



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:45 pm BST

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

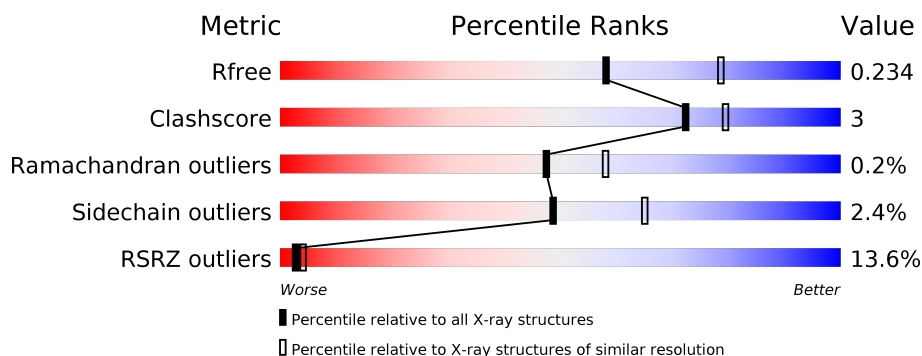
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 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	301	<div> <div>18%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	B	301	<div> <div>18%</div> <div>84%</div> <div>8%</div> <div>.</div> <div>7%</div> </div>
1	C	301	<div> <div>8%</div> <div>89%</div> <div>6%</div> <div>.</div> <div>.</div> </div>
1	D	301	<div> <div>7%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition [i](#)

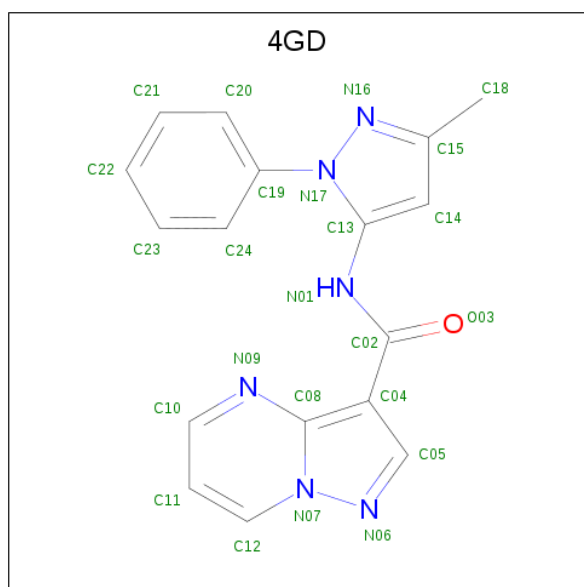
There are 3 unique types of molecules in this entry. The entry contains 9319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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

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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		

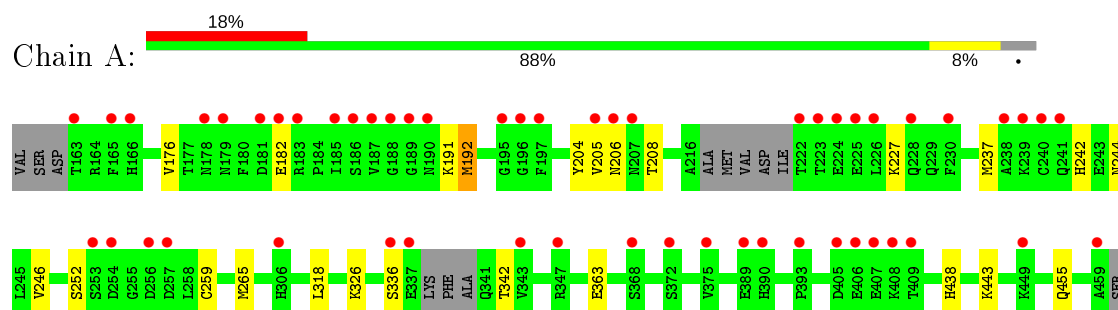
- Molecule 3 is water.

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		

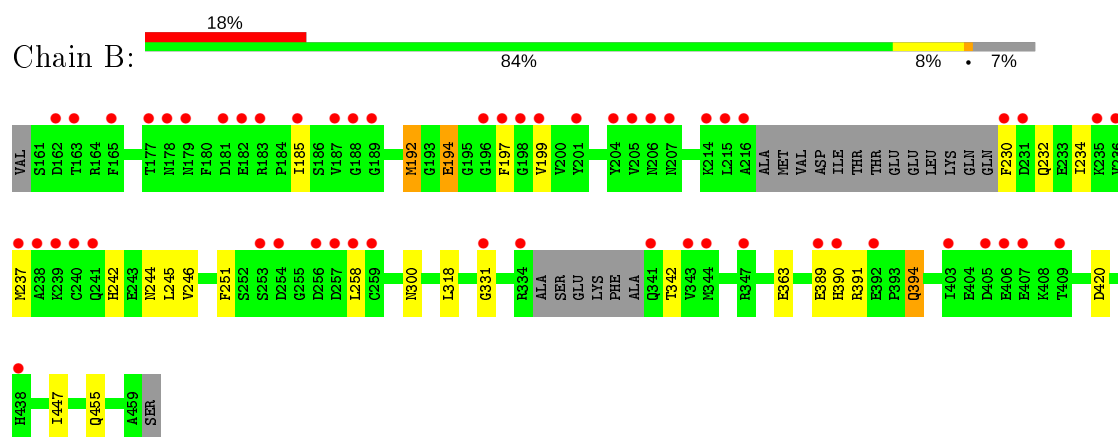
3 Residue-property plots [i](#)

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.

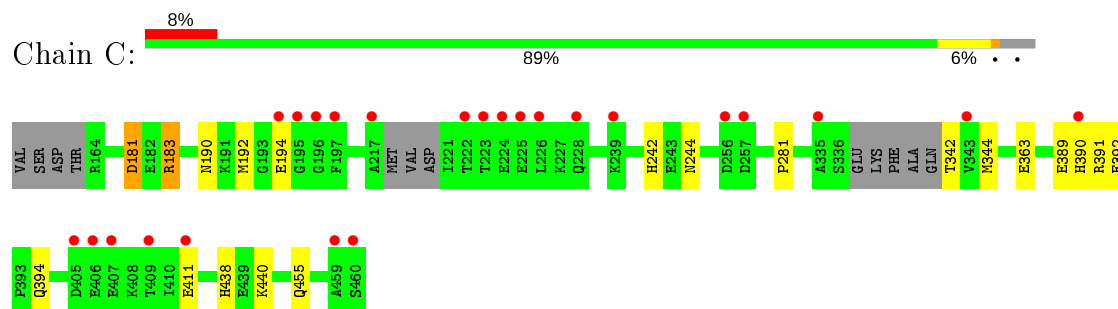
- Molecule 1: Interleukin-1 receptor-associated kinase 4



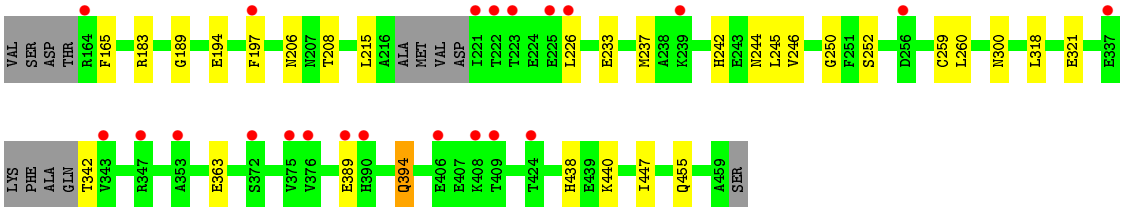
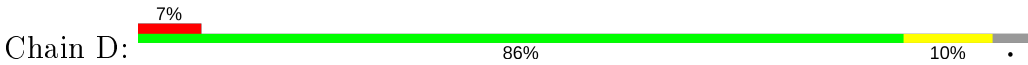
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

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 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.23-2.32) 99.4 (34.23-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.31Å)	Xtriage
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 (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.090 for -h-2*k,l	Xtriage
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

Xtriage'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, 4GD, SEP

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	0.48	0/2268	0.66	0/3054
1	B	0.48	0/2200	0.67	0/2963
1	C	0.51	0/2263	0.67	1/3050 (0.0%)
1	D	0.52	0/2280	0.66	0/3072
All	All	0.50	0/9011	0.66	1/12139 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	CB-CA-C	5.07	120.54	110.40

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	2218	13	0
1	B	2197	0	2150	25	0
1	C	2259	0	2215	14	0
1	D	2275	0	2234	20	0
2	A	24	0	14	1	0
2	B	24	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8887	62	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 3.

