79	0.46
1:B:863:TYR:CG	1:B:979:PHE:HE2	2.33	0.46
1:D:740:GLN:NE2	1:D:1112:LYS:O	2.49	0.46
1:A:653:LEU:HD13	1:A:725:ALA:HB2	1.97	0.46
1:B:1207:MET:HE2	1:C:1207:MET:CE	2.45	0.46
1:C:740:GLN:NE2	1:C:1112:LYS:O	2.49	0.46
2:D:1303:Y01:HAB3	2:D:1303:Y01:HAO2	1.98	0.46
1:A:477:LEU:HD21	1:A:628:TRP:CD2	2.50	0.46
1:B:477:LEU:O	1:B:628:TRP:NE1	2.49	0.46
1:D:983:ASN:HB3	2:D:1303:Y01:HAN2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:MET:HE3	1:A:787:GLN:HE21	1.80	0.45
1:B:740:GLN:NE2	1:B:1112:LYS:O	2.49	0.45
1:B:854:VAL:O	1:B:858:PHE:HB2	2.16	0.45
1:B:860:THR:HG22	1:B:979:PHE:CD1	2.52	0.45
1:B:1090:ASN:HD21	1:C:1093:ILE:HA	1.81	0.45
2:B:1302:Y01:HAC3	2:B:1302:Y01:HAJ1	1.79	0.45
2:A:1305:Y01:HAB3	2:A:1305:Y01:HBB	1.98	0.45
1:C:860:THR:HG22	1:C:979:PHE:CD1	2.51	0.45
1:B:1060:SER:OG	1:B:1061:THR:O	2.34	0.45
1:D:774:LEU:CD2	1:D:774:LEU:N	2.79	0.45
1:A:298:LEU:CD1	1:A:400:LEU:HD12	2.45	0.45
1:A:980:LEU:CD2	1:A:986:ALA:HB3	2.45	0.45
2:A:1304:Y01:HAK1	1:D:1033:ALA:HB2	1.98	0.45
1:A:1090:ASN:HD21	1:B:1093:ILE:HA	1.81	0.45
1:C:980:LEU:CD2	1:C:980:LEU:C	2.89	0.45
1:C:1090:ASN:HD21	1:D:1093:ILE:HA	1.81	0.45
2:D:1302:Y01:HAA3	2:D:1303:Y01:HAR2	1.86	0.45
2:D:1303:Y01:HAU2	2:D:1303:Y01:HAC1	1.99	0.45
1:B:983:ASN:ND2	2:B:1302:Y01:HAC3	2.31	0.45
2:A:1302:Y01:HAB1	1:D:1014:PHE:HB2	1.98	0.45
1:C:653:LEU:HD13	1:C:725:ALA:HB2	1.97	0.45
2:A:1305:Y01:CAI	1:D:1009:LEU:HD11	2.37	0.45
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.71	0.45
1:D:653:LEU:HD13	1:D:725:ALA:HB2	1.97	0.45
1:D:710:THR:HG21	1:D:786:PRO:HG3	1.98	0.45
1:A:774:LEU:HG	1:A:775:GLU:H	1.83	0.44
1:A:476:GLU:C	1:A:478:TYR:H	2.26	0.44
1:A:854:VAL:O	1:A:858:PHE:HB2	2.16	0.44
1:A:860:THR:HG22	1:A:979:PHE:CD1	2.51	0.44
1:A:1060:SER:OG	1:A:1061:THR:O	2.34	0.44
1:B:474:LEU:C	1:B:476:GLU:O	2.61	0.44
1:C:854:VAL:O	1:C:858:PHE:HB2	2.16	0.44
1:A:1093:ILE:HA	1:D:1090:ASN:HD21	1.81	0.44
1:C:474:LEU:C	1:C:476:GLU:O	2.61	0.44
1:D:856:PHE:CE2	2:D:1303:Y01:CAC	2.87	0.44
1:C:895:THR:OG1	1:C:1130:PRO:O	2.27	0.44
1:A:1033:ALA:HB2	2:A:1303:Y01:CAK	2.46	0.44
1:C:1129:PRO:HD2	1:C:1132:LEU:HD12	1.99	0.44
1:D:474:LEU:C	1:D:476:GLU:O	2.61	0.44
1:A:700:GLN:HE22	1:A:1180:MET:HG3	1.83	0.44
1:B:1129:PRO:HD2	1:B:1132:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:LEU:HG	1:C:775:GLU:H	1.83	0.44
1:C:1203:ARG:O	1:C:1207:MET:HB2	2.18	0.44
1:D:980:LEU:HD23	2:D:1303:Y01:HBG	1.99	0.44
1:B:1203:ARG:O	1:B:1207:MET:HB2	2.17	0.44
1:D:1203:ARG:O	1:D:1207:MET:HB2	2.18	0.44
1:B:746:MET:HB3	1:B:1123:HIS:HE1	1.83	0.44
1:B:870:TYR:O	1:B:874:VAL:HG23	2.17	0.44
1:C:700:GLN:HE22	1:C:1180:MET:HG3	1.83	0.43
1:D:746:MET:HB3	1:D:1123:HIS:HE1	1.83	0.43
1:D:854:VAL:O	1:D:858:PHE:HB2	2.16	0.43
1:A:746:MET:HB3	1:A:1123:HIS:HE1	1.83	0.43
1:B:691:VAL:HG21	1:B:732:PRO:HB2	2.00	0.43
2:C:1302:Y01:CAC	2:C:1302:Y01:HAU2	2.48	0.43
1:C:858:PHE:CE2	1:C:1129:PRO:HD3	2.53	0.43
1:D:298:LEU:HD23	1:D:298:LEU:HA	1.80	0.43
2:D:1303:Y01:OAG	2:D:1303:Y01:HAV2	2.17	0.43
1:A:870:TYR:O	1:A:874:VAL:HG23	2.18	0.43
1:B:858:PHE:CE2	1:B:1129:PRO:HD3	2.53	0.43
1:C:680:LYS:HE3	1:C:680:LYS:HB2	1.86	0.43
1:C:870:TYR:O	1:C:874:VAL:HG23	2.18	0.43
2:B:1301:Y01:HAJ1	2:B:1301:Y01:HAC3	1.77	0.43
1:D:691:VAL:HG21	1:D:732:PRO:HB2	2.00	0.43
1:D:870:TYR:O	1:D:874:VAL:HG23	2.18	0.43
1:C:1033:ALA:HB2	2:D:1302:Y01:HAK1	2.00	0.43
1:A:469:LEU:HD11	1:A:625:LEU:HG	2.01	0.43
1:A:871:THR:HG21	1:A:973:TYR:OH	2.19	0.43
1:B:469:LEU:HD11	1:B:625:LEU:HG	2.01	0.43
1:C:871:THR:HG21	1:C:973:TYR:OH	2.19	0.43
1:D:700:GLN:HE22	1:D:1180:MET:HG3	1.83	0.43
1:D:871:THR:HG21	1:D:973:TYR:OH	2.19	0.43
1:B:871:THR:HG21	1:B:973:TYR:OH	2.19	0.43
1:C:691:VAL:HG21	1:C:732:PRO:HB2	2.00	0.43
1:D:774:LEU:HD23	1:D:774:LEU:N	2.34	0.42
1:A:477:LEU:HD23	1:A:628:TRP:NE1	2.34	0.42
2:A:1301:Y01:HAC1	2:A:1301:Y01:HAE2	2.01	0.42
1:B:892:TYR:CE2	1:B:1131:PRO:HD3	2.55	0.42
1:C:469:LEU:HD11	1:C:625:LEU:HG	2.01	0.42
1:D:868:MET:HG2	2:D:1302:Y01:HAE2	2.00	0.42
2:A:1303:Y01:HAB2	2:B:1302:Y01:HAV2	2.00	0.42
1:B:774:LEU:HG	1:B:775:GLU:N	2.30	0.42
1:C:746:MET:HB3	1:C:1123:HIS:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:LEU:HD11	1:D:625:LEU:HG	2.01	0.42
1:D:992:MET:HG3	1:D:1103:VAL:HG12	2.02	0.42
1:A:691:VAL:HG21	1:A:732:PRO:HB2	2.00	0.42
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.71	0.42
1:A:892:TYR:CE2	1:A:1131:PRO:HD3	2.55	0.42
1:A:959:VAL:HG11	1:D:1068:PRO:HB2	2.02	0.42
1:B:700:GLN:HE22	1:B:1180:MET:HG3	1.83	0.42
1:D:774:LEU:HG	1:D:775:GLU:N	2.30	0.42
1:A:1207:MET:HE1	1:D:1207:MET:SD	2.60	0.42
1:A:1068:PRO:HB2	1:B:959:VAL:HG11	2.02	0.42
1:B:288:LEU:HB3	1:B:294:PRO:HG2	2.02	0.42
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.71	0.42
1:C:983:ASN:HB3	2:C:1302:Y01:HAN2	2.02	0.42
1:B:746:MET:HE2	1:B:786:PRO:HG2	2.01	0.42
1:B:1160:LEU:HD13	1:B:1162:LEU:HG	2.02	0.42
1:D:474:LEU:HD23	1:D:474:LEU:HA	1.71	0.42
1:D:1160:LEU:HD22	1:D:1160:LEU:C	2.45	0.42
2:A:1303:Y01:HAD2	2:A:1303:Y01:HAS2	1.81	0.42
2:A:1305:Y01:HAJ1	2:A:1305:Y01:HAB3	1.82	0.42
1:B:288:LEU:O	1:B:294:PRO:CD	2.68	0.42
1:C:288:LEU:O	1:C:294:PRO:CD	2.68	0.42
1:D:288:LEU:HB3	1:D:294:PRO:HG2	2.02	0.41
2:A:1305:Y01:CAM	1:D:1012:LEU:HD11	2.51	0.41
1:B:980:LEU:HA	2:B:1302:Y01:HAE2	2.02	0.41
1:C:892:TYR:CE2	1:C:1131:PRO:HD3	2.55	0.41
1:C:1012:LEU:HD11	2:D:1303:Y01:HAM1	2.01	0.41
1:D:483:GLY:O	1:D:485:THR:HG23	2.20	0.41
1:D:892:TYR:CE2	1:D:1131:PRO:HD3	2.55	0.41
1:A:288:LEU:O	1:A:294:PRO:CD	2.68	0.41
1:A:746:MET:HE2	1:A:786:PRO:HG2	2.01	0.41
1:C:1160:LEU:HD13	1:C:1162:LEU:HG	2.02	0.41
1:C:483:GLY:O	1:C:485:THR:HG23	2.20	0.41
1:A:288:LEU:HB3	1:A:294:PRO:HG2	2.02	0.41
1:A:483:GLY:O	1:A:485:THR:HG23	2.20	0.41
1:A:1011:LEU:HD23	1:A:1011:LEU:C	2.44	0.41
1:B:992:MET:HG3	1:B:1103:VAL:HG12	2.02	0.41
1:C:1060:SER:OG	1:C:1061:THR:O	2.34	0.41
1:A:992:MET:HG3	1:A:1103:VAL:HG12	2.02	0.41
1:B:1068:PRO:HB2	1:C:959:VAL:HG11	2.02	0.41
1:C:869:LEU:HD23	1:C:869:LEU:HA	1.90	0.41
2:D:1301:Y01:HAD2	2:D:1301:Y01:HAS2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:MET:HE2	1:C:786:PRO:HG2	2.01	0.41
1:C:774:LEU:CG	1:C:775:GLU:H	2.34	0.41
1:D:746:MET:HE2	1:D:786:PRO:HG2	2.01	0.41
1:A:892:TYR:CD2	1:A:1131:PRO:HD3	2.56	0.41
1:D:717:SER:O	1:D:717:SER:OG	2.30	0.41
1:A:694:LEU:HD12	1:A:709:LEU:HD21	1.97	0.41
1:A:774:LEU:CG	1:A:775:GLU:H	2.34	0.41
1:C:1068:PRO:HB2	1:D:959:VAL:HG11	2.02	0.41
1:C:1160:LEU:HD22	1:C:1160:LEU:C	2.45	0.41
1:D:288:LEU:O	1:D:294:PRO:CD	2.68	0.41
1:A:456:LYS:HG2	1:A:640:PHE:CE1	2.56	0.41
1:B:869:LEU:HD23	1:B:869:LEU:HA	1.90	0.41
1:C:456:LYS:HG2	1:C:640:PHE:CE1	2.56	0.41
1:D:1160:LEU:HD13	1:D:1162:LEU:HG	2.02	0.41
1:A:730:LEU:HD22	1:A:730:LEU:HA	1.91	0.40
1:B:456:LYS:HG2	1:B:640:PHE:CE1	2.56	0.40
1:B:730:LEU:HD22	1:B:730:LEU:HA	1.91	0.40
1:C:288:LEU:HB3	1:C:294:PRO:HG2	2.02	0.40
1:C:298:LEU:HD23	1:C:298:LEU:HA	1.80	0.40
1:C:867:LEU:HA	1:C:867:LEU:HD23	1.89	0.40
1:D:892:TYR:CD2	1:D:1131:PRO:HD3	2.56	0.40
1:A:1207:MET:HE1	1:D:1207:MET:HE2	2.02	0.40
1:C:892:TYR:CD2	1:C:1131:PRO:HD3	2.56	0.40
1:C:992:MET:HG3	1:C:1103:VAL:HG12	2.02	0.40
1:B:421:ASP:O	1:B:425:ASN:ND2	2.55	0.40
1:B:483:GLY:O	1:B:485:THR:HG23	2.20	0.40
1:B:892:TYR:CD2	1:B:1131:PRO:HD3	2.56	0.40
1:A:298:LEU:HD13	1:A:400:LEU:HD12	2.03	0.40
1:A:516:ILE:CD1	1:A:627:ILE:HG21	2.51	0.40
1:A:1160:LEU:HD13	1:A:1162:LEU:HG	2.03	0.40
2:A:1305:Y01:HAM1	1:D:1012:LEU:HD11	2.04	0.40
1:B:874:VAL:CG1	1:B:969:ILE:HD11	2.41	0.40
1:C:421:ASP:O	1:C:425:ASN:ND2	2.55	0.40
1:A:1011:LEU:HD21	1:A:1040:PRO:HG2	2.02	0.40
1:A:1207:MET:HE2	1:B:1207:MET:HE2	2.04	0.40
1:B:477:LEU:HD23	1:B:477:LEU:C	2.46	0.40
1:C:412:ILE:HG21	1:C:412:ILE:HD13	1.90	0.40
2:C:1302:Y01:HAE2	2:C:1302:Y01:CAC	2.30	0.40
1:D:456:LYS:HG2	1:D:640:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	784/1229 (64%)	750 (96%)	32 (4%)	2 (0%)	36	66
1	B	784/1229 (64%)	751 (96%)	32 (4%)	1 (0%)	48	76
1	C	784/1229 (64%)	750 (96%)	32 (4%)	2 (0%)	36	66
1	D	784/1229 (64%)	753 (96%)	30 (4%)	1 (0%)	48	76
All	All	3136/4916 (64%)	3004 (96%)	126 (4%)	6 (0%)	44	71

