Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 12:39 PM EST

PDB ID	:	2I3I
Title	:	Structure of an ML-IAP/XIAP chimera bound to a peptidomimetic
Authors	:	Fairbrother, W.J.; Franklin, M.C.
Deposited on	:	2006-08-18
Resolution	:	2.30 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 (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:

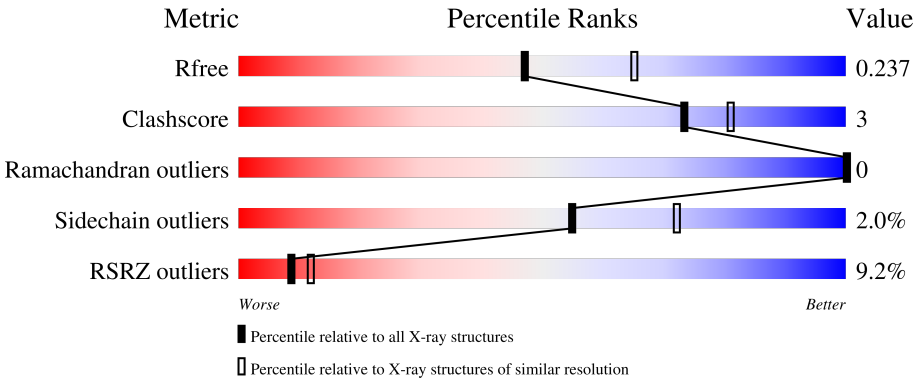
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	133	6% 65% 32%
1	B	133	7% 65% 5% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BTB	B	301	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 1724 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 Baculoviral IAP repeat-containing protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			727	473	124	126	4			
1	B	95	Total	C	N	O	S	0	0	0
			767	498	131	134	4			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	initiating methionine	UNP Q96CA5
A	41	GLY	-	expression tag	UNP Q96CA5
A	42	SER	-	expression tag	UNP Q96CA5
A	43	SER	-	expression tag	UNP Q96CA5
A	44	HIS	-	expression tag	UNP Q96CA5
A	45	HIS	-	expression tag	UNP Q96CA5
A	46	HIS	-	expression tag	UNP Q96CA5
A	47	HIS	-	expression tag	UNP Q96CA5
A	48	HIS	-	expression tag	UNP Q96CA5
A	49	HIS	-	expression tag	UNP Q96CA5
A	50	SER	-	expression tag	UNP Q96CA5
A	51	SER	-	expression tag	UNP Q96CA5
A	52	GLY	-	expression tag	UNP Q96CA5
A	53	GLU	-	expression tag	UNP Q96CA5
A	54	VAL	-	expression tag	UNP Q96CA5
A	55	PRO	-	expression tag	UNP Q96CA5
A	56	ARG	-	expression tag	UNP Q96CA5
A	57	GLY	-	expression tag	UNP Q96CA5
A	58	SER	-	expression tag	UNP Q96CA5
A	59	HIS	-	expression tag	UNP Q96CA5
A	60	MET	-	expression tag	UNP Q96CA5
A	61	LEU	-	expression tag	UNP Q96CA5
A	62	GLU	-	expression tag	UNP Q96CA5
A	150	GLY	SER	SEE REMARK 999	UNP Q96CA5
A	160	GLN	ARG	SEE REMARK 999	UNP Q96CA5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	161	GLU	ASP	SEE REMARK 999	UNP Q96CA5
A	162	TYR	PHE	SEE REMARK 999	UNP Q96CA5
A	163	ILE	VAL	SEE REMARK 999	UNP Q96CA5
A	164	ASN	HIS	SEE REMARK 999	UNP Q96CA5
A	165	ASN	SER	SEE REMARK 999	UNP Q96CA5
A	166	ILE	VAL	SEE REMARK 999	UNP Q96CA5
A	167	HIS	GLN	SEE REMARK 999	UNP Q96CA5
A	168	LEU	GLU	SEE REMARK 999	UNP Q96CA5
A	172	LEU	GLN	SEE REMARK 999	UNP Q96CA5
B	40	MET	-	initiating methionine	UNP Q96CA5
B	41	GLY	-	expression tag	UNP Q96CA5
B	42	SER	-	expression tag	UNP Q96CA5
B	43	SER	-	expression tag	UNP Q96CA5
B	44	HIS	-	expression tag	UNP Q96CA5
B	45	HIS	-	expression tag	UNP Q96CA5
B	46	HIS	-	expression tag	UNP Q96CA5
B	47	HIS	-	expression tag	UNP Q96CA5
B	48	HIS	-	expression tag	UNP Q96CA5
B	49	HIS	-	expression tag	UNP Q96CA5
B	50	SER	-	expression tag	UNP Q96CA5
B	51	SER	-	expression tag	UNP Q96CA5
B	52	GLY	-	expression tag	UNP Q96CA5
B	53	GLU	-	expression tag	UNP Q96CA5
B	54	VAL	-	expression tag	UNP Q96CA5
B	55	PRO	-	expression tag	UNP Q96CA5
B	56	ARG	-	expression tag	UNP Q96CA5
B	57	GLY	-	expression tag	UNP Q96CA5
B	58	SER	-	expression tag	UNP Q96CA5
B	59	HIS	-	expression tag	UNP Q96CA5
B	60	MET	-	expression tag	UNP Q96CA5
B	61	LEU	-	expression tag	UNP Q96CA5
B	62	GLU	-	expression tag	UNP Q96CA5
B	150	GLY	SER	SEE REMARK 999	UNP Q96CA5
B	160	GLN	ARG	SEE REMARK 999	UNP Q96CA5
B	161	GLU	ASP	SEE REMARK 999	UNP Q96CA5
B	162	TYR	PHE	SEE REMARK 999	UNP Q96CA5
B	163	ILE	VAL	SEE REMARK 999	UNP Q96CA5
B	164	ASN	HIS	SEE REMARK 999	UNP Q96CA5
B	165	ASN	SER	SEE REMARK 999	UNP Q96CA5
B	166	ILE	VAL	SEE REMARK 999	UNP Q96CA5
B	167	HIS	GLN	SEE REMARK 999	UNP Q96CA5
B	168	LEU	GLU	SEE REMARK 999	UNP Q96CA5

