Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 06:39 PM EST

PDB ID	:	6CNK
EMDB ID	:	EMD-7536
Title	:	Structure of the 3alpha2beta stiochiometry of the human Alpha4Beta2 nicotinic receptor
Authors	:	Walsh Jr, R.M.; Roh, S.H.; Gharpure, A.; Morales-Perez, C.L.; Hibbs, R.E.
Deposited on	:	2018-03-08
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

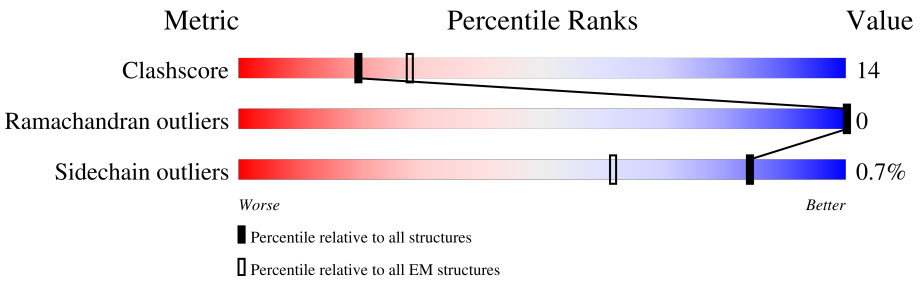
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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	386	64% 31% •
1	B	386	65% 29% • 5%
1	D	386	65% 31% •
2	C	403	63% 26% 11%
2	E	403	62% 26% • 11%
3	F	238	18% 69% 21% • 8%
3	J	238	18% 72% 19% 8%
4	G	462	8% 37% 10% 53%

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Mol	Chain	Length	Quality of chain
4	K	462	8% 34% 13% 53%
5	H	3	33% 67%
5	I	3	33% 67%

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
9	NCT	A	405	-	-	X	-
9	NCT	D	401	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 22080 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 Neuronal acetylcholine receptor subunit alpha-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	370	3049	2009	496	526	18	0	0
1	B	366	3016	1990	489	519	18	0	0
1	D	370	3048	2008	496	526	18	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	-	linker	UNP P43681
A	340	THR	-	linker	UNP P43681
A	341	ASP	-	linker	UNP P43681
A	342	PHE	-	linker	UNP P43681
A	343	GLU	-	linker	UNP P43681
A	344	ARG	-	linker	UNP P43681
B	339	ASP	-	linker	UNP P43681
B	340	THR	-	linker	UNP P43681
B	341	ASP	-	linker	UNP P43681
B	342	PHE	-	linker	UNP P43681
B	343	GLU	-	linker	UNP P43681
B	344	ARG	-	linker	UNP P43681
D	339	ASP	-	linker	UNP P43681
D	340	THR	-	linker	UNP P43681
D	341	ASP	-	linker	UNP P43681
D	342	PHE	-	linker	UNP P43681
D	343	GLU	-	linker	UNP P43681
D	344	ARG	-	linker	UNP P43681

- Molecule 2 is a protein called Neuronal acetylcholine receptor subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	358	2917	1915	461	522	19	0	0
2	E	358	2917	1915	461	522	19	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	329	HIS	-	linker	UNP P17787
C	330	HIS	-	linker	UNP P17787
C	331	ASP	-	linker	UNP P17787
C	332	ASP	-	linker	UNP P17787
C	333	ASP	-	linker	UNP P17787
C	334	GLN	-	linker	UNP P17787
C	335	GLU	-	linker	UNP P17787
C	336	ARG	-	linker	UNP P17787
C	394	SER	-	expression tag	UNP P17787
C	395	ALA	-	expression tag	UNP P17787
C	396	TRP	-	expression tag	UNP P17787
C	397	SER	-	expression tag	UNP P17787
C	398	HIS	-	expression tag	UNP P17787
C	399	PRO	-	expression tag	UNP P17787
C	400	GLN	-	expression tag	UNP P17787
C	401	PHE	-	expression tag	UNP P17787
C	402	GLU	-	expression tag	UNP P17787
C	403	LYS	-	expression tag	UNP P17787
E	329	HIS	-	linker	UNP P17787
E	330	HIS	-	linker	UNP P17787
E	331	ASP	-	linker	UNP P17787
E	332	ASP	-	linker	UNP P17787
E	333	ASP	-	linker	UNP P17787
E	334	GLN	-	linker	UNP P17787
E	335	GLU	-	linker	UNP P17787
E	336	ARG	-	linker	UNP P17787
E	394	SER	-	expression tag	UNP P17787
E	395	ALA	-	expression tag	UNP P17787
E	396	TRP	-	expression tag	UNP P17787
E	397	SER	-	expression tag	UNP P17787
E	398	HIS	-	expression tag	UNP P17787
E	399	PRO	-	expression tag	UNP P17787
E	400	GLN	-	expression tag	UNP P17787
E	401	PHE	-	expression tag	UNP P17787
E	402	GLU	-	expression tag	UNP P17787
E	403	LYS	-	expression tag	UNP P17787

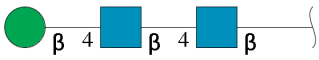
- Molecule 3 is a protein called IgG1 Kappa Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	218	1695	1061	287	341	6	0	0
3	J	218	1695	1061	287	341	6	0	0

- Molecule 4 is a protein called IgG1 Heavy Chain.

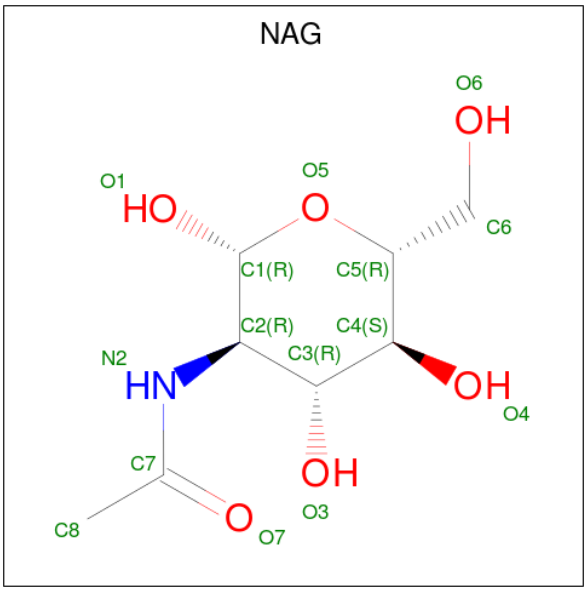
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	218	1653	1050	270	325	8	0	0
4	K	218	1653	1050	270	325	8	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



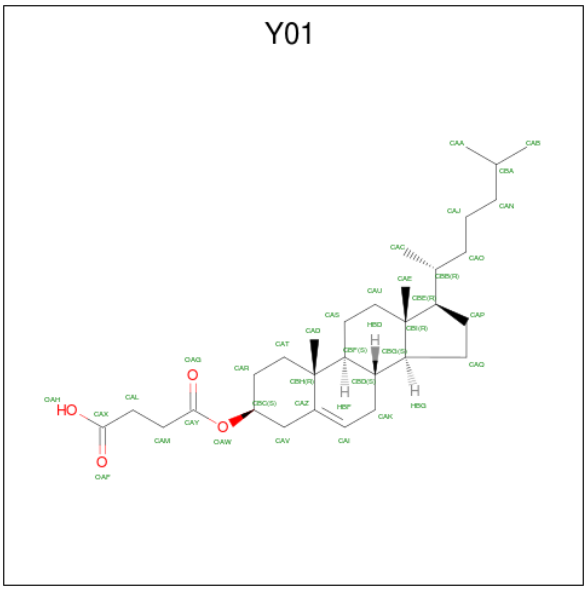
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	H	3	39	22	2	15	0	0
5	I	3	39	22	2	15	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			56	54	2	

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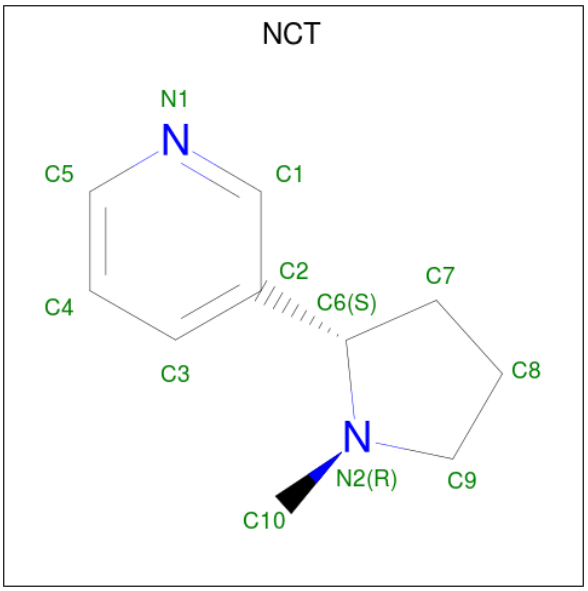
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	A	1	56	54	2	0
7	B	1	56	54	2	0
7	B	1	56	54	2	0
7	C	1	56	54	2	0
7	C	1	56	54	2	0
7	D	1	56	54	2	0
7	D	1	56	54	2	0
7	E	1	56	54	2	0
7	E	1	56	54	2	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
8	A	1	1	1	0

- Molecule 9 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$).



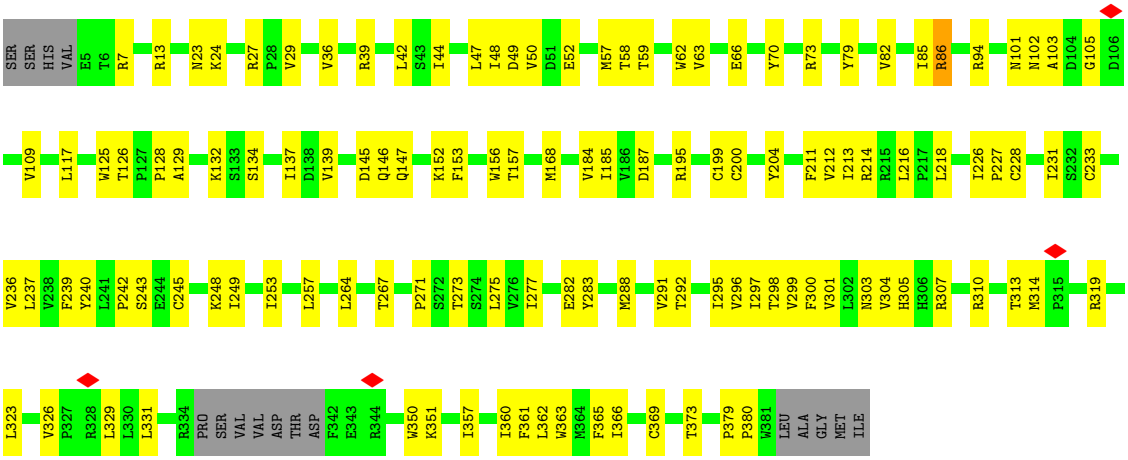
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
9	A	1	12	10	2	0
9	B	1	12	10	2	0
9	D	1	12	10	2	0

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.

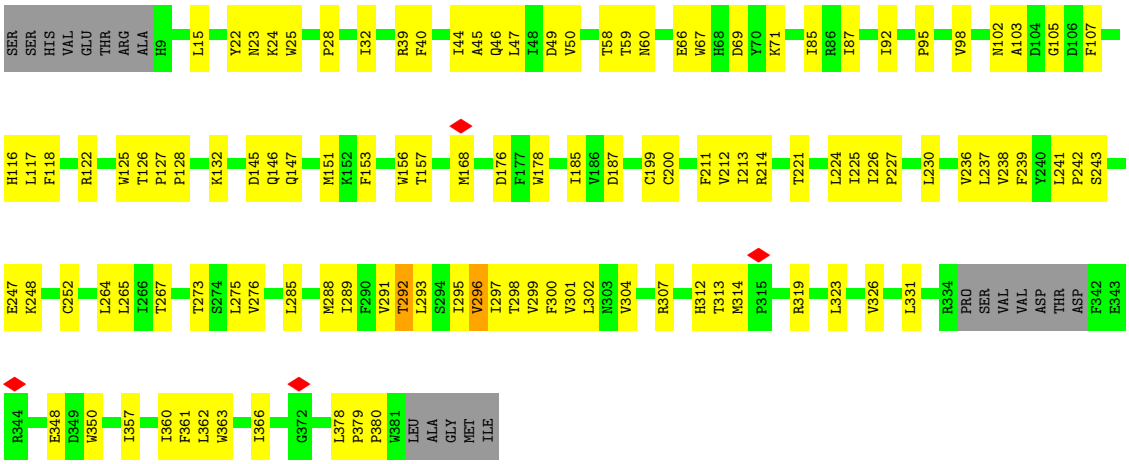
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain A: 64% 31%



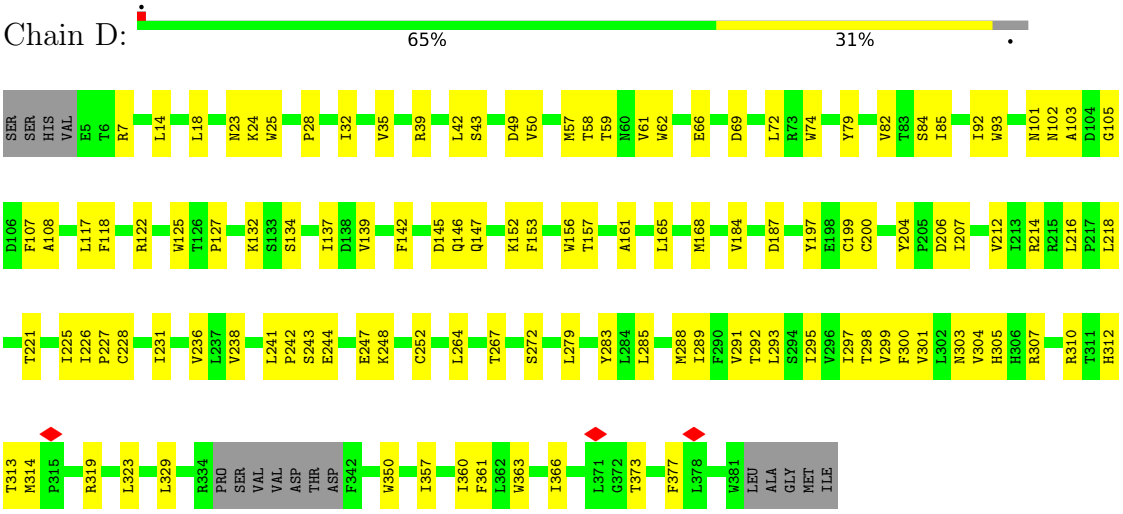
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain B: 65% 29% 5%



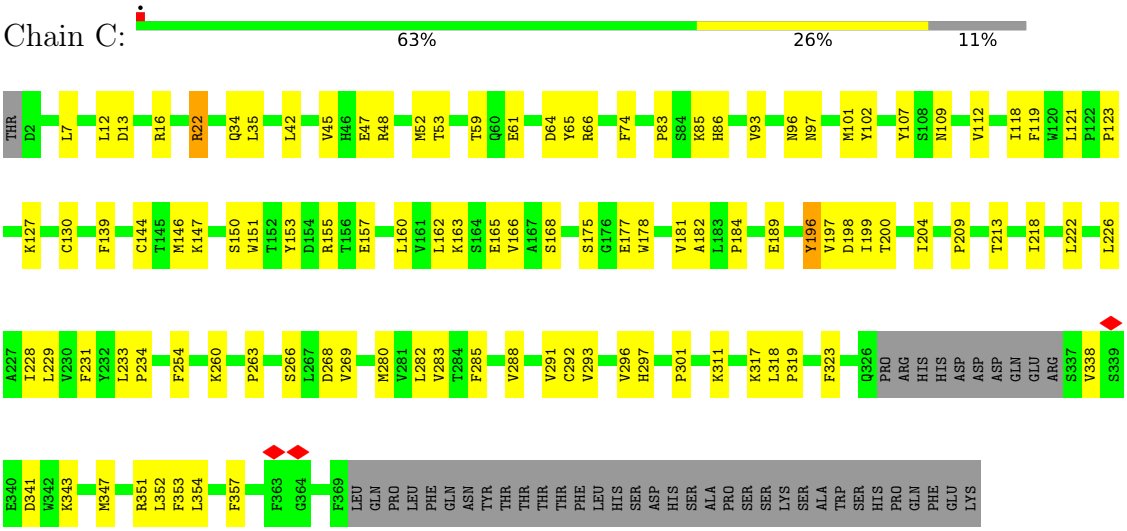
• Molecule 1: Neuronal acetylcholine receptor subunit alpha-4

Chain D:



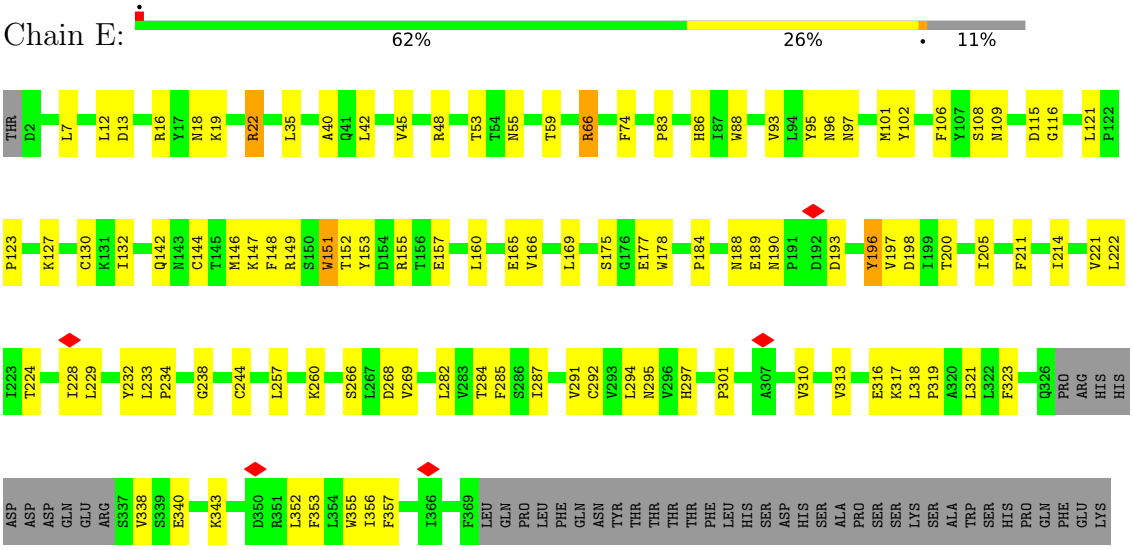
• Molecule 2: Neuronal acetylcholine receptor subunit beta-2

Chain C:



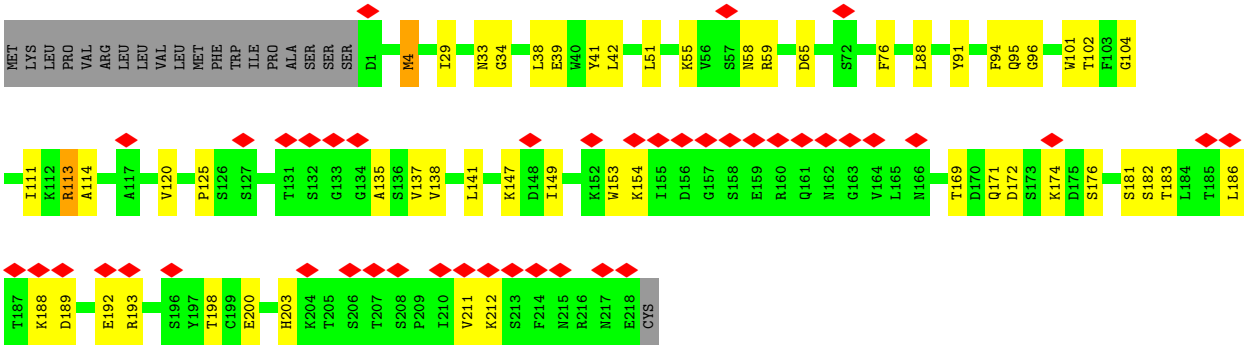
• Molecule 2: Neuronal acetylcholine receptor subunit beta-2

Chain E:



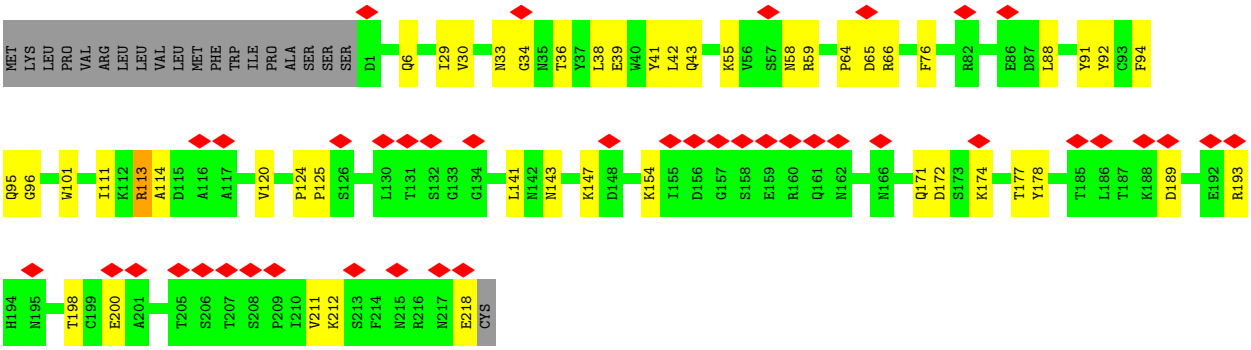
- Molecule 3: IgG1 Kappa Light Chain

Chain F:



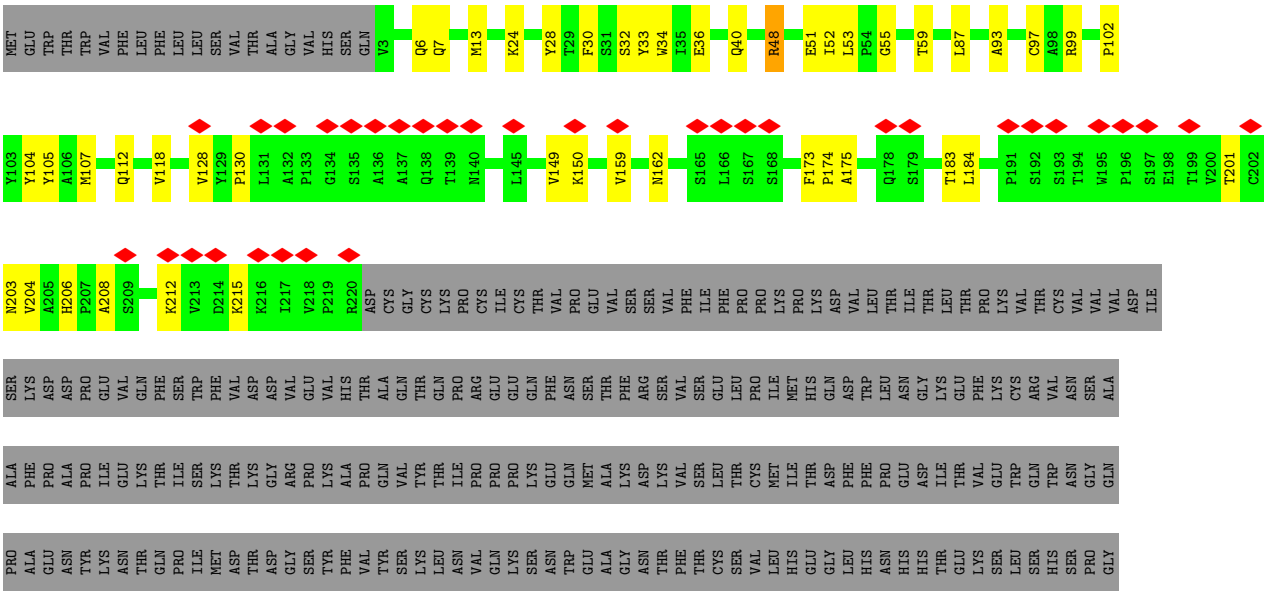
- Molecule 3: IgG1 Kappa Light Chain

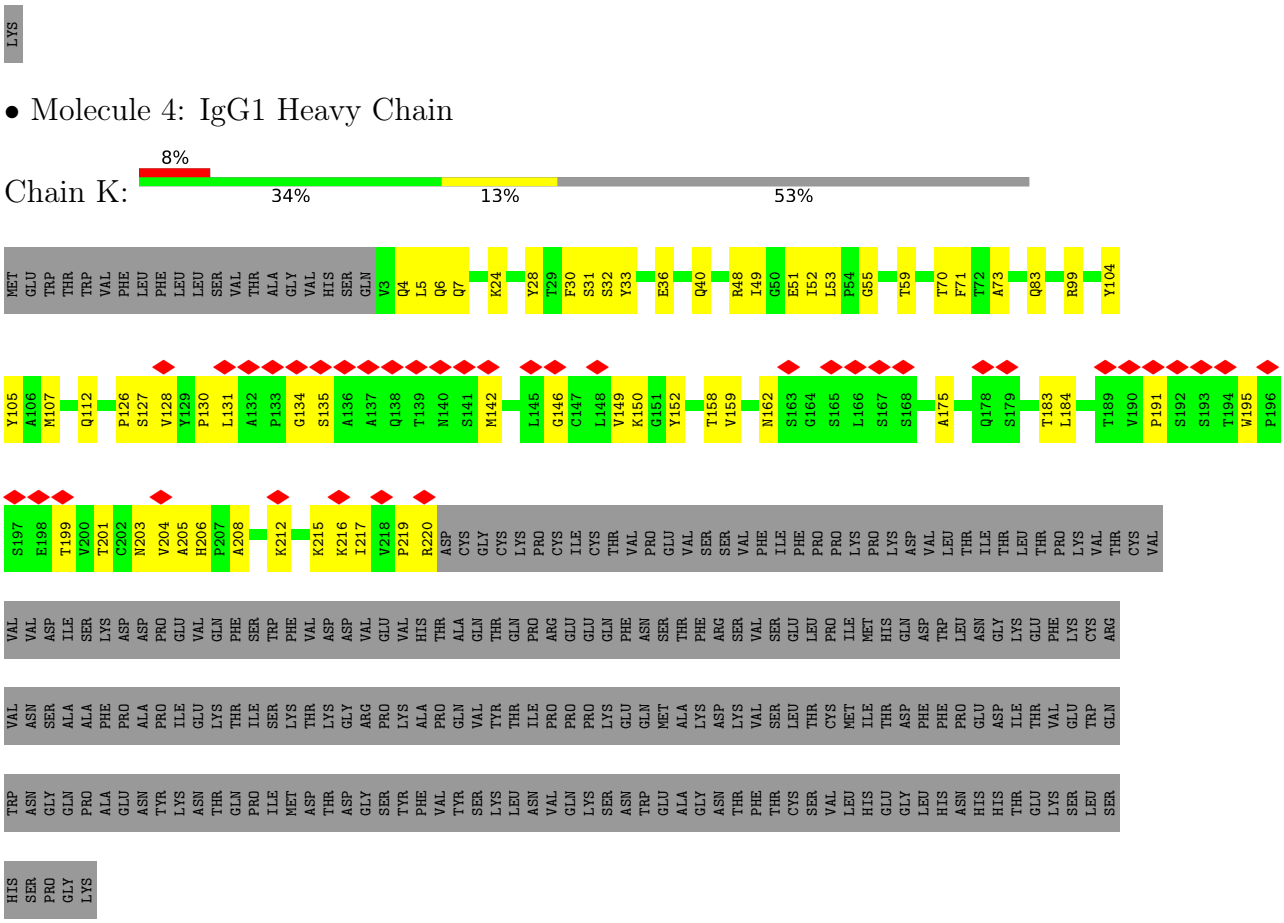
Chain J:



- Molecule 4: IgG1 Heavy Chain

Chain G:




LYS
• Molecule 4: IgG1 Heavy Chain
Chain K:
8%
34%
13%
53%
MET GLU TRP THR TRP VAL PHE LEU PHE LEU LEU SER VAL THR ALA GLY VAL HIS SER GLN V3 Q4 L5 Q6 Q7 K24 Y28 T29 F30 S31 S32 Y33 E36 Q40 R48 I49 G50 E51 I52 L53 P54 G55 T59 T70 F71 T72 A73 Q83 R99 Y104
Y105 A106 M107 Q112 P126 S127 V128 Y129 P130 L131 A132 P133 G134 S135 A136 A137 Q138 T139 N140 S141 M142 L145 G146 C147 L148 V149 K150 G151 Y152 T158 V159 N162 S163 G164 S165 L166 S167 S168 A175 Q178 S179 T183 L184 T189 V190 P191 S192 S193 T194 W195 P196
S197 E198 T199 V200 T201 C202 N203 V204 A205 H206 P207 A208 K212 K215 K216 I217 V218 P219 R220 ASP CYS GLY CYS LYS PRO CYS ILE CYS THR VAL PRO GLU VAL SER SER VAL PHE ILE PHE PRO PRO LYS PRO LYS ASP VAL LEU THR ILE THR LEU THR PRO LYS VAL THR CYS VAL
VAL VAL ASP ILE SER LYS ASP ASP PRO GLU VAL GLN PHE SER TRP PHE VAL ASP ASP VAL GLU VAL HIS THR ALA GLN THR GLN PRO ARG GLU GLU GLN PHE ASN SER THR PHE ARG SER VAL SER GLU LEU PRO ILE MET HIS GLN ASP TRP LEU ASN GLY LYS GLU PHE LYS CYS ARG
VAL ASN SER ALA ALA PHE PRO ALA PRO ILE GLU LYS THR ILE SER LYS THR LYS GLY ARG PRO LYS ALA PRO GLN VAL TYR THR ILE PRO PRO PRO LYS GLU GLN MET ALA LYS ASP LYS VAL SER LEU THR CYS MET ILE THR ASP PHE PHE PRO GLU ASP ILE THR VAL GLU TRP GLN
TRP ASN GLY GLN PRO ALA GLU ASN TYR LYS ASN THR GLN PRO ILE MET ASP THR ASP GLY SER TYR PHE VAL TYR SER LYS LEU ASN VAL GLN LYS SER ASN TRP GLU ALA GLY ASN THR PHE THR CYS SER VAL LEU HIS GLU GLY LEU HIS ASN HIS HIS THR GLU LYS SER LEU SER
HIS SER PRO GLY LYS
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
Chain H:
33%
67%
NAG1 NAG2 BMA3
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
Chain I:
33%
67%
NAG1 NAG2 BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0325	Depositor
Map size (Å)	267.5, 267.5, 267.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NA, NCT, Y01, NAG

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	0.31	0/3135	0.47	0/4278
1	B	0.40	2/3102 (0.1%)	0.48	0/4233
1	D	0.30	0/3134	0.47	0/4276
2	C	0.32	0/2996	0.49	0/4089
2	E	0.39	3/2996 (0.1%)	0.52	1/4089 (0.0%)
3	F	0.26	0/1735	0.43	0/2355
3	J	0.26	0/1735	0.44	0/2355
4	G	0.28	0/1699	0.47	0/2320
4	K	0.28	0/1699	0.48	0/2320
All	All	0.32	5/22231 (0.0%)	0.47	1/30315 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	ILE	C-N	11.40	1.60	1.34
2	E	356	ILE	C-N	8.98	1.54	1.34
1	B	296	VAL	C-N	8.53	1.53	1.34
2	E	238	GLY	C-N	7.81	1.52	1.34
2	E	148	PHE	C-N	-5.85	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	148	PHE	O-C-N	6.11	132.48	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3049	0	3085	104	0
1	B	3016	0	3050	107	0
1	D	3048	0	3081	104	0
2	C	2917	0	2938	88	0
2	E	2917	0	2937	100	0
3	F	1695	0	1632	34	0
3	J	1695	0	1632	34	0
4	G	1653	0	1614	40	0
4	K	1653	0	1614	53	0
5	H	39	0	32	0	0
5	I	39	0	31	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	D	14	0	13	0	0
7	A	56	0	78	12	0
7	B	56	0	78	19	0
7	C	56	0	78	13	0
7	D	56	0	78	16	0
7	E	56	0	78	9	0
8	A	1	0	0	0	0
9	A	12	0	14	9	0
9	B	12	0	14	1	0
9	D	12	0	14	8	0
All	All	22080	0	22117	614	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 14.

