



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:15 am BST

PDB ID : 6OXD  
Title : Structure of Mycobacterium tuberculosis methylmalonyl-CoA mutase with adenosyl cobalamin  
Authors : Purchal, M.; Ruetz, M.; Banerjee, R.; Koutmos, M.  
Deposited on : 2019-05-13  
Resolution : 2.00 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](mailto: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.

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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

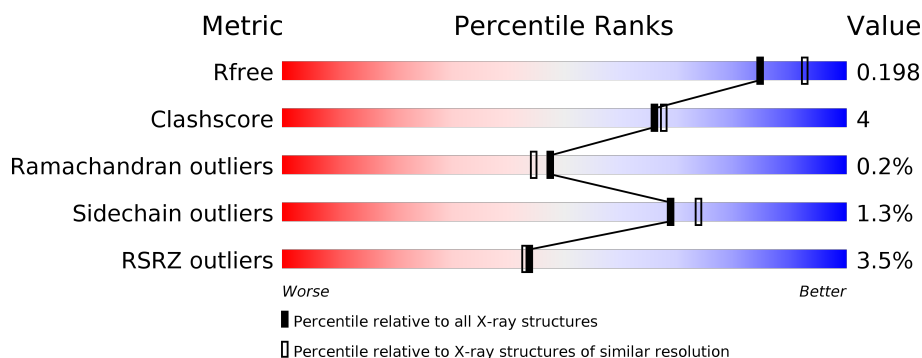
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	750	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
2	B	616	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21256 atoms, of which 9990 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 large subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	736	11127	3527	5528	996	1061	15	0	2	0

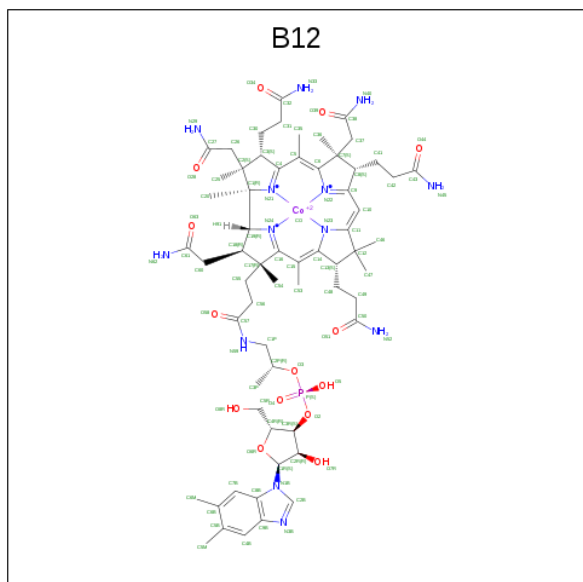
- Molecule 2 is a protein called Methylmalonyl-CoA mutase small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	590	8746	2746	4365	806	819	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

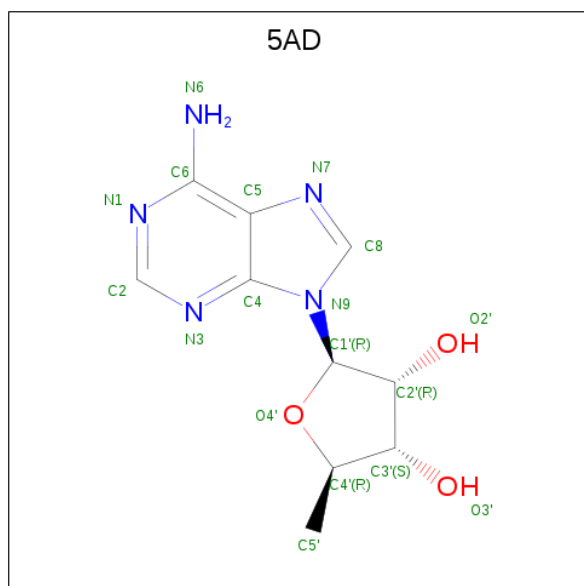
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP A0A045IZR3
B	2	VAL	MET	variant	UNP A0A045IZR3

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ) (labeled as "Ligand of Interest" by author).



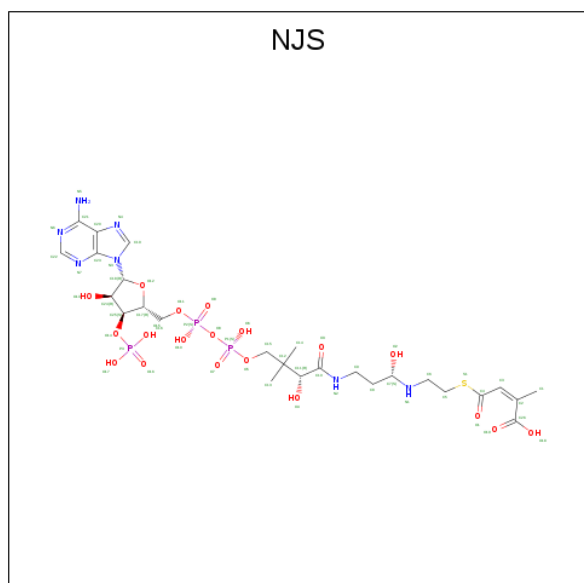
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Co	H	N	O	P	0	0
			177	62	1	86	13	14	1		

- Molecule 4 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			29	10	11	5	3		

- Molecule 5 is Itaconyl coenzyme A (three-letter code: NJS) (formula:  $C_{26}H_{42}N_7O_{19}P_3S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			56	26	7	19	3	1	
								0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K		
			1	1	0	0

