



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:47 am BST

PDB ID : 2XIQ
Title : Crystal structure of human methylmalonyl-CoA mutase in complex with adenosylcobalamin and malonyl-CoA
Authors : Yue, W.W.; Froese, D.S.; Kochan, G.; Chaikuad, A.; Krojer, T.; Muniz, J.; Ugochukwu, E.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; Bountra, C.; Oppermann, U.
Deposited on : 2010-06-30
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

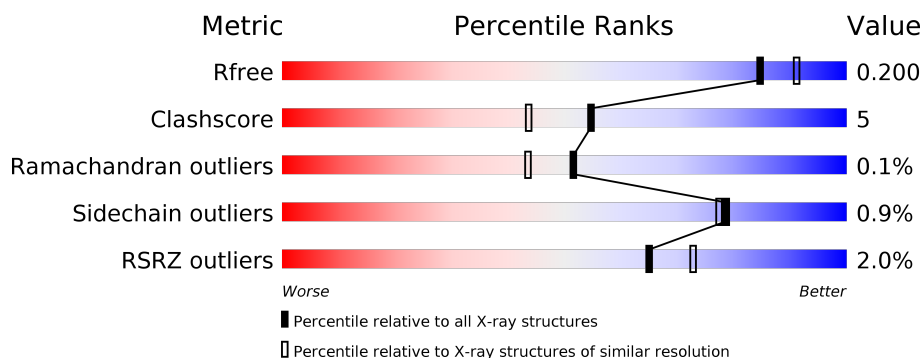
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	762	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	B	762	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>6%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B12	A	3001	X	-	X	-
2	B12	B	3001	X	-	-	-
3	5AD	A	4001[A]	-	-	-	X
3	5AD	A	4001[B]	-	-	X	X
3	5AD	B	4001[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12511 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 METHYLMALONYL-COA MUTASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	714	Total	C	N	O	S	0	3	0
			5531	3497	957	1045	32			
1	B	713	Total	C	N	O	S	0	2	0
			5512	3486	953	1041	32			

There are 48 discrepancies between the modelled and reference sequences:

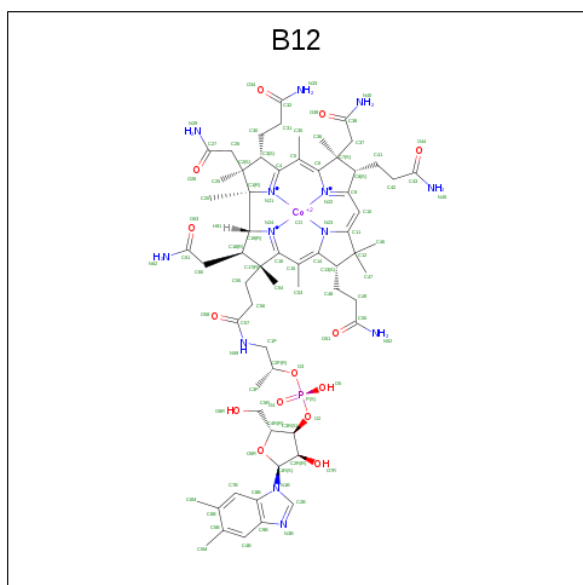
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P22033
A	751	ALA	-	expression tag	UNP P22033
A	752	GLU	-	expression tag	UNP P22033
A	753	ASN	-	expression tag	UNP P22033
A	754	LEU	-	expression tag	UNP P22033
A	755	TYR	-	expression tag	UNP P22033
A	756	PHE	-	expression tag	UNP P22033
A	757	GLN	-	expression tag	UNP P22033
A	758	SER	-	expression tag	UNP P22033
A	759	HIS	-	expression tag	UNP P22033
A	760	HIS	-	expression tag	UNP P22033
A	761	HIS	-	expression tag	UNP P22033
A	762	HIS	-	expression tag	UNP P22033
A	763	HIS	-	expression tag	UNP P22033
A	764	HIS	-	expression tag	UNP P22033
A	765	ASP	-	expression tag	UNP P22033
A	766	TYR	-	expression tag	UNP P22033
A	767	LYS	-	expression tag	UNP P22033
A	768	ASP	-	expression tag	UNP P22033
A	769	ASP	-	expression tag	UNP P22033
A	770	ASP	-	expression tag	UNP P22033
A	771	ASP	-	expression tag	UNP P22033
A	772	LYS	-	expression tag	UNP P22033
A	499	THR	ALA	conflict	UNP P22033
B	11	MET	-	expression tag	UNP P22033

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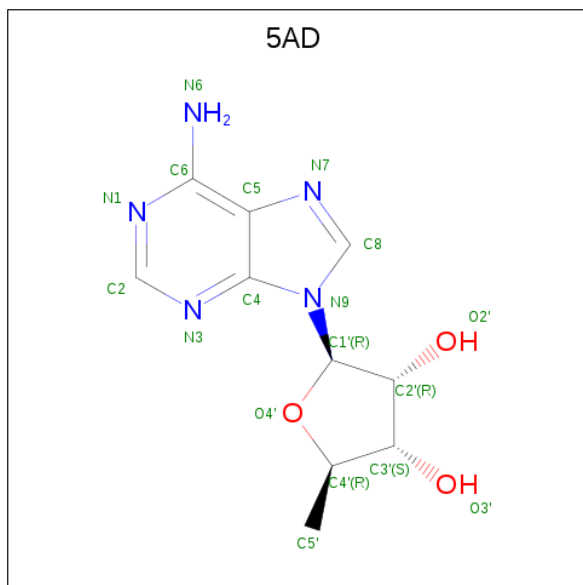
Chain	Residue	Modelled	Actual	Comment	Reference
B	751	ALA	-	expression tag	UNP P22033
B	752	GLU	-	expression tag	UNP P22033
B	753	ASN	-	expression tag	UNP P22033
B	754	LEU	-	expression tag	UNP P22033
B	755	TYR	-	expression tag	UNP P22033
B	756	PHE	-	expression tag	UNP P22033
B	757	GLN	-	expression tag	UNP P22033
B	758	SER	-	expression tag	UNP P22033
B	759	HIS	-	expression tag	UNP P22033
B	760	HIS	-	expression tag	UNP P22033
B	761	HIS	-	expression tag	UNP P22033
B	762	HIS	-	expression tag	UNP P22033
B	763	HIS	-	expression tag	UNP P22033
B	764	HIS	-	expression tag	UNP P22033
B	765	ASP	-	expression tag	UNP P22033
B	766	TYR	-	expression tag	UNP P22033
B	767	LYS	-	expression tag	UNP P22033
B	768	ASP	-	expression tag	UNP P22033
B	769	ASP	-	expression tag	UNP P22033
B	770	ASP	-	expression tag	UNP P22033
B	771	ASP	-	expression tag	UNP P22033
B	772	LYS	-	expression tag	UNP P22033
B	499	THR	ALA	conflict	UNP P22033

- Molecule 2 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



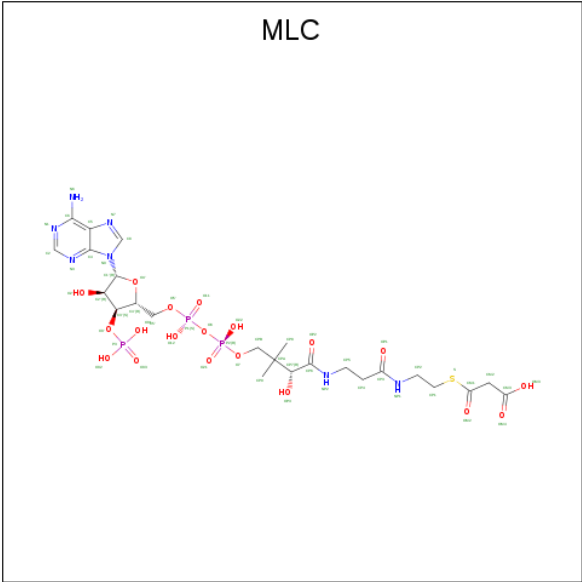
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
2	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 3 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			36	20	10	6		
3	B	1	Total	C	N	O	0	1
			36	20	10	6		

- Molecule 4 is MALONYL-COENZYME A (three-letter code: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

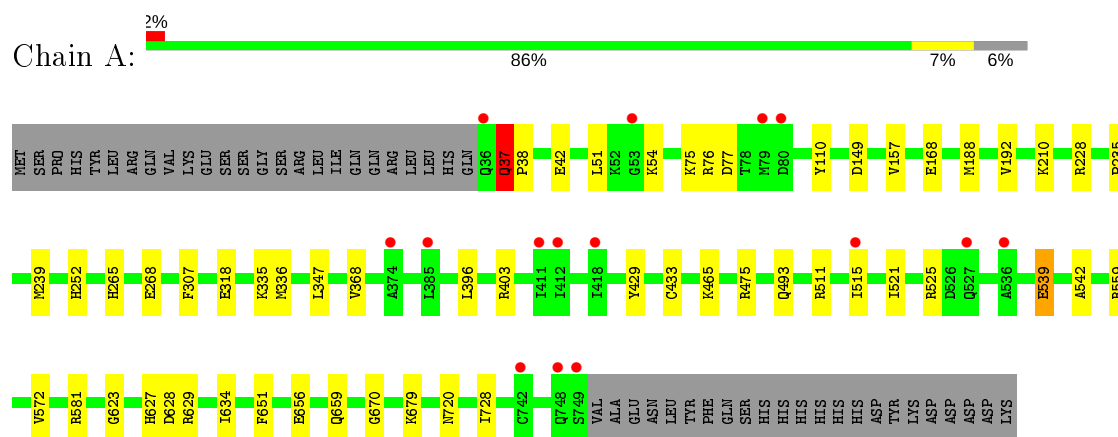
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	494	Total	O	0	0
			494	494		
5	B	612	Total	O	0	0
			612	612		