All (614) 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:300:PHE:CE1	7:D:404:Y01:CAD	1.80	1.59
7:A:403:Y01:CAP	7:A:403:Y01:CAQ	1.81	1.58
7:C:504:Y01:CAP	7:C:504:Y01:CAQ	1.81	1.57
7:E:505:Y01:CAP	7:E:505:Y01:CAQ	1.81	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:402:Y01:CAQ	7:A:402:Y01:CAP	1.81	1.57
7:C:505:Y01:CAQ	7:C:505:Y01:CAP	1.81	1.57
7:D:404:Y01:CAP	7:D:404:Y01:CAQ	1.81	1.54
7:B:403:Y01:CAP	7:B:403:Y01:CAQ	1.81	1.52
7:E:504:Y01:CAP	7:E:504:Y01:CAQ	1.81	1.51
7:B:404:Y01:CAP	7:B:404:Y01:CAQ	1.81	1.51
7:D:403:Y01:CAP	7:D:403:Y01:CAQ	1.81	1.50
1:D:300:PHE:CE1	7:D:404:Y01:HAD1	1.39	1.47
1:A:204:TYR:CE2	9:A:405:NCT:H101	1.53	1.40
1:A:204:TYR:CE2	9:A:405:NCT:C10	2.15	1.29
1:D:300:PHE:CZ	7:D:404:Y01:CAD	2.25	1.19
4:K:128:VAL:HG11	4:K:215:LYS:CE	1.77	1.15
4:K:128:VAL:HG11	4:K:215:LYS:HE2	1.19	1.15
1:D:300:PHE:CE1	7:D:404:Y01:HAD2	1.70	1.11
1:A:204:TYR:CD2	9:A:405:NCT:H101	1.86	1.10
1:D:300:PHE:CD1	7:D:404:Y01:HAD2	1.92	1.03
1:D:300:PHE:CZ	7:D:404:Y01:HAD3	1.99	0.94
1:B:300:PHE:CE1	7:B:403:Y01:HAV1	2.03	0.94
4:K:128:VAL:CG1	4:K:215:LYS:CE	2.47	0.93
1:B:288:MET:O	1:B:292:THR:HG22	1.71	0.89
1:B:300:PHE:CE1	7:B:403:Y01:HAD1	2.07	0.88
1:D:300:PHE:CZ	7:D:404:Y01:HAD1	2.00	0.87
1:A:204:TYR:CZ	9:A:405:NCT:C10	2.58	0.86
1:A:218:LEU:HD21	2:E:269:VAL:CG2	2.07	0.85
1:A:300:PHE:CE1	7:A:403:Y01:HAV1	2.11	0.84
1:A:204:TYR:CE2	9:A:405:NCT:H102	2.13	0.82
1:A:218:LEU:HD23	1:A:218:LEU:O	1.79	0.82
2:E:228:ILE:HG22	2:E:357:PHE:HB3	1.62	0.82
1:B:304:VAL:O	1:B:350:TRP:NE1	2.14	0.81
3:F:153:TRP:HE1	3:F:182:SER:HG	1.27	0.81
1:B:299:VAL:HG11	2:C:229:LEU:HD11	1.62	0.79
1:B:248:LYS:HD2	1:B:302:LEU:HD12	1.63	0.79
2:C:139:PHE:HB3	2:C:209:PRO:HB3	1.65	0.78
2:E:97:ASN:ND2	2:E:101:MET:O	2.16	0.77
2:C:53:THR:HG22	2:C:127:LYS:HG2	1.67	0.77
1:D:204:TYR:CD2	9:D:401:NCT:H101	2.19	0.77
1:D:204:TYR:CE2	9:D:401:NCT:H102	2.19	0.77
2:E:147:LYS:HG2	2:E:200:THR:HG22	1.67	0.77
1:B:146:GLN:HG2	1:B:214:ARG:HG2	1.65	0.76
2:C:147:LYS:HG2	2:C:200:THR:HG22	1.69	0.75
9:B:402:NCT:HC72	2:C:121:LEU:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:TYR:C	2:E:196:TYR:HD1	1.90	0.74
1:D:204:TYR:CE2	9:D:401:NCT:C10	2.69	0.74
2:E:196:TYR:HD1	2:E:197:VAL:N	1.84	0.74
4:G:48:ARG:NH1	4:G:51:GLU:OE1	2.20	0.74
2:C:93:VAL:HG11	2:C:102:TYR:HB3	1.67	0.74
2:C:184:PRO:HG2	4:G:104:TYR:CE2	2.23	0.74
3:F:154:LYS:HB2	3:F:198:THR:HB	1.70	0.74
2:C:196:TYR:HD1	2:C:197:VAL:N	1.86	0.73
1:B:300:PHE:CZ	7:B:403:Y01:HAV1	2.21	0.73
1:B:151:MET:CE	1:B:211:PHE:HE2	2.00	0.73
4:K:33:TYR:HE1	4:K:99:ARG:HB2	1.52	0.73
1:B:363:TRP:HE1	7:B:404:Y01:HAR1	1.53	0.72
4:K:162:ASN:HD21	4:K:201:THR:HB	1.54	0.72
4:K:6:GLN:HB2	4:K:24:LYS:HB3	1.70	0.72
1:D:300:PHE:HE1	7:D:404:Y01:HAD1	0.98	0.72
1:B:44:ILE:HD11	1:B:211:PHE:CE1	2.24	0.72
1:B:293:LEU:O	1:B:293:LEU:HD23	1.89	0.72
2:C:97:ASN:ND2	2:C:101:MET:O	2.23	0.72
1:A:304:VAL:O	1:A:350:TRP:NE1	2.23	0.71
1:D:146:GLN:HG2	1:D:214:ARG:HG2	1.72	0.71
2:E:93:VAL:HG11	2:E:102:TYR:HB3	1.71	0.71
2:E:175:SER:OG	2:E:178:TRP:O	2.08	0.71
1:D:145:ASP:OD2	1:D:147:GLN:NE2	2.23	0.71
4:G:33:TYR:HE1	4:G:99:ARG:HB2	1.56	0.71
3:J:88:LEU:HD21	3:J:111:ILE:HG23	1.72	0.71
1:D:84:SER:HA	1:D:117:LEU:O	1.91	0.71
4:G:150:LYS:HG2	4:G:183:THR:HG23	1.73	0.70
3:F:169:THR:HG22	4:G:174:PRO:HD3	1.73	0.70
1:D:157:THR:HG21	2:E:109:ASN:HB2	1.74	0.70
1:B:39:ARG:HB2	1:B:66:GLU:HB3	1.72	0.69
1:B:264:LEU:O	1:B:267:THR:HG22	1.92	0.69
2:C:196:TYR:HD1	2:C:196:TYR:C	1.95	0.69
2:C:22:ARG:HE	2:C:157:GLU:HB3	1.57	0.69
2:C:96:ASN:HD21	2:C:146:MET:HA	1.58	0.69
2:E:95:TYR:CE1	2:E:149:ARG:HD3	2.28	0.68
1:A:58:THR:HG22	1:A:132:LYS:HG2	1.73	0.68
1:B:58:THR:HG22	1:B:132:LYS:HG2	1.76	0.68
2:E:166:VAL:CG1	4:K:32:SER:HB3	2.24	0.68
1:B:300:PHE:CE1	7:B:403:Y01:CAD	2.77	0.68
1:A:300:PHE:CZ	7:A:403:Y01:HAV1	2.28	0.68
1:B:151:MET:HE2	1:B:211:PHE:HE2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:311:LYS:NZ	2:C:341:ASP:OD2	2.27	0.68
2:E:48:ARG:NH1	2:E:260:LYS:O	2.27	0.68
2:E:53:THR:HG22	2:E:127:LYS:HG2	1.76	0.67
3:F:171:GLN:HE21	3:F:176:SER:HB3	1.60	0.67
1:A:204:TYR:CZ	9:A:405:NCT:H102	2.29	0.67
2:E:353:PHE:HD2	2:E:357:PHE:HE2	1.41	0.67
2:E:184:PRO:HG3	4:K:104:TYR:CE2	2.30	0.67
1:A:300:PHE:CD1	7:A:403:Y01:HAD1	2.30	0.67
2:E:151:TRP:HD1	2:E:152:THR:N	1.93	0.66
4:K:175:ALA:HA	4:K:184:LEU:HD21	1.77	0.66
1:A:39:ARG:HB2	1:A:66:GLU:HB3	1.76	0.66
2:C:196:TYR:C	2:C:196:TYR:CD1	2.68	0.66
1:D:199:CYS:SG	9:D:401:NCT:HC3	2.36	0.66
1:B:157:THR:HG21	2:C:109:ASN:HB2	1.77	0.66
2:E:196:TYR:C	2:E:196:TYR:CD1	2.64	0.65
1:A:145:ASP:OD2	1:A:147:GLN:NE2	2.30	0.65
1:D:236:VAL:HG11	1:D:366:ILE:HD13	1.79	0.65
4:G:53:LEU:HD13	4:G:55:GLY:H	1.62	0.65
1:A:184:VAL:HG13	1:A:216:LEU:HD21	1.78	0.65
1:D:313:THR:HG23	1:D:314:MET:H	1.61	0.64
2:C:112:VAL:HG22	2:C:118:ILE:HG12	1.79	0.64
2:E:233:LEU:HD12	2:E:234:PRO:HD2	1.80	0.64
3:J:96:GLY:HA2	3:J:101:TRP:CD1	2.33	0.64
1:D:39:ARG:HB2	1:D:66:GLU:HB3	1.80	0.64
2:C:233:LEU:HD12	2:C:234:PRO:HD2	1.78	0.64
1:D:279:LEU:HD21	1:D:377:PHE:CE1	2.33	0.64
4:K:7:GLN:H	4:K:112:GLN:HE22	1.46	0.64
4:K:128:VAL:CG1	4:K:215:LYS:HD2	2.26	0.64
4:K:128:VAL:CG1	4:K:215:LYS:HE2	2.09	0.64
1:A:218:LEU:HD23	1:A:218:LEU:C	2.17	0.63
4:K:53:LEU:HD13	4:K:55:GLY:H	1.62	0.63
4:K:128:VAL:HG11	4:K:215:LYS:CD	2.28	0.63
4:K:33:TYR:OH	4:K:99:ARG:NE	2.24	0.63
1:B:25:TRP:CD1	2:C:83:PRO:HG3	2.34	0.62
1:D:14:LEU:HD12	1:D:79:TYR:HD2	1.63	0.62
4:G:130:PRO:HD3	4:G:215:LYS:HD3	1.81	0.62
1:A:218:LEU:HD21	2:E:269:VAL:HG23	1.80	0.62
2:C:282:LEU:HD11	2:C:357:PHE:CE2	2.34	0.62
1:D:299:VAL:HG11	2:E:229:LEU:HD11	1.81	0.62
2:E:221:VAL:HA	2:E:224:THR:HG22	1.81	0.62
1:D:304:VAL:O	1:D:350:TRP:NE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HD11	1:B:361:PHE:CZ	2.35	0.61
3:J:39:GLU:HB2	3:J:94:PHE:HB3	1.83	0.61
4:G:7:GLN:H	4:G:112:GLN:HE22	1.48	0.61
4:K:128:VAL:CG1	4:K:215:LYS:CD	2.77	0.61
2:E:155:ARG:NH1	2:E:189:GLU:OE2	2.34	0.61
4:G:87:LEU:HD12	4:G:118:VAL:HG11	1.83	0.61
1:B:363:TRP:NE1	7:B:404:Y01:HAR1	2.15	0.61
4:K:158:THR:HB	4:K:205:ALA:HB3	1.81	0.61
3:F:39:GLU:HB2	3:F:94:PHE:HB3	1.82	0.60
3:J:120:VAL:O	3:J:212:LYS:NZ	2.34	0.60
2:C:165:GLU:HB3	4:G:105:TYR:OH	2.01	0.60
3:F:96:GLY:HA2	3:F:101:TRP:CD1	2.36	0.60
1:A:237:LEU:HD21	2:E:291:VAL:HG21	1.81	0.60
1:B:39:ARG:HH21	1:B:168:MET:HG3	1.67	0.60
4:G:6:GLN:HB2	4:G:24:LYS:HB3	1.83	0.60
1:A:298:THR:HA	1:A:301:VAL:HG12	1.83	0.60
1:A:313:THR:HG23	1:A:314:MET:H	1.67	0.60
1:B:292:THR:O	1:B:295:ILE:HG22	2.02	0.59
1:B:293:LEU:HD23	1:B:293:LEU:C	2.23	0.59
1:D:200:CYS:SG	9:D:401:NCT:HC3	2.42	0.59
1:D:204:TYR:CZ	9:D:401:NCT:H102	2.38	0.59
2:E:292:CYS:SG	7:E:504:Y01:HAD2	2.42	0.59
2:C:351:ARG:NH2	7:C:504:Y01:OAW	2.35	0.59
4:K:4:GLN:NE2	4:K:5:LEU:O	2.35	0.59
2:E:165:GLU:HB3	4:K:105:TYR:OH	2.03	0.59
1:A:264:LEU:HD11	1:B:265:LEU:HG	1.85	0.59
4:K:142:MET:HA	4:K:191:PRO:HA	1.84	0.59
1:A:146:GLN:HG2	1:A:214:ARG:HG2	1.85	0.59
1:A:156:TRP:HD1	1:A:157:THR:HG23	1.67	0.59
2:E:317:LYS:HZ3	2:E:352:LEU:HD22	1.67	0.59
1:A:319:ARG:HA	1:A:323:LEU:HD23	1.86	0.58
1:B:185:ILE:HA	1:B:213:ILE:HG22	1.85	0.58
3:J:189:ASP:OD2	3:J:193:ARG:NH2	2.35	0.58
1:B:289:ILE:O	1:B:292:THR:HG23	2.01	0.58
1:D:204:TYR:CD2	9:D:401:NCT:C10	2.84	0.58
4:K:128:VAL:CG1	4:K:215:LYS:HE3	2.31	0.58
1:A:218:LEU:HD21	2:E:269:VAL:HG22	1.85	0.58
3:F:101:TRP:HB2	4:G:48:ARG:HH22	1.69	0.58
1:A:102:ASN:HD21	1:A:105:GLY:C	2.07	0.58
1:A:326:VAL:HG13	1:A:331:LEU:HB3	1.86	0.58
2:E:151:TRP:CD1	2:E:152:THR:N	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:317:LYS:NZ	2:C:352:LEU:HD22	2.18	0.58
1:A:185:ILE:HA	1:A:213:ILE:HG22	1.85	0.57
1:D:297:ILE:HG21	1:D:361:PHE:CE2	2.39	0.57
2:E:282:LEU:HD11	2:E:357:PHE:CD1	2.39	0.57
1:B:236:VAL:HG21	1:B:366:ILE:HD13	1.86	0.57
1:B:300:PHE:CD1	7:B:403:Y01:CAD	2.87	0.57
2:C:42:LEU:HD21	2:C:45:VAL:HG23	1.86	0.57
3:J:29:ILE:HD11	3:J:76:PHE:HE2	1.68	0.57
1:A:297:ILE:HD13	7:A:403:Y01:CAE	2.33	0.57
1:B:313:THR:HG23	1:B:314:MET:H	1.67	0.57
4:K:52:ILE:HG22	4:K:59:THR:HG22	1.85	0.57
1:A:13:ARG:HE	1:A:79:TYR:HE1	1.51	0.57
2:E:22:ARG:HE	2:E:157:GLU:HB3	1.69	0.57
1:A:102:ASN:OD1	1:A:103:ALA:N	2.38	0.57
3:F:95:GLN:HE21	3:F:102:THR:HG22	1.69	0.57
1:B:300:PHE:CD1	7:B:403:Y01:HAD1	2.40	0.57
1:B:379:PRO:HG2	1:B:380:PRO:HD3	1.87	0.57
2:C:226:LEU:HA	2:C:229:LEU:HB3	1.86	0.57
1:D:310:ARG:NH1	2:E:340:GLU:OE1	2.38	0.56
1:A:264:LEU:O	1:A:267:THR:HG22	2.05	0.56
2:C:175:SER:OG	2:C:178:TRP:O	2.23	0.56
1:D:145:ASP:OD1	1:D:146:GLN:N	2.37	0.56
1:B:275:LEU:HD23	1:B:276:VAL:HG13	1.87	0.56
1:D:58:THR:HG22	1:D:132:LYS:HG2	1.88	0.56
2:E:268:ASP:OD1	2:E:269:VAL:N	2.38	0.56
3:F:101:TRP:O	4:G:48:ARG:NH2	2.37	0.56
1:D:39:ARG:HH21	1:D:168:MET:HG3	1.71	0.56
2:E:196:TYR:HE1	2:E:198:ASP:CG	2.08	0.56
1:D:236:VAL:HG21	1:D:366:ILE:HB	1.87	0.56
1:D:102:ASN:OD1	1:D:103:ALA:N	2.39	0.56
1:B:118:PHE:CD2	1:B:122:ARG:HD3	2.41	0.56
2:E:12:LEU:HD11	2:E:86:HIS:HB3	1.88	0.56
3:F:120:VAL:O	3:F:212:LYS:NZ	2.39	0.56
1:D:298:THR:HA	1:D:301:VAL:HG12	1.87	0.56
3:J:154:LYS:HB2	3:J:198:THR:HB	1.87	0.56
1:D:247:GLU:HA	1:D:247:GLU:OE1	2.05	0.55
2:E:166:VAL:HG12	4:K:32:SER:HB3	1.88	0.55
3:F:120:VAL:HG22	3:F:141:LEU:HG	1.88	0.55
2:E:88:TRP:HZ2	2:E:153:TYR:HE2	1.54	0.55
3:J:42:LEU:HD13	3:J:91:TYR:HE1	1.71	0.55
2:E:40:ALA:HB3	2:E:55:ASN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ILE:HD12	1:D:93:TRP:O	2.07	0.55
4:K:150:LYS:HG2	4:K:183:THR:HG23	1.88	0.55
1:A:297:ILE:HG21	1:A:361:PHE:CE2	2.42	0.55
1:A:109:VAL:HG12	1:A:129:ALA:HB2	1.89	0.54
1:D:102:ASN:HB3	1:D:107:PHE:HE1	1.72	0.54
1:B:300:PHE:HE1	7:B:403:Y01:HAV1	1.62	0.54
2:C:301:PRO:HB3	2:C:338:VAL:HB	1.88	0.54
3:J:94:PHE:HE1	4:K:48:ARG:HH22	1.54	0.54
4:K:130:PRO:HB3	4:K:217:ILE:HG12	1.90	0.54
3:J:38:LEU:HD13	3:J:76:PHE:CD2	2.43	0.54
2:E:22:ARG:HH21	2:E:157:GLU:HG2	1.72	0.54
3:J:43:GLN:HE22	4:K:40:GLN:HE22	1.56	0.54
2:C:12:LEU:HD11	2:C:86:HIS:HB3	1.89	0.54
1:A:218:LEU:HB3	2:E:266:SER:OG	2.07	0.54
1:B:145:ASP:OD2	1:B:147:GLN:NE2	2.40	0.54
1:D:85:ILE:HD11	1:D:117:LEU:HD12	1.90	0.54
3:J:59:ARG:NH1	3:J:65:ASP:OD1	2.41	0.54
4:G:33:TYR:OH	4:G:99:ARG:NE	2.29	0.54
2:C:266:SER:HB2	1:D:216:LEU:HB3	1.88	0.54
1:B:288:MET:HA	1:B:291:VAL:HG12	1.91	0.53
2:C:292:CYS:SG	7:C:505:Y01:HAD2	2.48	0.53
2:C:189:GLU:OE1	2:C:197:VAL:HG12	2.08	0.53
1:D:49:ASP:OD1	1:D:50:VAL:N	2.42	0.53
1:A:195:ARG:NH2	1:B:176:ASP:OD1	2.36	0.53
2:C:166:VAL:CG1	4:G:32:SER:HB3	2.38	0.53
2:E:310:VAL:HA	2:E:313:VAL:HG12	1.90	0.53
1:A:300:PHE:CE1	7:A:403:Y01:HAD1	2.43	0.53
1:B:46:GLN:HB3	1:B:178:TRP:HB3	1.91	0.53
1:D:197:TYR:N	1:D:197:TYR:CD1	2.76	0.53
3:J:55:LYS:O	3:J:58:ASN:N	2.33	0.53
1:D:66:GLU:OE2	1:D:122:ARG:NE	2.31	0.53
4:K:203:ASN:HD21	4:K:212:LYS:HD2	1.74	0.53
2:E:318:LEU:HD21	2:E:323:PHE:HD2	1.73	0.52
3:J:200:GLU:HG2	3:J:211:VAL:HG22	1.91	0.52
2:C:318:LEU:HD21	2:C:323:PHE:CD2	2.45	0.52
1:D:288:MET:HA	1:D:291:VAL:HG12	1.92	0.52
1:B:145:ASP:OD1	1:B:146:GLN:N	2.43	0.52
1:A:249:ILE:HD11	1:B:247:GLU:HB3	1.90	0.52
1:A:369:CYS:SG	7:A:402:Y01:HAB3	2.49	0.52
1:A:379:PRO:HG2	1:A:380:PRO:HD3	1.90	0.52
2:C:48:ARG:NH1	2:C:260:LYS:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:TYR:HE1	2:C:198:ASP:CG	2.13	0.52
2:C:292:CYS:SG	7:C:505:Y01:HAE1	2.50	0.52
2:E:13:ASP:HB3	2:E:16:ARG:HB3	1.92	0.52
4:K:49:ILE:HG23	4:K:71:PHE:HZ	1.75	0.52
2:C:150:SER:OG	2:C:153:TYR:O	2.27	0.52
2:C:184:PRO:HG2	4:G:104:TYR:CZ	2.44	0.52
3:J:171:GLN:HB2	3:J:178:TYR:HE1	1.73	0.52
4:K:126:PRO:HA	4:K:152:TYR:HB3	1.92	0.52
1:B:296:VAL:O	1:B:299:VAL:HG12	2.10	0.52
2:C:155:ARG:NH1	2:C:189:GLU:OE2	2.43	0.52
2:C:317:LYS:HZ3	2:C:352:LEU:HD22	1.74	0.52
2:E:355:TRP:CZ2	7:E:505:Y01:OAW	2.62	0.52
1:B:300:PHE:CZ	7:B:403:Y01:CAV	2.90	0.52
4:G:128:VAL:HG22	4:G:149:VAL:HG22	1.91	0.52
2:C:318:LEU:HD21	2:C:323:PHE:HD2	1.74	0.51
1:A:288:MET:HA	1:A:291:VAL:HG12	1.92	0.51
1:D:152:LYS:HE3	1:D:206:ASP:OD2	2.10	0.51
1:A:62:TRP:CZ3	1:A:128:PRO:HG3	2.44	0.51
2:C:177:GLU:HG3	2:C:178:TRP:CD1	2.46	0.51
2:E:95:TYR:CD1	2:E:149:ARG:HD3	2.46	0.51
4:K:159:VAL:HG22	4:K:204:VAL:HG22	1.92	0.51
1:A:273:THR:HG22	1:A:275:LEU:H	1.75	0.51
1:D:23:ASN:OD1	1:D:24:LYS:N	2.43	0.51
3:F:42:LEU:HD13	3:F:91:TYR:HE1	1.76	0.51
1:A:49:ASP:OD1	1:A:50:VAL:N	2.44	0.51
1:A:101:ASN:OD1	1:A:134:SER:OG	2.27	0.51
1:D:137:ILE:HG22	1:D:139:VAL:HG23	1.93	0.51
1:D:244:GLU:OE2	1:D:305:HIS:NE2	2.41	0.51
4:G:175:ALA:HA	4:G:184:LEU:HD11	1.93	0.51
1:A:145:ASP:OD1	1:A:146:GLN:N	2.44	0.51
1:A:233:CYS:SG	7:A:402:Y01:HAA1	2.50	0.51
1:A:295:ILE:HA	1:A:298:THR:HG22	1.92	0.51
3:J:124:PRO:HG3	4:K:134:GLY:HA2	1.93	0.51
1:A:70:TYR:HA	1:A:73:ARG:HH21	1.76	0.51
1:A:305:HIS:HE2	1:A:351:LYS:HG3	1.76	0.51
2:C:22:ARG:HH21	2:C:157:GLU:HG2	1.75	0.51
1:A:86:ARG:H	1:A:86:ARG:HD2	1.75	0.51
1:B:102:ASN:HD21	1:B:105:GLY:C	2.14	0.51
1:B:151:MET:HE1	1:B:211:PHE:HE2	1.76	0.51
1:B:187:ASP:OD1	1:B:212:VAL:HB	2.11	0.51
1:B:298:THR:HA	1:B:301:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:LEU:HB3	2:C:199:ILE:HD11	1.93	0.51
2:E:130:CYS:HB2	2:E:144:CYS:HA	1.92	0.51
1:B:221:THR:HA	1:B:225:ILE:HG13	1.93	0.50
1:B:264:LEU:HD11	2:C:254:PHE:HE1	1.77	0.50
4:G:52:ILE:HG22	4:G:59:THR:HG22	1.92	0.50
4:K:128:VAL:HG12	4:K:215:LYS:CE	2.40	0.50
2:E:166:VAL:HG11	4:K:32:SER:HB3	1.91	0.50
2:E:282:LEU:HD11	2:E:357:PHE:CE1	2.45	0.50
3:J:218:GLU:OE2	4:K:135:SER:OG	2.29	0.50
4:G:36:GLU:HB3	4:G:51:GLU:HB3	1.93	0.50
2:E:196:TYR:CD1	2:E:197:VAL:N	2.72	0.50
4:K:195:TRP:HE1	4:K:219:PRO:HG3	1.77	0.50
9:A:405:NCT:C5	1:B:126:THR:OG1	2.60	0.50
2:E:196:TYR:OH	2:E:198:ASP:OD2	2.20	0.50
1:D:228:CYS:HA	1:D:231:ILE:HG12	1.92	0.50
4:K:36:GLU:HB3	4:K:51:GLU:HB3	1.93	0.50
1:B:47:LEU:HD12	1:B:59:THR:HG22	1.93	0.50
1:B:102:ASN:HD22	1:B:107:PHE:HD1	1.58	0.49
2:C:282:LEU:CD1	2:C:357:PHE:CE2	2.95	0.49
3:F:51:LEU:HD21	4:G:107:MET:HG3	1.93	0.49
2:C:291:VAL:HG23	1:D:241:LEU:HD12	1.93	0.49
1:D:165:LEU:HB3	1:D:207:ILE:HD11	1.94	0.49
1:D:184:VAL:HG13	1:D:216:LEU:HD21	1.94	0.49
1:D:238:VAL:HG21	1:D:252:CYS:SG	2.53	0.49
2:C:293:VAL:HA	2:C:296:VAL:HG22	1.95	0.49
1:D:108:ALA:HB2	2:E:106:PHE:HE1	1.78	0.49
2:E:96:ASN:HD21	2:E:146:MET:HA	1.76	0.49
1:A:299:VAL:HG11	1:B:237:LEU:HD21	1.94	0.49
2:E:244:CYS:HB3	2:E:287:ILE:HD13	1.95	0.49
4:G:162:ASN:HD21	4:G:201:THR:HB	1.78	0.49
1:B:102:ASN:HB3	1:B:107:PHE:HE1	1.77	0.49
2:C:59:THR:HG22	2:C:121:LEU:HD22	1.95	0.49
2:C:181:VAL:HB	2:C:204:ILE:HG13	1.95	0.49
3:F:55:LYS:O	3:F:58:ASN:N	2.38	0.49
4:G:28:TYR:CE1	4:G:30:PHE:HA	2.47	0.49
2:C:47:GLU:O	2:C:263:PRO:HB3	2.13	0.48
1:D:295:ILE:HA	1:D:298:THR:HG22	1.95	0.48
1:D:307:ARG:HD2	1:D:312:HIS:CG	2.48	0.48
2:E:317:LYS:NZ	2:E:352:LEU:HD22	2.27	0.48
1:A:156:TRP:O	9:A:405:NCT:HC1	2.12	0.48
2:C:64:ASP:OD1	2:C:65:TYR:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:CYS:SG	1:D:200:CYS:N	2.86	0.48
4:G:203:ASN:HD21	4:G:212:LYS:HD2	1.77	0.48
4:K:52:ILE:HD13	4:K:73:ALA:HB2	1.96	0.48
1:A:187:ASP:OD1	1:A:212:VAL:HB	2.12	0.48
1:D:18:LEU:HD11	1:D:72:LEU:HA	1.95	0.48
3:F:189:ASP:OD2	3:F:193:ARG:NH2	2.39	0.48
1:B:98:VAL:HG13	1:B:107:PHE:HB3	1.96	0.48
3:F:88:LEU:HD21	3:F:111:ILE:HG23	1.96	0.48
2:C:35:LEU:HA	2:C:59:THR:O	2.14	0.48
1:D:243:SER:HA	1:D:248:LYS:HE3	1.96	0.48
1:D:329:LEU:HD11	1:D:363:TRP:CD1	2.49	0.48
2:C:297:HIS:NE2	2:C:343:LYS:HG2	2.28	0.48
1:D:292:THR:O	1:D:295:ILE:HG22	2.13	0.48
3:F:42:LEU:HD13	3:F:91:TYR:CE1	2.48	0.48
3:J:6:GLN:HE22	3:J:92:TYR:HA	1.79	0.48
2:E:355:TRP:CZ2	7:E:505:Y01:HAR1	2.49	0.48
3:F:200:GLU:HG2	3:F:211:VAL:HG22	1.95	0.48
1:A:94:ARG:HD2	1:A:125:TRP:CH2	2.49	0.47
1:B:23:ASN:OD1	1:B:24:LYS:N	2.45	0.47
2:C:85:LYS:HZ3	2:C:107:TYR:HD2	1.61	0.47
2:C:162:LEU:HD21	2:C:199:ILE:HG21	1.95	0.47
1:D:125:TRP:CH2	1:D:127:PRO:HG3	2.49	0.47
1:D:264:LEU:HD11	2:E:257:LEU:HD22	1.96	0.47
1:D:289:ILE:HD13	2:E:222:LEU:HD12	1.96	0.47
1:B:289:ILE:HD13	2:C:222:LEU:HD12	1.95	0.47
1:D:285:LEU:HD13	2:E:214:ILE:HG23	1.95	0.47
4:K:28:TYR:CE1	4:K:30:PHE:HA	2.49	0.47
1:A:27:ARG:NH1	1:A:29:VAL:HG21	2.30	0.47
1:B:22:TYR:HE2	1:B:92:ILE:HA	1.79	0.47
1:B:295:ILE:HA	1:B:298:THR:HG22	1.97	0.47
7:C:505:Y01:HAE2	7:C:505:Y01:HBB	1.69	0.47
1:A:357:ILE:HA	1:A:360:ILE:HG22	1.96	0.47
1:B:118:PHE:HD2	1:B:122:ARG:HD3	1.78	0.47
1:D:272:SER:OG	2:E:177:GLU:OE1	2.32	0.47
2:E:285:PHE:HE1	7:E:504:Y01:HAN1	1.79	0.47
2:C:288:VAL:HG21	7:D:403:Y01:HAQ1	1.96	0.47
2:C:166:VAL:HG12	4:G:32:SER:HB3	1.97	0.47
1:D:187:ASP:OD1	1:D:212:VAL:HB	2.15	0.47
3:J:42:LEU:HD13	3:J:91:TYR:CE1	2.50	0.47
1:B:40:PHE:CZ	1:B:153:PHE:HD2	2.32	0.47
1:B:357:ILE:O	1:B:360:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:ASP:OD1	2:E:116:GLY:N	2.48	0.47
3:F:29:ILE:HD11	3:F:76:PHE:CE2	2.50	0.47
3:F:38:LEU:HD13	3:F:76:PHE:CD2	2.50	0.47
3:F:125:PRO:HD3	3:F:137:VAL:HG22	1.96	0.47
3:F:41:TYR:CZ	4:G:107:MET:HG2	2.50	0.47
1:B:239:PHE:HB2	1:B:362:LEU:HD12	1.96	0.47
1:A:277:ILE:CD1	1:A:282:GLU:HB2	2.46	0.46
1:A:299:VAL:HG23	1:B:241:LEU:HD12	1.96	0.46
1:D:102:ASN:HD21	1:D:105:GLY:C	2.18	0.46
1:D:156:TRP:CZ2	2:E:123:PRO:HD3	2.50	0.46
2:E:18:ASN:OD1	2:E:19:LYS:N	2.47	0.46
7:E:504:Y01:HBB	7:E:504:Y01:HAE2	1.75	0.46
4:K:199:THR:HG23	4:K:216:LYS:HE3	1.96	0.46
2:C:61:GLU:OE2	2:C:163:LYS:NZ	2.41	0.46
2:C:182:ALA:HB3	2:C:204:ILE:HD11	1.98	0.46
2:C:266:SER:HB3	1:D:218:LEU:HB3	1.97	0.46
1:A:233:CYS:SG	7:A:402:Y01:HAN1	2.55	0.46
2:E:7:LEU:HD23	2:E:74:PHE:CE2	2.50	0.46
4:G:159:VAL:HG22	4:G:204:VAL:HG22	1.96	0.46
1:B:289:ILE:O	1:B:292:THR:CG2	2.64	0.46
1:D:264:LEU:O	1:D:267:THR:HG22	2.15	0.46
2:E:151:TRP:CD1	2:E:152:THR:OG1	2.60	0.46
1:B:28:PRO:HB2	1:B:69:ASP:HB2	1.98	0.46
1:B:49:ASP:OD1	1:B:50:VAL:N	2.48	0.46
1:B:238:VAL:HG21	1:B:252:CYS:SG	2.55	0.46
2:C:196:TYR:CD1	2:C:197:VAL:N	2.76	0.46
3:J:125:PRO:O	4:K:220:ARG:NH2	2.49	0.46
4:K:128:VAL:HG12	4:K:215:LYS:HE3	1.97	0.46
2:C:285:PHE:HE1	7:C:505:Y01:HAN1	1.80	0.46
3:J:143:ASN:HA	3:J:177:THR:HB	1.98	0.46
1:B:292:THR:HB	2:C:222:LEU:HD21	1.98	0.46
2:E:188:ASN:HB2	2:E:198:ASP:OD1	2.16	0.46
1:A:236:VAL:HG21	1:A:366:ILE:HD13	1.98	0.46
1:B:357:ILE:HG12	1:B:361:PHE:CE2	2.51	0.46
2:E:132:ILE:HG23	2:E:142:GLN:NE2	2.31	0.46
7:D:404:Y01:HAC2	7:D:404:Y01:HAJ1	1.68	0.46
2:E:196:TYR:CE1	2:E:198:ASP:CG	2.89	0.46
3:F:181:SER:HB2	4:G:173:PHE:HE2	1.80	0.46
7:B:404:Y01:HAB1	7:B:404:Y01:HAJ1	1.79	0.46
1:D:303:ASN:ND2	2:E:232:TYR:O	2.49	0.46
1:A:152:LYS:NZ	1:A:195:ARG:HH11	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HD12	1:B:32:ILE:H	1.81	0.45
2:E:42:LEU:HD21	2:E:45:VAL:HG23	1.97	0.45
4:G:175:ALA:HA	4:G:184:LEU:HD21	1.98	0.45
1:A:57:MET:HG2	1:A:59:THR:HG23	1.98	0.45
1:D:299:VAL:HG23	2:E:233:LEU:HD13	1.98	0.45
3:J:113:ARG:HD3	3:J:114:ALA:O	2.15	0.45
1:D:42:LEU:HD21	1:D:153:PHE:HE2	1.79	0.45
3:F:96:GLY:HA2	3:F:101:TRP:HD1	1.80	0.45
1:B:297:ILE:HD13	7:B:403:Y01:HAQ1	1.99	0.45
1:D:32:ILE:H	1:D:32:ILE:HD12	1.81	0.45
2:C:7:LEU:HD13	2:C:74:PHE:CD2	2.51	0.45
2:E:190:ASN:ND2	2:E:193:ASP:OD2	2.49	0.45
1:A:85:ILE:HD11	1:A:117:LEU:HD12	1.98	0.45
2:C:318:LEU:HB3	2:C:319:PRO:HD3	1.99	0.45
1:D:357:ILE:HA	1:D:360:ILE:HG22	1.97	0.45
1:A:39:ARG:HH21	1:A:168:MET:HG3	1.82	0.45
1:A:63:VAL:O	1:A:126:THR:HA	2.16	0.45
1:A:239:PHE:HB2	1:A:362:LEU:HD12	1.98	0.45
1:B:102:ASN:HB3	1:B:107:PHE:CE1	2.51	0.45
7:C:504:Y01:HAE2	7:C:504:Y01:HBB	1.69	0.45
1:D:57:MET:HG2	1:D:59:THR:HG23	1.97	0.45
3:F:113:ARG:HD3	3:F:114:ALA:O	2.17	0.45
1:A:156:TRP:CD1	1:A:157:THR:HG23	2.50	0.45
1:B:102:ASN:OD1	1:B:103:ALA:N	2.50	0.45
2:C:231:PHE:HB2	2:C:354:LEU:HD12	1.98	0.45
1:D:279:LEU:HD21	1:D:377:PHE:CD1	2.52	0.45
1:A:218:LEU:C	1:A:218:LEU:CD2	2.86	0.45
1:A:292:THR:O	1:A:295:ILE:HG22	2.17	0.45
2:E:7:LEU:HD23	2:E:74:PHE:CD2	2.52	0.45
3:J:64:PRO:HG2	3:J:66:ARG:HH12	1.82	0.45
1:A:137:ILE:HG22	1:A:139:VAL:HG23	1.99	0.44
7:B:403:Y01:HAT2	7:C:504:Y01:HAQ1	1.99	0.44
2:E:169:LEU:HB2	4:K:31:SER:O	2.17	0.44
1:B:87:ILE:HD13	1:B:117:LEU:HD11	1.99	0.44
1:B:151:MET:CE	1:B:211:PHE:CE2	2.90	0.44
2:E:284:THR:O	2:E:287:ILE:HG22	2.17	0.44
2:E:297:HIS:CE1	2:E:343:LYS:HG2	2.52	0.44
2:C:268:ASP:OD1	2:C:269:VAL:N	2.44	0.44
1:D:14:LEU:HD12	1:D:79:TYR:CD2	2.49	0.44
2:E:178:TRP:HE3	2:E:205:ILE:HG22	1.82	0.44
1:A:23:ASN:HD21	1:B:15:LEU:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:MET:HE1	1:B:211:PHE:CE2	2.52	0.44
1:A:52:GLU:O	1:A:271:PRO:HB3	2.17	0.44
1:A:313:THR:HG23	1:A:314:MET:N	2.33	0.44
1:D:283:TYR:HE1	1:D:373:THR:HG22	1.82	0.44
1:D:307:ARG:HB2	1:D:350:TRP:HE1	1.82	0.44
2:E:301:PRO:HB3	2:E:338:VAL:HB	1.99	0.44
1:A:47:LEU:HD12	1:A:59:THR:HG22	2.00	0.44
1:B:273:THR:HG22	1:B:275:LEU:H	1.83	0.44
7:D:403:Y01:HBB	7:D:403:Y01:HAE2	1.74	0.44
3:F:138:VAL:HG22	3:F:183:THR:HG23	2.00	0.44
3:J:96:GLY:HA2	3:J:101:TRP:HD1	1.81	0.44
4:K:206:HIS:NE2	4:K:208:ALA:HB3	2.33	0.44
1:D:299:VAL:HG11	2:E:229:LEU:HD21	1.98	0.44
2:E:151:TRP:HD1	2:E:152:THR:H	1.65	0.44
2:E:321:LEU:HD11	2:E:355:TRP:CD1	2.52	0.44
4:G:13:MET:O	4:G:118:VAL:HG13	2.18	0.44
7:C:504:Y01:HAO2	7:C:504:Y01:HAP1	1.63	0.44
1:D:319:ARG:O	1:D:323:LEU:HB2	2.18	0.44
3:J:154:LYS:NZ	3:J:200:GLU:OE1	2.46	0.44
1:A:242:PRO:HG3	2:E:295:ASN:HA	2.00	0.43
1:B:22:TYR:HD1	1:B:71:LYS:HG2	1.83	0.43
2:C:155:ARG:HB2	2:C:197:VAL:HG13	2.00	0.43
2:C:353:PHE:HZ	7:C:505:Y01:HAQ1	1.82	0.43
1:D:28:PRO:HB2	1:D:69:ASP:HB2	2.00	0.43
2:E:355:TRP:HZ2	7:E:505:Y01:OAW	2.01	0.43
4:G:51:GLU:OE1	4:G:51:GLU:N	2.51	0.43
1:A:245:CYS:HB2	2:E:294:LEU:HD21	2.00	0.43
1:A:253:ILE:HG23	1:A:257:LEU:HD13	2.00	0.43
1:B:299:VAL:HG23	2:C:233:LEU:HD13	2.00	0.43
2:C:130:CYS:HB2	2:C:144:CYS:HA	2.00	0.43
3:J:95:GLN:O	3:J:101:TRP:HD1	2.01	0.43
7:B:403:Y01:HBB	7:B:403:Y01:HAE2	1.76	0.43
1:D:43:SER:HB2	1:D:62:TRP:HB2	2.01	0.43
7:D:404:Y01:HAP1	7:D:404:Y01:HAO2	1.52	0.43
1:A:199:CYS:SG	1:A:200:CYS:N	2.92	0.43
1:A:218:LEU:HB3	2:E:266:SER:HG	1.82	0.43
1:A:283:TYR:HE1	1:A:373:THR:HG22	1.83	0.43
1:D:204:TYR:CZ	9:D:401:NCT:C10	2.99	0.43
2:E:316:GLU:O	2:E:319:PRO:HD2	2.19	0.43
4:G:201:THR:HG23	4:G:215:LYS:C	2.39	0.43
4:K:127:SER:H	4:K:149:VAL:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:NH1	1:B:348:GLU:HG3	2.34	0.43
1:D:221:THR:HA	1:D:225:ILE:HG13	2.00	0.43
1:D:307:ARG:HB2	1:D:350:TRP:NE1	2.34	0.43
1:A:42:LEU:HD11	1:A:153:PHE:HE2	1.84	0.43
1:B:224:LEU:O	1:B:227:PRO:HD2	2.18	0.43
1:B:243:SER:HA	1:B:248:LYS:NZ	2.33	0.43
2:C:196:TYR:CE1	2:C:198:ASP:CG	2.91	0.43
1:A:204:TYR:CD2	9:A:405:NCT:C10	2.73	0.43
1:A:243:SER:HA	1:A:248:LYS:HE3	2.01	0.43
2:C:13:ASP:HB3	2:C:16:ARG:HB3	2.01	0.43
1:B:293:LEU:C	1:B:293:LEU:CD2	2.86	0.43
3:F:59:ARG:NH1	3:F:65:ASP:OD1	2.52	0.43
4:G:7:GLN:NE2	4:G:97:CYS:SG	2.69	0.43
3:J:33:ASN:OD1	3:J:34:GLY:N	2.52	0.43
1:A:156:TRP:CZ2	1:B:128:PRO:HD3	2.53	0.42
1:D:101:ASN:OD1	1:D:134:SER:OG	2.30	0.42
2:E:35:LEU:HD23	2:E:160:LEU:HD22	2.01	0.42
2:C:351:ARG:HH21	7:C:504:Y01:CAR	2.32	0.42
1:A:329:LEU:HD11	1:A:363:TRP:CD1	2.54	0.42
4:G:206:HIS:NE2	4:G:208:ALA:HB3	2.34	0.42
1:A:23:ASN:OD1	1:A:24:LYS:N	2.52	0.42
1:B:313:THR:HG23	1:B:314:MET:N	2.33	0.42
1:A:310:ARG:HH11	1:B:348:GLU:HG3	1.83	0.42
1:D:7:ARG:CZ	1:D:82:VAL:HG12	2.49	0.42
2:E:285:PHE:CD2	2:E:357:PHE:HZ	2.38	0.42
4:K:128:VAL:HG12	4:K:215:LYS:HD2	1.99	0.42
1:D:108:ALA:HB2	2:E:106:PHE:CE1	2.53	0.42
1:D:139:VAL:HG13	1:D:142:PHE:HB2	2.02	0.42
3:J:101:TRP:O	4:K:48:ARG:NE	2.53	0.42
1:A:44:ILE:HD11	1:A:211:PHE:CE1	2.54	0.42
7:A:403:Y01:HAE2	7:A:403:Y01:HBB	1.72	0.42
1:B:45:ALA:HB3	1:B:60:ASN:HB3	2.01	0.42
1:B:312:HIS:NE2	2:C:347:MET:SD	2.83	0.42
1:D:319:ARG:HA	1:D:323:LEU:HD23	2.02	0.42
1:B:39:ARG:NH2	1:B:168:MET:HG3	2.32	0.42
1:B:156:TRP:CZ2	2:C:123:PRO:HD3	2.54	0.42
1:B:226:ILE:HG22	1:B:227:PRO:HD3	2.02	0.42
1:D:272:SER:HA	2:E:211:PHE:CZ	2.54	0.42
3:F:135:ALA:O	3:F:186:LEU:N	2.34	0.42
4:K:201:THR:HG23	4:K:215:LYS:C	2.40	0.42
1:A:29:VAL:HG22	1:A:36:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:LEU:HD23	1:D:242:PRO:O	2.20	0.42
1:D:313:THR:HG23	1:D:314:MET:N	2.32	0.42
2:E:95:TYR:CE1	2:E:149:ARG:CD	3.02	0.42
3:F:4:MET:HB2	3:F:104:GLY:HA2	2.01	0.42
3:F:33:ASN:OD1	3:F:34:GLY:N	2.53	0.42
1:A:42:LEU:HD11	1:A:153:PHE:CE2	2.55	0.42
1:A:236:VAL:HG23	1:A:365:PHE:HD2	1.85	0.42
1:B:241:LEU:HD23	1:B:242:PRO:O	2.20	0.42
7:B:403:Y01:HAC3	7:B:403:Y01:HAJ1	1.73	0.42
4:G:40:GLN:O	4:G:93:ALA:HB1	2.19	0.42
3:J:41:TYR:CZ	4:K:107:MET:HG2	2.55	0.42
3:J:120:VAL:HG22	3:J:141:LEU:HG	2.02	0.42
1:B:357:ILE:HA	1:B:360:ILE:HG22	2.02	0.41
7:D:403:Y01:HAC3	7:D:403:Y01:HAJ1	1.72	0.41
2:E:108:SER:OG	2:E:109:ASN:N	2.53	0.41
2:E:151:TRP:HD1	2:E:152:THR:HG1	1.55	0.41
3:F:149:ILE:HD12	3:F:203:HIS:CD2	2.55	0.41
1:A:297:ILE:HD13	7:A:403:Y01:HAE1	2.01	0.41
1:B:307:ARG:CZ	1:B:350:TRP:HZ2	2.32	0.41
1:D:14:LEU:HD11	1:D:74:TRP:CE2	2.55	0.41
1:A:228:CYS:HA	1:A:231:ILE:HG12	2.01	0.41
1:B:67:TRP:CH2	1:B:95:PRO:HD2	2.55	0.41
1:B:125:TRP:CH2	1:B:127:PRO:HG3	2.55	0.41
1:B:247:GLU:OE1	1:B:247:GLU:HA	2.19	0.41
2:C:184:PRO:CG	4:G:104:TYR:CE2	3.00	0.41
3:F:188:LYS:NZ	3:F:192:GLU:OE2	2.52	0.41
3:J:94:PHE:HE1	4:K:48:ARG:NH2	2.18	0.41
1:D:125:TRP:CZ2	1:D:127:PRO:HG3	2.55	0.41
7:E:505:Y01:HAJ1	7:E:505:Y01:HAC3	1.69	0.41
4:K:131:LEU:HB2	4:K:146:GLY:HA3	2.01	0.41
2:C:34:GLN:HB3	2:C:163:LYS:HG3	2.01	0.41
3:J:172:ASP:OD2	3:J:174:LYS:HG2	2.21	0.41
1:B:378:LEU:N	1:B:379:PRO:HD2	2.35	0.41
2:C:61:GLU:HG2	2:C:119:PHE:HD1	1.86	0.41
2:C:204:ILE:HG13	2:C:204:ILE:O	2.20	0.41
2:E:121:LEU:HD12	2:E:121:LEU:O	2.21	0.41
1:A:7:ARG:NH2	1:A:82:VAL:HG12	2.36	0.41
1:A:245:CYS:SG	2:E:294:LEU:HD11	2.60	0.41
1:A:296:VAL:O	1:A:299:VAL:HG12	2.21	0.41
2:C:213:THR:O	2:C:218:ILE:HG12	2.21	0.41
2:C:288:VAL:O	2:C:291:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:66:ARG:H	2:E:66:ARG:HD3	1.85	0.41
1:B:118:PHE:HB2	1:B:122:ARG:HB3	2.03	0.41
1:B:319:ARG:HA	1:B:323:LEU:HD23	2.03	0.41
2:E:59:THR:HG22	2:E:121:LEU:HD22	2.02	0.41
1:B:326:VAL:HG13	1:B:331:LEU:HB3	2.03	0.41
2:C:168:SER:HA	4:G:32:SER:OG	2.21	0.41
1:D:42:LEU:HD22	1:D:61:VAL:HG11	2.03	0.41
1:D:226:ILE:CG2	1:D:227:PRO:HD3	2.50	0.41
3:J:30:VAL:HG22	3:J:36:THR:OG1	2.21	0.41
3:J:64:PRO:HG2	3:J:66:ARG:NH1	2.36	0.41
1:B:300:PHE:CD1	7:B:403:Y01:HAD3	2.55	0.40
2:C:45:VAL:HG22	2:C:52:MET:HG3	2.02	0.40
2:C:228:ILE:CD1	7:C:504:Y01:CAC	2.98	0.40
2:E:284:THR:HA	2:E:287:ILE:HG22	2.03	0.40
3:F:154:LYS:O	3:F:198:THR:N	2.54	0.40
4:G:162:ASN:ND2	4:G:201:THR:O	2.54	0.40
4:K:7:GLN:N	4:K:112:GLN:HE22	2.17	0.40
1:A:48:ILE:HB	1:A:58:THR:O	2.22	0.40
1:A:226:ILE:CG2	1:A:227:PRO:HD3	2.51	0.40
1:A:240:TYR:O	2:E:295:ASN:ND2	2.54	0.40
1:A:292:THR:HB	1:B:230:LEU:HD21	2.03	0.40
2:C:280:MET:HA	2:C:283:VAL:HG12	2.04	0.40
1:A:303:ASN:O	1:A:307:ARG:HG3	2.21	0.40
1:B:199:CYS:SG	1:B:200:CYS:N	2.94	0.40
7:B:404:Y01:HAE2	7:B:404:Y01:HBB	1.75	0.40
1:D:218:LEU:HA	1:D:221:THR:HG22	2.02	0.40
2:E:285:PHE:HD2	2:E:357:PHE:CZ	2.39	0.40
4:G:34:TRP:CD1	4:G:102:PRO:HD3	2.56	0.40
4:G:128:VAL:O	4:G:215:LYS:HE3	2.22	0.40
1:B:285:LEU:HD11	2:C:218:ILE:HG21	2.03	0.40
1:D:25:TRP:CE2	2:E:83:PRO:HG3	2.57	0.40
1:D:35:VAL:HG12	1:D:161:ALA:O	2.21	0.40
1:D:293:LEU:HD21	7:D:404:Y01:HAB2	2.02	0.40
3:F:172:ASP:OD2	3:F:174:LYS:HG2	2.21	0.40
1:D:118:PHE:CD2	1:D:122:ARG:HD3	2.57	0.40
4:K:70:THR:O	4:K:83:GLN:N	2.54	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	366/386 (95%)	347 (95%)	19 (5%)	0	100	100
1	B	362/386 (94%)	345 (95%)	17 (5%)	0	100	100
1	D	366/386 (95%)	349 (95%)	17 (5%)	0	100	100
2	C	354/403 (88%)	338 (96%)	16 (4%)	0	100	100
2	E	354/403 (88%)	336 (95%)	18 (5%)	0	100	100
3	F	216/238 (91%)	211 (98%)	5 (2%)	0	100	100
3	J	216/238 (91%)	204 (94%)	12 (6%)	0	100	100
4	G	216/462 (47%)	203 (94%)	13 (6%)	0	100	100
4	K	216/462 (47%)	201 (93%)	15 (7%)	0	100	100
All	All	2666/3364 (79%)	2534 (95%)	132 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/359 (96%)	344 (100%)	1 (0%)	92	96
1	B	342/359 (95%)	340 (99%)	2 (1%)	86	93
1	D	345/359 (96%)	345 (100%)	0	100	100
2	C	336/379 (89%)	332 (99%)	4 (1%)	71	84
2	E	336/379 (89%)	332 (99%)	4 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	195/214 (91%)	192 (98%)	3 (2%)	65	81
3	J	195/214 (91%)	193 (99%)	2 (1%)	76	86
4	G	186/412 (45%)	185 (100%)	1 (0%)	88	94
4	K	186/412 (45%)	186 (100%)	0	100	100
All	All	2466/3087 (80%)	2449 (99%)	17 (1%)	84	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	B	116	HIS
1	B	292	THR
2	C	22	ARG
2	C	66	ARG
2	C	151	TRP
2	C	196	TYR
2	E	22	ARG
2	E	66	ARG
2	E	151	TRP
2	E	196	TYR
3	F	4	MET
3	F	113	ARG
3	F	147	LYS
4	G	48	ARG
3	J	113	ARG
3	J	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	142	GLN
3	F	95	GLN
3	F	98	HIS
3	F	171	GLN
3	J	43	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)