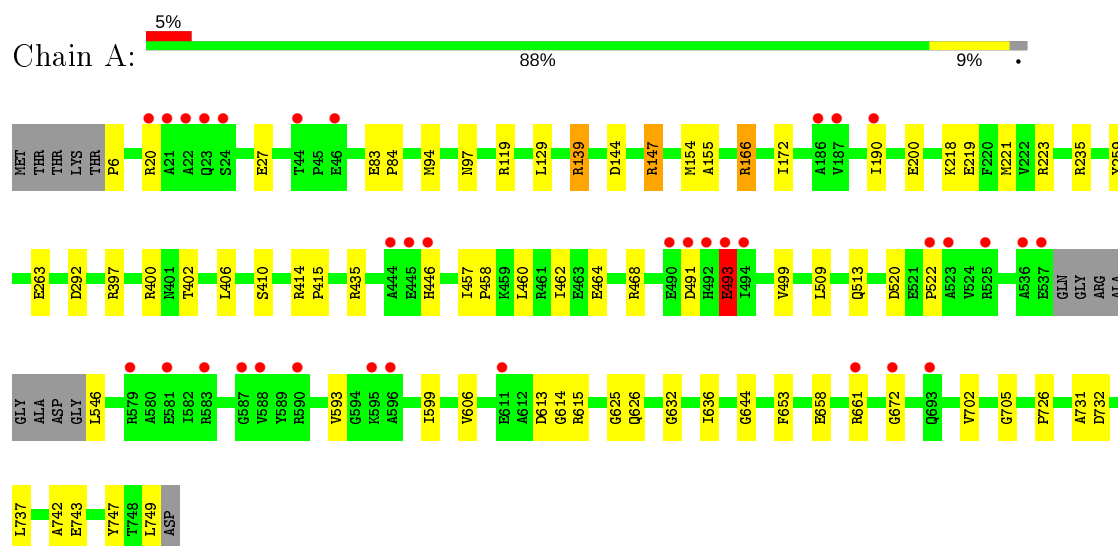
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	555	Total	O		
			555	555	0	0
7	B	565	Total	O		
			565	565	0	0

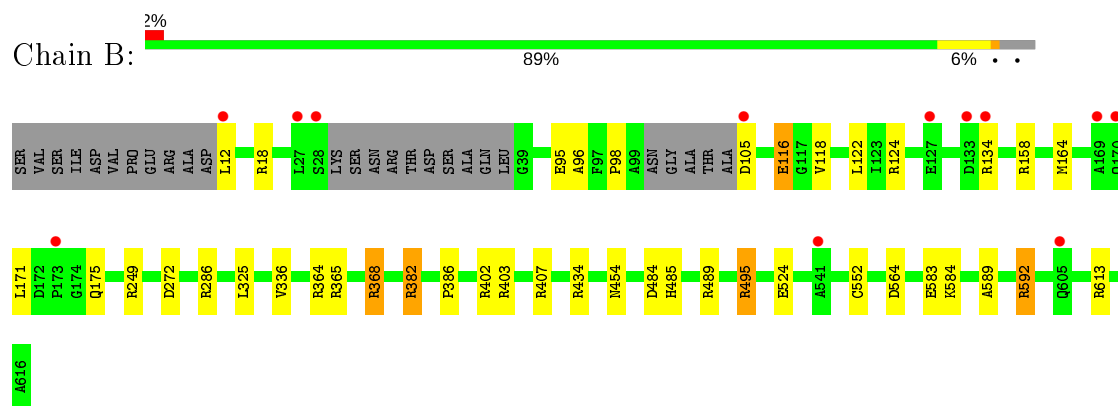
### 3 Residue-property plots [i](#)

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 large subunit



#### • Molecule 2: Methylmalonyl-CoA mutase small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.58Å 104.96Å 194.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 2.00 29.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.80-2.00) 97.9 (29.80-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.159 , 0.197 0.161 , 0.198	Depositor DCC
$R_{free}$ test set	5352 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NJS, K, 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	0.75	7/5722 (0.1%)	0.84	11/7787 (0.1%)
2	B	0.77	4/4467 (0.1%)	0.91	13/6094 (0.2%)
All	All	0.76	11/10189 (0.1%)	0.87	24/13881 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	493	GLU	CD-OE1	10.68	1.37	1.25
2	B	382	ARG	CB-CG	-8.43	1.29	1.52
2	B	116	GLU	CG-CD	7.38	1.63	1.51
1	A	493	GLU	CB-CG	6.56	1.64	1.52
2	B	368	ARG	CD-NE	-5.96	1.36	1.46
1	A	97	ASN	CB-CG	5.61	1.64	1.51
1	A	435	ARG	CB-CG	-5.58	1.37	1.52
1	A	27[A]	GLU	CG-CD	5.46	1.60	1.51
1	A	27[B]	GLU	CG-CD	5.46	1.60	1.51
2	B	552	CYS	CB-SG	-5.23	1.73	1.81
1	A	493	GLU	CG-CD	5.04	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	368	ARG	NE-CZ-NH1	16.51	128.56	120.30
2	B	368	ARG	NE-CZ-NH2	-16.47	112.06	120.30
1	A	147	ARG	NE-CZ-NH1	11.38	125.99	120.30
2	B	402	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	400	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	147	ARG	NE-CZ-NH2	-9.67	115.46	120.30
2	B	382	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	435	ARG	CG-CD-NE	-8.27	94.44	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	400	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	166	ARG	NE-CZ-NH2	-6.55	117.02	120.30
2	B	286	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	402	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	B	272	ASP	CB-CG-OD1	5.41	123.16	118.30
2	B	365	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	468	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	B	484	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	593	VAL	C-N-CA	-5.17	111.43	122.30
2	B	164	MET	CG-SD-CE	5.17	108.48	100.20
1	A	139	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	B	434	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	249	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	B	286	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	493	GLU	CG-CD-OE1	5.01	128.33	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5599	5528	5533	48	0
2	B	4381	4365	4364	26	0
3	A	91	86	87	10	0
4	A	18	11	11	1	0
5	A	56	0	0	1	0
6	A	1	0	0	0	0
7	A	555	0	0	10	0
7	B	565	0	0	12	0
All	All	11266	9990	9995	81	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 4.