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	625/1094 (57%)	612 (98%)	13 (2%)	47	67
1	B	625/1094 (57%)	612 (98%)	13 (2%)	47	67
1	C	625/1094 (57%)	612 (98%)	13 (2%)	47	67
1	D	625/1094 (57%)	611 (98%)	14 (2%)	45	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2500/4376 (57%)	2447 (98%)	53 (2%)	46 67

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	LEU
1	A	722	LEU
1	A	724	LEU
1	A	730	LEU
1	A	756	ASN
1	A	774	LEU
1	A	980	LEU
1	A	995	LYS
1	A	1011	LEU
1	A	1055	VAL
1	A	1097	ASN
1	A	1128	LEU
1	A	1160	LEU
1	B	458	LEU
1	B	722	LEU
1	B	724	LEU
1	B	730	LEU
1	B	756	ASN
1	B	774	LEU
1	B	980	LEU
1	B	995	LYS
1	B	1011	LEU
1	B	1055	VAL
1	B	1097	ASN
1	B	1128	LEU
1	B	1160	LEU
1	C	458	LEU
1	C	722	LEU
1	C	724	LEU
1	C	730	LEU
1	C	756	ASN
1	C	774	LEU
1	C	980	LEU
1	C	995	LYS
1	C	1011	LEU
1	C	1055	VAL
1	C	1097	ASN

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Mol	Chain	Res	Type
1	C	1128	LEU
1	C	1160	LEU
1	D	458	LEU
1	D	710	THR
1	D	722	LEU
1	D	724	LEU
1	D	730	LEU
1	D	756	ASN
1	D	774	LEU
1	D	980	LEU
1	D	995	LYS
1	D	1011	LEU
1	D	1055	VAL
1	D	1097	ASN
1	D	1128	LEU
1	D	1160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	276	HIS
1	A	425	ASN
1	A	491	HIS
1	A	700	GLN
1	A	756	ASN
1	A	787	GLN
1	A	789	GLN
1	A	1090	ASN
1	A	1098	ASN
1	A	1117	HIS
1	A	1123	HIS
1	B	276	HIS
1	B	425	ASN
1	B	491	HIS
1	B	700	GLN
1	B	756	ASN
1	B	787	GLN
1	B	789	GLN
1	B	1090	ASN
1	B	1098	ASN
1	B	1117	HIS

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Mol	Chain	Res	Type
1	B	1123	HIS
1	C	276	HIS
1	C	425	ASN
1	C	491	HIS
1	C	700	GLN
1	C	756	ASN
1	C	787	GLN
1	C	789	GLN
1	C	1090	ASN
1	C	1098	ASN
1	C	1117	HIS
1	C	1123	HIS
1	D	276	HIS
1	D	425	ASN
1	D	491	HIS
1	D	688	GLN
1	D	700	GLN
1	D	756	ASN
1	D	787	GLN
1	D	789	GLN
1	D	1090	ASN
1	D	1098	ASN
1	D	1117	HIS
1	D	1123	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	Y01	A	1301	-	38,38,38	1.88	5 (13%)	57,57,57	1.61	9 (15%)
2	Y01	A	1302	-	38,38,38	1.80	5 (13%)	57,57,57	1.86	13 (22%)
2	Y01	B	1301	-	38,38,38	1.87	5 (13%)	57,57,57	1.68	11 (19%)
2	Y01	D	1303	-	38,38,38	1.84	6 (15%)	57,57,57	1.70	14 (24%)
2	Y01	A	1304	-	38,38,38	2.38	8 (21%)	57,57,57	2.68	19 (33%)
2	Y01	B	1302	-	38,38,38	1.94	8 (21%)	57,57,57	2.11	18 (31%)
2	Y01	D	1302	-	38,38,38	2.31	6 (15%)	57,57,57	2.65	21 (36%)
2	Y01	C	1302	-	38,38,38	2.00	6 (15%)	57,57,57	1.55	6 (10%)
2	Y01	D	1301	-	38,38,38	1.86	7 (18%)	57,57,57	1.81	13 (22%)
2	Y01	C	1301	-	38,38,38	2.30	6 (15%)	57,57,57	2.61	20 (35%)
2	Y01	A	1303	-	38,38,38	2.19	7 (18%)	57,57,57	2.49	19 (33%)
2	Y01	A	1305	-	38,38,38	1.94	6 (15%)	57,57,57	1.59	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	1301	-	-	5/19/77/77	0/4/4/4
2	Y01	A	1302	-	-	5/19/77/77	0/4/4/4
2	Y01	B	1301	-	-	3/19/77/77	0/4/4/4
2	Y01	D	1303	-	-	5/19/77/77	0/4/4/4
2	Y01	A	1304	-	-	10/19/77/77	0/4/4/4
2	Y01	B	1302	-	-	10/19/77/77	0/4/4/4
2	Y01	D	1302	-	-	12/19/77/77	0/4/4/4
2	Y01	C	1302	-	-	9/19/77/77	0/4/4/4
2	Y01	D	1301	-	-	4/19/77/77	0/4/4/4
2	Y01	C	1301	-	-	10/19/77/77	0/4/4/4
2	Y01	A	1303	-	-	10/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	1305	-	-	9/19/77/77	0/4/4/4

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1304	Y01	CAV-CAZ	-6.50	1.38	1.51
2	C	1302	Y01	CAV-CAZ	-6.45	1.38	1.51
2	D	1302	Y01	CAK-CAI	-6.43	1.37	1.50
2	A	1303	Y01	CBH-CAZ	-6.41	1.40	1.52
2	A	1304	Y01	CAK-CAI	-6.38	1.37	1.50
2	A	1304	Y01	CBH-CAZ	-6.38	1.40	1.52
2	D	1302	Y01	CAV-CAZ	-6.36	1.39	1.51
2	C	1301	Y01	CAV-CAZ	-6.26	1.39	1.51
2	C	1301	Y01	CBH-CAZ	-6.24	1.41	1.52
2	C	1301	Y01	CAK-CAI	-6.23	1.37	1.50
2	D	1302	Y01	CBH-CAZ	-6.18	1.41	1.52
2	A	1303	Y01	CAV-CAZ	-6.18	1.39	1.51
2	A	1301	Y01	CAV-CAZ	-6.01	1.39	1.51
2	A	1305	Y01	CAV-CAZ	-5.92	1.39	1.51
2	D	1303	Y01	CAV-CAZ	-5.92	1.39	1.51
2	A	1303	Y01	CAK-CAI	-5.86	1.38	1.50
2	B	1301	Y01	CAV-CAZ	-5.76	1.40	1.51
2	A	1305	Y01	CBH-CAZ	-5.76	1.41	1.52
2	C	1302	Y01	CBH-CAZ	-5.74	1.41	1.52
2	B	1302	Y01	CBH-CAZ	-5.74	1.41	1.52
2	D	1301	Y01	CAV-CAZ	-5.63	1.40	1.51
2	A	1301	Y01	CBH-CAZ	-5.62	1.42	1.52
2	B	1301	Y01	CAK-CAI	-5.58	1.38	1.50
2	B	1301	Y01	CBH-CAZ	-5.55	1.42	1.52
2	B	1302	Y01	CAV-CAZ	-5.46	1.40	1.51
2	D	1301	Y01	CBH-CAZ	-5.45	1.42	1.52
2	D	1301	Y01	CAK-CAI	-5.41	1.39	1.50
2	A	1302	Y01	CBH-CAZ	-5.38	1.42	1.52
2	D	1303	Y01	CBH-CAZ	-5.32	1.42	1.52
2	A	1304	Y01	CAK-CBD	-5.27	1.44	1.53
2	D	1302	Y01	CAK-CBD	-5.07	1.44	1.53
2	A	1302	Y01	CAV-CAZ	-5.07	1.41	1.51
2	A	1302	Y01	CAK-CAI	-4.98	1.40	1.50
2	C	1301	Y01	CAK-CBD	-4.88	1.45	1.53
2	C	1302	Y01	CAK-CAI	-4.82	1.40	1.50
2	A	1304	Y01	CBI-CBG	-4.76	1.46	1.55
2	D	1303	Y01	CAK-CAI	-4.69	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	Y01	CAK-CAI	-4.68	1.40	1.50
2	D	1302	Y01	CBI-CBG	-4.63	1.46	1.55
2	C	1301	Y01	CBI-CBG	-4.57	1.46	1.55
2	A	1305	Y01	CAK-CAI	-4.46	1.41	1.50
2	B	1302	Y01	CAK-CAI	-4.31	1.41	1.50
2	A	1303	Y01	CBI-CBG	-4.18	1.47	1.55
2	A	1305	Y01	CAI-CAZ	3.58	1.40	1.33
2	C	1302	Y01	CAI-CAZ	3.52	1.40	1.33
2	A	1303	Y01	CAK-CBD	-3.48	1.47	1.53
2	B	1302	Y01	CAI-CAZ	3.46	1.40	1.33
2	D	1303	Y01	CAI-CAZ	3.42	1.40	1.33
2	A	1301	Y01	CAI-CAZ	3.31	1.39	1.33
2	A	1302	Y01	CAI-CAZ	3.13	1.39	1.33
2	D	1301	Y01	CAI-CAZ	3.01	1.39	1.33
2	A	1305	Y01	CAQ-CBG	-2.95	1.48	1.54
2	B	1301	Y01	CAI-CAZ	2.84	1.38	1.33
2	A	1303	Y01	CAI-CAZ	2.83	1.38	1.33
2	C	1302	Y01	CBD-CBG	-2.71	1.48	1.53
2	C	1302	Y01	CBI-CBG	-2.64	1.50	1.55
2	B	1302	Y01	CBI-CBG	-2.64	1.50	1.55
2	B	1302	Y01	CBI-CBE	-2.63	1.50	1.55
2	C	1301	Y01	CAI-CAZ	2.60	1.38	1.33
2	D	1302	Y01	CAI-CAZ	2.51	1.38	1.33
2	D	1303	Y01	CBI-CBG	-2.48	1.50	1.55
2	A	1301	Y01	CBI-CBG	-2.41	1.50	1.55
2	A	1304	Y01	CAI-CAZ	2.40	1.37	1.33
2	A	1305	Y01	CBI-CBG	-2.35	1.50	1.55
2	D	1303	Y01	CBD-CBG	-2.30	1.49	1.53
2	D	1301	Y01	OAW-CBC	-2.22	1.41	1.46
2	B	1302	Y01	CBD-CBG	-2.15	1.49	1.53
2	D	1301	Y01	CAQ-CBG	-2.12	1.50	1.54
2	B	1302	Y01	CAT-CBH	-2.12	1.50	1.54
2	A	1303	Y01	CBI-CBE	-2.11	1.51	1.55
2	A	1304	Y01	CBD-CBG	-2.04	1.49	1.53
2	B	1301	Y01	OAW-CBC	-2.04	1.41	1.46
2	D	1301	Y01	CBH-CBF	-2.03	1.52	1.56
2	A	1304	Y01	CBD-CBF	-2.02	1.49	1.53
2	A	1302	Y01	CAQ-CBG	-2.01	1.50	1.54