6 monosaccharides 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	$\#\|Z\| > 2$
5	NAG	H	1	2,5	14,14,15	1.91	5 (35%)	17,19,21	1.31	3 (17%)
5	NAG	H	2	2,5	14,14,15	1.87	4 (28%)	17,19,21	1.24	3 (17%)
5	BMA	H	3	5	11,11,12	0.56	0	15,15,17	0.74	0
5	NAG	I	1	2,5	14,14,15	1.93	6 (42%)	17,19,21	1.30	2 (11%)
5	NAG	I	2	2,5	14,14,15	1.80	4 (28%)	17,19,21	1.27	1 (5%)
5	BMA	I	3	5	11,11,12	0.57	0	15,15,17	0.79	0

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
5	NAG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	2,5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	NAG	I	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	2,5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-3.65	1.37	1.43
5	I	1	NAG	O5-C1	-3.63	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	NAG	O5-C1	-3.52	1.38	1.43
5	I	2	NAG	O5-C1	-3.24	1.38	1.43
5	I	1	NAG	O5-C5	-2.80	1.37	1.43
5	H	1	NAG	O5-C5	-2.76	1.37	1.43
5	H	2	NAG	O5-C5	-2.76	1.37	1.43
5	I	2	NAG	O5-C5	-2.73	1.37	1.43
5	H	2	NAG	C7-N2	2.59	1.43	1.34
5	I	2	NAG	C7-N2	2.58	1.43	1.34
5	I	1	NAG	C7-N2	2.49	1.42	1.34
5	H	1	NAG	C7-N2	2.45	1.42	1.34
5	I	1	NAG	O3-C3	-2.23	1.37	1.43
5	H	1	NAG	O3-C3	-2.20	1.37	1.43
5	I	2	NAG	O3-C3	-2.17	1.37	1.43
5	H	2	NAG	O3-C3	-2.16	1.37	1.43
5	I	1	NAG	C1-C2	-2.04	1.49	1.52
5	I	1	NAG	O4-C4	-2.02	1.38	1.43
5	H	1	NAG	O4-C4	-2.01	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	1	NAG	C2-N2-C7	-3.09	118.50	122.90
5	H	1	NAG	C2-N2-C7	-2.81	118.91	122.90
5	I	2	NAG	C8-C7-N2	2.73	120.72	116.10
5	H	2	NAG	C2-N2-C7	-2.40	119.48	122.90
5	H	1	NAG	C8-C7-N2	2.37	120.12	116.10
5	H	2	NAG	C8-C7-N2	2.29	119.97	116.10
5	I	1	NAG	C8-C7-N2	2.24	119.90	116.10
5	H	2	NAG	O5-C1-C2	-2.23	107.76	111.29
5	H	1	NAG	O5-C5-C6	2.04	110.41	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

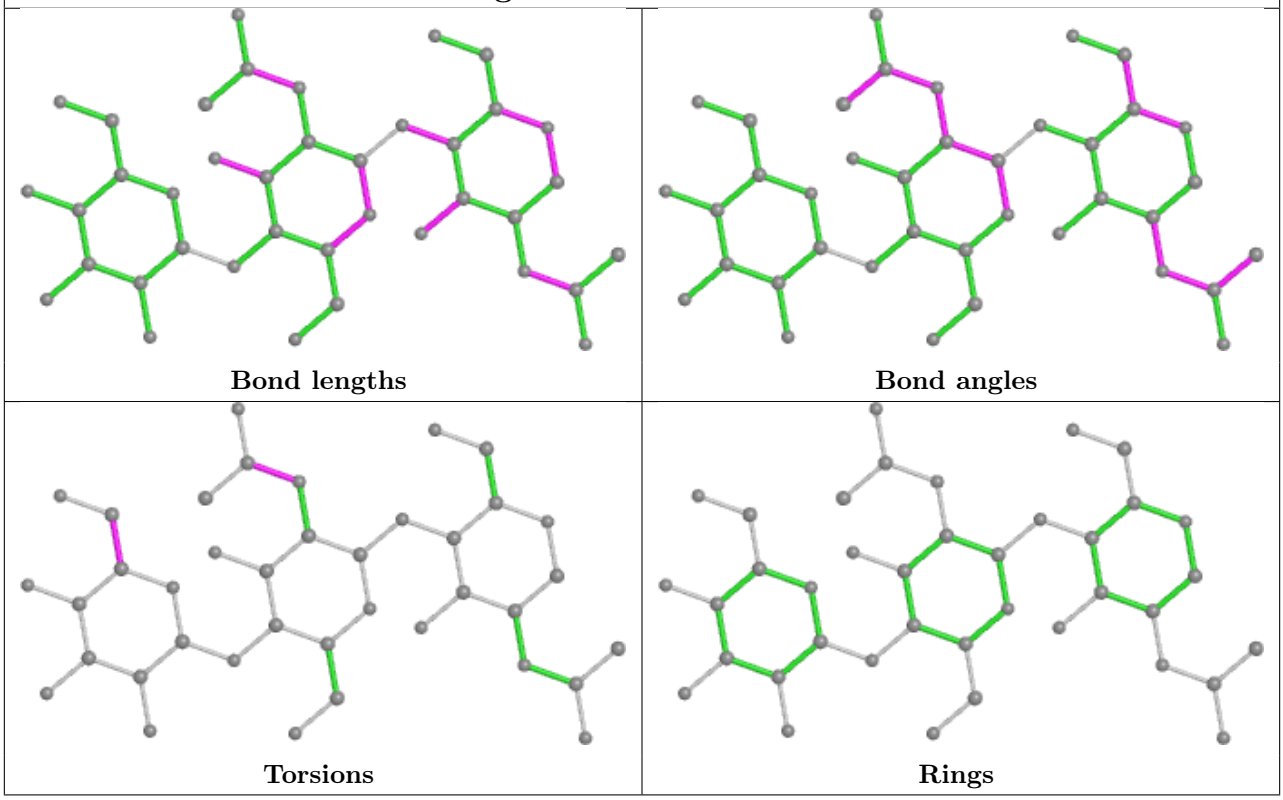
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	H	3	BMA	O5-C5-C6-O6

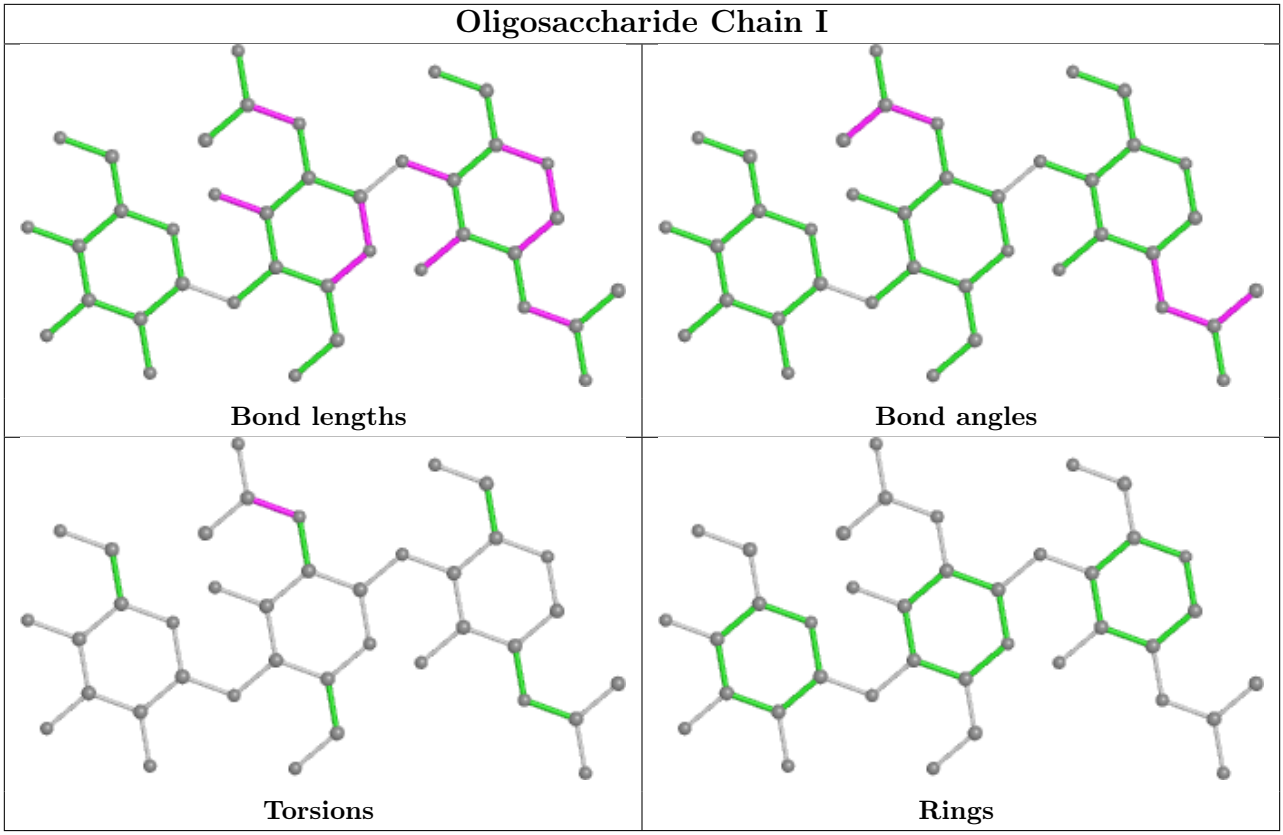
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain H