All (81) 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)
5:A:1002:NJS:O12	5:A:1002:NJS:C17	1.64	1.27
1:A:221:MET:SD	7:A:1403:HOH:O	2.09	1.10
1:A:154:MET:SD	7:A:1258:HOH:O	2.11	1.09
1:A:513:GLN:OE1	7:A:1101:HOH:O	1.88	0.89
2:B:407:ARG:NH2	7:B:701:HOH:O	2.06	0.87
1:A:292:ASP:OD2	7:A:1102:HOH:O	1.96	0.84
3:A:1000:B12:H531	3:A:1000:B12:H552	1.60	0.84
2:B:118:VAL:HG23	2:B:368:ARG:HD2	1.69	0.74
2:B:403:ARG:HD2	7:B:996:HOH:O	1.88	0.72
1:A:493:GLU:OE2	7:A:1103:HOH:O	2.08	0.71
1:A:166:ARG:HD3	1:A:200:GLU:OE1	1.93	0.68
1:A:263:GLU:HB3	3:A:1000:B12:H532	1.77	0.66
3:A:1000:B12:H531	3:A:1000:B12:C55	2.26	0.66
2:B:564:ASP:OD2	7:B:702:HOH:O	2.15	0.65
1:A:154:MET:HE1	1:A:499:VAL:HG12	1.77	0.64
2:B:95:GLU:OE2	2:B:368:ARG:HD3	1.99	0.62
2:B:613:ARG:HD3	7:B:712:HOH:O	2.00	0.62
1:A:144:ASP:HB3	1:A:509:LEU:CD2	2.31	0.60
2:B:116:GLU:HG2	7:B:1143:HOH:O	2.04	0.58
2:B:98:PRO:HB3	2:B:105:ASP:HA	1.84	0.58
2:B:485:HIS:NE2	2:B:489:ARG:HD2	2.19	0.58
1:A:460:LEU:O	1:A:464[B]:GLU:HG3	2.07	0.55
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.69	0.55
4:A:1001:5AD:H8	4:A:1001:5AD:H5'2	1.89	0.55
3:A:1000:B12:H473	3:A:1000:B12:H492	1.89	0.54
1:A:147:ARG:NH2	1:A:658:GLU:OE2	2.32	0.54
2:B:171:LEU:HB3	2:B:175:GLN:HG3	1.90	0.53
1:A:491:ASP:OD2	7:A:1104:HOH:O	2.19	0.53
1:A:520:ASP:OD1	1:A:522:PRO:HD2	2.09	0.53
2:B:583:GLU:HG2	2:B:592:ARG:NH2	2.23	0.53
2:B:18:ARG:NH1	7:B:710:HOH:O	2.43	0.52
2:B:118:VAL:CG2	2:B:368:ARG:HD2	2.37	0.51
2:B:583:GLU:CG	2:B:592:ARG:NH2	2.75	0.50
1:A:6:PRO:HG2	7:B:990:HOH:O	2.12	0.50
1:A:464[A]:GLU:HG2	7:A:1571:HOH:O	2.11	0.49
2:B:134:ARG:HB3	7:B:971:HOH:O	2.12	0.49
1:A:219:GLU:OE2	1:A:223:ARG:HD3	2.12	0.49
1:A:606:VAL:HG11	1:A:644:GLY:HA3	1.94	0.49
2:B:124:ARG:CZ	2:B:124:ARG:HB2	2.43	0.49
3:A:1000:B12:H351	3:A:1000:B12:H372	1.95	0.48
2:B:583:GLU:HB2	7:B:992:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASP:HB3	1:A:509:LEU:HD22	1.95	0.48
2:B:407:ARG:NE	7:B:713:HOH:O	2.45	0.48
1:A:20:ARG:NH2	7:A:1113:HOH:O	2.47	0.48
1:A:259:TYR:CE2	1:A:263:GLU:HG3	2.48	0.48
1:A:702:VAL:HG11	1:A:737:LEU:HD21	1.96	0.47
1:A:599:ILE:HD13	1:A:731:ALA:HB2	1.97	0.47
1:A:397:ARG:CZ	2:B:454:ASN:HB2	2.44	0.47
1:A:139:ARG:HD3	1:A:626:GLN:OE1	2.14	0.47
3:A:1000:B12:H351	3:A:1000:B12:H362	1.97	0.47
2:B:583:GLU:HG2	2:B:592:ARG:HH22	1.80	0.46
1:A:218:LYS:HE2	1:A:223:ARG:HD2	1.97	0.46
1:A:446:HIS:O	1:A:446:HIS:CD2	2.69	0.46
3:A:1000:B12:C47	3:A:1000:B12:H492	2.46	0.46
2:B:592:ARG:HD2	7:B:768:HOH:O	2.14	0.45
1:A:625:GLY:O	1:A:653:PHE:HA	2.17	0.45
3:A:1000:B12:C49	3:A:1000:B12:H473	2.43	0.45
2:B:364:ARG:HD3	7:B:1090:HOH:O	2.16	0.45
2:B:495:ARG:HA	2:B:524:GLU:O	2.18	0.45
1:A:546:LEU:N	7:A:1116:HOH:O	2.48	0.44
1:A:672:GLY:HA3	3:A:1000:B12:HM53	2.00	0.44
1:A:83:GLU:HG3	1:A:84:PRO:HD2	2.00	0.44
1:A:154:MET:CE	1:A:499:VAL:CG1	2.96	0.44
1:A:491:ASP:O	1:A:493:GLU:HG3	2.19	0.43
1:A:154:MET:CE	1:A:499:VAL:HG12	2.46	0.43
1:A:732:ASP:OD2	7:A:1105:HOH:O	2.21	0.43
1:A:144:ASP:HB3	1:A:509:LEU:HD21	2.01	0.43
1:A:613:ASP:O	1:A:614:GLY:C	2.57	0.43
2:B:336:VAL:HG13	2:B:386:PRO:HG2	2.01	0.42
1:A:613:ASP:OD1	1:A:747:TYR:OH	2.29	0.42
1:A:155:ALA:HB1	3:A:1000:B12:H362	2.02	0.42
1:A:129:LEU:HD11	1:A:172:ILE:HD13	2.02	0.42
1:A:221:MET:HE3	1:A:462:ILE:HD11	2.02	0.41
1:A:406:LEU:HA	1:A:410:SER:HB3	2.01	0.41
1:A:402:THR:HA	2:B:325:LEU:HD13	2.02	0.41
1:A:705:GLY:O	1:A:726:PRO:HD3	2.20	0.41
1:A:190:ILE:HD13	1:A:190:ILE:HA	1.96	0.41
1:A:632:GLY:O	1:A:636:ILE:HG12	2.21	0.41
2:B:96:ALA:HA	2:B:122:LEU:O	2.21	0.41
1:A:457:ILE:HB	1:A:458:PRO:HD3	2.03	0.40
1:A:742:ALA:HB2	1:A:749:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 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	734/750 (98%)	713 (97%)	20 (3%)	1 (0%)	51	49
2	B	584/616 (95%)	582 (100%)	1 (0%)	1 (0%)	47	44
All	All	1318/1366 (96%)	1295 (98%)	21 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	589	ALA
1	A	94	MET

