Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 09:41 PM JST

PDB ID	:	6JD1
EMDB ID	:	EMD-9801
Title	:	Cryo-EM Structure of Sulfolobus solfataricus ketol-acid reductoisomerase (SsoKARI) in complex with Mg2+, NADH, and CPD at pH7.5
Authors	:	Chen, C.Y.; Chang, Y.C.; Lin, K.F.; Huang, C.H.; Lin, B.L.; Ko, T.P.; Hsieh, D.L.; Tsai, M.D.
Deposited on	:	2019-01-30
Resolution	:	3.38 Å(reported)
Based on initial model	:	6JCV

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

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

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

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

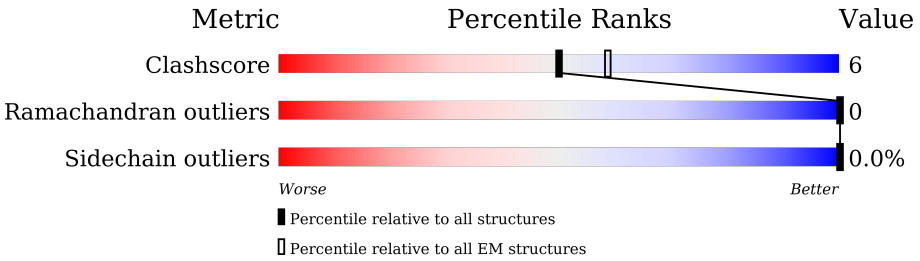
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.38 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	333	8% 83% 17% •
1	B	333	8% 87% 13% •
1	C	333	8% 85% 15% •
1	D	333	7% 84% 15% •
1	E	333	7% 83% 16% •
1	F	333	8% 80% 18% •
1	G	333	8% 81% 18% •
1	H	333	6% 81% 18% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	333	8% 81% 17%
1	J	333	8% 83% 16%
1	K	333	9% 83% 16%
1	L	333	8% 79% 19%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 63799 atoms, of which 31841 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 Putative ketol-acid reductoisomerase 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	330	5225	1678	2629	427	481	10	0	0
1	B	331	5237	1682	2633	428	484	10	0	0
1	C	331	5236	1682	2632	428	484	10	0	0
1	D	330	5225	1678	2629	427	481	10	0	0
1	E	329	5211	1674	2623	425	479	10	0	0
1	F	330	5223	1678	2627	426	482	10	0	0
1	G	330	5223	1678	2627	426	482	10	0	0
1	H	329	5211	1674	2623	425	479	10	0	0
1	I	328	5189	1668	2610	423	478	10	0	0
1	J	329	5211	1674	2623	425	479	10	0	0
1	K	328	5184	1667	2604	423	480	10	0	0
1	L	328	5188	1668	2609	423	478	10	0	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
2	A	3	3	3	0
2	B	3	3	3	0
2	C	3	3	3	0

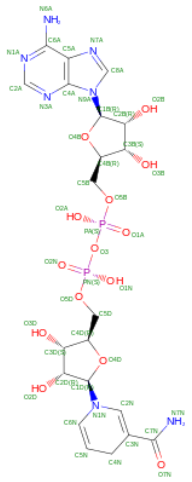
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
2	D	3	3	3	0
2	E	2	2	2	0
2	F	4	4	4	0
2	G	3	3	3	0
2	H	3	3	3	0
2	I	3	3	3	0
2	J	3	3	3	0
2	K	3	3	3	0
2	L	3	3	3	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

NAI



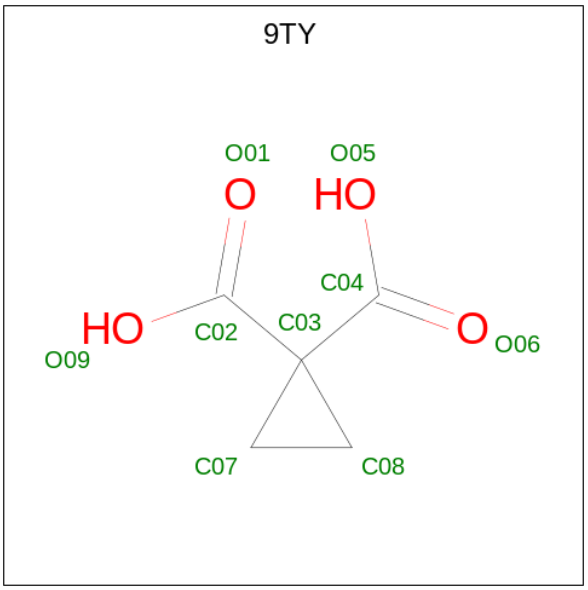
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	71	21	27	7	14	2	0
3	B	1	71	21	27	7	14	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	C	1	71	21	27	7	14	2	0
3	D	1	71	21	27	7	14	2	0
3	E	1	71	21	27	7	14	2	0
3	F	1	71	21	27	7	14	2	0
3	G	1	71	21	27	7	14	2	0
3	H	1	71	21	27	7	14	2	0
3	I	1	71	21	27	7	14	2	0
3	J	1	71	21	27	7	14	2	0
3	K	1	71	21	27	7	14	2	0
3	L	1	71	21	27	7	14	2	0

- Molecule 4 is cyclopropane-1,1-dicarboxylic acid (three-letter code: 9TY) (formula: $C_5H_6O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	13	5	4	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	B	1	13	5	4	4	0
4	C	1	13	5	4	4	0
4	D	1	13	5	4	4	0
4	E	1	13	5	4	4	0
4	F	1	13	5	4	4	0
4	G	1	13	5	4	4	0
4	H	1	13	5	4	4	0
4	I	1	13	5	4	4	0
4	J	1	13	5	4	4	0
4	K	1	13	5	4	4	0
4	L	1	13	5	4	4	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	A	15	15	15	0
5	B	21	21	21	0
5	C	16	16	16	0
5	D	18	18	18	0
5	E	17	17	17	0
5	F	20	20	20	0
5	G	16	16	16	0
5	H	12	12	12	0

Continued on next page...

Continued from previous page...

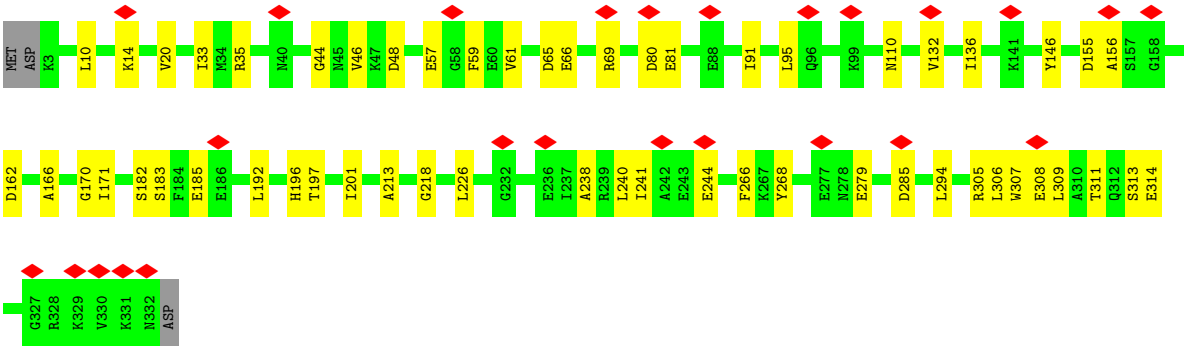
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
5	I	15	15	15	0
			Total	O	
5	J	14	14	14	0
			Total	O	
5	K	10	10	10	0
			Total	O	
5	L	18	18	18	0

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.

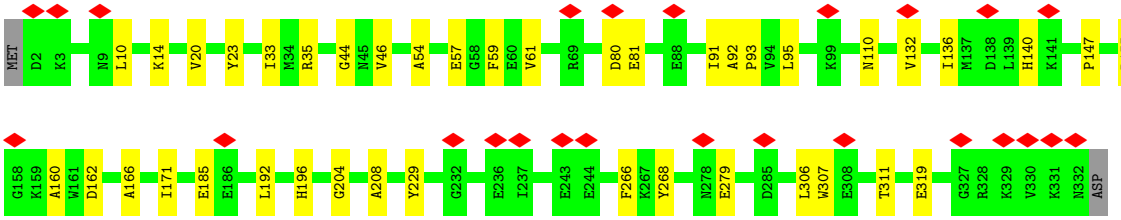
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain A:



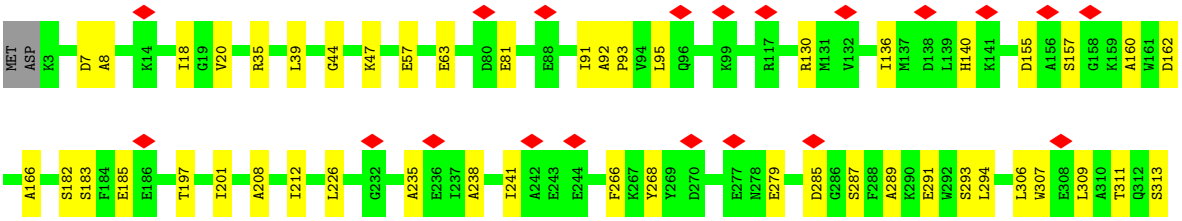
• Molecule 1: Putative ketol-acid reductoisomerase 2

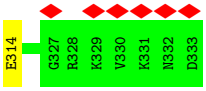
Chain B:



• Molecule 1: Putative ketol-acid reductoisomerase 2

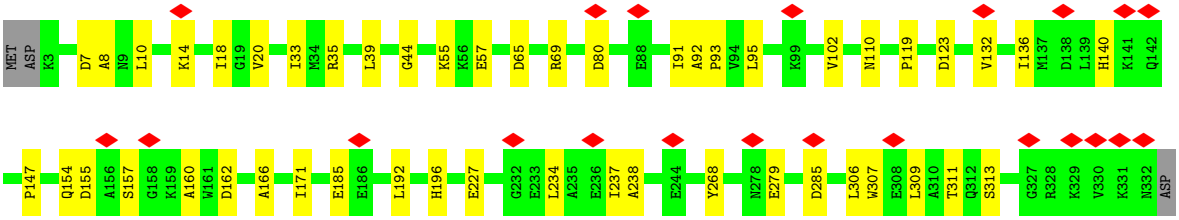
Chain C:





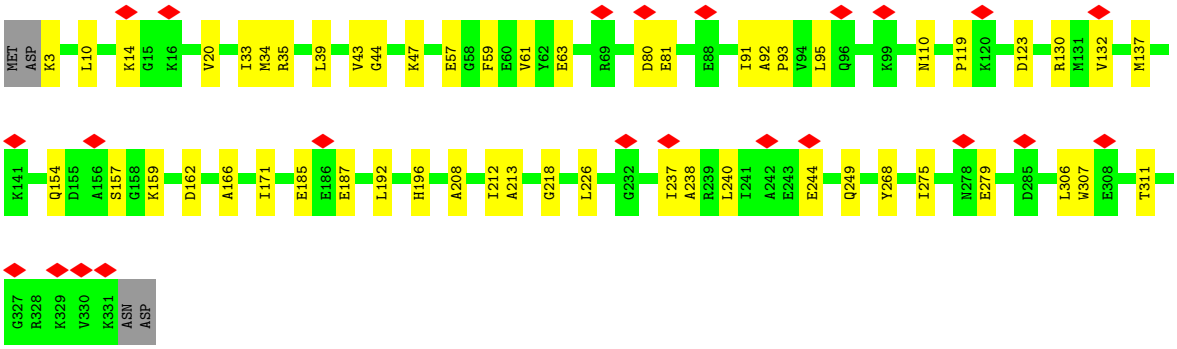
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain D:



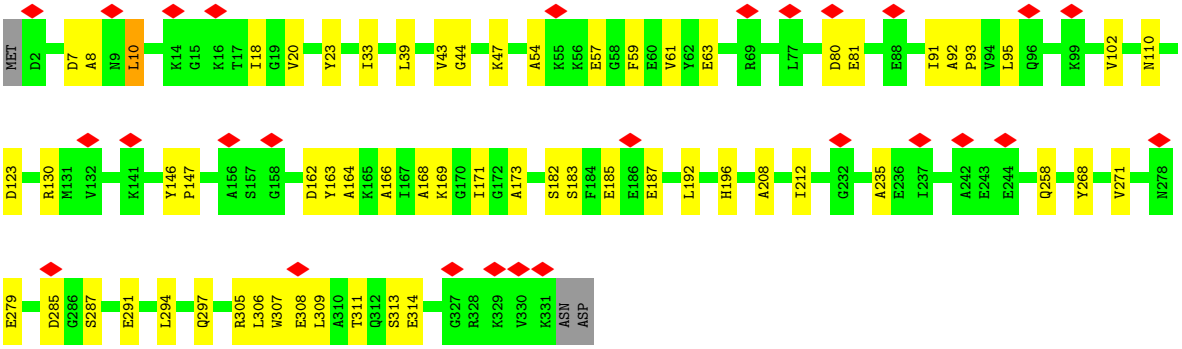
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain E:



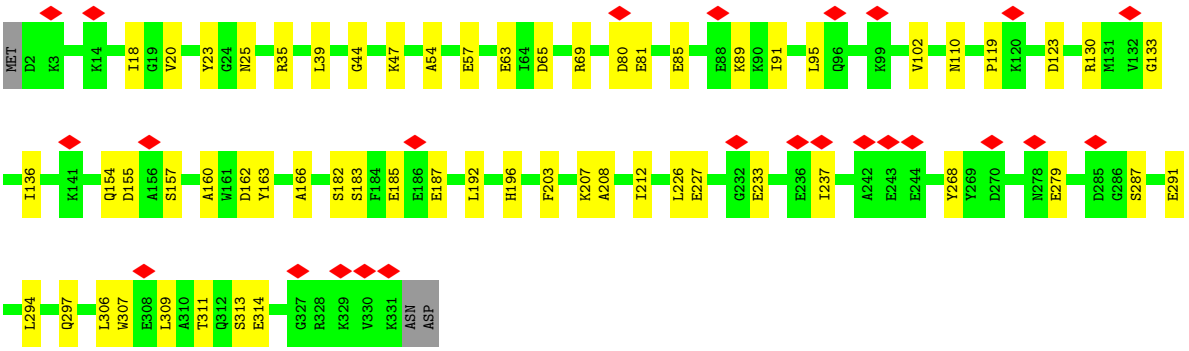
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain F:



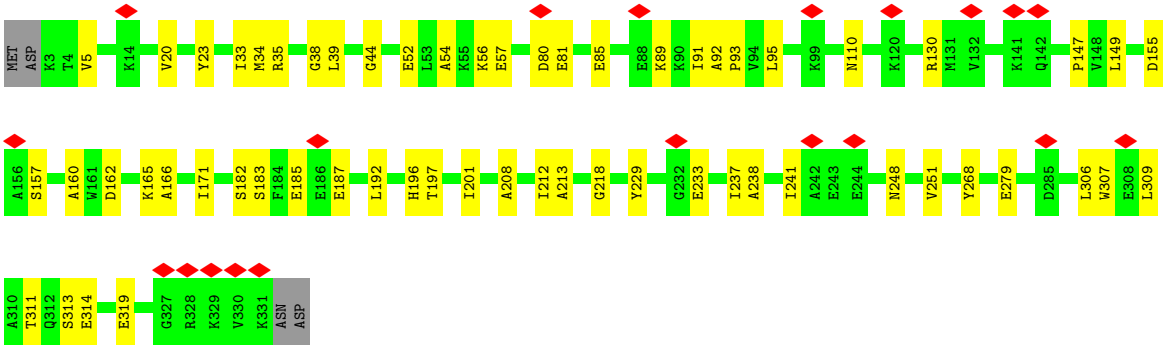
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain G:



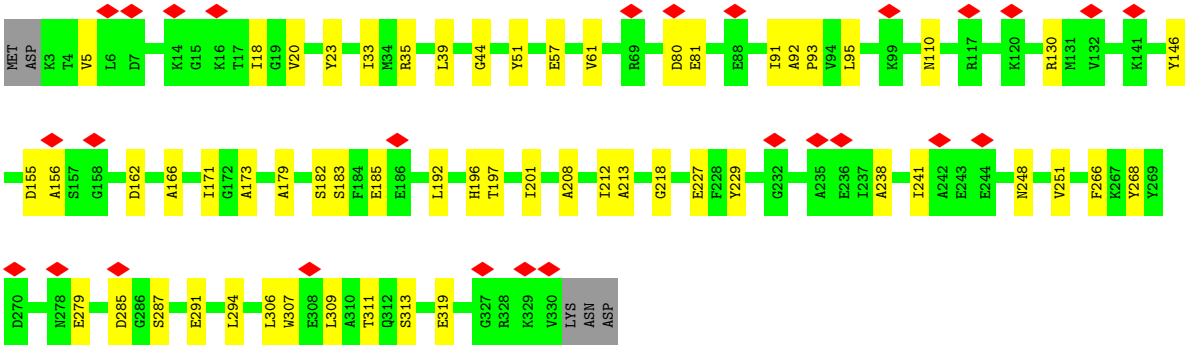
• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain H:



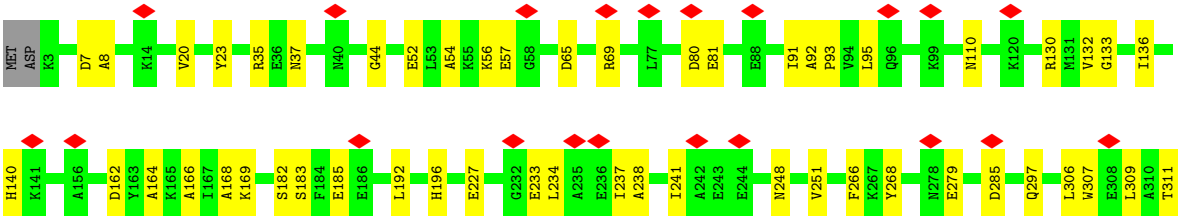
• Molecule 1: Putative ketol-acid reductoisomerase 2

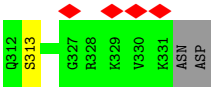
Chain I:



• Molecule 1: Putative ketol-acid reductoisomerase 2

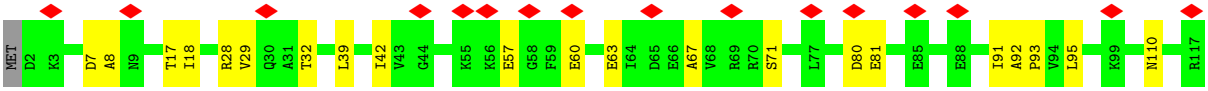
Chain J:

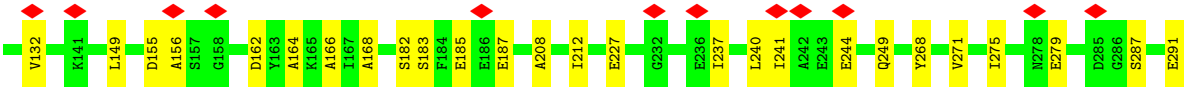


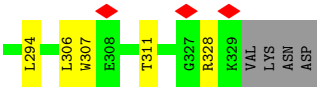


• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain K:

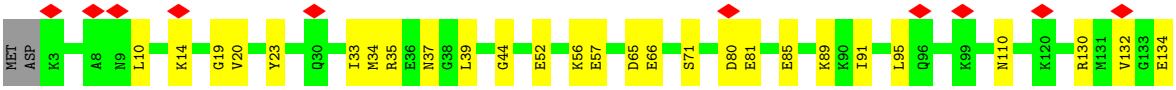


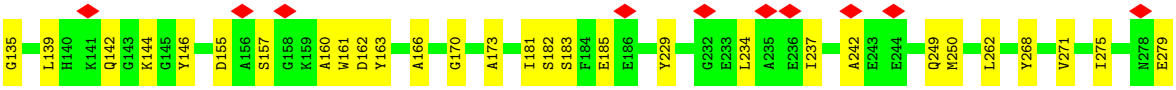


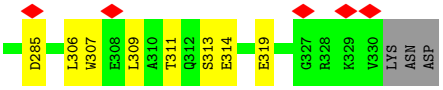


• Molecule 1: Putative ketol-acid reductoisomerase 2

Chain L:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.31	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	6.346	Depositor
Minimum map value	-2.333	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.361	Depositor
Recommended contour level	1.88	Depositor
Map size (Å)	281.88, 281.88, 281.88	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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: MG, NAI, 9TY

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	0.33	0/2649	0.54	0/3576
1	B	0.33	0/2657	0.54	0/3587
1	C	0.34	0/2657	0.52	0/3587
1	D	0.33	0/2649	0.52	0/3576
1	E	0.34	0/2641	0.52	0/3565
1	F	0.34	0/2649	0.53	1/3576 (0.0%)
1	G	0.33	0/2649	0.52	0/3576
1	H	0.34	0/2641	0.54	0/3565
1	I	0.33	0/2632	0.53	0/3554
1	J	0.33	0/2641	0.52	0/3565
1	K	0.33	0/2633	0.54	0/3555
1	L	0.33	0/2632	0.53	0/3554
All	All	0.33	0/31730	0.53	1/42836 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	10	LEU	CA-CB-CG	5.29	127.47	115.30

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	2596	2629	2628	38	0
1	B	2604	2633	2632	30	0
1	C	2604	2632	2632	35	0
1	D	2596	2629	2628	32	0
1	E	2588	2623	2622	34	0
1	F	2596	2627	2626	41	0
1	G	2596	2627	2626	38	0
1	H	2588	2623	2622	36	0
1	I	2579	2610	2609	34	0
1	J	2588	2623	2622	35	0
1	K	2580	2604	2604	36	0
1	L	2579	2609	2609	43	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	4	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	44	27	26	1	0
3	B	44	27	26	3	0
3	C	44	27	26	0	0
3	D	44	27	26	1	0
3	E	44	27	26	1	0
3	F	44	27	26	0	0
3	G	44	27	26	2	0
3	H	44	27	26	0	0
3	I	44	27	26	0	0
3	J	44	27	26	1	0
3	K	44	27	26	1	0
3	L	44	27	26	1	0
4	A	9	4	0	0	0
4	B	9	4	0	0	0
4	C	9	4	0	0	0
4	D	9	4	0	0	0
4	E	9	4	0	0	0
4	F	9	4	0	0	0
4	G	9	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	9	4	0	0	0
4	I	9	4	0	0	0
4	J	9	4	0	0	0
4	K	9	4	0	0	0
4	L	9	4	0	0	0
5	A	15	0	0	0	0
5	B	21	0	0	0	0
5	C	16	0	0	0	0
5	D	18	0	0	0	0
5	E	17	0	0	0	0
5	F	20	0	0	0	0
5	G	16	0	0	0	0
5	H	12	0	0	0	0
5	I	15	0	0	0	0
5	J	14	0	0	0	0
5	K	10	0	0	0	0
5	L	18	0	0	0	0
All	All	31958	31841	31772	383	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 6.