5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
7	Y01	D	404	-	31,31,38	8.94	22 (70%)	48,48,57	2.19	15 (31%)
7	Y01	B	404	-	31,31,38	8.95	22 (70%)	48,48,57	2.19	15 (31%)
6	NAG	A	401	1	14,14,15	1.86	5 (35%)	17,19,21	1.35	3 (17%)
7	Y01	E	504	-	31,31,38	8.95	22 (70%)	48,48,57	2.16	16 (33%)
9	NCT	D	401	-	13,13,13	0.95	0	17,17,17	1.30	1 (5%)
7	Y01	D	403	-	31,31,38	8.96	22 (70%)	48,48,57	2.21	17 (35%)
7	Y01	E	505	-	31,31,38	8.95	22 (70%)	48,48,57	2.17	15 (31%)
9	NCT	A	405	-	13,13,13	0.94	0	17,17,17	1.30	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	Y01	B	403	-	31,31,38	8.95	22 (70%)	48,48,57	2.19	16 (33%)
9	NCT	B	402	-	13,13,13	1.09	0	17,17,17	1.40	2 (11%)
6	NAG	D	402	1	14,14,15	1.86	5 (35%)	17,19,21	1.35	3 (17%)
7	Y01	C	505	-	31,31,38	8.95	22 (70%)	48,48,57	2.17	17 (35%)
7	Y01	C	504	-	31,31,38	8.93	22 (70%)	48,48,57	2.17	17 (35%)
6	NAG	B	401	1	14,14,15	1.84	4 (28%)	17,19,21	1.18	2 (11%)
7	Y01	A	403	-	31,31,38	8.95	22 (70%)	48,48,57	2.20	16 (33%)
7	Y01	A	402	-	31,31,38	8.95	22 (70%)	48,48,57	2.21	16 (33%)

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
7	Y01	D	404	-	-	8/10/68/77	0/4/4/4
7	Y01	B	404	-	-	6/10/68/77	0/4/4/4
6	NAG	A	401	1	-	0/6/23/26	0/1/1/1
7	Y01	E	504	-	-	6/10/68/77	0/4/4/4
9	NCT	D	401	-	-	0/4/14/14	0/2/2/2
7	Y01	D	403	-	-	5/10/68/77	0/4/4/4
7	Y01	E	505	-	-	6/10/68/77	0/4/4/4
9	NCT	A	405	-	-	0/4/14/14	0/2/2/2
7	Y01	B	403	-	-	6/10/68/77	0/4/4/4
9	NCT	B	402	-	-	0/4/14/14	0/2/2/2
6	NAG	D	402	1	-	0/6/23/26	0/1/1/1
7	Y01	C	505	-	-	7/10/68/77	0/4/4/4
7	Y01	C	504	-	-	6/10/68/77	0/4/4/4
6	NAG	B	401	1	-	0/6/23/26	0/1/1/1
7	Y01	A	403	-	-	8/10/68/77	0/4/4/4
7	Y01	A	402	-	-	5/10/68/77	0/4/4/4

All (234) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	403	Y01	CBD-CBG	-27.94	1.00	1.53
7	A	402	Y01	CBD-CBG	-27.94	1.00	1.53
7	E	504	Y01	CBD-CBG	-27.88	1.00	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	403	Y01	CBD-CBG	-27.88	1.00	1.53
7	C	505	Y01	CBD-CBG	-27.87	1.00	1.53
7	B	404	Y01	CBD-CBG	-27.86	1.00	1.53
7	D	404	Y01	CBD-CBG	-27.86	1.00	1.53
7	E	505	Y01	CBD-CBG	-27.84	1.00	1.53
7	B	403	Y01	CBD-CBG	-27.83	1.00	1.53
7	C	504	Y01	CBD-CBG	-27.81	1.00	1.53
7	C	505	Y01	CAU-CAS	-17.03	1.17	1.53
7	A	402	Y01	CAU-CAS	-17.02	1.17	1.53
7	A	403	Y01	CAU-CAS	-17.02	1.17	1.53
7	B	403	Y01	CAU-CAS	-17.02	1.17	1.53
7	D	403	Y01	CAU-CAS	-17.00	1.17	1.53
7	E	504	Y01	CAU-CAS	-16.99	1.17	1.53
7	B	404	Y01	CAU-CAS	-16.97	1.17	1.53
7	E	505	Y01	CAU-CAS	-16.97	1.17	1.53
7	D	404	Y01	CAU-CAS	-16.96	1.17	1.53
7	C	504	Y01	CAU-CAS	-16.96	1.17	1.53
7	E	504	Y01	CAU-CBI	-16.51	1.24	1.54
7	D	403	Y01	CAU-CBI	-16.45	1.24	1.54
7	D	404	Y01	CAU-CBI	-16.45	1.24	1.54
7	A	402	Y01	CAU-CBI	-16.44	1.24	1.54
7	B	404	Y01	CAU-CBI	-16.44	1.24	1.54
7	C	505	Y01	CAU-CBI	-16.42	1.24	1.54
7	B	403	Y01	CAU-CBI	-16.40	1.24	1.54
7	E	505	Y01	CAU-CBI	-16.39	1.24	1.54
7	C	504	Y01	CAU-CBI	-16.32	1.24	1.54
7	A	403	Y01	CAU-CBI	-16.29	1.24	1.54
7	D	404	Y01	CAK-CBD	-15.42	1.27	1.53
7	D	403	Y01	CAK-CBD	-15.41	1.27	1.53
7	A	402	Y01	CAK-CBD	-15.33	1.27	1.53
7	B	404	Y01	CAK-CBD	-15.33	1.27	1.53
7	E	505	Y01	CAK-CBD	-15.32	1.27	1.53
7	E	504	Y01	CAK-CBD	-15.32	1.27	1.53
7	A	403	Y01	CAK-CBD	-15.31	1.27	1.53
7	B	403	Y01	CAK-CBD	-15.30	1.27	1.53
7	C	505	Y01	CAK-CBD	-15.30	1.27	1.53
7	C	504	Y01	CAK-CBD	-15.25	1.27	1.53
7	C	505	Y01	CBH-CAZ	-12.74	1.27	1.52
7	E	504	Y01	CBH-CAZ	-12.71	1.27	1.52
7	E	505	Y01	CBH-CAZ	-12.70	1.27	1.52
7	C	504	Y01	CBH-CAZ	-12.70	1.27	1.52
7	B	403	Y01	CBH-CAZ	-12.69	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	403	Y01	CBH-CAZ	-12.69	1.27	1.52
7	B	404	Y01	CBH-CAZ	-12.66	1.27	1.52
7	A	403	Y01	CBH-CAZ	-12.64	1.27	1.52
7	D	404	Y01	CBH-CAZ	-12.63	1.27	1.52
7	A	402	Y01	CBH-CAZ	-12.62	1.27	1.52
7	B	403	Y01	CAQ-CAP	10.02	1.81	1.54
7	A	402	Y01	CAQ-CAP	9.99	1.81	1.54
7	D	403	Y01	CAQ-CAP	9.99	1.81	1.54
7	A	403	Y01	CAQ-CAP	9.97	1.81	1.54
7	E	504	Y01	CAQ-CAP	9.96	1.81	1.54
7	E	505	Y01	CAQ-CAP	9.96	1.81	1.54
7	C	504	Y01	CAQ-CAP	9.96	1.81	1.54
7	C	505	Y01	CAQ-CAP	9.95	1.81	1.54
7	D	404	Y01	CAQ-CAP	9.92	1.81	1.54
7	B	404	Y01	CAQ-CAP	9.92	1.81	1.54
7	A	402	Y01	CBB-CBE	-9.76	1.37	1.54
7	D	403	Y01	CBB-CBE	-9.76	1.37	1.54
7	C	505	Y01	CBB-CBE	-9.71	1.37	1.54
7	B	404	Y01	CBB-CBE	-9.70	1.37	1.54
7	E	504	Y01	CBB-CBE	-9.69	1.37	1.54
7	E	505	Y01	CBB-CBE	-9.69	1.37	1.54
7	D	404	Y01	CBB-CBE	-9.64	1.37	1.54
7	B	403	Y01	CBB-CBE	-9.62	1.37	1.54
7	A	403	Y01	CBB-CBE	-9.58	1.37	1.54
7	C	504	Y01	CBB-CBE	-9.56	1.37	1.54
7	E	505	Y01	CBH-CBF	9.10	1.71	1.56
7	C	504	Y01	CBH-CBF	9.06	1.71	1.56
7	B	404	Y01	CBH-CBF	9.03	1.71	1.56
7	D	404	Y01	CBH-CBF	9.03	1.71	1.56
7	C	504	Y01	CBD-CBF	-9.02	1.36	1.53
7	A	403	Y01	CBI-CBE	9.02	1.72	1.55
7	A	403	Y01	CBD-CBF	-9.02	1.36	1.53
7	C	505	Y01	CBD-CBF	-9.01	1.36	1.53
7	B	403	Y01	CBI-CBE	9.00	1.72	1.55
7	A	402	Y01	CBD-CBF	-9.00	1.36	1.53
7	A	402	Y01	CBH-CBF	9.00	1.71	1.56
7	B	403	Y01	CBD-CBF	-8.98	1.36	1.53
7	E	504	Y01	CBD-CBF	-8.98	1.36	1.53
7	C	504	Y01	CBI-CBE	8.98	1.72	1.55
7	D	403	Y01	CBI-CBE	8.97	1.72	1.55
7	B	404	Y01	CBD-CBF	-8.96	1.36	1.53
7	B	403	Y01	CBH-CBF	8.95	1.71	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	404	Y01	CBD-CBF	-8.95	1.36	1.53
7	E	505	Y01	CBD-CBF	-8.94	1.36	1.53
7	D	403	Y01	CBD-CBF	-8.94	1.36	1.53
7	E	504	Y01	CBH-CBF	8.94	1.71	1.56
7	D	403	Y01	CBH-CBF	8.94	1.71	1.56
7	E	504	Y01	CBI-CBE	8.93	1.72	1.55
7	C	505	Y01	CBH-CBF	8.92	1.71	1.56
7	A	403	Y01	CBH-CBF	8.92	1.71	1.56
7	E	505	Y01	CBI-CBE	8.90	1.72	1.55
7	C	505	Y01	CBI-CBE	8.88	1.71	1.55
7	B	404	Y01	CBI-CBE	8.87	1.71	1.55
7	D	404	Y01	CBI-CBE	8.82	1.71	1.55
7	A	402	Y01	CBI-CBE	8.81	1.71	1.55
7	D	404	Y01	CAQ-CBG	8.25	1.71	1.54
7	A	403	Y01	CAQ-CBG	8.23	1.71	1.54
7	B	404	Y01	CAQ-CBG	8.22	1.71	1.54
7	E	505	Y01	CAQ-CBG	8.21	1.71	1.54
7	A	402	Y01	CAQ-CBG	8.20	1.71	1.54
7	E	504	Y01	CAQ-CBG	8.20	1.71	1.54
7	C	505	Y01	CAQ-CBG	8.20	1.71	1.54
7	B	403	Y01	CAQ-CBG	8.19	1.71	1.54
7	C	504	Y01	CAQ-CBG	8.18	1.71	1.54
7	D	403	Y01	CAQ-CBG	8.08	1.71	1.54
7	E	504	Y01	CAK-CAI	7.72	1.66	1.50
7	C	505	Y01	CAK-CAI	7.71	1.66	1.50
7	A	403	Y01	CAK-CAI	7.69	1.66	1.50
7	B	403	Y01	CAK-CAI	7.68	1.66	1.50
7	D	404	Y01	CAK-CAI	7.67	1.66	1.50
7	A	402	Y01	CAK-CAI	7.65	1.66	1.50
7	C	504	Y01	CAK-CAI	7.64	1.66	1.50
7	E	505	Y01	CAK-CAI	7.64	1.66	1.50
7	B	404	Y01	CAK-CAI	7.62	1.66	1.50
7	D	403	Y01	CAK-CAI	7.61	1.66	1.50
7	D	403	Y01	CAT-CBH	6.45	1.66	1.54
7	B	404	Y01	CAT-CBH	6.43	1.66	1.54
7	E	504	Y01	CAT-CBH	6.38	1.66	1.54
7	E	505	Y01	CAT-CBH	6.37	1.66	1.54
7	C	505	Y01	CAT-CBH	6.36	1.66	1.54
7	A	403	Y01	CAT-CBH	6.34	1.66	1.54
7	C	504	Y01	CAT-CBH	6.31	1.66	1.54
7	B	403	Y01	CAT-CBH	6.29	1.66	1.54
7	D	404	Y01	CAT-CBH	6.29	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	402	Y01	CAT-CBH	6.28	1.66	1.54
7	B	404	Y01	CAR-CBC	-6.27	1.36	1.51
7	B	403	Y01	CAR-CBC	-6.25	1.36	1.51
7	E	505	Y01	CAR-CBC	-6.21	1.36	1.51
7	C	505	Y01	CAR-CBC	-6.20	1.36	1.51
7	E	504	Y01	CAR-CBC	-6.20	1.36	1.51
7	C	504	Y01	CAR-CBC	-6.20	1.36	1.51
7	A	403	Y01	CAR-CBC	-6.19	1.36	1.51
7	D	403	Y01	CAR-CBC	-6.19	1.36	1.51
7	A	402	Y01	CAR-CBC	-6.18	1.36	1.51
7	D	404	Y01	CAR-CBC	-6.17	1.36	1.51
7	C	504	Y01	CBI-CBG	5.85	1.66	1.55
7	B	403	Y01	CBI-CBG	5.80	1.66	1.55
7	A	403	Y01	CBI-CBG	5.78	1.66	1.55
7	C	505	Y01	CBI-CBG	5.78	1.66	1.55
7	E	505	Y01	CBI-CBG	5.76	1.66	1.55
7	E	504	Y01	CBI-CBG	5.76	1.66	1.55
7	D	403	Y01	CBI-CBG	5.72	1.65	1.55
7	B	404	Y01	CBI-CBG	5.69	1.65	1.55
7	A	402	Y01	CBI-CBG	5.68	1.65	1.55
7	D	404	Y01	CBI-CBG	5.66	1.65	1.55
7	E	505	Y01	CAP-CBE	4.00	1.62	1.54
7	A	403	Y01	CAP-CBE	4.00	1.62	1.54
7	B	404	Y01	CAP-CBE	3.92	1.62	1.54
7	B	403	Y01	CAP-CBE	3.92	1.62	1.54
7	C	504	Y01	CAP-CBE	3.91	1.62	1.54
7	A	402	Y01	CAP-CBE	3.90	1.62	1.54
7	C	505	Y01	CAP-CBE	3.90	1.62	1.54
7	D	404	Y01	CAP-CBE	3.85	1.62	1.54
7	E	504	Y01	CAP-CBE	3.85	1.62	1.54
7	D	403	Y01	CAP-CBE	3.80	1.62	1.54
7	C	505	Y01	CAI-CAZ	3.74	1.41	1.33
7	B	404	Y01	CAI-CAZ	3.67	1.41	1.33
7	A	402	Y01	CAI-CAZ	3.66	1.41	1.33
7	A	403	Y01	CAI-CAZ	3.65	1.41	1.33
7	B	403	Y01	CAI-CAZ	3.65	1.41	1.33
7	C	504	Y01	CAI-CAZ	3.63	1.41	1.33
7	D	404	Y01	CAI-CAZ	3.62	1.40	1.33
7	D	403	Y01	CAI-CAZ	3.61	1.40	1.33
7	E	504	Y01	CAI-CAZ	3.60	1.40	1.33
7	E	505	Y01	CAI-CAZ	3.60	1.40	1.33
7	A	403	Y01	CAV-CAZ	3.46	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	504	Y01	CAV-CAZ	3.45	1.59	1.51
7	B	403	Y01	CAV-CAZ	3.45	1.59	1.51
7	D	404	Y01	CAO-CBB	3.44	1.63	1.54
7	B	404	Y01	CAV-CAZ	3.44	1.59	1.51
7	A	403	Y01	CAO-CBB	3.43	1.63	1.54
7	D	403	Y01	CAV-CAZ	3.43	1.59	1.51
7	A	402	Y01	CAV-CAZ	3.43	1.59	1.51
6	B	401	NAG	O5-C1	-3.41	1.38	1.43
7	C	505	Y01	CAV-CAZ	3.41	1.59	1.51
7	C	504	Y01	CAO-CBB	3.40	1.63	1.54
7	C	504	Y01	CAV-CAZ	3.39	1.59	1.51
6	A	401	NAG	O5-C1	-3.38	1.38	1.43
7	D	404	Y01	CAV-CAZ	3.37	1.59	1.51
7	B	403	Y01	CAV-CBC	3.36	1.58	1.52
7	B	404	Y01	CAO-CBB	3.35	1.63	1.54
7	B	404	Y01	CAV-CBC	3.35	1.58	1.52
7	C	505	Y01	CAV-CBC	3.35	1.58	1.52
6	D	402	NAG	O5-C1	-3.35	1.38	1.43
7	E	505	Y01	CAV-CAZ	3.35	1.58	1.51
7	D	404	Y01	CAV-CBC	3.35	1.58	1.52
7	A	402	Y01	CAV-CBC	3.33	1.58	1.52
7	A	403	Y01	CAV-CBC	3.32	1.57	1.52
7	E	505	Y01	CAO-CBB	3.31	1.62	1.54
7	E	505	Y01	CAV-CBC	3.29	1.57	1.52
7	D	403	Y01	CAV-CBC	3.28	1.57	1.52
7	E	504	Y01	CAV-CBC	3.27	1.57	1.52
7	B	403	Y01	CAO-CBB	3.27	1.62	1.54
7	A	402	Y01	CAO-CBB	3.26	1.62	1.54
7	C	504	Y01	CAV-CBC	3.26	1.57	1.52
7	E	504	Y01	CAO-CBB	3.25	1.62	1.54
7	C	505	Y01	CAO-CBB	3.25	1.62	1.54
7	D	403	Y01	CAO-CBB	3.23	1.62	1.54
6	B	401	NAG	O5-C5	-2.90	1.37	1.43
6	D	402	NAG	O5-C5	-2.75	1.37	1.43
6	A	401	NAG	O5-C5	-2.72	1.37	1.43
6	B	401	NAG	C7-N2	2.59	1.43	1.34
6	D	402	NAG	C7-N2	2.56	1.43	1.34
6	A	401	NAG	C7-N2	2.54	1.43	1.34
7	D	404	Y01	CAS-CBF	2.35	1.57	1.53
7	C	504	Y01	CAS-CBF	2.30	1.57	1.53
7	E	505	Y01	CAS-CBF	2.30	1.57	1.53
7	B	404	Y01	CAS-CBF	2.30	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	403	Y01	CAS-CBF	2.28	1.57	1.53
7	A	402	Y01	CAS-CBF	2.26	1.57	1.53
7	A	403	Y01	CAS-CBF	2.26	1.57	1.53
7	C	505	Y01	CAS-CBF	2.22	1.57	1.53
7	B	403	Y01	CAS-CBF	2.21	1.57	1.53
7	E	504	Y01	CAS-CBF	2.16	1.57	1.53
6	A	401	NAG	O3-C3	-2.14	1.37	1.43
7	C	505	Y01	OAW-CBC	2.10	1.49	1.43
7	A	403	Y01	OAW-CBC	2.10	1.49	1.43
7	E	505	Y01	OAW-CBC	2.10	1.49	1.43
6	D	402	NAG	O3-C3	-2.10	1.38	1.43
6	D	402	NAG	O4-C4	-2.10	1.38	1.43
7	B	404	Y01	OAW-CBC	2.09	1.49	1.43
7	D	404	Y01	OAW-CBC	2.08	1.49	1.43
7	C	504	Y01	OAW-CBC	2.08	1.49	1.43
7	B	403	Y01	OAW-CBC	2.07	1.49	1.43
6	B	401	NAG	O3-C3	-2.07	1.38	1.43
7	D	403	Y01	OAW-CBC	2.07	1.49	1.43
7	A	402	Y01	OAW-CBC	2.07	1.49	1.43
6	A	401	NAG	O4-C4	-2.06	1.38	1.43
7	E	504	Y01	OAW-CBC	2.04	1.49	1.43

