



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:38 AM UTC

PDB ID : 4YO6 / pdb_00004yo6
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2015-03-11
Resolution : 2.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

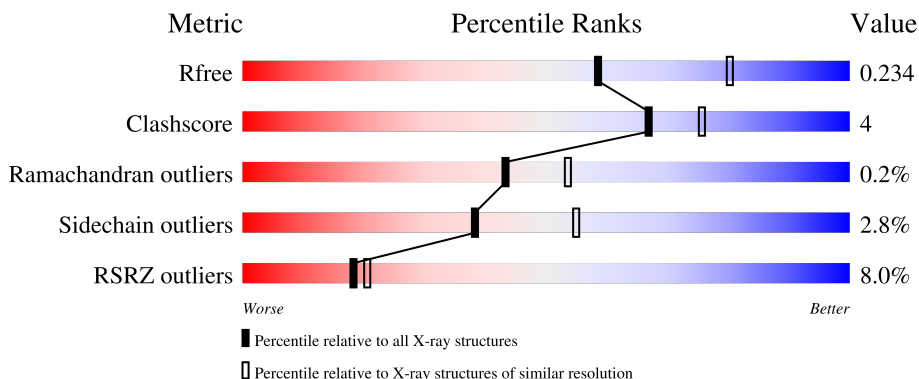
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of 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	301	 9% 84% 11% . .
1	B	301	 10% 81% 11% . 7%
1	C	301	 5% 86% 9% . .
1	D	301	 5% 83% 12% . .

2 Entry composition [i](#)

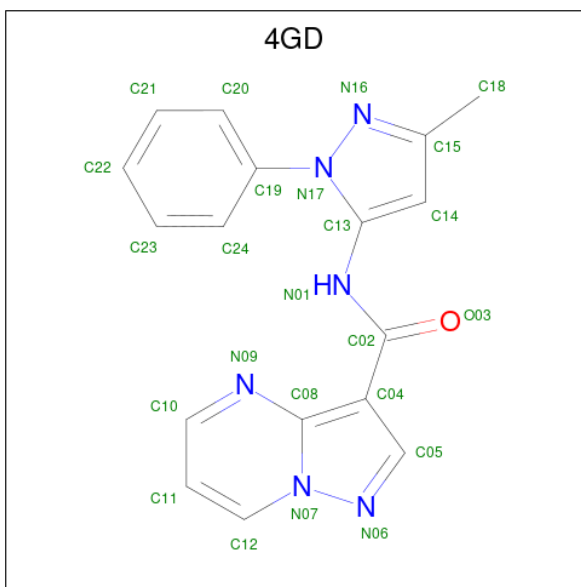
There are 3 unique types of molecules in this entry. The entry contains 9319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	289	Total 2265	C 1417	N 382	O 449	P 3	S 14	0	0	3
1	B	280	Total 2197	C 1378	N 369	O 433	P 3	S 14	0	0	1
1	C	289	Total 2259	C 1416	N 378	O 448	P 3	S 14	0	0	1
1	D	288	Total 2275	C 1425	N 385	O 448	P 3	S 14	0	1	2

- Molecule 2 is N-(3-methyl-1-phenyl-1H-pyrazol-5-yl)pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: 4GD) (formula: C₁₇H₁₄N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 24	C 17	N 6	O 1	0	0
2	B	1	Total 24	C 17	N 6	O 1	0	0

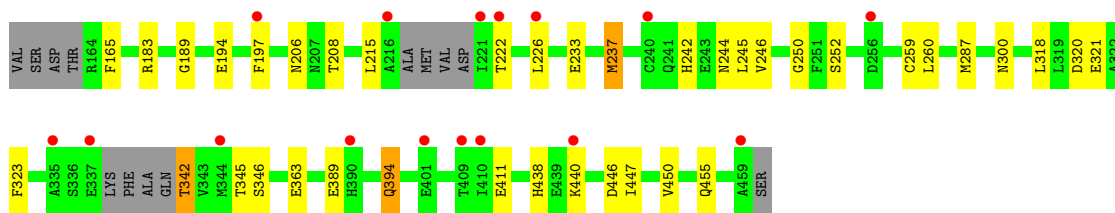
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			24	17	6	1		
2	D	1	Total	C	N	O	0	0
			24	17	6	1		
2	D	1	Total	C	N	O	0	0
			24	17	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	44	Total	O	0	0
			44	44		
3	C	69	Total	O	0	0
			69	69		
3	D	55	Total	O	0	0
			55	55		



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.71Å 139.55Å 87.62Å 90.00° 124.97° 90.00°	Depositor
Resolution (Å)	34.23 – 2.32 34.23 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.23-2.32) 99.4 (34.23-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.31Å)	Xtrriage
Refinement program	BUSTER-TNT 2.9.3	Depositor
R, R_{free}	0.197 , 0.225 0.203 , 0.234	Depositor DCC
R_{free} test set	3093 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.090 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9319	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.62% 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: TPO, SEP, 4GD

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	0.81	0/2268	1.32	7/3054 (0.2%)
1	B	0.82	0/2200	1.34	10/2963 (0.3%)
1	C	0.86	0/2263	1.33	8/3050 (0.3%)
1	D	0.86	1/2280 (0.0%)	1.33	6/3072 (0.2%)
All	All	0.84	1/9011 (0.0%)	1.33	31/12139 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	MET	SD-CE	-6.47	1.63	1.79

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	CB-CA-C	6.87	120.54	109.41
1	D	222	THR	CA-C-N	6.46	128.84	120.44
1	D	222	THR	C-N-CA	6.46	128.84	120.44
1	B	196	GLY	CA-C-N	5.98	128.78	120.29
1	B	196	GLY	C-N-CA	5.98	128.78	120.29

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	2265	0	2219	14	0
1	B	2197	0	2151	26	0
1	C	2259	0	2215	15	0
1	D	2275	0	2234	21	0
2	A	24	0	14	1	0
2	B	24	0	14	0	0
2	C	24	0	14	0	0
2	D	48	0	28	0	0
3	A	35	0	0	0	0
3	B	44	0	0	0	0
3	C	69	0	0	0	0
3	D	55	0	0	0	0
All	All	9319	0	8889	66	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.