All (383) 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:L:10:LEU:O	1:L:14:LYS:NZ	2.19	0.75
1:J:35:ARG:NH2	1:J:57:GLU:O	2.19	0.75
1:L:23:TYR:OH	1:L:57:GLU:OE2	2.03	0.75
1:B:132:VAL:O	3:B:404:NAI:N7N	2.20	0.74
1:A:132:VAL:O	3:A:404:NAI:N7N	2.21	0.73
1:K:28:ARG:NH1	1:K:57:GLU:OE2	2.22	0.72
1:J:52:GLU:O	1:J:56:LYS:NZ	2.21	0.72
1:K:132:VAL:O	3:K:404:NAI:N7N	2.22	0.72
1:J:37:ASN:ND2	1:J:169:LYS:O	2.23	0.71
1:J:132:VAL:O	3:J:404:NAI:N7N	2.23	0.71
1:I:227:GLU:OE1	1:J:130:ARG:NH1	2.23	0.71
1:K:227:GLU:OE1	1:L:130:ARG:NH1	2.23	0.71
1:K:307:TRP:O	1:K:311:THR:OG1	2.09	0.71
1:L:132:VAL:O	3:L:404:NAI:N7N	2.23	0.71
1:L:142:GLN:OE1	1:L:144:LYS:NZ	2.24	0.71
1:A:35:ARG:NH1	1:A:57:GLU:O	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:TRP:O	1:G:311:THR:OG1	2.09	0.70
1:I:130:ARG:NH1	1:J:227:GLU:OE1	2.25	0.69
1:A:20:VAL:O	1:A:44:GLY:N	2.26	0.69
1:D:80:ASP:O	1:D:110:ASN:ND2	2.26	0.69
1:I:20:VAL:O	1:I:44:GLY:N	2.26	0.68
1:E:47:LYS:NZ	1:E:63:GLU:OE2	2.27	0.68
1:H:80:ASP:O	1:H:110:ASN:ND2	2.27	0.68
1:J:80:ASP:O	1:J:110:ASN:ND2	2.27	0.67
1:I:51:TYR:OH	1:I:61:VAL:O	2.08	0.67
1:H:20:VAL:O	1:H:44:GLY:N	2.27	0.67
1:C:279:GLU:OE2	1:D:268:TYR:OH	2.09	0.67
1:G:80:ASP:O	1:G:110:ASN:ND2	2.28	0.67
1:G:268:TYR:OH	1:H:279:GLU:OE2	2.09	0.66
1:J:65:ASP:O	1:J:69:ARG:NH1	2.27	0.66
1:D:192:LEU:O	1:D:196:HIS:ND1	2.28	0.66
1:H:192:LEU:O	1:H:196:HIS:ND1	2.27	0.66
1:B:20:VAL:O	1:B:44:GLY:N	2.29	0.66
1:I:307:TRP:O	1:I:311:THR:OG1	2.14	0.66
1:E:80:ASP:O	1:E:110:ASN:ND2	2.29	0.66
1:F:192:LEU:O	1:F:196:HIS:ND1	2.27	0.66
1:E:268:TYR:OH	1:F:279:GLU:OE2	2.10	0.66
1:C:289:ALA:O	1:C:293:SER:OG	2.08	0.66
1:F:10:LEU:HD22	1:F:169:LYS:HG2	1.76	0.66
1:C:35:ARG:NH2	1:C:57:GLU:O	2.28	0.65
1:I:192:LEU:O	1:I:196:HIS:ND1	2.30	0.65
1:J:20:VAL:O	1:J:44:GLY:N	2.29	0.65
1:D:20:VAL:O	1:D:44:GLY:N	2.30	0.65
1:F:307:TRP:O	1:F:311:THR:OG1	2.12	0.65
1:A:192:LEU:O	1:A:196:HIS:ND1	2.30	0.65
1:B:46:VAL:HG22	3:B:404:NAI:H2A	1.78	0.65
1:D:65:ASP:O	1:D:69:ARG:NH1	2.30	0.64
1:L:80:ASP:O	1:L:110:ASN:ND2	2.30	0.64
1:B:80:ASP:O	1:B:110:ASN:ND2	2.30	0.64
1:L:166:ALA:O	1:L:170:GLY:N	2.30	0.64
1:G:192:LEU:O	1:G:196:HIS:ND1	2.30	0.64
1:J:192:LEU:O	1:J:196:HIS:ND1	2.31	0.64
1:F:20:VAL:O	1:F:44:GLY:N	2.30	0.64
1:C:155:ASP:OD1	1:C:157:SER:OG	2.16	0.64
1:F:23:TYR:OH	1:F:57:GLU:OE1	2.16	0.64
1:L:155:ASP:OD1	1:L:160:ALA:HB2	1.98	0.64
1:K:268:TYR:OH	1:L:279:GLU:OE2	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:O	1:A:110:ASN:ND2	2.31	0.63
1:F:80:ASP:O	1:F:110:ASN:ND2	2.31	0.63
1:E:279:GLU:OE2	1:F:268:TYR:OH	2.10	0.63
1:H:23:TYR:CD2	1:H:54:ALA:HB2	2.34	0.63
1:E:159:LYS:NZ	1:E:162:ASP:OD2	2.20	0.62
1:C:18:ILE:HD11	1:C:39:LEU:HD13	1.81	0.62
1:L:307:TRP:O	1:L:311:THR:OG1	2.14	0.62
1:D:307:TRP:O	1:D:311:THR:OG1	2.15	0.62
1:K:80:ASP:O	1:K:110:ASN:ND2	2.32	0.62
1:E:307:TRP:O	1:E:311:THR:OG1	2.17	0.62
1:C:20:VAL:O	1:C:44:GLY:N	2.33	0.61
1:L:20:VAL:O	1:L:44:GLY:N	2.33	0.61
1:L:134:GLU:OE1	1:L:134:GLU:N	2.33	0.61
1:J:23:TYR:CD2	1:J:54:ALA:HB2	2.36	0.61
1:H:307:TRP:O	1:H:311:THR:OG1	2.14	0.61
1:I:279:GLU:OE2	1:J:268:TYR:OH	2.13	0.61
1:B:192:LEU:O	1:B:196:HIS:ND1	2.34	0.61
1:I:35:ARG:NH1	1:I:57:GLU:O	2.34	0.61
1:A:279:GLU:OE2	1:B:268:TYR:OH	2.09	0.61
1:I:268:TYR:OH	1:J:279:GLU:OE2	2.10	0.61
1:B:155:ASP:OD1	1:B:160:ALA:HB2	2.01	0.60
1:K:182:SER:OG	1:K:183:SER:N	2.31	0.60
1:E:10:LEU:O	1:E:14:LYS:NZ	2.27	0.60
1:K:279:GLU:OE2	1:L:268:TYR:OH	2.10	0.60
1:F:130:ARG:NH2	1:F:187:GLU:OE2	2.34	0.60
1:I:238:ALA:HA	1:I:241:ILE:HD12	1.84	0.60
1:C:307:TRP:O	1:C:311:THR:OG1	2.14	0.60
1:G:20:VAL:O	1:G:44:GLY:N	2.34	0.60
1:J:233:GLU:HG2	1:J:237:ILE:HD12	1.83	0.59
1:L:182:SER:OG	1:L:183:SER:N	2.37	0.58
1:I:23:TYR:OH	1:I:57:GLU:OE2	2.18	0.58
1:E:192:LEU:O	1:E:196:HIS:ND1	2.37	0.58
1:B:23:TYR:CE2	1:B:54:ALA:HB2	2.39	0.57
1:C:268:TYR:OH	1:D:279:GLU:OE2	2.14	0.57
1:E:162:ASP:O	1:E:166:ALA:N	2.38	0.57
1:H:233:GLU:O	1:H:237:ILE:N	2.38	0.57
1:I:80:ASP:O	1:I:110:ASN:ND2	2.37	0.57
1:J:234:LEU:O	1:J:238:ALA:N	2.38	0.56
1:C:185:GLU:N	1:C:185:GLU:OE1	2.37	0.56
1:C:155:ASP:OD1	1:C:160:ALA:HB2	2.06	0.56
1:D:10:LEU:O	1:D:14:LYS:NZ	2.32	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:ARG:NH1	1:H:187:GLU:OE2	2.37	0.56
1:D:155:ASP:OD1	1:D:160:ALA:HB2	2.06	0.56
1:G:65:ASP:O	1:G:69:ARG:NE	2.38	0.56
1:G:279:GLU:OE2	1:H:268:TYR:OH	2.13	0.56
1:F:185:GLU:N	1:F:185:GLU:OE1	2.37	0.56
1:J:307:TRP:O	1:J:311:THR:OG1	2.21	0.56
1:A:91:ILE:HG22	1:A:95:LEU:HG	1.88	0.55
1:G:91:ILE:O	1:G:95:LEU:N	2.38	0.55
1:G:185:GLU:N	1:G:185:GLU:OE1	2.38	0.55
1:A:268:TYR:OH	1:B:279:GLU:OE2	2.13	0.55
1:K:185:GLU:OE1	1:K:185:GLU:N	2.37	0.55
1:H:35:ARG:NH2	1:H:57:GLU:O	2.39	0.55
1:K:162:ASP:O	1:K:166:ALA:N	2.38	0.55
1:C:47:LYS:NZ	1:C:63:GLU:OE2	2.40	0.54
1:A:91:ILE:O	1:A:95:LEU:N	2.40	0.54
1:D:185:GLU:OE1	1:D:185:GLU:N	2.41	0.54
1:A:307:TRP:O	1:A:311:THR:OG1	2.23	0.54
1:H:185:GLU:N	1:H:185:GLU:OE1	2.40	0.54
1:E:123:ASP:OD1	1:E:157:SER:OG	2.26	0.54
1:G:91:ILE:HG22	1:G:95:LEU:HG	1.88	0.53
1:A:314:GLU:N	1:A:314:GLU:OE1	2.42	0.53
1:E:119:PRO:O	1:E:154:GLN:NE2	2.42	0.53
1:K:18:ILE:CD1	1:K:39:LEU:HD13	2.39	0.53
1:F:18:ILE:CD1	1:F:39:LEU:HD13	2.39	0.53
1:A:238:ALA:HA	1:A:241:ILE:HD12	1.90	0.53
1:D:91:ILE:HG22	1:D:95:LEU:HG	1.91	0.53
1:C:7:ASP:OD1	1:C:8:ALA:N	2.41	0.53
1:C:238:ALA:HA	1:C:241:ILE:HD12	1.90	0.53
1:B:33:ILE:HD13	1:B:171:ILE:O	2.09	0.53
1:I:91:ILE:O	1:I:95:LEU:N	2.40	0.53
1:G:314:GLU:N	1:G:314:GLU:OE1	2.42	0.53
1:K:7:ASP:OD1	1:K:8:ALA:N	2.41	0.53
1:K:63:GLU:O	1:K:67:ALA:HB2	2.08	0.53
1:A:136:ILE:HD11	1:A:146:TYR:CE1	2.44	0.53
1:K:91:ILE:O	1:K:95:LEU:N	2.43	0.52
1:A:66:GLU:OE1	1:A:69:ARG:NH1	2.43	0.52
1:E:20:VAL:O	1:E:44:GLY:N	2.42	0.52
1:C:266:PHE:CE2	1:D:306:LEU:HD22	2.45	0.52
1:I:285:ASP:OD1	1:K:306:LEU:HD21	2.09	0.52
1:G:130:ARG:NH1	1:G:187:GLU:OE2	2.42	0.52
1:H:314:GLU:N	1:H:314:GLU:OE1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:294:LEU:HD13	1:K:294:LEU:HD13	1.91	0.52
1:D:91:ILE:O	1:D:95:LEU:N	2.43	0.52
1:E:81:GLU:N	1:E:81:GLU:OE1	2.43	0.52
1:L:81:GLU:N	1:L:81:GLU:OE1	2.43	0.52
1:E:33:ILE:HD13	1:E:171:ILE:O	2.10	0.51
1:G:18:ILE:CD1	1:G:39:LEU:HD13	2.40	0.51
1:F:314:GLU:N	1:F:314:GLU:OE1	2.43	0.51
1:J:185:GLU:N	1:J:185:GLU:OE1	2.43	0.51
1:C:91:ILE:HG22	1:C:95:LEU:HG	1.91	0.51
1:G:226:LEU:HD13	1:H:147:PRO:HB2	1.93	0.51
1:H:5:VAL:HG11	1:H:165:LYS:NZ	2.26	0.51
1:B:35:ARG:NH2	1:B:57:GLU:O	2.43	0.51
1:F:306:LEU:HD21	1:J:285:ASP:OD1	2.11	0.51
1:L:314:GLU:OE1	1:L:314:GLU:N	2.44	0.51
1:A:285:ASP:OD1	1:C:306:LEU:HD21	2.11	0.51
1:C:314:GLU:OE1	1:C:314:GLU:N	2.43	0.51
1:K:149:LEU:HD12	1:K:187:GLU:HG2	1.93	0.51
1:B:155:ASP:OD1	1:B:157:SER:OG	2.29	0.50
1:E:208:ALA:O	1:E:212:ILE:N	2.43	0.50
1:H:306:LEU:HD21	1:L:285:ASP:OD1	2.11	0.50
1:A:185:GLU:N	1:A:185:GLU:OE1	2.43	0.50
1:B:307:TRP:O	1:B:311:THR:OG1	2.28	0.50
1:E:185:GLU:N	1:E:185:GLU:OE1	2.42	0.50
1:K:155:ASP:OD1	1:K:156:ALA:N	2.44	0.50
1:L:185:GLU:N	1:L:185:GLU:OE1	2.42	0.50
1:F:91:ILE:O	1:F:95:LEU:N	2.45	0.50
1:F:59:PHE:O	1:F:61:VAL:HG23	2.12	0.50
1:J:81:GLU:OE1	1:J:81:GLU:N	2.45	0.50
1:D:155:ASP:OD1	1:D:157:SER:OG	2.28	0.50
1:G:155:ASP:OD1	1:G:157:SER:OG	2.30	0.50
1:B:81:GLU:N	1:B:81:GLU:OE1	2.44	0.50
1:G:81:GLU:N	1:G:81:GLU:OE1	2.44	0.50
1:H:162:ASP:O	1:H:166:ALA:N	2.42	0.50
1:A:81:GLU:OE1	1:A:81:GLU:N	2.45	0.50
1:C:91:ILE:O	1:C:95:LEU:N	2.43	0.50
1:F:81:GLU:N	1:F:81:GLU:OE1	2.45	0.50
1:K:81:GLU:N	1:K:81:GLU:OE1	2.45	0.49
1:E:237:ILE:O	1:E:249:GLN:NE2	2.44	0.49
1:K:208:ALA:O	1:K:212:ILE:N	2.45	0.49
1:I:81:GLU:N	1:I:81:GLU:OE1	2.44	0.49
1:B:136:ILE:O	1:B:140:HIS:N	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:GLU:OE2	1:L:89:LYS:NZ	2.45	0.49
1:C:18:ILE:CD1	1:C:39:LEU:HD13	2.43	0.49
1:C:285:ASP:OD1	1:E:306:LEU:HD21	2.12	0.49
1:F:285:ASP:OD1	1:G:306:LEU:HD21	2.12	0.49
1:G:287:SER:O	1:G:291:GLU:N	2.46	0.49
1:H:52:GLU:O	1:H:56:LYS:N	2.43	0.49
1:J:91:ILE:HG22	1:J:95:LEU:HG	1.95	0.49
1:H:81:GLU:OE1	1:H:81:GLU:N	2.45	0.49
1:A:266:PHE:CE2	1:B:306:LEU:HD22	2.48	0.49
1:G:25:ASN:N	3:G:404:NAI:O1N	2.43	0.49
1:L:155:ASP:OD1	1:L:157:SER:OG	2.26	0.49
1:C:81:GLU:OE1	1:C:81:GLU:N	2.46	0.49
1:D:123:ASP:OD1	1:D:157:SER:OG	2.24	0.49
1:E:137:MET:SD	1:E:137:MET:N	2.86	0.48
1:G:162:ASP:O	1:G:166:ALA:N	2.42	0.48
1:A:306:LEU:HD22	1:B:266:PHE:CD2	2.48	0.48
1:C:130:ARG:NH1	1:D:227:GLU:OE1	2.47	0.48
1:B:10:LEU:O	1:B:14:LYS:NZ	2.37	0.48
1:A:166:ALA:O	1:A:170:GLY:N	2.45	0.48
1:D:285:ASP:OD1	1:L:306:LEU:HD21	2.13	0.48
1:E:34:MET:HB3	1:E:39:LEU:HD12	1.96	0.48
1:F:146:TYR:CZ	1:F:173:ALA:HB2	2.48	0.48
1:B:23:TYR:OH	1:B:57:GLU:OE1	2.21	0.48
1:I:185:GLU:OE1	1:I:185:GLU:N	2.45	0.48
1:E:91:ILE:HG22	1:E:95:LEU:HG	1.95	0.47
1:H:155:ASP:OD1	1:H:157:SER:OG	2.32	0.47
1:B:185:GLU:OE1	1:B:185:GLU:N	2.44	0.47
1:E:240:LEU:O	1:E:244:GLU:N	2.46	0.47
1:G:119:PRO:O	1:G:154:GLN:NE2	2.47	0.47
1:G:133:GLY:HA2	1:G:136:ILE:HD12	1.96	0.47
1:D:162:ASP:O	1:D:166:ALA:N	2.44	0.47
1:E:132:VAL:O	3:E:403:NAI:N7N	2.46	0.47
1:H:149:LEU:HD12	1:H:187:GLU:HG2	1.97	0.47
1:H:91:ILE:O	1:H:95:LEU:N	2.48	0.47
1:L:139:LEU:HD22	1:L:146:TYR:HB3	1.96	0.47
1:G:233:GLU:O	1:G:237:ILE:N	2.48	0.47
1:C:162:ASP:O	1:C:166:ALA:N	2.44	0.46
1:J:133:GLY:HA2	1:J:136:ILE:HD12	1.97	0.46
1:E:59:PHE:O	1:E:61:VAL:HG23	2.15	0.46
1:K:42:ILE:HG22	1:K:60:GLU:CB	2.45	0.46
1:B:162:ASP:O	1:B:166:ALA:N	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ILE:O	1:C:140:HIS:N	2.44	0.46
1:H:34:MET:HB3	1:H:39:LEU:HD12	1.96	0.46
1:I:266:PHE:CE2	1:J:306:LEU:HD22	2.51	0.46
1:A:59:PHE:O	1:A:61:VAL:HG23	2.16	0.46
1:J:182:SER:OG	1:J:183:SER:N	2.48	0.46
1:K:17:THR:HG23	1:K:71:SER:HA	1.98	0.46
1:A:33:ILE:HD13	1:A:171:ILE:O	2.16	0.46
1:D:136:ILE:O	1:D:140:HIS:N	2.47	0.46
1:H:33:ILE:HD13	1:H:171:ILE:O	2.15	0.46
1:I:162:ASP:O	1:I:166:ALA:N	2.45	0.46
1:F:102:VAL:HG21	1:F:163:TYR:CD2	2.51	0.46
1:G:123:ASP:OD1	1:G:157:SER:OG	2.28	0.46
1:I:146:TYR:CZ	1:I:173:ALA:HB2	2.51	0.46
1:J:248:ASN:O	1:J:251:VAL:HG12	2.16	0.46
1:D:102:VAL:HG22	1:D:123:ASP:HB2	1.97	0.45
1:F:54:ALA:HB1	1:F:59:PHE:HB2	1.98	0.45
1:G:208:ALA:O	1:G:212:ILE:N	2.47	0.45
1:A:65:ASP:O	1:A:69:ARG:NH2	2.49	0.45
1:A:226:LEU:HD13	1:B:147:PRO:HB2	1.97	0.45
1:B:229:TYR:OH	1:B:319:GLU:OE1	2.27	0.45
1:L:91:ILE:HG22	1:L:95:LEU:HD23	1.97	0.45
1:B:91:ILE:HG22	1:B:95:LEU:HG	1.98	0.45
1:C:235:ALA:HB2	1:D:238:ALA:CB	2.47	0.45
1:D:132:VAL:O	3:D:404:NAI:N7N	2.49	0.45
1:F:43:VAL:HB	1:F:61:VAL:HG22	1.98	0.45
1:F:309:LEU:O	1:F:313:SER:N	2.50	0.45
1:G:23:TYR:CD2	1:G:54:ALA:HB2	2.52	0.45
1:G:182:SER:OG	1:G:183:SER:N	2.48	0.45
1:D:33:ILE:HD13	1:D:171:ILE:O	2.16	0.45
1:G:155:ASP:OD1	1:G:160:ALA:HB2	2.16	0.45
1:H:208:ALA:O	1:H:212:ILE:N	2.48	0.45
1:I:208:ALA:O	1:I:212:ILE:N	2.46	0.45
1:K:42:ILE:HG22	1:K:60:GLU:HB3	1.99	0.45
1:A:306:LEU:HD22	1:B:266:PHE:CE2	2.51	0.45
1:C:309:LEU:O	1:C:313:SER:N	2.50	0.45
1:K:328:ARG:NH1	1:L:242:ALA:O	2.50	0.45
1:J:7:ASP:OD1	1:J:8:ALA:N	2.50	0.45
1:A:136:ILE:HD11	1:A:146:TYR:CZ	2.52	0.44
1:D:119:PRO:O	1:D:154:GLN:NE2	2.50	0.44
1:D:18:ILE:HD11	1:D:39:LEU:HD13	1.99	0.44
1:I:5:VAL:HG22	1:I:179:ALA:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:ALA:HA	1:H:241:ILE:HD12	1.98	0.44
1:K:237:ILE:O	1:K:249:GLN:NE2	2.47	0.44
1:F:91:ILE:HG22	1:F:95:LEU:HG	1.98	0.44
1:E:3:LYS:HD3	1:E:3:LYS:N	2.33	0.44
1:E:213:ALA:O	1:E:218:GLY:N	2.51	0.44
1:L:19:GLY:N	1:L:71:SER:OG	2.51	0.44
1:L:309:LEU:O	1:L:313:SER:N	2.50	0.44
1:I:213:ALA:O	1:I:218:GLY:N	2.51	0.44
1:A:294:LEU:HD13	1:C:294:LEU:HD13	2.00	0.44
1:F:208:ALA:O	1:F:212:ILE:N	2.45	0.44
1:A:10:LEU:O	1:A:14:LYS:NZ	2.34	0.44
1:F:33:ILE:HD13	1:F:171:ILE:O	2.17	0.44
1:J:238:ALA:HA	1:J:241:ILE:HD12	2.00	0.44
1:K:271:VAL:HG11	1:L:275:ILE:HD11	1.98	0.44
1:G:35:ARG:NH1	1:G:57:GLU:O	2.49	0.44
1:C:18:ILE:HD12	1:C:39:LEU:HB3	2.00	0.43
1:F:162:ASP:O	1:F:166:ALA:N	2.45	0.43
1:G:102:VAL:HG21	1:G:163:TYR:CD2	2.53	0.43
1:L:237:ILE:O	1:L:249:GLN:OE1	2.36	0.43
1:E:43:VAL:HB	1:E:61:VAL:HG22	1.98	0.43
1:F:297:GLN:O	1:J:297:GLN:NE2	2.48	0.43
1:L:35:ARG:NH2	1:L:57:GLU:O	2.46	0.43
1:B:92:ALA:HB3	1:B:93:PRO:HD3	2.00	0.43
1:F:294:LEU:HD13	1:G:294:LEU:HD13	2.00	0.43
1:I:287:SER:O	1:I:291:GLU:N	2.47	0.43
1:D:35:ARG:NH1	1:D:57:GLU:O	2.48	0.43
1:J:162:ASP:O	1:J:166:ALA:N	2.46	0.43
1:L:161:TRP:CZ3	1:L:181:ILE:HG23	2.54	0.43
1:A:162:ASP:O	1:A:166:ALA:N	2.46	0.43
1:C:208:ALA:O	1:C:212:ILE:N	2.48	0.43
1:E:307:TRP:NE1	1:F:258:GLN:OE1	2.52	0.43
1:H:92:ALA:HB3	1:H:93:PRO:HD3	2.00	0.43
1:I:155:ASP:OD1	1:I:156:ALA:N	2.52	0.43
3:G:404:NAI:H2N	3:G:404:NAI:O5D	2.19	0.43
1:C:197:THR:O	1:C:201:ILE:HD12	2.19	0.43
1:G:85:GLU:OE2	1:G:89:LYS:NZ	2.52	0.43
1:K:240:LEU:O	1:K:244:GLU:N	2.52	0.43
1:A:240:LEU:O	1:A:244:GLU:N	2.48	0.42
1:A:266:PHE:CD2	1:B:306:LEU:HD22	2.54	0.42
1:J:23:TYR:CE2	1:J:54:ALA:HB2	2.53	0.42
1:I:229:TYR:OH	1:I:319:GLU:OE1	2.24	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:ASN:O	1:I:251:VAL:HG12	2.19	0.42
1:K:92:ALA:HB3	1:K:93:PRO:HD3	2.01	0.42
1:L:65:ASP:OD1	1:L:66:GLU:N	2.52	0.42
1:K:29:VAL:O	1:K:32:THR:N	2.53	0.42
1:K:275:ILE:HD11	1:L:271:VAL:HG11	2.00	0.42
1:L:52:GLU:N	1:L:52:GLU:OE1	2.52	0.42
1:B:59:PHE:O	1:B:61:VAL:HG23	2.18	0.42
1:D:234:LEU:HA	1:D:237:ILE:HG22	2.01	0.42
1:I:92:ALA:HB3	1:I:93:PRO:HD3	2.01	0.42
1:G:47:LYS:NZ	1:G:63:GLU:OE2	2.52	0.42
1:H:182:SER:OG	1:H:183:SER:N	2.51	0.42
1:A:46:VAL:O	1:A:48:ASP:N	2.52	0.42
1:G:102:VAL:HG22	1:G:123:ASP:HB2	2.01	0.42
1:L:52:GLU:O	1:L:56:LYS:N	2.50	0.42
1:D:7:ASP:OD1	1:D:8:ALA:N	2.52	0.42
1:F:47:LYS:NZ	1:F:63:GLU:OE1	2.50	0.42
1:G:309:LEU:O	1:G:313:SER:N	2.52	0.42
1:L:250:MET:CE	1:L:262:LEU:HD21	2.49	0.42
1:J:136:ILE:O	1:J:140:HIS:N	2.52	0.42
1:A:309:LEU:O	1:A:313:SER:N	2.52	0.42
1:C:226:LEU:HD13	1:D:147:PRO:CB	2.49	0.42
1:C:235:ALA:HB2	1:D:238:ALA:HB3	2.02	0.42
1:E:130:ARG:NH1	1:E:187:GLU:OE2	2.50	0.42
1:K:241:ILE:CD1	1:L:234:LEU:HD23	2.50	0.42
1:A:182:SER:OG	1:A:183:SER:N	2.52	0.42
1:B:46:VAL:HG22	3:B:404:NAI:C2A	2.48	0.42
1:K:287:SER:O	1:K:291:GLU:N	2.47	0.42
1:A:155:ASP:OD1	1:A:156:ALA:N	2.53	0.41
1:J:164:ALA:O	1:J:168:ALA:N	2.50	0.41
1:L:162:ASP:OD1	1:L:163:TYR:N	2.53	0.41
1:F:287:SER:O	1:F:291:GLU:N	2.50	0.41
1:H:229:TYR:OH	1:H:319:GLU:OE1	2.32	0.41
1:K:91:ILE:HG22	1:K:95:LEU:HG	2.02	0.41
1:A:197:THR:O	1:A:201:ILE:HD12	2.20	0.41
1:C:182:SER:OG	1:C:183:SER:N	2.52	0.41
1:H:85:GLU:OE2	1:H:89:LYS:NZ	2.53	0.41
1:H:213:ALA:O	1:H:218:GLY:N	2.53	0.41
1:I:306:LEU:HD22	1:J:266:PHE:CD2	2.55	0.41
1:I:182:SER:OG	1:I:183:SER:N	2.54	0.41
1:L:146:TYR:CE2	1:L:173:ALA:HB2	2.55	0.41
1:A:305:ARG:O	1:A:308:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:SER:OG	1:F:183:SER:N	2.53	0.41
1:H:155:ASP:OD1	1:H:160:ALA:HB2	2.19	0.41
1:H:309:LEU:O	1:H:313:SER:N	2.53	0.41
1:E:275:ILE:HD11	1:F:271:VAL:HG11	2.02	0.41
1:G:227:GLU:OE1	1:H:130:ARG:NE	2.54	0.41
1:K:241:ILE:HG23	1:K:249:GLN:OE1	2.21	0.41
1:H:248:ASN:O	1:H:251:VAL:HG12	2.21	0.41
1:D:309:LEU:O	1:D:313:SER:N	2.54	0.41
1:E:92:ALA:HB3	1:E:93:PRO:HD3	2.03	0.41
1:F:102:VAL:HG22	1:F:123:ASP:HB2	2.03	0.41
1:F:164:ALA:O	1:F:168:ALA:N	2.47	0.41
1:I:18:ILE:CD1	1:I:39:LEU:HD13	2.50	0.41
1:I:309:LEU:O	1:I:313:SER:N	2.54	0.41
1:K:241:ILE:HD12	1:L:234:LEU:HD23	2.02	0.41
1:L:33:ILE:O	1:L:37:ASN:N	2.54	0.41
1:L:229:TYR:OH	1:L:319:GLU:OE1	2.24	0.41
1:C:287:SER:O	1:C:291:GLU:N	2.54	0.41
1:F:7:ASP:OD1	1:F:8:ALA:N	2.49	0.41
1:F:92:ALA:HB3	1:F:93:PRO:HD3	2.03	0.41
1:H:38:GLY:O	1:H:39:LEU:HD23	2.21	0.41
1:J:309:LEU:O	1:J:313:SER:N	2.54	0.40
1:E:35:ARG:NH2	1:E:57:GLU:O	2.51	0.40
1:E:238:ALA:HB3	1:F:235:ALA:HB2	2.03	0.40
1:F:23:TYR:CD2	1:F:54:ALA:HB2	2.55	0.40
1:G:203:PHE:O	1:G:207:LYS:N	2.54	0.40
1:L:34:MET:HB3	1:L:39:LEU:HD12	2.03	0.40
1:A:213:ALA:O	1:A:218:GLY:N	2.54	0.40
1:G:297:GLN:NE2	1:J:297:GLN:O	2.49	0.40
1:H:197:THR:O	1:H:201:ILE:HD12	2.21	0.40
1:I:33:ILE:HD13	1:I:171:ILE:O	2.21	0.40
1:J:92:ALA:HB3	1:J:93:PRO:HD3	2.03	0.40
1:D:92:ALA:HB3	1:D:93:PRO:HD3	2.03	0.40
1:E:226:LEU:HD13	1:F:147:PRO:HB2	2.03	0.40
1:F:305:ARG:O	1:F:308:GLU:N	2.54	0.40
1:I:197:THR:O	1:I:201:ILE:HD12	2.21	0.40
1:L:135:GLY:O	1:L:139:LEU:HD12	2.21	0.40
1:B:204:GLY:O	1:B:208:ALA:N	2.54	0.40
1:C:92:ALA:HB3	1:C:93:PRO:HD3	2.04	0.40
1:K:164:ALA:O	1:K:168:ALA:N	2.52	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	328/333 (98%)	307 (94%)	21 (6%)	0	100	100
1	B	329/333 (99%)	306 (93%)	23 (7%)	0	100	100
1	C	329/333 (99%)	305 (93%)	24 (7%)	0	100	100
1	D	328/333 (98%)	303 (92%)	25 (8%)	0	100	100
1	E	327/333 (98%)	302 (92%)	25 (8%)	0	100	100
1	F	328/333 (98%)	308 (94%)	20 (6%)	0	100	100
1	G	328/333 (98%)	302 (92%)	26 (8%)	0	100	100
1	H	327/333 (98%)	301 (92%)	26 (8%)	0	100	100
1	I	326/333 (98%)	304 (93%)	22 (7%)	0	100	100
1	J	327/333 (98%)	305 (93%)	22 (7%)	0	100	100
1	K	326/333 (98%)	303 (93%)	23 (7%)	0	100	100
1	L	326/333 (98%)	298 (91%)	28 (9%)	0	100	100
All	All	3929/3996 (98%)	3644 (93%)	285 (7%)	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	269/272 (99%)	269 (100%)	0	100	100
1	B	270/272 (99%)	270 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	270/272 (99%)	270 (100%)	0	100	100
1	D	269/272 (99%)	268 (100%)	1 (0%)	91	95
1	E	268/272 (98%)	268 (100%)	0	100	100
1	F	269/272 (99%)	269 (100%)	0	100	100
1	G	269/272 (99%)	269 (100%)	0	100	100
1	H	268/272 (98%)	268 (100%)	0	100	100
1	I	267/272 (98%)	267 (100%)	0	100	100
1	J	268/272 (98%)	268 (100%)	0	100	100
1	K	267/272 (98%)	267 (100%)	0	100	100
1	L	267/272 (98%)	267 (100%)	0	100	100
All	All	3221/3264 (99%)	3220 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAI	E	403	-	42,48,48	4.90	19 (45%)	47,73,73	1.95	6 (12%)
4	9TY	D	405	2	9,9,9	1.00	0	13,14,14	1.43	1 (7%)
4	9TY	I	405	2	9,9,9	1.00	0	13,14,14	1.44	1 (7%)
3	NAI	F	405	-	42,48,48	4.89	19 (45%)	47,73,73	1.94	6 (12%)
3	NAI	B	404	-	42,48,48	4.91	20 (47%)	47,73,73	1.88	5 (10%)
4	9TY	A	405	2	9,9,9	1.00	0	13,14,14	1.44	1 (7%)
4	9TY	E	404	2	9,9,9	0.99	0	13,14,14	1.43	2 (15%)
3	NAI	H	404	-	42,48,48	4.89	19 (45%)	47,73,73	1.95	6 (12%)
4	9TY	G	405	2	9,9,9	1.00	0	13,14,14	1.44	1 (7%)
3	NAI	G	404	-	42,48,48	4.89	18 (42%)	47,73,73	1.94	5 (10%)
4	9TY	J	405	2	9,9,9	1.01	0	13,14,14	1.47	1 (7%)
3	NAI	C	404	-	42,48,48	4.89	19 (45%)	47,73,73	1.95	6 (12%)
4	9TY	L	405	2	9,9,9	1.00	0	13,14,14	1.44	1 (7%)
4	9TY	K	405	2	9,9,9	1.00	0	13,14,14	1.46	1 (7%)
3	NAI	I	404	-	42,48,48	4.92	19 (45%)	47,73,73	1.90	6 (12%)
3	NAI	J	404	-	42,48,48	4.89	18 (42%)	47,73,73	1.95	5 (10%)
3	NAI	K	404	-	42,48,48	4.91	19 (45%)	47,73,73	1.93	5 (10%)
3	NAI	L	404	-	42,48,48	4.90	19 (45%)	47,73,73	1.97	6 (12%)
3	NAI	D	404	-	42,48,48	4.89	18 (42%)	47,73,73	1.89	5 (10%)
4	9TY	C	405	2	9,9,9	0.99	0	13,14,14	1.42	1 (7%)
3	NAI	A	404	-	42,48,48	4.90	19 (45%)	47,73,73	1.97	5 (10%)
4	9TY	F	406	2	9,9,9	1.00	0	13,14,14	1.43	1 (7%)
4	9TY	B	405	2	9,9,9	1.00	0	13,14,14	1.49	2 (15%)
4	9TY	H	405	2	9,9,9	1.01	0	13,14,14	1.44	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAI	E	403	-	-	9/25/72/72	0/5/5/5
4	9TY	D	405	2	-	4/12/16/16	0/1/1/1
4	9TY	I	405	2	-	3/12/16/16	0/1/1/1
3	NAI	F	405	-	-	9/25/72/72	0/5/5/5
3	NAI	B	404	-	-	13/25/72/72	0/5/5/5
4	9TY	A	405	2	-	4/12/16/16	0/1/1/1
4	9TY	E	404	2	-	6/12/16/16	0/1/1/1
3	NAI	H	404	-	-	11/25/72/72	0/5/5/5
4	9TY	G	405	2	-	4/12/16/16	0/1/1/1
3	NAI	G	404	-	-	6/25/72/72	0/5/5/5
4	9TY	J	405	2	-	4/12/16/16	0/1/1/1
3	NAI	C	404	-	-	9/25/72/72	0/5/5/5
4	9TY	L	405	2	-	4/12/16/16	0/1/1/1
4	9TY	K	405	2	-	3/12/16/16	0/1/1/1
3	NAI	I	404	-	-	7/25/72/72	0/5/5/5
3	NAI	J	404	-	-	7/25/72/72	0/5/5/5
3	NAI	K	404	-	-	15/25/72/72	0/5/5/5
3	NAI	L	404	-	-	12/25/72/72	0/5/5/5
3	NAI	D	404	-	-	11/25/72/72	0/5/5/5
4	9TY	C	405	2	-	4/12/16/16	0/1/1/1
3	NAI	A	404	-	-	14/25/72/72	0/5/5/5
4	9TY	F	406	2	-	3/12/16/16	0/1/1/1
4	9TY	B	405	2	-	3/12/16/16	0/1/1/1
4	9TY	H	405	2	-	4/12/16/16	0/1/1/1