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	404	Y01	CBI-CBE-CBB	-5.80	110.41	119.49
7	C	505	Y01	CBI-CBE-CBB	-5.47	110.92	119.49
7	B	404	Y01	CBI-CBE-CBB	-5.40	111.03	119.49
7	A	402	Y01	CBI-CBE-CBB	-5.40	111.03	119.49
7	E	504	Y01	CBI-CBE-CBB	-5.32	111.15	119.49
7	E	505	Y01	CBI-CBE-CBB	-5.27	111.23	119.49
7	D	403	Y01	CBI-CBE-CBB	-5.25	111.26	119.49
7	A	403	Y01	CBI-CBE-CBB	-5.22	111.32	119.49
7	C	504	Y01	CBI-CBE-CBB	-5.21	111.32	119.49
7	D	403	Y01	CAK-CAI-CAZ	-5.19	115.48	125.06
7	B	404	Y01	CAK-CAI-CAZ	-5.19	115.49	125.06
7	B	403	Y01	CBI-CBE-CBB	-5.19	111.36	119.49
7	E	505	Y01	CAK-CAI-CAZ	-5.14	115.57	125.06
7	C	504	Y01	CAK-CAI-CAZ	-5.07	115.71	125.06
7	A	403	Y01	CAK-CAI-CAZ	-5.05	115.74	125.06
7	D	404	Y01	CAK-CAI-CAZ	-5.03	115.78	125.06
7	A	402	Y01	CAK-CAI-CAZ	-5.01	115.82	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	404	Y01	CAE-CBI-CBE	-4.98	102.43	111.71
7	B	403	Y01	CAK-CAI-CAZ	-4.91	116.01	125.06
7	E	505	Y01	CAU-CBI-CBG	4.90	114.87	107.27
7	C	505	Y01	CAE-CBI-CBE	-4.89	102.59	111.71
7	B	403	Y01	CAU-CBI-CBG	4.87	114.83	107.27
7	C	505	Y01	CAK-CAI-CAZ	-4.80	116.20	125.06
7	A	402	Y01	CAU-CBI-CBG	4.80	114.72	107.27
7	E	504	Y01	CAK-CAI-CAZ	-4.78	116.23	125.06
7	C	504	Y01	CAE-CBI-CBE	-4.75	102.85	111.71
7	B	404	Y01	CAU-CBI-CBG	4.74	114.62	107.27
7	A	403	Y01	CAE-CBI-CBE	-4.72	102.92	111.71
7	E	504	Y01	CAE-CBI-CBE	-4.66	103.03	111.71
7	D	403	Y01	CAU-CBI-CBG	4.65	114.48	107.27
7	D	403	Y01	CAE-CBI-CBE	-4.62	103.11	111.71
7	B	404	Y01	CAE-CBI-CBE	-4.60	103.13	111.71
7	E	504	Y01	CAU-CBI-CBG	4.58	114.38	107.27
7	A	403	Y01	CAU-CBI-CBG	4.58	114.38	107.27
7	B	403	Y01	CAE-CBI-CBE	-4.55	103.23	111.71
7	A	402	Y01	CAE-CBI-CBE	-4.51	103.31	111.71
7	E	505	Y01	CAE-CBI-CBE	-4.48	103.35	111.71
7	C	505	Y01	CAU-CBI-CBG	4.41	114.12	107.27
7	C	504	Y01	CAU-CBI-CBG	4.39	114.09	107.27
7	A	403	Y01	CBH-CAZ-CAI	-4.31	116.31	122.90
7	D	404	Y01	CAU-CBI-CBG	4.31	113.95	107.27
7	D	403	Y01	CBH-CAZ-CAI	-4.27	116.36	122.90
7	C	505	Y01	CBH-CAZ-CAI	-4.27	116.37	122.90
7	E	504	Y01	CBH-CAZ-CAI	-4.23	116.43	122.90
7	B	403	Y01	CBH-CAZ-CAI	-4.20	116.47	122.90
7	B	404	Y01	CBH-CAZ-CAI	-4.13	116.58	122.90
7	A	402	Y01	CBH-CAZ-CAI	-4.12	116.60	122.90
7	E	505	Y01	CBH-CAZ-CAI	-4.09	116.64	122.90
7	C	504	Y01	CBH-CAZ-CAI	-4.07	116.68	122.90
7	A	403	Y01	CAS-CBF-CBH	-4.04	107.76	113.08
7	B	403	Y01	CAS-CBF-CBH	-4.02	107.78	113.08
7	C	505	Y01	CAS-CBF-CBH	-3.99	107.82	113.08
7	A	403	Y01	CAD-CBH-CBF	-3.96	106.96	111.68
7	D	404	Y01	CBH-CAZ-CAI	-3.94	116.88	122.90
7	D	403	Y01	CAS-CBF-CBH	-3.91	107.93	113.08
7	A	402	Y01	CAS-CBF-CBH	-3.86	108.00	113.08
7	E	504	Y01	CAS-CBF-CBH	-3.80	108.07	113.08
7	A	403	Y01	CAU-CBI-CBE	3.79	122.24	116.57
7	B	403	Y01	CAU-CBI-CBE	3.79	122.24	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	402	Y01	CAU-CBI-CBE	3.78	122.24	116.57
7	C	504	Y01	CAU-CBI-CBE	3.78	122.24	116.57
9	A	405	NCT	C10-N2-C6	-3.77	101.38	112.83
7	D	404	Y01	CAS-CBF-CBH	-3.75	108.13	113.08
7	D	403	Y01	CAD-CBH-CBF	-3.75	107.21	111.68
9	B	402	NCT	C10-N2-C6	-3.75	101.43	112.83
7	C	504	Y01	CAS-CBF-CBH	-3.75	108.14	113.08
7	B	404	Y01	CAS-CBF-CBH	-3.72	108.18	113.08
7	A	402	Y01	CAD-CBH-CBF	-3.71	107.26	111.68
7	E	504	Y01	CAU-CBI-CBE	3.70	122.12	116.57
7	E	505	Y01	CAU-CBI-CBE	3.70	122.12	116.57
9	D	401	NCT	C10-N2-C6	-3.70	101.60	112.83
7	D	403	Y01	CAU-CBI-CBE	3.66	122.04	116.57
7	C	505	Y01	CAU-CBI-CBE	3.62	121.99	116.57
7	D	404	Y01	CAU-CBI-CBE	3.61	121.98	116.57
7	C	504	Y01	CAD-CBH-CBF	-3.59	107.40	111.68
7	B	404	Y01	CAU-CBI-CBE	3.58	121.93	116.57
7	D	404	Y01	CAD-CBH-CBF	-3.58	107.41	111.68
7	B	404	Y01	CAD-CBH-CBF	-3.54	107.47	111.68
7	B	403	Y01	CAD-CBH-CBF	-3.53	107.47	111.68
7	D	404	Y01	CBF-CBD-CBG	3.46	113.73	109.09
7	E	505	Y01	CAS-CBF-CBH	-3.44	108.55	113.08
7	E	504	Y01	CAD-CBH-CBF	-3.30	107.74	111.68
7	E	505	Y01	CAD-CBH-CBF	-3.30	107.75	111.68
7	C	505	Y01	CAD-CBH-CBF	-3.25	107.81	111.68
7	B	403	Y01	CAQ-CBG-CBD	3.02	124.06	119.08
7	C	505	Y01	CBF-CBD-CBG	3.00	113.11	109.09
7	E	505	Y01	CAQ-CBG-CBD	2.98	123.99	119.08
7	D	403	Y01	CAQ-CBG-CBD	2.95	123.94	119.08
7	A	402	Y01	CAQ-CBG-CBD	2.91	123.87	119.08
7	B	404	Y01	CAQ-CBG-CBD	2.87	123.80	119.08
7	E	504	Y01	CBF-CBD-CBG	2.83	112.88	109.09
7	A	403	Y01	CAQ-CBG-CBD	2.82	123.72	119.08
7	A	403	Y01	CAE-CBI-CAU	-2.80	106.16	110.59
7	B	403	Y01	CAE-CBI-CAU	-2.79	106.18	110.59
7	E	505	Y01	CAE-CBI-CAU	-2.75	106.25	110.59
7	A	402	Y01	CAE-CBI-CAU	-2.74	106.26	110.59
7	B	404	Y01	CAE-CBI-CAU	-2.74	106.26	110.59
7	C	504	Y01	CAE-CBI-CAU	-2.74	106.26	110.59
7	E	504	Y01	CAQ-CBG-CBD	2.74	123.59	119.08
7	C	504	Y01	CAQ-CBG-CBD	2.71	123.55	119.08
7	B	404	Y01	CAC-CBB-CBE	-2.71	108.77	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	403	Y01	CAE-CBI-CAU	-2.71	106.32	110.59
9	B	402	NCT	C10-N2-C9	-2.70	104.23	112.70
7	C	505	Y01	CAQ-CBG-CBD	2.69	123.51	119.08
7	C	504	Y01	CBF-CBD-CBG	2.67	112.66	109.09
7	A	402	Y01	CAC-CBB-CBE	-2.67	108.84	112.92
7	E	504	Y01	CAE-CBI-CAU	-2.66	106.39	110.59
7	E	505	Y01	CAC-CBB-CBE	-2.65	108.86	112.92
6	D	402	NAG	O5-C5-C6	2.62	111.32	107.20
6	A	401	NAG	O5-C5-C6	2.61	111.29	107.20
6	A	401	NAG	C2-N2-C7	-2.56	119.26	122.90
7	E	504	Y01	CAC-CBB-CBE	-2.56	109.01	112.92
7	E	505	Y01	CAK-CBD-CBF	2.55	112.80	109.71
7	D	403	Y01	CAK-CBD-CBF	2.54	112.79	109.71
7	B	404	Y01	CAK-CBD-CBF	2.53	112.78	109.71
6	D	402	NAG	C2-N2-C7	-2.51	119.32	122.90
7	D	403	Y01	CAC-CBB-CBE	-2.49	109.11	112.92
7	C	505	Y01	CAE-CBI-CAU	-2.47	106.68	110.59
7	D	404	Y01	CBG-CBI-CBE	2.47	103.00	100.07
7	D	404	Y01	CAQ-CBG-CBD	2.47	123.14	119.08
6	D	402	NAG	C8-C7-N2	2.46	120.27	116.10
6	A	401	NAG	C8-C7-N2	2.44	120.23	116.10
7	D	403	Y01	CAE-CBI-CBG	-2.44	107.17	111.71
7	A	403	Y01	CAK-CBD-CBF	2.44	112.66	109.71
7	A	402	Y01	CBF-CBD-CBG	2.42	112.33	109.09
7	A	403	Y01	CAE-CBI-CBG	-2.41	107.21	111.71
7	D	404	Y01	CAC-CBB-CBE	-2.41	109.23	112.92
7	B	403	Y01	CAK-CBD-CBF	2.40	112.62	109.71
7	A	403	Y01	CBF-CBD-CBG	2.40	112.30	109.09
7	E	505	Y01	CAE-CBI-CBG	-2.38	107.28	111.71
7	B	403	Y01	CAE-CBI-CBG	-2.37	107.29	111.71
7	D	404	Y01	CAE-CBI-CAU	-2.36	106.86	110.59
7	C	504	Y01	CAV-CAZ-CBH	-2.35	113.29	116.42
7	D	404	Y01	CAE-CBI-CBG	-2.34	107.35	111.71
6	B	401	NAG	C2-N2-C7	-2.33	119.58	122.90
7	B	404	Y01	CBF-CBD-CBG	2.33	112.21	109.09
7	C	505	Y01	CAC-CBB-CBE	-2.33	109.35	112.92
7	E	504	Y01	CAV-CAZ-CBH	-2.31	113.35	116.42
6	B	401	NAG	C8-C7-N2	2.30	120.00	116.10
7	B	403	Y01	CAC-CBB-CBE	-2.30	109.40	112.92
7	B	404	Y01	CAE-CBI-CBG	-2.30	107.43	111.71
7	C	504	Y01	CAK-CBD-CBF	2.29	112.49	109.71
7	A	402	Y01	CAE-CBI-CBG	-2.28	107.46	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	505	Y01	CAE-CBI-CBG	-2.27	107.48	111.71
7	B	403	Y01	CBF-CBD-CBG	2.27	112.12	109.09
7	C	504	Y01	CAC-CBB-CBE	-2.26	109.45	112.92
7	C	505	Y01	CBG-CBI-CBE	2.26	102.75	100.07
7	A	402	Y01	CAK-CBD-CBF	2.25	112.44	109.71
7	C	504	Y01	CAE-CBI-CBG	-2.23	107.55	111.71
7	A	402	Y01	CAV-CAZ-CBH	-2.22	113.47	116.42
7	E	504	Y01	CAE-CBI-CBG	-2.21	107.58	111.71
7	C	505	Y01	CAV-CAZ-CBH	-2.21	113.48	116.42
7	D	404	Y01	CAV-CAZ-CBH	-2.21	113.49	116.42
7	D	403	Y01	CAV-CAZ-CBH	-2.18	113.52	116.42
7	C	504	Y01	CBG-CBI-CBE	2.17	102.64	100.07
7	A	403	Y01	CBG-CBI-CBE	2.16	102.63	100.07
7	A	403	Y01	CAC-CBB-CBE	-2.12	109.67	112.92
7	E	504	Y01	CAJ-CAO-CBB	-2.10	109.00	115.03
7	C	504	Y01	CBF-CBH-CAZ	2.09	112.92	109.65
7	A	402	Y01	CAJ-CAO-CBB	-2.09	109.04	115.03
7	C	505	Y01	CAT-CBH-CAZ	2.08	112.57	108.75
7	B	404	Y01	CAV-CAZ-CBH	-2.08	113.65	116.42
7	D	403	Y01	CBF-CBD-CBG	2.06	111.86	109.09
7	E	505	Y01	CBF-CBD-CBG	2.06	111.85	109.09
7	A	403	Y01	CAT-CBH-CAZ	2.06	112.52	108.75
7	E	504	Y01	CAT-CBH-CAZ	2.05	112.50	108.75
7	E	505	Y01	CAT-CBH-CAZ	2.04	112.50	108.75
7	B	403	Y01	CAJ-CAO-CBB	-2.04	109.16	115.03
7	B	403	Y01	CAV-CAZ-CBH	-2.04	113.72	116.42
7	C	505	Y01	CAJ-CAO-CBB	-2.03	109.19	115.03
7	D	403	Y01	CBG-CBI-CBE	2.01	102.45	100.07
7	D	403	Y01	CAJ-CAO-CBB	-2.00	109.27	115.03

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	404	Y01	CAC-CBB-CBE-CBI
7	A	402	Y01	CAC-CBB-CBE-CAP
7	B	404	Y01	CAC-CBB-CBE-CAP
7	E	505	Y01	CAC-CBB-CBE-CAP
7	A	402	Y01	CAC-CBB-CBE-CBI
7	A	403	Y01	CAC-CBB-CBE-CBI
7	B	403	Y01	CAC-CBB-CBE-CBI
7	B	404	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
7	C	504	Y01	CAC-CBB-CBE-CBI
7	C	505	Y01	CAC-CBB-CBE-CBI
7	D	403	Y01	CAC-CBB-CBE-CBI
7	E	504	Y01	CAC-CBB-CBE-CBI
7	E	505	Y01	CAC-CBB-CBE-CBI
7	B	403	Y01	CAO-CBB-CBE-CBI
7	C	504	Y01	CAO-CBB-CBE-CBI
7	C	505	Y01	CAO-CBB-CBE-CBI
7	C	505	Y01	CAC-CBB-CBE-CAP
7	D	403	Y01	CAC-CBB-CBE-CAP
7	D	404	Y01	CAC-CBB-CBE-CAP
7	E	504	Y01	CAC-CBB-CBE-CAP
7	A	402	Y01	CAO-CBB-CBE-CBI
7	A	403	Y01	CAO-CBB-CBE-CBI
7	B	404	Y01	CAO-CBB-CBE-CBI
7	D	403	Y01	CAO-CBB-CBE-CBI
7	D	404	Y01	CAO-CBB-CBE-CBI
7	E	504	Y01	CAO-CBB-CBE-CBI
7	E	505	Y01	CAO-CBB-CBE-CBI
7	A	403	Y01	CAC-CBB-CBE-CAP
7	B	403	Y01	CAC-CBB-CBE-CAP
7	D	404	Y01	CAO-CBB-CBE-CAP
7	C	504	Y01	CAC-CBB-CBE-CAP
7	E	505	Y01	CAO-CBB-CBE-CAP
7	A	403	Y01	CAJ-CAO-CBB-CAC
7	C	504	Y01	CAJ-CAO-CBB-CAC
7	D	404	Y01	CAJ-CAO-CBB-CAC
7	B	404	Y01	CAO-CBB-CBE-CAP
7	A	403	Y01	CAJ-CAO-CBB-CBE
7	C	504	Y01	CAJ-CAO-CBB-CBE
7	D	404	Y01	CAJ-CAO-CBB-CBE
7	A	402	Y01	CAO-CBB-CBE-CAP
7	A	402	Y01	CAN-CAJ-CAO-CBB
7	B	404	Y01	CAJ-CAO-CBB-CAC
7	A	403	Y01	CAN-CAJ-CAO-CBB
7	C	505	Y01	CAN-CAJ-CAO-CBB
7	D	404	Y01	CAO-CAJ-CAN-CBA
7	D	404	Y01	CAN-CAJ-CAO-CBB
7	E	504	Y01	CAO-CBB-CBE-CAP
7	E	504	Y01	CAN-CAJ-CAO-CBB
7	B	403	Y01	CAN-CAJ-CAO-CBB
7	D	403	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
7	A	403	Y01	CAO-CBB-CBE-CAP
7	D	403	Y01	CAO-CBB-CBE-CAP
7	C	505	Y01	CAJ-CAN-CBA-CAA
7	C	504	Y01	CAO-CBB-CBE-CAP
7	C	505	Y01	CAO-CBB-CBE-CAP
7	B	403	Y01	CAO-CBB-CBE-CAP
7	E	505	Y01	CAJ-CAO-CBB-CAC
7	C	505	Y01	CAJ-CAN-CBA-CAB
7	B	404	Y01	CAO-CAJ-CAN-CBA
7	E	505	Y01	CAN-CAJ-CAO-CBB
7	B	403	Y01	CAJ-CAN-CBA-CAB
7	A	403	Y01	CAJ-CAN-CBA-CAA
7	E	504	Y01	CAJ-CAN-CBA-CAB

There are no ring outliers.

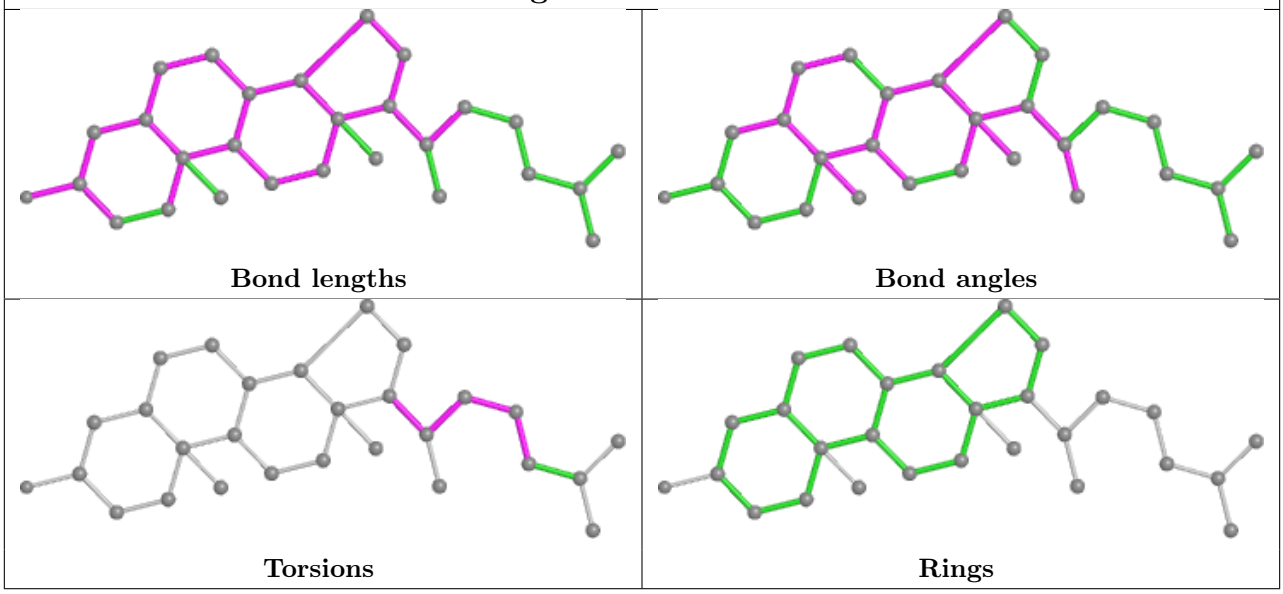
13 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	404	Y01	12	0
7	B	404	Y01	5	0
7	E	504	Y01	4	0
9	D	401	NCT	8	0
7	D	403	Y01	4	0
7	E	505	Y01	5	0
9	A	405	NCT	9	0
7	B	403	Y01	14	0
9	B	402	NCT	1	0
7	C	505	Y01	6	0
7	C	504	Y01	7	0
7	A	403	Y01	8	0
7	A	402	Y01	4	0

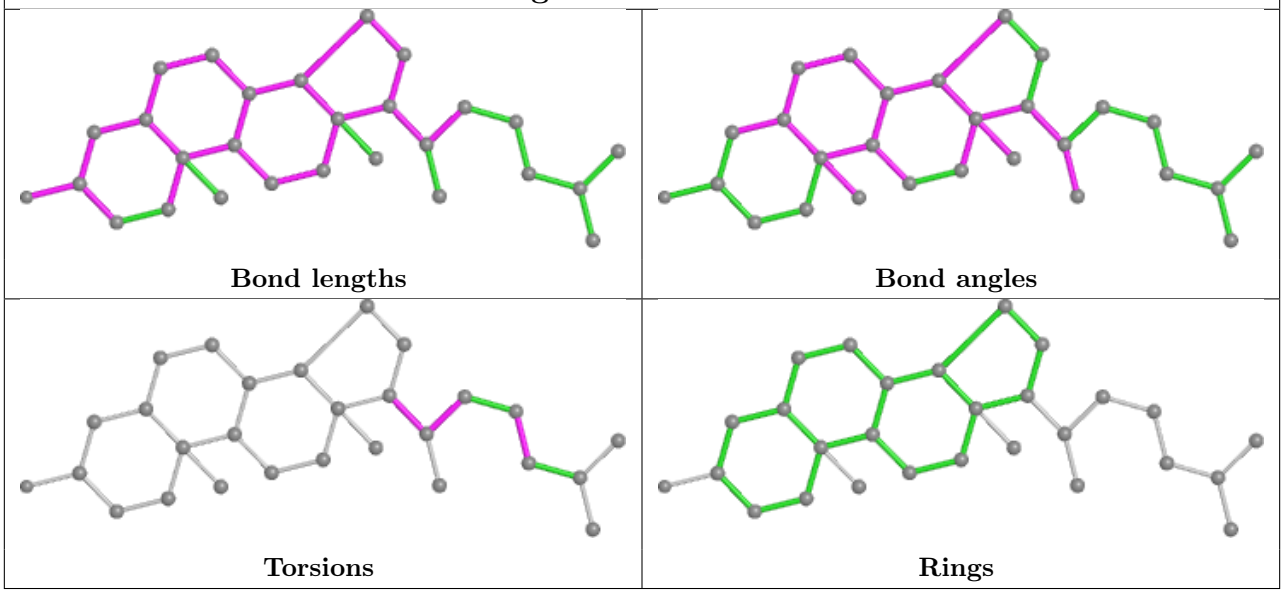
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

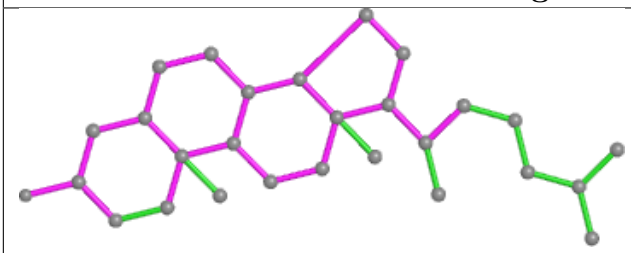
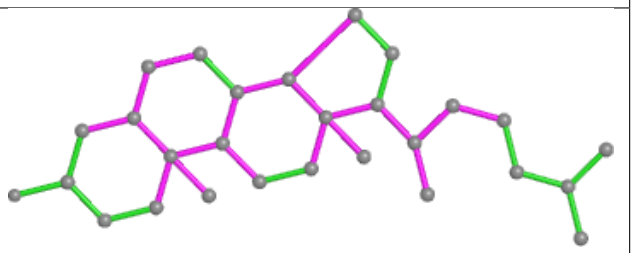
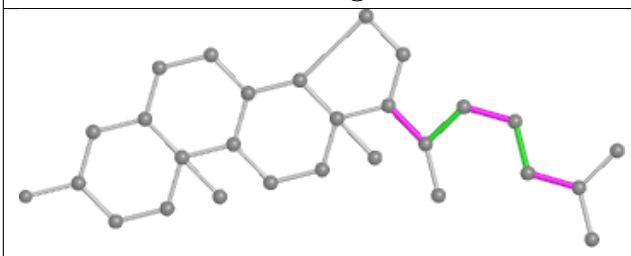
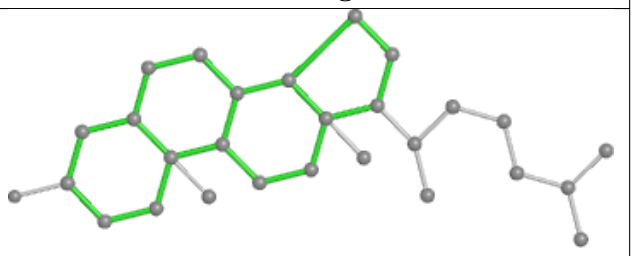
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

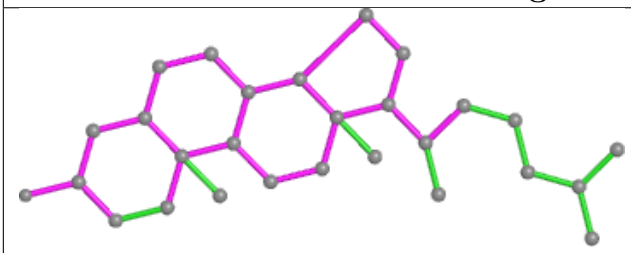
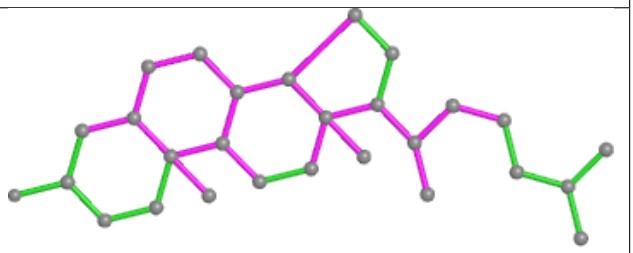
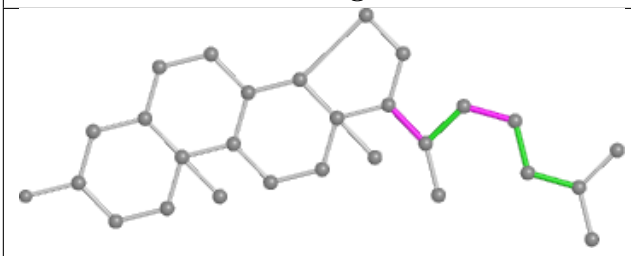
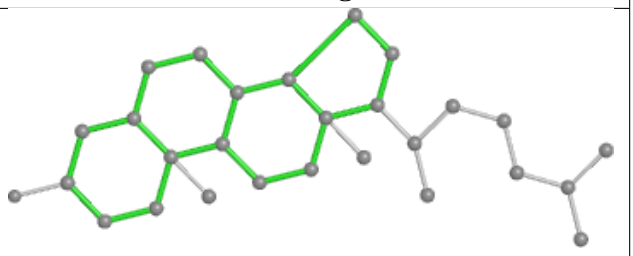
Ligand Y01 D 404