The worst 5 of 66 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:A:438:HIS:HD2	1:A:443:LYS:HB2	1.06	1.09
1:A:438:HIS:CD2	1:A:443:LYS:HB2	1.98	0.98
1:A:438:HIS:HD2	1:A:443:LYS:CB	1.77	0.96
1:B:230:PHE:HE1	1:B:234:ILE:HD11	1.43	0.83
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.58	0.83

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 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	280/301 (93%)	271 (97%)	8 (3%)	1 (0%)	30 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	271/301 (90%)	259 (96%)	12 (4%)	0	100	100
1	C	281/301 (93%)	273 (97%)	7 (2%)	1 (0%)	30	37
1	D	281/301 (93%)	275 (98%)	6 (2%)	0	100	100
All	All	1113/1204 (92%)	1078 (97%)	33 (3%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	181	ASP
1	A	206	ASN

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 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	247/259 (95%)	239 (97%)	8 (3%)	34	50
1	B	239/259 (92%)	233 (98%)	6 (2%)	42	59
1	C	245/259 (95%)	237 (97%)	8 (3%)	33	48
1	D	248/259 (96%)	243 (98%)	5 (2%)	48	66
All	All	979/1036 (94%)	952 (97%)	27 (3%)	38	55

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	183	ARG
1	C	227	LYS
1	D	394	GLN
1	C	194	GLU
1	C	344	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	438	HIS
1	D	178	ASN
1	D	394	GLN
1	D	175	ASN
1	D	190	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
1	SEP	B	346	1	8,9,10	0.98	0	7,12,14	1.91	1 (14%)
1	TPO	C	345	1	8,10,11	1.37	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	C	342	1	8,10,11	1.24	1 (12%)	10,14,16	1.42	1 (10%)
1	SEP	D	346	1	8,9,10	0.99	0	7,12,14	2.26	1 (14%)
1	TPO	D	342	1	8,10,11	1.51	1 (12%)	10,14,16	1.39	1 (10%)
1	TPO	A	342	1	8,10,11	1.32	1 (12%)	10,14,16	1.49	1 (10%)
1	TPO	B	342	1	8,10,11	1.29	1 (12%)	10,14,16	1.44	1 (10%)
1	TPO	B	345	1	8,10,11	1.20	1 (12%)	10,14,16	1.33	1 (10%)
1	SEP	C	346	1	8,9,10	1.02	0	7,12,14	1.93	1 (14%)
1	TPO	D	345	1	8,10,11	0.86	0	10,14,16	1.36	2 (20%)
1	TPO	A	345	1	8,10,11	1.25	1 (12%)	10,14,16	1.49	3 (30%)
1	SEP	A	346	1	8,9,10	0.90	0	7,12,14	1.85	2 (28%)

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
1	SEP	B	346	1	-	2/6/8/10	-
1	TPO	C	345	1	-	2/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	2/6/8/10	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	2/6/8/10	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-3.65	1.53	1.59
1	A	342	TPO	P-OG1	-3.17	1.54	1.59
1	B	342	TPO	P-OG1	-3.02	1.54	1.59
1	C	342	TPO	P-OG1	-2.84	1.54	1.59
1	C	345	TPO	P-OG1	-2.81	1.54	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	5.33	113.34	108.14
1	C	346	SEP	OG-CB-CA	4.86	112.88	108.14
1	B	346	SEP	OG-CB-CA	4.82	112.83	108.14
1	A	346	SEP	OG-CB-CA	4.29	112.32	108.14
1	A	342	TPO	P-OG1-CB	-3.47	113.89	123.33

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	B	346	SEP	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	342	TPO	1	0
1	D	342	TPO	1	0
1	A	342	TPO	1	0
1	B	342	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4GD	B	501	-	27,27,27	2.34	13 (48%)	33,38,38	1.39	4 (12%)
2	4GD	D	501	-	27,27,27	2.16	12 (44%)	33,38,38	1.93	8 (24%)
2	4GD	C	501	-	27,27,27	2.17	12 (44%)	33,38,38	1.62	5 (15%)
2	4GD	D	502	-	27,27,27	2.21	10 (37%)	33,38,38	2.06	9 (27%)
2	4GD	A	501	-	27,27,27	2.17	12 (44%)	33,38,38	1.40	7 (21%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4GD	B	501	-	-	0/12/12/12	0/4/4/4
2	4GD	D	501	-	-	0/12/12/12	0/4/4/4
2	4GD	C	501	-	-	0/12/12/12	0/4/4/4
2	4GD	D	502	-	-	0/12/12/12	0/4/4/4
2	4GD	A	501	-	-	0/12/12/12	0/4/4/4

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4GD	C08-N07	5.51	1.48	1.38
2	D	502	4GD	C21-C20	4.45	1.46	1.38
2	D	502	4GD	C13-N17	4.26	1.40	1.36
2	A	501	4GD	C14-C13	3.99	1.42	1.37
2	B	501	4GD	C12-C11	3.96	1.43	1.35

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4GD	C14-C13-N17	6.26	111.18	107.01
2	D	502	4GD	C10-N09-C08	5.69	119.97	115.55
2	D	502	4GD	C04-C08-N09	4.50	135.56	132.07
2	D	502	4GD	C13-N17-N16	-4.14	108.23	111.82
2	D	502	4GD	C15-N16-N17	3.89	107.10	104.57

There are no chirality outliers.