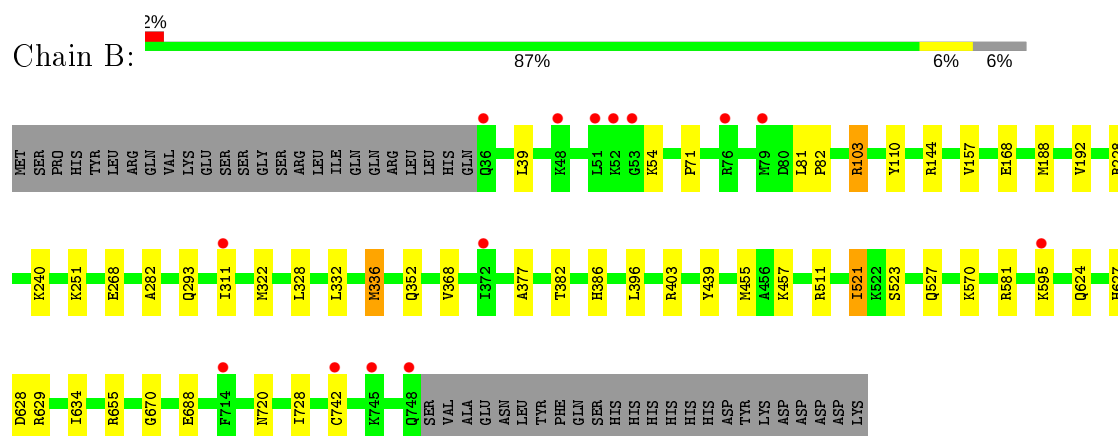
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: METHYLMALONYL-COA MUTASE, MITOCHONDRIAL



• Molecule 1: METHYLMALONYL-COA MUTASE, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.65Å 143.62Å 163.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.82 – 1.95 52.08 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (107.82-1.95) 99.2 (52.08-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0066	Depositor
R, R_{free}	0.161 , 0.201 0.161 , 0.200	Depositor DCC
R_{free} test set	6447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.825	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12511	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MLC, B12, 5AD

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	0.68	2/5646 (0.0%)	0.51	0/7634
1	B	0.71	0/5624	0.54	0/7606
All	All	0.70	2/11270 (0.0%)	0.52	0/15240

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	GLU	CD-OE2	10.63	1.37	1.25
1	A	539	GLU	CD-OE1	-6.50	1.18	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5531	0	5521	46	0
1	B	5512	0	5497	39	0
2	A	91	0	87	21	0
2	B	91	0	87	18	0
3	A	36	0	26	11	0
3	B	36	0	26	12	0
4	A	54	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	54	0	34	4	0
5	A	494	0	0	17	1
5	B	612	0	0	11	1
All	All	12511	0	11311	117	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (117) 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)
2:B:3001:B12:H531	2:B:3001:B12:H552	1.34	1.09
2:A:3001:B12:H552	2:A:3001:B12:H531	1.45	0.97
1:A:465:LYS:NZ	5:A:2296:HOH:O	1.94	0.95
1:A:656:GLU:HG3	5:A:2428:HOH:O	1.71	0.90
2:A:3001:B12:H372	3:A:4001[B]:5AD:H2	1.52	0.89
2:B:3001:B12:H372	3:B:4001[B]:5AD:H2	1.55	0.87
1:B:368:VAL:HG23	5:B:2298:HOH:O	1.76	0.84
2:B:3001:B12:H531	2:B:3001:B12:C55	2.10	0.82
3:B:4001[B]:5AD:H8	5:B:2308:HOH:O	1.80	0.80
1:B:403[B]:ARG:HD3	5:B:2324:HOH:O	1.79	0.80
1:B:634:ILE:HD13	1:B:728:ILE:HD13	1.64	0.80
2:B:3001:B12:H261	3:B:4001[B]:5AD:H3'	1.63	0.79
1:A:368:VAL:HG23	5:A:2226:HOH:O	1.86	0.75
3:A:4001[B]:5AD:H8	5:A:2493:HOH:O	1.86	0.75
2:A:3001:B12:H261	3:A:4001[B]:5AD:H3'	1.68	0.75
1:A:42:GLU:HB2	5:A:2004:HOH:O	1.86	0.74
3:A:4001[B]:5AD:O4'	3:A:4001[B]:5AD:N3	2.20	0.73
2:A:3001:B12:C55	2:A:3001:B12:H531	2.17	0.73
3:B:4001[B]:5AD:N3	3:B:4001[B]:5AD:O4'	2.16	0.73
1:A:37:GLN:H	1:A:38:PRO:HD2	1.53	0.72
1:A:525:ARG:HD2	5:A:2359:HOH:O	1.89	0.72
1:A:525:ARG:HB2	5:A:2359:HOH:O	1.89	0.71
1:A:168:GLU:HG3	1:A:521:ILE:HD11	1.73	0.70
1:A:403[A]:ARG:HD3	5:A:2251:HOH:O	1.90	0.69
2:B:3001:B12:H351	2:B:3001:B12:H362	1.75	0.69
1:B:168:GLU:HG3	1:B:521:ILE:HD11	1.74	0.67
1:A:37:GLN:H	1:A:38:PRO:CD	2.07	0.67
1:A:629:ARG:H	2:A:3001:B12:H522	1.41	0.66
1:A:581:ARG:HD2	5:A:2371:HOH:O	1.94	0.66
1:B:629:ARG:H	2:B:3001:B12:H522	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:HG3	5:A:2323:HOH:O	1.96	0.65
1:B:628:ASP:H	2:B:3001:B12:H522	1.45	0.64
1:B:240:LYS:NZ	5:B:2211:HOH:O	2.31	0.63
1:B:527:GLN:HB2	5:B:2441:HOH:O	1.99	0.62
1:B:570:LYS:NZ	5:B:2485:HOH:O	2.33	0.61
1:B:54:LYS:HB3	5:B:2005:HOH:O	2.00	0.61
2:A:3001:B12:H362	2:A:3001:B12:H351	1.82	0.61
1:B:332:LEU:O	1:B:336:MET:HG2	2.00	0.60
1:B:634:ILE:HD13	1:B:728:ILE:CD1	2.32	0.59
1:B:627:HIS:NE2	2:B:3001:B12:N21	2.49	0.59
2:A:3001:B12:H372	2:A:3001:B12:H351	1.85	0.58
1:B:168:GLU:CG	1:B:521:ILE:HD11	2.34	0.57
1:B:742:CYS:HB2	5:B:2596:HOH:O	2.06	0.56
1:B:396:LEU:HD22	3:B:4001[A]:5AD:N6	2.22	0.55
2:B:3001:B12:N22	3:B:4001[B]:5AD:H5'2	2.21	0.55
1:B:457:LYS:NZ	5:B:2370:HOH:O	2.40	0.55
1:A:627:HIS:NE2	2:A:3001:B12:N21	2.54	0.55
1:A:559:ARG:HB2	5:A:2359:HOH:O	2.07	0.54
1:A:628:ASP:H	2:A:3001:B12:H522	1.54	0.53
2:B:3001:B12:H291	3:B:4001[A]:5AD:C8	2.22	0.53
1:B:332:LEU:O	1:B:336:MET:CG	2.56	0.53
2:A:3001:B12:N29	3:A:4001[B]:5AD:H2'	2.23	0.53
1:A:228:ARG:NH2	2:A:3001:B12:H401	2.07	0.52
1:A:670:GLY:HA3	2:A:3001:B12:HM53	1.92	0.52
1:A:268:GLU:HB3	2:A:3001:B12:H532	1.91	0.51
1:B:268:GLU:HB3	2:B:3001:B12:H532	1.92	0.51
1:A:396:LEU:HD22	3:A:4001[A]:5AD:N6	2.26	0.51
1:A:403[B]:ARG:NH1	5:A:2250:HOH:O	2.44	0.49
3:B:4001[A]:5AD:H5'1	4:B:5001:MLC:HM22	1.95	0.49
1:A:37:GLN:N	1:A:38:PRO:HD2	2.24	0.49
1:A:335:LYS:HG2	1:A:336:MET:CE	2.43	0.49
2:A:3001:B12:N22	3:A:4001[B]:5AD:C5'	2.75	0.48
1:B:157:VAL:HG11	1:B:511:ARG:HA	1.96	0.48
2:A:3001:B12:N22	3:A:4001[B]:5AD:H5'2	2.28	0.48
1:A:307:PHE:CD1	1:A:347:LEU:HG	2.48	0.48
2:B:3001:B12:C35	2:B:3001:B12:H362	2.43	0.48
5:A:2423:HOH:O	1:B:581:ARG:HD2	2.14	0.48
1:B:251:LYS:HD3	1:B:251:LYS:HA	1.74	0.47
1:B:655:ARG:HD3	1:B:688:GLU:OE1	2.15	0.47
2:A:3001:B12:H362	2:A:3001:B12:C35	2.46	0.46
1:B:110:TYR:CE2	4:B:5001:MLC:HM21	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:HD3	4:B:5001:MLC:C8	2.45	0.46
1:A:188:MET:HG3	1:A:192:VAL:HA	1.98	0.46
1:A:623:GLY:O	1:A:651:PHE:HA	2.15	0.46
1:A:51:LEU:HB3	1:A:54:LYS:HB2	1.98	0.46
1:B:188:MET:HG3	1:B:192:VAL:HA	1.97	0.46
2:A:3001:B12:N22	3:A:4001[A]:5AD:H5'2	2.32	0.45
1:A:634:ILE:HD13	1:A:728:ILE:HG12	1.99	0.45
2:B:3001:B12:N22	3:B:4001[A]:5AD:H5'2	2.32	0.45
2:B:3001:B12:N22	3:B:4001[B]:5AD:C5'	2.79	0.45
1:B:144:ARG:HD3	1:B:624:GLN:OE1	2.17	0.45
1:B:670:GLY:HA3	2:B:3001:B12:HM53	1.98	0.45
1:A:542:ALA:HA	1:A:572:VAL:HG11	1.99	0.45
1:B:228:ARG:NH2	2:B:3001:B12:H401	2.15	0.45
1:A:149:ASP:HB3	1:A:515:ILE:HG12	1.98	0.44
2:A:3001:B12:C5	3:A:4001[A]:5AD:H8	2.47	0.44
1:B:311:ILE:HG13	1:B:377:ALA:HB2	2.00	0.44
1:A:110:TYR:CE2	4:A:5001:MLC:HM21	2.53	0.44
3:A:4001[A]:5AD:H5'1	4:A:5001:MLC:HM22	2.00	0.44
1:B:352:GLN:HG3	1:B:386:HIS:CD2	2.53	0.44
1:A:210:LYS:HD2	1:A:252:HIS:HB3	2.00	0.43
1:A:210:LYS:HG2	5:A:2126:HOH:O	2.18	0.43
1:B:328:LEU:HG	1:B:439:TYR:CD2	2.54	0.43
1:A:539:GLU:OE1	1:A:539:GLU:HA	2.19	0.43
1:A:157:VAL:HG11	1:A:511:ARG:HA	2.01	0.43
1:B:627:HIS:CD2	2:B:3001:B12:N23	2.86	0.43
1:A:77:ASP:HB3	1:A:433:CYS:SG	2.59	0.43
1:A:659:GLN:NE2	5:B:2370:HOH:O	2.52	0.43
2:B:3001:B12:C53	2:B:3001:B12:C55	2.90	0.43
1:B:322:MET:HE1	1:B:382:THR:HB	2.00	0.43
1:A:656:GLU:CG	5:A:2428:HOH:O	2.47	0.42
1:A:525:ARG:CB	5:A:2359:HOH:O	2.61	0.42
1:A:235:PRO:O	1:A:239:MET:HG2	2.20	0.42
1:A:37:GLN:HE21	1:A:37:GLN:HB2	1.75	0.41
1:B:352:GLN:HE22	3:B:4001[B]:5AD:H4'	1.85	0.41
1:B:39:LEU:HD21	1:B:71:PRO:HD2	2.02	0.41
1:A:228:ARG:HD2	1:A:265:HIS:CD2	2.55	0.41
1:B:282:ALA:HB1	1:B:455:MET:HG2	2.02	0.41
1:A:75:LYS:HA	1:A:429:TYR:CE1	2.56	0.41
1:A:318:GLU:OE1	1:A:318:GLU:HA	2.21	0.41
1:B:81:LEU:HA	1:B:82:PRO:HD3	1.97	0.40
2:A:3001:B12:C53	2:A:3001:B12:C55	2.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3001:B12:H253	2:A:3001:B12:H301	1.76	0.40
1:A:627:HIS:CE1	2:A:3001:B12:H421	2.57	0.40
1:A:679:LYS:HB2	5:A:2446:HOH:O	2.22	0.40
3:B:4001[A]:5AD:H5'1	4:B:5001:MLC:CM2	2.51	0.40
1:B:595:LYS:HG2	5:B:2220:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2219:HOH:O	5:B:2334:HOH:O[2_565]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	715/762 (94%)	702 (98%)	12 (2%)	1 (0%)	51	43
1	B	713/762 (94%)	699 (98%)	14 (2%)	0	100	100
All	All	1428/1524 (94%)	1401 (98%)	26 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	583/636 (92%)	579 (99%)	4 (1%)	84	82
1	B	580/636 (91%)	574 (99%)	6 (1%)	76	74
All	All	1163/1272 (91%)	1153 (99%)	10 (1%)	78	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	76	ARG
1	A	475	ARG
1	A	720	ASN
1	B	103	ARG
1	B	293	GLN
1	B	336	MET
1	B	521	ILE
1	B	523	SER
1	B	720	ASN