### 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	568/575 (99%)	561 (99%)	7 (1%)	71	76
2	B	434/455 (95%)	428 (99%)	6 (1%)	67	72
All	All	1002/1030 (97%)	989 (99%)	13 (1%)	69	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ARG
1	A	414	ARG
1	A	415	PRO
1	A	493	GLU

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Mol	Chain	Res	Type
1	A	615	ARG
1	A	661	ARG
1	A	743	GLU
2	B	12	LEU
2	B	158	ARG
2	B	382	ARG
2	B	495	ARG
2	B	584	LYS
2	B	592	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
4	5AD	A	1001	5	17,20,20	4.45	7 (41%)	15,30,30	3.46	7 (46%)
3	B12	A	1000	1	80,101,101	1.19	10 (12%)	101,166,166	2.42	20 (19%)
5	NJS	A	1002	4	45,58,58	2.40	9 (20%)	56,86,86	2.41	14 (25%)

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
4	5AD	A	1001	5	-	0/0/20/20	0/3/3/3
3	B12	A	1000	1	-	8/51/223/223	0/3/11/11
5	NJS	A	1002	4	-	7/49/75/75	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	5AD	O4'-C1'	12.29	1.58	1.41
4	A	1001	5AD	C3'-C4'	9.11	1.65	1.52
5	A	1002	NJS	O12-C17	8.52	1.64	1.45
5	A	1002	NJS	C25-C17	-6.65	1.35	1.52
4	A	1001	5AD	C3'-C2'	-6.44	1.35	1.53
5	A	1002	NJS	O12-C18	-5.98	1.32	1.41
4	A	1001	5AD	O4'-C4'	-5.01	1.29	1.44
5	A	1002	NJS	C10-N2	4.92	1.44	1.33
5	A	1002	NJS	O13-C24	-4.36	1.32	1.43
3	A	1000	B12	C11-C10	-3.89	1.34	1.40
5	A	1002	NJS	P3-O14	3.70	1.66	1.59
3	A	1000	B12	C6B-C5B	3.15	1.48	1.40
4	A	1001	5AD	C2-N3	2.93	1.36	1.32
3	A	1000	B12	C8B-C9B	2.85	1.46	1.40
5	A	1002	NJS	C21-N5	2.80	1.44	1.34
5	A	1002	NJS	C3-C4	2.74	1.51	1.47
3	A	1000	B12	C1-C19	-2.63	1.49	1.55
4	A	1001	5AD	C6-N6	2.47	1.43	1.34
4	A	1001	5AD	O2'-C2'	2.44	1.48	1.43
3	A	1000	B12	C2-C3	-2.39	1.54	1.58
3	A	1000	B12	C1-C2	-2.38	1.53	1.58
3	A	1000	B12	C25-C2	-2.26	1.49	1.54
5	A	1002	NJS	C24-C18	2.21	1.57	1.53
3	A	1000	B12	C14-C15	2.15	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	B12	C56-C57	2.14	1.55	1.51
3	A	1000	B12	P-O3	2.07	1.65	1.60

