



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:14 AM UTC

PDB ID : 7T0U / pdb_00007t0u
Title : Crystal structure of the BCL6 BTB domain in complex with OICR-12387
Authors : Kuntz, D.A.; Prive, G.G.
Deposited on : 2021-11-30
Resolution : 1.49 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 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)
Xtriage (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

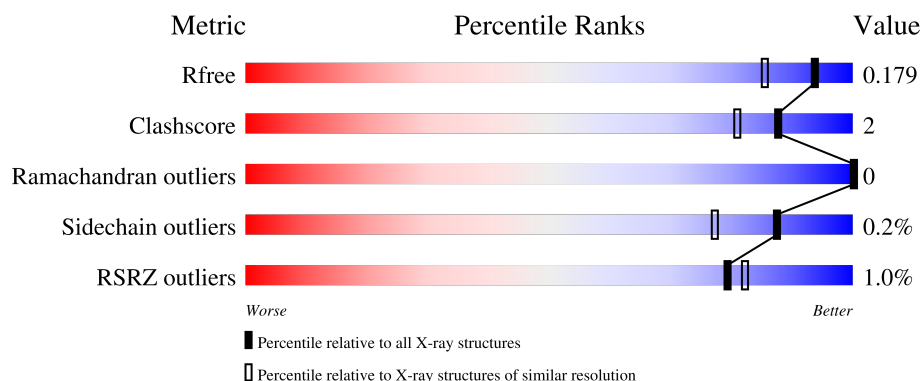
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	127	 93%
1	B	127	 2% 95%
1	C	127	 1% 92% 5%
1	D	127	 2% 87% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8925 atoms, of which 4292 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.

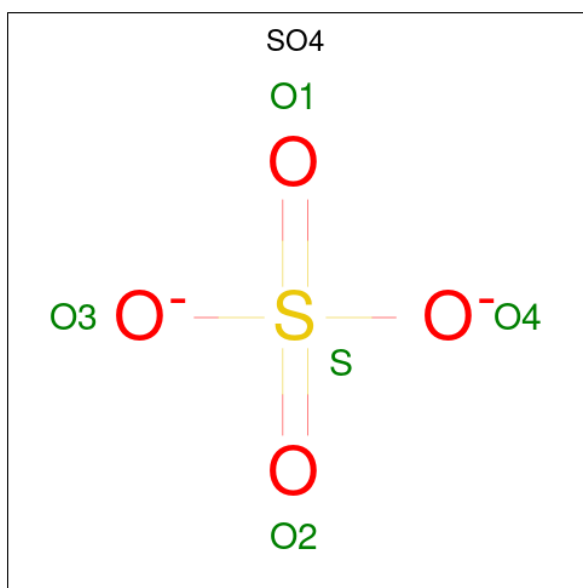
- Molecule 1 is a protein called Isoform 2 of B-cell lymphoma 6 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	122	Total	C	H	N	O	S	0	6	0
			1995	633	1006	168	180	8			
1	B	124	Total	C	H	N	O	S	0	7	0
			2059	647	1042	178	184	8			
1	C	121	Total	C	H	N	O	S	0	6	0
			2037	636	1034	178	181	8			
1	D	123	Total	C	H	N	O	S	0	7	0
			2077	647	1057	181	184	8			

There are 20 discrepancies between the modelled and reference sequences:

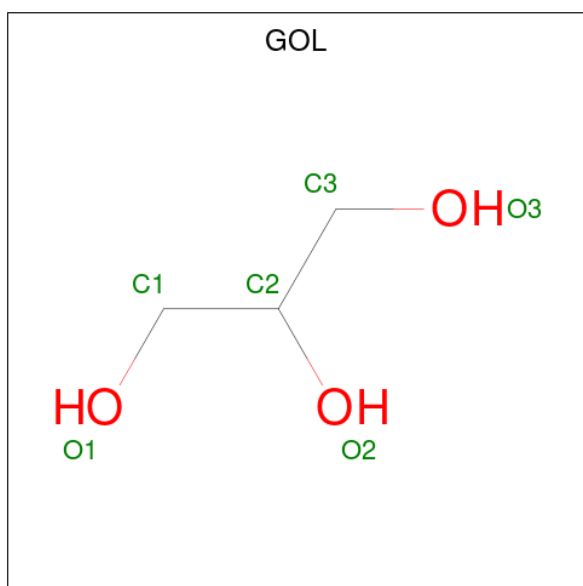
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P41182
A	4	SER	-	expression tag	UNP P41182
A	8	GLN	CYS	engineered mutation	UNP P41182
A	67	ARG	CYS	engineered mutation	UNP P41182
A	84	ASN	CYS	engineered mutation	UNP P41182
B	3	GLY	-	expression tag	UNP P41182
B	4	SER	-	expression tag	UNP P41182
B	8	GLN	CYS	engineered mutation	UNP P41182
B	67	ARG	CYS	engineered mutation	UNP P41182
B	84	ASN	CYS	engineered mutation	UNP P41182
C	3	GLY	-	expression tag	UNP P41182
C	4	SER	-	expression tag	UNP P41182
C	8	GLN	CYS	engineered mutation	UNP P41182
C	67	ARG	CYS	engineered mutation	UNP P41182
C	84	ASN	CYS	engineered mutation	UNP P41182
D	3	GLY	-	expression tag	UNP P41182
D	4	SER	-	expression tag	UNP P41182
D	8	GLN	CYS	engineered mutation	UNP P41182
D	67	ARG	CYS	engineered mutation	UNP P41182
D	84	ASN	CYS	engineered mutation	UNP P41182

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	1
			27	6	15	6		

Continued on next page...