There are no torsion outliers.

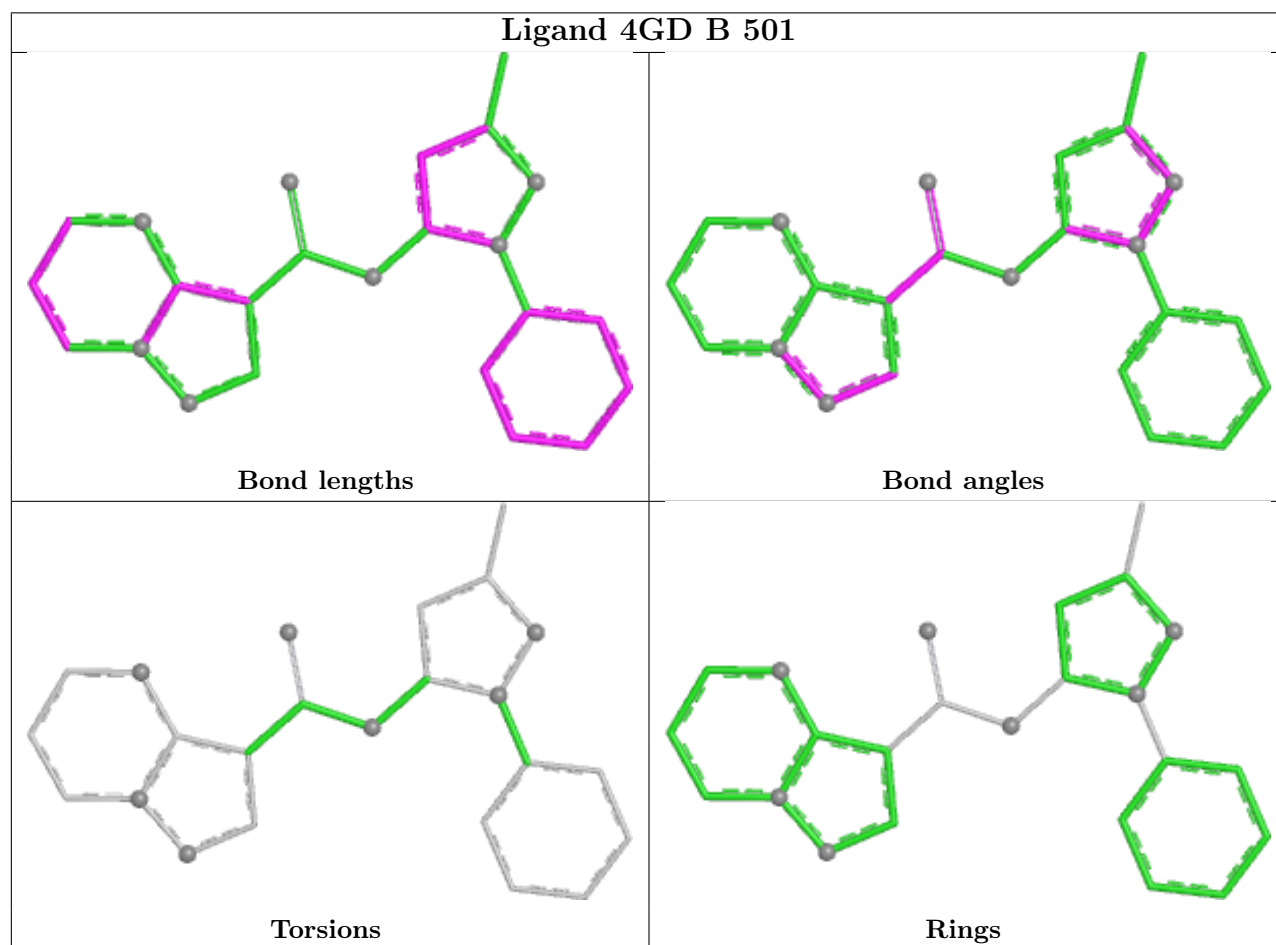
There are no ring outliers.