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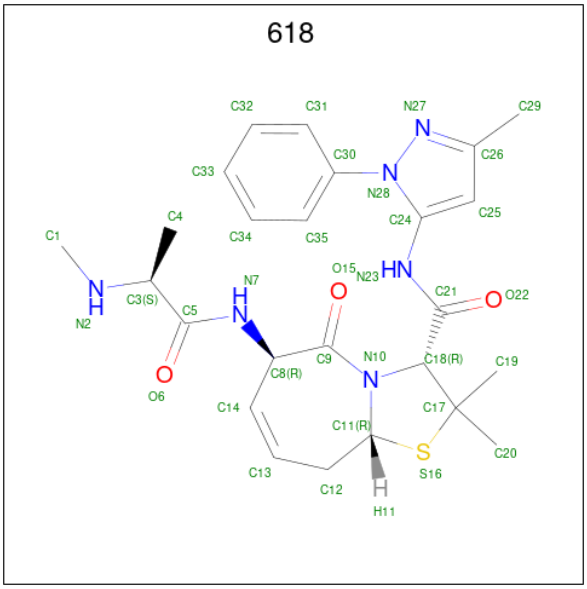
Chain	Residue	Modelled	Actual	Comment	Reference
B	172	LEU	GLN	SEE REMARK 999	UNP Q96CA5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is (3R,6R,9AR)-2,2-DIMETHYL-6-[(N-METHYL-L-ALANYL)AMINO]-N-(3-METHYL-1-PHENYL-1H-PYRAZOL-5-YL)-5-OXO-2,3,5,6,9,9A-HEXAHYDRO[1,3]THIAZOLO[3,2-A]AZEPINE-3-CARBOXAMIDE (three-letter code: 618) (formula: $C_{25}H_{32}N_6O_3S$).

