wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 11:02 AM EDT

PDB ID	:	6EMH
Title	:	Crystal structure of JNK3 in complex with a pyridinylimidazole inhibitor
Authors	:	Macedo, J.T.; Stehle, T.; Blaum, B.S.
Deposited on	:	2017-10-02
Resolution	:	1.76 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 (i) 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 (i)) were used in the production of this report:

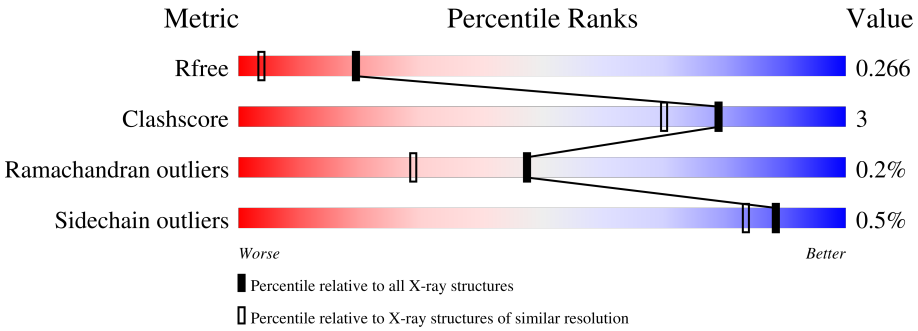
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	367	86% 7% 6%
1	B	367	86% 7% 6%
1	C	367	83% 7% • 9%
1	D	367	84% 6% 10%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12089 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.

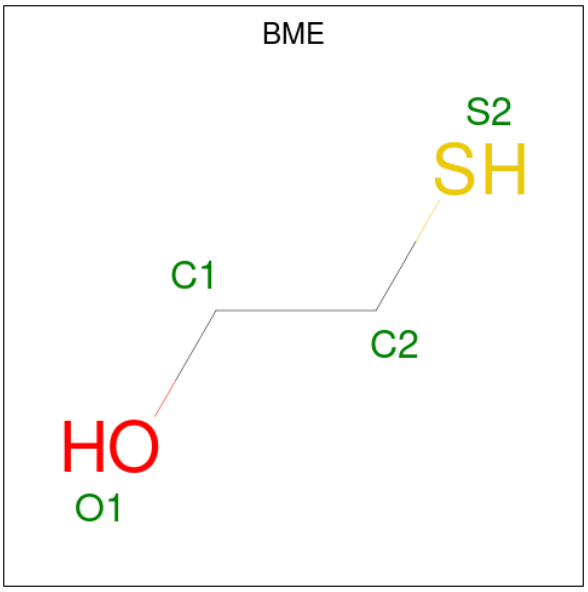
- Molecule 1 is a protein called Mitogen-activated protein kinase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	16	0
			2826	1826	469	506	25			
1	B	344	Total	C	N	O	S	0	16	0
			2826	1821	469	511	25			
1	C	334	Total	C	N	O	S	0	13	0
			2700	1745	446	485	24			
1	D	331	Total	C	N	O	S	0	9	0
			2665	1721	442	480	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP P53779
A	37	GLY	-	expression tag	UNP P53779
A	38	SER	-	expression tag	UNP P53779
B	36	GLY	-	expression tag	UNP P53779
B	37	GLY	-	expression tag	UNP P53779
B	38	SER	-	expression tag	UNP P53779
C	36	GLY	-	expression tag	UNP P53779
C	37	GLY	-	expression tag	UNP P53779
C	38	SER	-	expression tag	UNP P53779
D	36	GLY	-	expression tag	UNP P53779
D	37	GLY	-	expression tag	UNP P53779
D	38	SER	-	expression tag	UNP P53779

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).

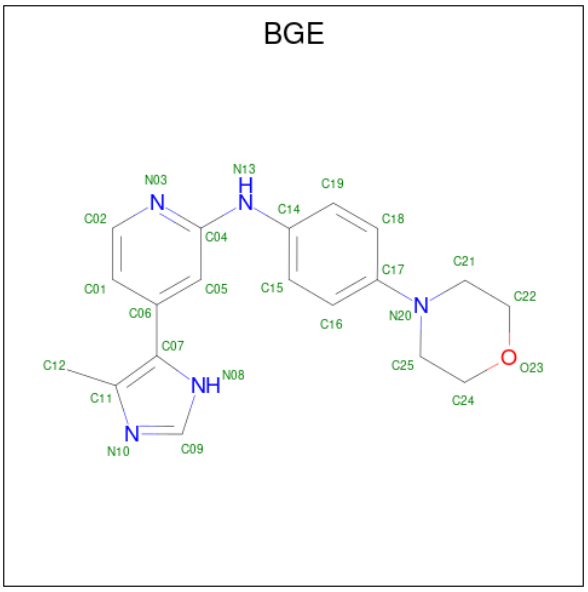


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 4 2 1 1	0	0
2	A	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

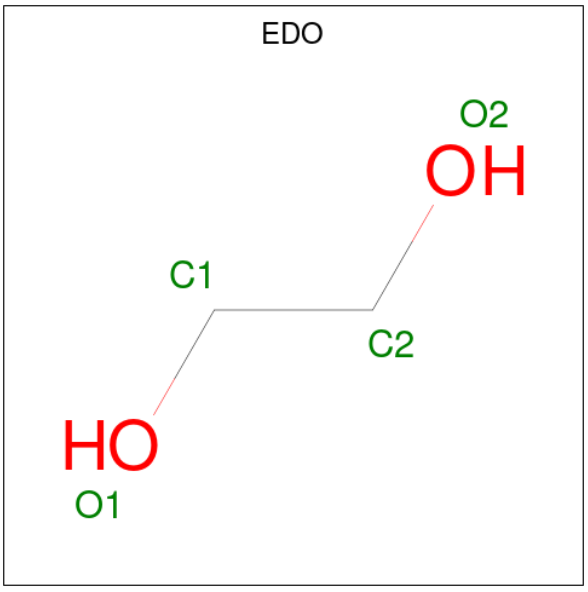
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is 4-(4-methyl-1 {H}-imidazol-5-yl)- {N}-(4-morpholin-4-ylphenyl)pyridin-2-amine (three-letter code: BGE) (formula: $C_{19}H_{21}N_5O$) (labeled as "Ligand of Interest" by depositor).