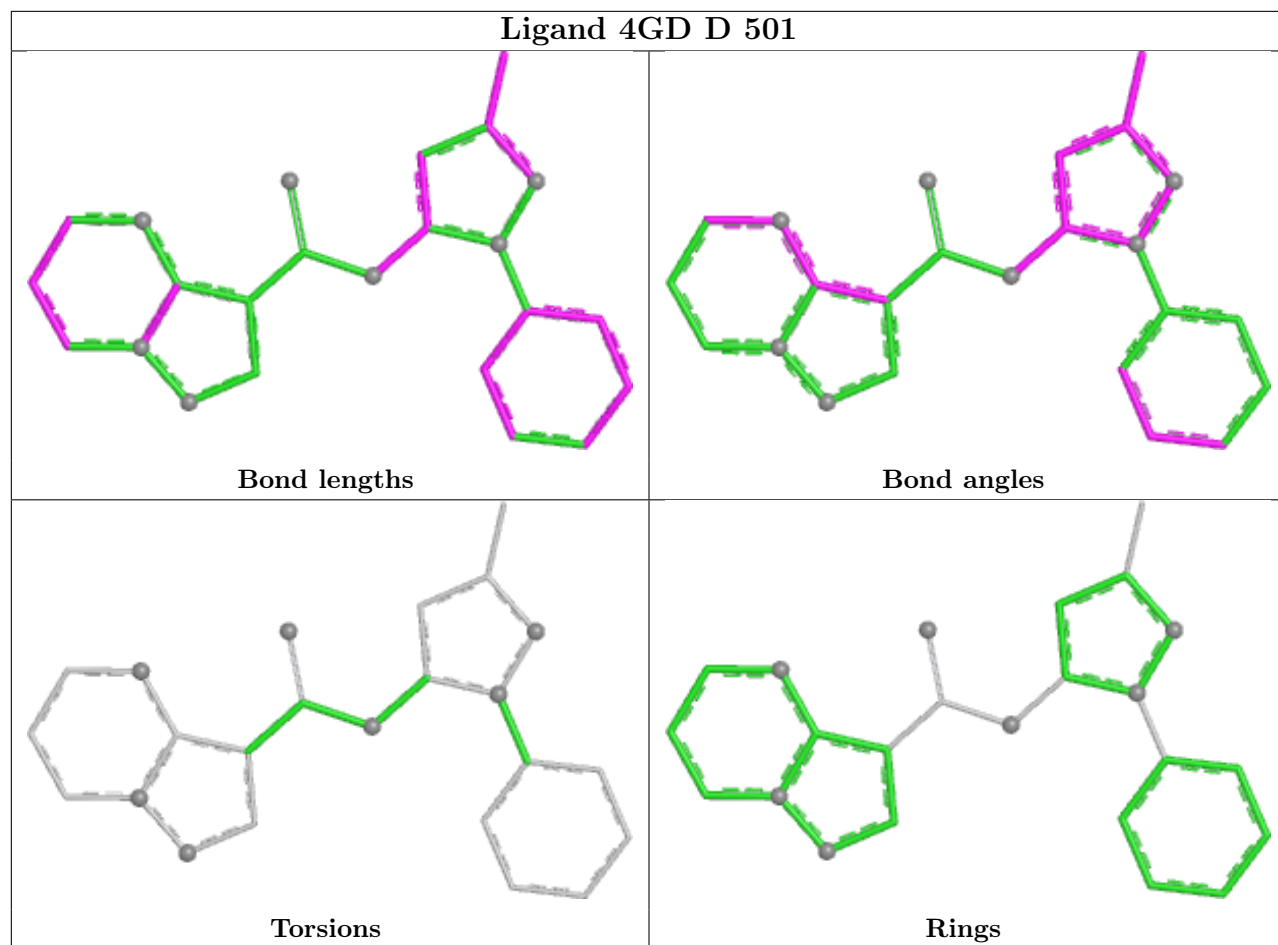
1 monomer is involved in 1 short contact:

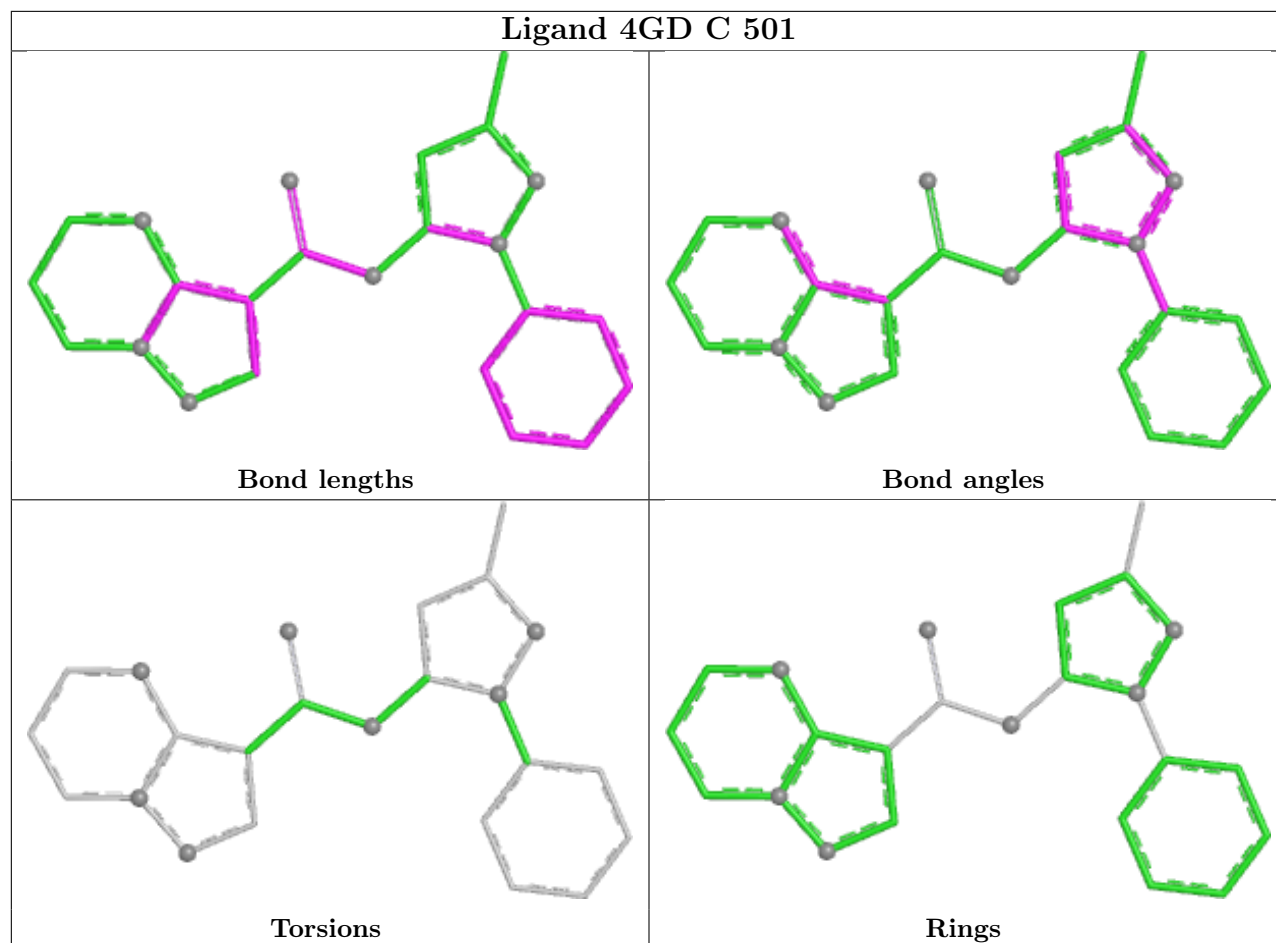
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4GD	1	0