All (226) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	404	NAI	C2B-C1B	-16.54	1.28	1.53
3	B	404	NAI	C2B-C1B	-16.39	1.28	1.53
3	K	404	NAI	C2B-C1B	-16.33	1.29	1.53
3	A	404	NAI	C2B-C1B	-16.27	1.29	1.53
3	L	404	NAI	C2B-C1B	-16.20	1.29	1.53
3	E	403	NAI	C2B-C1B	-16.10	1.29	1.53
3	F	405	NAI	C2B-C1B	-16.10	1.29	1.53
3	H	404	NAI	C2B-C1B	-16.09	1.29	1.53
3	G	404	NAI	C2B-C1B	-16.09	1.29	1.53
3	J	404	NAI	C2B-C1B	-16.08	1.29	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	404	NAI	C2B-C1B	-16.05	1.29	1.53
3	D	404	NAI	C2B-C1B	-16.02	1.29	1.53
3	F	405	NAI	O4B-C1B	15.29	1.62	1.41
3	I	404	NAI	O4B-C1B	15.26	1.62	1.41
3	E	403	NAI	O4B-C1B	15.23	1.62	1.41
3	G	404	NAI	O4B-C1B	15.22	1.62	1.41
3	J	404	NAI	O4B-C1B	15.21	1.62	1.41
3	C	404	NAI	O4B-C1B	15.18	1.62	1.41
3	H	404	NAI	O4B-C1B	15.16	1.62	1.41
3	K	404	NAI	O4B-C1B	15.13	1.62	1.41
3	D	404	NAI	O4B-C1B	15.12	1.62	1.41
3	L	404	NAI	O4B-C1B	15.10	1.62	1.41
3	B	404	NAI	O4B-C1B	15.10	1.62	1.41
3	A	404	NAI	O4B-C1B	15.08	1.62	1.41
3	L	404	NAI	C6N-C5N	11.44	1.53	1.33
3	B	404	NAI	C6N-C5N	11.43	1.53	1.33
3	J	404	NAI	C6N-C5N	11.41	1.53	1.33
3	I	404	NAI	C6N-C5N	11.40	1.53	1.33
3	D	404	NAI	C6N-C5N	11.40	1.53	1.33
3	A	404	NAI	C6N-C5N	11.40	1.53	1.33
3	K	404	NAI	C6N-C5N	11.37	1.53	1.33
3	C	404	NAI	C6N-C5N	11.37	1.53	1.33
3	E	403	NAI	C6N-C5N	11.37	1.53	1.33
3	H	404	NAI	C6N-C5N	11.35	1.53	1.33
3	F	405	NAI	C6N-C5N	11.33	1.53	1.33
3	G	404	NAI	C6N-C5N	11.31	1.53	1.33
3	C	404	NAI	O4D-C1D	8.89	1.63	1.42
3	G	404	NAI	O4D-C1D	8.86	1.63	1.42
3	D	404	NAI	O4D-C1D	8.84	1.62	1.42
3	J	404	NAI	O4D-C1D	8.82	1.62	1.42
3	I	404	NAI	O4D-C1D	8.82	1.62	1.42
3	F	405	NAI	O4D-C1D	8.80	1.62	1.42
3	E	403	NAI	O4D-C1D	8.80	1.62	1.42
3	B	404	NAI	O4D-C1D	8.78	1.62	1.42
3	H	404	NAI	O4D-C1D	8.76	1.62	1.42
3	K	404	NAI	O4D-C1D	8.75	1.62	1.42
3	A	404	NAI	O4D-C1D	8.70	1.62	1.42
3	L	404	NAI	O4D-C1D	8.67	1.62	1.42
3	D	404	NAI	C2N-C3N	7.14	1.54	1.34
3	E	403	NAI	C2N-C3N	7.12	1.54	1.34
3	I	404	NAI	C2N-C3N	7.11	1.54	1.34
3	C	404	NAI	C2N-C3N	7.11	1.54	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	404	NAI	C2N-C3N	7.08	1.54	1.34
3	K	404	NAI	C2N-C3N	7.08	1.54	1.34
3	J	404	NAI	C2N-C3N	7.07	1.54	1.34
3	B	404	NAI	C2N-C3N	7.06	1.54	1.34
3	H	404	NAI	C2N-C3N	7.06	1.54	1.34
3	F	405	NAI	C2N-C3N	7.05	1.54	1.34
3	A	404	NAI	C2N-C3N	7.05	1.54	1.34
3	G	404	NAI	C2N-C3N	7.00	1.54	1.34
3	K	404	NAI	C2D-C1D	-6.83	1.31	1.53
3	A	404	NAI	C2D-C1D	-6.81	1.31	1.53
3	L	404	NAI	C2D-C1D	-6.80	1.31	1.53
3	H	404	NAI	C2D-C1D	-6.78	1.31	1.53
3	B	404	NAI	C2D-C1D	-6.77	1.31	1.53
3	E	403	NAI	C2D-C1D	-6.75	1.31	1.53
3	J	404	NAI	C2D-C1D	-6.73	1.32	1.53
3	I	404	NAI	C2D-C1D	-6.73	1.32	1.53
3	D	404	NAI	C2D-C1D	-6.70	1.32	1.53
3	F	405	NAI	C2D-C1D	-6.70	1.32	1.53
3	C	404	NAI	C2D-C1D	-6.69	1.32	1.53
3	G	404	NAI	C2D-C1D	-6.67	1.32	1.53
3	A	404	NAI	O4D-C4D	-6.54	1.30	1.45
3	G	404	NAI	O4D-C4D	-6.50	1.30	1.45
3	F	405	NAI	O4D-C4D	-6.49	1.30	1.45
3	H	404	NAI	O4D-C4D	-6.48	1.30	1.45
3	L	404	NAI	O4D-C4D	-6.48	1.30	1.45
3	J	404	NAI	O4D-C4D	-6.45	1.30	1.45
3	I	404	NAI	O4D-C4D	-6.44	1.30	1.45
3	K	404	NAI	O4D-C4D	-6.43	1.30	1.45
3	B	404	NAI	O4D-C4D	-6.43	1.30	1.45
3	E	403	NAI	O4D-C4D	-6.42	1.30	1.45
3	D	404	NAI	O4D-C4D	-6.41	1.30	1.45
3	C	404	NAI	O4D-C4D	-6.38	1.30	1.45
3	D	404	NAI	O4B-C4B	-5.99	1.31	1.45
3	E	403	NAI	O4B-C4B	-5.95	1.31	1.45
3	H	404	NAI	O4B-C4B	-5.94	1.31	1.45
3	A	404	NAI	O4B-C4B	-5.91	1.31	1.45
3	K	404	NAI	O4B-C4B	-5.91	1.31	1.45
3	C	404	NAI	O4B-C4B	-5.90	1.31	1.45
3	J	404	NAI	O4B-C4B	-5.89	1.31	1.45
3	G	404	NAI	O4B-C4B	-5.88	1.31	1.45
3	F	405	NAI	O4B-C4B	-5.87	1.31	1.45
3	L	404	NAI	O4B-C4B	-5.84	1.32	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	NAI	O4B-C4B	-5.62	1.32	1.45
3	I	404	NAI	O4B-C4B	-5.54	1.32	1.45
3	A	404	NAI	C7N-N7N	4.30	1.44	1.33
3	D	404	NAI	C7N-N7N	4.30	1.44	1.33
3	B	404	NAI	C7N-N7N	4.29	1.44	1.33
3	E	403	NAI	C7N-N7N	4.28	1.44	1.33
3	I	404	NAI	C7N-N7N	4.28	1.44	1.33
3	G	404	NAI	C7N-N7N	4.28	1.44	1.33
3	C	404	NAI	C7N-N7N	4.28	1.44	1.33
3	L	404	NAI	C7N-N7N	4.27	1.44	1.33
3	F	405	NAI	C7N-N7N	4.25	1.44	1.33
3	K	404	NAI	C7N-N7N	4.24	1.44	1.33
3	H	404	NAI	C7N-N7N	4.22	1.44	1.33
3	J	404	NAI	C7N-N7N	4.22	1.44	1.33
3	A	404	NAI	O3D-C3D	-3.76	1.34	1.43
3	G	404	NAI	O3D-C3D	-3.71	1.34	1.43
3	J	404	NAI	O3D-C3D	-3.69	1.34	1.43
3	H	404	NAI	O3D-C3D	-3.68	1.34	1.43
3	B	404	NAI	O3D-C3D	-3.68	1.34	1.43
3	L	404	NAI	O3D-C3D	-3.66	1.34	1.43
3	K	404	NAI	O3D-C3D	-3.65	1.34	1.43
3	F	405	NAI	O3D-C3D	-3.63	1.34	1.43
3	D	404	NAI	O3D-C3D	-3.63	1.34	1.43
3	E	403	NAI	O3D-C3D	-3.62	1.34	1.43
3	C	404	NAI	O3D-C3D	-3.62	1.34	1.43
3	B	404	NAI	C7N-C3N	3.60	1.56	1.48
3	I	404	NAI	O3D-C3D	-3.58	1.34	1.43
3	L	404	NAI	C7N-C3N	3.58	1.56	1.48
3	A	404	NAI	C7N-C3N	3.57	1.56	1.48
3	D	404	NAI	C7N-C3N	3.55	1.56	1.48
3	I	404	NAI	C7N-C3N	3.53	1.56	1.48
3	G	404	NAI	C7N-C3N	3.53	1.56	1.48
3	E	403	NAI	C7N-C3N	3.52	1.56	1.48
3	C	404	NAI	C7N-C3N	3.52	1.56	1.48
3	J	404	NAI	C7N-C3N	3.51	1.56	1.48
3	F	405	NAI	C7N-C3N	3.51	1.56	1.48
3	K	404	NAI	C7N-C3N	3.49	1.56	1.48
3	H	404	NAI	C7N-C3N	3.48	1.56	1.48
3	L	404	NAI	C6N-N1N	3.45	1.45	1.37
3	B	404	NAI	C6N-N1N	3.40	1.45	1.37
3	A	404	NAI	C6N-N1N	3.37	1.45	1.37
3	J	404	NAI	C6N-N1N	3.35	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	404	NAI	C6N-N1N	3.34	1.45	1.37
3	C	404	NAI	C6N-N1N	3.34	1.45	1.37
3	I	404	NAI	C5A-C4A	-3.33	1.32	1.40
3	I	404	NAI	C6N-N1N	3.33	1.45	1.37
3	H	404	NAI	C6N-N1N	3.33	1.45	1.37
3	D	404	NAI	C6N-N1N	3.33	1.45	1.37
3	F	405	NAI	C6N-N1N	3.32	1.45	1.37
3	E	403	NAI	C6N-N1N	3.32	1.45	1.37
3	B	404	NAI	C5A-C4A	-3.31	1.32	1.40
3	G	404	NAI	C6N-N1N	3.29	1.45	1.37
3	E	403	NAI	C5A-C4A	-3.27	1.32	1.40
3	J	404	NAI	C5A-C4A	-3.26	1.32	1.40
3	A	404	NAI	C5A-C4A	-3.25	1.32	1.40
3	K	404	NAI	C5A-C4A	-3.25	1.32	1.40
3	H	404	NAI	C5A-C4A	-3.25	1.32	1.40
3	C	404	NAI	C5A-C4A	-3.24	1.32	1.40
3	L	404	NAI	C5A-C4A	-3.24	1.32	1.40
3	G	404	NAI	C5A-C4A	-3.24	1.32	1.40
3	F	405	NAI	C5A-C4A	-3.23	1.32	1.40
3	D	404	NAI	C5A-C4A	-3.20	1.32	1.40
3	K	404	NAI	O2D-C2D	2.48	1.48	1.43
3	L	404	NAI	O2D-C2D	2.48	1.48	1.43
3	J	404	NAI	O2D-C2D	2.47	1.48	1.43
3	E	403	NAI	O2D-C2D	2.46	1.48	1.43
3	A	404	NAI	O2D-C2D	2.45	1.48	1.43
3	C	404	NAI	O2D-C2D	2.45	1.48	1.43
3	H	404	NAI	O2D-C2D	2.44	1.48	1.43
3	G	404	NAI	O2D-C2D	2.44	1.48	1.43
3	B	404	NAI	O2D-C2D	2.44	1.48	1.43
3	D	404	NAI	O2D-C2D	2.44	1.48	1.43
3	F	405	NAI	O2D-C2D	2.44	1.48	1.43
3	I	404	NAI	O2D-C2D	2.42	1.48	1.43
3	K	404	NAI	O3B-C3B	-2.41	1.37	1.43
3	E	403	NAI	O3B-C3B	-2.40	1.37	1.43
3	G	404	NAI	O3B-C3B	-2.38	1.37	1.43
3	A	404	NAI	O3B-C3B	-2.36	1.37	1.43
3	F	405	NAI	O3B-C3B	-2.36	1.37	1.43
3	L	404	NAI	O3B-C3B	-2.34	1.37	1.43
3	B	404	NAI	O3B-C3B	-2.34	1.37	1.43
3	I	404	NAI	O3B-C3B	-2.33	1.37	1.43
3	C	404	NAI	O3B-C3B	-2.33	1.37	1.43
3	H	404	NAI	O3B-C3B	-2.31	1.37	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	NAI	O3B-C3B	-2.30	1.37	1.43
3	K	404	NAI	C6A-N6A	2.29	1.42	1.34
3	J	404	NAI	O3B-C3B	-2.28	1.37	1.43
3	A	404	NAI	C6A-N6A	2.25	1.42	1.34
3	I	404	NAI	C6A-N6A	2.25	1.42	1.34
3	B	404	NAI	C6A-N6A	2.24	1.42	1.34
3	L	404	NAI	C6A-N6A	2.22	1.42	1.34
3	E	403	NAI	C6A-N6A	2.22	1.42	1.34
3	G	404	NAI	C6A-N6A	2.22	1.42	1.34
3	F	405	NAI	C6A-N6A	2.20	1.42	1.34
3	D	404	NAI	C6A-N6A	2.20	1.42	1.34
3	C	404	NAI	C6A-N6A	2.20	1.42	1.34
3	H	404	NAI	C6A-N6A	2.18	1.42	1.34
3	J	404	NAI	C6A-N6A	2.17	1.41	1.34
3	J	404	NAI	O5D-C5D	-2.16	1.36	1.44
3	G	404	NAI	O5D-C5D	-2.16	1.36	1.44
3	A	404	NAI	C4N-C5N	2.14	1.54	1.48
3	L	404	NAI	C4N-C5N	2.12	1.54	1.48
3	H	404	NAI	C4N-C5N	2.12	1.54	1.48
3	C	404	NAI	O5D-C5D	-2.11	1.36	1.44
3	K	404	NAI	O5D-C5D	-2.11	1.36	1.44
3	I	404	NAI	O5D-C5D	-2.11	1.36	1.44
3	D	404	NAI	O5D-C5D	-2.11	1.36	1.44
3	B	404	NAI	O5D-C5D	-2.10	1.36	1.44
3	H	404	NAI	O5D-C5D	-2.10	1.36	1.44
3	F	405	NAI	O5D-C5D	-2.10	1.36	1.44
3	D	404	NAI	C4N-C5N	2.09	1.54	1.48
3	E	403	NAI	O5D-C5D	-2.09	1.36	1.44
3	A	404	NAI	O5D-C5D	-2.09	1.36	1.44
3	I	404	NAI	C4N-C5N	2.08	1.54	1.48
3	E	403	NAI	C4N-C5N	2.08	1.54	1.48
3	L	404	NAI	O5D-C5D	-2.07	1.36	1.44
3	C	404	NAI	C4N-C5N	2.07	1.54	1.48
3	B	404	NAI	C4N-C5N	2.07	1.54	1.48
3	K	404	NAI	C4N-C5N	2.07	1.54	1.48
3	G	404	NAI	C4N-C5N	2.06	1.54	1.48
3	F	405	NAI	C4N-C5N	2.06	1.54	1.48
3	J	404	NAI	C4N-C5N	2.05	1.54	1.48
3	A	404	NAI	PN-O5D	2.04	1.67	1.59
3	B	404	NAI	PN-O5D	2.04	1.67	1.59
3	K	404	NAI	PN-O5D	2.04	1.67	1.59
3	F	405	NAI	PN-O5D	2.03	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	404	NAI	PN-O5D	2.03	1.67	1.59
3	I	404	NAI	PN-O5D	2.02	1.67	1.59
3	E	403	NAI	PN-O5D	2.02	1.67	1.59
3	B	404	NAI	O2B-C2B	2.01	1.47	1.43
3	H	404	NAI	PN-O5D	2.01	1.67	1.59
3	C	404	NAI	PN-O5D	2.00	1.67	1.59