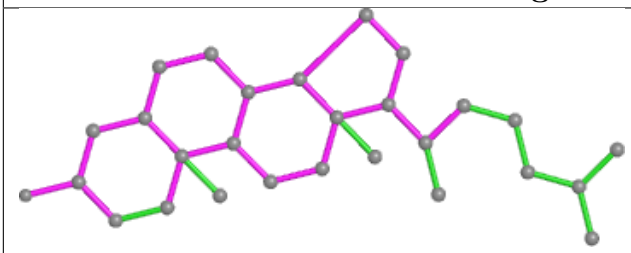
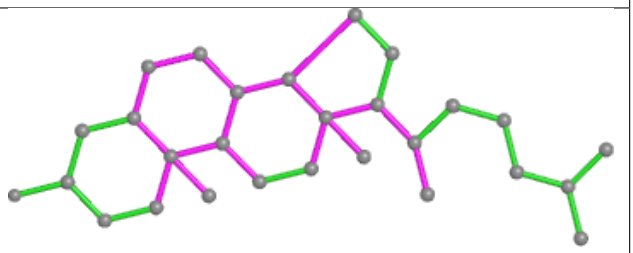
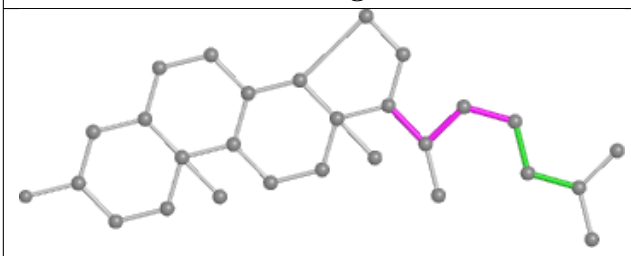
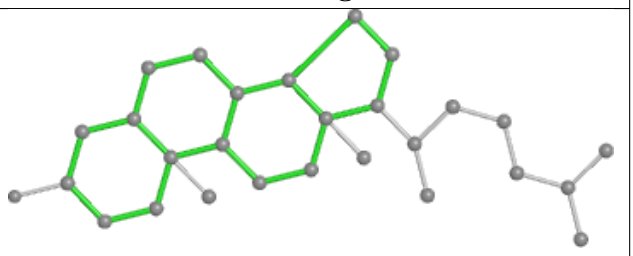


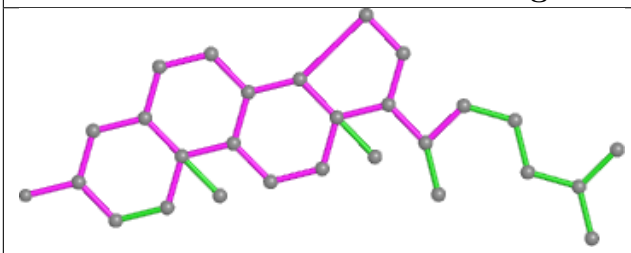
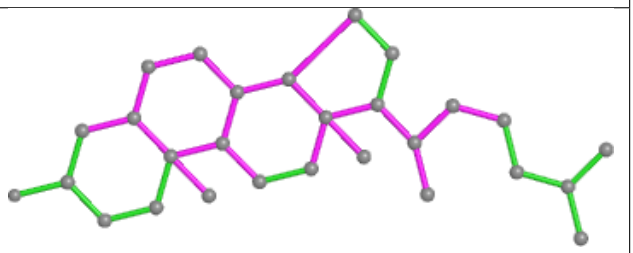
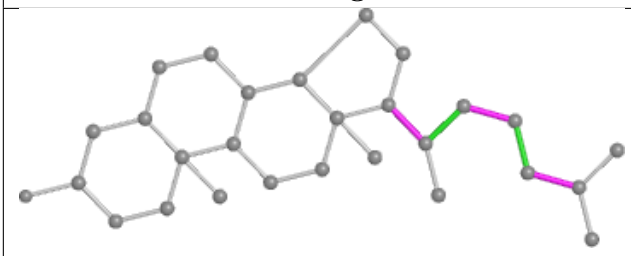
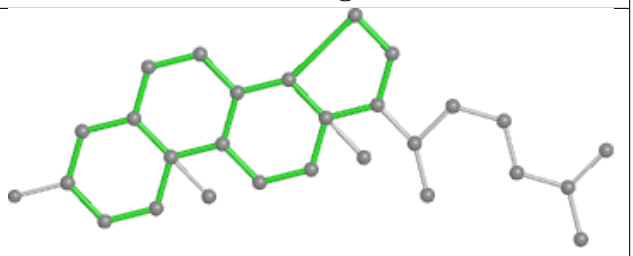
Ligand Y01 B 404

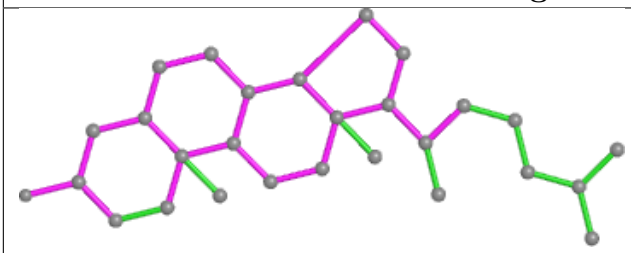
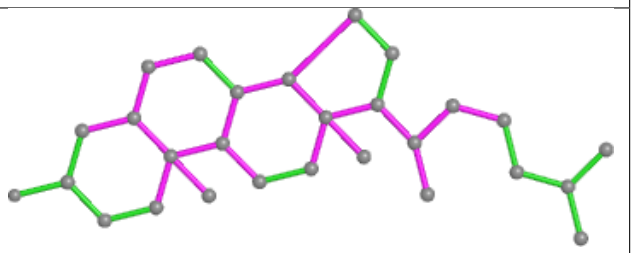
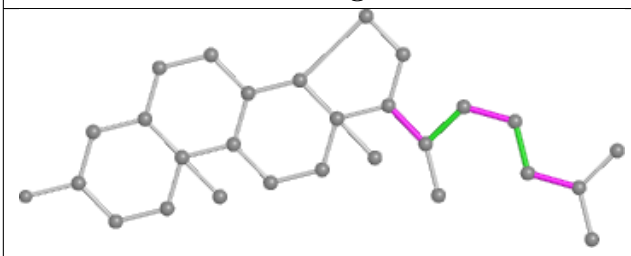
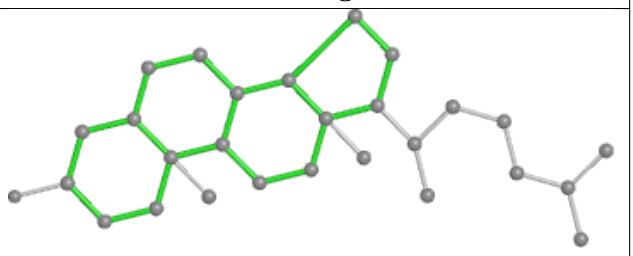


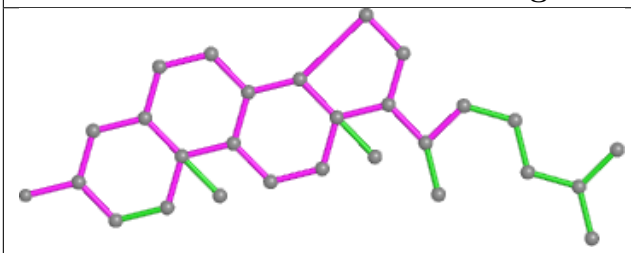
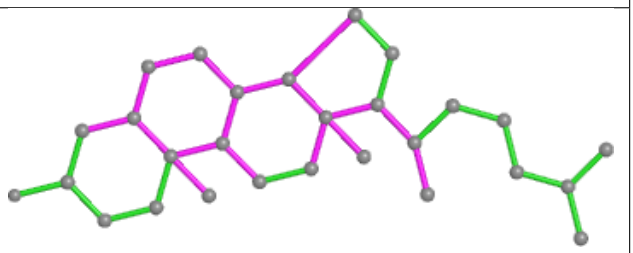
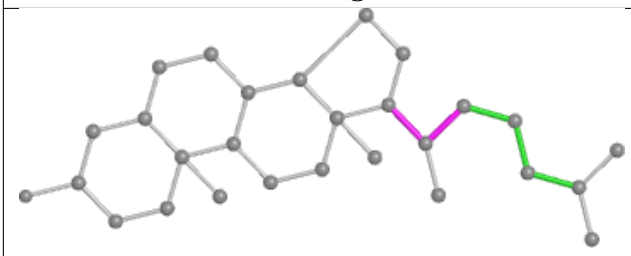
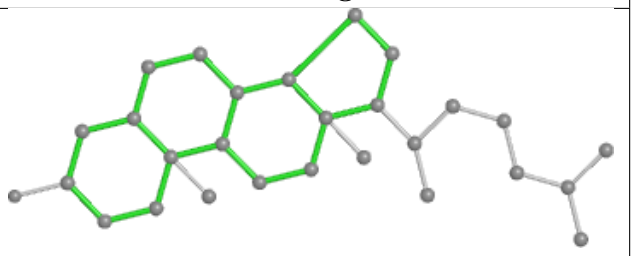
Ligand Y01 E 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

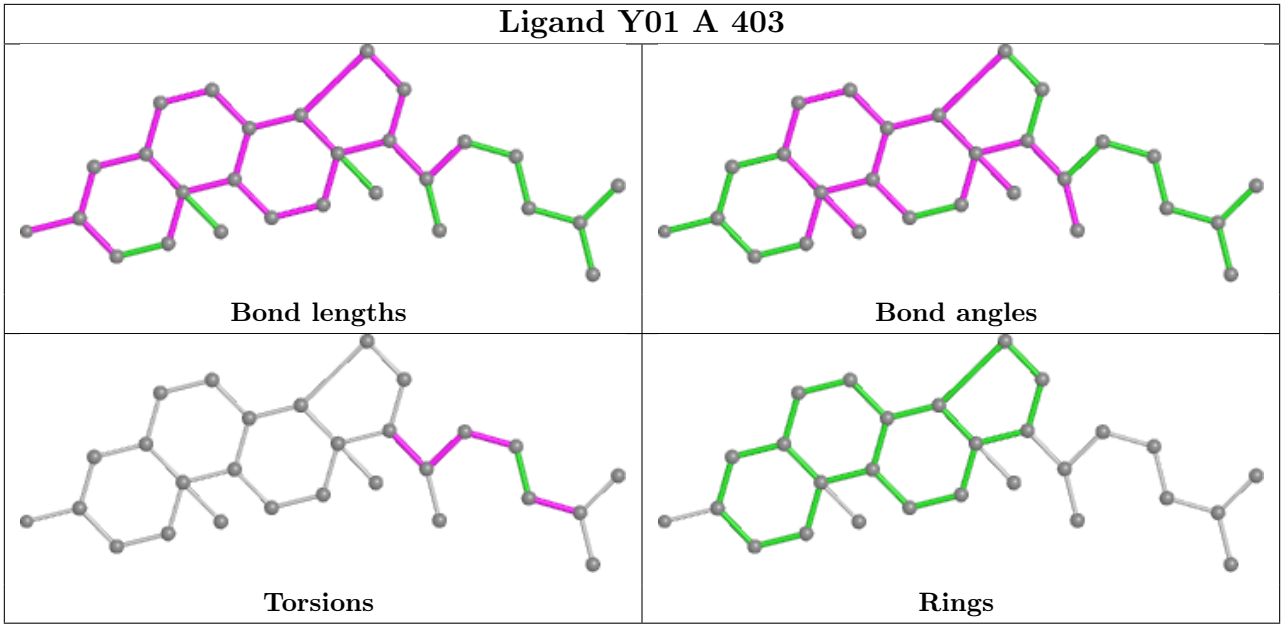
Ligand Y01 D 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

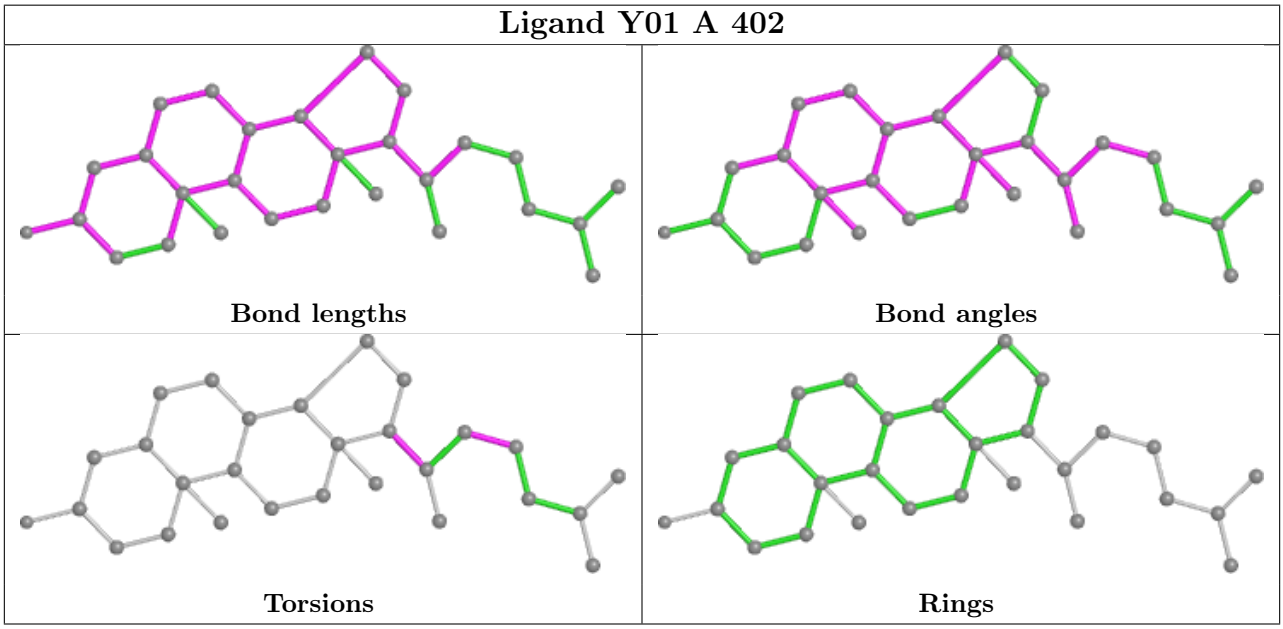
Ligand Y01 E 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 B 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

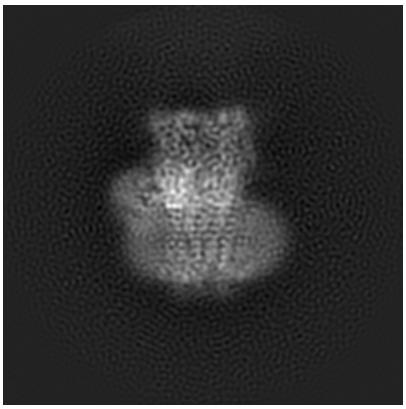
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7536. These allow visual inspection of the internal detail of the map and identification of artifacts.

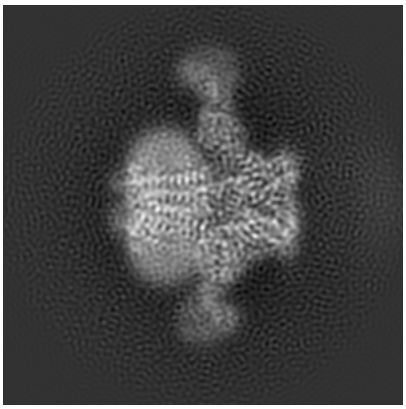
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

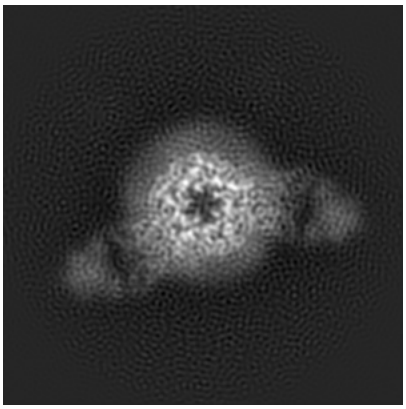
6.1.1 Primary map



X

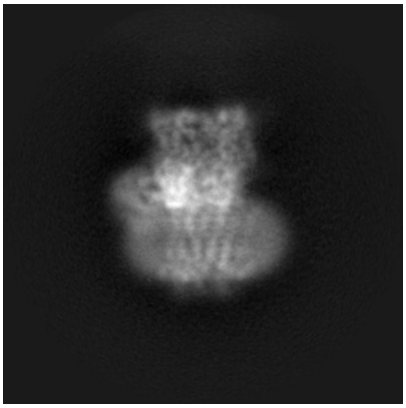


Y

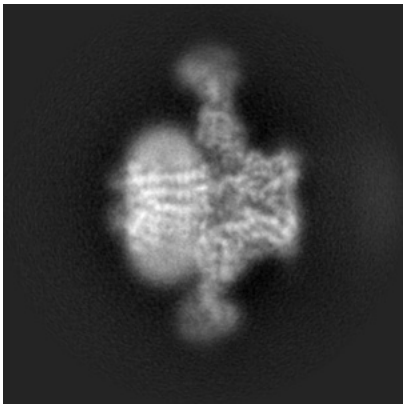


Z

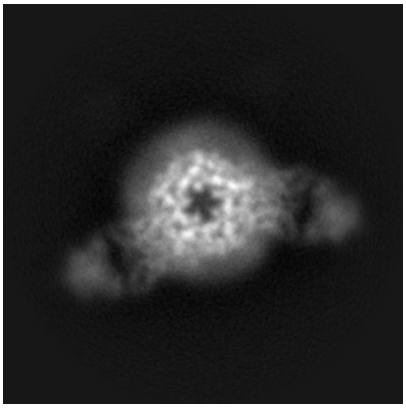
6.1.2 Raw map



X



Y

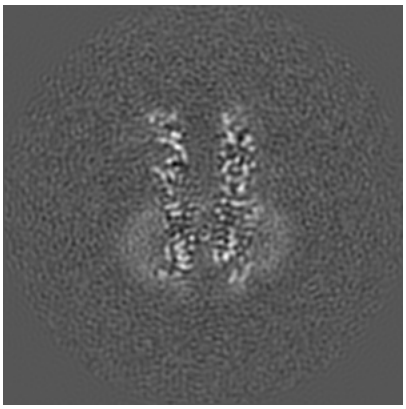


Z

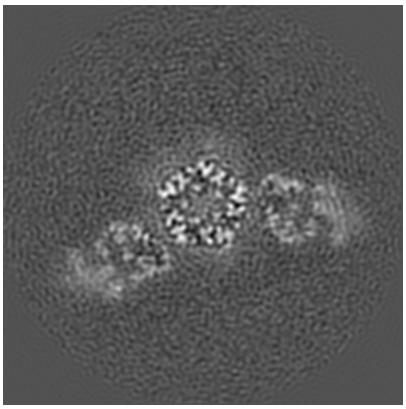
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

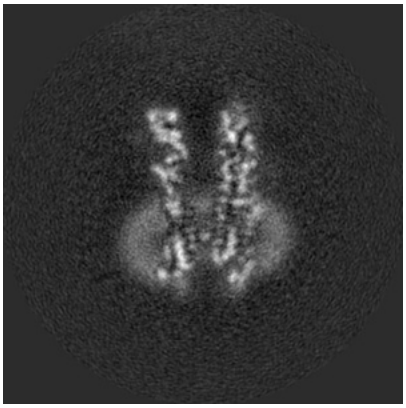
6.2.1 Primary map

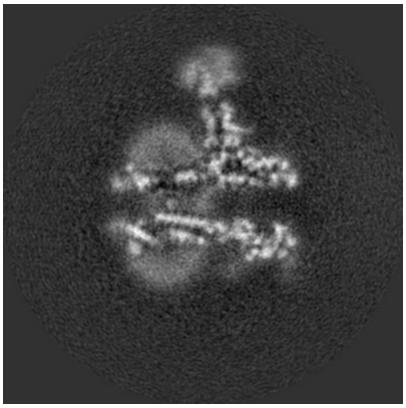

X Index: 125

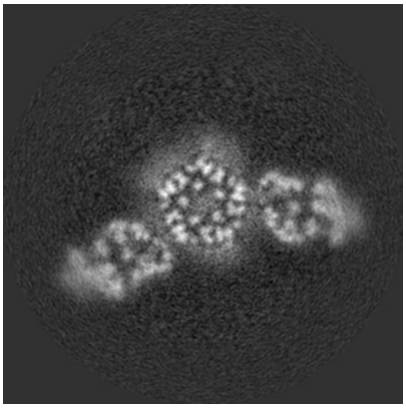
Y Index: 125


Z Index: 125

6.2.2 Raw map


X Index: 125

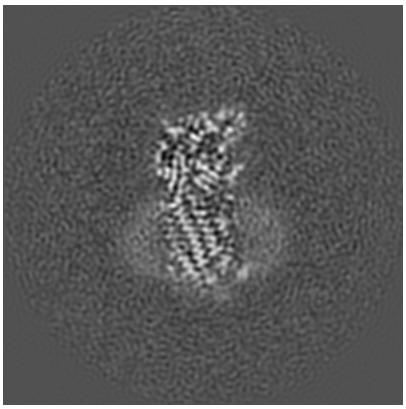

Y Index: 125

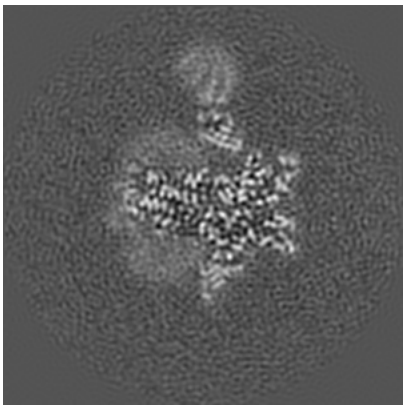

Z Index: 125

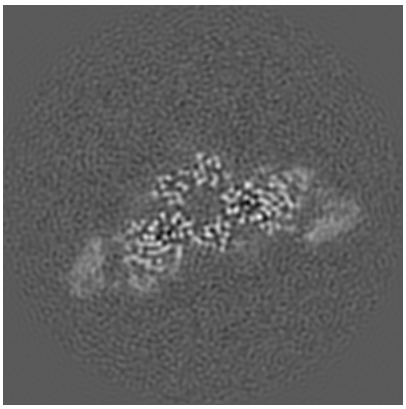
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

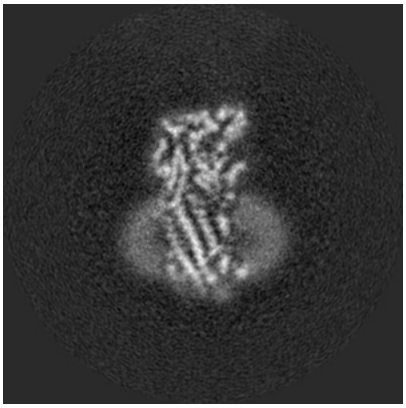
6.3.1 Primary map

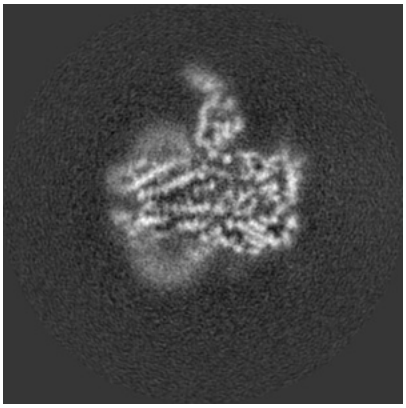

X Index: 140

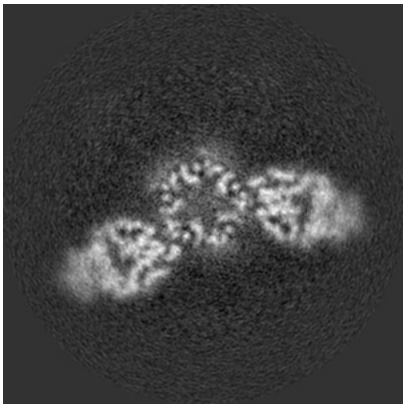

Y Index: 111


Z Index: 140

6.3.2 Raw map


X Index: 140

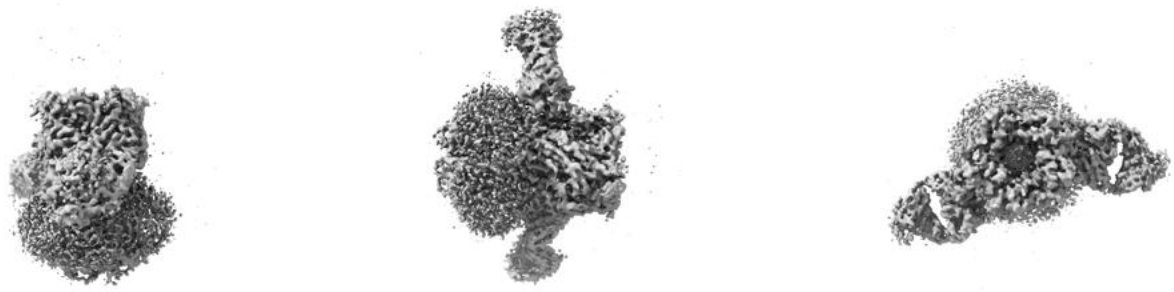

Y Index: 137


Z Index: 130

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 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