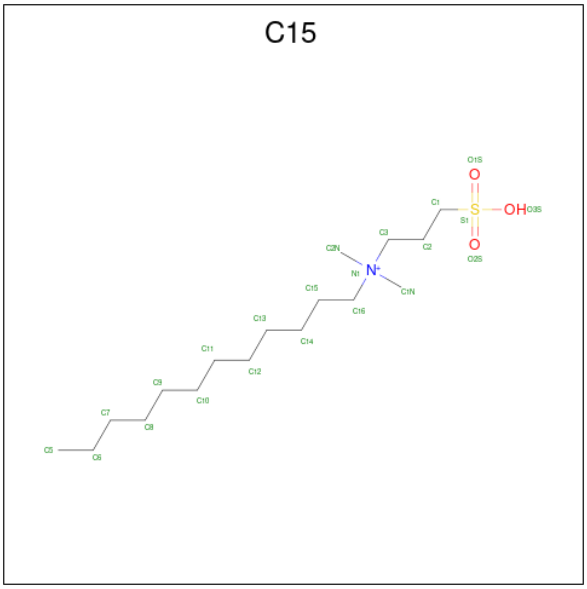
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 25 19 5 1	0	0
4	B	1	Total C N O 25 19 5 1	0	0
4	C	1	Total C N O 25 19 5 1	0	0
4	D	1	Total C N O 25 19 5 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



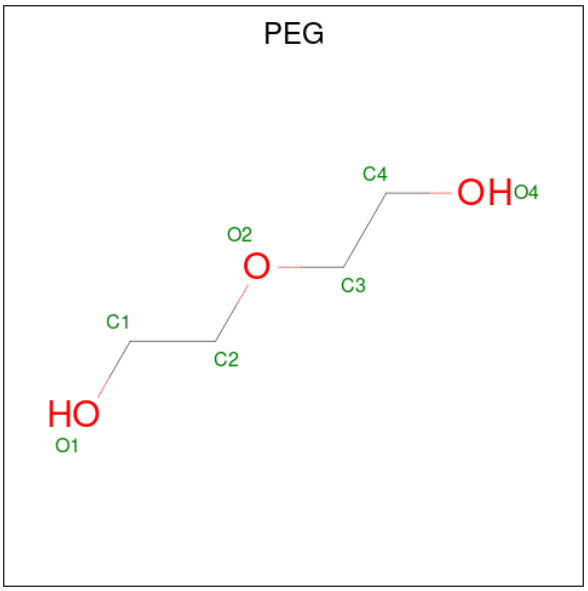
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is N-DODECYL-N,N-DIMETHYL-3-AMMONIO-1-PROPANESULFONATE (three-letter code: C15) (formula: $C_{17}H_{38}NO_3S$).



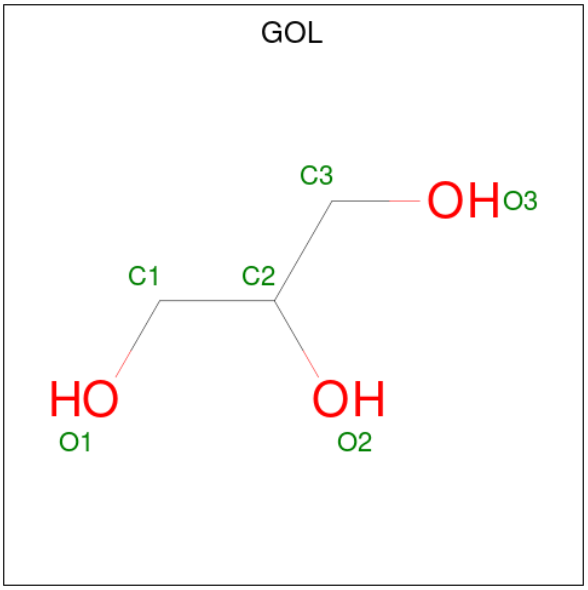
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O S 22 17 1 3 1	0	0
6	B	1	Total C N O S 22 17 1 3 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is water.

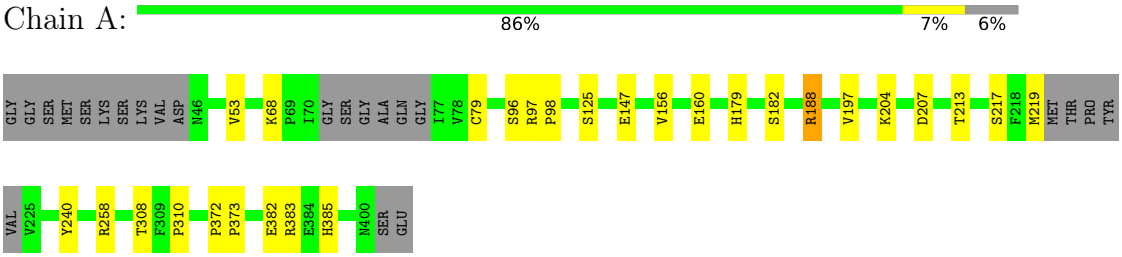
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	247	Total	O	0	0
			247	247		
9	B	246	Total	O	0	0
			246	246		
9	C	191	Total	O	0	0
			191	191		
9	D	177	Total	O	0	0
			177	177		

3 Residue-property plots (i)

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. 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. 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.

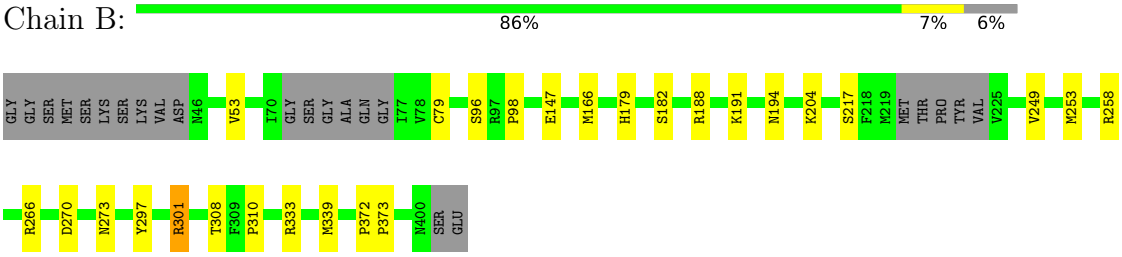
• Molecule 1: Mitogen-activated protein kinase 10

Chain A:



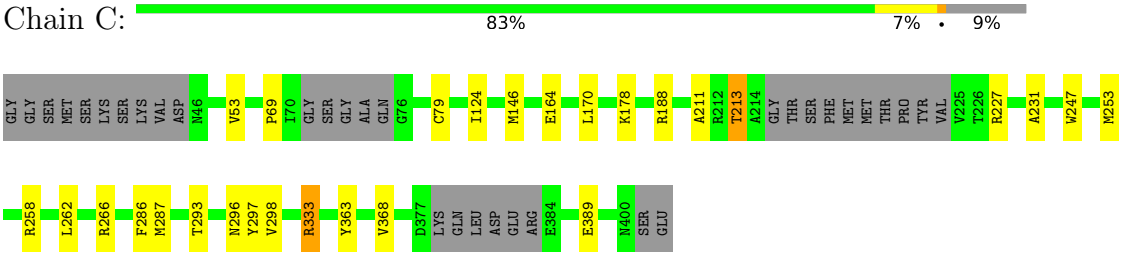
• Molecule 1: Mitogen-activated protein kinase 10