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

Mol	Chain	Res	Type
1	A	37	GLN
1	A	314	ASN
1	A	605	HIS
1	B	293	GLN
1	B	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	5AD	A	4001[B]	-	17,20,20	2.55	7 (41%)	15,30,30	4.01	4 (26%)
2	B12	B	3001	1	80,101,101	1.07	5 (6%)	101,166,166	1.77	16 (15%)
3	5AD	B	4001[B]	-	17,20,20	2.61	6 (35%)	15,30,30	4.00	4 (26%)
4	MLC	B	5001	-	44,56,56	1.94	7 (15%)	56,83,83	1.90	7 (12%)
3	5AD	A	4001[A]	-	17,20,20	2.74	6 (35%)	15,30,30	4.52	4 (26%)
4	MLC	A	5001	-	44,56,56	2.14	9 (20%)	56,83,83	2.00	5 (8%)
2	B12	A	3001	1	80,101,101	1.09	4 (5%)	101,166,166	1.77	16 (15%)
3	5AD	B	4001[A]	-	17,20,20	2.72	7 (41%)	15,30,30	4.46	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5AD	A	4001[B]	-	-	0/0/20/20	0/3/3/3
2	B12	B	3001	1	1/1/36/38	14/51/223/223	0/3/11/11
3	5AD	B	4001[B]	-	-	0/0/20/20	0/3/3/3
4	MLC	B	5001	-	-	2/48/71/71	0/3/3/3
3	5AD	A	4001[A]	-	-	0/0/20/20	0/3/3/3
4	MLC	A	5001	-	-	6/48/71/71	0/3/3/3
2	B12	A	3001	1	1/1/36/38	11/51/223/223	0/3/11/11
3	5AD	B	4001[A]	-	-	0/0/20/20	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	MLC	OM2-CM1	9.44	1.36	1.21
4	B	5001	MLC	OM2-CM1	9.29	1.36	1.21
3	A	4001[A]	5AD	C3'-C4'	-8.15	1.41	1.52
3	B	4001[A]	5AD	C3'-C4'	-7.90	1.41	1.52
3	B	4001[B]	5AD	C3'-C4'	-7.68	1.41	1.52
3	A	4001[B]	5AD	C3'-C4'	-7.23	1.42	1.52
3	A	4001[A]	5AD	C3'-C2'	-5.03	1.39	1.53
3	B	4001[A]	5AD	C3'-C2'	-4.98	1.39	1.53
3	B	4001[B]	5AD	C3'-C2'	-4.85	1.40	1.53
3	A	4001[B]	5AD	C3'-C2'	-4.82	1.40	1.53
4	A	5001	MLC	CP3-NP1	4.57	1.43	1.33
4	A	5001	MLC	CP6-NP2	4.52	1.43	1.33
2	A	3001	B12	C6B-C5B	4.04	1.51	1.40
2	A	3001	B12	C11-C10	-4.01	1.34	1.40
2	A	3001	B12	C8B-C9B	3.94	1.48	1.40
2	B	3001	B12	C11-C10	-3.57	1.34	1.40
2	B	3001	B12	C2-C3	-3.52	1.52	1.58
4	B	5001	MLC	CP6-NP2	3.50	1.41	1.33
4	A	5001	MLC	C2'-C3'	-3.07	1.46	1.52
4	B	5001	MLC	CP3-NP1	3.05	1.40	1.33
3	A	4001[A]	5AD	C5'-C4'	-2.99	1.44	1.51
2	B	3001	B12	C6B-C5B	2.98	1.48	1.40
4	A	5001	MLC	OP3-CP7	-2.98	1.36	1.42
3	B	4001[A]	5AD	C5'-C4'	-2.95	1.44	1.51
2	B	3001	B12	C8B-C9B	2.92	1.46	1.40
3	B	4001[B]	5AD	C5'-C4'	-2.92	1.44	1.51
3	A	4001[B]	5AD	C5'-C4'	-2.73	1.45	1.51
3	B	4001[A]	5AD	C2'-C1'	-2.73	1.49	1.53
2	A	3001	B12	C2-C3	-2.67	1.54	1.58
4	B	5001	MLC	C2'-C1'	-2.66	1.49	1.53
4	A	5001	MLC	C6-N6	2.66	1.43	1.34
3	B	4001[A]	5AD	C6-N6	2.61	1.43	1.34
3	A	4001[A]	5AD	C6-N6	2.56	1.43	1.34
3	A	4001[B]	5AD	C2'-C1'	-2.54	1.49	1.53
2	B	3001	B12	O6R-C1R	2.47	1.44	1.41
3	A	4001[A]	5AD	C2'-C1'	-2.46	1.50	1.53
4	B	5001	MLC	C6-N6	2.32	1.42	1.34
3	A	4001[B]	5AD	C6-N6	2.31	1.42	1.34
3	B	4001[B]	5AD	C6-N6	2.30	1.42	1.34
3	B	4001[A]	5AD	O4'-C4'	2.29	1.51	1.44
4	A	5001	MLC	CP8-CPA	-2.26	1.48	1.53
4	B	5001	MLC	C5'-C4'	-2.15	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4001[A]	5AD	O4'-C4'	2.14	1.50	1.44
4	A	5001	MLC	O2'-C2'	-2.13	1.38	1.43
3	B	4001[B]	5AD	C4-N3	2.13	1.38	1.35
4	A	5001	MLC	C5'-C4'	-2.13	1.45	1.51
3	B	4001[B]	5AD	C2'-C1'	-2.12	1.50	1.53
4	B	5001	MLC	CP8-CPA	-2.12	1.49	1.53
3	A	4001[B]	5AD	C2-N3	2.07	1.35	1.32
3	A	4001[B]	5AD	O4'-C4'	2.04	1.50	1.44
3	B	4001[A]	5AD	C4-N3	2.04	1.38	1.35