All (171) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1304	Y01	CBG-CBI-CBE	-9.62	89.06	100.10
2	A	1303	Y01	CAC-CBB-CBE	-8.82	99.65	112.88
2	C	1301	Y01	CAC-CBB-CBE	-8.34	100.36	112.88
2	D	1302	Y01	CAC-CBB-CBE	-8.20	100.58	112.88
2	C	1301	Y01	CBG-CBI-CBE	-8.08	90.83	100.10
2	A	1304	Y01	CAC-CBB-CBE	-7.72	101.29	112.88
2	D	1302	Y01	CBG-CBI-CBE	-7.72	91.25	100.10
2	A	1303	Y01	CBG-CBI-CBE	-7.68	91.28	100.10
2	D	1302	Y01	CAV-CAZ-CBH	6.05	124.17	116.42
2	C	1301	Y01	CAV-CAZ-CBH	5.28	123.18	116.42
2	A	1304	Y01	CAK-CBD-CBG	-5.25	103.50	110.93
2	D	1302	Y01	CAV-CAZ-CAI	-5.22	113.49	120.57
2	A	1304	Y01	CAV-CAZ-CBH	5.19	123.07	116.42
2	B	1302	Y01	CBI-CBE-CBB	-5.19	111.49	119.50
2	B	1302	Y01	CAV-CAZ-CBH	5.02	122.86	116.42
2	D	1302	Y01	CAK-CBD-CBG	-4.99	103.87	110.93
2	A	1303	Y01	CAV-CAZ-CBH	4.83	122.61	116.42
2	B	1301	Y01	CAV-CAZ-CBH	4.82	122.60	116.42
2	D	1303	Y01	CAQ-CBG-CBD	-4.75	111.52	119.10
2	C	1301	Y01	CAK-CBD-CBG	-4.74	104.22	110.93
2	A	1304	Y01	CAK-CBD-CBF	-4.73	104.25	109.72
2	C	1302	Y01	CAQ-CBG-CBD	-4.69	111.62	119.10
2	D	1301	Y01	CAV-CAZ-CBH	4.68	122.41	116.42
2	A	1302	Y01	CAV-CAZ-CBH	4.50	122.18	116.42
2	A	1301	Y01	CBI-CBE-CBB	-4.45	112.62	119.50
2	C	1301	Y01	CAV-CAZ-CAI	-4.45	114.54	120.57
2	A	1303	Y01	CBH-CBF-CBD	-4.44	106.22	112.71
2	C	1301	Y01	CBH-CBF-CBD	-4.33	106.38	112.71
2	A	1304	Y01	CAV-CAZ-CAI	-4.32	114.71	120.57
2	D	1302	Y01	CBH-CBF-CBD	-4.18	106.60	112.71
2	A	1302	Y01	CBH-CBF-CBD	-4.14	106.66	112.71
2	B	1301	Y01	CAQ-CBG-CBD	-4.11	112.54	119.10
2	A	1304	Y01	CBH-CBF-CBD	-4.10	106.72	112.71
2	A	1305	Y01	CBI-CBG-CBD	-4.09	108.60	114.41
2	A	1303	Y01	CAV-CAZ-CAI	-4.09	115.02	120.57
2	D	1301	Y01	CAQ-CBG-CBD	-4.09	112.58	119.10
2	B	1302	Y01	CAQ-CBG-CBD	-4.08	112.58	119.10
2	C	1302	Y01	CBI-CBG-CBD	-4.07	108.63	114.41
2	A	1302	Y01	CAQ-CBG-CBD	-4.07	112.61	119.10
2	D	1303	Y01	CBI-CBE-CBB	-4.07	113.22	119.50
2	B	1301	Y01	CAV-CAZ-CAI	-3.93	115.24	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1302	Y01	CBI-CBG-CBD	-3.92	108.84	114.41
2	A	1301	Y01	CAQ-CBG-CBD	-3.90	112.87	119.10
2	B	1302	Y01	CBC-CAV-CAZ	3.89	117.20	111.45
2	A	1303	Y01	CBI-CBG-CBD	-3.89	108.89	114.41
2	A	1305	Y01	CAQ-CBG-CBD	-3.89	112.90	119.10
2	C	1302	Y01	CBI-CBE-CBB	-3.88	113.50	119.50
2	A	1302	Y01	CAP-CBE-CBB	-3.87	106.32	112.18
2	D	1301	Y01	CAP-CBE-CBB	-3.78	106.46	112.18
2	C	1301	Y01	CBI-CBG-CBD	-3.76	109.08	114.41
2	A	1305	Y01	CBF-CBH-CAZ	3.71	115.08	109.65
2	D	1302	Y01	CBI-CBG-CBD	-3.70	109.16	114.41
2	A	1302	Y01	CAD-CBH-CBF	-3.67	107.54	111.66
2	D	1302	Y01	CAD-CBH-CBF	-3.66	107.55	111.66
2	C	1301	Y01	CAK-CBD-CBF	-3.64	105.51	109.72
2	A	1304	Y01	CAJ-CAO-CBB	-3.63	104.94	115.08
2	A	1303	Y01	CAK-CBD-CBG	-3.62	105.81	110.93
2	D	1301	Y01	CBG-CBI-CBE	-3.60	95.97	100.10
2	A	1302	Y01	CBG-CBI-CBE	-3.59	95.98	100.10
2	D	1301	Y01	CBH-CBF-CBD	-3.59	107.47	112.71
2	B	1302	Y01	CAD-CBH-CBF	-3.57	107.65	111.66
2	D	1301	Y01	CAV-CAZ-CAI	-3.57	115.73	120.57
2	A	1304	Y01	CAE-CBI-CBE	3.55	118.12	111.68
2	A	1305	Y01	CAP-CAQ-CBG	-3.54	98.21	105.14
2	A	1304	Y01	CBI-CBG-CBD	-3.52	109.42	114.41
2	C	1301	Y01	CAD-CBH-CBF	-3.50	107.73	111.66
2	A	1304	Y01	CAD-CBH-CBF	-3.48	107.75	111.66
2	B	1302	Y01	CBF-CBH-CAZ	3.48	114.75	109.65
2	B	1302	Y01	CBC-OAW-CAY	-3.47	109.48	117.80
2	C	1301	Y01	CAJ-CAO-CBB	-3.47	105.36	115.08
2	D	1302	Y01	CAJ-CAO-CBB	-3.43	105.49	115.08
2	D	1303	Y01	CBI-CBG-CBD	-3.42	109.56	114.41
2	C	1302	Y01	CAP-CBE-CBB	-3.39	107.05	112.18
2	B	1302	Y01	CAV-CAZ-CAI	-3.38	115.98	120.57
2	A	1303	Y01	CAO-CBB-CBE	3.36	117.30	110.33
2	B	1302	Y01	CBH-CBF-CBD	-3.36	107.80	112.71
2	D	1302	Y01	CAK-CBD-CBF	-3.34	105.86	109.72
2	A	1301	Y01	CBF-CBH-CAZ	3.31	114.50	109.65
2	A	1303	Y01	CAD-CBH-CBF	-3.28	107.98	111.66
2	C	1301	Y01	CAO-CBB-CBE	3.28	117.12	110.33
2	A	1301	Y01	CBI-CBG-CBD	-3.23	109.83	114.41
2	D	1302	Y01	CAO-CBB-CBE	3.22	117.00	110.33
2	D	1301	Y01	CAC-CBB-CAO	-3.19	105.41	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1302	Y01	CBC-CAV-CAZ	3.16	116.12	111.45
2	B	1302	Y01	CAC-CBB-CBE	-3.16	108.14	112.88
2	C	1301	Y01	CAQ-CBG-CBD	-3.15	114.07	119.10
2	C	1302	Y01	CBF-CBH-CAZ	3.14	114.25	109.65
2	D	1303	Y01	CAD-CBH-CBF	-3.13	108.15	111.66
2	A	1304	Y01	CAQ-CAP-CBE	-3.13	99.02	105.14
2	A	1303	Y01	CAJ-CAO-CBB	-3.11	106.39	115.08
2	D	1302	Y01	CAQ-CBG-CBD	-3.08	114.18	119.10
2	A	1304	Y01	CAQ-CBG-CBD	-3.08	114.18	119.10
2	A	1305	Y01	CBC-OAW-CAY	-3.05	110.49	117.80
2	D	1302	Y01	CBC-OAW-CAY	-3.04	110.53	117.80
2	A	1302	Y01	CAC-CBB-CAO	-3.03	105.65	110.34
2	C	1301	Y01	CAC-CBB-CAO	-3.03	105.65	110.34
2	A	1304	Y01	CAO-CBB-CBE	2.98	116.52	110.33
2	B	1301	Y01	CBH-CBF-CBD	-2.98	108.36	112.71
2	A	1303	Y01	CAQ-CBG-CBD	-2.96	114.37	119.10
2	D	1301	Y01	CAD-CBH-CBF	-2.96	108.34	111.66
2	A	1303	Y01	CBC-CAV-CAZ	2.94	115.80	111.45
2	D	1302	Y01	CAC-CBB-CAO	-2.92	105.82	110.34
2	B	1301	Y01	CBG-CBI-CBE	-2.92	96.75	100.10
2	B	1302	Y01	CAS-CAU-CBI	-2.91	107.83	112.74
2	A	1304	Y01	CAK-CAI-CAZ	-2.90	120.12	125.02
2	A	1302	Y01	CAV-CAZ-CAI	-2.89	116.66	120.57
2	A	1301	Y01	CAS-CAU-CBI	-2.88	107.88	112.74
2	A	1305	Y01	CBI-CBE-CBB	-2.88	115.05	119.50
2	B	1302	Y01	CAR-CBC-CAV	2.86	114.95	110.97
2	C	1301	Y01	CBC-OAW-CAY	-2.83	111.02	117.80
2	C	1301	Y01	CBC-CAV-CAZ	2.81	115.61	111.45
2	D	1303	Y01	CBF-CBH-CAZ	2.78	113.73	109.65
2	A	1302	Y01	CAC-CBB-CBE	2.78	117.06	112.88
2	A	1305	Y01	CAQ-CBG-CBI	-2.75	100.61	103.84
2	B	1301	Y01	CAP-CBE-CBB	-2.75	108.02	112.18
2	D	1302	Y01	CAS-CBF-CBD	-2.74	107.96	111.78
2	A	1303	Y01	CBC-OAW-CAY	-2.72	111.28	117.80
2	A	1304	Y01	CBC-CAV-CAZ	2.68	115.41	111.45
2	D	1303	Y01	CAP-CBE-CBB	-2.68	108.13	112.18
2	A	1303	Y01	CAQ-CAP-CBE	-2.67	99.92	105.14
2	D	1303	Y01	CAC-CBB-CBE	-2.66	108.89	112.88
2	C	1301	Y01	CAQ-CAP-CBE	-2.66	99.94	105.14
2	A	1304	Y01	CBC-OAW-CAY	-2.65	111.44	117.80
2	C	1301	Y01	CAS-CBF-CBD	-2.61	108.14	111.78
2	B	1301	Y01	CAD-CBH-CBF	-2.59	108.75	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	Y01	CAC-CBB-CBE	-2.59	109.00	112.88
2	C	1302	Y01	CAC-CBB-CBE	-2.54	109.07	112.88
2	A	1303	Y01	CAS-CBF-CBD	-2.53	108.24	111.78
2	D	1302	Y01	CAQ-CAP-CBE	-2.53	100.19	105.14
2	C	1301	Y01	CAE-CBI-CBE	2.52	116.25	111.68
2	A	1303	Y01	CAE-CBI-CBE	2.49	116.19	111.68
2	A	1302	Y01	CAK-CBD-CBF	-2.44	106.90	109.72
2	A	1302	Y01	CAS-CBF-CBH	-2.43	110.08	113.08
2	D	1303	Y01	CAT-CAR-CBC	-2.43	106.37	110.33
2	B	1301	Y01	CAK-CBD-CBG	-2.40	107.54	110.93
2	D	1303	Y01	CAS-CAU-CBI	-2.39	108.71	112.74
2	A	1301	Y01	CAP-CBE-CBB	-2.38	108.58	112.18
2	A	1302	Y01	CAP-CBE-CBI	-2.35	101.08	103.84
2	A	1305	Y01	CAJ-CAO-CBB	-2.34	108.53	115.08
2	D	1303	Y01	CAV-CAZ-CBH	2.34	119.41	116.42
2	C	1301	Y01	CAK-CAI-CAZ	-2.32	121.09	125.02
2	D	1302	Y01	CBI-CBE-CBB	-2.31	115.93	119.50
2	D	1302	Y01	CAK-CAI-CAZ	-2.31	121.13	125.02
2	D	1302	Y01	CAE-CBI-CBE	2.30	115.86	111.68
2	D	1303	Y01	CAR-CBC-CAV	-2.30	107.78	110.97
2	A	1303	Y01	CAK-CBD-CBF	-2.29	107.07	109.72
2	B	1302	Y01	CBD-CAK-CAI	2.29	115.94	112.76
2	C	1301	Y01	CBI-CBE-CBB	-2.29	115.96	119.50
2	A	1304	Y01	CAS-CBF-CBD	-2.28	108.60	111.78
2	A	1301	Y01	CAV-CAZ-CBH	2.28	119.34	116.42
2	D	1303	Y01	CAP-CAQ-CBG	-2.22	100.80	105.14
2	D	1301	Y01	CAP-CBE-CBI	-2.22	101.23	103.84
2	D	1303	Y01	CBH-CBF-CBD	-2.22	109.48	112.71
2	D	1301	Y01	CAS-CBF-CBH	-2.21	110.36	113.08
2	A	1303	Y01	CAC-CBB-CAO	-2.20	106.93	110.34
2	D	1301	Y01	CAC-CBB-CBE	2.19	116.17	112.88
2	A	1303	Y01	CBI-CBE-CBB	-2.15	116.17	119.50
2	A	1302	Y01	CAR-CAT-CBH	-2.14	108.23	112.78
2	A	1304	Y01	CBF-CBH-CAZ	2.14	112.78	109.65
2	B	1302	Y01	CBF-CBD-CBG	-2.10	106.34	109.09
2	D	1301	Y01	CAJ-CAN-CBA	-2.10	106.58	115.94
2	B	1301	Y01	CAP-CAQ-CBG	-2.08	101.08	105.14
2	A	1301	Y01	CAD-CBH-CBF	-2.05	109.36	111.66
2	B	1302	Y01	CAP-CBE-CBI	-2.03	101.45	103.84
2	B	1302	Y01	CAT-CBH-CBF	-2.03	106.05	108.74
2	D	1302	Y01	CAR-CBC-CAV	-2.03	108.15	110.97
2	B	1302	Y01	OAW-CAY-CAM	2.02	115.85	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	Y01	CAP-CBE-CBI	-2.01	101.47	103.84
2	D	1301	Y01	CAM-CAL-CAX	-2.01	108.33	113.67
2	B	1301	Y01	CAM-CAL-CAX	-2.01	108.33	113.67
2	D	1303	Y01	OAF-CAX-CAL	-2.00	116.74	123.09