All (62) 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:420:ASP:HA	1:D:208:THR:HG21	1.61	0.83
1:B:390:HIS:O	1:C:390:HIS:O	2.00	0.79
1:A:438:HIS:CD2	1:A:443:LYS:CB	2.63	0.76
1:B:390:HIS:HB3	1:C:391:ARG:HA	1.75	0.68
1:B:391:ARG:HA	1:C:390:HIS:HB3	1.80	0.63
1:B:389:GLU:HA	1:B:394:GLN:NE2	2.16	0.60
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.84	0.60
1:B:420:ASP:HA	1:D:208:THR:CG2	2.29	0.59
1:B:230:PHE:HE1	1:B:234:ILE:CD1	2.16	0.59
1:B:230:PHE:CD2	1:B:258:LEU:HB3	2.39	0.58
1:C:242:HIS:CD2	1:C:244:ASN:H	2.22	0.56
1:D:206:ASN:O	1:D:208:THR:HG23	2.06	0.56
1:D:389:GLU:HA	1:D:394:GLN:NE2	2.19	0.56
1:D:438:HIS:HD2	1:D:440:LYS:H	1.54	0.56
1:C:389:GLU:HA	1:C:394:GLN:NE2	2.20	0.56
1:B:185:ILE:HD11	1:B:192:MET:HG3	1.87	0.55
1:B:230:PHE:HD2	1:B:258:LEU:HB3	1.72	0.55
1:C:242:HIS:HD2	1:C:244:ASN:H	1.55	0.55
1:B:230:PHE:CE1	1:B:234:ILE:HD11	2.33	0.54
1:C:438:HIS:HD2	1:C:440:LYS:H	1.55	0.53
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.92	0.52
1:D:237:MET:HE1	1:D:246:VAL:HG23	1.92	0.51
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:HIS:CD2	1:B:244:ASN:H	2.27	0.51
1:C:281:PRO:CD	1:D:321:GLU:HG3	2.42	0.50
1:A:192:MET:HG2	2:A:501:4GD:C15	2.43	0.49
1:B:194:GLU:HG3	1:B:199:VAL:HG22	1.95	0.49
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.96	0.48
1:B:237:MET:CE	1:B:246:VAL:HG23	2.42	0.48
1:D:215:LEU:HB3	1:D:226:LEU:HD22	1.95	0.48
1:C:281:PRO:HD3	1:D:321:GLU:HG3	1.96	0.48
1:B:390:HIS:ND1	1:C:392:GLU:HB3	2.30	0.47
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.95	0.47
1:C:181:ASP:HB3	1:C:190:ASN:HB2	1.96	0.47
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.96	0.46
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.98	0.46
1:A:182:GLU:HG2	1:A:191:LYS:HD2	1.96	0.46
1:C:394:GLN:HB3	1:C:394:GLN:HE21	1.63	0.45
1:D:237:MET:CE	1:D:246:VAL:HG23	2.46	0.45
1:B:420:ASP:CA	1:D:208:THR:HG21	2.40	0.45
1:A:242:HIS:CD2	1:A:244:ASN:H	2.34	0.45
1:B:230:PHE:CE2	1:B:258:LEU:HD22	2.52	0.45
1:B:342:TPO:HG21	1:B:363:GLU:OE1	2.17	0.45
1:A:342:TPO:HG21	1:A:363:GLU:OE1	2.17	0.44
1:D:342:TPO:HG21	1:D:363:GLU:OE1	2.17	0.43
1:A:237:MET:CE	1:A:246:VAL:HG23	2.48	0.43
1:C:342:TPO:HG21	1:C:363:GLU:OE1	2.18	0.43
1:B:242:HIS:HB3	1:B:245:LEU:HG	2.00	0.43
1:D:242:HIS:CD2	1:D:244:ASN:H	2.37	0.42
1:A:265:MET:SD	1:A:326:LYS:HG3	2.59	0.42
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.01	0.41
1:B:232:GLN:HG2	1:B:331:GLY:O	2.21	0.41
1:D:183:ARG:HB2	1:D:189:GLY:HA3	2.03	0.41
1:A:176:VAL:HB	1:A:204:TYR:H	1.86	0.41
1:D:242:HIS:HB3	1:D:245:LEU:HG	2.03	0.40
1:D:246:VAL:HG11	1:D:318:LEU:HD12	2.03	0.40
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.03	0.40
1:B:390:HIS:HB3	1:C:392:GLU:H	1.86	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	280/301 (93%)	271 (97%)	8 (3%)	1 (0%)	34	41
1	B	271/301 (90%)	259 (96%)	12 (4%)	0	100	100
1	C	281/301 (93%)	273 (97%)	7 (2%)	1 (0%)	34	41
1	D	281/301 (93%)	275 (98%)	6 (2%)	0	100	100
All	All	1113/1204 (92%)	1078 (97%)	33 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

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

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	247/259 (95%)	240 (97%)	7 (3%)	43	59
1	B	239/259 (92%)	233 (98%)	6 (2%)	47	64
1	C	245/259 (95%)	239 (98%)	6 (2%)	49	65
1	D	248/259 (96%)	244 (98%)	4 (2%)	62	77
All	All	979/1036 (94%)	956 (98%)	23 (2%)	49	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	MET
1	A	205	VAL
1	A	208	THR
1	A	227	LYS
1	A	318	LEU
1	A	336	SER
1	A	455	GLN
1	B	192	MET
1	B	194	GLU
1	B	197	PHE
1	B	251	PHE
1	B	394	GLN
1	B	455	GLN
1	C	183	ARG
1	C	192	MET
1	C	194	GLU
1	C	344	MET
1	C	411	GLU
1	C	455	GLN
1	D	194	GLU
1	D	197	PHE
1	D	394	GLN
1	D	455	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	232	GLN
1	A	242	HIS
1	A	419	ASN
1	A	438	HIS
1	B	242	HIS
1	B	394	GLN
1	C	166	HIS
1	C	190	ASN
1	C	242	HIS
1	C	394	GLN
1	C	419	ASN
1	C	438	HIS
1	D	242	HIS
1	D	394	GLN
1	D	438	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TPO	B	345	1	8,10,11	1.11	1 (12%)	10,14,16	1.20	1 (10%)
1	SEP	D	346	1	8,9,10	0.95	0	8,12,14	2.48	2 (25%)
1	SEP	C	346	1	8,9,10	0.97	0	8,12,14	2.05	2 (25%)
1	SEP	B	346	1	8,9,10	0.94	0	8,12,14	2.06	2 (25%)
1	SEP	A	346	1	8,9,10	0.86	0	8,12,14	2.10	3 (37%)
1	TPO	C	342	1	8,10,11	1.14	1 (12%)	10,14,16	1.29	1 (10%)
1	TPO	C	345	1	8,10,11	1.27	1 (12%)	10,14,16	1.12	1 (10%)
1	TPO	A	345	1	8,10,11	1.17	0	10,14,16	1.37	2 (20%)
1	TPO	D	345	1	8,10,11	0.80	0	10,14,16	1.23	1 (10%)
1	TPO	D	342	1	8,10,11	1.38	1 (12%)	10,14,16	1.25	1 (10%)
1	TPO	A	342	1	8,10,11	1.21	1 (12%)	10,14,16	1.36	1 (10%)
1	TPO	B	342	1	8,10,11	1.19	1 (12%)	10,14,16	1.31	1 (10%)