Chain B:



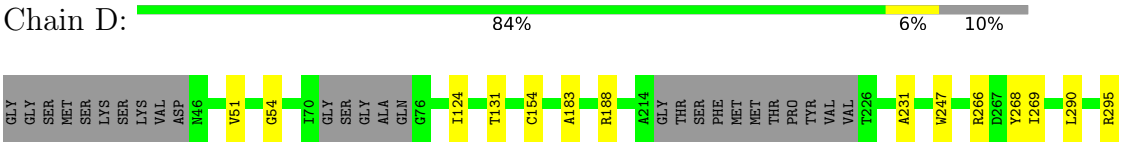
• Molecule 1: Mitogen-activated protein kinase 10

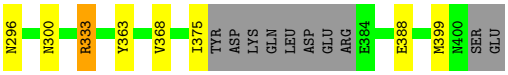
Chain C:



• Molecule 1: Mitogen-activated protein kinase 10

Chain D:




N296
N300
R333
Y363
V368
I375
TYR
ASP
LYS
GLN
LEU
ASP
GLU
ARG
E384
E388
M399
N400
SER
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.56Å 114.26Å 157.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 1.76 48.01 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.01-1.76) 99.9 (48.01-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	(Not available) , (Not available) 0.222 , 0.266	Depositor DCC
R_{free} test set	1580 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12089	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 82.20 % 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 2.9551e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, EDO, GOL, C15, BME, BGE, PEG

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	0.71	0/2936	0.79	5/3977 (0.1%)
1	B	0.68	0/2936	0.76	4/3978 (0.1%)
1	C	0.74	1/2799 (0.0%)	0.74	2/3799 (0.1%)
1	D	0.71	0/2752	0.75	4/3735 (0.1%)
All	All	0.71	1/11423 (0.0%)	0.76	15/15489 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	GLU	CD-OE2	5.59	1.31	1.25

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	333	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	D	188	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	258[A]	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	258[B]	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	C	188	ARG	NE-CZ-NH2	6.13	123.36	120.30

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	2826	0	2838	15	0
1	B	2826	0	2823	18	0
1	C	2700	0	2653	22	0
1	D	2665	0	2623	16	0
2	A	8	0	10	0	0
2	B	4	0	5	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	25	0	0	0	0
4	D	25	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
5	D	8	0	12	0	0
6	A	22	0	38	0	0
6	B	22	0	38	0	0
7	C	7	0	10	0	0
7	D	7	0	10	0	0
8	C	6	0	8	0	0
8	D	12	0	16	0	0
9	A	247	0	0	2	1
9	B	246	0	0	2	0
9	C	191	0	0	2	0
9	D	177	0	0	2	1
All	All	12089	0	11102	63	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 63 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:B:166:MET:CE	1:B:253:MET:HG3	2.17	0.73
1:B:266:ARG:NH2	1:B:270[A]:ASP:OD2	2.24	0.71
1:A:53:VAL:HG11	1:A:79[A]:CYS:SG	2.32	0.68
1:B:53:VAL:HG11	1:B:79[A]:CYS:SG	2.35	0.67
1:A:156:VAL:HG21	1:A:197[A]:VAL:HG21	1.78	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:630:HOH:O	9:D:651:HOH:O[2_455]	1.69	0.51

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	354/367 (96%)	349 (99%)	4 (1%)	1 (0%)	41 22
1	B	354/367 (96%)	349 (99%)	5 (1%)	0	100 100
1	C	339/367 (92%)	328 (97%)	10 (3%)	1 (0%)	41 22
1	D	332/367 (90%)	321 (97%)	10 (3%)	1 (0%)	41 22
All	All	1379/1468 (94%)	1347 (98%)	29 (2%)	3 (0%)	47 29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	THR
1	D	54	GLY
1	A	97	ARG

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	312/330 (94%)	310 (99%)	2 (1%)	86 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	313/330 (95%)	312 (100%)	1 (0%)	92 89
1	C	288/330 (87%)	287 (100%)	1 (0%)	92 89
1	D	286/330 (87%)	284 (99%)	2 (1%)	84 75
All	All	1199/1320 (91%)	1193 (100%)	6 (0%)	88 83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	333	ARG
1	D	51	VAL
1	D	124	ILE
1	A	219	MET
1	A	217	SER

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

Mol	Chain	Res	Type
1	B	291	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
2	BME	B	501	1	3,3,3	0.28	0	1,2,2	0.33	0
4	BGE	D	503	-	23,28,28	1.77	3 (13%)	31,38,38	1.47	4 (12%)
5	EDO	B	503	-	3,3,3	0.44	0	2,2,2	0.21	0
4	BGE	B	502	-	23,28,28	1.76	4 (17%)	31,38,38	1.52	5 (16%)
8	GOL	C	505	-	5,5,5	0.36	0	5,5,5	0.32	0
5	EDO	D	504	-	3,3,3	0.43	0	2,2,2	0.36	0
7	PEG	C	502	-	6,6,6	0.46	0	5,5,5	0.26	0
4	BGE	A	504	-	23,28,28	1.74	3 (13%)	31,38,38	1.56	7 (22%)
8	GOL	D	506	-	5,5,5	0.41	0	5,5,5	0.20	0
6	C15	A	506	-	21,21,21	1.93	2 (9%)	25,26,26	1.43	2 (8%)
5	EDO	A	505	-	3,3,3	0.47	0	2,2,2	0.46	0
4	BGE	C	503	-	23,28,28	1.78	3 (13%)	31,38,38	1.67	6 (19%)
2	BME	A	501	1	3,3,3	0.27	0	1,2,2	0.40	0
8	GOL	D	507	-	5,5,5	0.32	0	5,5,5	0.22	0
6	C15	B	504	-	21,21,21	2.16	4 (19%)	25,26,26	2.28	8 (32%)
7	PEG	D	502	-	6,6,6	0.45	0	5,5,5	0.27	0
2	BME	A	502	1	3,3,3	0.27	0	1,2,2	0.16	0
5	EDO	C	504	-	3,3,3	0.37	0	2,2,2	0.65	0
5	EDO	D	505	-	3,3,3	0.31	0	2,2,2	0.83	0