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4001[A]	5AD	C1'-N9-C4	-14.71	100.80	126.64
3	B	4001[A]	5AD	C1'-N9-C4	-14.46	101.23	126.64
3	B	4001[B]	5AD	C1'-N9-C4	-13.43	103.05	126.64
3	A	4001[B]	5AD	C1'-N9-C4	-13.27	103.33	126.64
2	B	3001	B12	C1-C19-N24	11.04	118.67	106.24
4	A	5001	MLC	OM2-CM1-S	-10.95	108.40	122.61
2	A	3001	B12	C1-C19-N24	10.72	118.30	106.24
4	B	5001	MLC	OM2-CM1-S	-10.13	109.46	122.61
3	A	4001[A]	5AD	C5'-C4'-C3'	-6.90	108.45	115.70
3	B	4001[A]	5AD	C5'-C4'-C3'	-6.73	108.63	115.70
4	A	5001	MLC	OM2-CM1-CM2	-5.53	113.77	123.35
3	A	4001[B]	5AD	C5'-C4'-C3'	-5.53	109.90	115.70
2	A	3001	B12	C19-C1-N21	5.12	107.41	102.16
4	B	5001	MLC	OM2-CM1-CM2	-4.98	114.72	123.35
3	B	4001[A]	5AD	N3-C2-N1	-4.74	121.28	128.68
3	A	4001[A]	5AD	N3-C2-N1	-4.73	121.29	128.68
3	B	4001[B]	5AD	C5'-C4'-C3'	-4.65	110.82	115.70
4	A	5001	MLC	N3-C2-N1	-4.60	121.49	128.68
2	B	3001	B12	C8-C9-N22	4.50	116.74	111.12
2	B	3001	B12	C26-C2-C1	4.43	116.91	110.02
3	B	4001[B]	5AD	N3-C2-N1	-4.29	121.97	128.68
2	B	3001	B12	C19-C1-N21	4.22	106.48	102.16
3	A	4001[B]	5AD	N3-C2-N1	-4.17	122.16	128.68
2	A	3001	B12	C8-C9-N22	4.15	116.31	111.12
4	B	5001	MLC	N3-C2-N1	-3.96	122.49	128.68
3	A	4001[A]	5AD	C3'-C2'-C1'	3.90	106.85	100.98
2	A	3001	B12	C20-C1-C19	-3.75	105.74	109.36
2	A	3001	B12	O6R-C1R-C2R	-3.74	101.46	106.93
2	A	3001	B12	C26-C2-C1	3.68	115.75	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4001[B]	5AD	C3'-C2'-C1'	3.47	106.20	100.98
3	A	4001[B]	5AD	C3'-C2'-C1'	3.36	106.04	100.98
3	B	4001[A]	5AD	C3'-C2'-C1'	3.34	106.01	100.98
2	B	3001	B12	C3-C4-C5	-3.10	120.43	131.68
2	B	3001	B12	C30-C3-C2	-3.03	112.70	119.13
2	A	3001	B12	C12-C11-C10	-3.00	119.56	124.64
2	B	3001	B12	C9-C10-C11	-2.98	120.50	130.91
2	A	3001	B12	C9-C10-C11	-2.97	120.56	130.91
2	A	3001	B12	C55-C17-C16	2.94	119.72	109.92
2	A	3001	B12	C3-C4-C5	-2.93	121.04	131.68
4	B	5001	MLC	C4-C5-N7	-2.82	106.46	109.40
2	B	3001	B12	O6R-C1R-C2R	-2.82	102.81	106.93
4	B	5001	MLC	CM2-CM1-S	-2.78	110.23	113.69
2	B	3001	B12	C12-C11-C10	-2.73	120.01	124.64
2	A	3001	B12	C2P-C1P-N59	-2.73	108.91	112.93
2	B	3001	B12	C55-C17-C16	2.65	118.73	109.92
2	A	3001	B12	C30-C3-C2	-2.63	113.55	119.13
4	A	5001	MLC	C4-C5-N7	-2.49	106.80	109.40
2	A	3001	B12	C25-C2-C3	-2.47	111.82	115.58
2	B	3001	B12	C25-C2-C3	-2.41	111.91	115.58
4	A	5001	MLC	O7-CPB-CPA	2.39	114.39	110.55
2	B	3001	B12	C16-C15-C14	-2.36	120.59	124.27
4	B	5001	MLC	P2-O6-P1	-2.36	124.74	132.83
2	B	3001	B12	C6-C5-C4	-2.31	120.66	124.27
2	B	3001	B12	C13-C14-C15	-2.25	123.52	131.68
2	A	3001	B12	C13-C14-C15	-2.15	123.87	131.68
2	A	3001	B12	C3R-C2R-C1R	2.14	104.64	99.89
2	B	3001	B12	C3R-C2R-C1R	2.11	104.56	99.89
2	A	3001	B12	C6-C5-C4	-2.09	121.01	124.27
4	B	5001	MLC	CP5-NP2-CP6	-2.06	118.92	122.59
2	B	3001	B12	C2P-C1P-N59	-2.02	109.95	112.93

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3001	B12	C19
2	A	3001	B12	C19

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3001	B12	C2P-O3-P-O5

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Mol	Chain	Res	Type	Atoms
4	B	5001	MLC	OM2-CM1-S-CP1
4	A	5001	MLC	C3'-O3'-P3-O33
4	A	5001	MLC	OM2-CM1-S-CP1
2	A	3001	B12	C2P-O3-P-O5
2	A	3001	B12	C7-C37-C38-O39
2	B	3001	B12	C48-C49-C50-O51
2	A	3001	B12	C48-C49-C50-O51
2	B	3001	B12	C48-C49-C50-N52
2	A	3001	B12	C48-C49-C50-N52
4	A	5001	MLC	P1-O6-P2-O7
2	B	3001	B12	C7-C37-C38-O39
2	A	3001	B12	C7-C37-C38-N40
4	A	5001	MLC	C3'-O3'-P3-O31
2	A	3001	B12	C2P-O3-P-O2
2	B	3001	B12	C7-C37-C38-N40
2	B	3001	B12	C4-C3-C30-C31
2	B	3001	B12	C42-C41-C8-C9
2	A	3001	B12	C42-C41-C8-C9
2	B	3001	B12	C2-C3-C30-C31
2	B	3001	B12	C2P-O3-P-O2
2	A	3001	B12	C30-C31-C32-N33
2	B	3001	B12	C38-C37-C7-C36
2	B	3001	B12	C38-C37-C7-C8
4	B	5001	MLC	CP2-CP1-S-CM1
4	A	5001	MLC	CP2-CP1-S-CM1
2	A	3001	B12	C30-C31-C32-O34
2	B	3001	B12	C30-C31-C32-N33
4	A	5001	MLC	P2-O6-P1-O12
2	B	3001	B12	C30-C31-C32-O34
2	A	3001	B12	C55-C56-C57-O58
2	A	3001	B12	C55-C56-C57-N59
2	B	3001	B12	C55-C56-C57-O58

There are no ring outliers.