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	B12	C20-C1-C19	-14.32	95.56	109.36
5	A	1002	NJS	C3-C4-S1	11.24	125.27	111.24
3	A	1000	B12	C19-C1-N21	8.14	110.50	102.16
5	A	1002	NJS	O1-C4-C3	-7.95	115.74	125.50
4	A	1001	5AD	C5-C6-N6	7.22	131.32	120.35
4	A	1001	5AD	C5'-C4'-C3'	-6.59	108.78	115.70
3	A	1000	B12	C47-C12-C46	6.01	122.32	109.73
3	A	1000	B12	C1-C19-C18	5.76	131.46	121.93
3	A	1000	B12	C12-C11-C10	-5.42	115.45	124.64
4	A	1001	5AD	N6-C6-N1	-5.26	107.66	118.57
3	A	1000	B12	C2P-C1P-N59	-5.21	105.26	112.93
4	A	1001	5AD	N3-C2-N1	-5.20	120.55	128.68
3	A	1000	B12	C2-C1-C19	5.08	126.61	118.60
3	A	1000	B12	C54-C17-C18	-4.73	106.00	112.98
5	A	1002	NJS	N7-C22-N6	-4.67	121.39	128.68
3	A	1000	B12	O6R-C1R-C2R	-3.67	101.56	106.93
5	A	1002	NJS	O5-C15-C12	-3.54	104.86	110.55
5	A	1002	NJS	C1-C2-C3	-3.51	117.39	123.03
4	A	1001	5AD	O4'-C1'-C2'	-3.16	102.31	106.93
5	A	1002	NJS	C5-C6-N1	-3.01	103.67	112.05
3	A	1000	B12	C25-C2-C3	-2.99	111.01	115.58
5	A	1002	NJS	C5-S1-C4	-2.66	96.45	99.80
3	A	1000	B12	C55-C17-C18	2.65	116.25	111.14
4	A	1001	5AD	O3'-C3'-C2'	2.58	120.18	111.82
3	A	1000	B12	C60-C18-C19	2.53	121.19	114.62
5	A	1002	NJS	C18-N3-C23	-2.50	122.25	126.64
5	A	1002	NJS	C14-C12-C15	2.47	112.27	108.23
5	A	1002	NJS	C9-N2-C10	-2.43	118.26	122.59
4	A	1001	5AD	C1'-N9-C4	-2.43	122.38	126.64
3	A	1000	B12	C54-C17-C55	-2.42	105.27	109.26
3	A	1000	B12	C26-C2-C3	2.36	111.82	107.47
3	A	1000	B12	C9-C10-C11	-2.21	123.18	130.91
5	A	1002	NJS	C24-C25-C17	2.19	107.11	103.22
5	A	1002	NJS	C9-C8-C7	-2.18	109.19	114.17
3	A	1000	B12	C36-C7-C37	2.15	114.50	110.83
5	A	1002	NJS	P2-O8-P1	-2.13	125.53	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	B12	C17-C18-C19	-2.09	99.18	102.37
3	A	1000	B12	C26-C2-C1	2.09	113.28	110.02
3	A	1000	B12	C55-C17-C16	2.06	116.78	109.92
5	A	1002	NJS	O6-P1-O5	2.04	117.24	107.75
3	A	1000	B12	C20-C1-C2	2.01	116.64	113.32

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1002	NJS	C3-C4-S1-C5
5	A	1002	NJS	O1-C4-S1-C5
5	A	1002	NJS	O2-C7-C8-C9
5	A	1002	NJS	N1-C7-C8-C9
5	A	1002	NJS	C25-O14-P3-O15
3	A	1000	B12	C4-C3-C30-C31
3	A	1000	B12	C42-C41-C8-C9
3	A	1000	B12	C2P-O3-P-O2
5	A	1002	NJS	P1-O8-P2-O10
3	A	1000	B12	C55-C56-C57-O58
3	A	1000	B12	C30-C31-C32-O34
3	A	1000	B12	C55-C56-C57-N59
5	A	1002	NJS	C6-C5-S1-C4
3	A	1000	B12	C30-C31-C32-N33
3	A	1000	B12	C3-C30-C31-C32

There are no ring outliers.