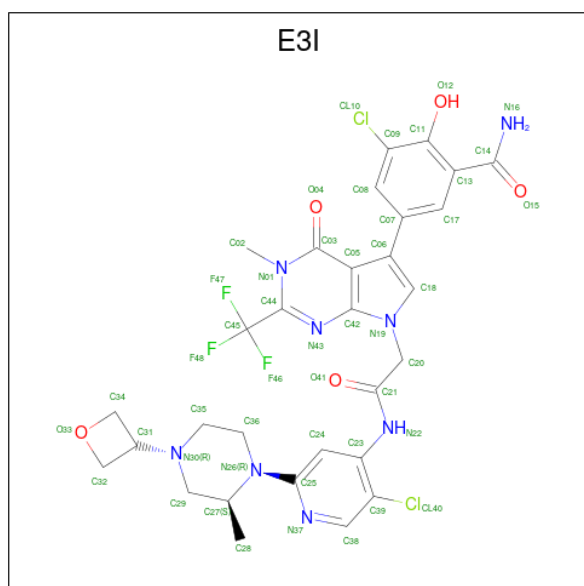
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	1
			28	6	16	6		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

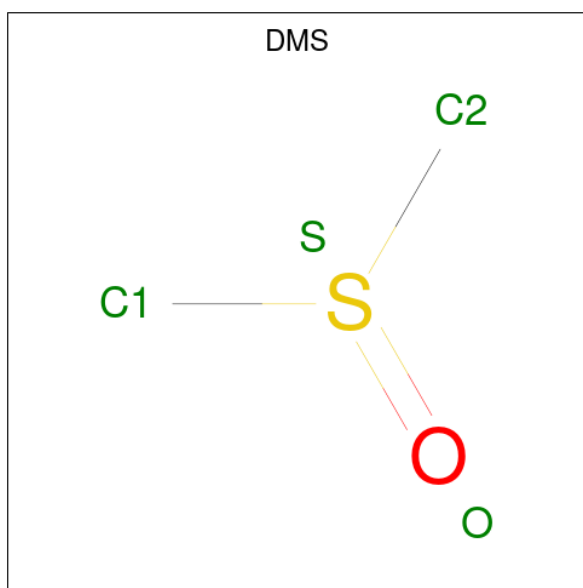
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 3-chloro-5-{7-[2-({5-chloro-2-[(2S)-2-methyl-4-(oxetan-3-yl)piperazin-1-yl]pyridin-4-yl}amino)-2-oxoethyl]-3-methyl-4-oxo-2-(trifluoromethyl)-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidin-5-yl}-2-hydroxybenzamide (CCD ID: E3I) (formula: C₃₀H₂₉Cl₂F₃N₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	H	N	O	0	0
			77	30	2	3	29	8	5		
5	B	1	Total	C	Cl	F	H	N	O	0	0
			77	30	2	3	29	8	5		
5	C	1	Total	C	Cl	F	H	N	O	0	0
			77	30	2	3	29	8	5		
5	D	1	Total	C	Cl	F	H	N	O	0	0
			77	30	2	3	29	8	5		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

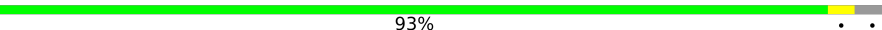
- Molecule 7 is water.

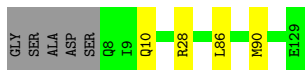
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	85	Total	O	0	5
			90	90		
7	B	81	Total	O	0	4
			85	85		
7	C	89	Total	O	0	10
			99	99		
7	D	94	Total	O	0	3
			97	97		

3 Residue-property plots

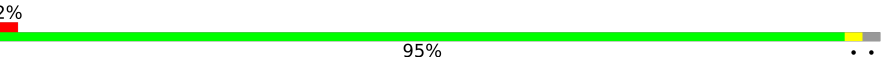
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoform 2 of B-cell lymphoma 6 protein

Chain A:  93% . .

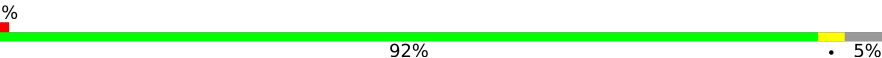


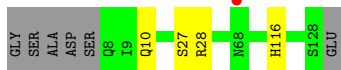
- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein

Chain B:  2% 95% . .



- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein

Chain C:  0% 92% . 5%



- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein

Chain D:  2% 87% 9% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.48Å 72.55Å 67.49Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	36.27 – 1.49 36.27 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.27-1.49) 99.7 (36.27-1.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.49Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.141 , 0.180 0.141 , 0.179	Depositor DCC
R_{free} test set	3970 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8925	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2619e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: E3I, DMS, CL, SO4, GOL

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	0.59	0/1024	0.62	0/1384
1	B	0.57	0/1060	0.64	0/1429
1	C	0.56	0/1038	0.66	0/1400
1	D	0.62	1/1061 (0.1%)	0.64	0/1430
All	All	0.59	1/4183 (0.0%)	0.64	0/5643

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	125	ILE	CG1-CD1	-5.18	1.31	1.51

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	989	1006	994	3	0
1	B	1017	1042	1024	2	0
1	C	1003	1034	1020	3	0
1	D	1020	1057	1046	11	0
2	A	5	0	0	0	0
2	D	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	15	16	0	0
3	C	12	16	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	48	29	0	0	0
5	B	48	29	0	0	0
5	C	48	29	0	0	0
5	D	48	29	0	0	0
6	D	4	6	6	0	0
7	A	90	0	0	0	0
7	B	85	0	0	1	0
7	C	99	0	0	2	0
7	D	97	0	0	1	0
All	All	4633	4292	4122	17	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 2.

All (17) 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:D:35[A]:VAL:CG1	1:D:71:VAL:HG22	2.29	0.63
1:D:123:LYS:HE2	1:D:124:PHE:CE2	2.35	0.61
1:A:28:ARG:HD2	7:B:329:HOH:O	2.04	0.57
1:D:125:ILE:O	1:D:129:GLU:N	2.39	0.54
3:C:201[B]:GOL:H12	1:D:48:THR:HG23	1.92	0.50
1:A:10:GLN:OE1	1:B:94:ARG:HG2	2.13	0.48
1:D:106:MET:HE1	1:D:125:ILE:CD1	2.45	0.46
1:A:86:LEU:O	1:A:90:MET:HG3	2.18	0.43
1:C:28:ARG:HD2	7:C:375:HOH:O	2.19	0.43
1:D:86:LEU:O	1:D:90:MET:HG3	2.18	0.43
1:D:128:SER:O	1:D:129:GLU:CB	2.67	0.42
1:C:10[A]:GLN:NE2	1:D:94:ARG:NH2	2.68	0.42
1:D:128:SER:HB2	7:D:329:HOH:O	2.20	0.41
1:D:35[A]:VAL:HG12	1:D:71:VAL:HG22	2.01	0.41
1:C:116[B]:HIS:HD2	7:C:328[B]:HOH:O	2.04	0.41
1:B:58:TYR:O	1:B:62:THR:HG23	2.20	0.41
1:D:128:SER:O	1:D:129:GLU:HB3	2.22	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	126/127 (99%)	123 (98%)	3 (2%)	0	100	100
1	B	129/127 (102%)	126 (98%)	3 (2%)	0	100	100
1	C	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
1	D	128/127 (101%)	124 (97%)	4 (3%)	0	100	100
All	All	508/508 (100%)	495 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	113/115 (98%)	113 (100%)	0	100	100
1	B	116/115 (101%)	116 (100%)	0	100	100
1	C	117/115 (102%)	115 (98%)	2 (2%)	53	26
1	D	119/115 (104%)	119 (100%)	0	100	100
All	All	465/460 (101%)	463 (100%)	2 (0%)	87	71