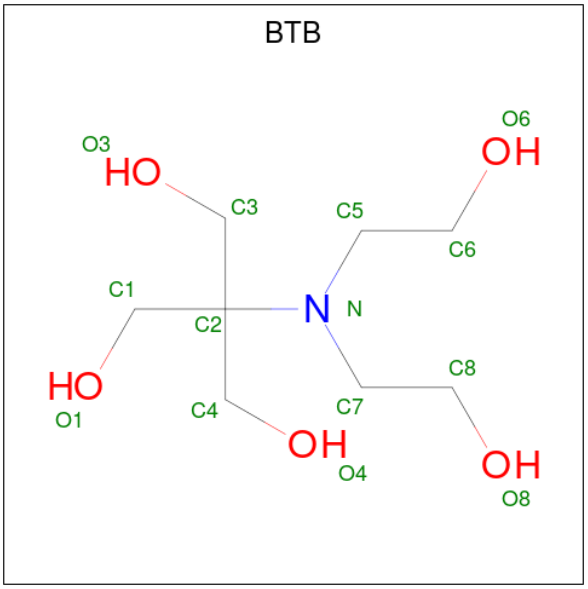


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 35 25 6 3 1	0	0
3	B	1	Total C N O S 35 25 6 3 1	0	0

- Molecule 4 is LITHIUM ION (three-letter code: LI) (formula: Li).

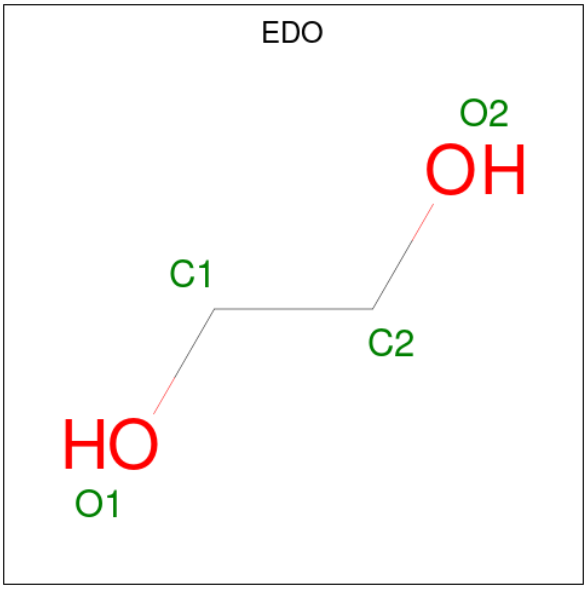
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Li 1 1	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

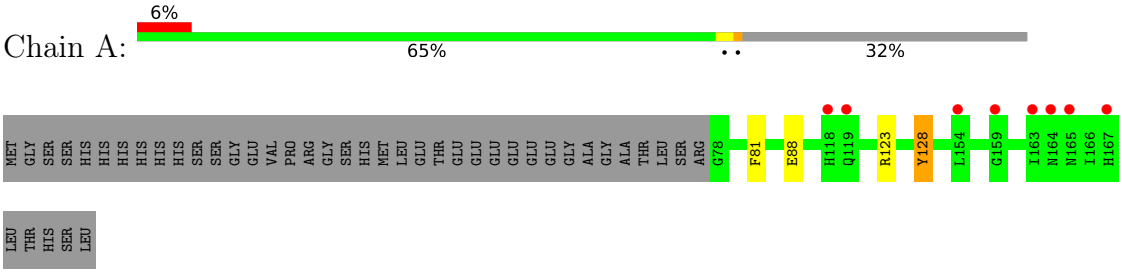
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	65	Total O 65 65	0	0

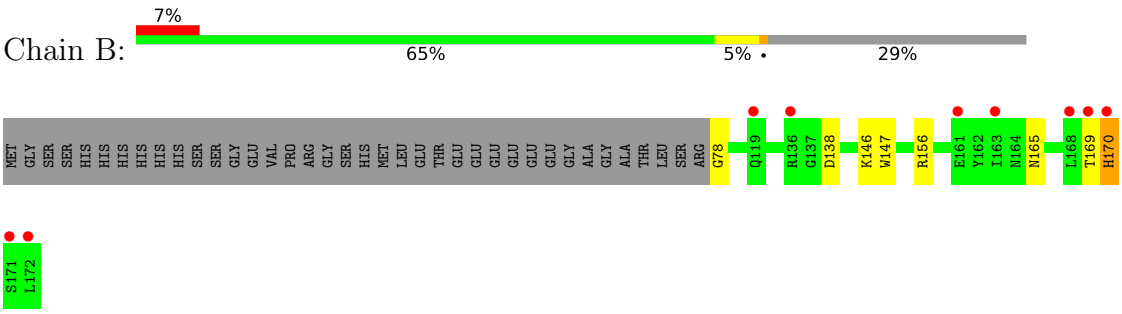
3 Residue-property plots (i)