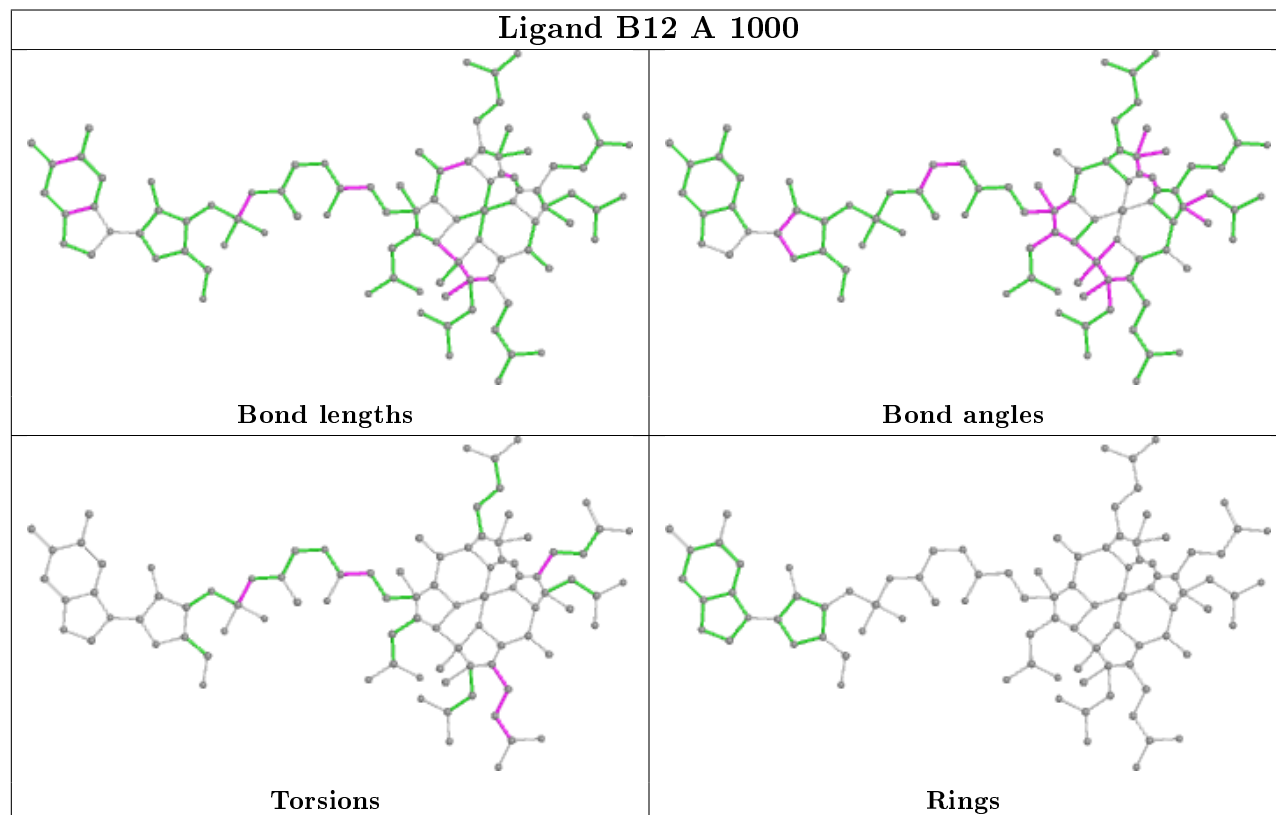
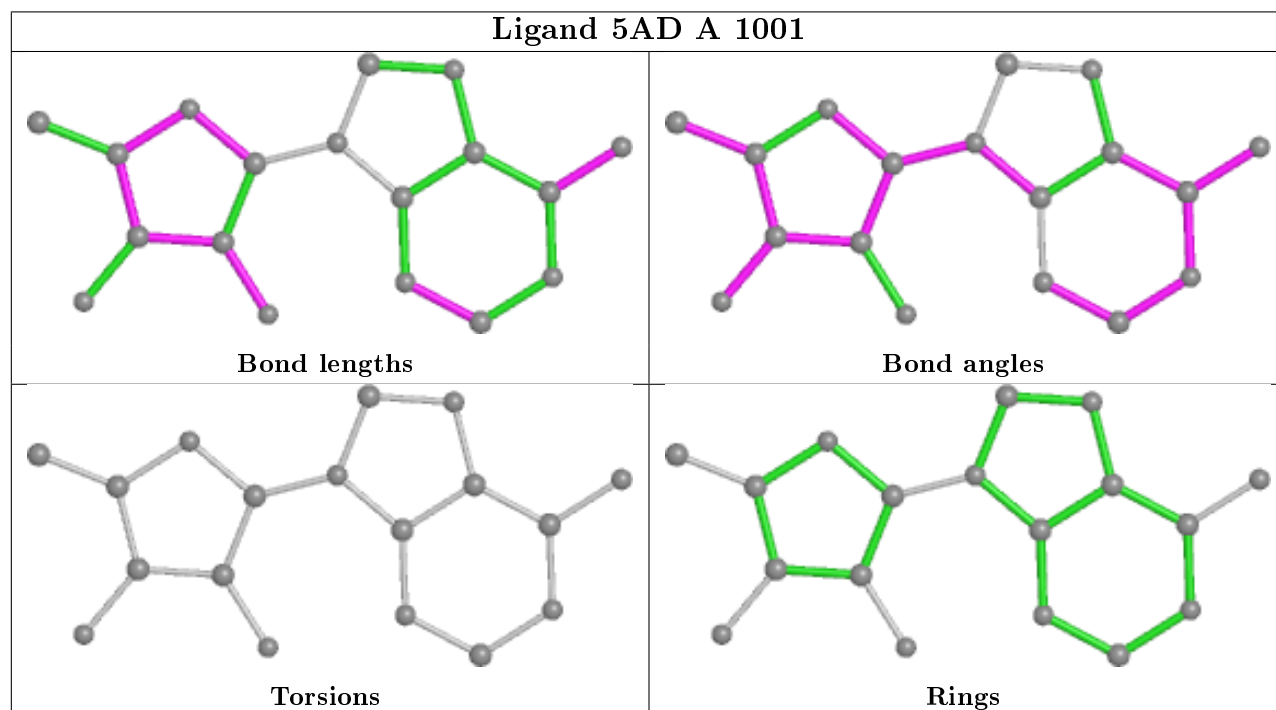
3 monomers are involved in 12 short contacts:

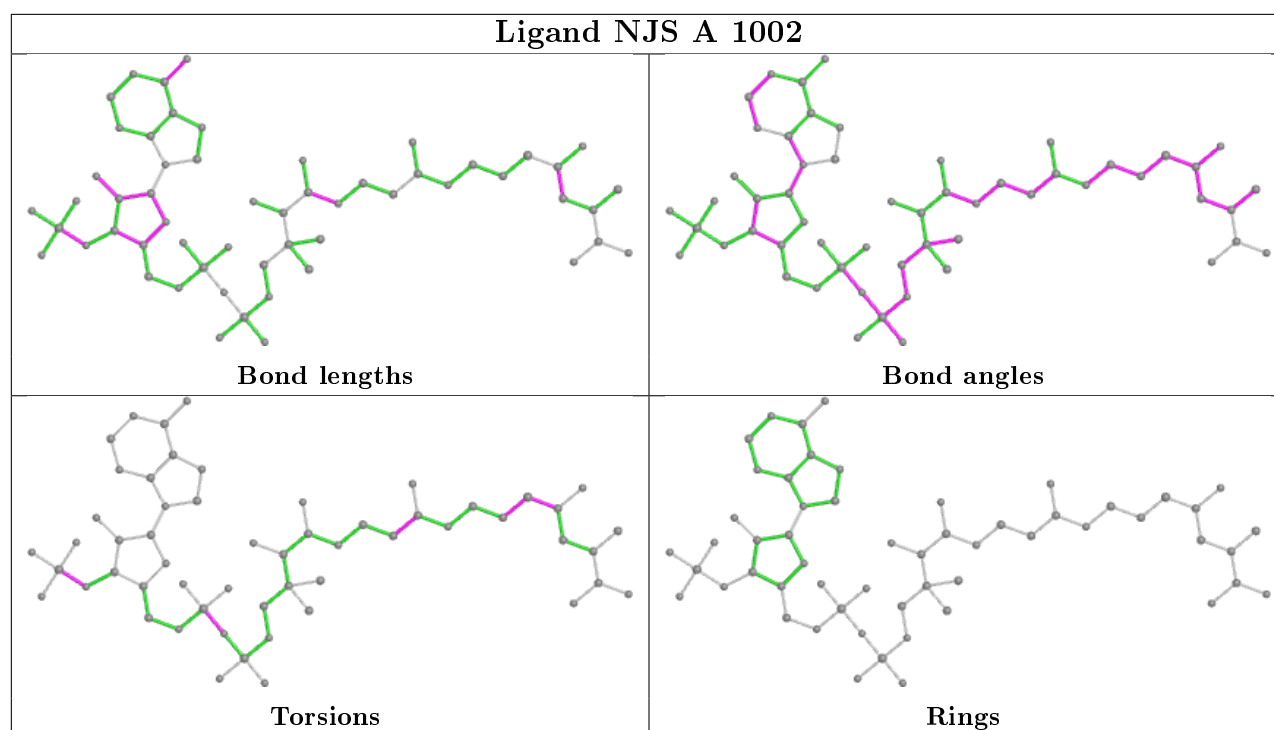
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	5AD	1	0
3	A	1000	B12	10	0
5	A	1002	NJS	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	736/750 (98%)	-0.02	35 (4%)	30 29	16, 31, 53, 87	0
2	B	590/616 (95%)	-0.26	12 (2%)	65 63	17, 27, 50, 78	0
All	All	1326/1366 (97%)	-0.13	47 (3%)	44 43	16, 30, 51, 87	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	ALA	8.3
1	A	492	HIS	5.9
1	A	22	ALA	5.3
1	A	23	GLN	4.9
1	A	24	SER	4.6
2	B	173	PRO	4.4
2	B	127	GLU	3.8
1	A	595	LYS	3.6
1	A	491	ASP	3.3
2	B	169	ALA	3.3
2	B	28	SER	3.2
1	A	522	PRO	3.1
1	A	490	GLU	3.1
1	A	693	GLN	3.0
1	A	661	ARG	2.9
2	B	105	ASP	2.9
1	A	20	ARG	2.9
1	A	536	ALA	2.9
1	A	588	VAL	2.6
2	B	170	GLN	2.6
1	A	445	GLU	2.5
1	A	579	ARG	2.5
1	A	583	ARG	2.5
1	A	494	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	12	LEU	2.4
2	B	134	ARG	2.4
1	A	537	GLU	2.4
1	A	446	HIS	2.4
1	A	187	VAL	2.4
1	A	596	ALA	2.4
1	A	587	GLY	2.4
1	A	672	GLY	2.4
2	B	541	ALA	2.3
1	A	444	ALA	2.3
1	A	190	ILE	2.3
2	B	605	GLN	2.3
1	A	581	GLU	2.3
1	A	611	GLU	2.3
1	A	46	GLU	2.2
1	A	525	ARG	2.2
2	B	133	ASP	2.2
1	A	44	THR	2.1
2	B	27	LEU	2.1
1	A	493	GLU	2.1
1	A	186	ALA	2.1
1	A	523	ALA	2.1
1	A	590	ARG	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, 95<sup>th</sup> 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.