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	404	NAI	C5A-C6A-N6A	8.71	133.59	120.35
3	A	404	NAI	C5A-C6A-N6A	8.69	133.56	120.35
3	I	404	NAI	C5A-C6A-N6A	8.57	133.38	120.35
3	K	404	NAI	C5A-C6A-N6A	8.51	133.28	120.35
3	B	404	NAI	C5A-C6A-N6A	8.45	133.19	120.35
3	H	404	NAI	C5A-C6A-N6A	8.12	132.69	120.35
3	G	404	NAI	C5A-C6A-N6A	8.11	132.68	120.35
3	E	403	NAI	C5A-C6A-N6A	8.11	132.67	120.35
3	J	404	NAI	C5A-C6A-N6A	8.10	132.66	120.35
3	F	405	NAI	C5A-C6A-N6A	8.02	132.54	120.35
3	C	404	NAI	C5A-C6A-N6A	8.01	132.53	120.35
3	D	404	NAI	C5A-C6A-N6A	7.93	132.40	120.35
3	L	404	NAI	N6A-C6A-N1A	-5.93	106.27	118.57
3	A	404	NAI	N6A-C6A-N1A	-5.83	106.47	118.57
3	I	404	NAI	N6A-C6A-N1A	-5.72	106.69	118.57
3	B	404	NAI	N6A-C6A-N1A	-5.70	106.75	118.57
3	K	404	NAI	N6A-C6A-N1A	-5.68	106.78	118.57
3	J	404	NAI	N6A-C6A-N1A	-5.52	107.12	118.57
3	K	404	NAI	N3A-C2A-N1A	-5.47	120.14	128.68
3	H	404	NAI	N6A-C6A-N1A	-5.46	107.24	118.57
3	E	403	NAI	N6A-C6A-N1A	-5.45	107.27	118.57
3	F	405	NAI	N6A-C6A-N1A	-5.44	107.29	118.57
3	B	404	NAI	N3A-C2A-N1A	-5.43	120.19	128.68
3	G	404	NAI	N6A-C6A-N1A	-5.43	107.30	118.57
3	I	404	NAI	N3A-C2A-N1A	-5.42	120.20	128.68
3	A	404	NAI	N3A-C2A-N1A	-5.41	120.22	128.68
3	C	404	NAI	N6A-C6A-N1A	-5.39	107.39	118.57
3	G	404	NAI	N3A-C2A-N1A	-5.38	120.27	128.68
3	J	404	NAI	N3A-C2A-N1A	-5.35	120.31	128.68
3	C	404	NAI	N3A-C2A-N1A	-5.34	120.33	128.68
3	E	403	NAI	N3A-C2A-N1A	-5.34	120.34	128.68
3	D	404	NAI	N6A-C6A-N1A	-5.32	107.52	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	405	NAI	N3A-C2A-N1A	-5.32	120.36	128.68
3	L	404	NAI	N3A-C2A-N1A	-5.31	120.37	128.68
3	D	404	NAI	N3A-C2A-N1A	-5.28	120.42	128.68
3	H	404	NAI	N3A-C2A-N1A	-5.27	120.43	128.68
3	J	404	NAI	C3B-C2B-C1B	4.53	107.79	100.98
3	F	405	NAI	C3B-C2B-C1B	4.37	107.55	100.98
3	H	404	NAI	C3B-C2B-C1B	4.36	107.54	100.98
3	C	404	NAI	C3B-C2B-C1B	4.34	107.51	100.98
3	E	403	NAI	C3B-C2B-C1B	4.29	107.44	100.98
3	G	404	NAI	C3B-C2B-C1B	4.16	107.24	100.98
3	D	404	NAI	C3B-C2B-C1B	4.00	106.99	100.98
4	K	405	9TY	C08-C03-C07	3.02	60.11	57.41
4	B	405	9TY	C08-C03-C07	2.96	60.07	57.41
4	A	405	9TY	C08-C03-C07	2.96	60.06	57.41
4	J	405	9TY	C08-C03-C07	2.95	60.05	57.41
4	H	405	9TY	C08-C03-C07	2.93	60.04	57.41
4	D	405	9TY	C08-C03-C07	2.93	60.03	57.41
4	L	405	9TY	C08-C03-C07	2.92	60.03	57.41
4	F	406	9TY	C08-C03-C07	2.92	60.03	57.41
4	C	405	9TY	C08-C03-C07	2.90	60.01	57.41
4	I	405	9TY	C08-C03-C07	2.90	60.01	57.41
4	G	405	9TY	C08-C03-C07	2.89	60.00	57.41
4	E	404	9TY	C08-C03-C07	2.86	59.97	57.41
3	L	404	NAI	C3B-C2B-C1B	2.62	104.93	100.98
3	G	404	NAI	PN-O3-PA	-2.60	123.90	132.83
3	K	404	NAI	O4B-C1B-C2B	-2.58	103.15	106.93
3	J	404	NAI	PN-O3-PA	-2.56	124.05	132.83
3	I	404	NAI	PN-O3-PA	-2.52	124.17	132.83
3	B	404	NAI	O4B-C1B-C2B	-2.51	103.25	106.93
3	C	404	NAI	PN-O3-PA	-2.44	124.45	132.83
3	A	404	NAI	PN-O3-PA	-2.41	124.54	132.83
3	I	404	NAI	O4B-C1B-C2B	-2.41	103.41	106.93
3	F	405	NAI	PN-O3-PA	-2.40	124.60	132.83
3	E	403	NAI	PN-O3-PA	-2.39	124.64	132.83
3	A	404	NAI	O4B-C1B-C2B	-2.26	103.62	106.93
3	K	404	NAI	PN-O3-PA	-2.22	125.22	132.83
3	B	404	NAI	PN-O3-PA	-2.20	125.29	132.83
3	H	404	NAI	PN-O3-PA	-2.17	125.38	132.83
3	F	405	NAI	C2B-C3B-C4B	2.16	106.83	102.64
3	D	404	NAI	PN-O3-PA	-2.14	125.48	132.83
3	L	404	NAI	PN-O3-PA	-2.11	125.59	132.83
4	E	404	9TY	O09-C02-C03	2.06	120.52	114.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	404	NAI	C1B-N9A-C4A	2.03	130.22	126.64
3	C	404	NAI	C2B-C3B-C4B	2.03	106.58	102.64
4	B	405	9TY	O09-C02-C03	2.02	120.41	114.91
3	I	404	NAI	C3N-C2N-N1N	-2.02	120.21	123.10
3	E	403	NAI	C2B-C3B-C4B	2.01	106.55	102.64
3	H	404	NAI	C2B-C3B-C4B	2.01	106.55	102.64