There are no chirality outliers.

All (92) torsion outliers are listed below:

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

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

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

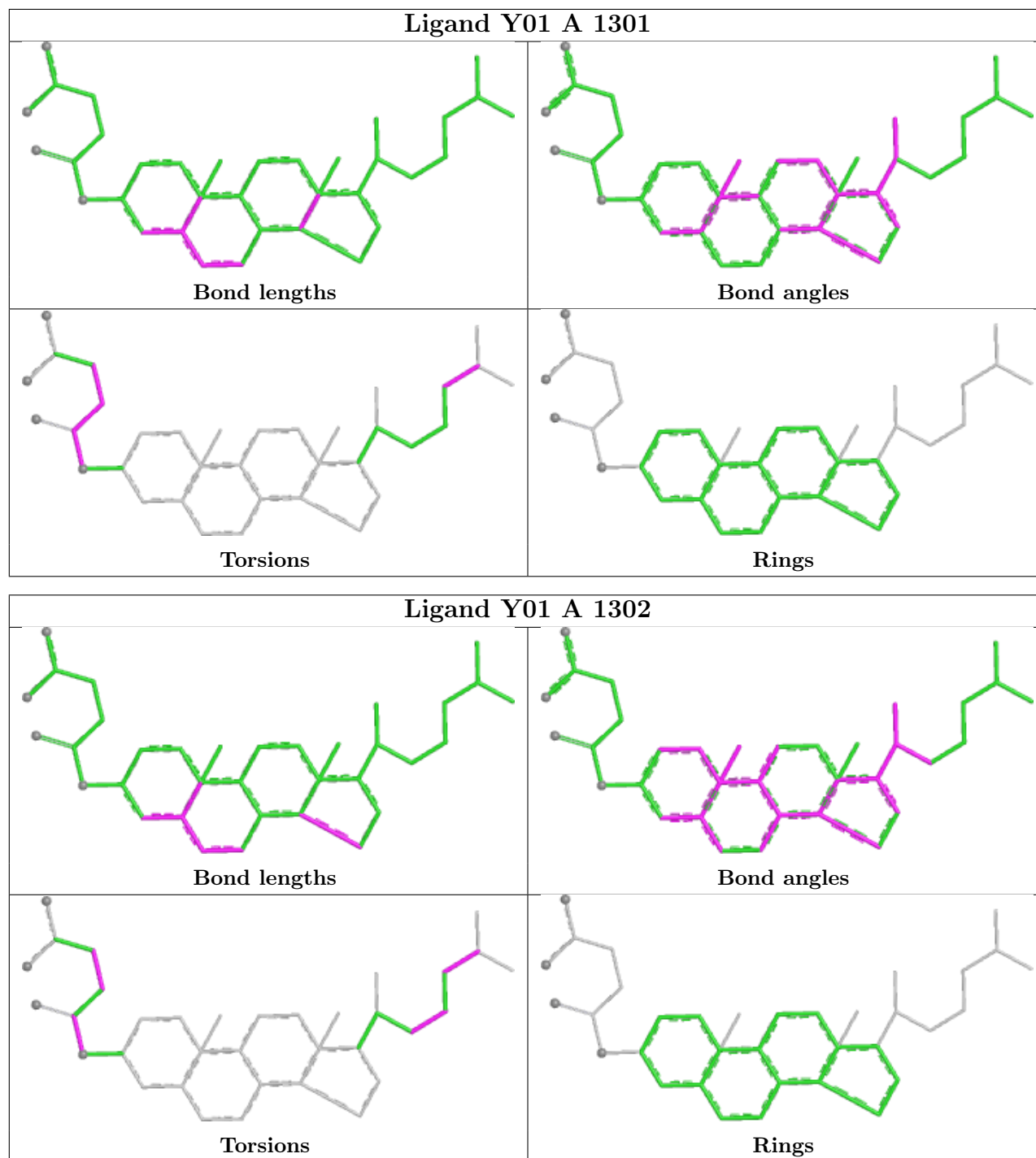
There are no ring outliers.

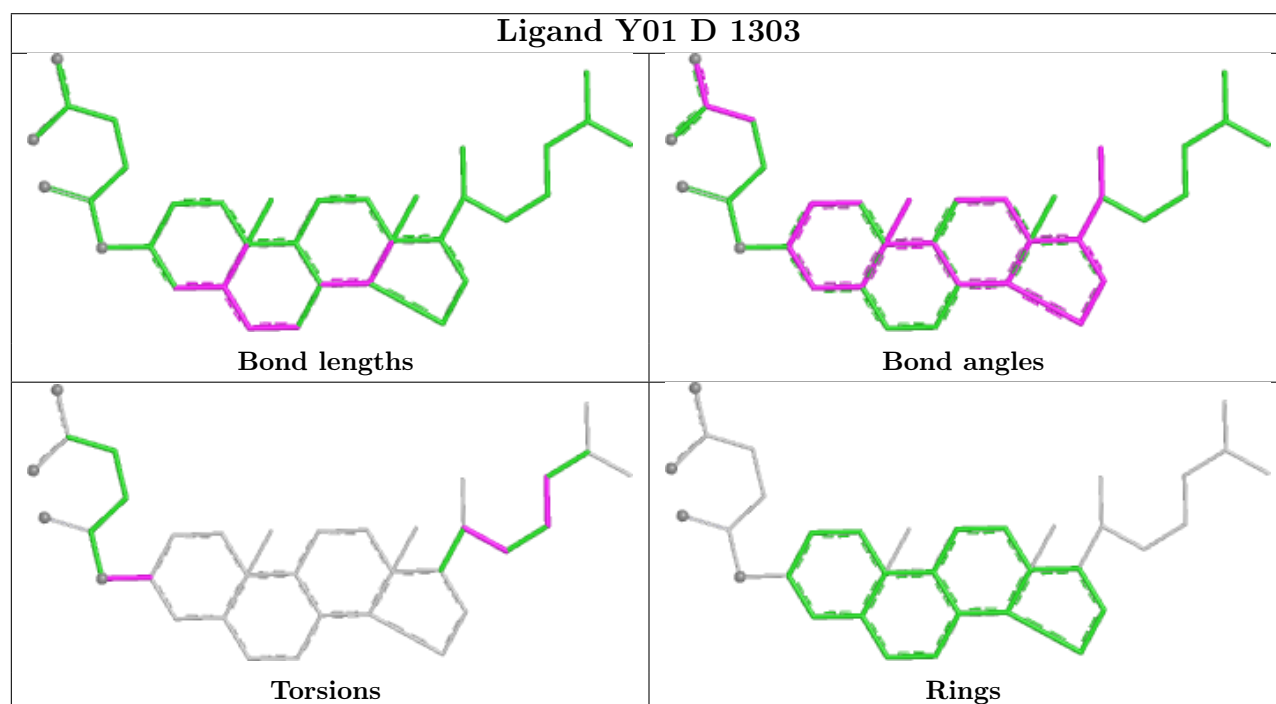
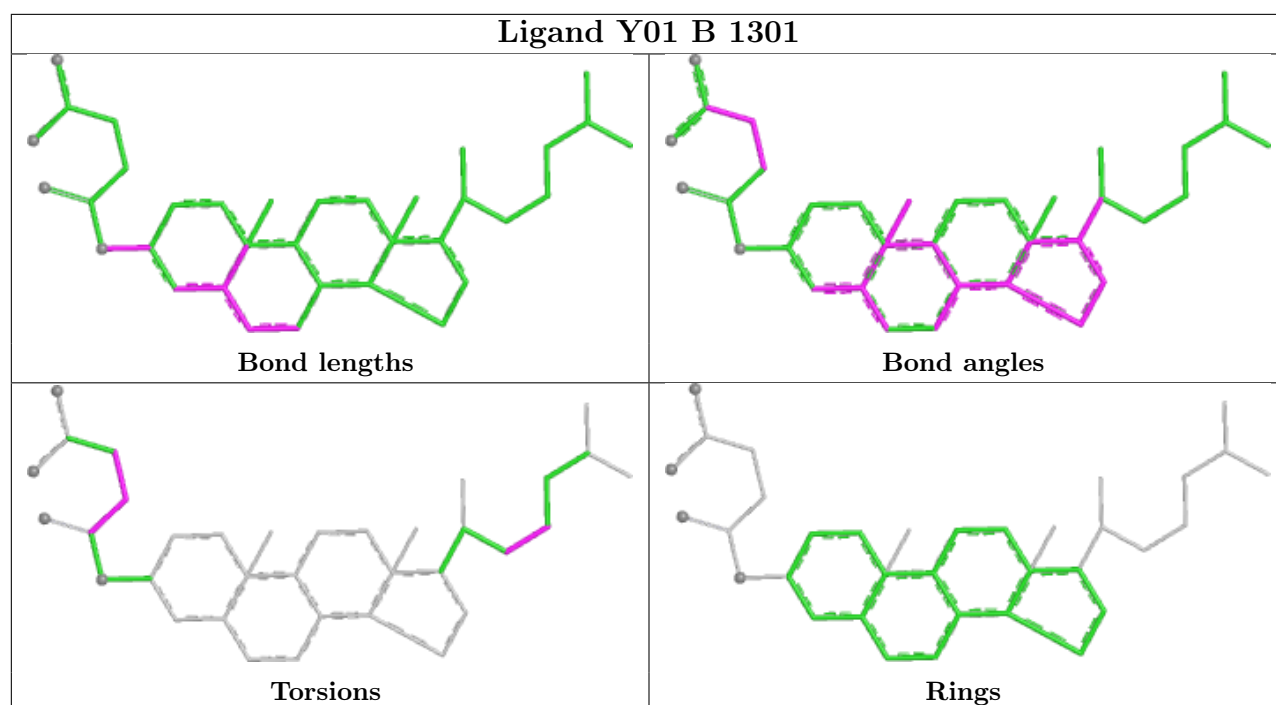
12 monomers are involved in 116 short contacts:

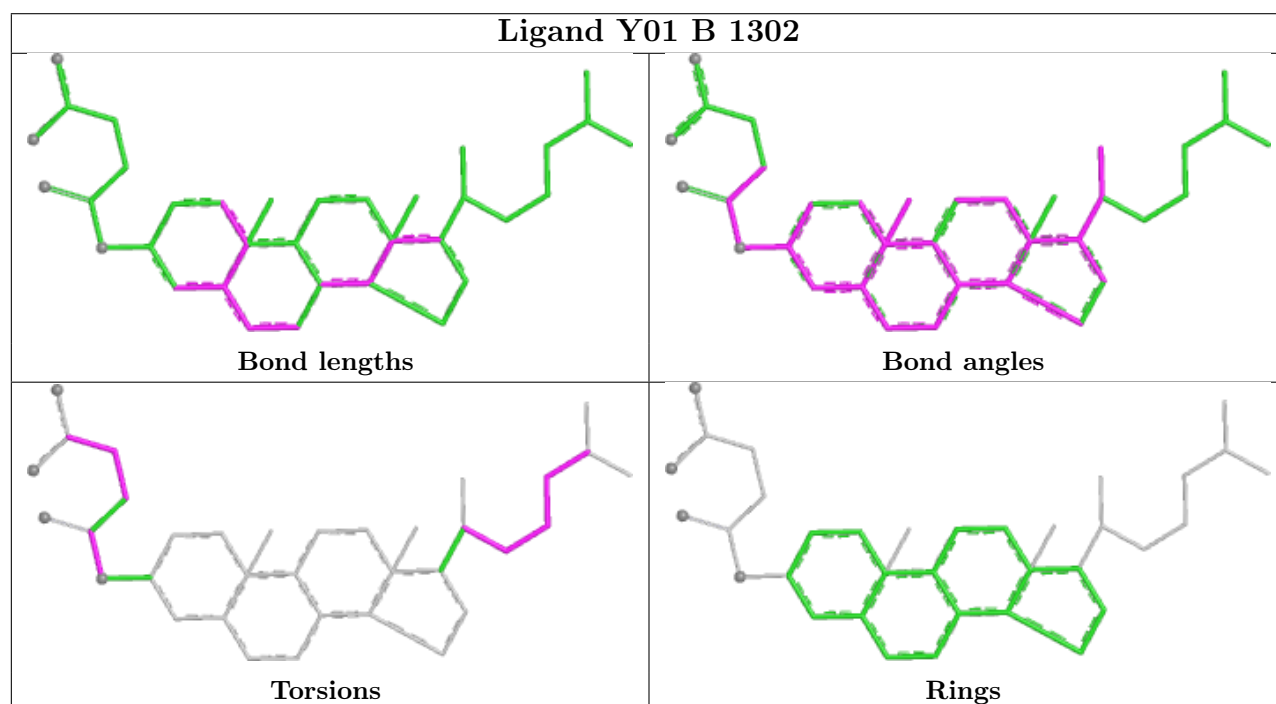
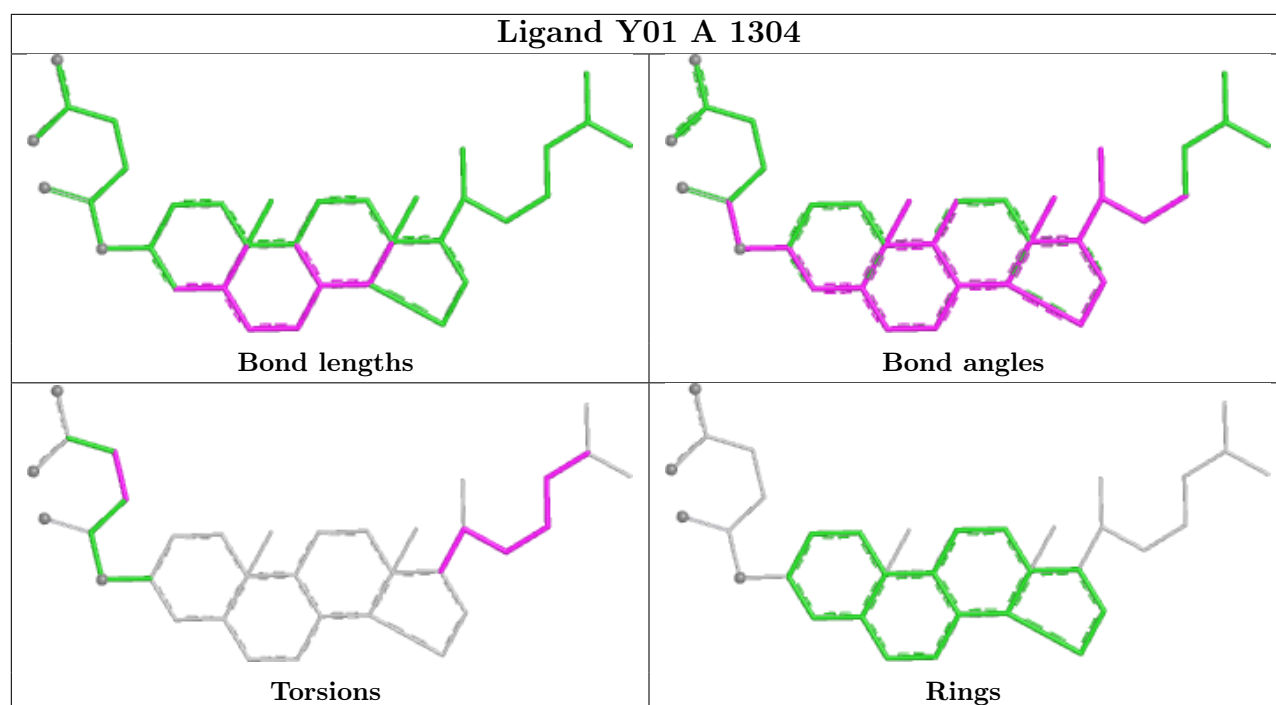
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	Y01	7	0
2	A	1302	Y01	1	0
2	B	1301	Y01	2	0
2	D	1303	Y01	29	0
2	A	1304	Y01	3	0
2	B	1302	Y01	15	0
2	D	1302	Y01	11	0
2	C	1302	Y01	12	0
2	D	1301	Y01	1	0
2	C	1301	Y01	6	0
2	A	1303	Y01	6	0
2	A	1305	Y01	42	0

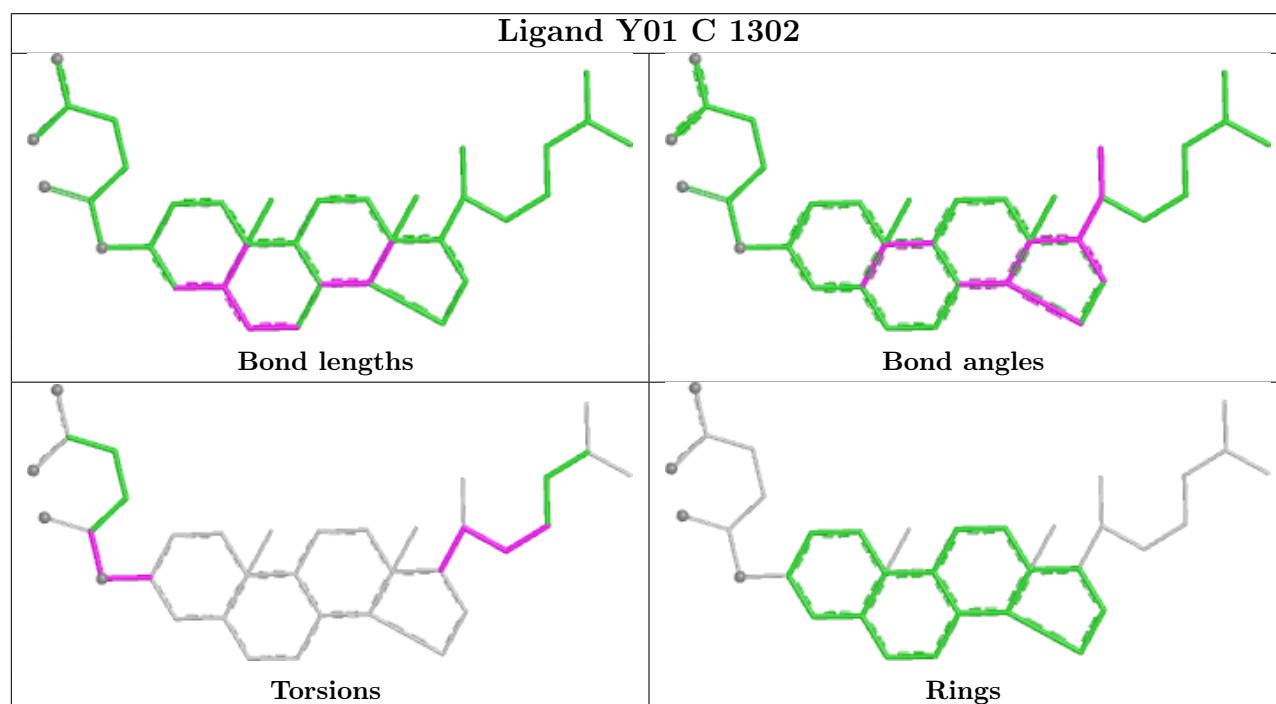
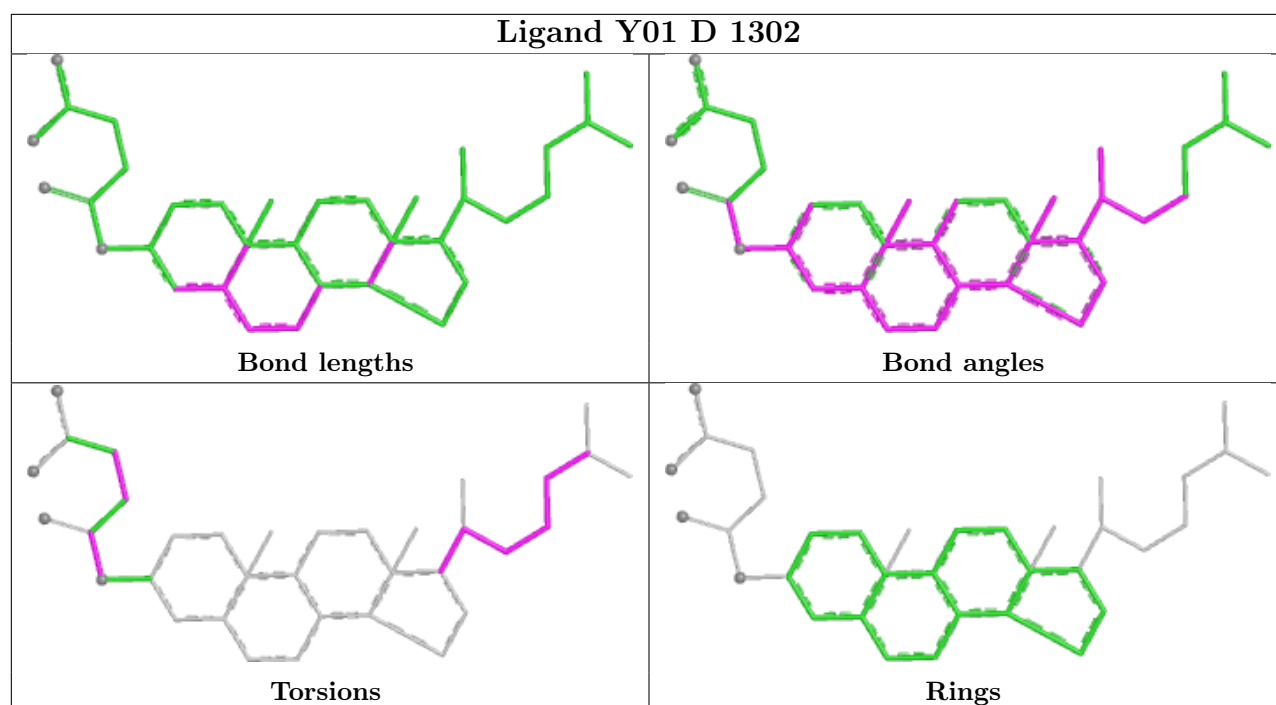
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