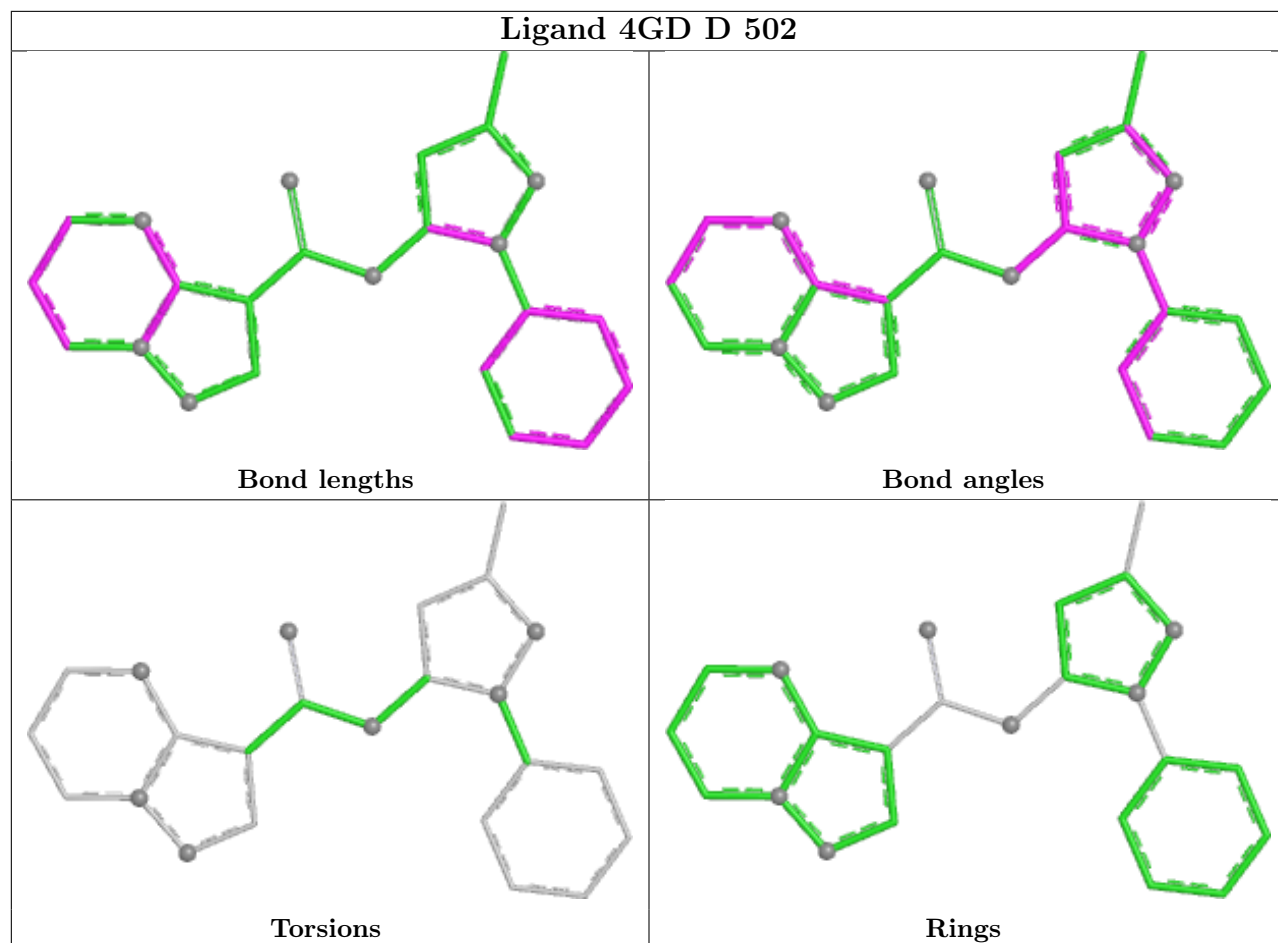
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