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	BME	B	501	1	-	0/1/1/1	-
4	BGE	D	503	-	-	2/12/20/20	0/4/4/4
5	EDO	B	503	-	-	0/1/1/1	-
4	BGE	B	502	-	-	0/12/20/20	0/4/4/4
8	GOL	C	505	-	-	3/4/4/4	-
5	EDO	D	504	-	-	1/1/1/1	-
7	PEG	C	502	-	-	1/4/4/4	-
4	BGE	A	504	-	-	0/12/20/20	0/4/4/4
8	GOL	D	506	-	-	2/4/4/4	-
6	C15	A	506	-	-	11/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	505	-	-	1/1/1/1	-
4	BGE	C	503	-	-	0/12/20/20	0/4/4/4
2	BME	A	501	1	-	0/1/1/1	-
8	GOL	D	507	-	-	2/4/4/4	-
6	C15	B	504	-	-	15/21/21/21	-
7	PEG	D	502	-	-	2/4/4/4	-
2	BME	A	502	1	-	1/1/1/1	-
5	EDO	C	504	-	-	1/1/1/1	-
5	EDO	D	505	-	-	1/1/1/1	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	504	C15	C1-S1	-7.32	1.67	1.77
6	A	506	C15	C1-S1	-7.00	1.67	1.77
4	D	503	BGE	C06-C07	-6.28	1.41	1.49
4	A	504	BGE	C06-C07	-6.28	1.41	1.49
4	B	502	BGE	C06-C07	-6.06	1.42	1.49

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	504	C15	O2S-S1-C1	5.45	113.48	106.92
6	A	506	C15	O3S-S1-C1	5.26	114.28	105.77
6	B	504	C15	C2N-N1-C3	4.95	122.07	109.46
4	C	503	BGE	C24-C25-N20	4.34	118.02	110.02
4	C	503	BGE	C22-C21-N20	4.11	117.60	110.02

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

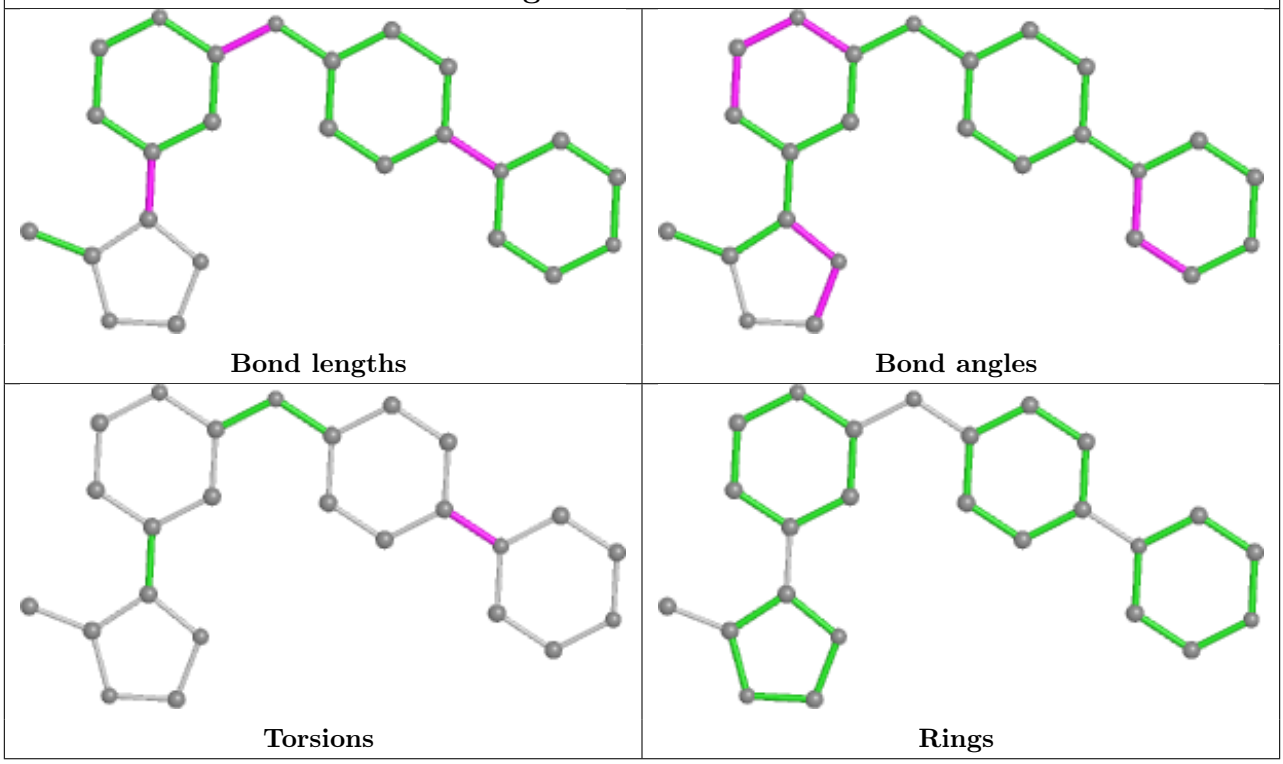
Mol	Chain	Res	Type	Atoms
2	A	502	BME	O1-C1-C2-S2
6	A	506	C15	C2-C1-S1-O1S
6	A	506	C15	C2-C1-S1-O3S
6	B	504	C15	S1-C1-C2-C3
6	B	504	C15	C2-C1-S1-O1S

There are no ring outliers.

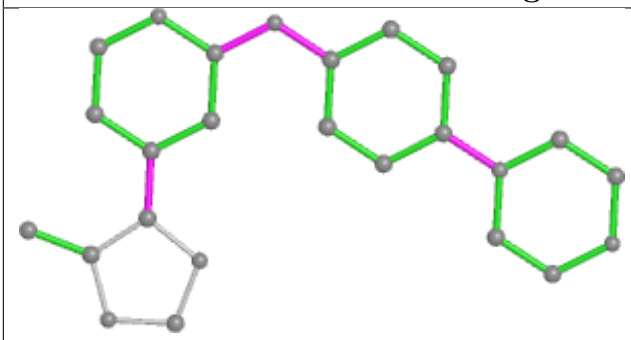
No monomer is involved in short contacts.

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 then 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.