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	NAI	C5B-O5B-PA-O1A
3	A	404	NAI	C5B-O5B-PA-O2A
3	A	404	NAI	PN-O3-PA-O5B
3	A	404	NAI	C5D-O5D-PN-O1N
3	A	404	NAI	C5D-O5D-PN-O2N
3	A	404	NAI	O4D-C4D-C5D-O5D
3	A	404	NAI	O4D-C1D-N1N-C6N
3	A	404	NAI	C2N-C3N-C7N-N7N
3	B	404	NAI	C5B-O5B-PA-O2A
3	B	404	NAI	C5B-O5B-PA-O3
3	B	404	NAI	C5D-O5D-PN-O2N
3	B	404	NAI	O4D-C4D-C5D-O5D
3	B	404	NAI	C2N-C3N-C7N-N7N
3	C	404	NAI	C5B-O5B-PA-O3
3	C	404	NAI	C5D-O5D-PN-O2N
3	C	404	NAI	O4D-C4D-C5D-O5D
3	D	404	NAI	C5B-O5B-PA-O1A
3	D	404	NAI	C5B-O5B-PA-O2A
3	D	404	NAI	C5D-O5D-PN-O2N
3	D	404	NAI	O4D-C4D-C5D-O5D
3	E	403	NAI	C5B-O5B-PA-O2A
3	E	403	NAI	C5B-O5B-PA-O3
3	E	403	NAI	C5D-O5D-PN-O2N
3	E	403	NAI	O4D-C4D-C5D-O5D
3	F	405	NAI	C5B-O5B-PA-O2A
3	F	405	NAI	C5B-O5B-PA-O3
3	F	405	NAI	C5D-O5D-PN-O2N
3	F	405	NAI	O4D-C4D-C5D-O5D
3	G	404	NAI	C5B-O5B-PA-O2A
3	G	404	NAI	C5B-O5B-PA-O3
3	G	404	NAI	O4D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	404	NAI	C3D-C4D-C5D-O5D
3	H	404	NAI	C5B-O5B-PA-O2A
3	H	404	NAI	C5B-O5B-PA-O3
3	H	404	NAI	C5D-O5D-PN-O2N
3	H	404	NAI	O4D-C4D-C5D-O5D
3	I	404	NAI	O4D-C4D-C5D-O5D
3	J	404	NAI	C5B-O5B-PA-O3
3	J	404	NAI	O4D-C4D-C5D-O5D
3	J	404	NAI	C3D-C4D-C5D-O5D
3	J	404	NAI	C2N-C3N-C7N-N7N
3	K	404	NAI	C5B-O5B-PA-O1A
3	K	404	NAI	C5B-O5B-PA-O2A
3	K	404	NAI	C5B-O5B-PA-O3
3	K	404	NAI	C5D-O5D-PN-O1N
3	K	404	NAI	C5D-O5D-PN-O2N
3	K	404	NAI	O4D-C4D-C5D-O5D
3	K	404	NAI	C2N-C3N-C7N-N7N
3	L	404	NAI	C5B-O5B-PA-O2A
3	L	404	NAI	C5B-O5B-PA-O3
3	L	404	NAI	PN-O3-PA-O5B
3	L	404	NAI	C5D-O5D-PN-O1N
3	L	404	NAI	C5D-O5D-PN-O2N
3	L	404	NAI	O4D-C4D-C5D-O5D
3	L	404	NAI	C2N-C3N-C7N-N7N
4	A	405	9TY	C02-C03-C04-O05
4	A	405	9TY	C02-C03-C04-O06
4	A	405	9TY	C07-C03-C04-O05
4	A	405	9TY	C07-C03-C04-O06
4	C	405	9TY	C02-C03-C04-O05
4	C	405	9TY	C02-C03-C04-O06
4	D	405	9TY	C02-C03-C04-O05
4	D	405	9TY	C02-C03-C04-O06
4	D	405	9TY	C07-C03-C04-O05
4	D	405	9TY	C07-C03-C04-O06
4	E	404	9TY	O01-C02-C03-C07
4	E	404	9TY	O09-C02-C03-C04
4	E	404	9TY	O09-C02-C03-C07
4	F	406	9TY	C02-C03-C04-O06
4	F	406	9TY	C07-C03-C04-O06
4	G	405	9TY	C02-C03-C04-O05
4	G	405	9TY	C02-C03-C04-O06
4	G	405	9TY	C07-C03-C04-O05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	405	9TY	C07-C03-C04-O06
4	H	405	9TY	C02-C03-C04-O06
4	H	405	9TY	C07-C03-C04-O05
4	H	405	9TY	C07-C03-C04-O06
4	I	405	9TY	C02-C03-C04-O06
4	I	405	9TY	C07-C03-C04-O06
4	J	405	9TY	C02-C03-C04-O06
4	J	405	9TY	C07-C03-C04-O05
4	J	405	9TY	C07-C03-C04-O06
4	L	405	9TY	C02-C03-C04-O05
4	L	405	9TY	C02-C03-C04-O06
4	L	405	9TY	C07-C03-C04-O05
4	L	405	9TY	C07-C03-C04-O06
3	A	404	NAI	C3D-C4D-C5D-O5D
3	B	404	NAI	C3D-C4D-C5D-O5D
3	C	404	NAI	C3D-C4D-C5D-O5D
3	D	404	NAI	C3D-C4D-C5D-O5D
3	E	403	NAI	C3D-C4D-C5D-O5D
3	F	405	NAI	C3D-C4D-C5D-O5D
3	H	404	NAI	C3D-C4D-C5D-O5D
3	I	404	NAI	C3D-C4D-C5D-O5D
3	K	404	NAI	C3D-C4D-C5D-O5D
3	L	404	NAI	C3D-C4D-C5D-O5D
3	B	404	NAI	O4D-C1D-N1N-C6N
3	H	404	NAI	O4D-C1D-N1N-C6N
3	J	404	NAI	O4D-C1D-N1N-C6N
3	K	404	NAI	O4D-C1D-N1N-C6N
3	L	404	NAI	O4D-C1D-N1N-C6N
3	E	403	NAI	O4D-C1D-N1N-C6N
3	G	404	NAI	O4D-C1D-N1N-C6N
3	I	404	NAI	O4D-C1D-N1N-C6N
3	A	404	NAI	C3B-C4B-C5B-O5B
3	K	404	NAI	C3B-C4B-C5B-O5B
3	F	405	NAI	O4D-C1D-N1N-C6N
3	D	404	NAI	O4D-C1D-N1N-C6N
3	A	404	NAI	O4B-C4B-C5B-O5B
3	K	404	NAI	O4B-C4B-C5B-O5B
3	B	404	NAI	PN-O3-PA-O5B
3	C	404	NAI	PN-O3-PA-O5B
3	D	404	NAI	PN-O3-PA-O5B
3	G	404	NAI	PN-O3-PA-O5B
3	H	404	NAI	PN-O3-PA-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	I	404	NAI	PN-O3-PA-O5B
3	J	404	NAI	PN-O3-PA-O5B
3	K	404	NAI	PN-O3-PA-O5B
3	A	404	NAI	C5B-O5B-PA-O3
3	A	404	NAI	C5D-O5D-PN-O3
3	C	404	NAI	C5D-O5D-PN-O3
3	D	404	NAI	C5D-O5D-PN-O3
3	E	403	NAI	C5D-O5D-PN-O3
3	F	405	NAI	C5D-O5D-PN-O3
3	H	404	NAI	C5D-O5D-PN-O3
3	H	404	NAI	PA-O3-PN-O2N
3	C	404	NAI	O4D-C1D-N1N-C6N
3	B	404	NAI	C5D-O5D-PN-O1N
3	C	404	NAI	C5B-O5B-PA-O2A
3	C	404	NAI	C5D-O5D-PN-O1N
3	D	404	NAI	C5D-O5D-PN-O1N
3	E	403	NAI	C5D-O5D-PN-O1N
3	F	405	NAI	C5D-O5D-PN-O1N
3	H	404	NAI	C5D-O5D-PN-O1N
3	I	404	NAI	C5D-O5D-PN-O1N
3	J	404	NAI	C5B-O5B-PA-O2A
4	B	405	9TY	C02-C03-C04-O06
4	E	404	9TY	O01-C02-C03-C04
4	K	405	9TY	C02-C03-C04-O06
4	B	405	9TY	C07-C03-C04-O05
4	B	405	9TY	C07-C03-C04-O06
4	C	405	9TY	C07-C03-C04-O05
4	C	405	9TY	C07-C03-C04-O06
4	E	404	9TY	O01-C02-C03-C08
4	E	404	9TY	O09-C02-C03-C08
4	F	406	9TY	C07-C03-C04-O05
4	I	405	9TY	C07-C03-C04-O05
4	K	405	9TY	C07-C03-C04-O05
4	K	405	9TY	C07-C03-C04-O06
3	B	404	NAI	C2N-C3N-C7N-O7N
3	K	404	NAI	C2N-C3N-C7N-O7N
3	L	404	NAI	C2N-C3N-C7N-O7N
4	H	405	9TY	C02-C03-C04-O05
4	J	405	9TY	C02-C03-C04-O05
3	B	404	NAI	PN-O3-PA-O2A
3	E	403	NAI	PN-O3-PA-O5B
3	F	405	NAI	PN-O3-PA-O5B

Continued on next page...

Continued from previous page...

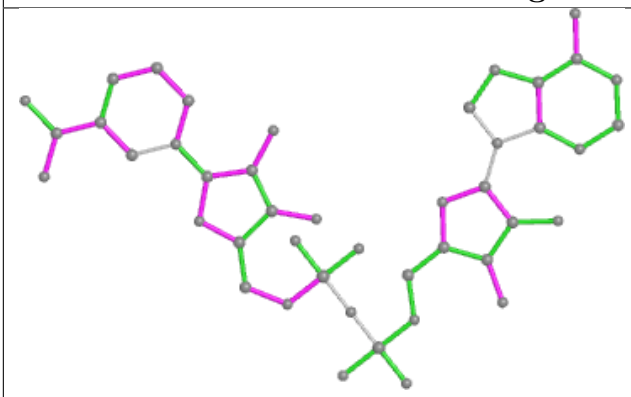
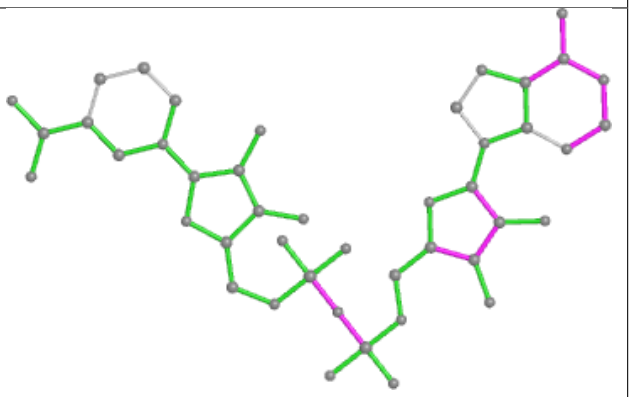
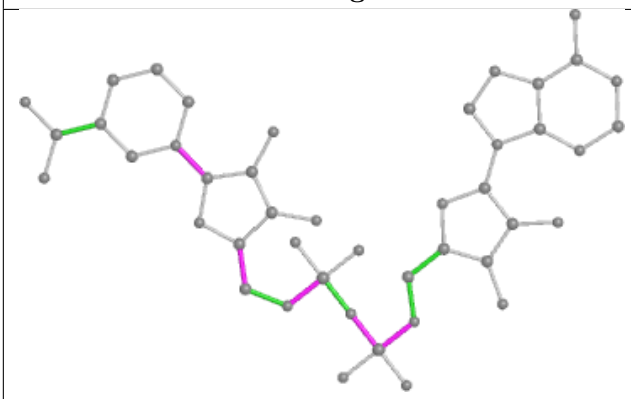
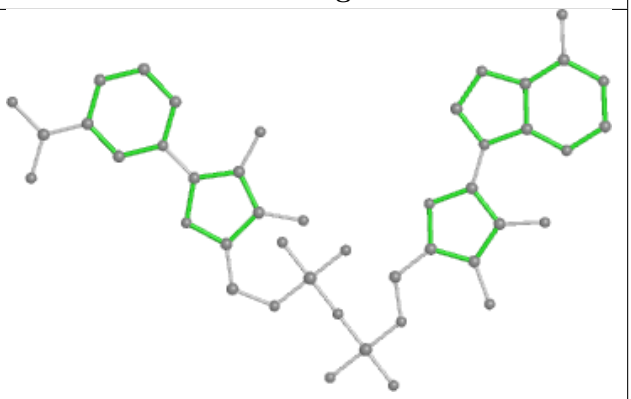
Mol	Chain	Res	Type	Atoms
3	B	404	NAI	C5D-O5D-PN-O3
3	D	404	NAI	C5B-O5B-PA-O3
3	I	404	NAI	C5B-O5B-PA-O3
3	I	404	NAI	C5D-O5D-PN-O3
3	K	404	NAI	C5D-O5D-PN-O3
3	L	404	NAI	C5D-O5D-PN-O3
3	A	404	NAI	PN-O3-PA-O1A
3	B	404	NAI	PA-O3-PN-O2N
3	D	404	NAI	PN-O3-PA-O2A
3	H	404	NAI	PN-O3-PA-O2A
3	K	404	NAI	PN-O3-PA-O1A
3	L	404	NAI	PA-O3-PN-O2N

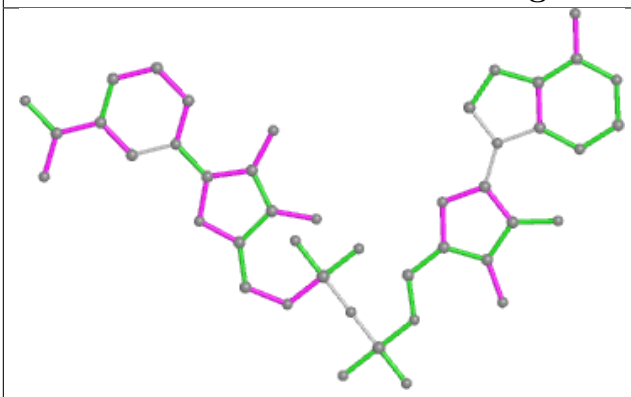
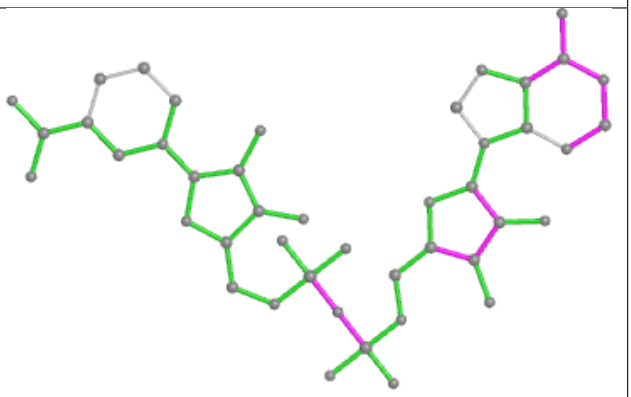
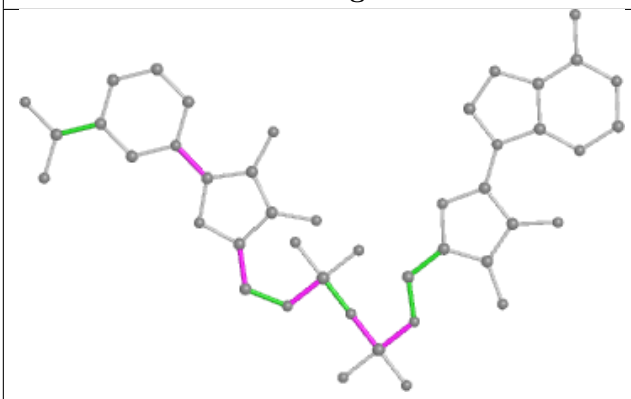
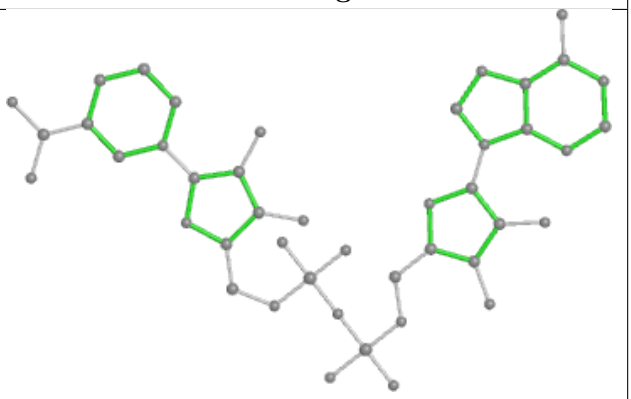
There are no ring outliers.