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	27[A]	SER
1	C	27[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	113	GLN
1	B	73	ASN
1	B	84	ASN
1	B	113	GLN
1	C	8	GLN
1	C	113	GLN
1	D	73	ASN
1	D	113	GLN
1	D	116	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	C	201[A]	-	5,5,5	1.33	0	5,5,5	1.20	1 (20%)
5	E3I	B	201	-	49,53,53	1.66	5 (10%)	60,81,81	1.96	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	202[B]	-	5,5,5	1.12	0	5,5,5	1.20	0
6	DMS	D	202	-	3,3,3	0.66	0	3,3,3	0.90	0
3	GOL	C	201[B]	-	5,5,5	1.24	0	5,5,5	1.19	1 (20%)
2	SO4	D	203	-	4,4,4	0.41	0	6,6,6	0.25	0
2	SO4	A	201	-	4,4,4	0.18	0	6,6,6	0.48	0
3	GOL	A	202[A]	-	5,5,5	0.84	0	5,5,5	1.04	0
5	E3I	C	202	-	49,53,53	2.00	16 (32%)	60,81,81	2.18	18 (30%)
5	E3I	A	204	-	49,53,53	1.60	7 (14%)	60,81,81	1.84	13 (21%)
5	E3I	D	201	-	49,53,53	1.68	7 (14%)	60,81,81	1.92	18 (30%)

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	GOL	C	201[A]	-	-	0/4/4/4	-
5	E3I	B	201	-	-	0/30/49/49	0/6/6/6
3	GOL	A	202[B]	-	-	2/4/4/4	-
3	GOL	C	201[B]	-	-	0/4/4/4	-
3	GOL	A	202[A]	-	-	0/4/4/4	-
5	E3I	C	202	-	-	0/30/49/49	0/6/6/6
5	E3I	A	204	-	-	0/30/49/49	0/6/6/6
5	E3I	D	201	-	-	0/30/49/49	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	E3I	C20-N19	-6.82	1.37	1.46
5	D	201	E3I	C20-N19	-6.39	1.38	1.46
5	C	202	E3I	C36-N26	6.20	1.56	1.46
5	A	204	E3I	C20-N19	-4.76	1.40	1.46
5	A	204	E3I	C36-N26	4.63	1.54	1.46
5	C	202	E3I	C27-N26	4.57	1.52	1.47
5	D	201	E3I	C07-C06	-4.37	1.41	1.48
5	D	201	E3I	C29-C27	4.05	1.60	1.52
5	D	201	E3I	C36-N26	3.92	1.52	1.46
5	C	202	E3I	C29-C27	3.89	1.59	1.52
5	C	202	E3I	C20-N19	-3.80	1.41	1.46
5	B	201	E3I	C27-N26	3.33	1.51	1.47
5	B	201	E3I	C35-N30	-3.22	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	204	E3I	C29-C27	3.13	1.58	1.52
5	C	202	E3I	C38-C39	3.13	1.42	1.39
5	B	201	E3I	C07-C06	-3.11	1.43	1.48
5	A	204	E3I	C08-C09	-3.06	1.33	1.38
5	C	202	E3I	C07-C06	-2.93	1.44	1.48
5	A	204	E3I	C27-N26	2.81	1.50	1.47
5	A	204	E3I	C35-N30	-2.77	1.42	1.47
5	C	202	E3I	C24-C23	-2.65	1.35	1.39
5	C	202	E3I	C08-C09	-2.57	1.34	1.38
5	C	202	E3I	C18-N19	-2.52	1.30	1.36
5	A	204	E3I	C07-C06	-2.50	1.44	1.48
5	C	202	E3I	C24-C25	2.43	1.43	1.39
5	D	201	E3I	C35-N30	-2.38	1.42	1.47
5	C	202	E3I	C21-N22	-2.34	1.30	1.35
5	B	201	E3I	C13-C14	-2.33	1.46	1.50
5	C	202	E3I	C39-CL40	-2.28	1.68	1.73
5	C	202	E3I	F48-C45	2.24	1.41	1.32
5	C	202	E3I	C23-C39	-2.21	1.34	1.39
5	D	201	E3I	C24-C25	2.17	1.42	1.39
5	C	202	E3I	C03-N01	2.10	1.44	1.40
5	C	202	E3I	C08-C07	2.09	1.42	1.39
5	D	201	E3I	C17-C07	2.04	1.42	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	E3I	C35-N30-C29	7.60	115.64	108.17
5	B	201	E3I	C18-C06-C05	-5.34	101.94	106.22
5	B	201	E3I	F47-C45-C44	5.33	119.28	111.95
5	D	201	E3I	C18-C06-C05	-4.83	102.36	106.22
5	C	202	E3I	C23-C39-CL40	4.81	124.73	119.52
5	A	204	E3I	C36-N26-C27	-4.75	106.41	114.63
5	C	202	E3I	C21-C20-N19	4.73	117.22	111.16
5	C	202	E3I	C18-C06-C05	-4.66	102.49	106.22
5	A	204	E3I	C18-C06-C05	-4.61	102.53	106.22
5	A	204	E3I	C29-N30-C31	-4.46	101.60	112.80
5	B	201	E3I	C17-C07-C08	-4.42	114.48	119.65
5	C	202	E3I	C29-N30-C31	-4.35	101.90	112.80
5	B	201	E3I	C17-C07-C06	4.35	127.28	120.65
5	C	202	E3I	C17-C07-C06	4.09	126.89	120.65
5	D	201	E3I	C21-C20-N19	4.07	116.36	111.16
5	C	202	E3I	F47-C45-C44	4.03	117.49	111.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	E3I	C29-N30-C31	-3.92	102.96	112.80
5	D	201	E3I	F47-C45-C44	3.86	117.27	111.95
5	D	201	E3I	C36-N26-C27	-3.85	107.97	114.63
5	B	201	E3I	C21-C20-N19	3.75	115.96	111.16
5	D	201	E3I	C29-N30-C31	-3.74	103.41	112.80
5	A	204	E3I	F47-C45-C44	3.69	117.03	111.95
5	A	204	E3I	C23-C39-CL40	3.65	123.48	119.52
5	D	201	E3I	F46-C45-C44	3.64	116.96	111.95
5	D	201	E3I	C35-N30-C31	-3.64	103.54	112.79
5	C	202	E3I	C35-N30-C31	-3.63	103.54	112.79
5	A	204	E3I	C36-C35-N30	-3.54	104.36	110.61
5	C	202	E3I	C17-C07-C08	-3.44	115.62	119.65
5	A	204	E3I	C35-N30-C31	-3.33	104.31	112.79
5	A	204	E3I	C21-C20-N19	3.33	115.42	111.16
5	D	201	E3I	C23-C39-CL40	3.14	122.93	119.52
5	D	201	E3I	C35-N30-C29	3.10	111.22	108.17
5	B	201	E3I	C35-N30-C31	-3.09	104.93	112.79
5	D	201	E3I	C17-C07-C06	2.97	125.18	120.65
5	B	201	E3I	C20-C21-N22	2.97	119.72	114.23
5	B	201	E3I	C23-C39-CL40	2.81	122.57	119.52
5	D	201	E3I	C34-O33-C32	2.77	93.97	91.34
5	A	204	E3I	C07-C06-C05	2.71	135.24	128.48
5	D	201	E3I	C38-N37-C25	2.61	121.69	117.41
5	B	201	E3I	C07-C08-C09	2.59	122.52	120.26
5	D	201	E3I	C07-C06-C05	2.57	134.90	128.48
5	A	204	E3I	C24-C25-N37	-2.55	118.58	122.82
5	D	201	E3I	C38-C39-C23	-2.54	118.61	120.07
5	C	202	E3I	C20-C21-N22	2.53	118.92	114.23
5	C	202	E3I	C24-C25-N37	-2.48	118.69	122.82
5	D	201	E3I	C24-C25-N37	-2.46	118.72	122.82
5	B	201	E3I	C13-C17-C07	2.45	124.75	120.70
5	C	202	E3I	O41-C21-C20	-2.44	116.75	121.02
5	B	201	E3I	O41-C21-C20	-2.42	116.78	121.02
5	C	202	E3I	C38-C39-CL40	-2.38	115.14	118.57
3	C	201[A]	GOL	C3-C2-C1	-2.36	103.14	111.80
5	B	201	E3I	C07-C06-C05	2.34	134.32	128.48
5	D	201	E3I	C17-C07-C08	-2.33	116.92	119.65
5	B	201	E3I	C35-N30-C29	2.33	110.46	108.17
5	B	201	E3I	C06-C05-C42	2.31	110.27	106.66
5	A	204	E3I	C17-C07-C08	-2.29	116.97	119.65
5	D	201	E3I	C36-C35-N30	-2.27	106.60	110.61
5	C	202	E3I	C13-C11-C09	-2.25	116.82	118.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	E3I	C24-C25-N26	-2.25	119.63	122.35
5	B	201	E3I	C24-C23-C39	-2.22	115.93	118.21
5	C	202	E3I	C13-C17-C07	2.18	124.30	120.70
5	D	201	E3I	C20-C21-N22	2.16	118.23	114.23
5	C	202	E3I	C08-C07-C06	-2.16	117.36	120.65
5	C	202	E3I	C07-C06-C05	2.13	133.81	128.48
5	A	204	E3I	C05-C03-N01	-2.12	112.61	116.10
5	B	201	E3I	C11-C09-CL10	2.12	121.44	118.81
3	C	201[B]	GOL	C3-C2-C1	-2.07	104.22	111.80
5	B	201	E3I	C24-C25-N37	-2.04	119.42	122.82
5	A	204	E3I	O15-C14-C13	2.03	122.63	120.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202[B]	GOL	O1-C1-C2-C3
3	A	202[B]	GOL	O1-C1-C2-O2