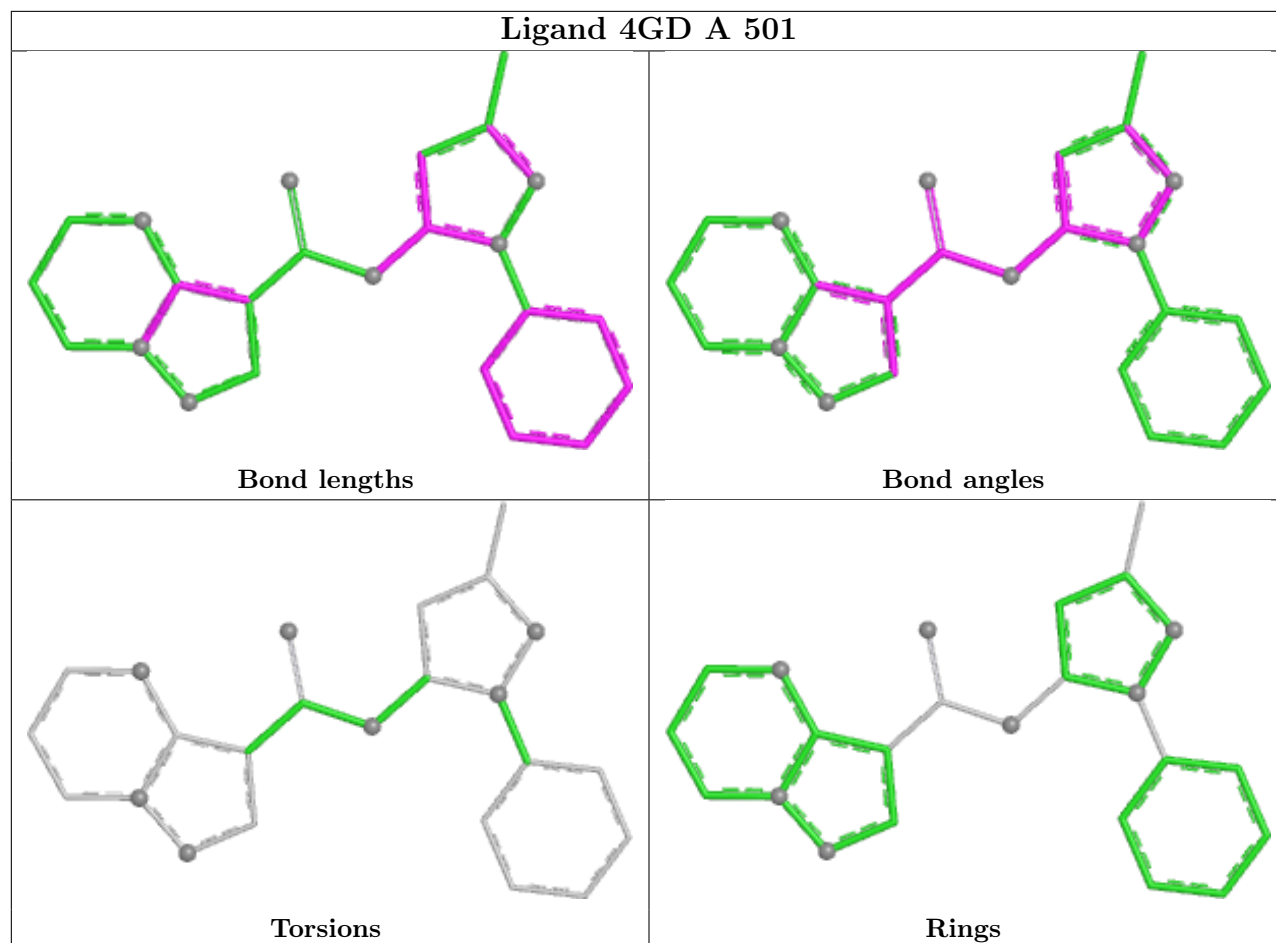
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	286/301 (95%)	0.64	28 (9%) 13 15	31, 57, 96, 107	0
1	B	277/301 (92%)	0.65	31 (11%) 10 11	31, 53, 101, 116	0
1	C	286/301 (95%)	0.22	16 (5%) 30 32	29, 47, 83, 100	0
1	D	285/301 (94%)	0.33	16 (5%) 30 32	27, 47, 82, 103	1 (0%)
All	All	1134/1204 (94%)	0.46	91 (8%) 18 20	27, 50, 94, 116	1 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	ILE	7.3
1	A	216	ALA	7.1
1	A	337	GLU	7.1
1	A	240	CYS	7.1
1	D	337	GLU	6.8

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	B	346	10/11	0.43	0.15	93,97,101,101	0
1	SEP	D	346	10/11	0.73	0.14	76,82,91,91	0
1	TPO	D	342	11/12	0.75	0.15	81,83,89,89	0
1	TPO	C	342	11/12	0.77	0.14	87,88,94,94	0
1	SEP	A	346	10/11	0.78	0.10	83,88,95,95	0
1	SEP	C	346	10/11	0.78	0.12	72,78,87,88	0
1	TPO	A	342	11/12	0.79	0.14	102,103,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	B	345	11/12	0.86	0.13	89,90,93,94	0
1	TPO	B	342	11/12	0.86	0.12	96,98,99,100	0
1	TPO	A	345	11/12	0.90	0.12	83,84,86,87	0
1	TPO	D	345	11/12	0.92	0.10	68,69,76,76	0
1	TPO	C	345	11/12	0.94	0.08	65,67,72,73	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