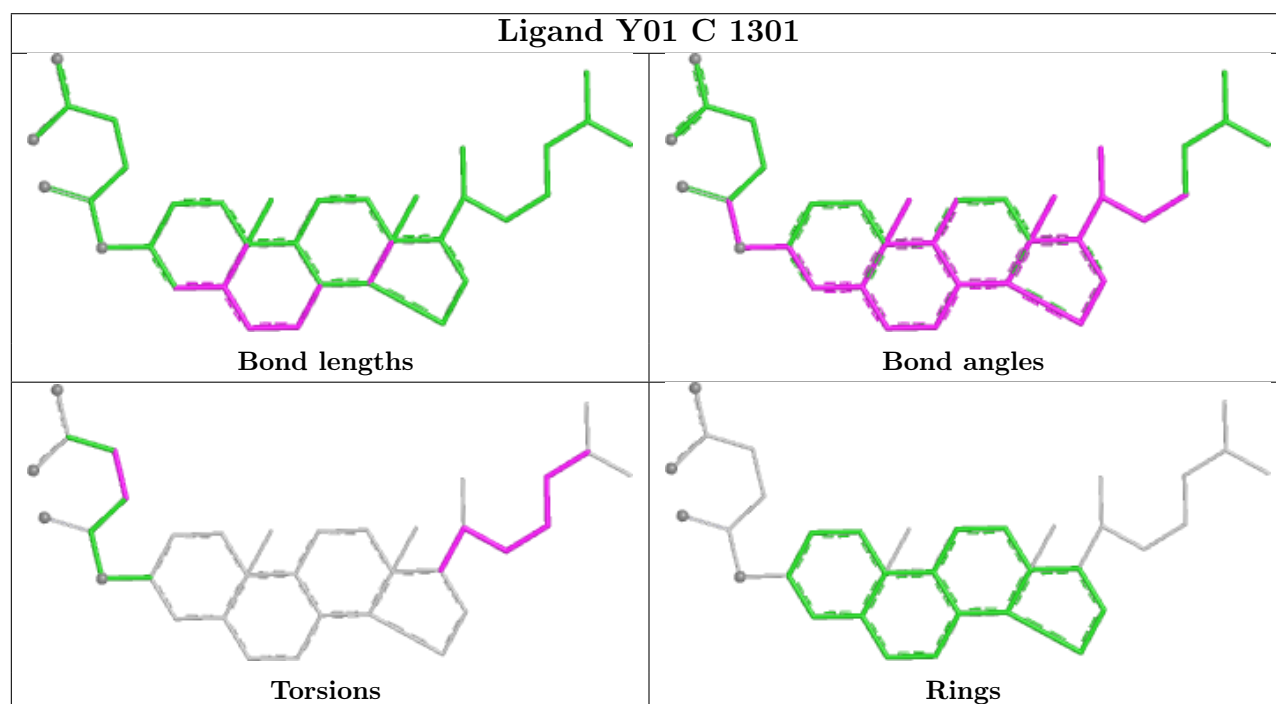
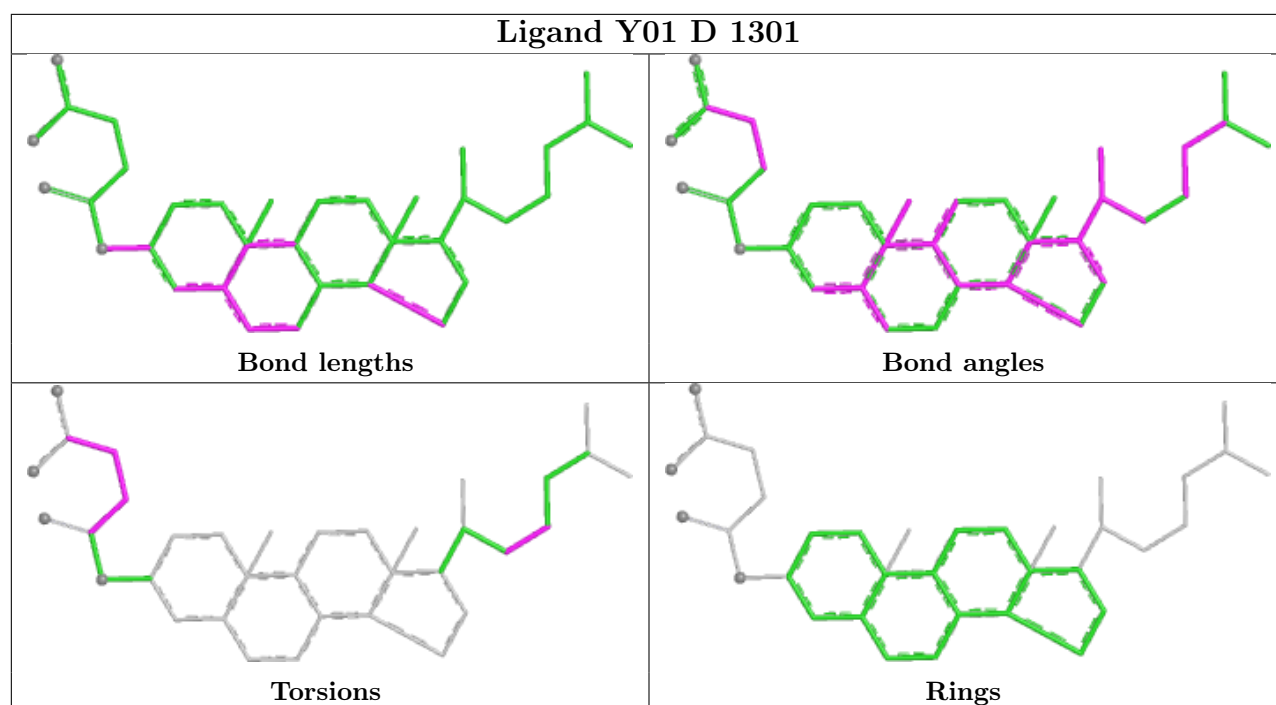
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

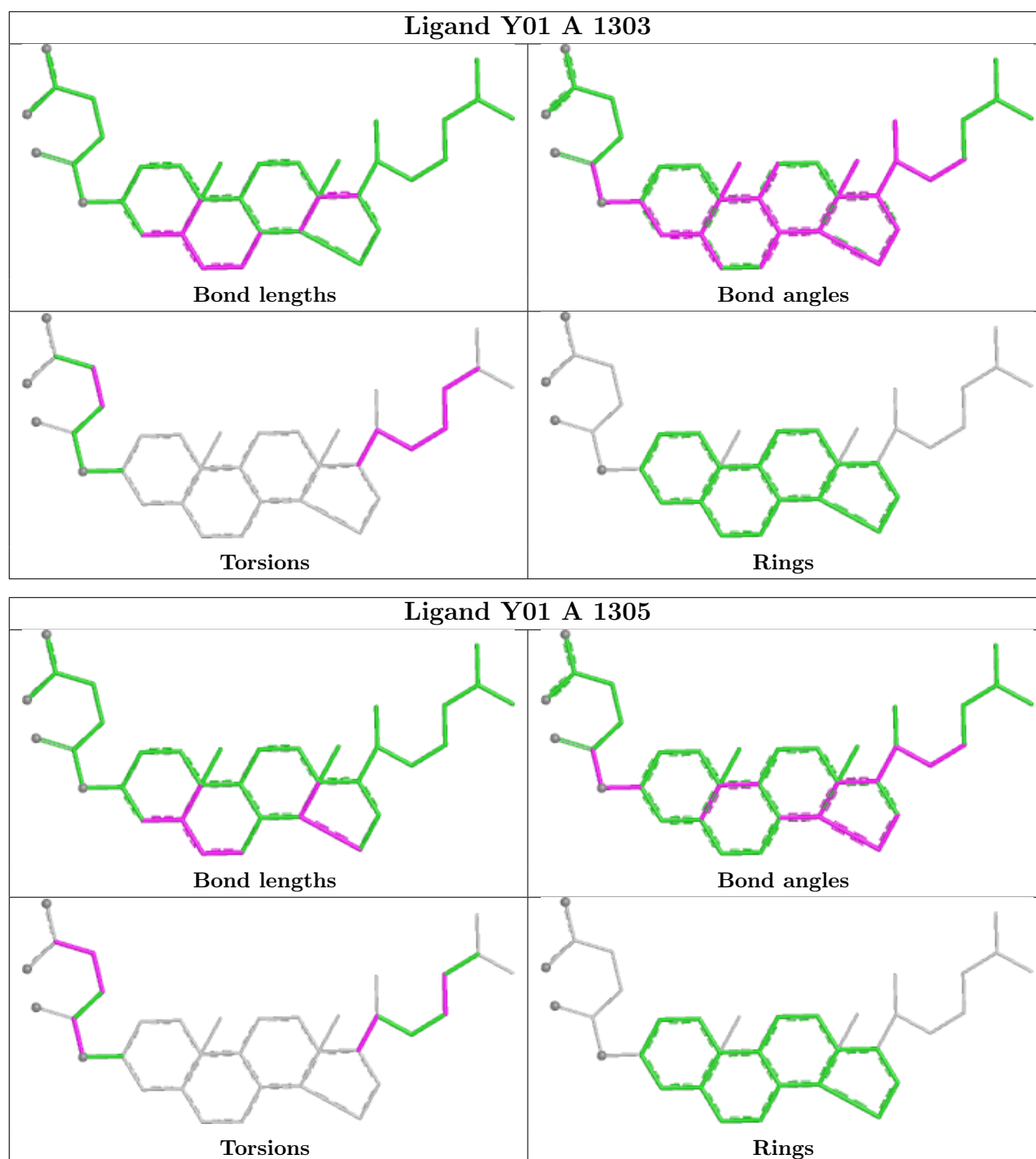












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

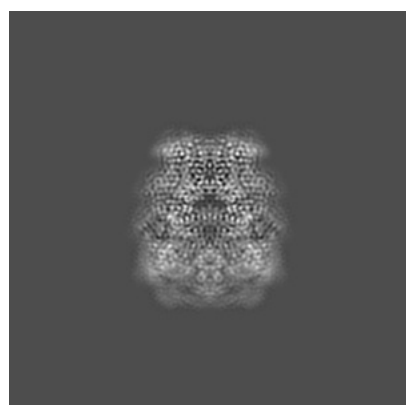
6 Map visualisation [i](#)

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

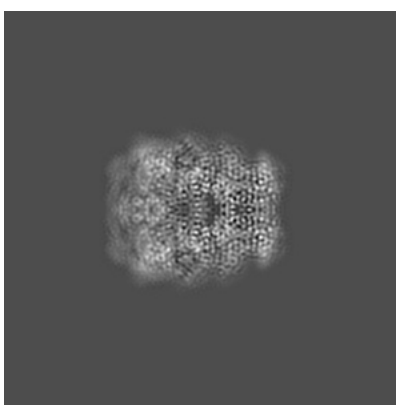
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

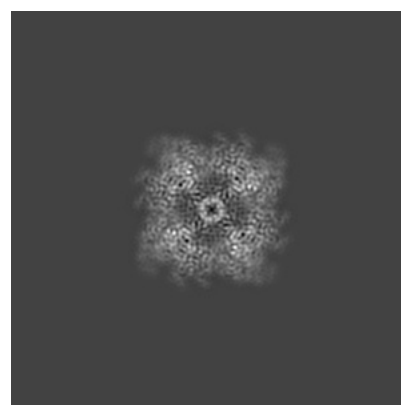
6.1.1 Primary map



X



Y

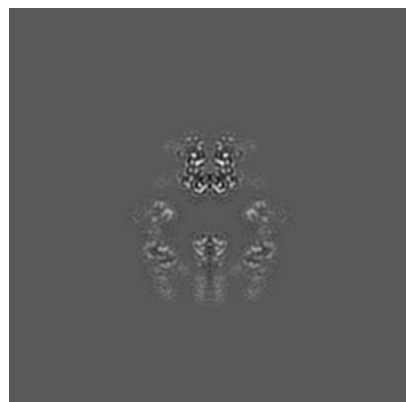


Z

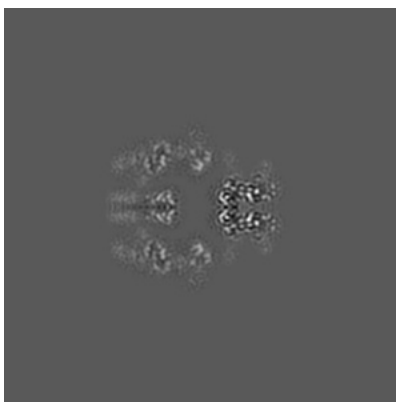
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

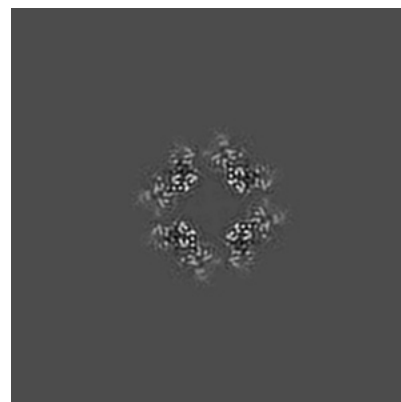
6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

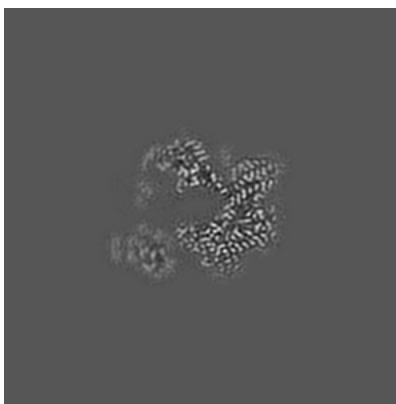
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

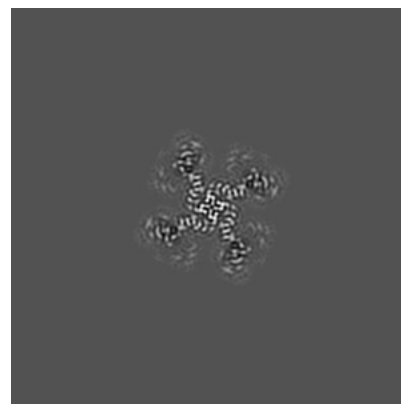
6.3.1 Primary map



X Index: 142



Y Index: 114

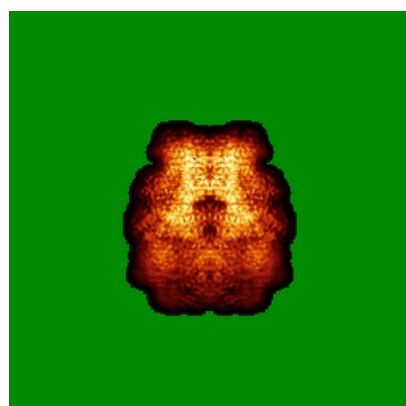


Z Index: 142

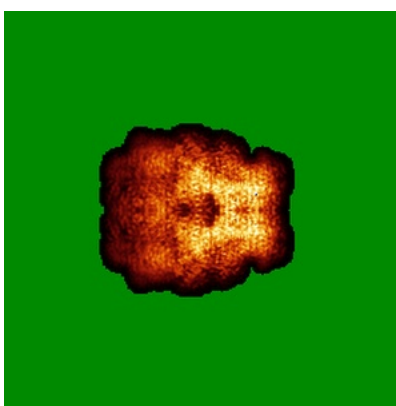
The images above show the largest variance slices of the map in three orthogonal directions.