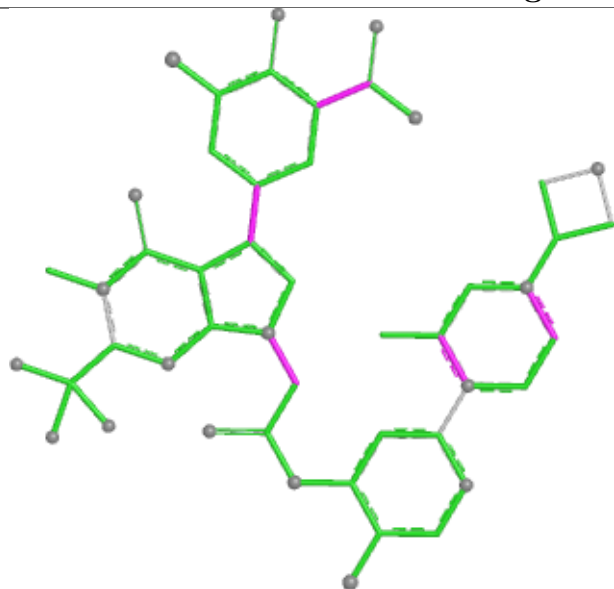
There are no ring outliers.

1 monomer is involved in 1 short contact:

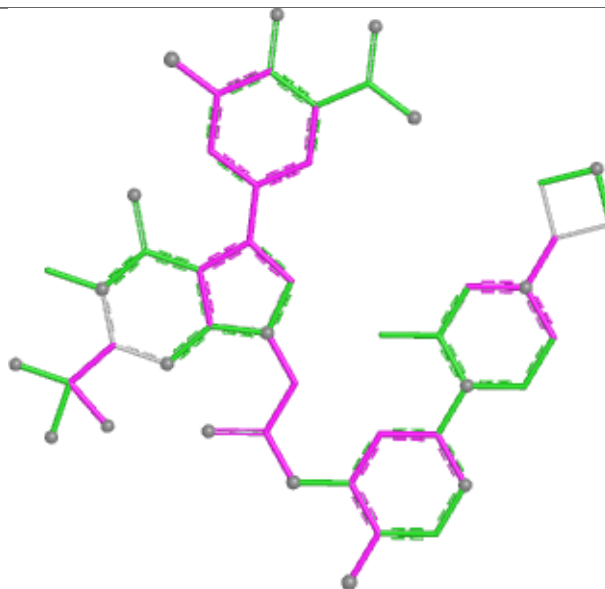
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201[B]	GOL	1	0

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.