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	TPO	B	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-
1	SEP	C	346	1	-	1/5/8/10	-
1	SEP	B	346	1	-	1/5/8/10	-
1	SEP	A	346	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	342	1	-	0/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	D	342	1	-	0/9/11/13	-
1	TPO	A	342	1	-	0/9/11/13	-
1	TPO	B	342	1	-	0/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-3.27	1.53	1.59
1	A	342	TPO	P-OG1	-2.82	1.54	1.59
1	B	342	TPO	P-OG1	-2.69	1.54	1.59
1	C	342	TPO	P-OG1	-2.52	1.54	1.59
1	C	345	TPO	P-OG1	-2.49	1.54	1.59
1	B	345	TPO	P-OG1	-2.10	1.55	1.59

All (18) 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	D	346	SEP	P-OG-CB	-3.72	108.05	118.30
1	A	346	SEP	P-OG-CB	-3.40	108.92	118.30
1	A	342	TPO	P-OG1-CB	-3.08	113.89	123.21
1	C	342	TPO	P-OG1-CB	-3.03	114.06	123.21
1	B	342	TPO	P-OG1-CB	-2.96	114.27	123.21
1	B	346	SEP	P-OG-CB	-2.93	110.23	118.30
1	D	342	TPO	P-OG1-CB	-2.80	114.76	123.21
1	C	346	SEP	P-OG-CB	-2.79	110.61	118.30
1	A	345	TPO	CG2-CB-CA	-2.41	108.41	113.16
1	B	345	TPO	O3P-P-OG1	2.25	116.08	105.99
1	D	345	TPO	O3P-P-OG1	2.19	115.79	105.99
1	A	346	SEP	O3P-P-OG	2.18	112.52	106.73
1	C	345	TPO	OG1-P-O1P	2.02	117.21	109.39
1	A	345	TPO	P-OG1-CB	-2.02	117.10	123.21

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	D	346	SEP	N-CA-CB-OG
1	C	346	SEP	N-CA-CB-OG
1	B	346	SEP	N-CA-CB-OG
1	A	346	SEP	N-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	A	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB

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 carbohydrates 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	A	501	-	22,27,27	1.84	9 (40%)	23,38,38	1.25	2 (8%)
2	4GD	D	501	-	22,27,27	1.98	11 (50%)	23,38,38	1.45	3 (13%)
2	4GD	D	502	-	22,27,27	2.07	10 (45%)	23,38,38	1.65	7 (30%)
2	4GD	B	501	-	22,27,27	1.99	10 (45%)	23,38,38	1.39	3 (13%)
2	4GD	C	501	-	22,27,27	2.02	10 (45%)	23,38,38	1.27	1 (4%)

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
2	4GD	A	501	-	-	0/8/12/12	0/4/4/4
2	4GD	D	501	-	-	0/8/12/12	0/4/4/4
2	4GD	D	502	-	-	0/8/12/12	0/4/4/4
2	4GD	B	501	-	-	0/8/12/12	0/4/4/4
2	4GD	C	501	-	-	0/8/12/12	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4GD	C20-C19	4.13	1.46	1.38
2	D	502	4GD	C20-C19	4.04	1.46	1.38
2	D	502	4GD	C21-C20	3.61	1.46	1.38
2	B	501	4GD	C11-C10	3.50	1.48	1.37
2	A	501	4GD	C24-C19	3.42	1.45	1.38
2	A	501	4GD	C20-C19	3.40	1.45	1.38
2	D	502	4GD	C13-N17	3.23	1.40	1.37
2	D	502	4GD	C08-N09	3.18	1.40	1.35
2	C	501	4GD	C20-C19	3.06	1.44	1.38
2	B	501	4GD	C12-C11	3.02	1.43	1.35
2	C	501	4GD	C23-C24	2.97	1.45	1.38
2	D	502	4GD	C12-C11	2.94	1.43	1.35
2	C	501	4GD	C13-N17	2.92	1.40	1.37
2	C	501	4GD	C04-C02	-2.91	1.45	1.50
2	D	501	4GD	C24-C19	2.90	1.44	1.38
2	C	501	4GD	C24-C19	2.86	1.44	1.38
2	C	501	4GD	C21-C20	2.82	1.44	1.38
2	D	501	4GD	C08-N09	2.78	1.39	1.35
2	D	502	4GD	C24-C19	2.77	1.43	1.38
2	C	501	4GD	C23-C22	2.73	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	4GD	C13-N01	-2.70	1.34	1.39
2	D	501	4GD	C11-C10	2.69	1.45	1.37
2	B	501	4GD	C10-N09	2.64	1.37	1.32
2	D	501	4GD	C12-C11	2.62	1.42	1.35
2	D	502	4GD	C11-C10	2.61	1.45	1.37
2	B	501	4GD	C23-C22	2.60	1.44	1.38
2	D	501	4GD	C20-C19	2.56	1.43	1.38
2	B	501	4GD	C14-C15	2.52	1.45	1.39
2	D	502	4GD	C22-C21	2.51	1.44	1.38
2	B	501	4GD	C24-C19	2.50	1.43	1.38
2	D	501	4GD	C10-N09	2.45	1.37	1.32
2	B	501	4GD	C23-C24	2.45	1.44	1.38
2	A	501	4GD	C22-C21	2.43	1.44	1.38
2	D	501	4GD	C21-C20	2.41	1.44	1.38
2	D	501	4GD	C22-C21	2.40	1.44	1.38
2	A	501	4GD	C23-C24	2.34	1.43	1.38
2	C	501	4GD	O03-C02	2.34	1.28	1.23
2	D	501	4GD	C04-C02	-2.31	1.46	1.50
2	A	501	4GD	C10-N09	2.29	1.37	1.32
2	A	501	4GD	C23-C22	2.28	1.44	1.38
2	A	501	4GD	C11-C10	2.23	1.44	1.37
2	B	501	4GD	C22-C21	2.23	1.43	1.38
2	A	501	4GD	C21-C20	2.23	1.43	1.38
2	C	501	4GD	C22-C21	2.20	1.43	1.38
2	D	502	4GD	C23-C22	2.17	1.43	1.38
2	A	501	4GD	C15-N16	2.14	1.38	1.33
2	B	501	4GD	C21-C20	2.14	1.43	1.38
2	D	501	4GD	C23-C24	2.13	1.43	1.38
2	D	502	4GD	C10-N09	2.07	1.36	1.32
2	C	501	4GD	N16-N17	-2.02	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4GD	C13-C14-C15	-4.43	102.66	107.23
2	D	501	4GD	C13-C14-C15	-4.02	103.08	107.23
2	A	501	4GD	O03-C02-C04	-3.56	116.80	121.72
2	B	501	4GD	C05-N06-N07	3.32	106.12	103.70
2	B	501	4GD	O03-C02-C04	-3.22	117.28	121.72
2	B	501	4GD	C13-C14-C15	-3.12	104.01	107.23
2	A	501	4GD	C13-C14-C15	-3.12	104.01	107.23
2	D	502	4GD	C23-C24-C19	2.83	122.31	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	4GD	C13-C14-C15	-2.69	104.46	107.23
2	D	502	4GD	C10-N09-C08	2.58	119.97	116.77
2	D	502	4GD	C13-N01-C02	2.52	133.18	126.46
2	D	502	4GD	O03-C02-C04	-2.40	118.40	121.72
2	D	501	4GD	C23-C24-C19	2.38	121.72	118.63
2	D	502	4GD	C24-C19-C20	-2.37	117.81	121.33
2	D	501	4GD	C13-N01-C02	2.26	132.48	126.46
2	D	502	4GD	C05-N06-N07	2.06	105.19	103.70

There are no chirality outliers.