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

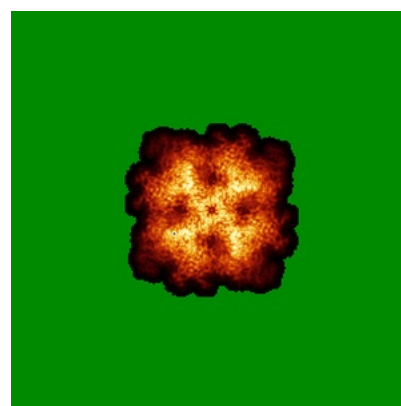
6.4.1 Primary map



X



Y



Z

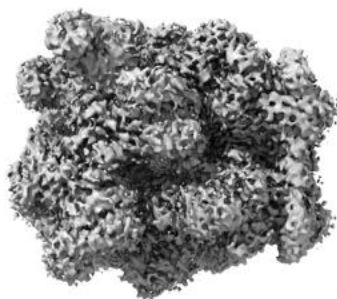
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

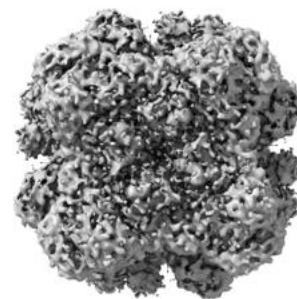
6.5.1 Primary map



X



Y



Z

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

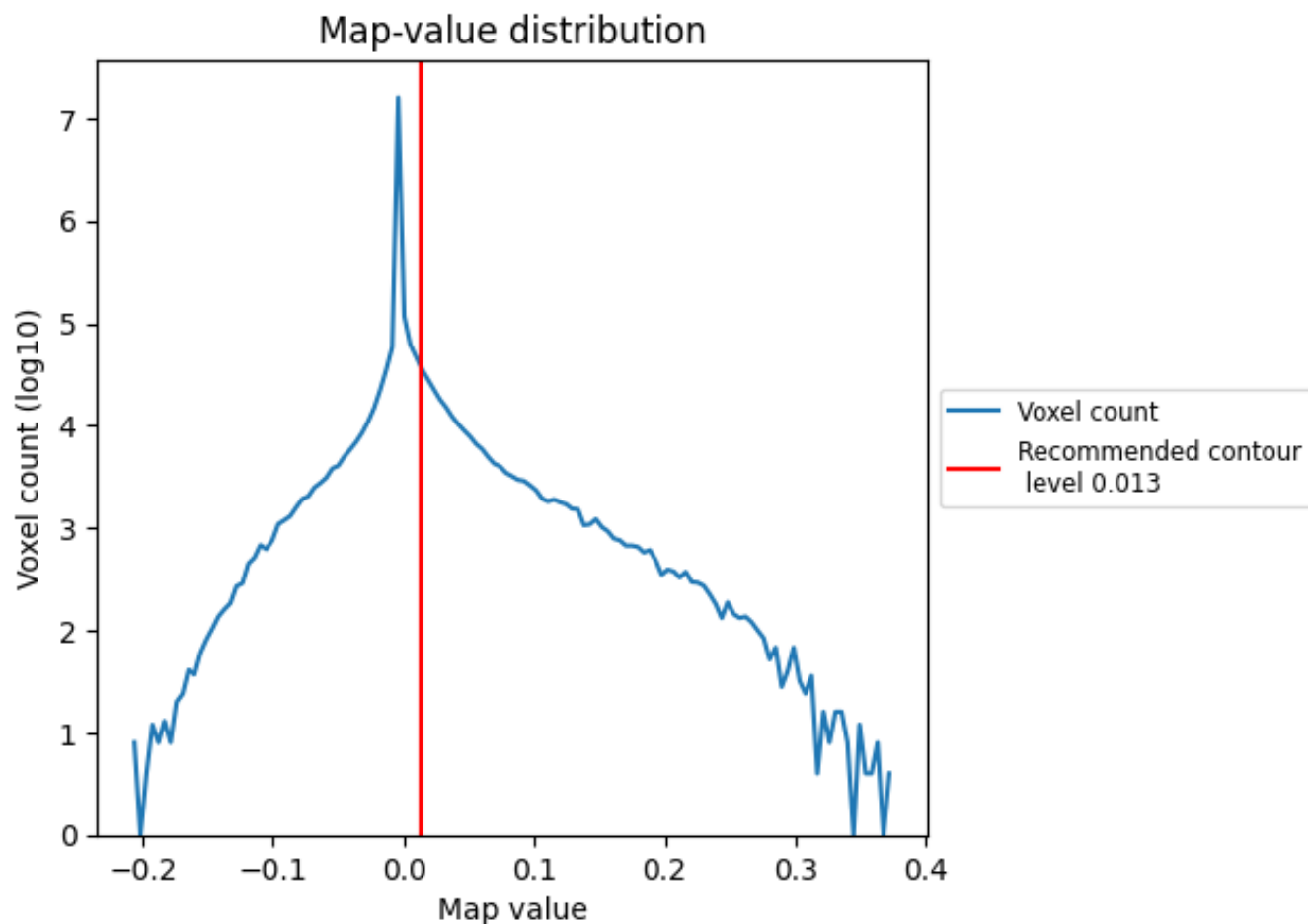
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

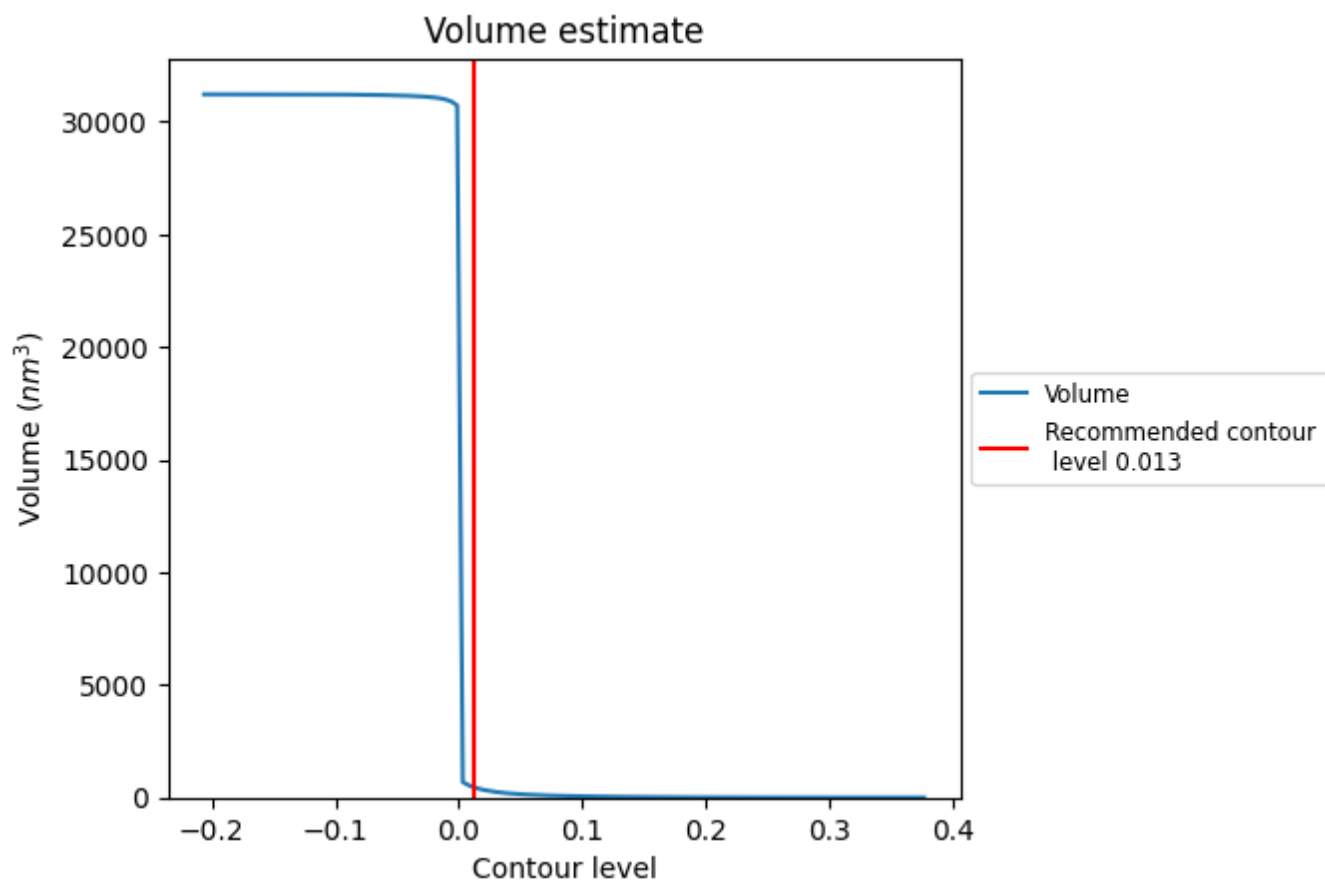
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

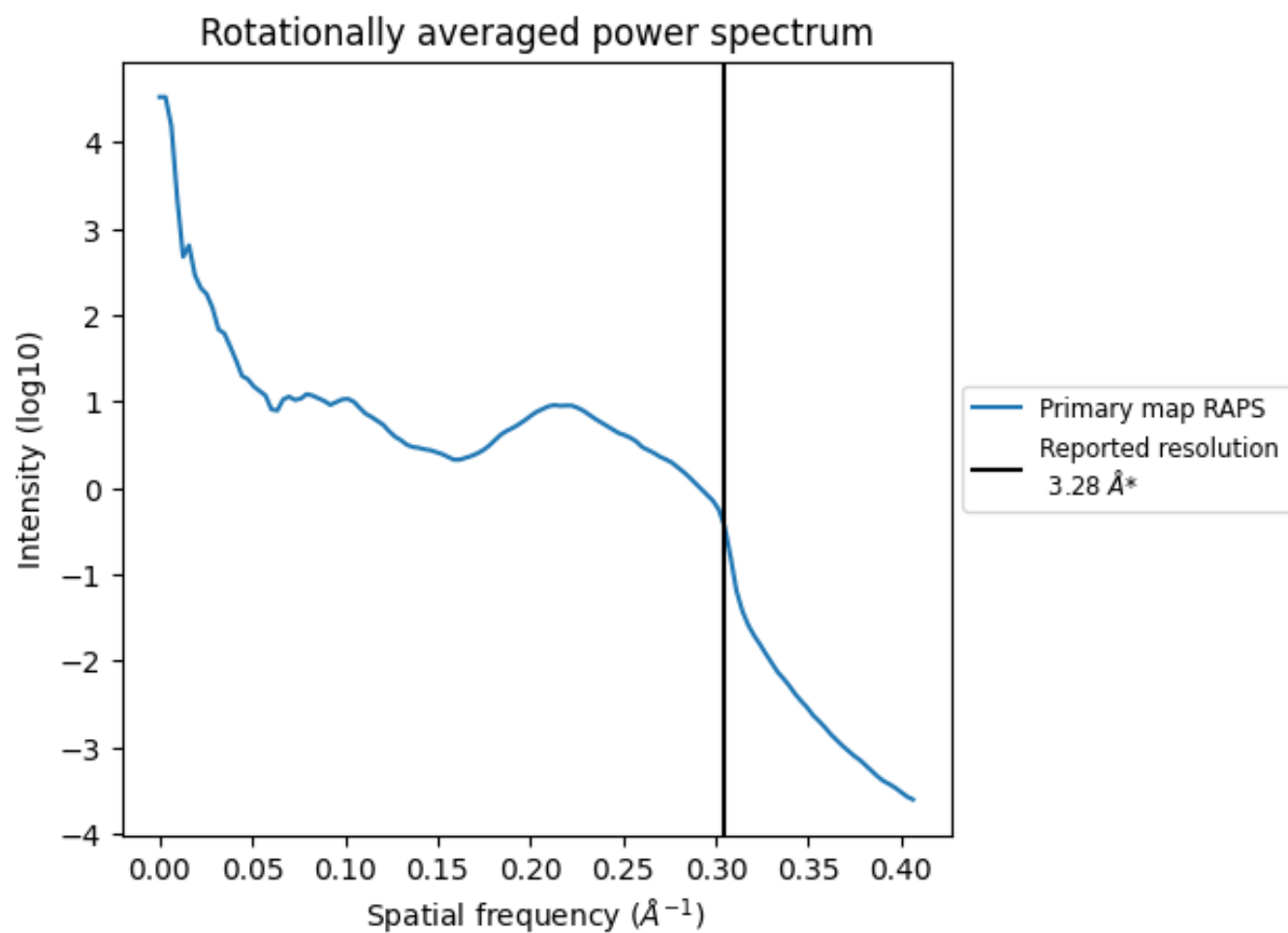
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