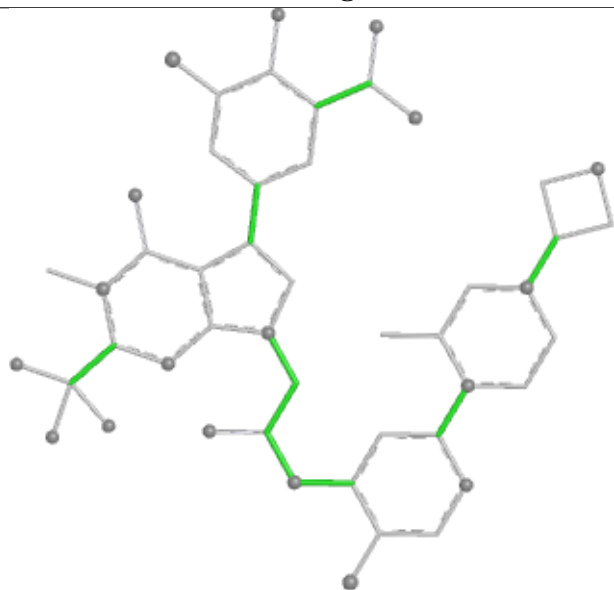
Ligand E3I B 201



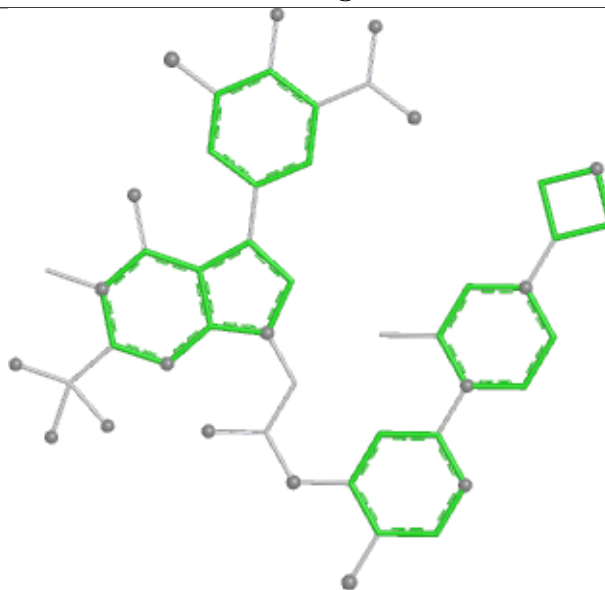
Bond lengths



Bond angles

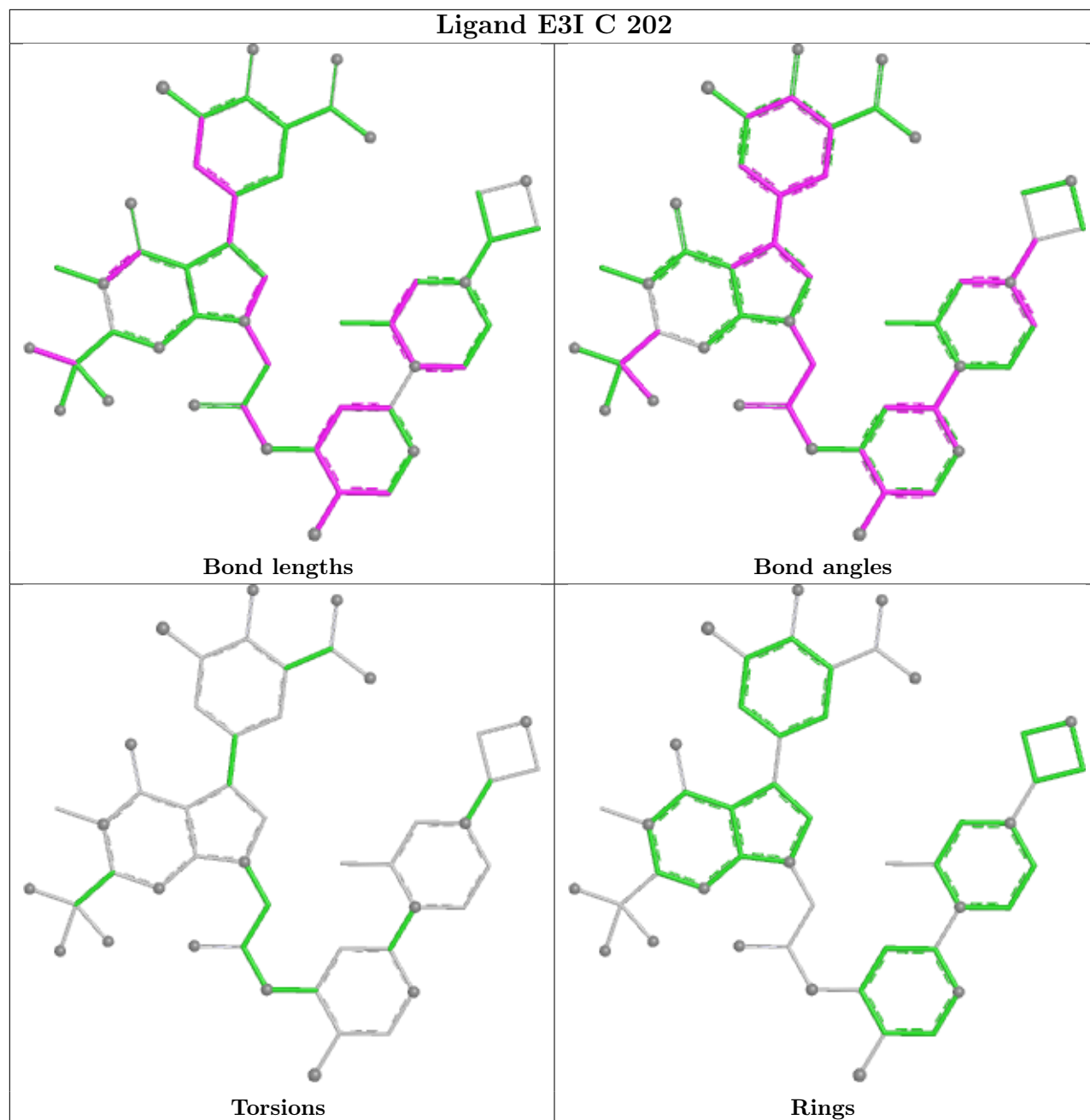


Torsions

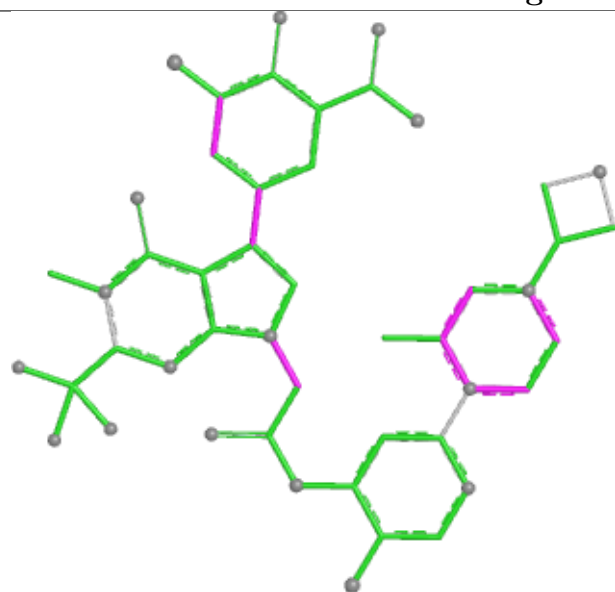


Rings

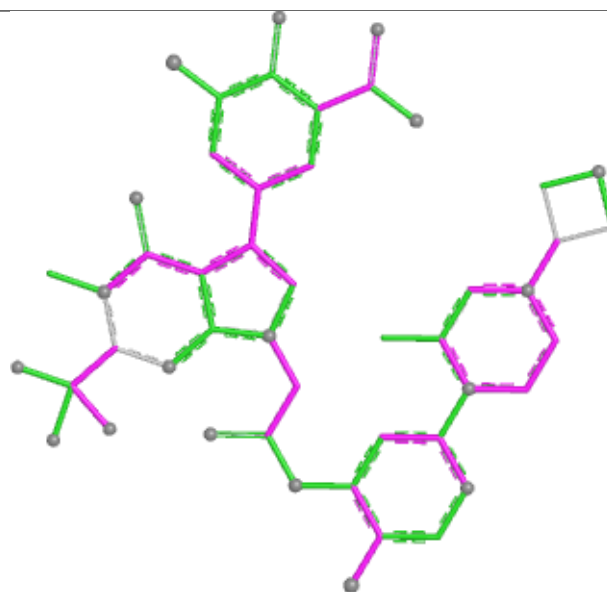
Ligand E3I C 202



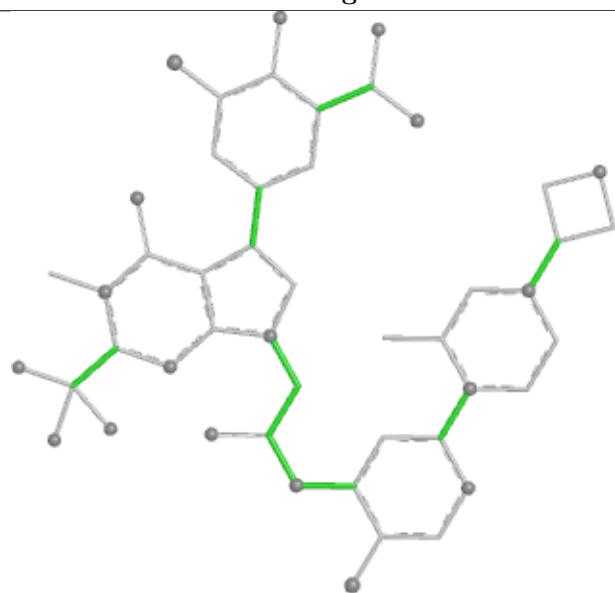
Ligand E3I A 204



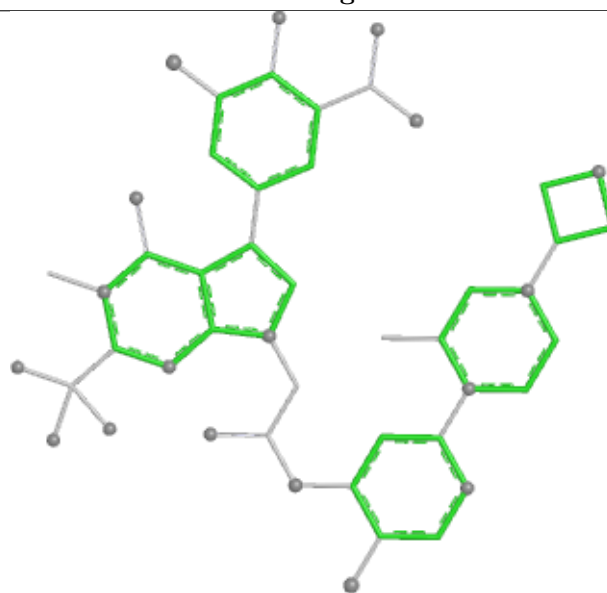
Bond lengths



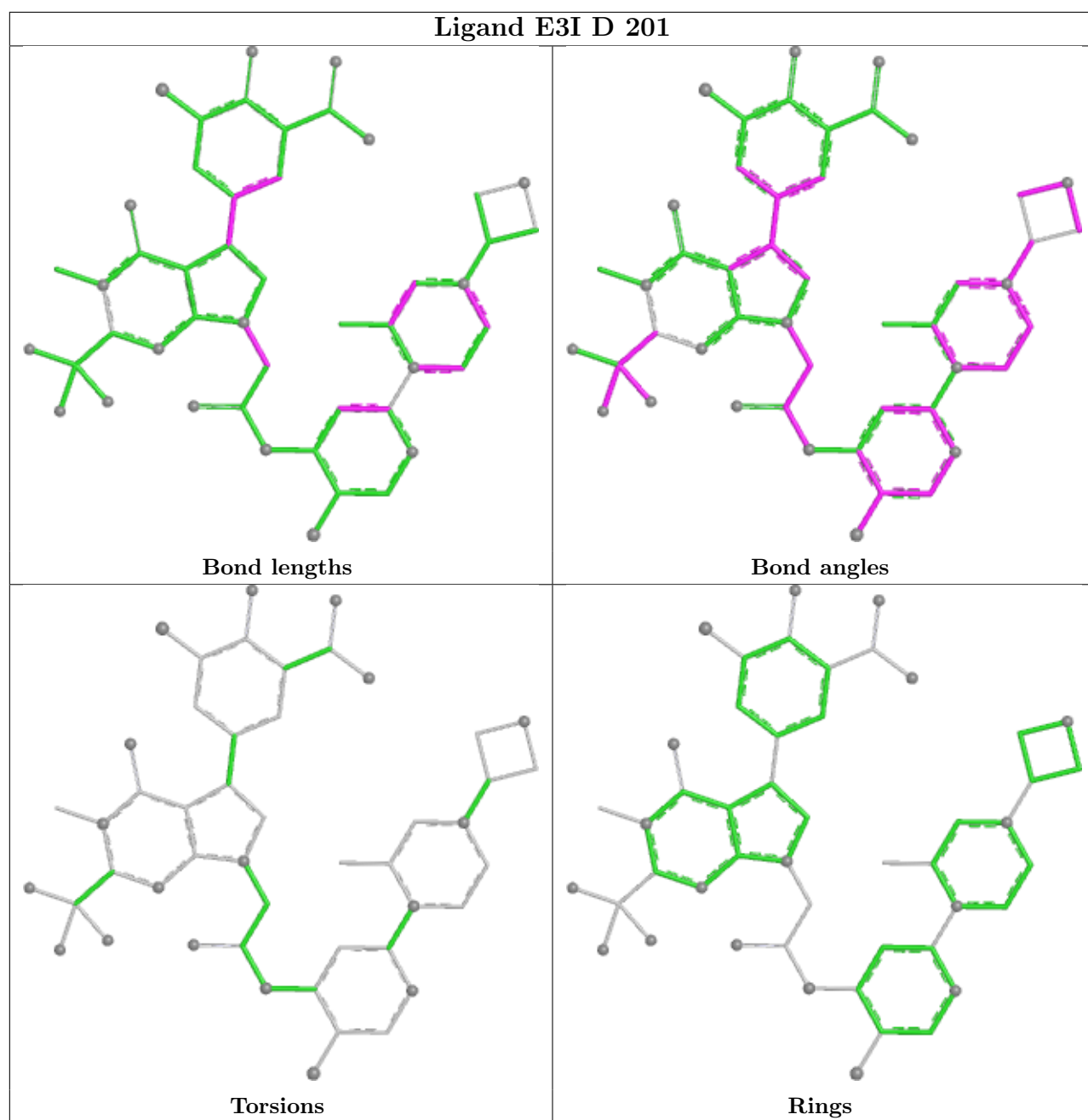
Bond angles



Torsions



Rings



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	122/127 (96%)	-0.38	0 100 100	9, 18, 36, 47	5 (4%)