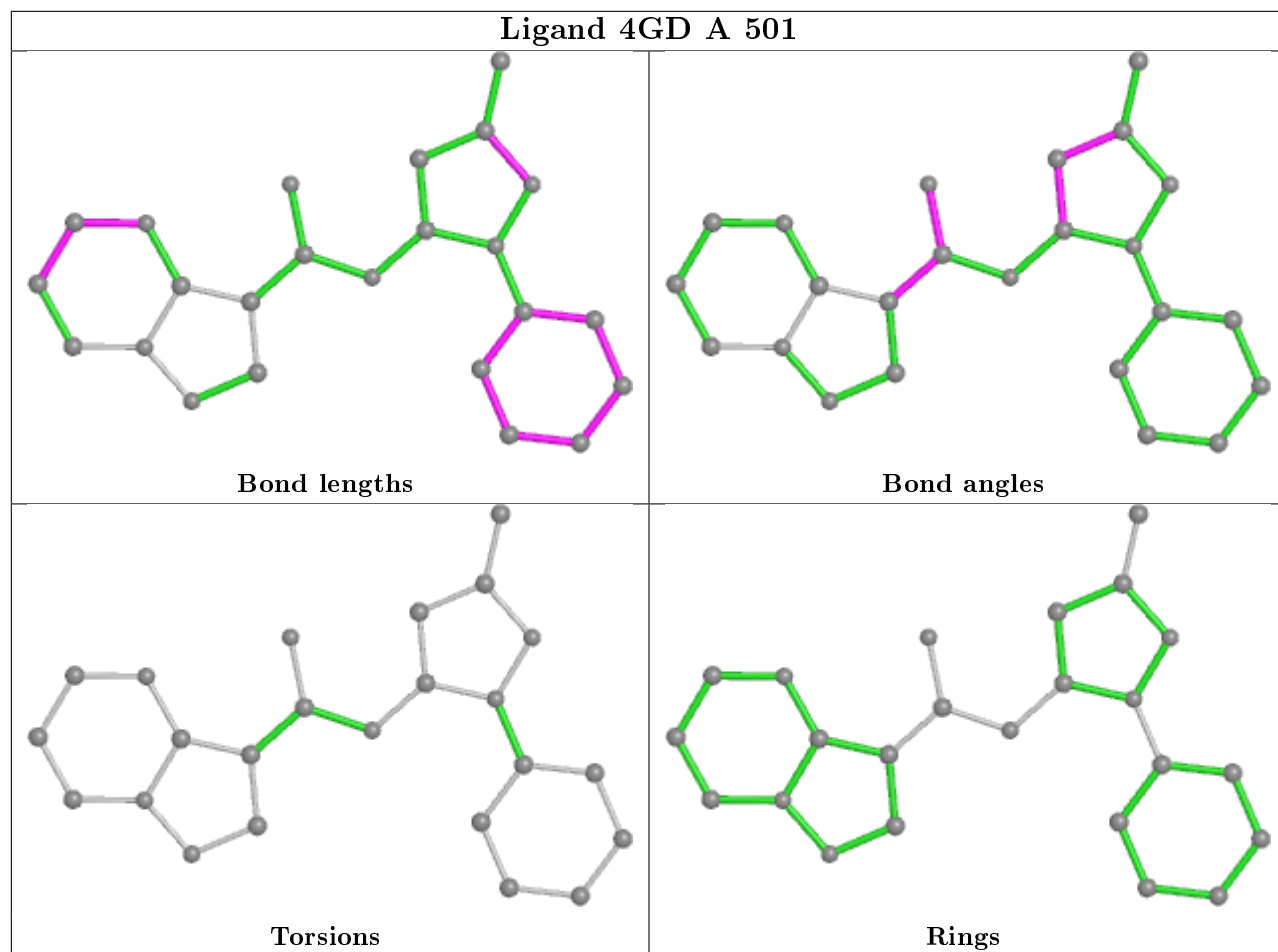
There are no torsion outliers.

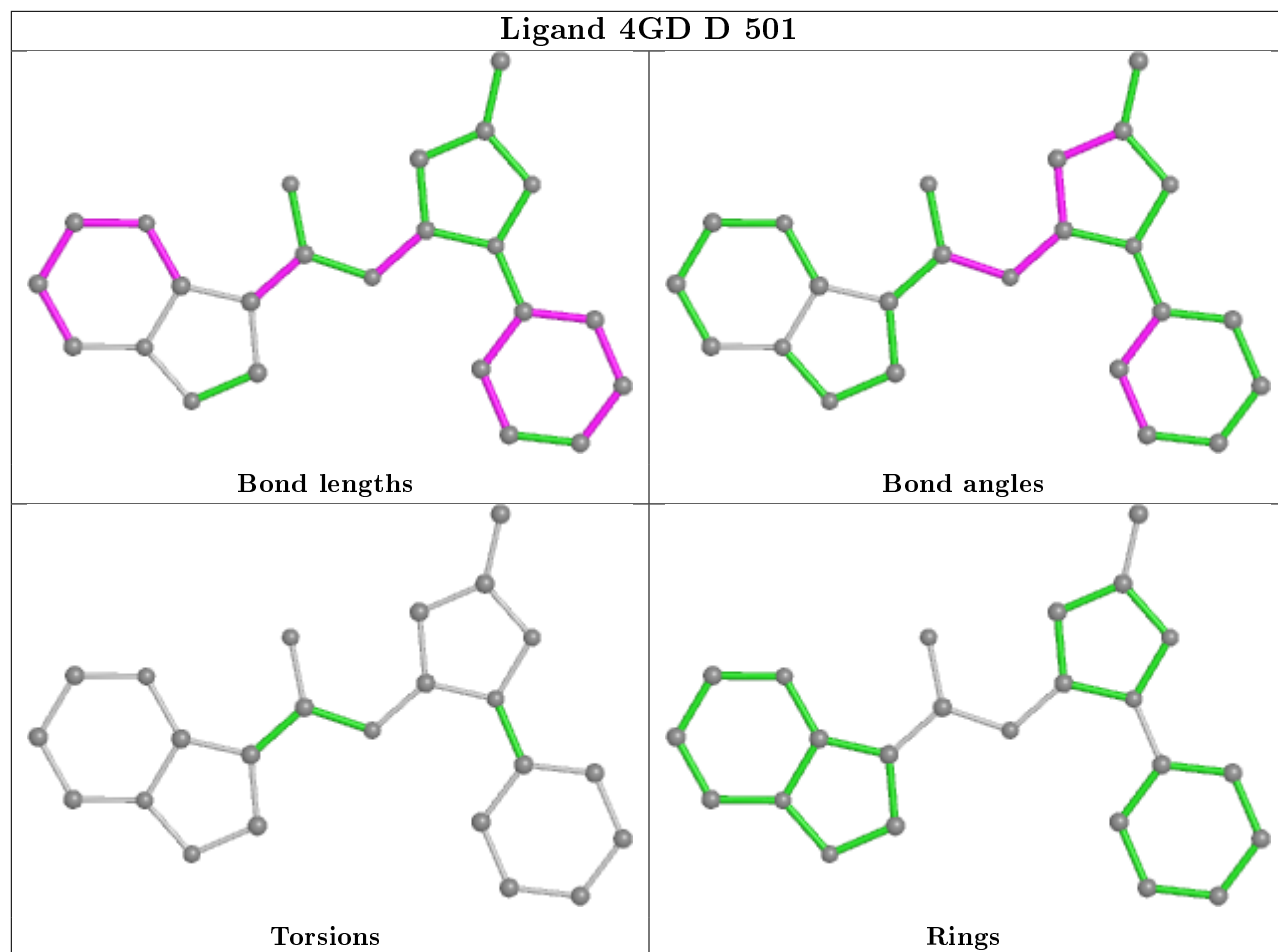
There are no ring outliers.