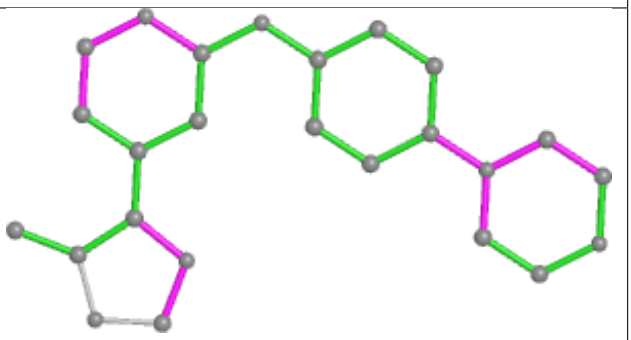
Ligand BGE D 503



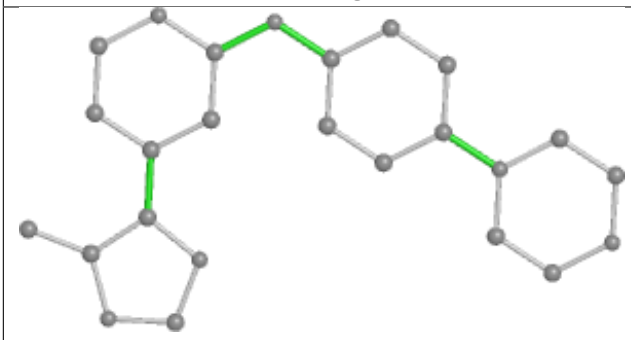
Ligand BGE B 502



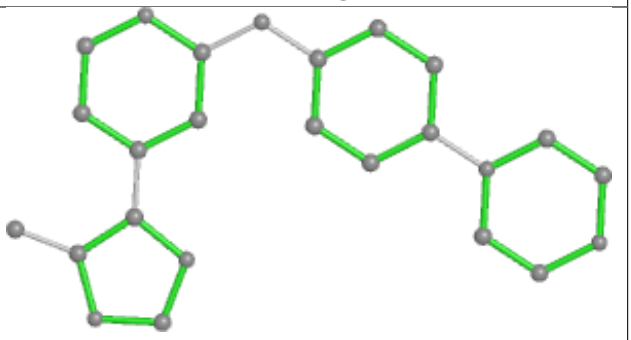
Bond lengths



Bond angles

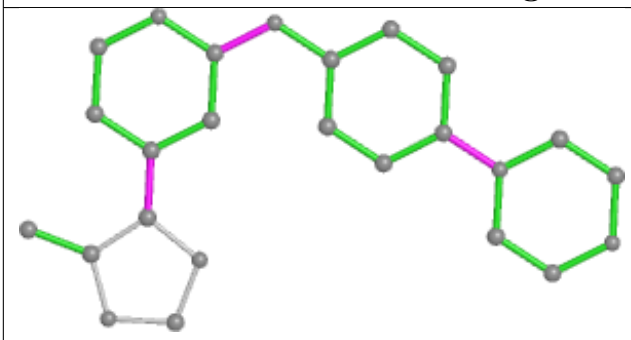


Torsions

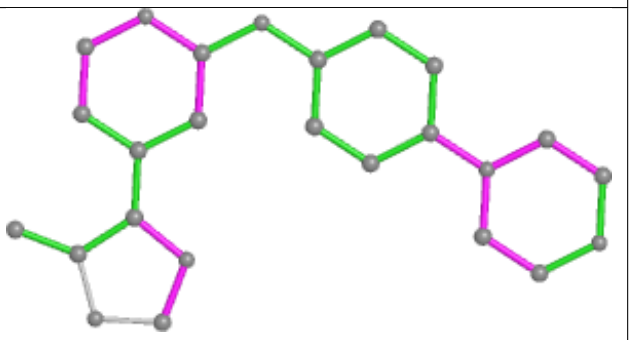


Rings

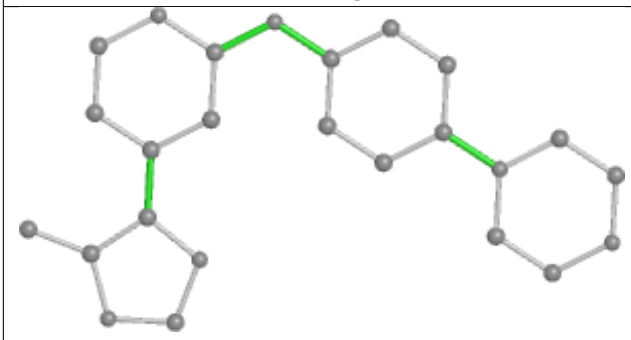
Ligand BGE A 504



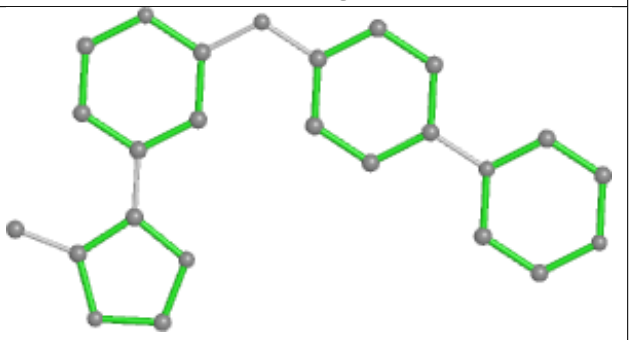
Bond lengths