1	B	124/127 (97%)	-0.26	2 (1%) 70 74	8, 20, 41, 54	5 (4%)
1	C	121/127 (95%)	-0.42	1 (0%) 82 86	9, 17, 35, 52	5 (4%)
1	D	123/127 (96%)	-0.39	2 (1%) 70 74	8, 17, 36, 72	6 (4%)
All	All	490/508 (96%)	-0.36	5 (1%) 79 82	8, 18, 38, 72	21 (4%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ALA	3.7
1	D	126	LYS	2.4
1	D	129	GLU	2.3
1	B	128	SER	2.2
1	C	68	ASN	2.1

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 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,

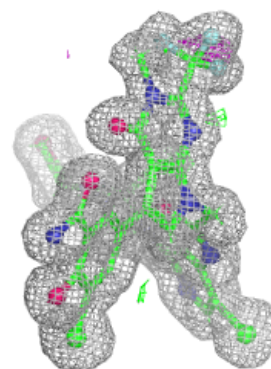
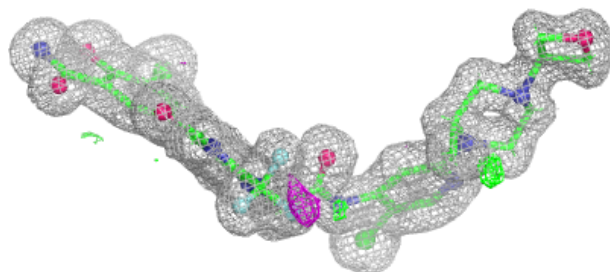
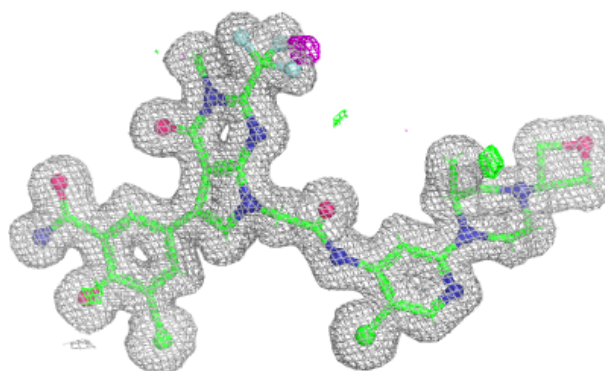
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	202	1/1	0.82	0.35	31,31,31,31	1
6	DMS	D	202	4/4	0.86	0.18	20,25,25,27	0
4	CL	A	203	1/1	0.87	0.22	31,31,31,31	1
3	GOL	C	201[B]	6/6	0.92	0.10	18,33,73,73	14
3	GOL	A	202[A]	6/6	0.92	0.11	13,26,33,42	13
3	GOL	A	202[B]	6/6	0.92	0.11	13,38,65,78	14
3	GOL	C	201[A]	6/6	0.92	0.10	15,26,41,46	14
2	SO4	A	201	5/5	0.95	0.09	21,22,31,34	5
2	SO4	D	203	5/5	0.96	0.09	20,27,30,39	5
5	E3I	B	201	48/48	0.98	0.05	7,10,19,25	0
5	E3I	C	202	48/48	0.98	0.07	7,13,66,89	77
5	E3I	D	201	48/48	0.98	0.05	9,12,26,33	0
5	E3I	A	204	48/48	0.98	0.05	8,12,33,34	0
4	CL	D	204	1/1	0.99	0.04	25,25,25,25	1

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.