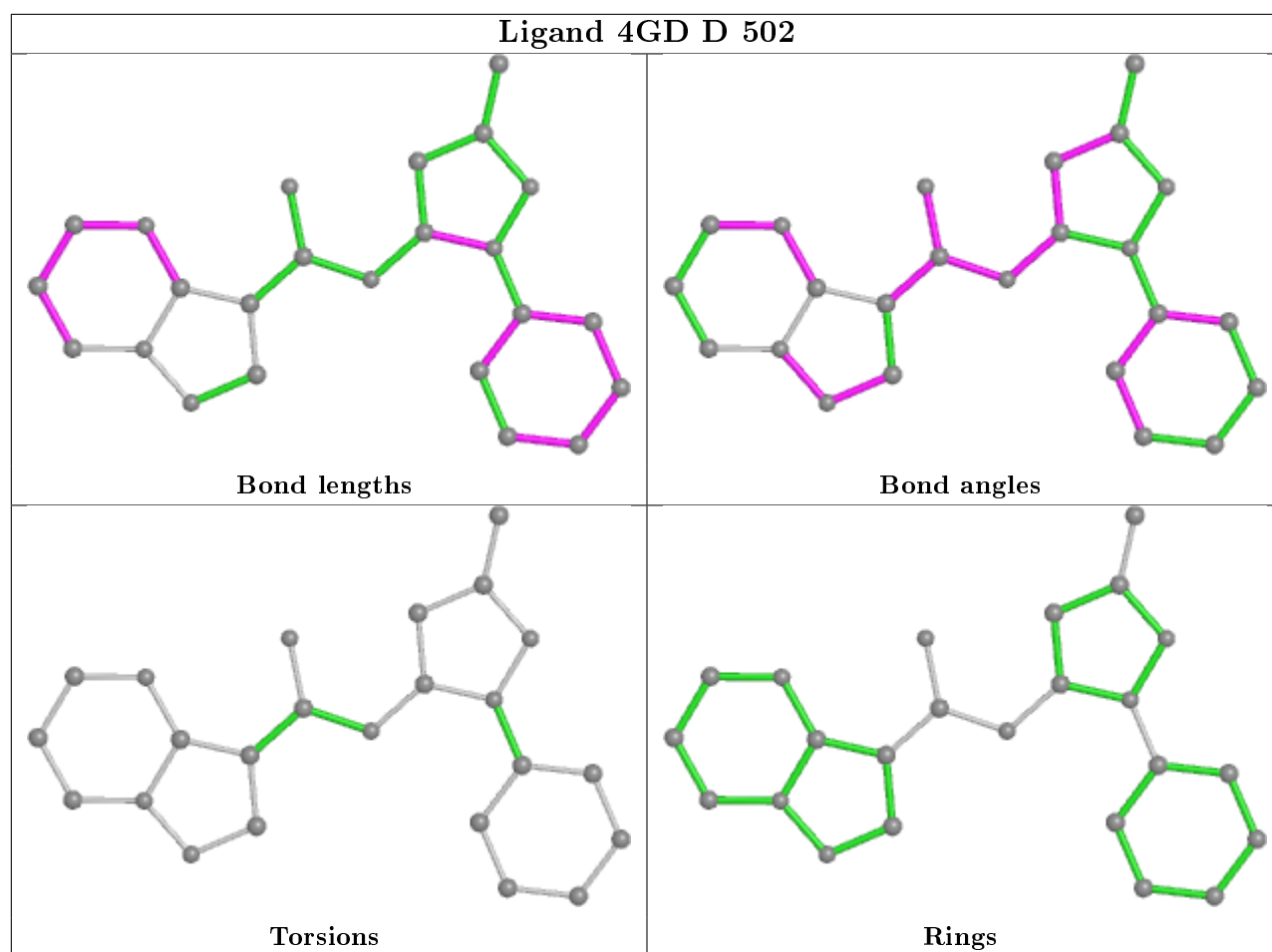
1 monomer is involved in 1 short contact:

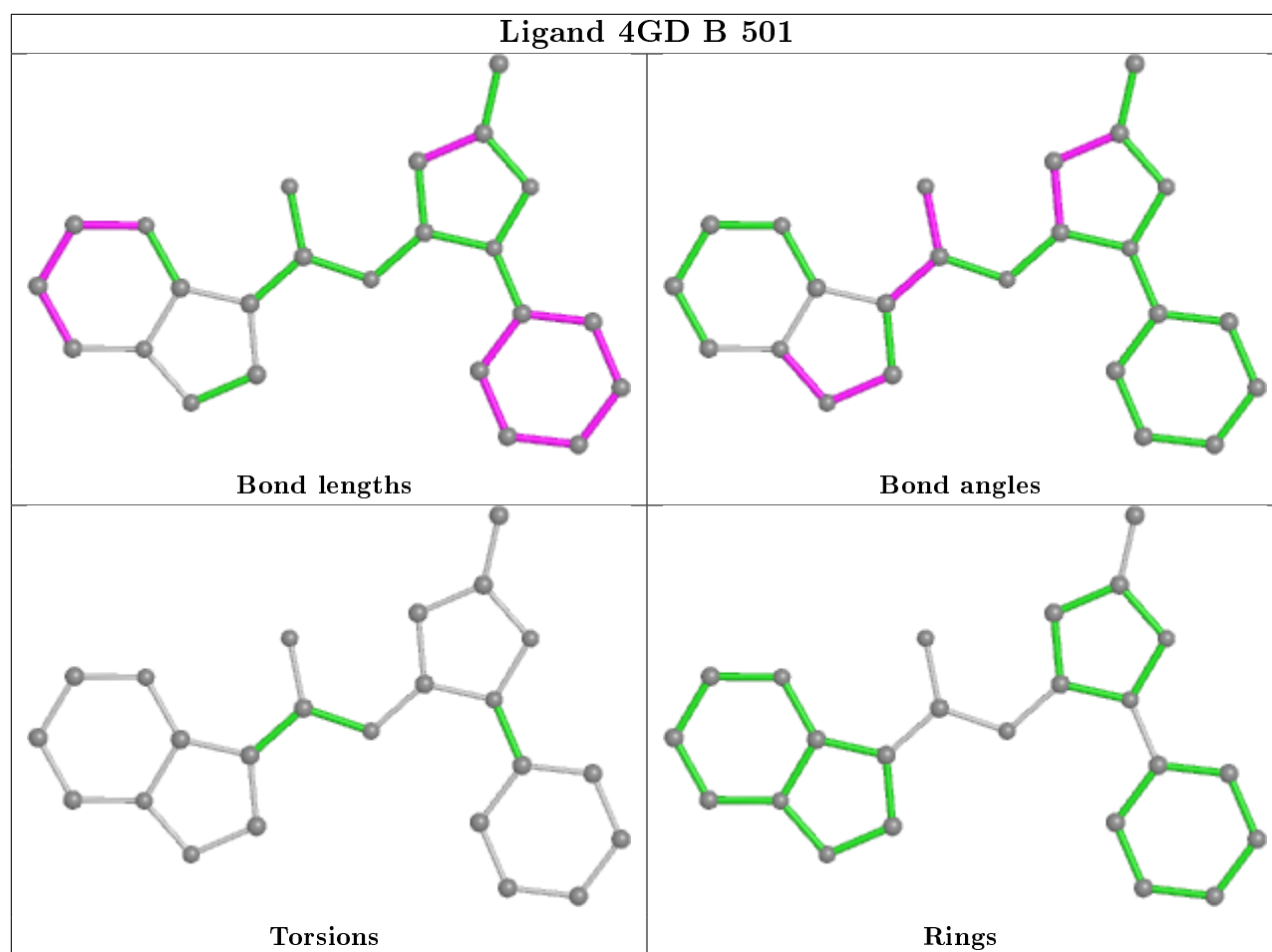
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4GD	1	0