8 monomers are involved in 52 short contacts:

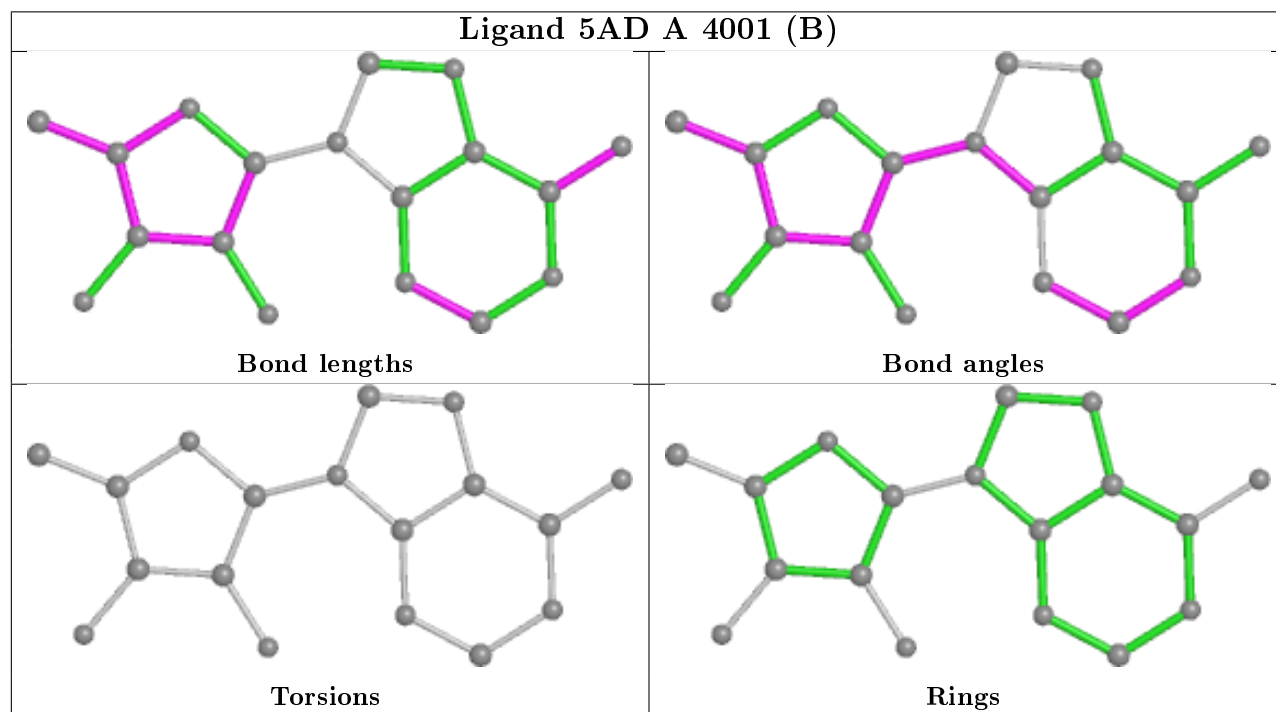
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4001[B]	5AD	7	0
2	B	3001	B12	18	0
3	B	4001[B]	5AD	7	0
4	B	5001	MLC	4	0
3	A	4001[A]	5AD	4	0