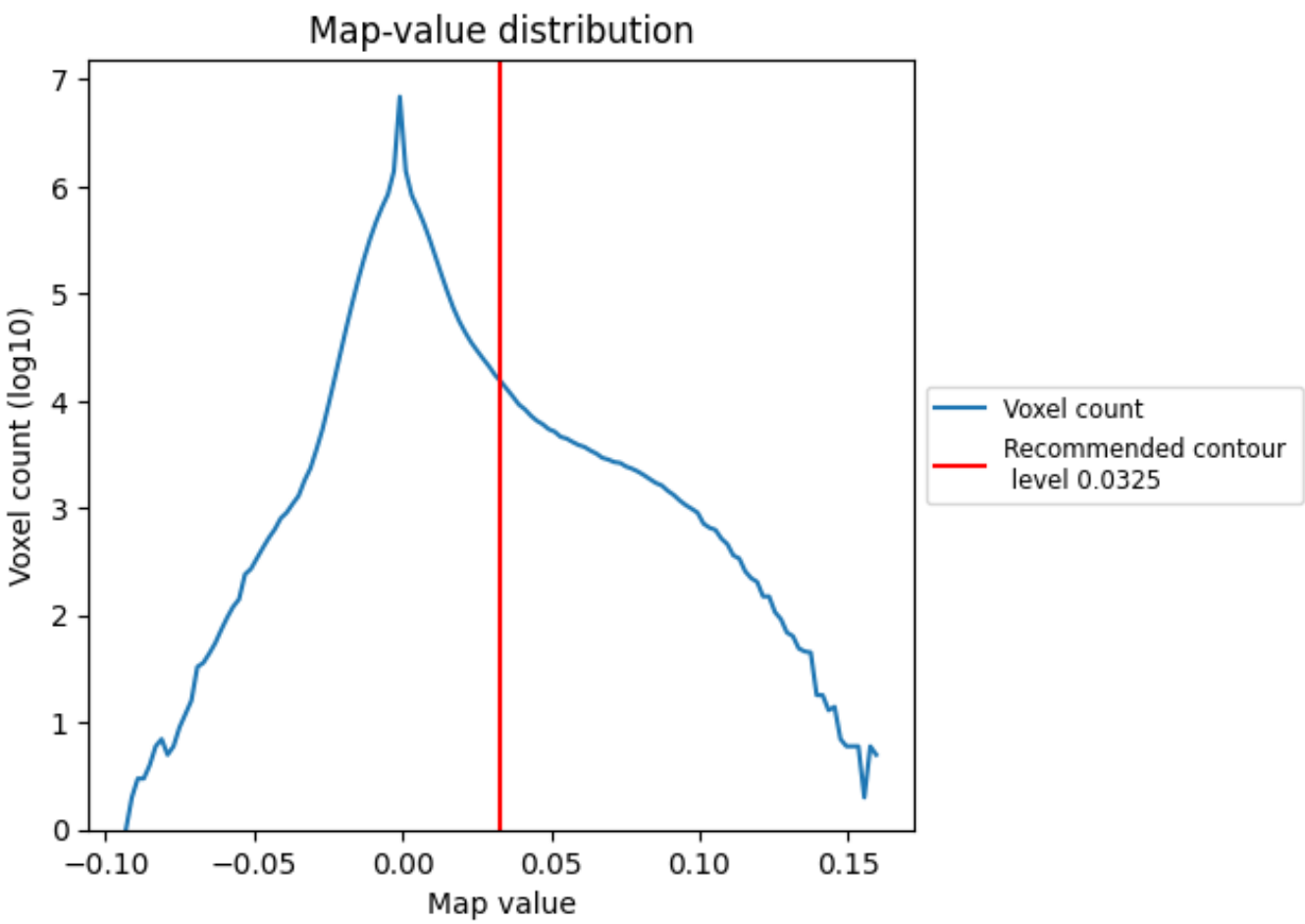
6.5 Mask visualisation (i)

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

7 Map analysis (i)

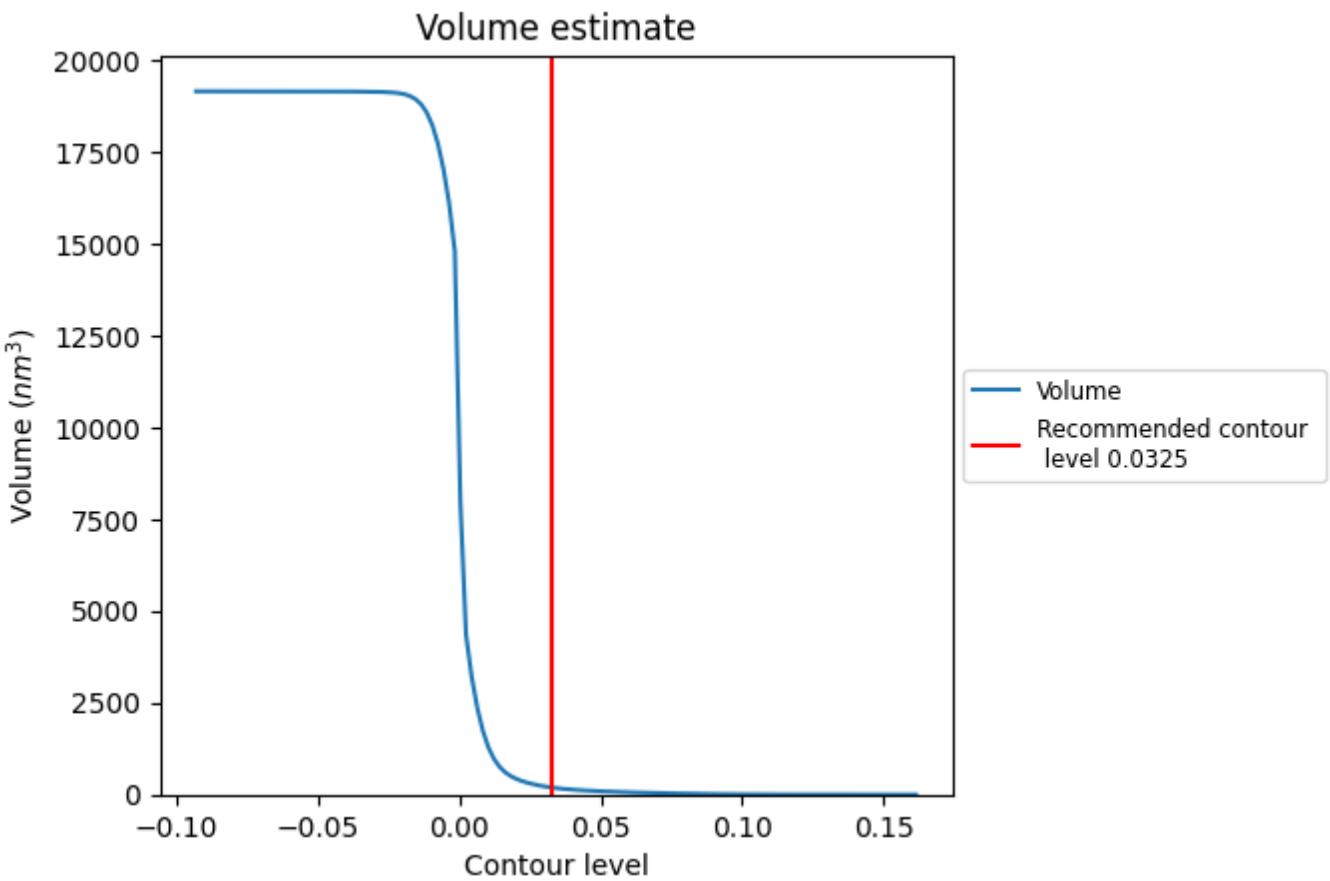
This section contains the results of statistical analysis of the map.

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.

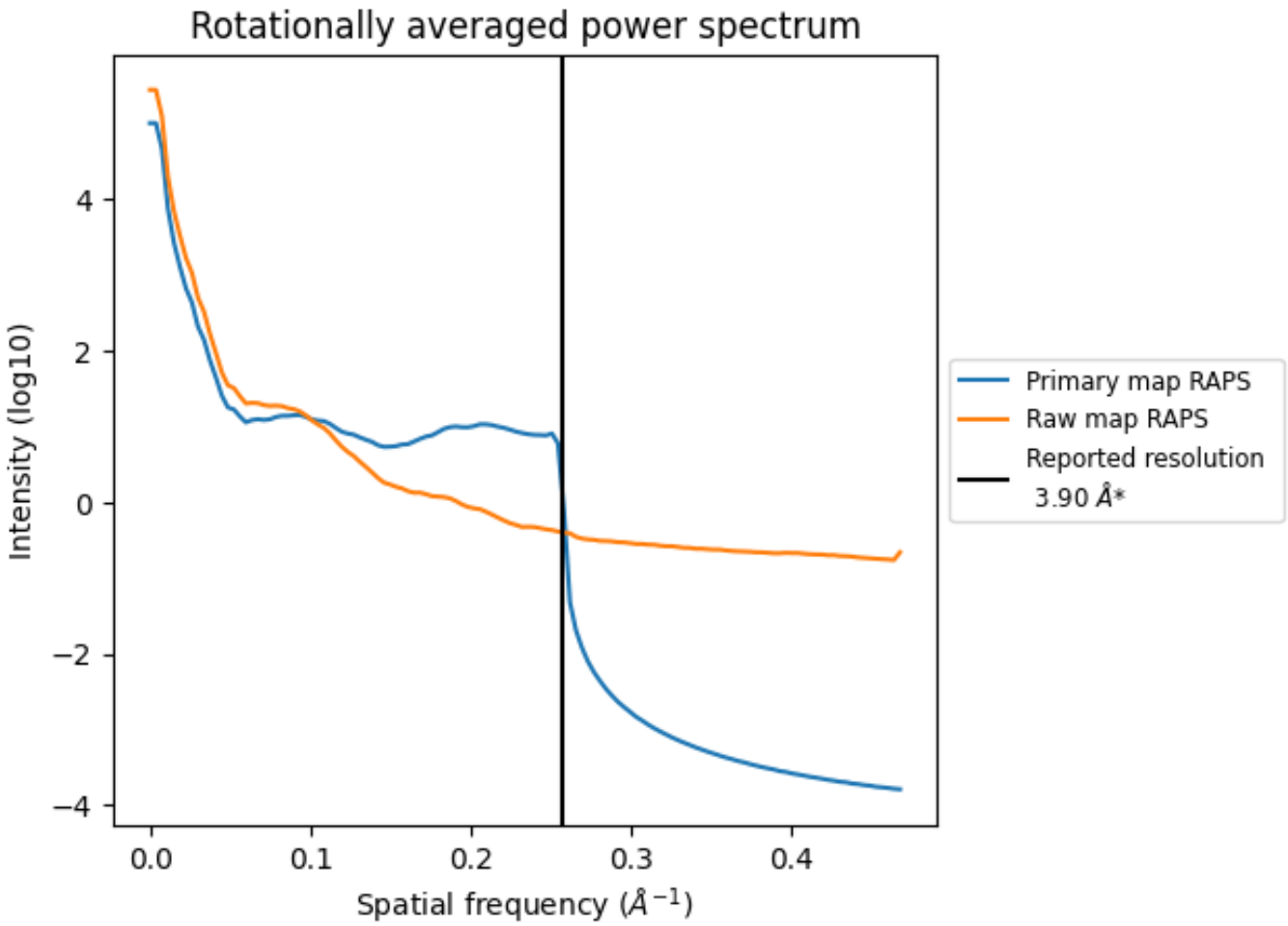
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

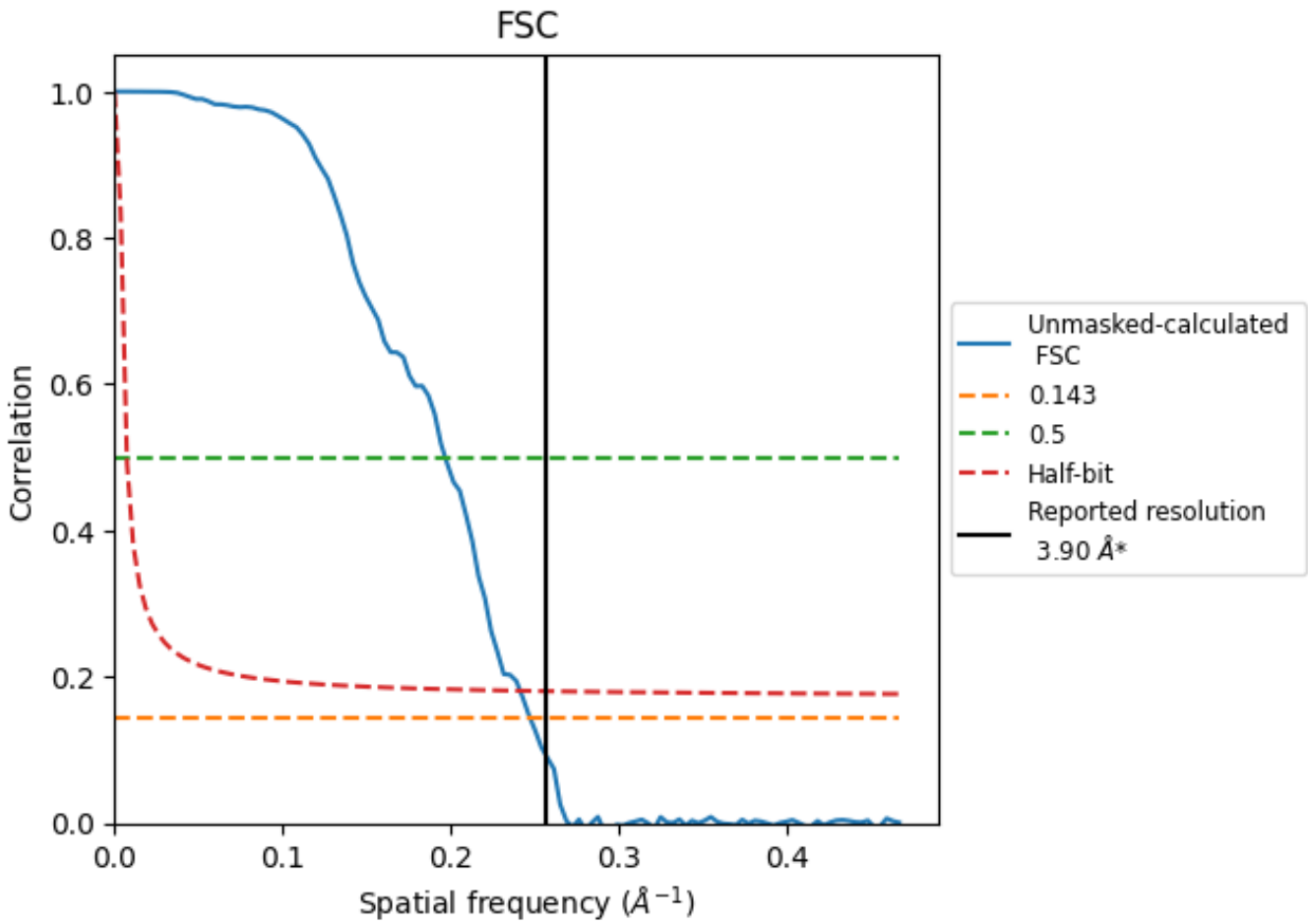


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

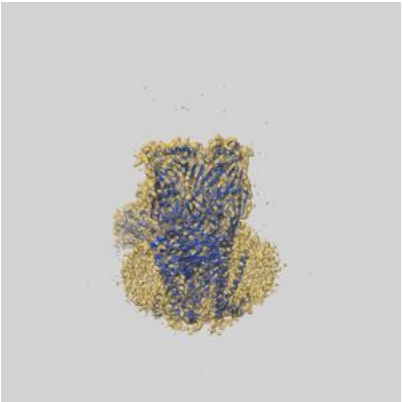
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	5.08	4.14

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

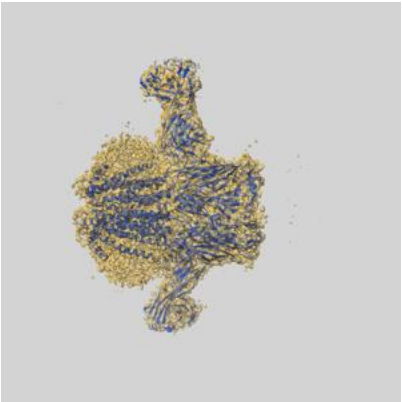
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7536 and PDB model 6CNK. Per-residue inclusion information can be found in section 3 on page 10.

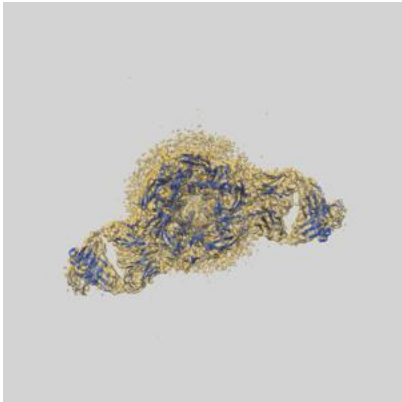
9.1 Map-model overlay (i)



X



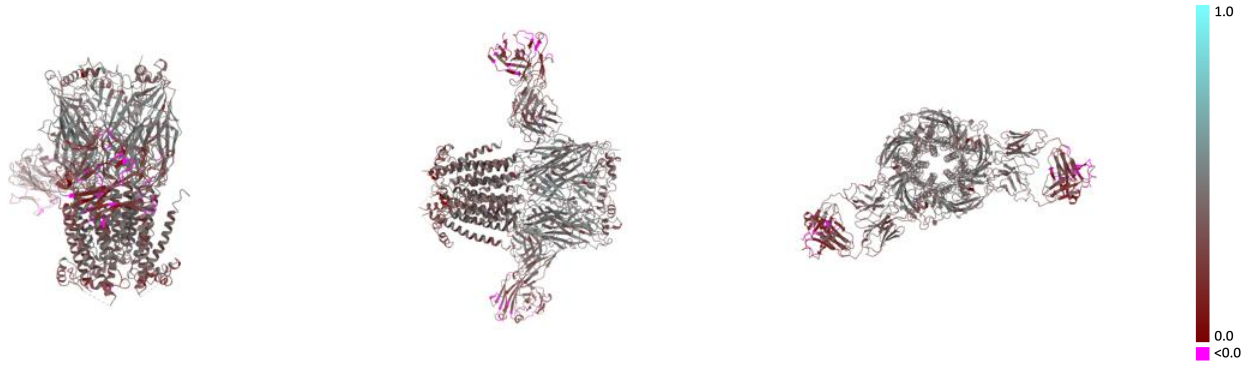
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0325 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

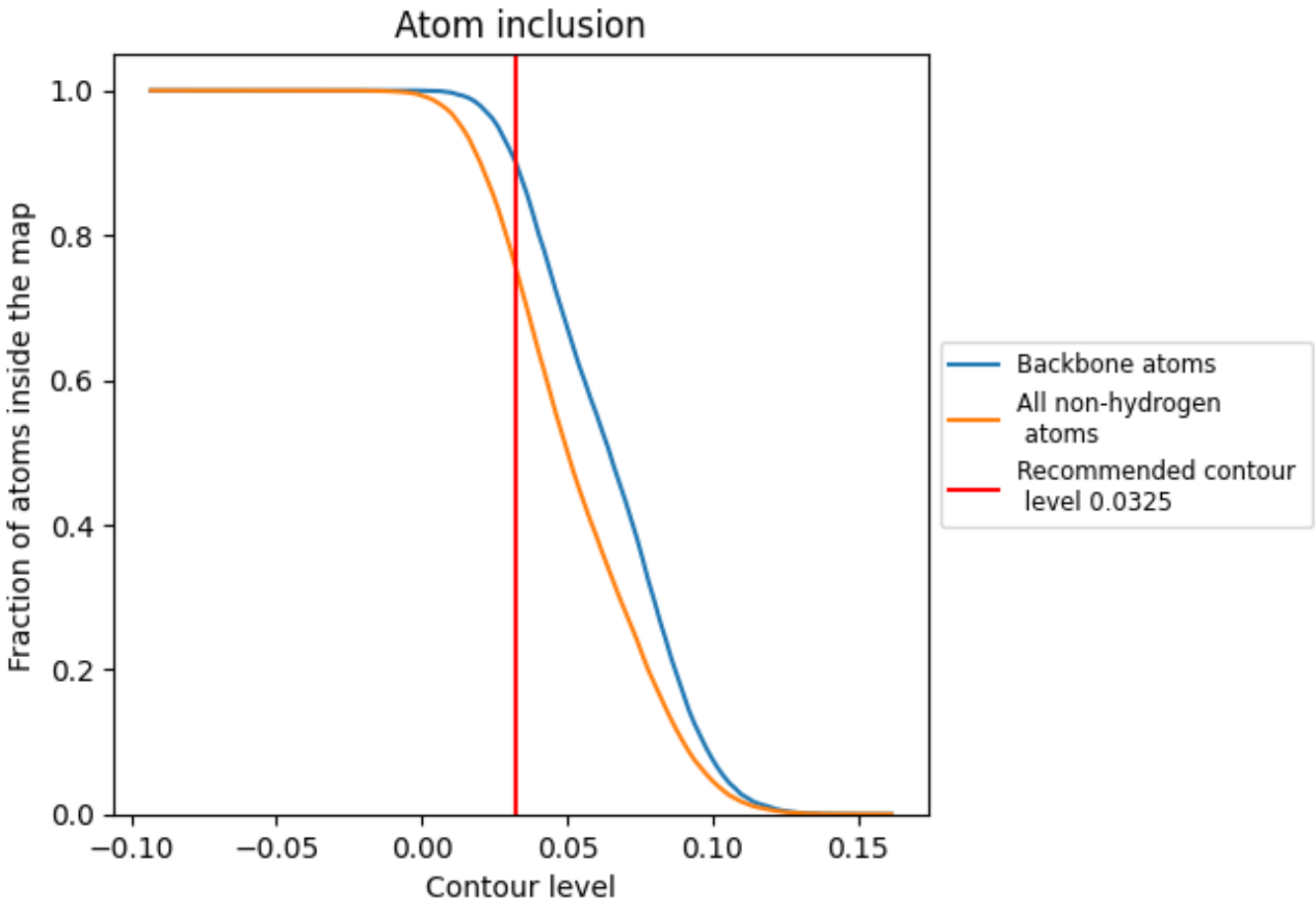
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0325).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7521	0.3770
A	0.7982	0.4130
B	0.7865	0.4080
C	0.7972	0.4130
D	0.8069	0.4110
E	0.7941	0.4150
F	0.6182	0.2760
G	0.6718	0.3120
H	0.8718	0.4520
I	0.8718	0.5050
J	0.6369	0.2830
K	0.6706	0.3110