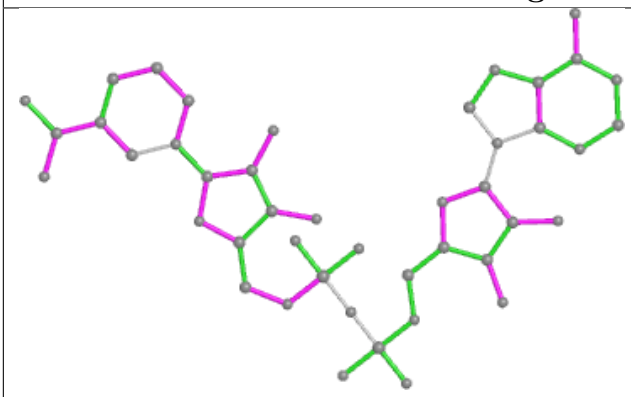
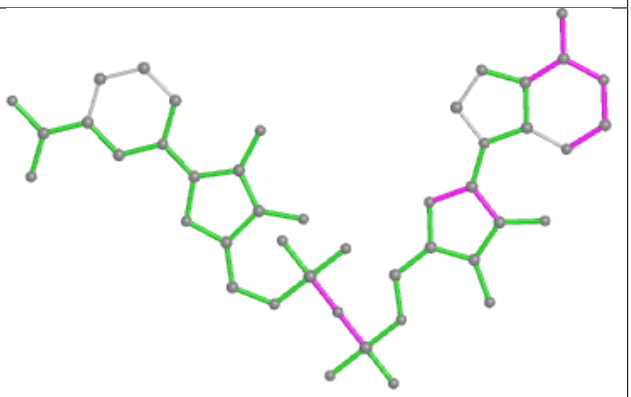
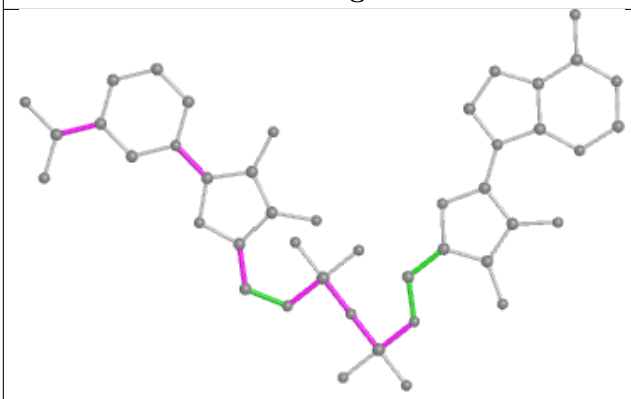
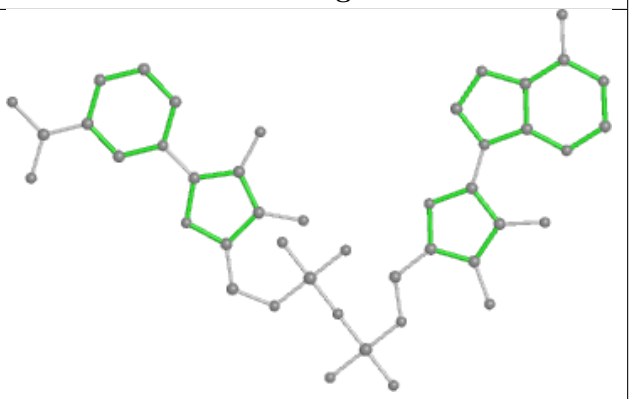
8 monomers are involved in 11 short contacts:

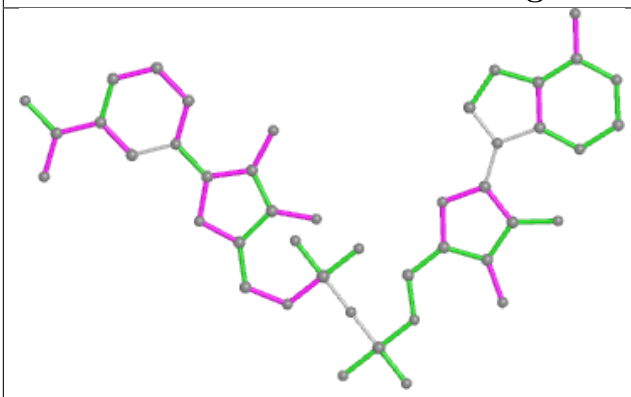
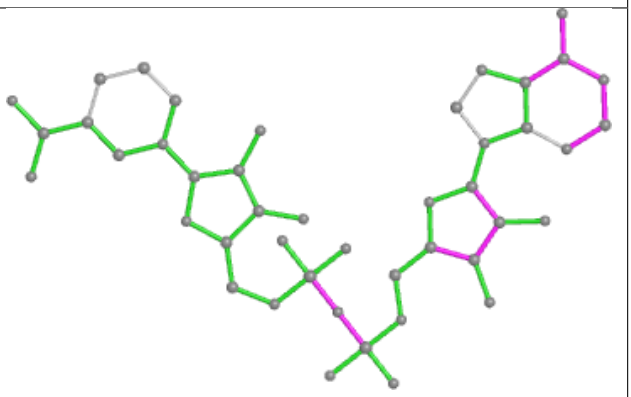
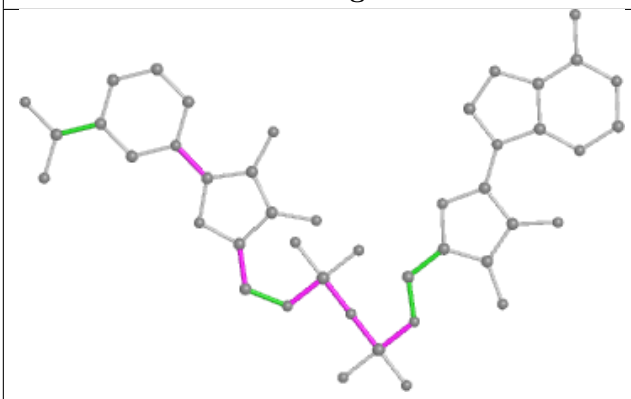
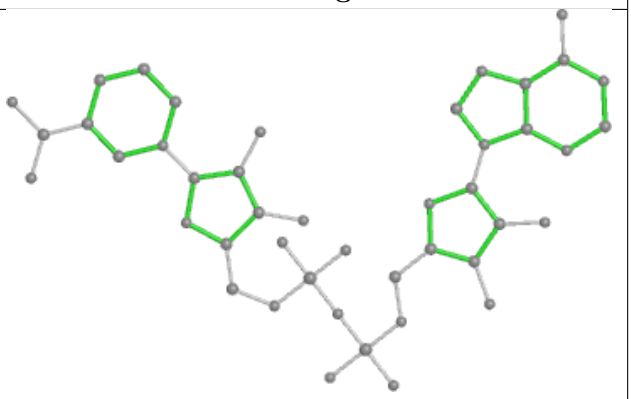
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	403	NAI	1	0
3	B	404	NAI	3	0
3	G	404	NAI	2	0
3	J	404	NAI	1	0
3	K	404	NAI	1	0
3	L	404	NAI	1	0
3	D	404	NAI	1	0
3	A	404	NAI	1	0

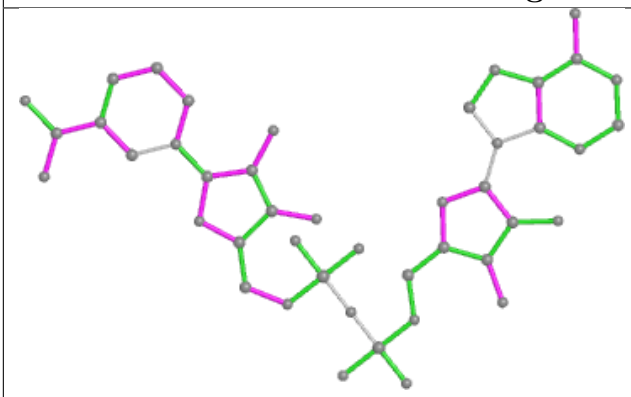
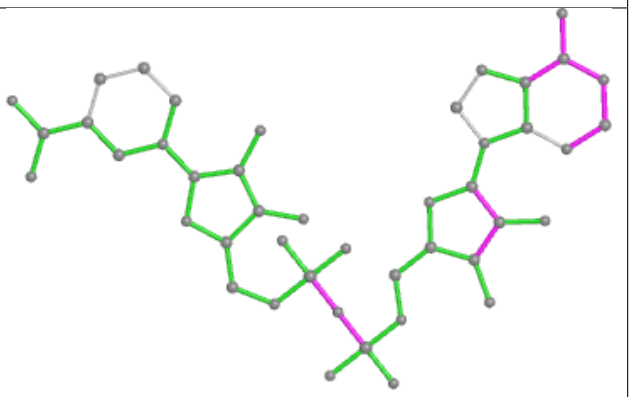
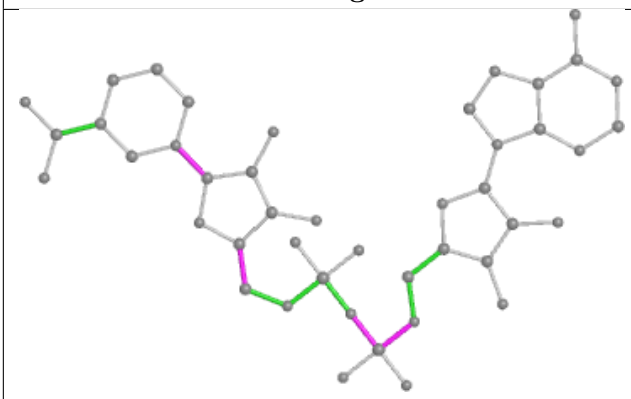
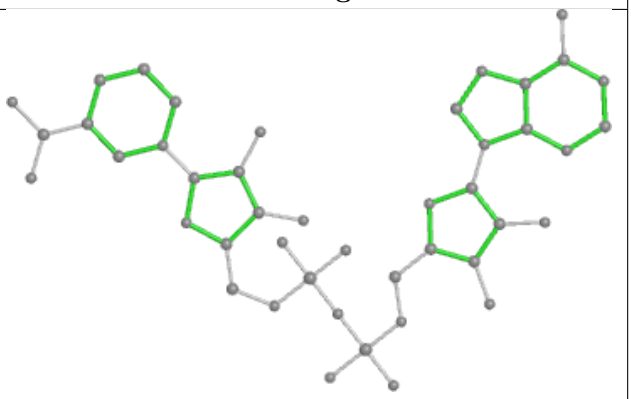
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

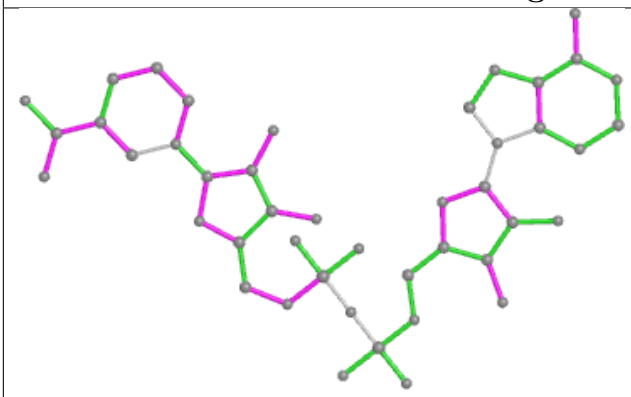
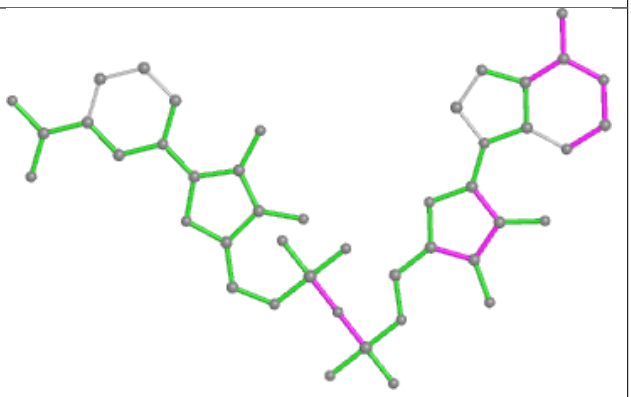
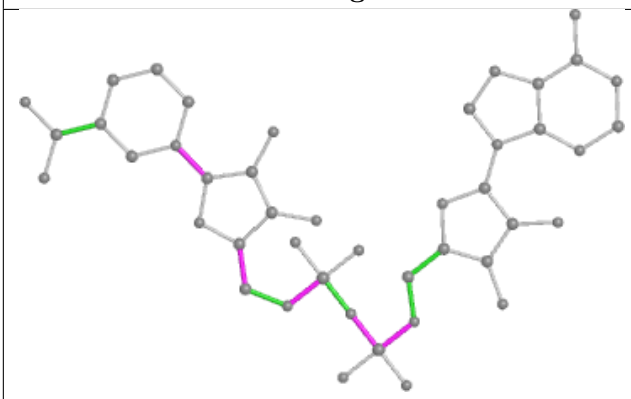
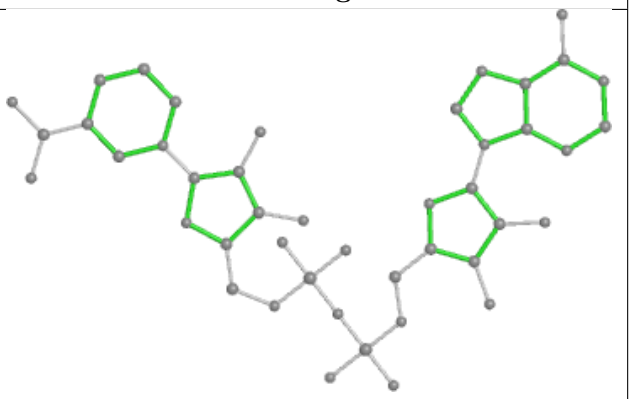
Ligand NAI E 403	
 Bond lengths	 Bond angles
 Torsions	 Rings

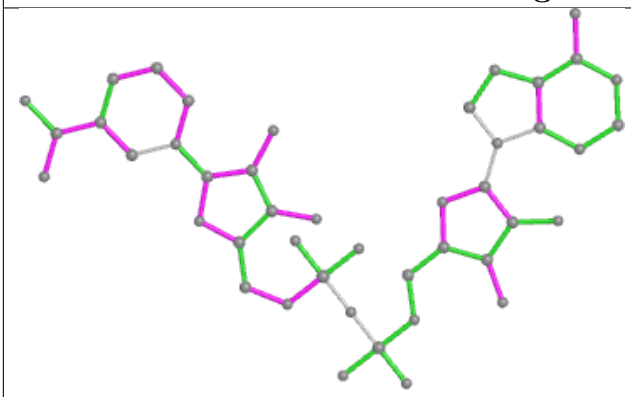
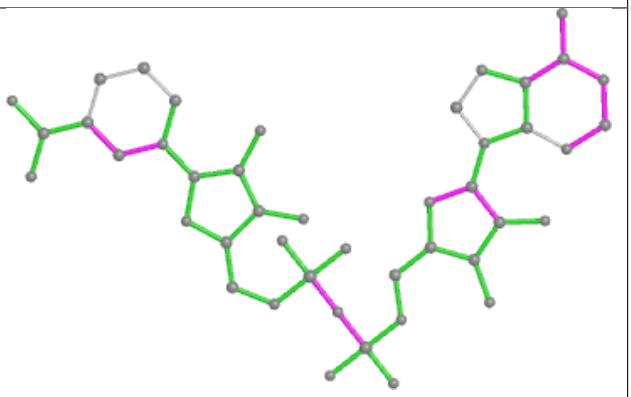
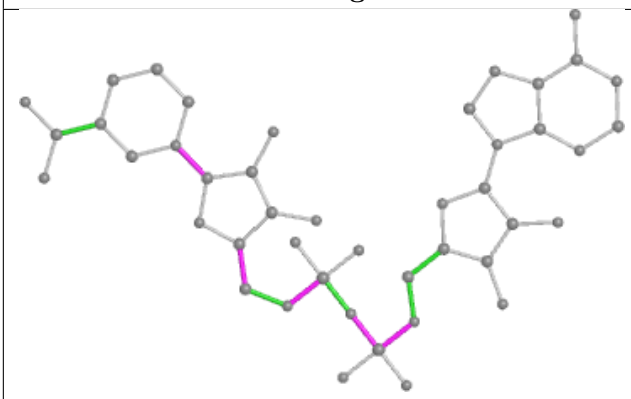
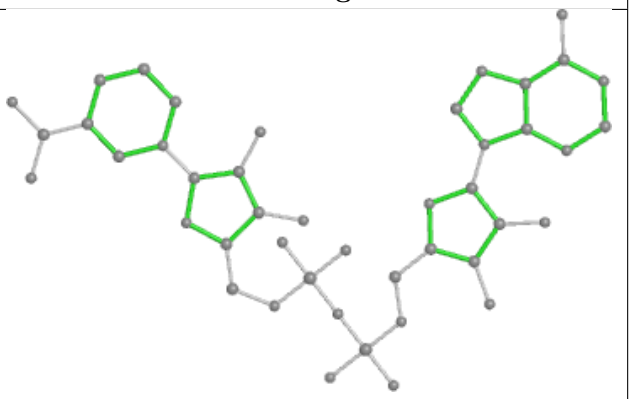
Ligand NAI F 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI B 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

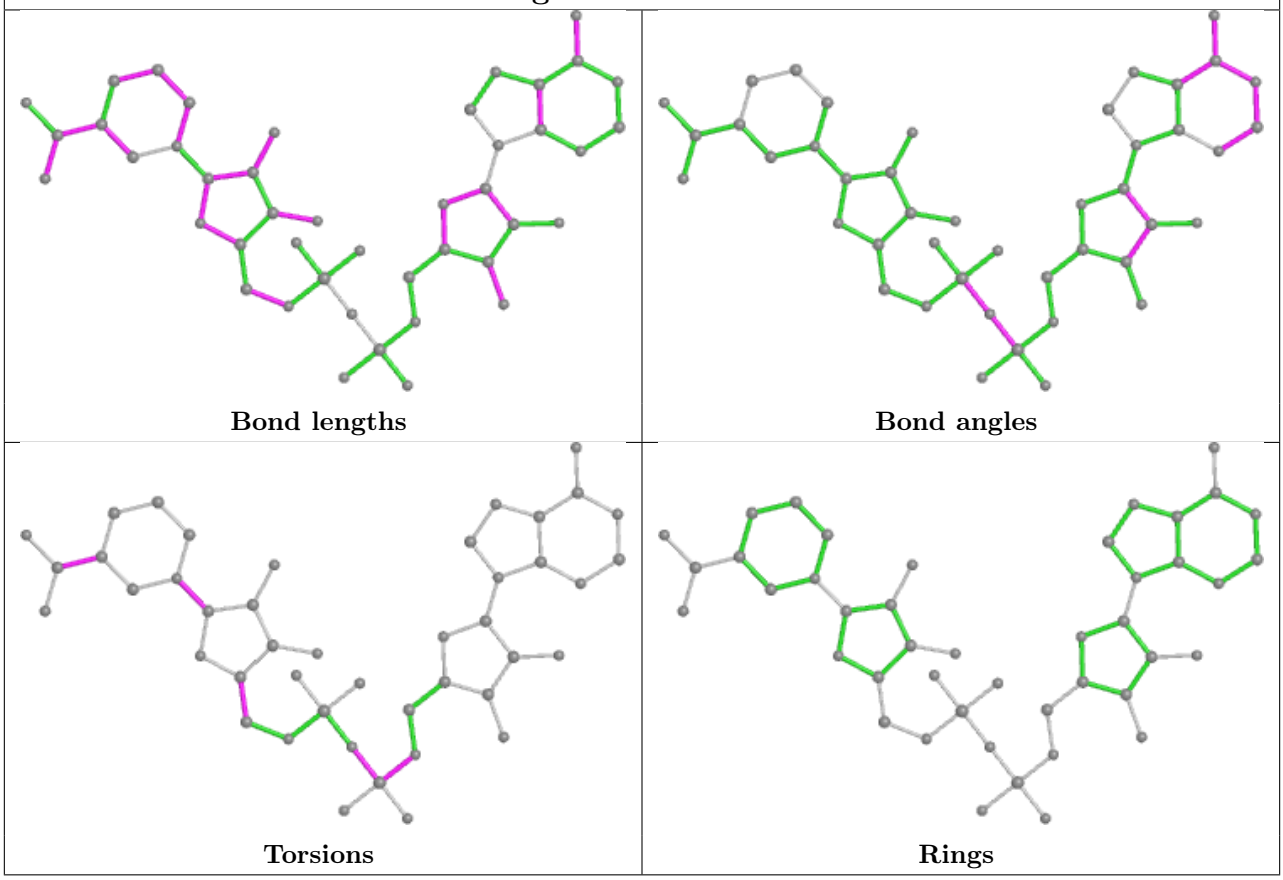
Ligand NAI H 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI G 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

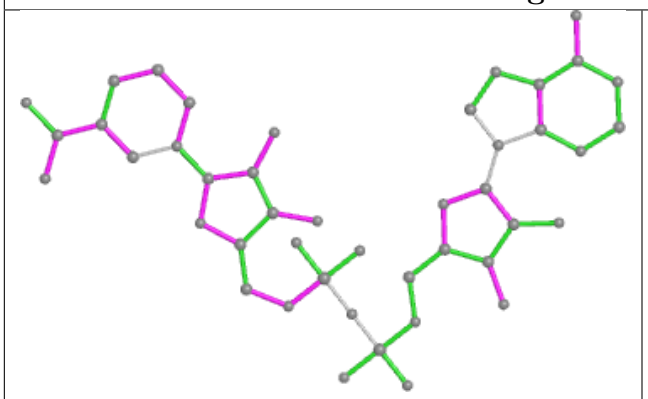
Ligand NAI C 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI I 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