Bond angles

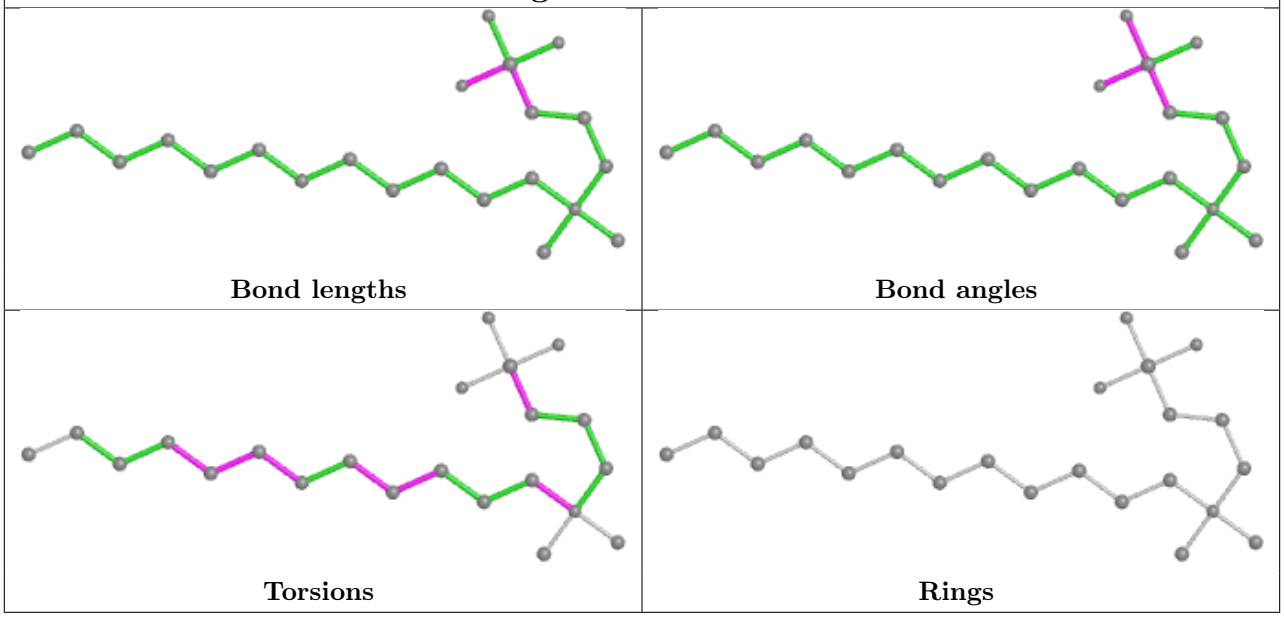


Torsions

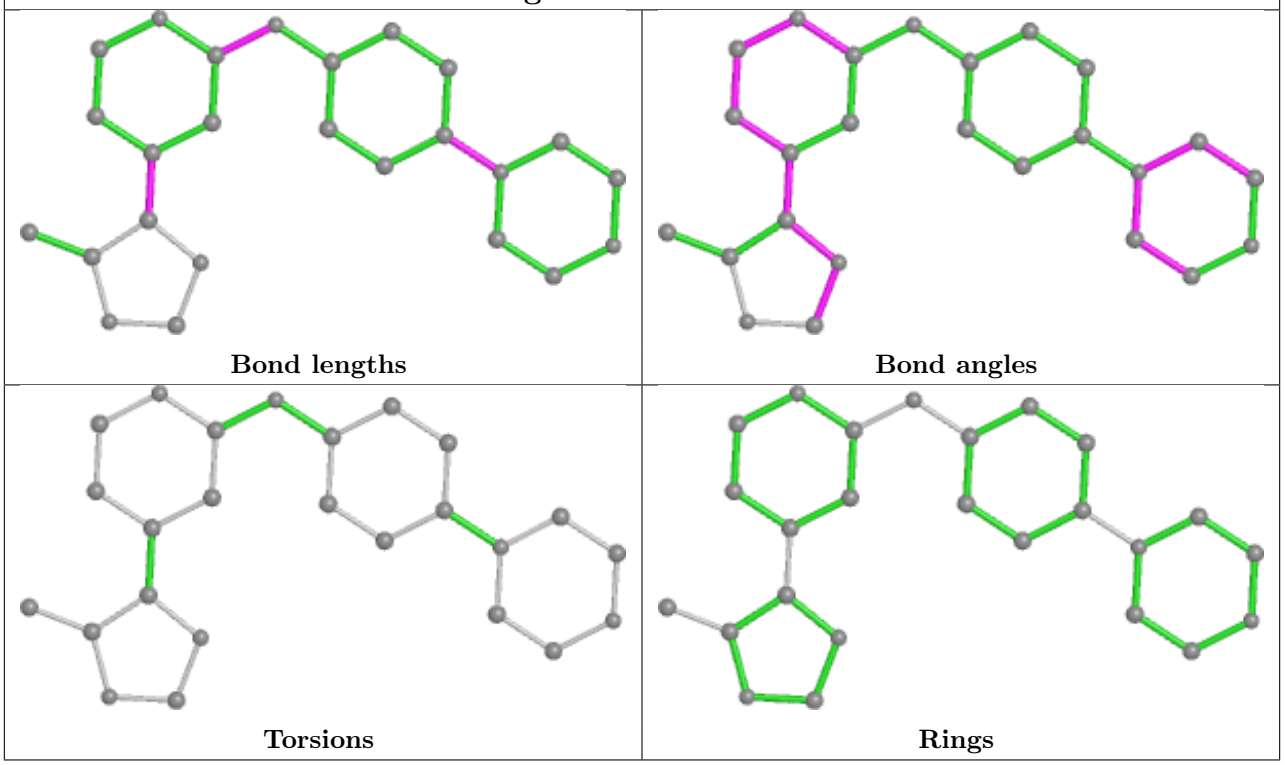


Rings

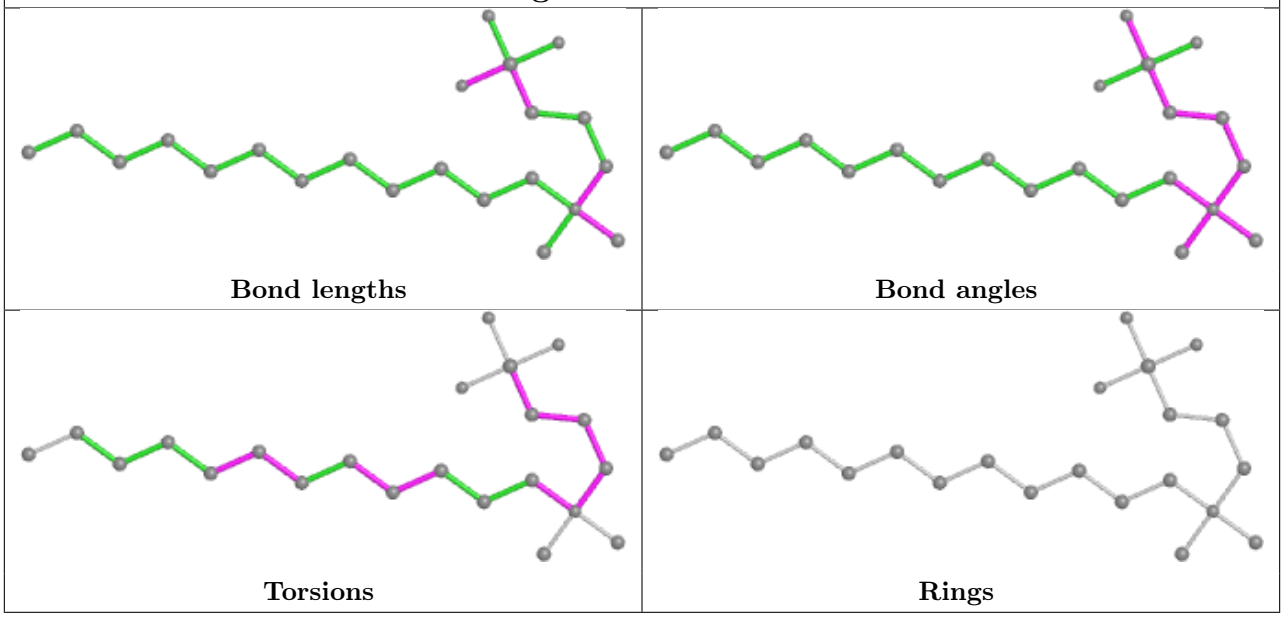
Ligand C15 A 506



Ligand BGE C 503



Ligand C15 B 504



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

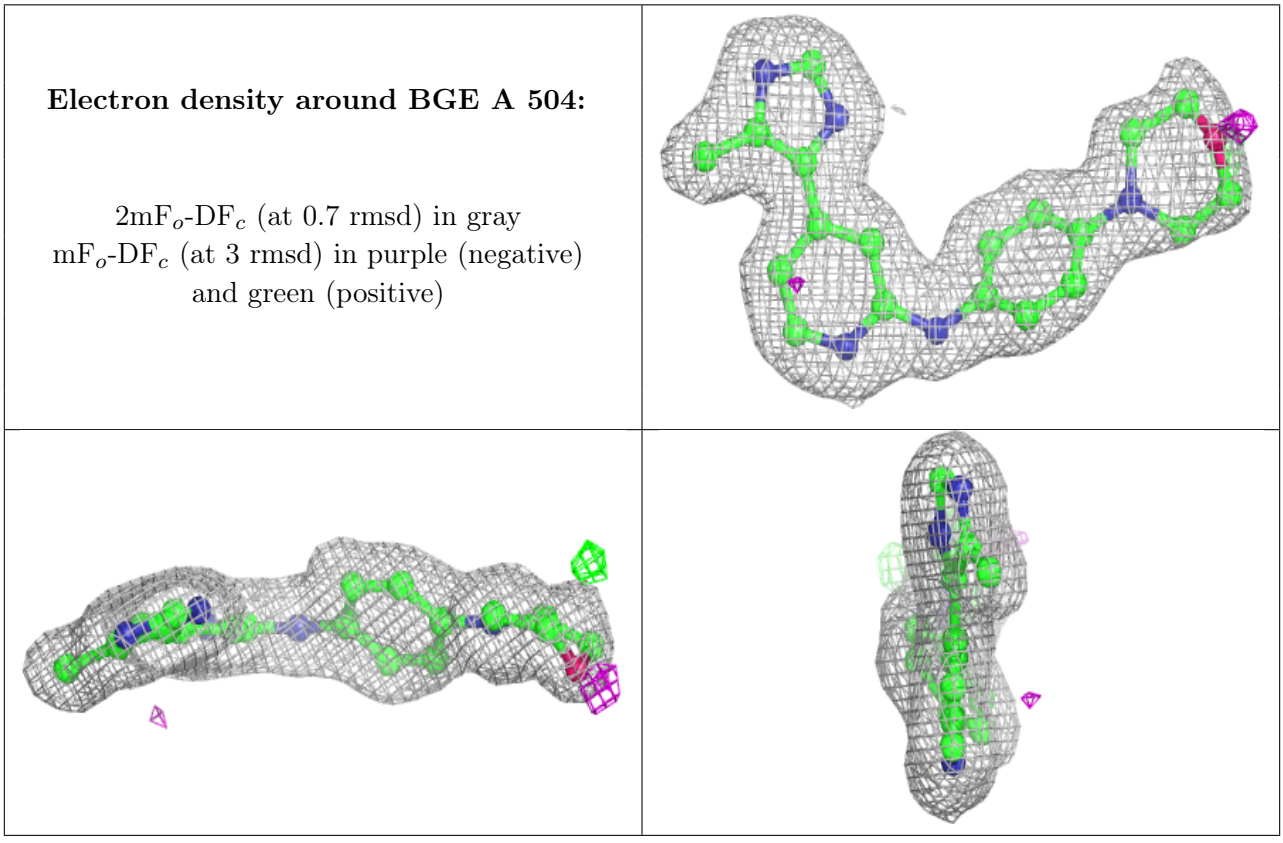
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

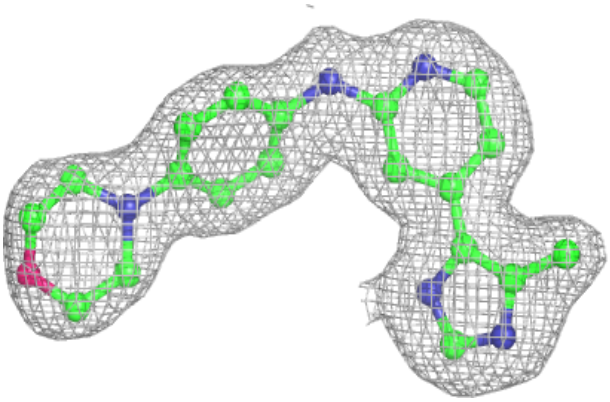