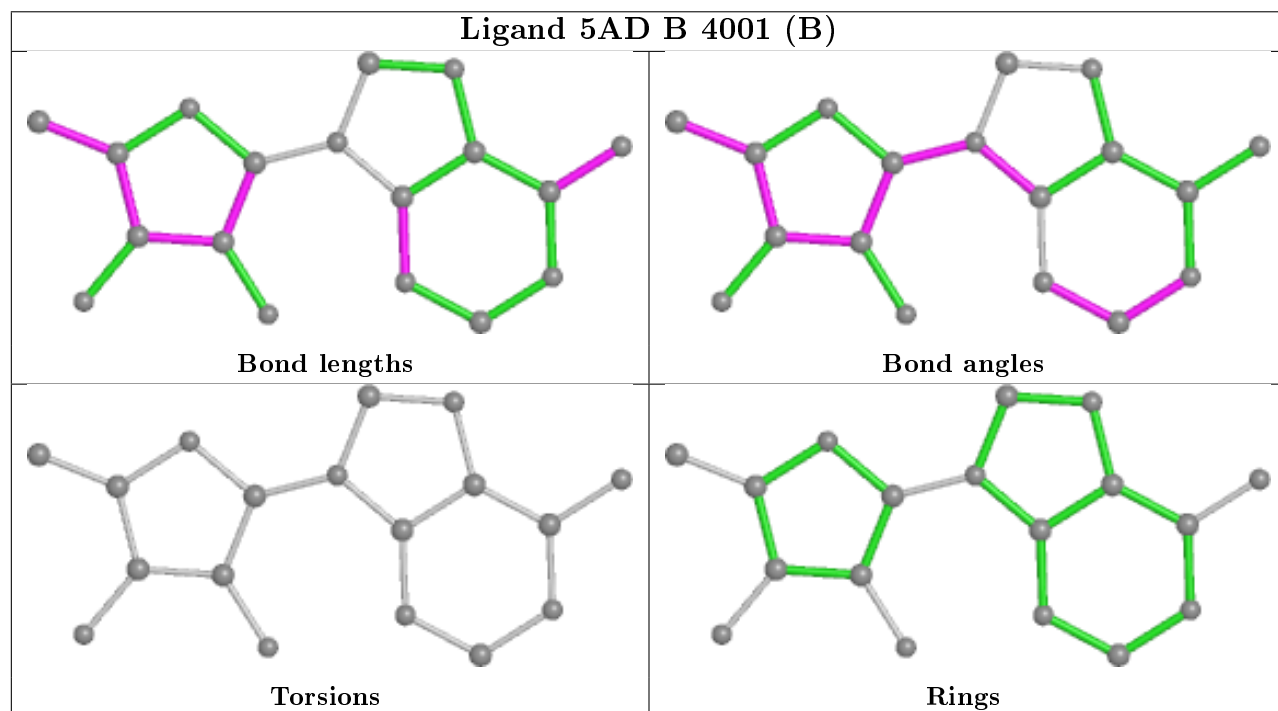
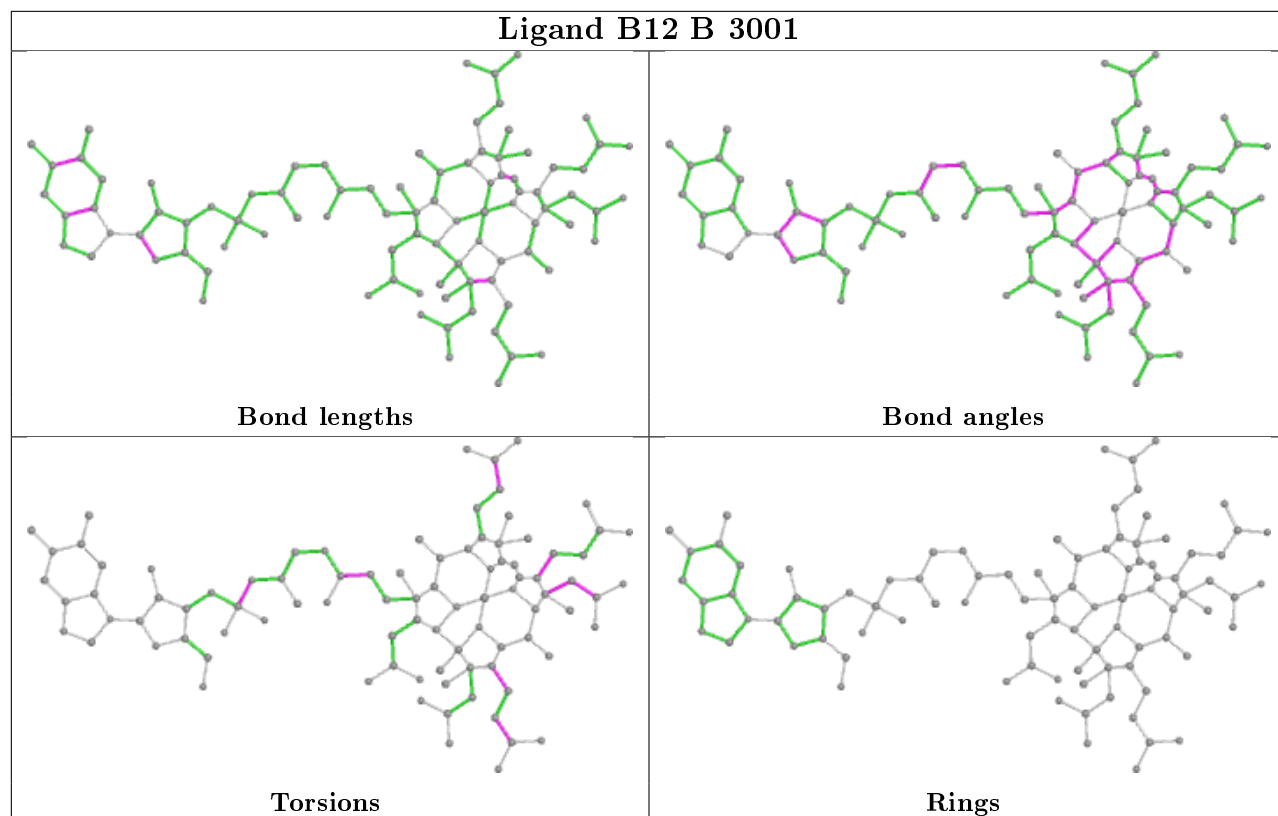
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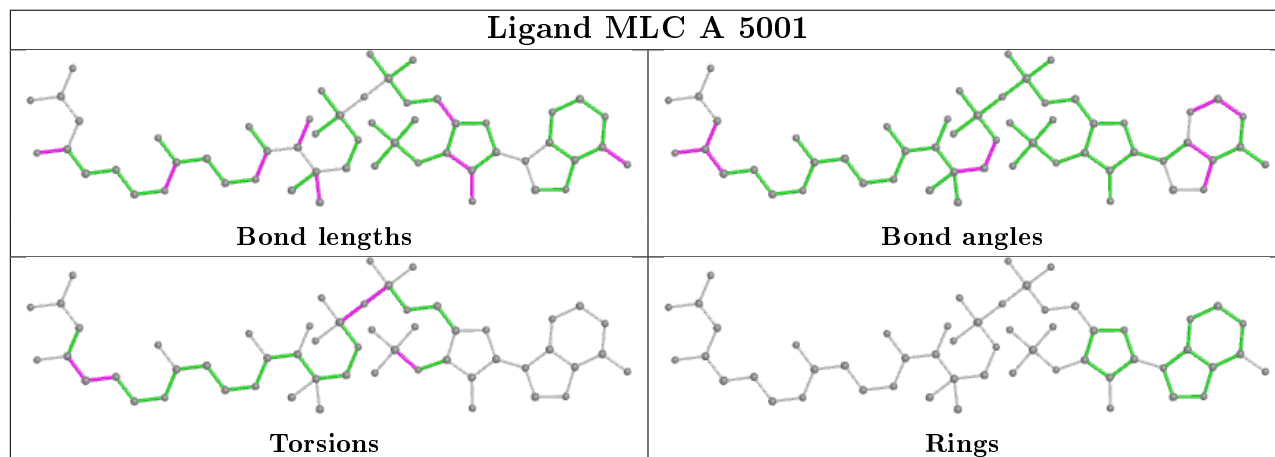
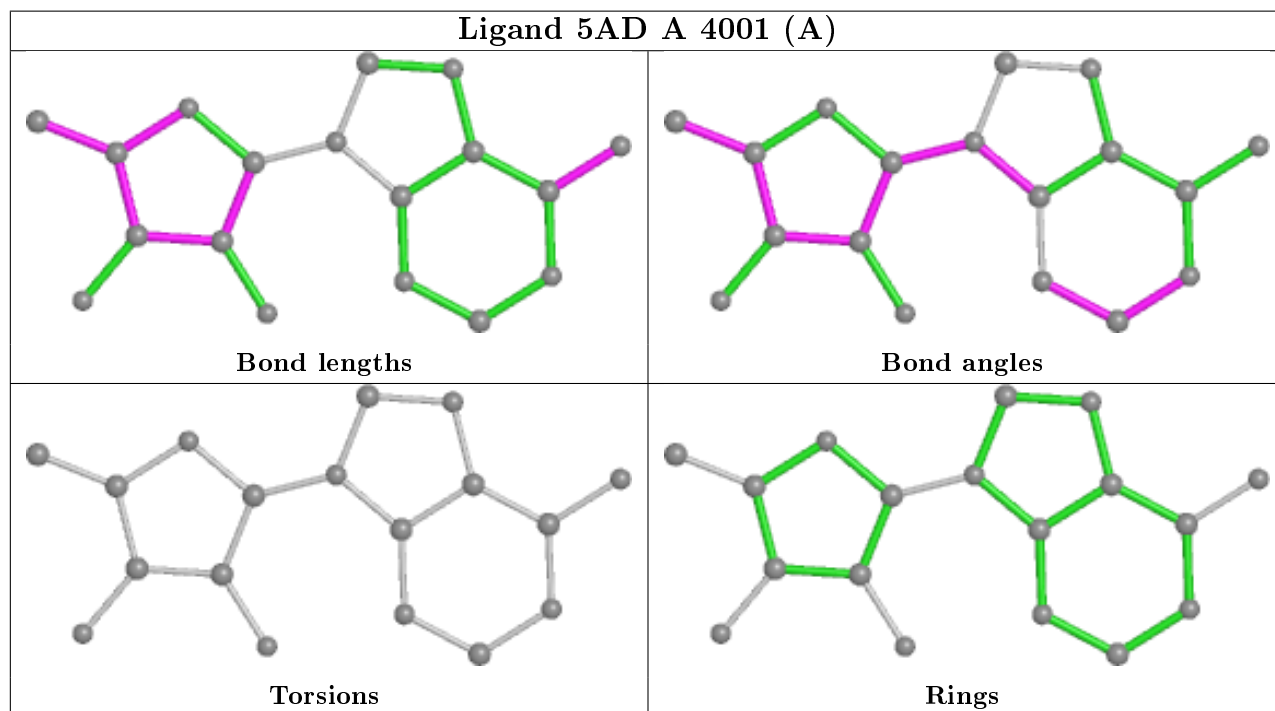
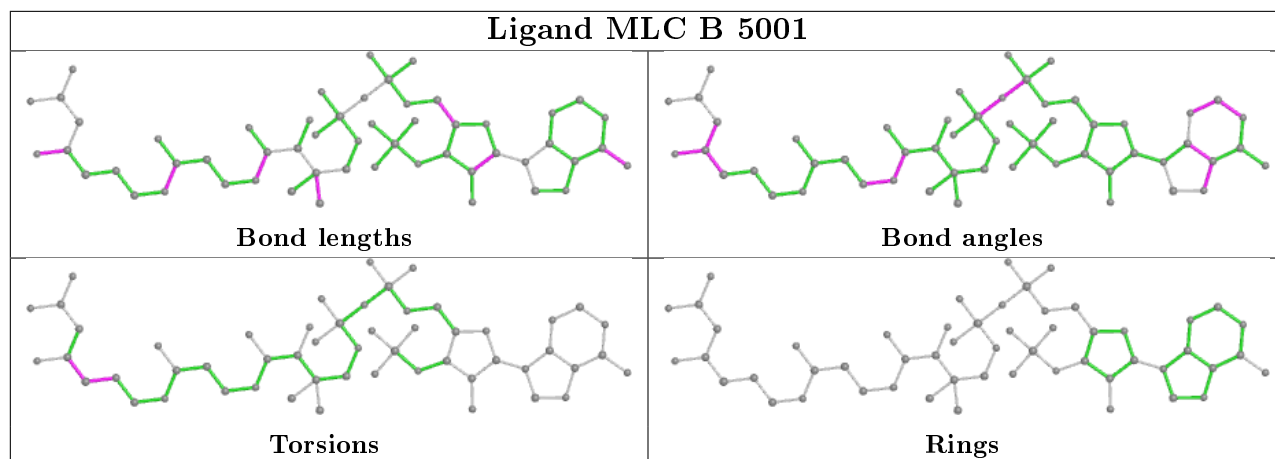
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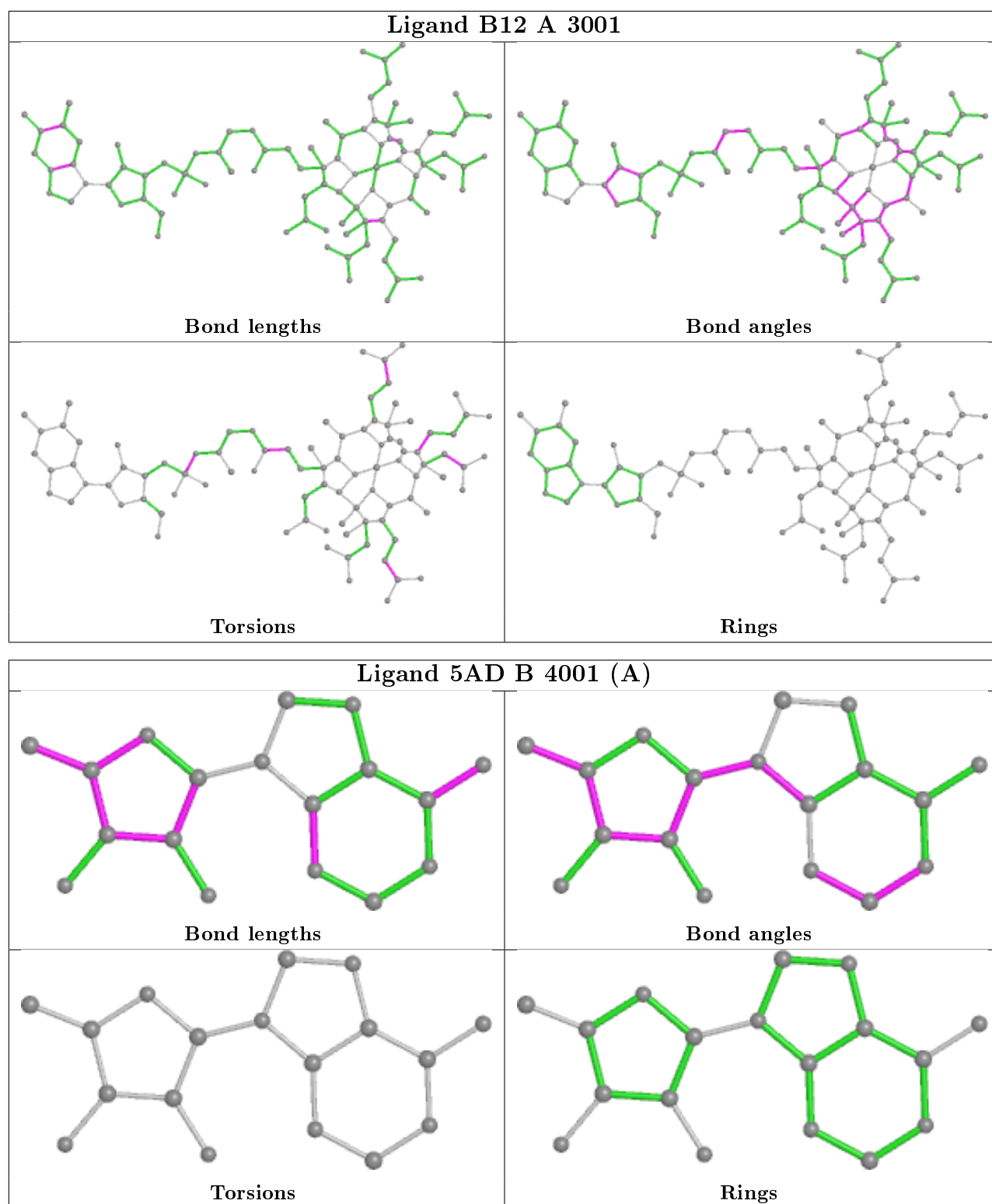
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5001	MLC	2	0
2	A	3001	B12	21	0
3	B	4001[A]	5AD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	714/762 (93%)	-0.02	15 (2%) 63 72	19, 33, 62, 93	0
1	B	713/762 (93%)	-0.21	14 (1%) 65 73	14, 26, 51, 87	0
All	All	1427/1524 (93%)	-0.11	29 (2%) 65 73	14, 30, 57, 93	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	GLN	5.0
1	A	36	GLN	4.7
1	A	749	SER	4.0
1	B	742	CYS	3.5
1	B	51	LEU	3.3
1	B	79	MET	3.1
1	A	748	GLN	3.1
1	A	79	MET	2.9
1	B	714	PHE	2.8
1	B	53	GLY	2.7
1	A	53	GLY	2.6
1	B	52	LYS	2.4
1	B	372	ILE	2.4
1	B	76	ARG	2.4
1	A	527	GLN	2.4
1	B	745	LYS	2.3
1	A	412	ILE	2.2
1	A	742	CYS	2.2
1	B	748	GLN	2.2
1	A	80	ASP	2.2
1	B	48	LYS	2.2
1	A	418	ILE	2.2
1	A	515	ILE	2.1
1	A	536	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	2.1
1	B	595	LYS	2.1
1	B	311	ILE	2.1
1	A	374	ALA	2.1
1	A	385	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