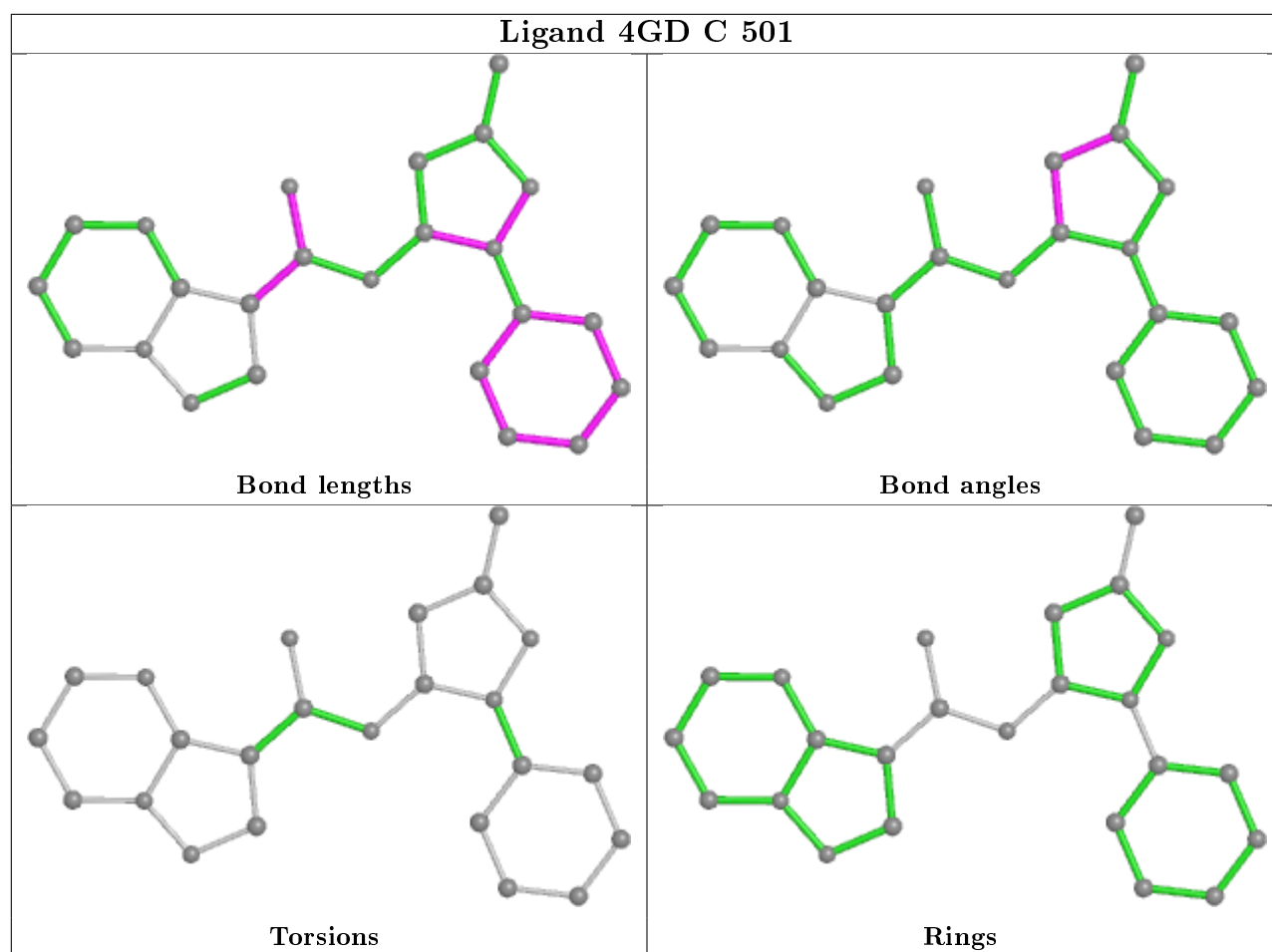
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	286/301 (95%)	0.95	53 (18%) 1 1	31, 57, 96, 107	0
1	B	277/301 (92%)	1.11	55 (19%) 1 1	31, 53, 101, 116	0
1	C	286/301 (95%)	0.37	24 (8%) 11 15	29, 47, 83, 100	0
1	D	285/301 (94%)	0.43	22 (7%) 13 18	28, 47, 82, 103	0
All	All	1134/1204 (94%)	0.71	154 (13%) 3 4	28, 50, 94, 116	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	CYS	9.4
1	C	460	SER	8.9
1	A	240	CYS	8.9
1	A	187	VAL	8.3
1	C	217	ALA	7.1
1	B	239	LYS	6.3
1	D	223	THR	6.3
1	C	196	GLY	6.3
1	B	187	VAL	6.1
1	D	221	ILE	6.1
1	A	226	LEU	6.0
1	B	343	VAL	6.0
1	C	459	ALA	5.9
1	B	230	PHE	5.8
1	C	390	HIS	5.6
1	A	189	GLY	5.6
1	B	178	ASN	5.6
1	A	336	SER	5.5
1	A	206	ASN	5.4
1	D	222	THR	5.3
1	A	223	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	5.3
1	A	188	GLY	5.3
1	B	236	VAL	5.2
1	B	238	ALA	5.1
1	D	390	HIS	5.0
1	B	235	LYS	4.9
1	B	253	SER	4.7
1	D	197	PHE	4.7
1	B	231	ASP	4.7
1	B	204	TYR	4.7
1	B	197	PHE	4.7
1	D	226	LEU	4.6
1	A	183	ARG	4.5
1	A	205	VAL	4.5
1	B	183	ARG	4.5
1	B	215	LEU	4.5
1	A	222	THR	4.4
1	A	225	GLU	4.2
1	A	407	GLU	4.2
1	B	241	GLN	4.2
1	D	389	GLU	4.2
1	A	178	ASN	4.1
1	A	239	LYS	4.1
1	A	337	GLU	4.1
1	B	196	GLY	4.1
1	B	256	ASP	4.0
1	A	207	ASN	3.9
1	B	188	GLY	3.9
1	B	216	ALA	3.9
1	C	256	ASP	3.9
1	A	182	GLU	3.8
1	A	228	GLN	3.7
1	A	390	HIS	3.7
1	A	254	ASP	3.7
1	B	257	ASP	3.7
1	B	163	THR	3.7
1	C	197	PHE	3.7
1	C	222	THR	3.7
1	C	343	VAL	3.7
1	B	177	THR	3.6
1	B	390	HIS	3.5
1	A	197	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	179	ASN	3.5
1	C	406	GLU	3.5
1	B	406	GLU	3.5
1	A	185	ILE	3.4
1	B	334	ARG	3.3
1	B	179	ASN	3.3
1	B	254	ASP	3.3
1	B	347	ARG	3.3
1	D	347	ARG	3.3
1	A	186	SER	3.2
1	A	406	GLU	3.2
1	B	199	VAL	3.2
1	D	256	ASP	3.2
1	B	258	LEU	3.2
1	B	407	GLU	3.1
1	C	226	LEU	3.1
1	A	181	ASP	3.1
1	B	198	GLY	3.1
1	B	206	ASN	3.0
1	D	337	GLU	3.0
1	C	223	THR	3.0
1	D	225	GLU	2.9
1	A	257	ASP	2.9
1	A	196	GLY	2.9
1	C	409	THR	2.8
1	B	201	TYR	2.8
1	A	347	ARG	2.8
1	D	239	LYS	2.8
1	C	257	ASP	2.8
1	B	185	ILE	2.8
1	D	409	THR	2.7
1	B	162	ASP	2.7
1	B	165	PHE	2.7
1	B	392	GLU	2.7
1	B	237	MET	2.7
1	A	408	LYS	2.7
1	D	375	VAL	2.7
1	B	214	LYS	2.6
1	B	403	ILE	2.6
1	D	406	GLU	2.5
1	A	306	HIS	2.5
1	A	372	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	368	SER	2.4
1	B	205	VAL	2.4
1	A	190	ASN	2.4
1	A	166	HIS	2.4
1	A	256	ASP	2.4
1	B	389	GLU	2.4
1	A	409	THR	2.4
1	D	164	ARG	2.3
1	B	341	GLN	2.3
1	A	165	PHE	2.3
1	A	405	ASP	2.3
1	A	163	THR	2.3
1	D	343	VAL	2.3
1	C	335	ALA	2.3
1	B	409	THR	2.3
1	B	438	HIS	2.3
1	C	239	LYS	2.3
1	A	230	PHE	2.3
1	A	241	GLN	2.2
1	D	353	ALA	2.2
1	B	259	CYS	2.2
1	C	224	GLU	2.2
1	C	405	ASP	2.2
1	A	343	VAL	2.2
1	C	194	GLU	2.2
1	C	195	GLY	2.2
1	D	424	THR	2.2
1	A	449	LYS	2.1
1	B	331	GLY	2.1
1	D	376	VAL	2.1
1	A	195	GLY	2.1
1	C	407	GLU	2.1
1	B	207	ASN	2.1
1	A	393	PRO	2.1
1	C	225	GLU	2.1
1	C	411	GLU	2.1
1	A	238	ALA	2.1
1	B	182	GLU	2.1
1	A	253	SER	2.1
1	A	389	GLU	2.0
1	B	344	MET	2.0
1	A	459	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	2.0
1	B	405	ASP	2.0
1	D	408	LYS	2.0
1	B	189	GLY	2.0
1	B	181	ASP	2.0
1	C	228	GLN	2.0
1	D	372	SER	2.0