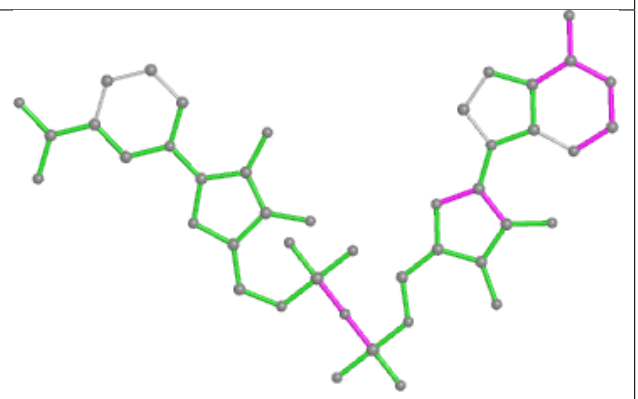
Ligand NAI J 404



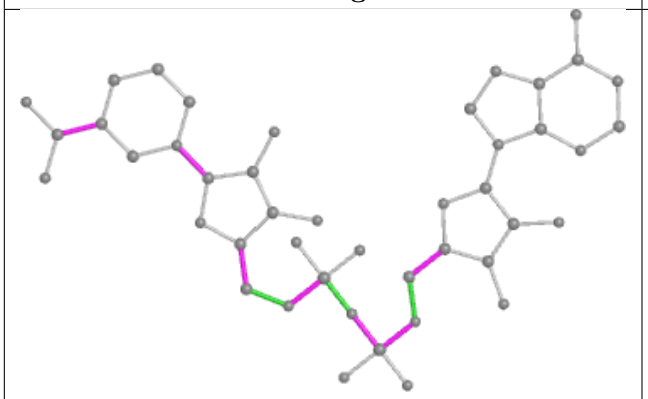
Ligand NAI K 404



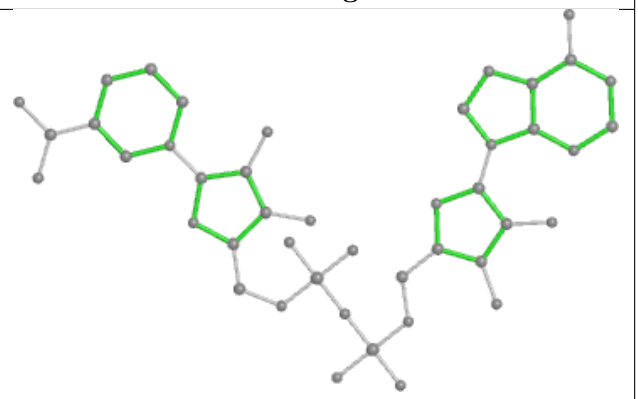
Bond lengths



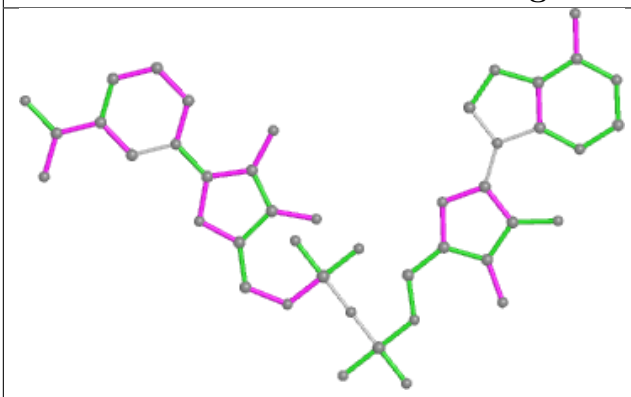
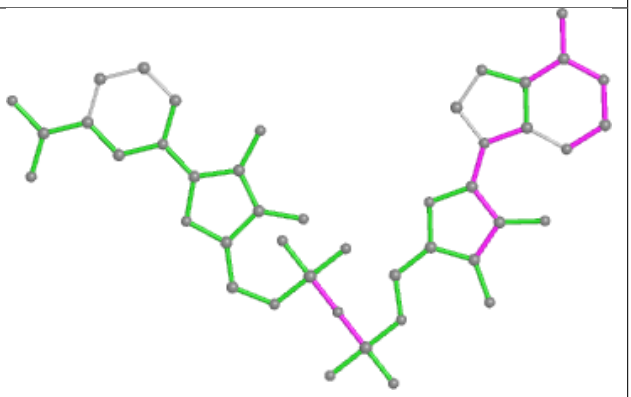
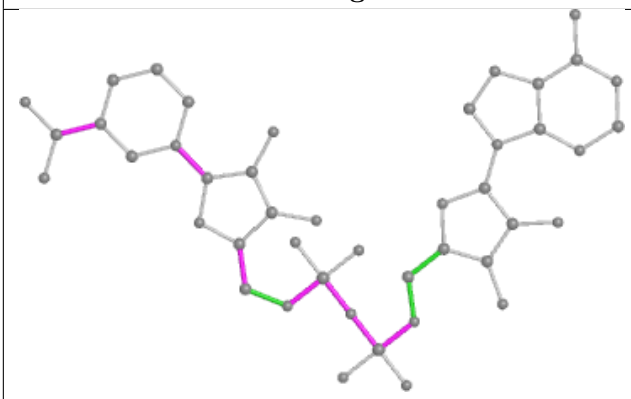
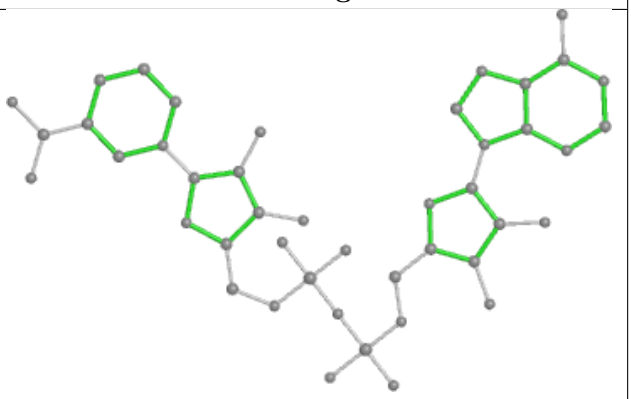
Bond angles

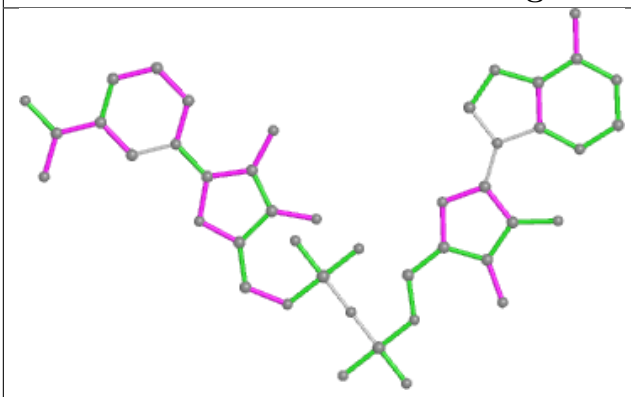
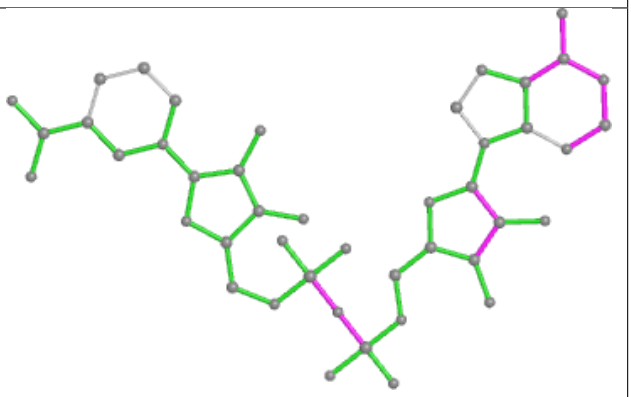
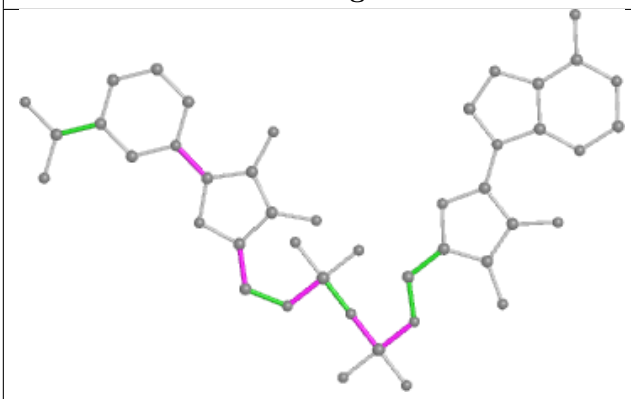
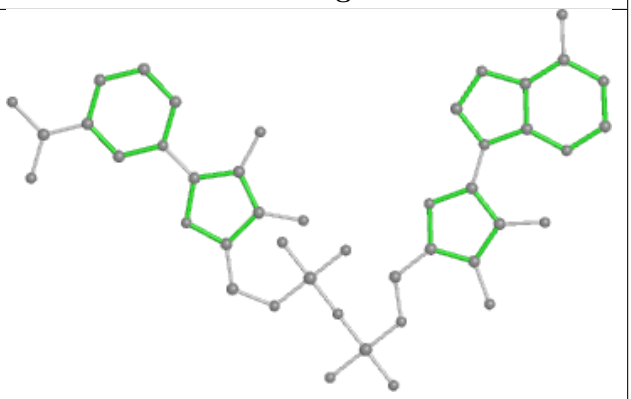


Torsions

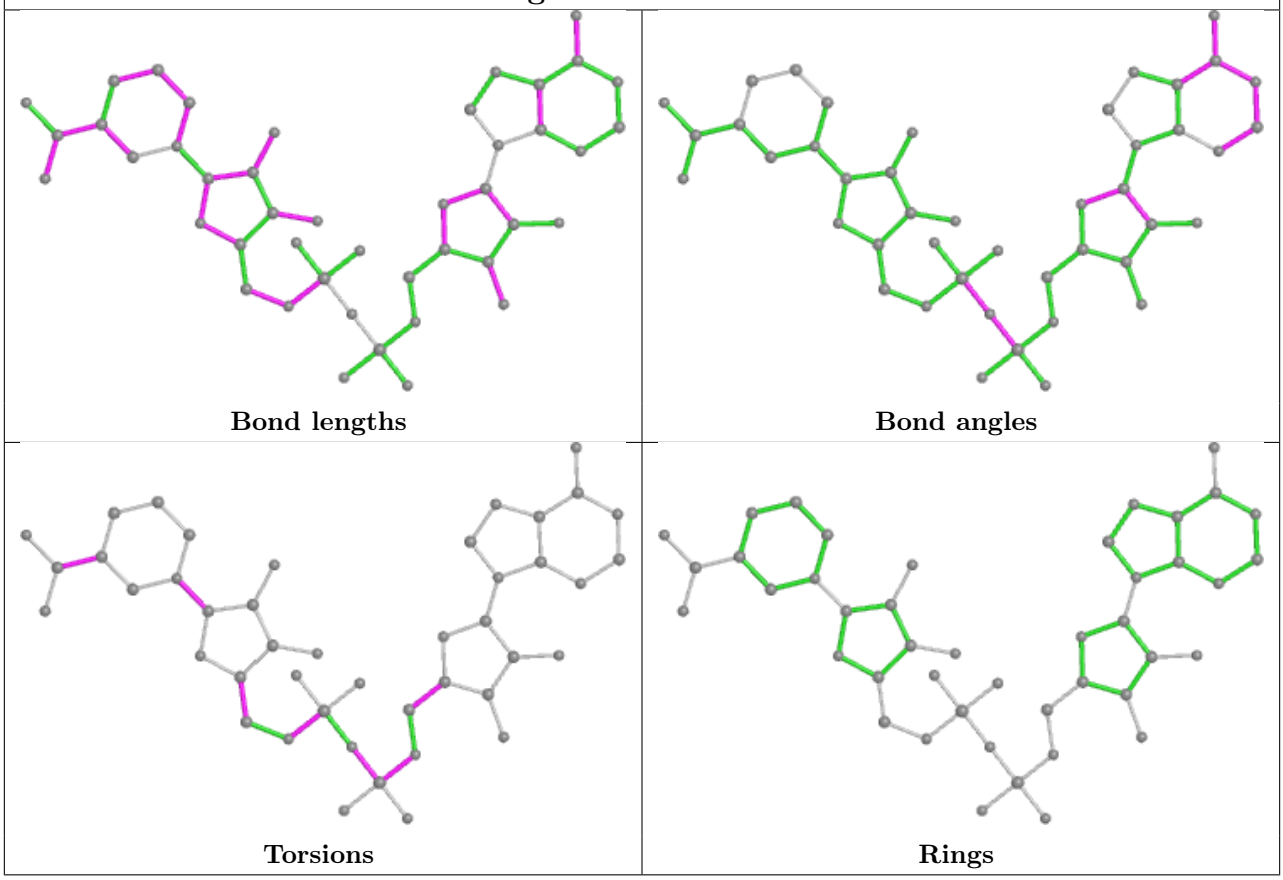


Rings

Ligand NAI L 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI D 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAI A 404



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.

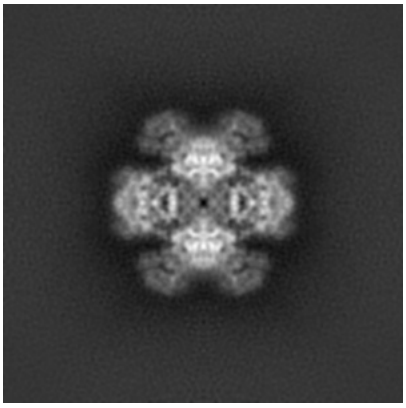
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9801. These allow visual inspection of the internal detail of the map and identification of artifacts.

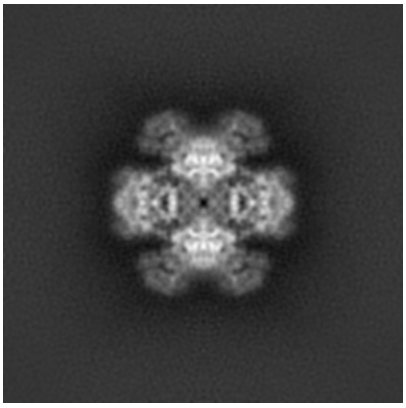
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

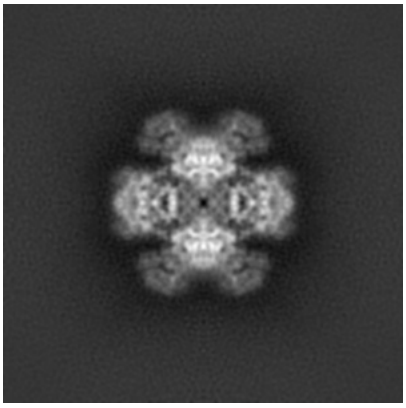
6.1.1 Primary map



X



Y

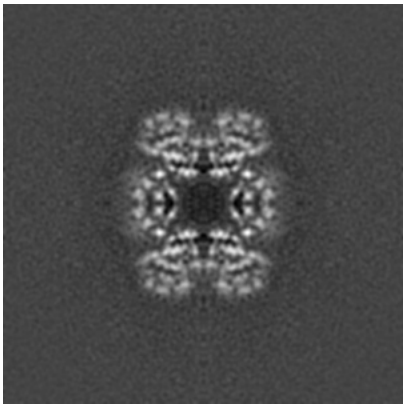


Z

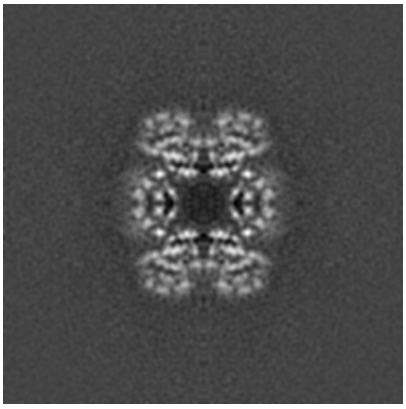
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

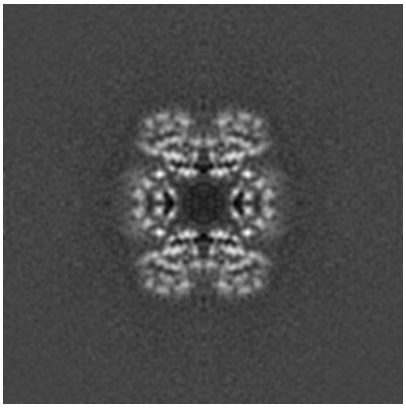
6.2.1 Primary map



X Index: 162



Y Index: 162

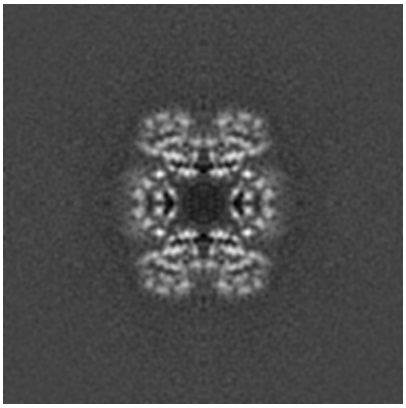


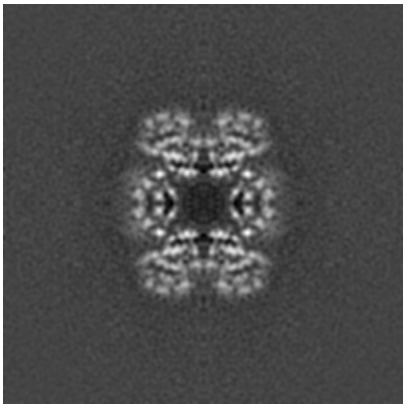
Z Index: 162

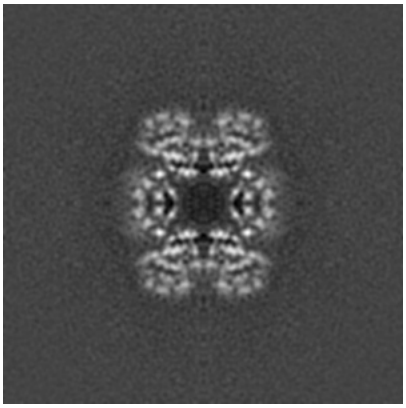
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 162

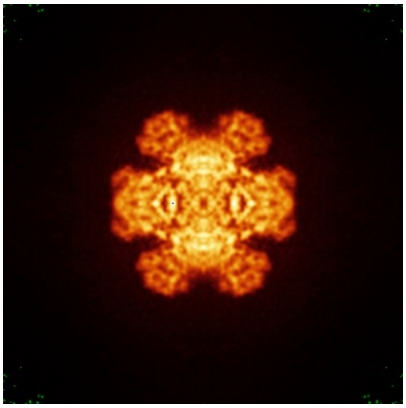

Y Index: 162

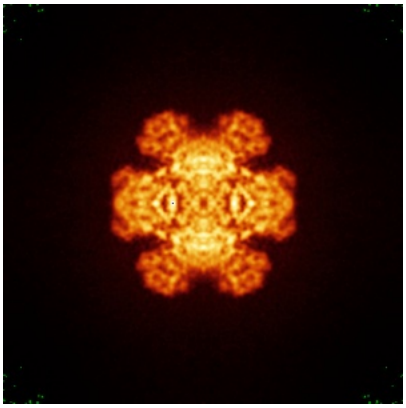

Z Index: 162

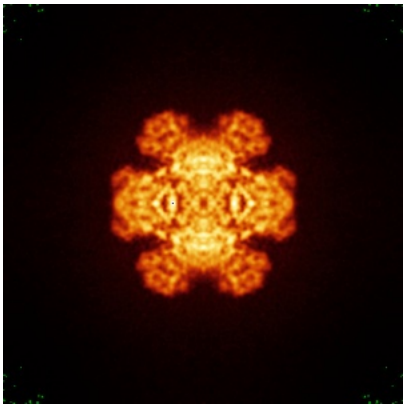
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

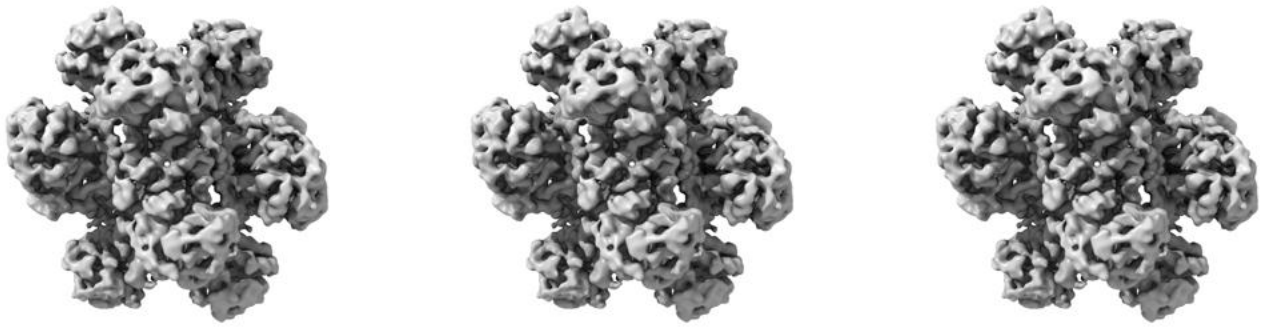

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.88. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