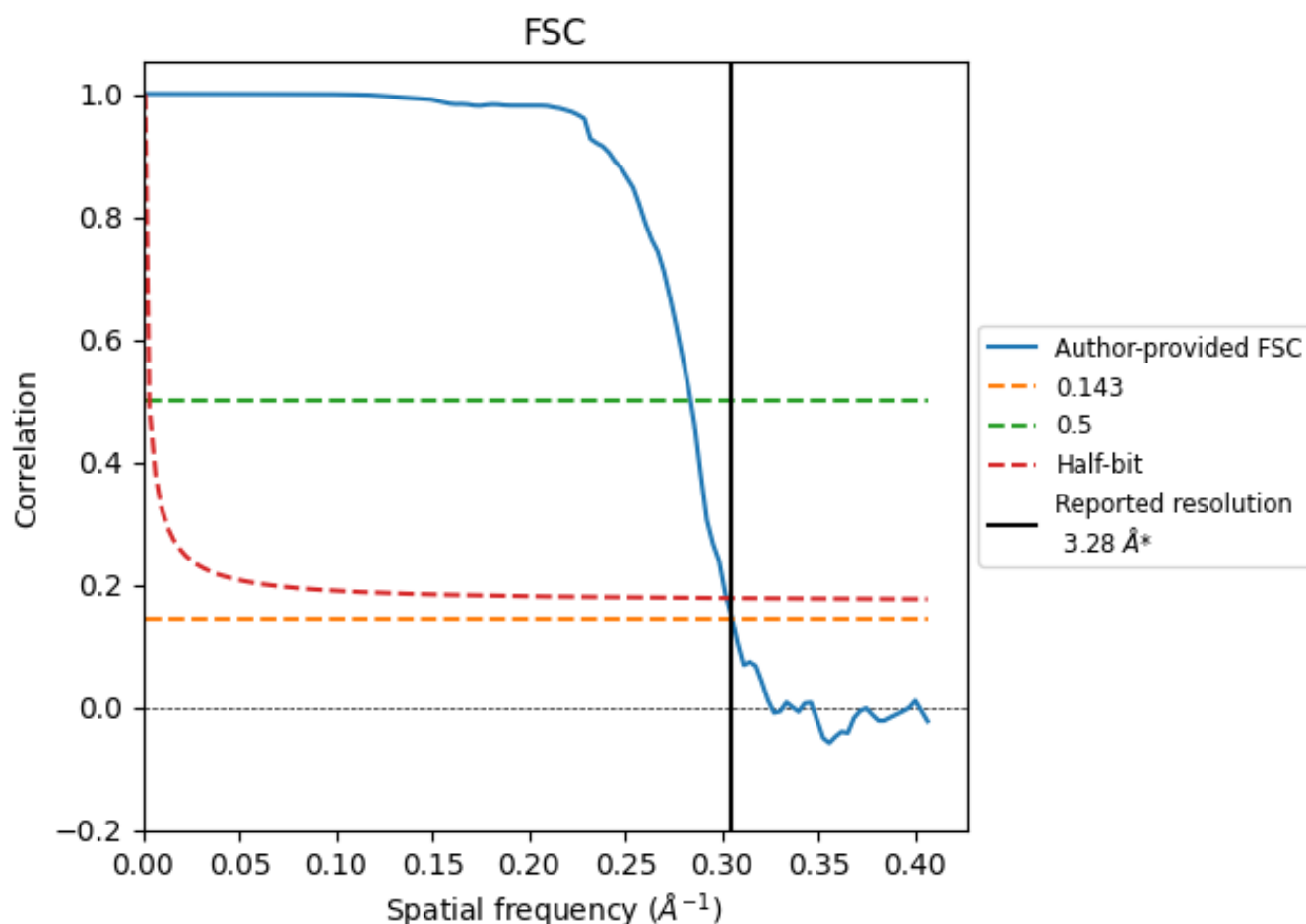


*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.305 Å⁻¹

8.2 Resolution estimates [i](#)

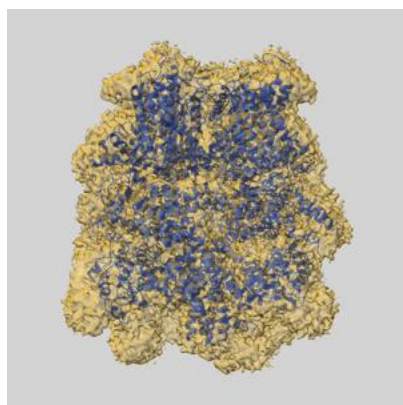
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.52	3.31
Unmasked-calculated*	-	-	-

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

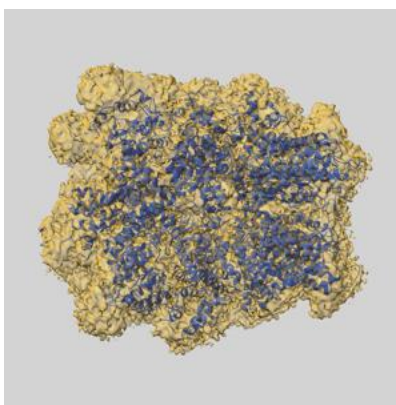
9 Map-model fit [i](#)

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

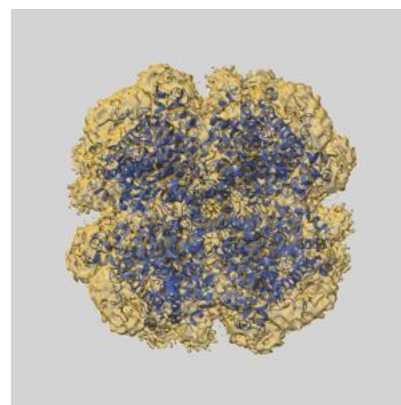
9.1 Map-model overlay [i](#)



X



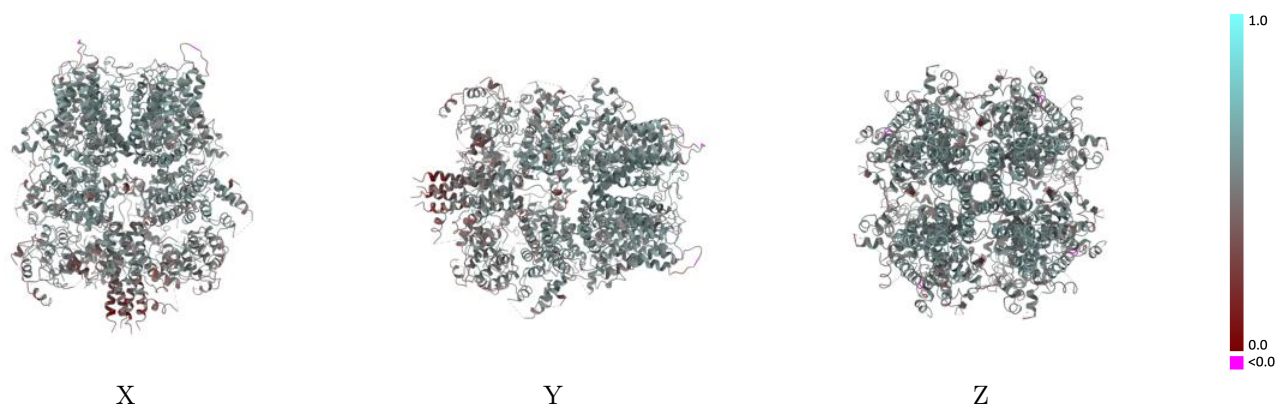
Y



Z

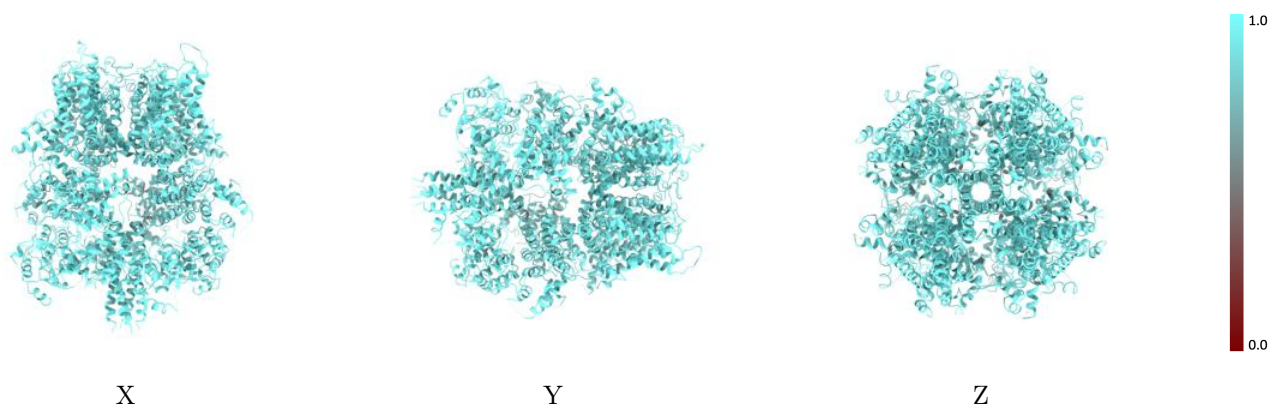
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



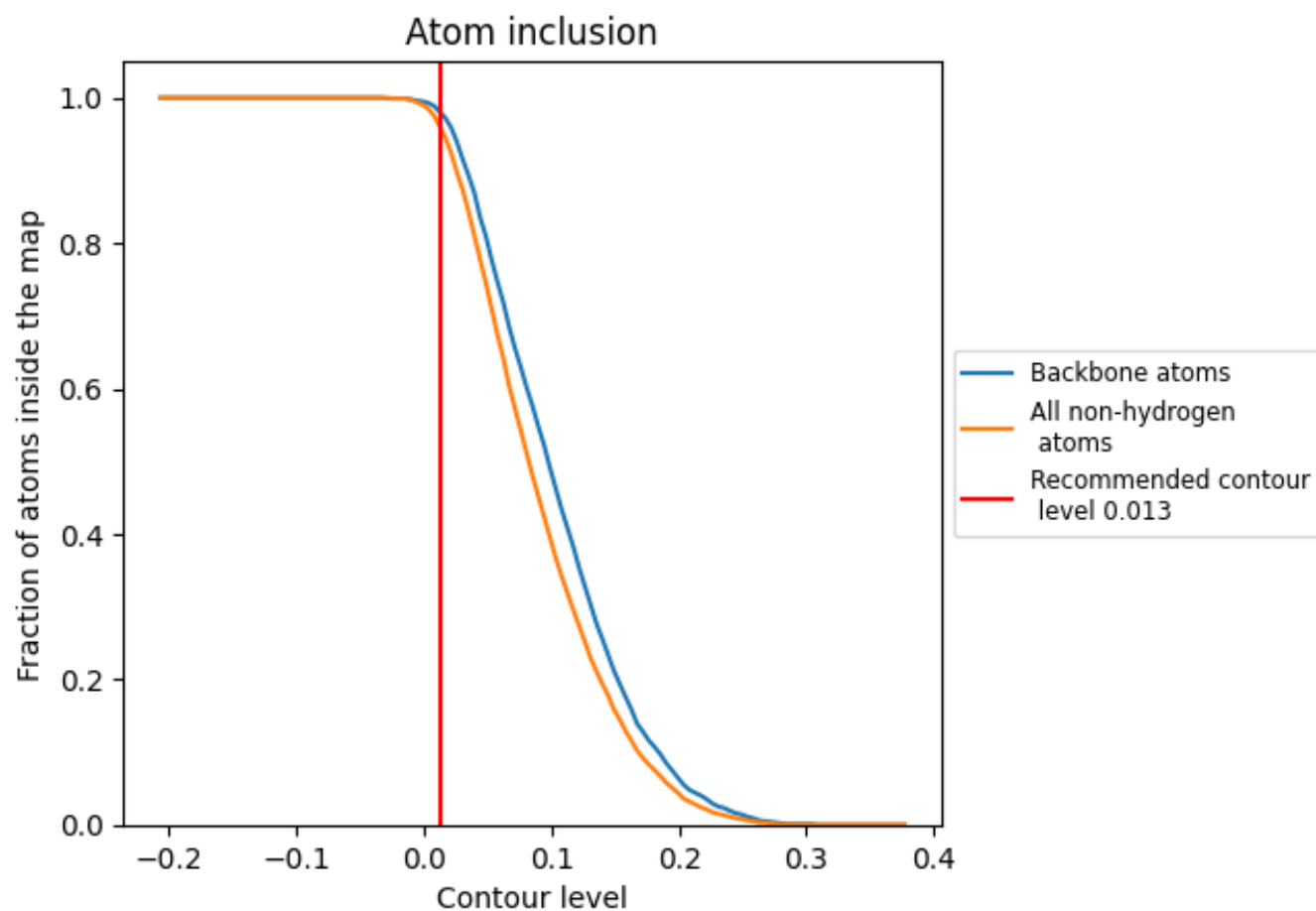
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.013).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

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