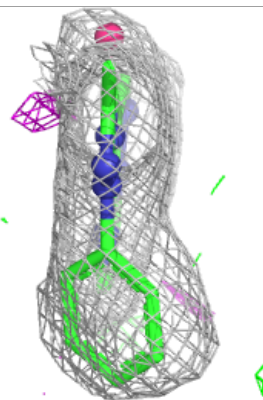
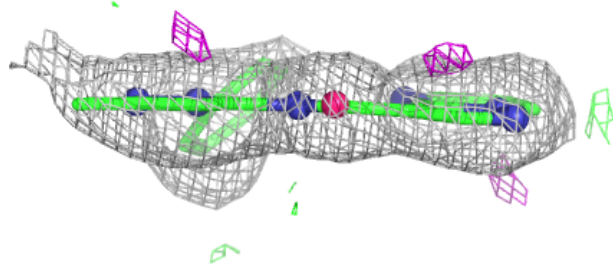
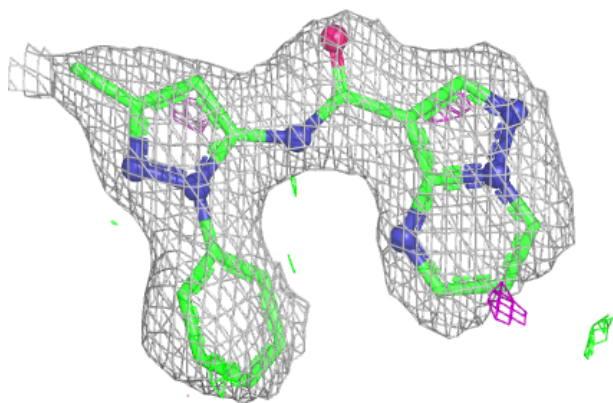
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4GD	D	502	24/24	0.90	0.11	52,56,58,59	0
2	4GD	B	501	24/24	0.92	0.09	40,43,55,56	0
2	4GD	A	501	24/24	0.93	0.09	40,46,55,55	0
2	4GD	C	501	24/24	0.95	0.07	33,38,45,45	0
2	4GD	D	501	24/24	0.96	0.07	30,36,42,43	0

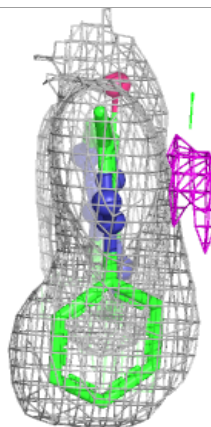
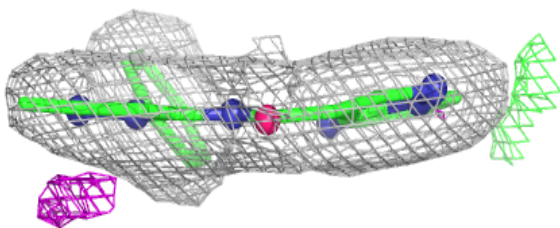
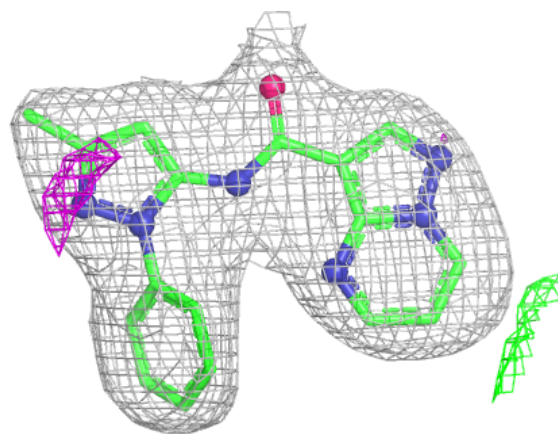
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4GD D 502:

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

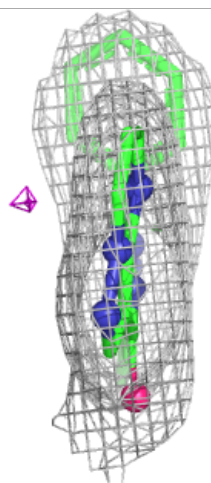
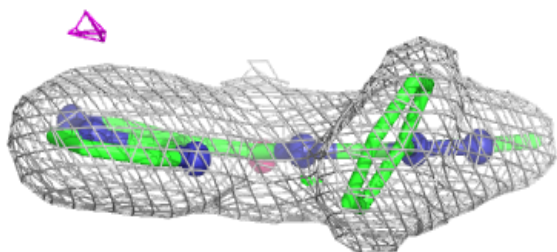
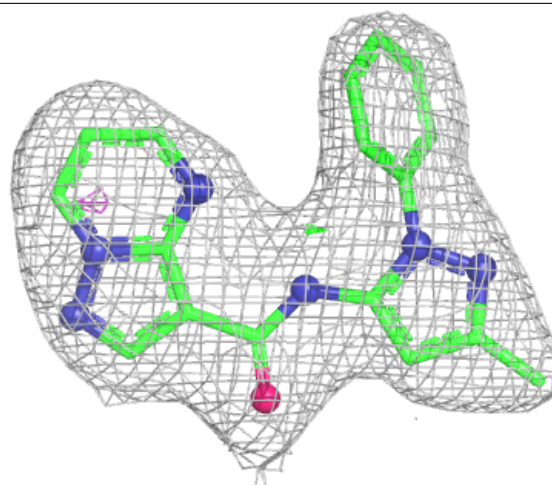
**Electron density around 4GD B 501:**