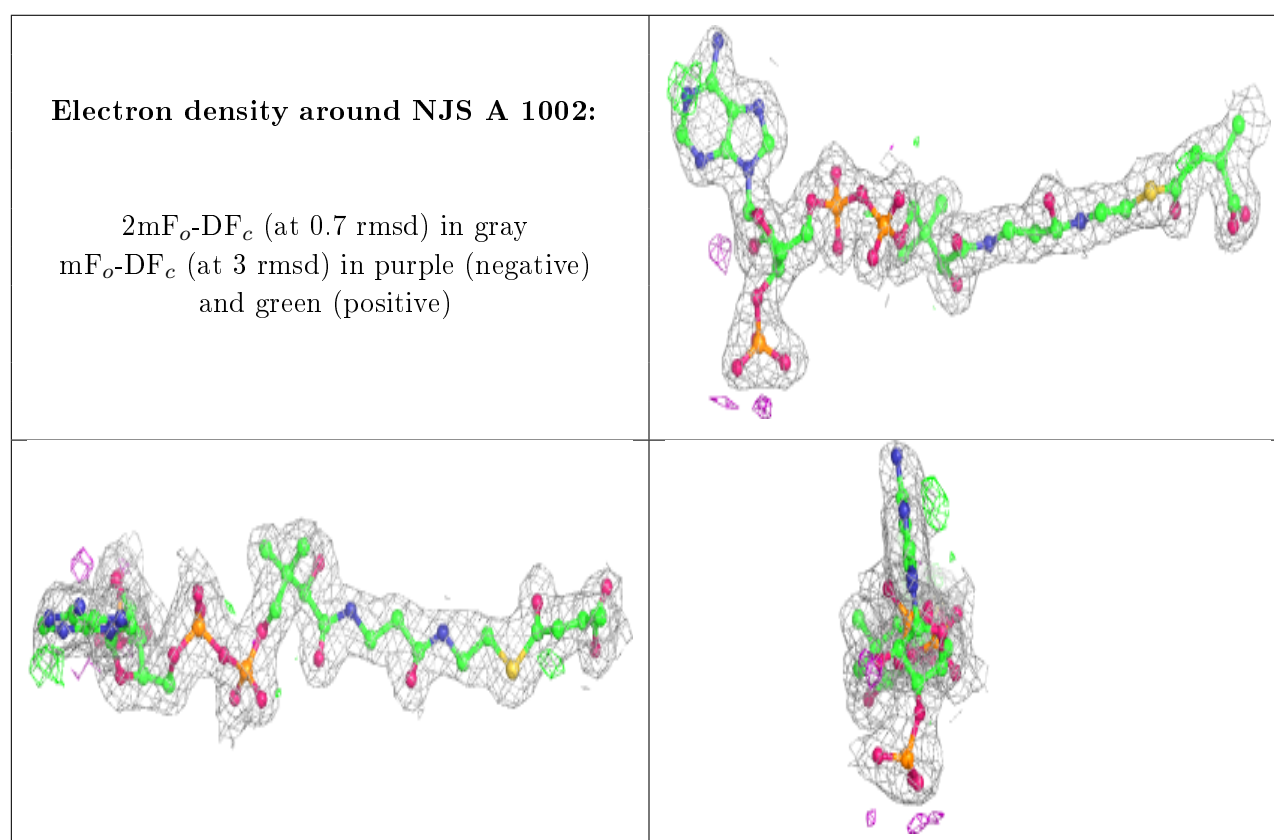
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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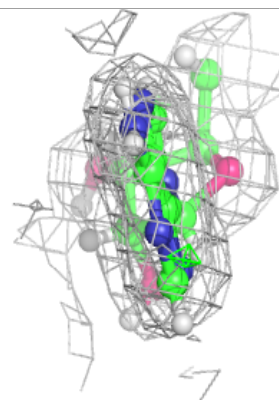
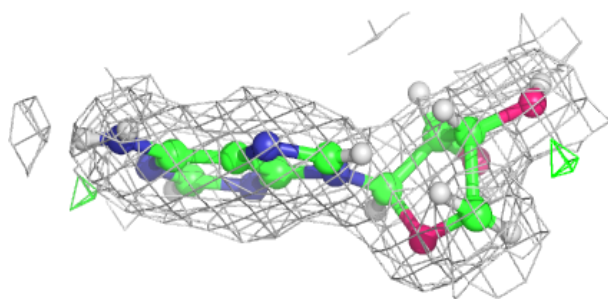
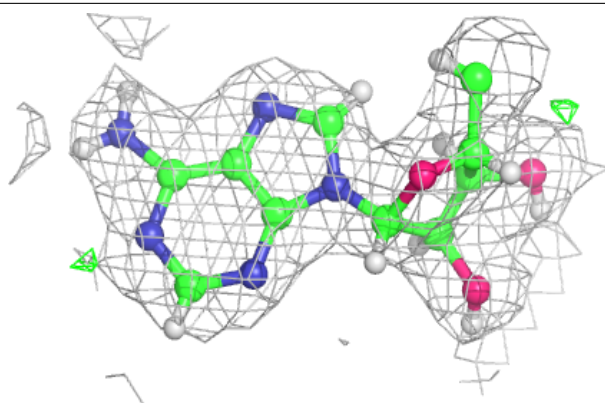
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NJS	A	1002	56/56	0.94	0.11	18,27,48,50	0
4	5AD	A	1001	18/18	0.97	0.09	20,25,30,31	0
3	B12	A	1000	91/91	0.98	0.14	19,28,36,39	0
6	K	A	1003	1/1	0.98	0.16	26,26,26,26	0

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.

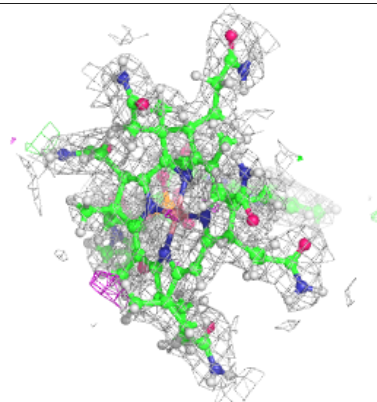
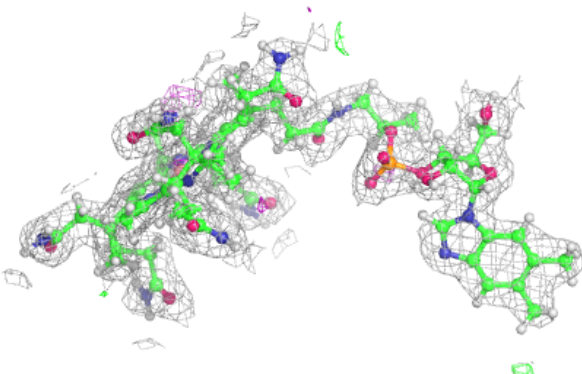
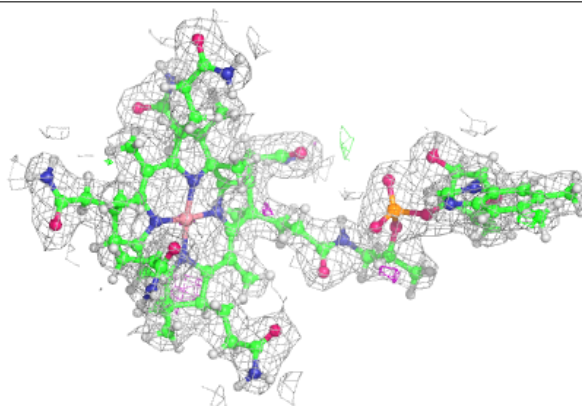


**Electron density around 5AD A 1001:**

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

**Electron density around B12 A 1000:**

$2mF_o-DF_c$  (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.