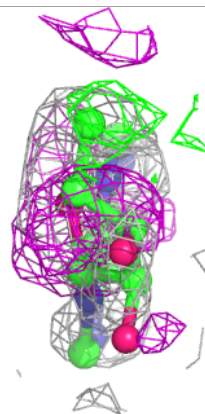
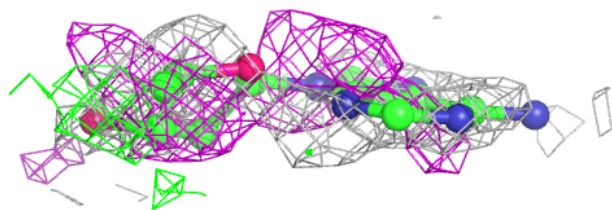
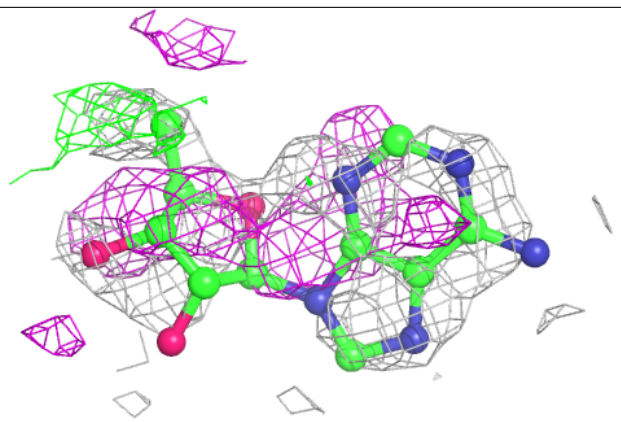
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5AD	A	4001[B]	18/18	0.57	0.45	36,58,87,88	18
3	5AD	A	4001[A]	18/18	0.57	0.45	56,106,143,145	18
3	5AD	B	4001[B]	18/18	0.64	0.40	33,75,120,137	18
3	5AD	B	4001[A]	18/18	0.64	0.40	38,58,74,78	18
4	MLC	A	5001	54/54	0.95	0.11	18,28,41,49	0
4	MLC	B	5001	54/54	0.97	0.10	13,21,34,53	0
2	B12	A	3001	91/91	0.97	0.12	15,22,31,35	0
2	B12	B	3001	91/91	0.97	0.12	12,19,24,33	0

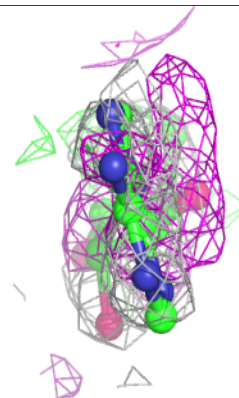
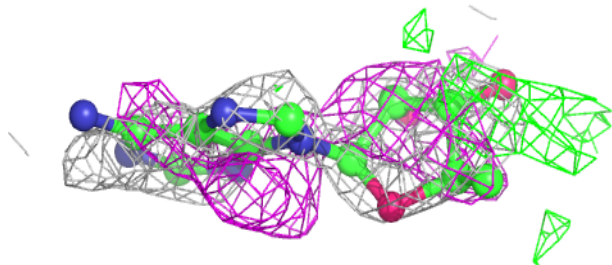
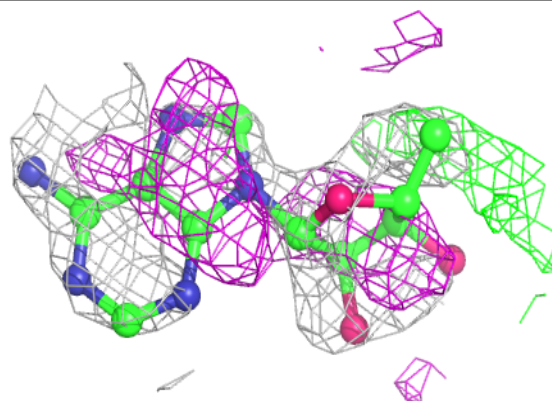
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5AD A 4001 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

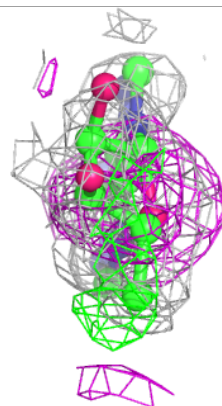
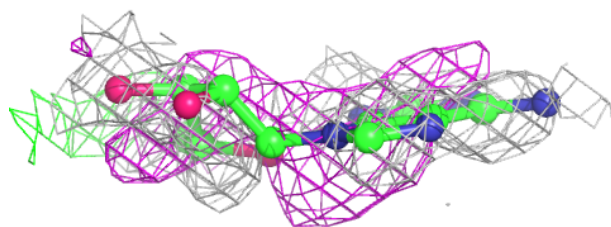
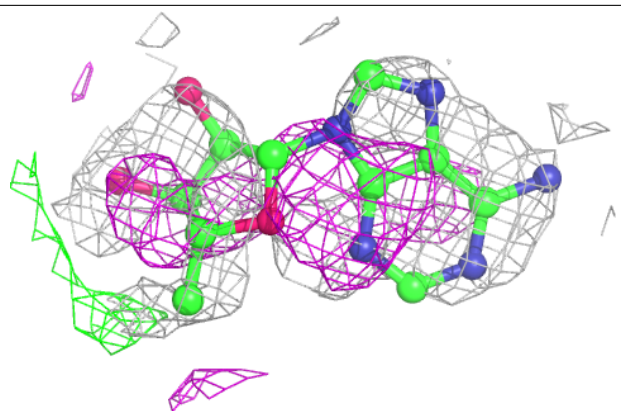
**Electron density around 5AD A 4001 (A):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