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



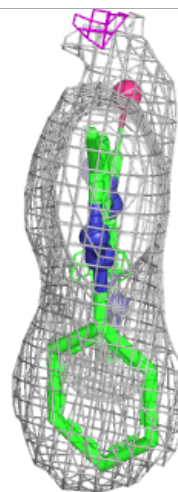
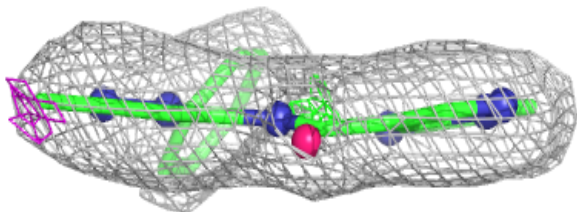
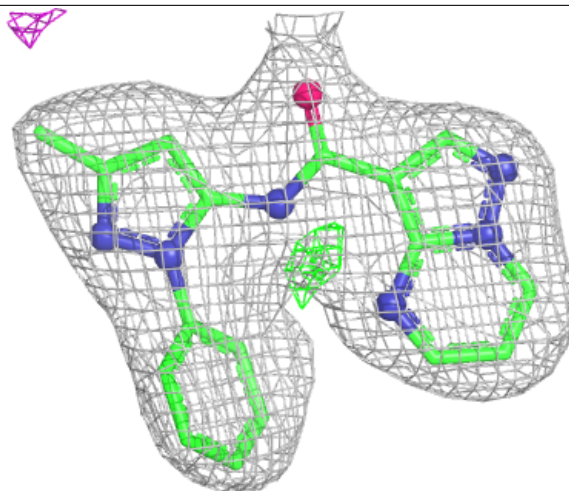
Electron density around 4GD A 501:

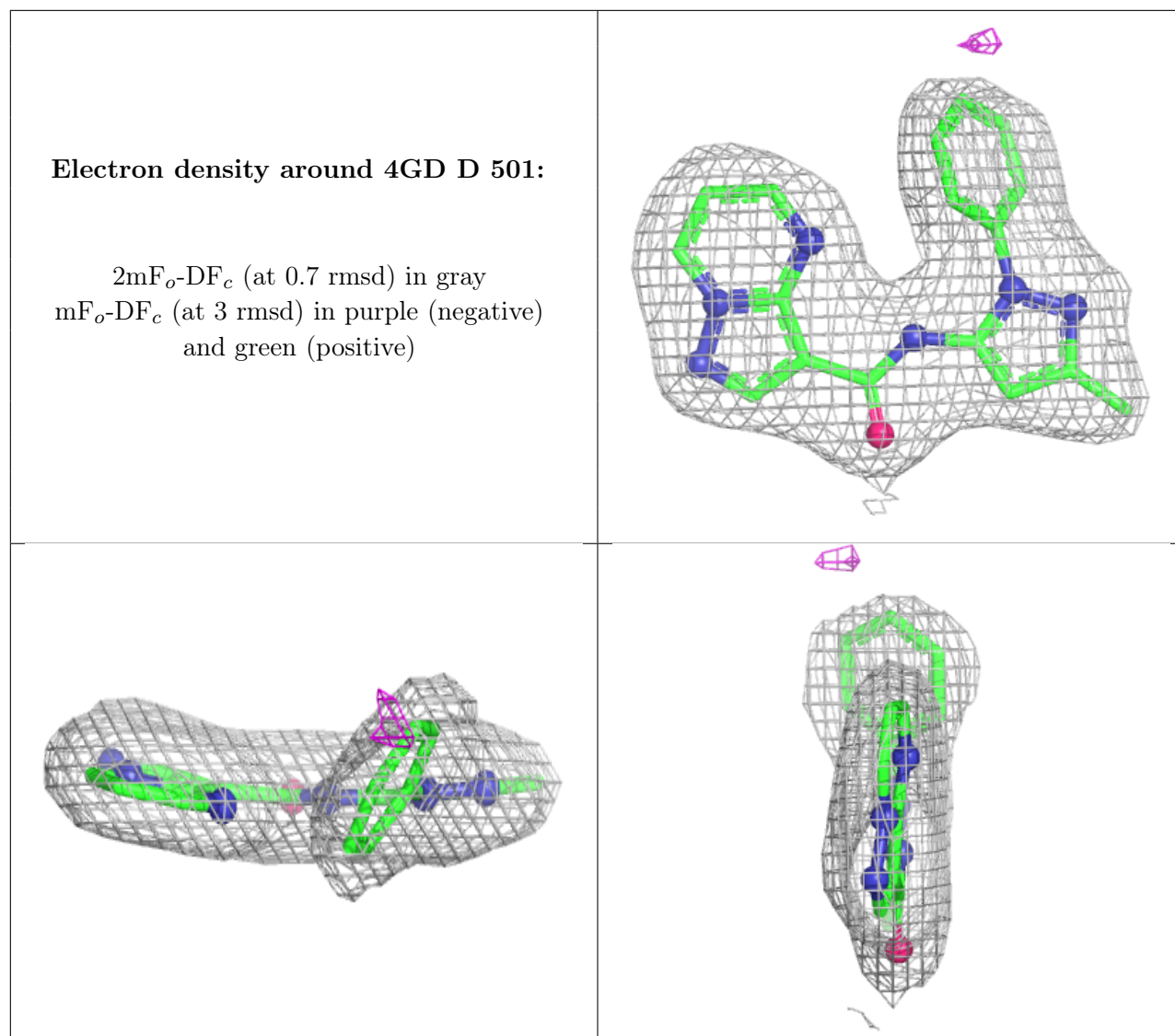
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4GD C 501:

$2mF_o-DF_c$ (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.