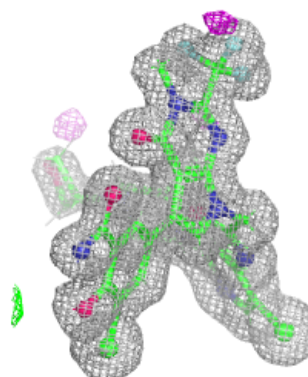
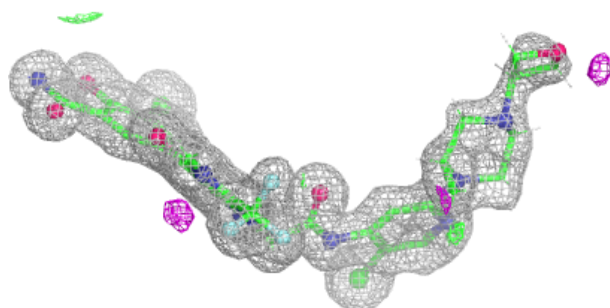
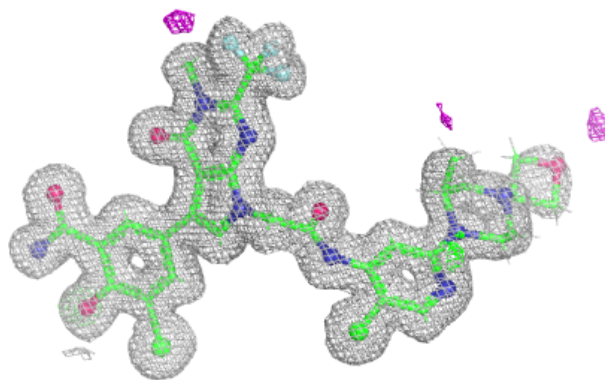
Electron density around E3I B 201:

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

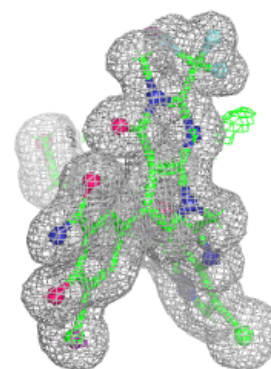
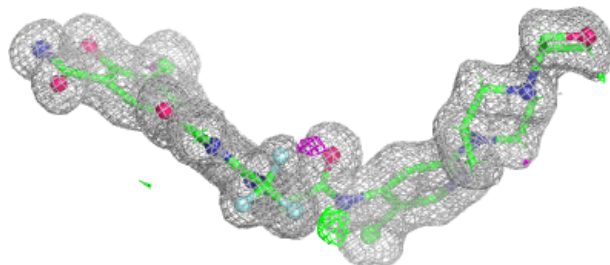
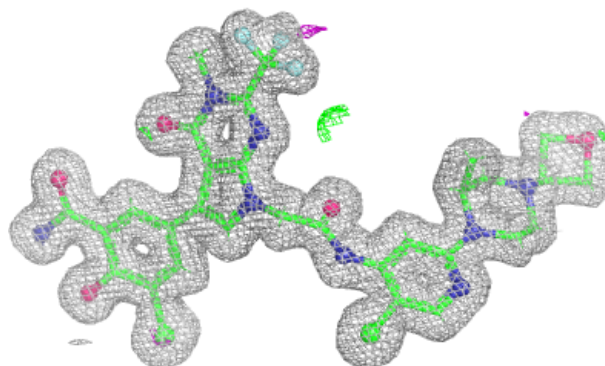


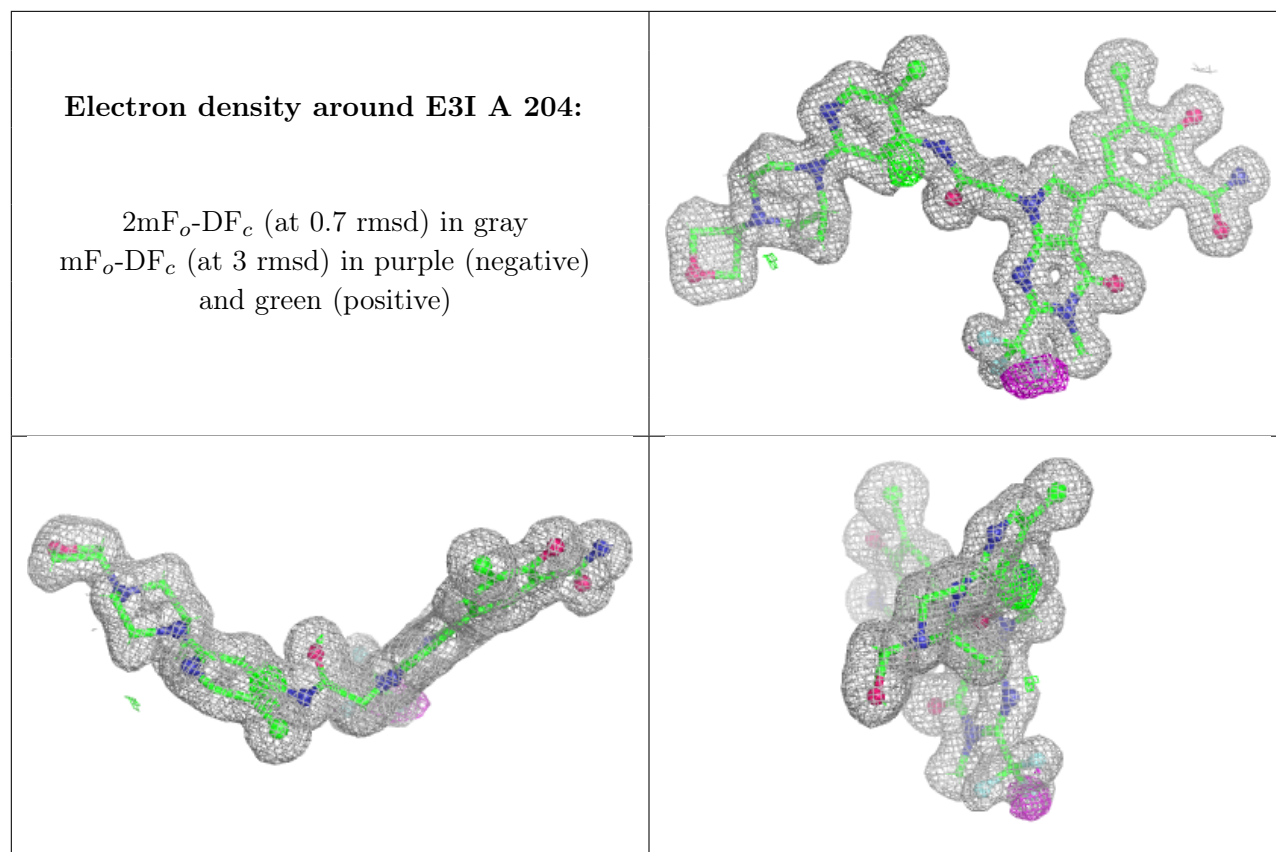
Electron density around E3I C 202:

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

**Electron density around E3I D 201:**

$2mF_o-DF_c$ (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.