Electron density around BGE A 504:

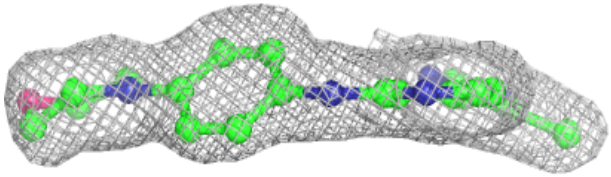
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

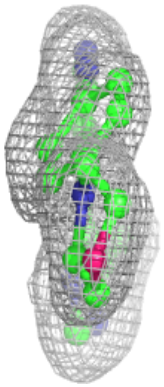


Electron density around BGE B 502:

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

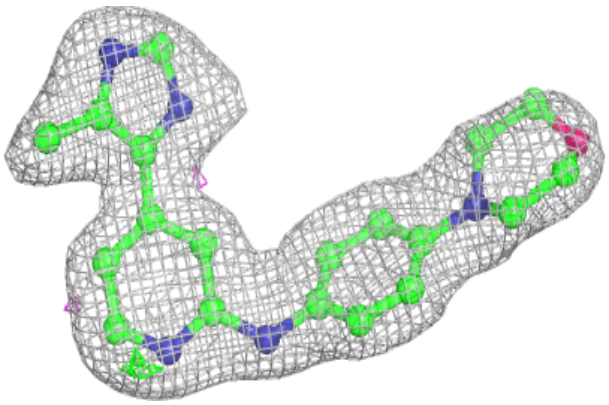


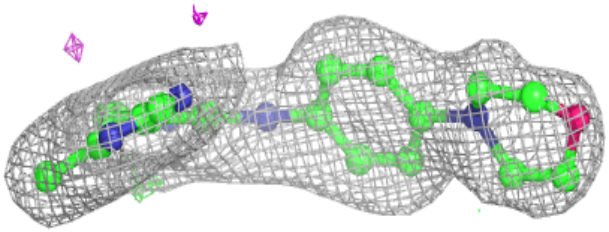


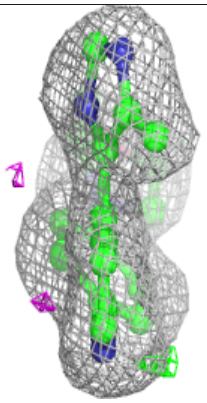


Electron density around BGE C 503:

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

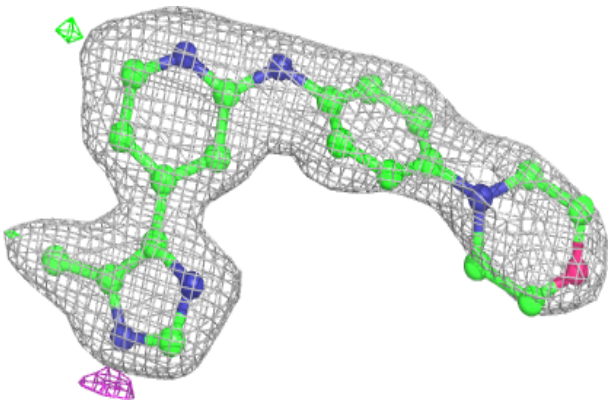


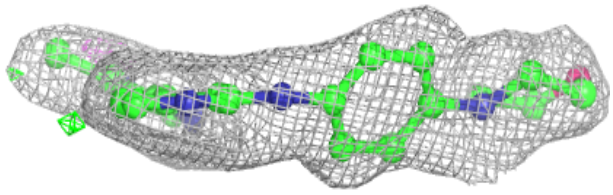


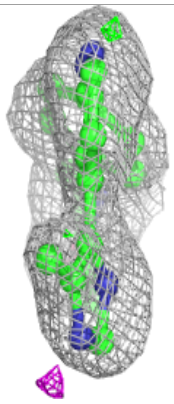


Electron density around BGE D 503:

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

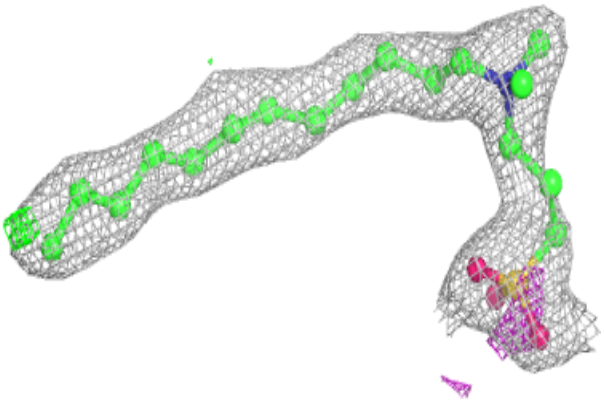


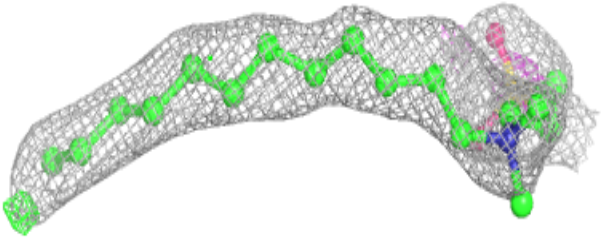


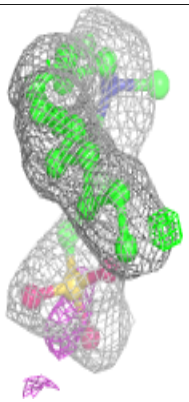


Electron density around C15 A 506:

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

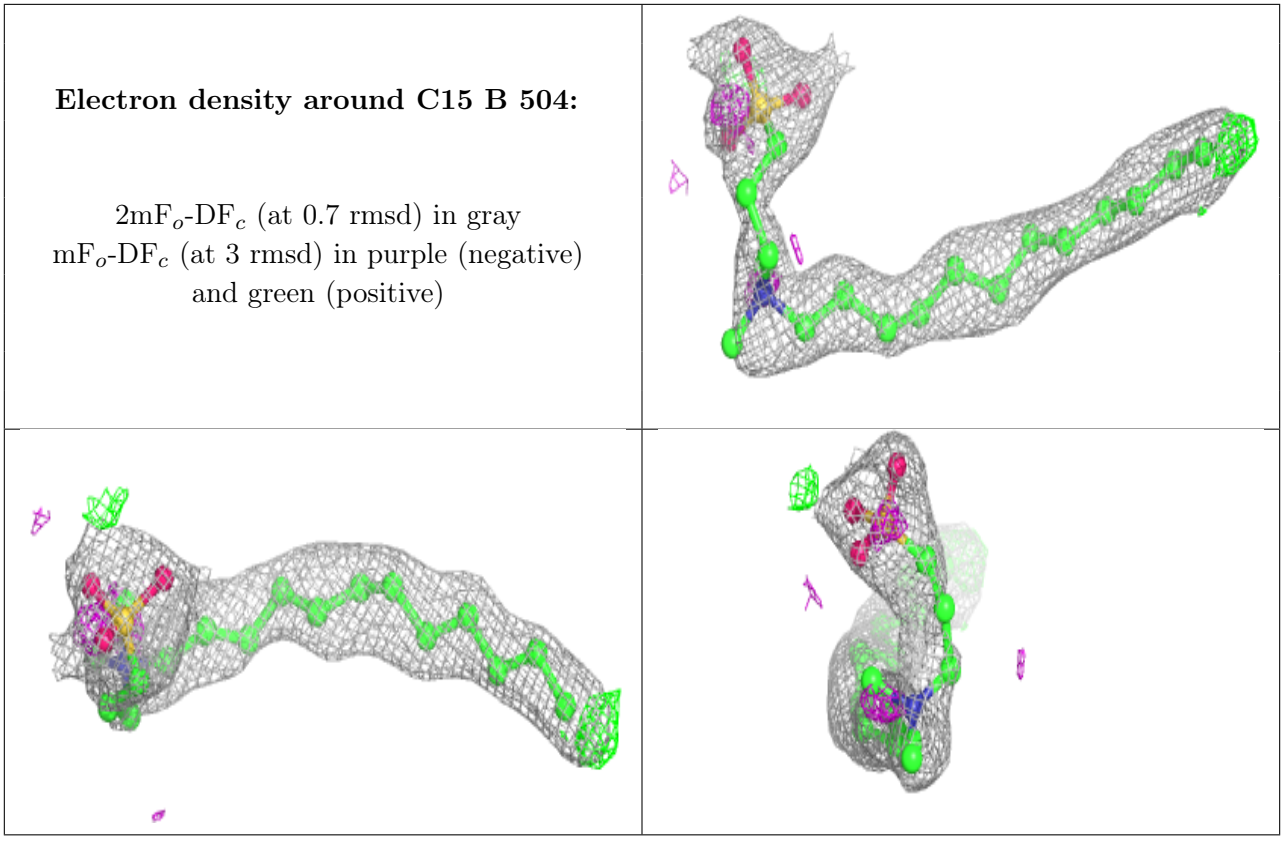






Electron density around C15 B 504:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.