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

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	0.59	0.34	93,97,101,101	0
1	SEP	D	346	10/11	0.70	0.29	76,82,91,91	0
1	SEP	C	346	10/11	0.76	0.27	72,78,87,88	0
1	TPO	D	342	11/12	0.84	0.19	81,83,89,89	0
1	TPO	A	342	11/12	0.85	0.26	102,103,108,108	0
1	TPO	B	345	11/12	0.89	0.23	89,90,93,94	0
1	SEP	A	346	10/11	0.90	0.27	83,88,95,95	0
1	TPO	C	342	11/12	0.90	0.21	87,88,94,94	0
1	TPO	B	342	11/12	0.91	0.22	96,98,99,100	0
1	TPO	A	345	11/12	0.92	0.18	83,84,86,87	0
1	TPO	D	345	11/12	0.95	0.14	68,69,76,76	0
1	TPO	C	345	11/12	0.95	0.14	65,67,72,73	0

6.3 Carbohydrates ⓘ

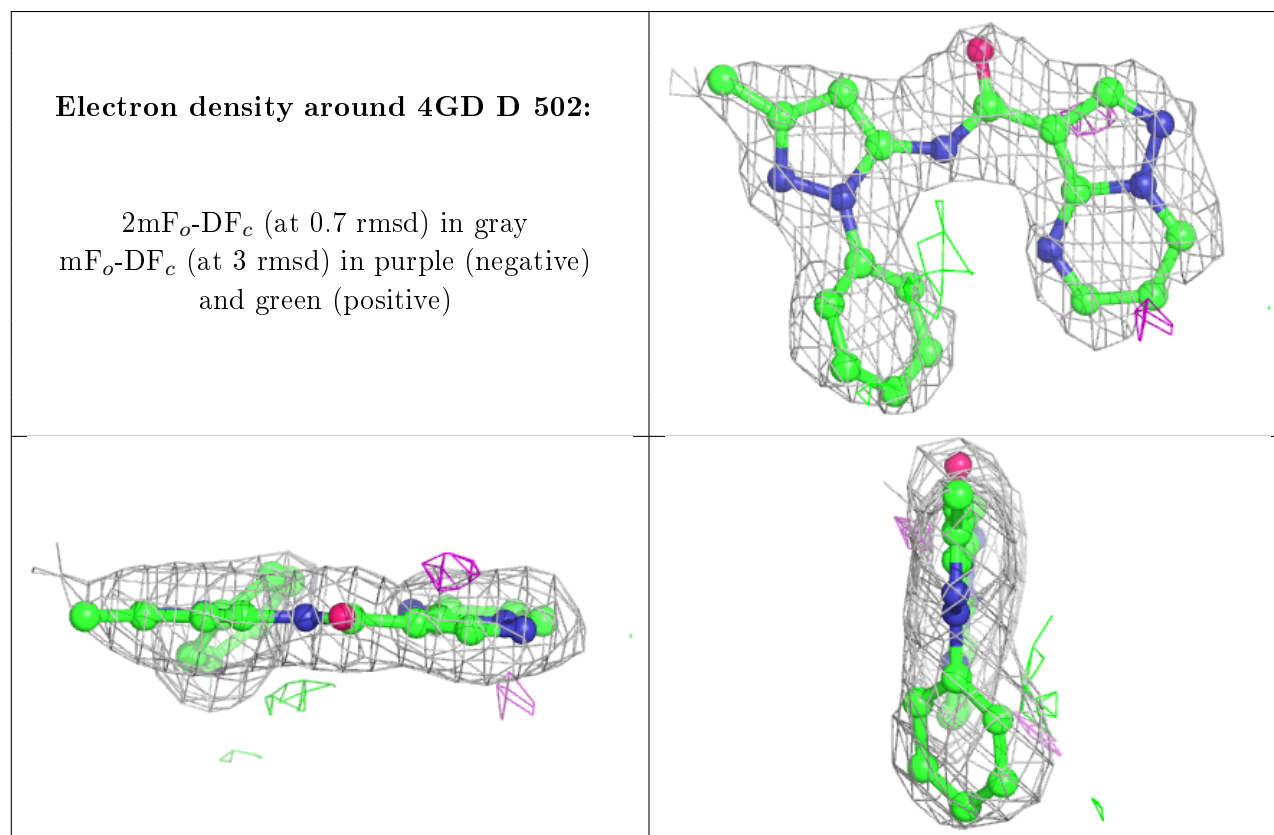
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

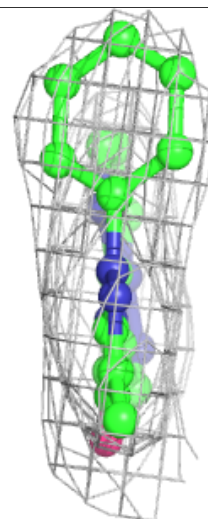
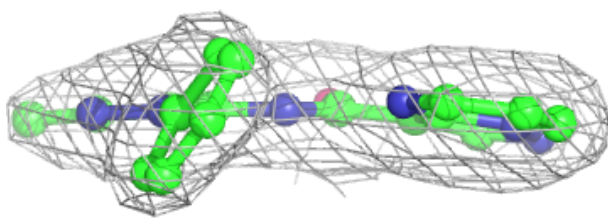
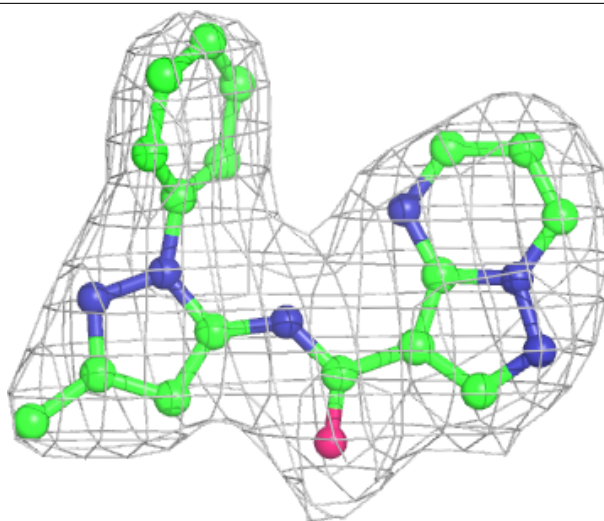
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4GD	D	502	24/24	0.94	0.15	52,56,58,59	0
2	4GD	A	501	24/24	0.95	0.10	40,46,55,55	0
2	4GD	B	501	24/24	0.95	0.11	40,43,55,56	0
2	4GD	C	501	24/24	0.97	0.11	33,38,45,45	0
2	4GD	D	501	24/24	0.98	0.11	30,36,42,43	0

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.