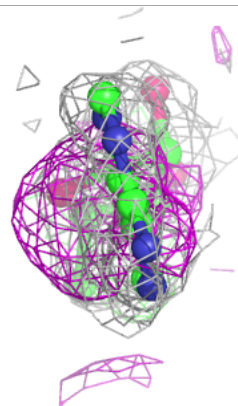
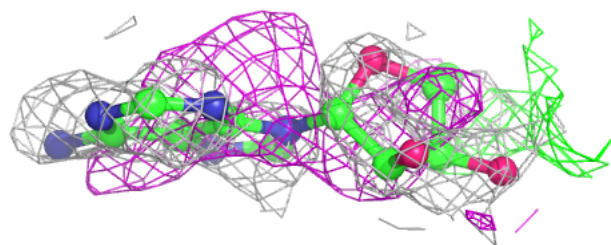
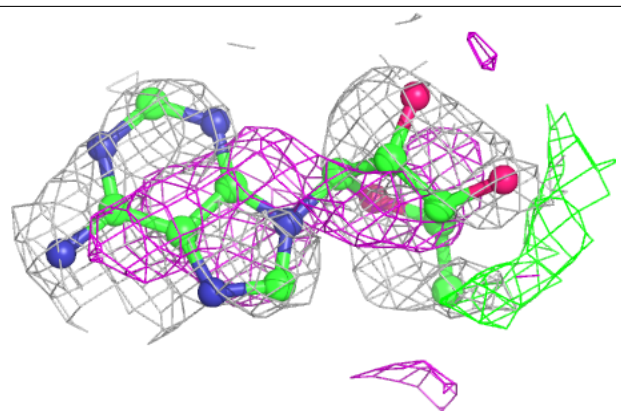


Electron density around 5AD B 4001 (B):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

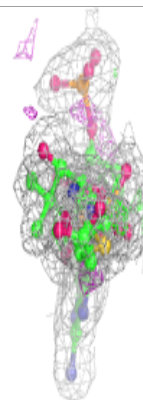
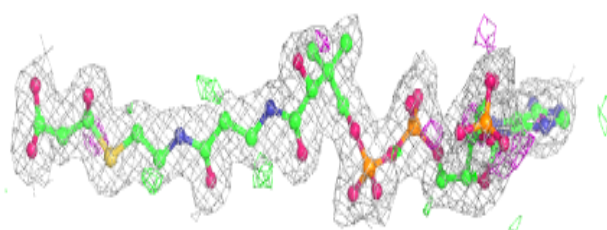
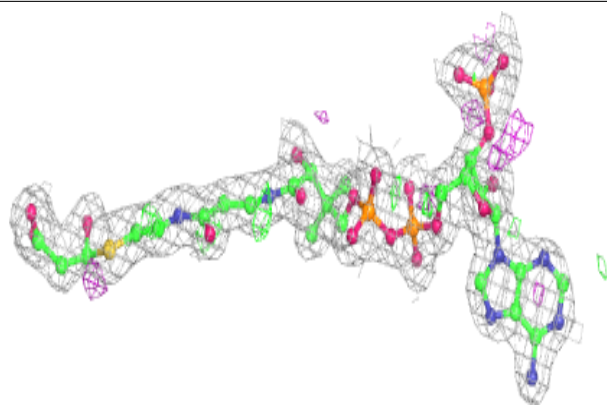
**Electron density around 5AD B 4001 (A):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

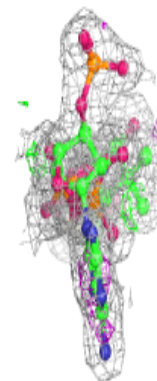
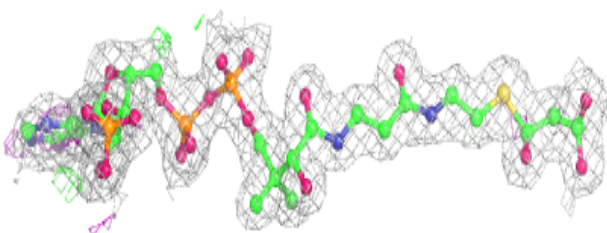
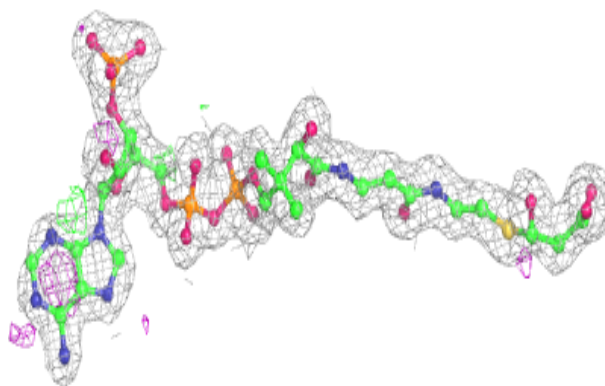


Electron density around MLC A 5001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

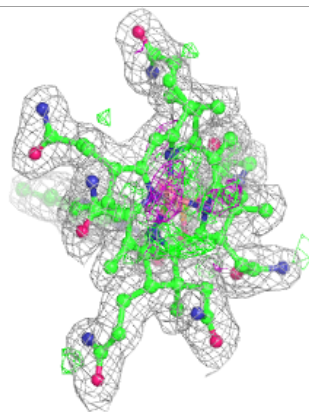
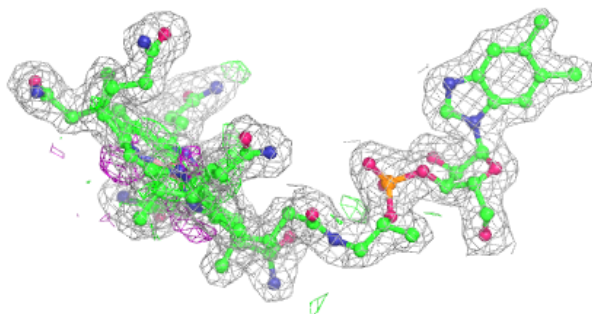
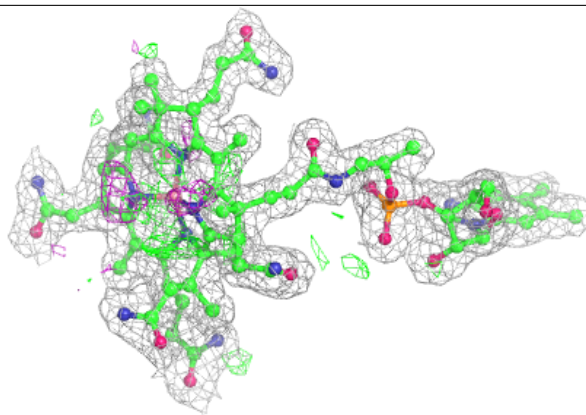
**Electron density around MLC B 5001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

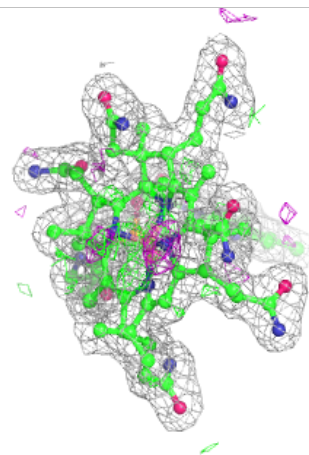
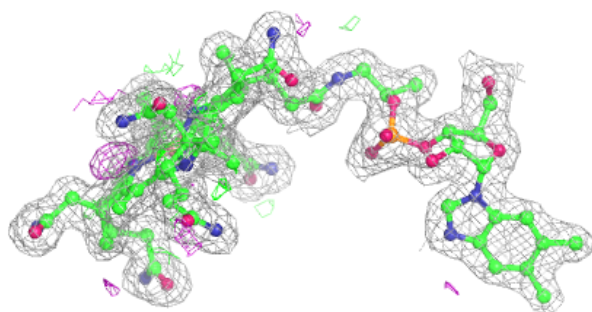
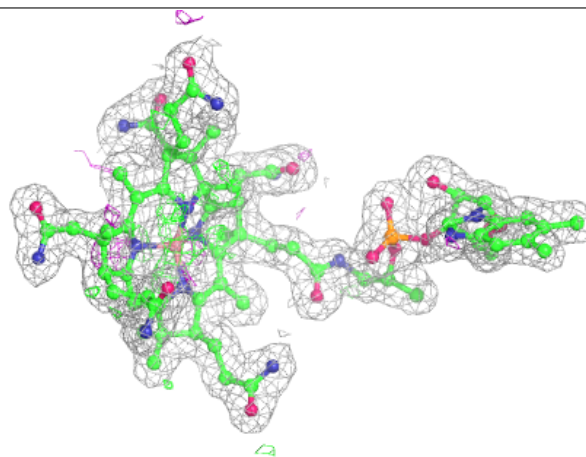


Electron density around B12 A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B12 B 3001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.