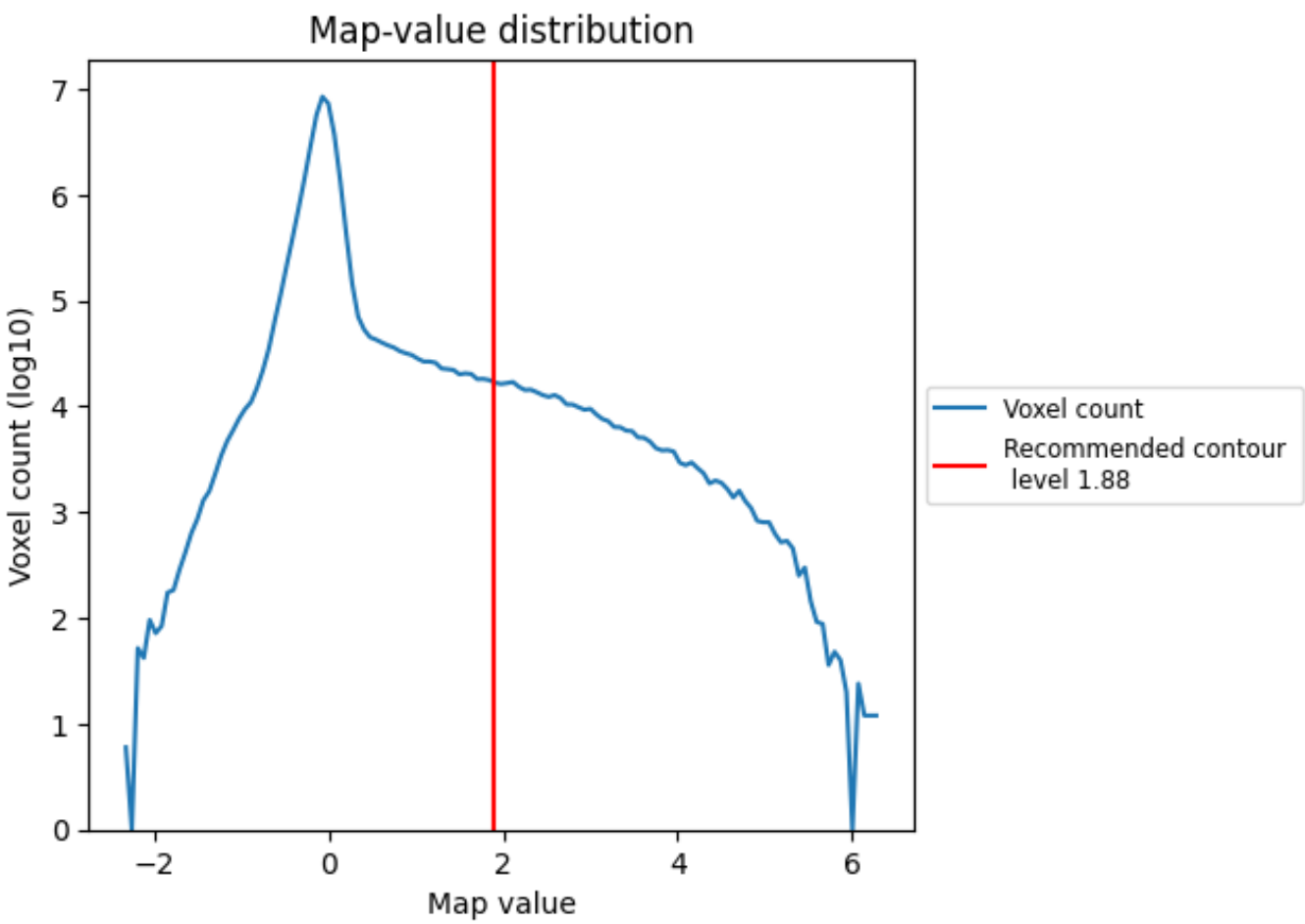
6.6 Mask visualisation (i)

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

7 Map analysis (i)

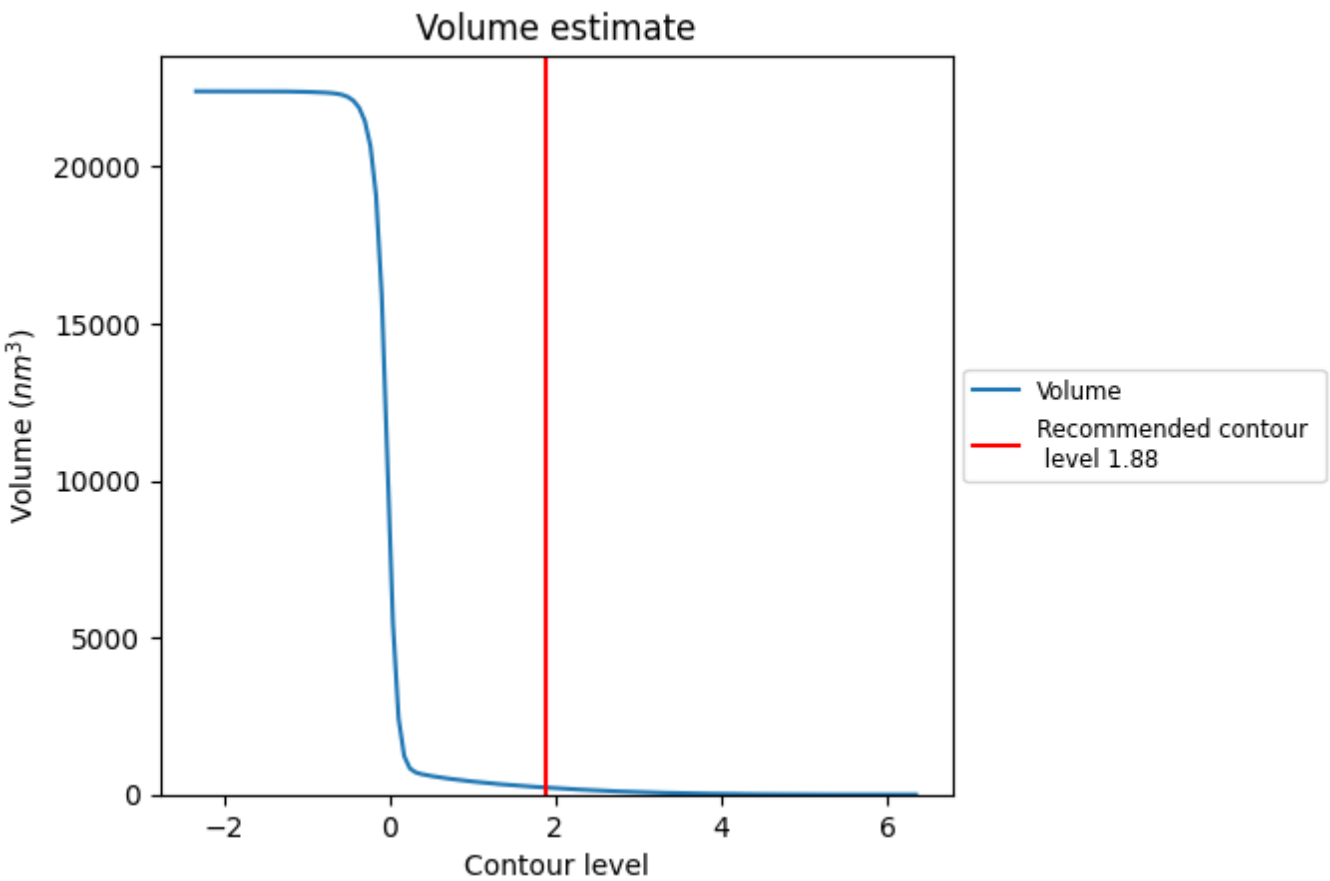
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

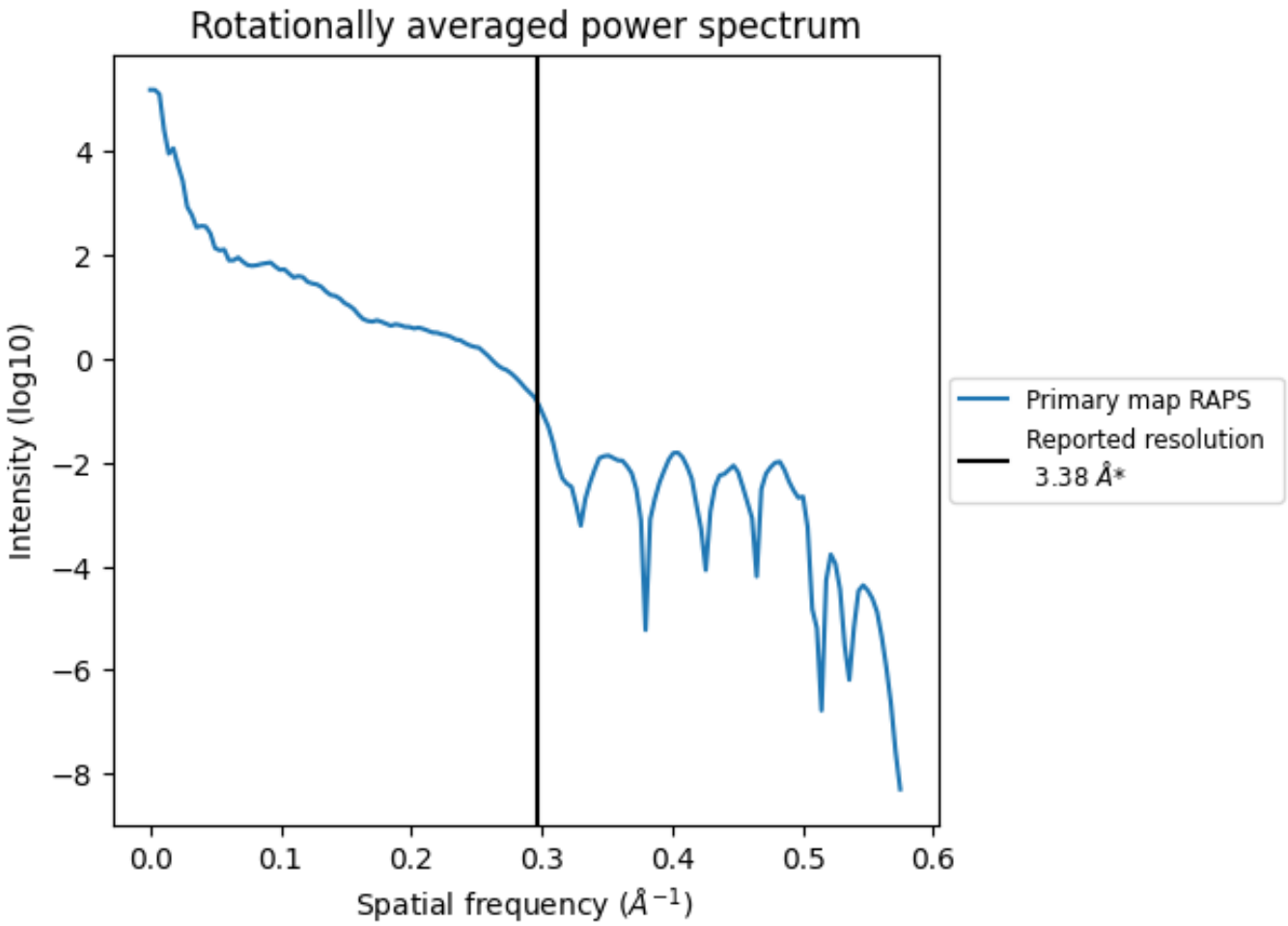
7.2 Volume estimate (i)



The volume at the recommended contour level is 224 nm^3; this corresponds to an approximate mass of 202 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 0.296 Å^{-1}

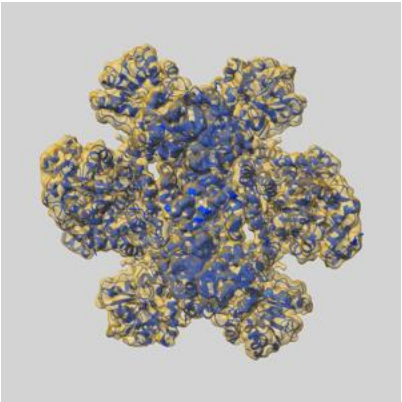
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

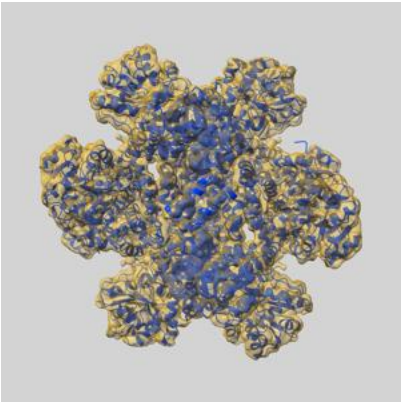
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9801 and PDB model 6JD1. Per-residue inclusion information can be found in section 3 on page 9.

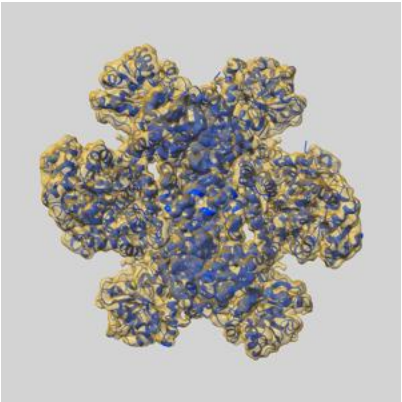
9.1 Map-model overlay (i)



X



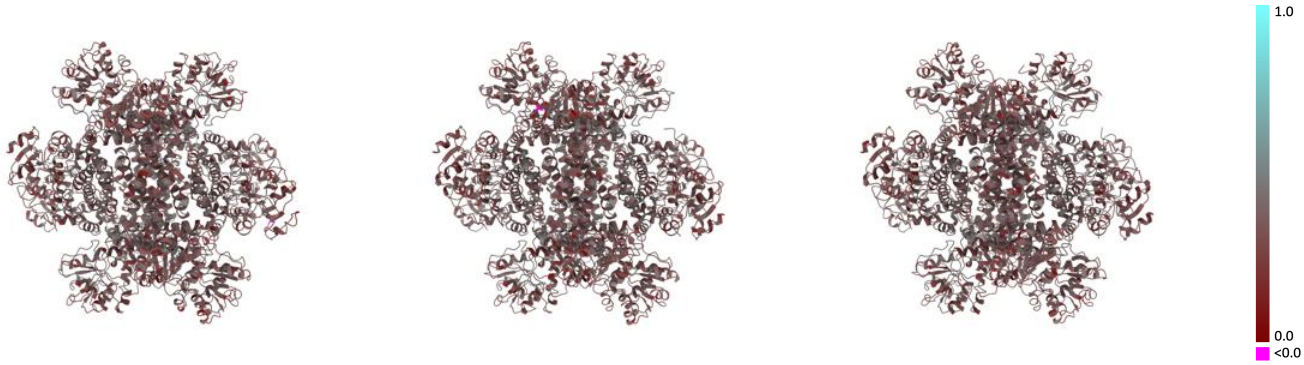
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.88 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.

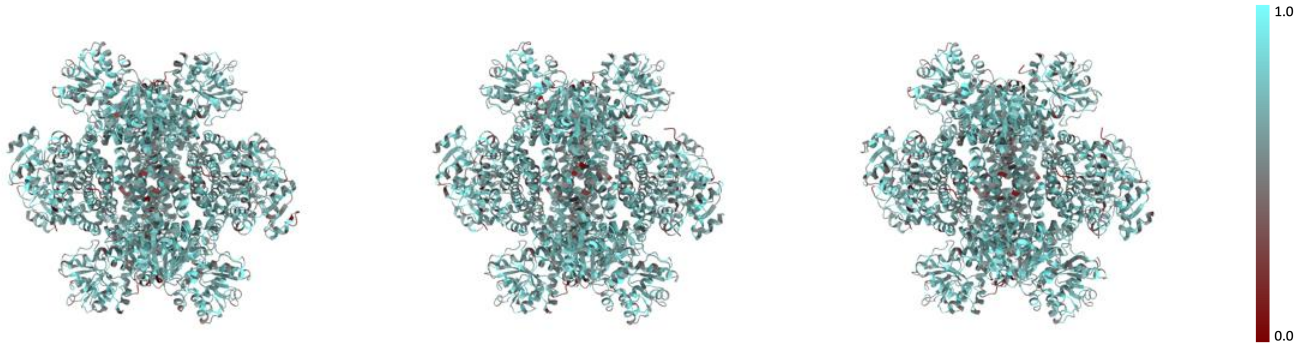
9.2 Q-score mapped to coordinate model (i)



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.

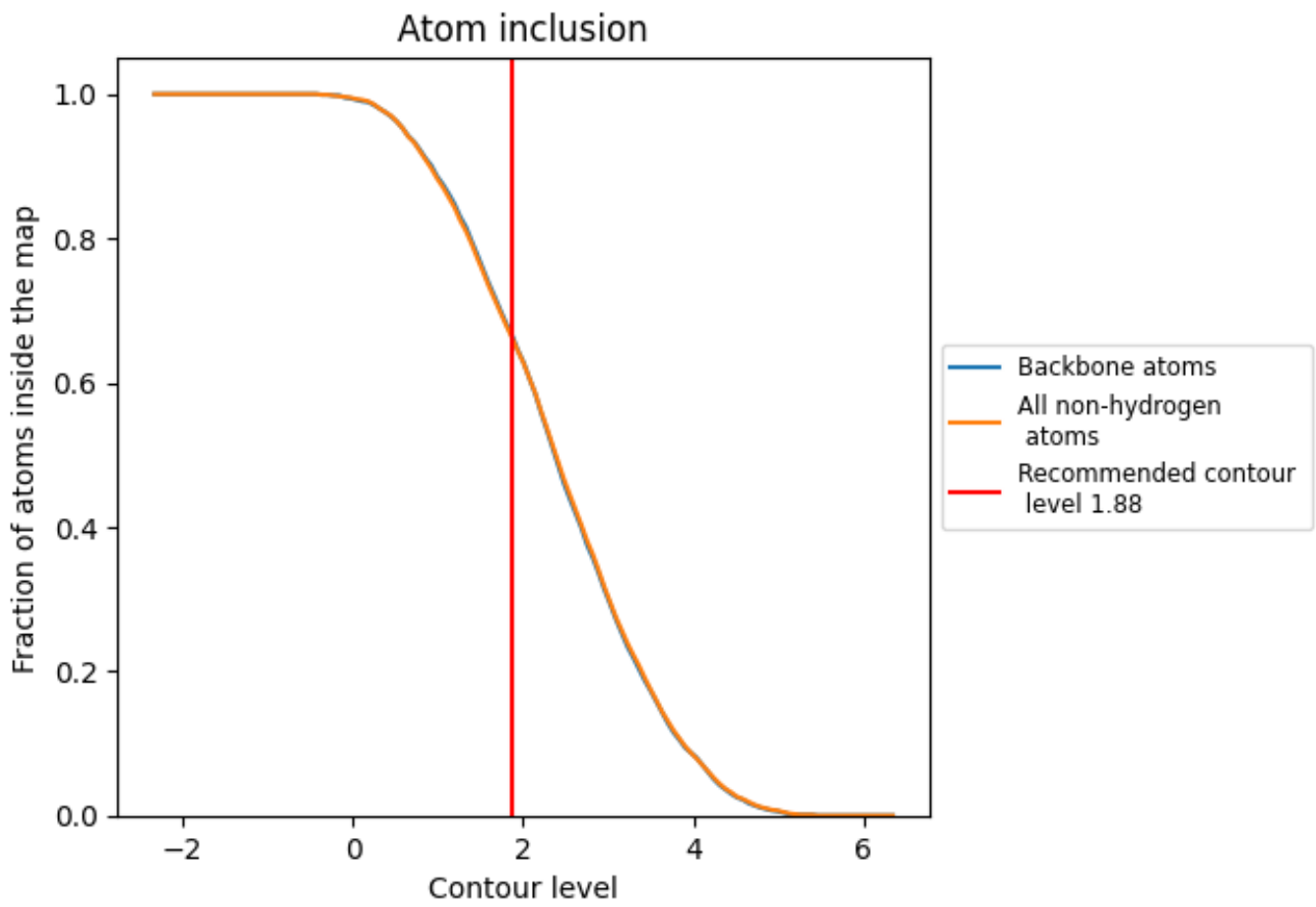
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.88).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (1.88) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6600	0.3510
A	0.6740	0.3540
B	0.6690	0.3510
C	0.6710	0.3560
D	0.6660	0.3500
E	0.6700	0.3510
F	0.6730	0.3520
G	0.6690	0.3510
H	0.6730	0.3540
I	0.6700	0.3510
J	0.6740	0.3500
K	0.6660	0.3480
L	0.6720	0.3510