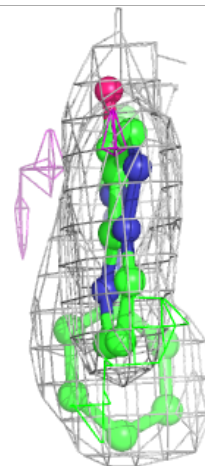
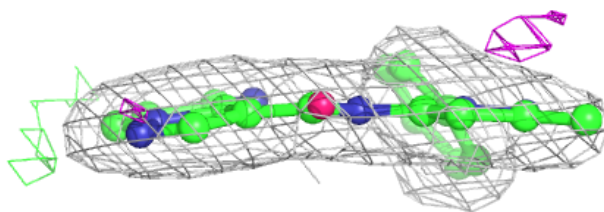
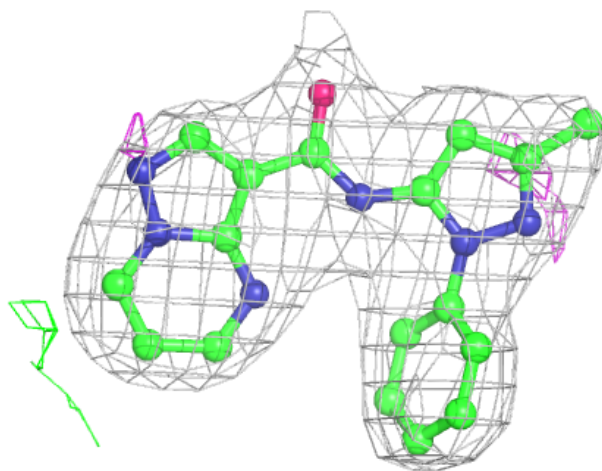
Electron density around 4GD A 501:

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



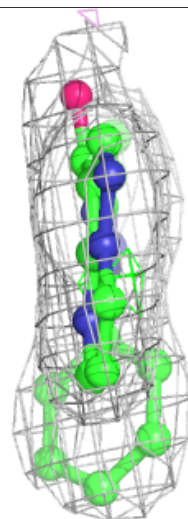
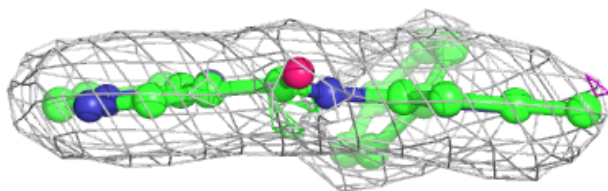
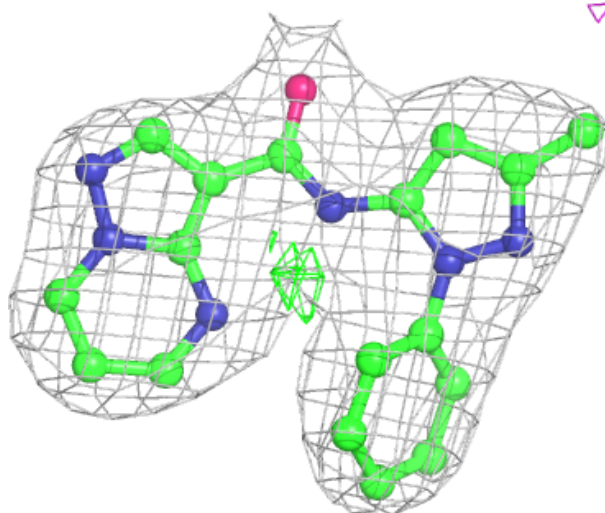
Electron density around 4GD B 501:

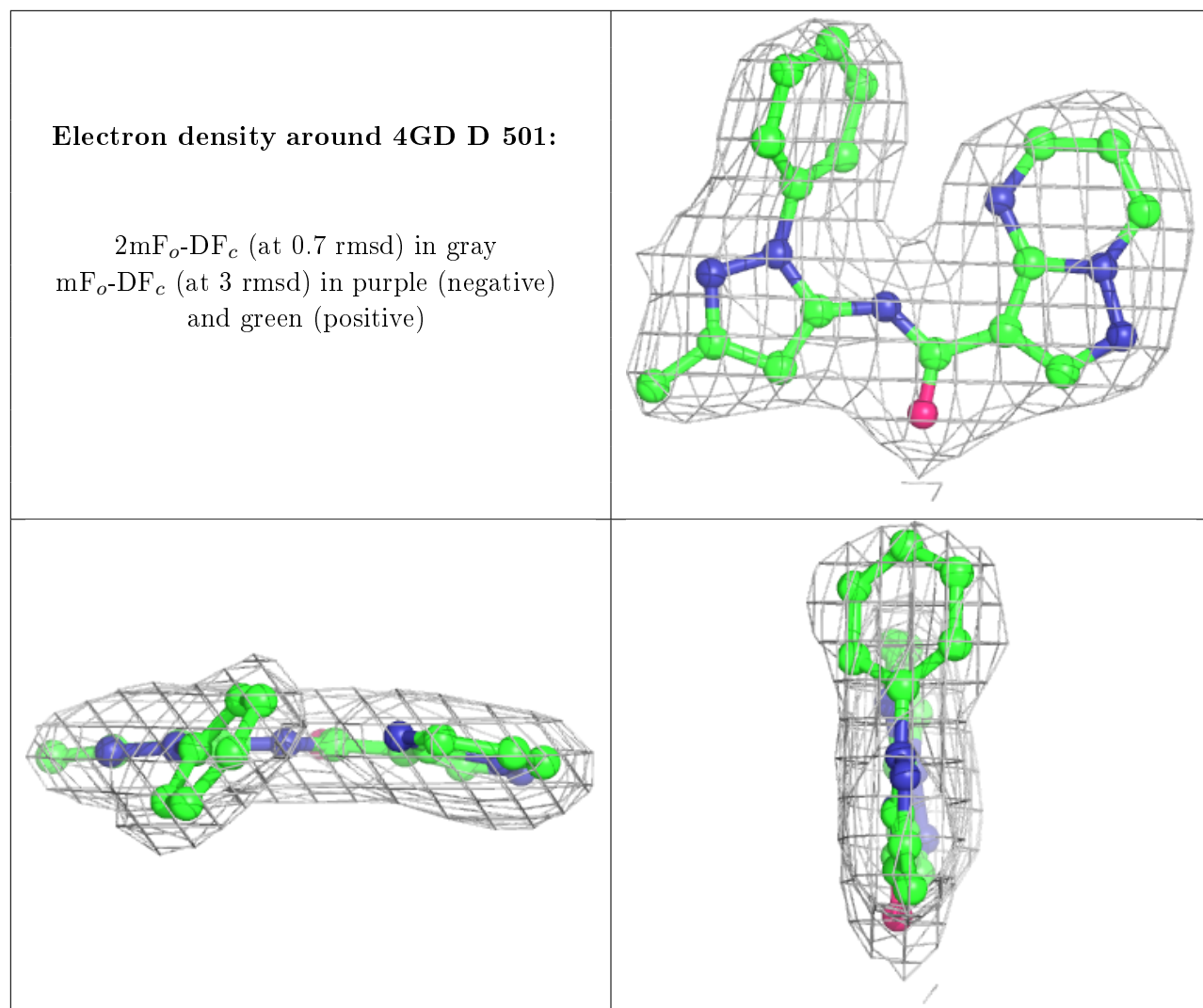
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4GD 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.