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 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: Baculoviral IAP repeat-containing protein 7



• Molecule 1: Baculoviral IAP repeat-containing protein 7



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.36Å 87.36Å 73.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.34 – 2.30 17.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.34-2.30) 99.9 (17.47-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.224 0.204 , 0.237	Depositor DCC
R_{free} test set	644 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 21.7	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	0.92	EDS
Total number of atoms	1724	wwPDB-VP
Average B, all atoms (Å^2)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN, 618, BTB, EDO, LI

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	0.62	0/756	0.60	0/1026
1	B	0.64	0/797	0.65	1/1081 (0.1%)
All	All	0.63	0/1553	0.62	1/2107 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	156	ARG	NE-CZ-NH2	-5.53	117.53	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	727	0	670	2	0
1	B	767	0	711	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	35	0	32	0	0
3	B	35	0	32	2	0
4	B	1	0	0	0	0
5	B	14	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	8	0	11	0	0
7	A	70	0	0	1	0
7	B	65	0	0	1	0
All	All	1724	0	1475	10	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 (10) 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:88:GLU:HG3	7:A:1061:HOH:O	1.56	1.03
1:B:78:GLY:N	7:B:1060:HOH:O	2.16	0.78
1:B:146:LYS:HE2	1:B:170:HIS:NE2	2.16	0.60
1:B:146:LYS:HE2	1:B:170:HIS:CD2	2.38	0.59
1:B:138:ASP:OD2	3:B:501:618:N2	2.42	0.53
1:B:146:LYS:HE2	1:B:170:HIS:HE2	1.77	0.49
1:B:165:ASN:O	1:B:169:THR:HG23	2.15	0.46
1:B:146:LYS:CE	1:B:170:HIS:HE2	2.30	0.44
1:A:123:ARG:HD3	1:A:128:TYR:CG	2.56	0.41
1:B:147:TRP:CH2	3:B:501:618:H11	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/133 (66%)	87 (99%)	1 (1%)	0	100	100
1	B	93/133 (70%)	90 (97%)	3 (3%)	0	100	100
All	All	181/266 (68%)	177 (98%)	4 (2%)	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	73/109 (67%)	71 (97%)	2 (3%)	44	61
1	B	78/109 (72%)	77 (99%)	1 (1%)	69	82
All	All	151/218 (69%)	148 (98%)	3 (2%)	55	72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	PHE
1	A	128	TYR
1	B	170	HIS

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

Mol	Chain	Res	Type
1	A	167	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	618	B	501	-	32,38,38	2.11	6 (18%)	36,56,56	1.93	9 (25%)
3	618	A	501	-	32,38,38	2.10	7 (21%)	36,56,56	2.11	9 (25%)
6	EDO	B	202	-	3,3,3	0.46	0	2,2,2	0.54	0
5	BTB	B	301	-	13,13,13	0.47	0	7,16,16	0.33	0
6	EDO	B	201	4	3,3,3	0.73	0	2,2,2	0.16	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
3	618	B	501	-	-	3/16/55/55	0/4/4/4
3	618	A	501	-	-	7/16/55/55	0/4/4/4
6	EDO	B	202	-	-	1/1/1/1	-
5	BTB	B	301	-	-	6/21/21/21	-
6	EDO	B	201	4	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	618	C14-C13	9.08	1.54	1.33
3	B	501	618	C14-C13	9.00	1.54	1.33
3	A	501	618	C24-N23	3.34	1.46	1.39
3	B	501	618	C24-N23	3.31	1.46	1.39
3	B	501	618	C18-C21	3.12	1.58	1.53
3	B	501	618	C17-S16	-2.69	1.79	1.85
3	A	501	618	C18-N10	2.55	1.50	1.46
3	A	501	618	C18-C21	2.54	1.57	1.53
3	B	501	618	C26-N27	2.51	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	618	C18-N10	2.44	1.50	1.46
3	A	501	618	C17-S16	-2.34	1.80	1.85
3	A	501	618	C12-C13	2.21	1.55	1.50
3	A	501	618	C26-N27	2.10	1.37	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	618	O15-C9-C8	-7.22	113.89	121.70
3	B	501	618	O15-C9-C8	-5.70	115.54	121.70
3	B	501	618	C12-C13-C14	-5.19	116.94	127.83
3	A	501	618	C12-C13-C14	-4.67	118.03	127.83
3	A	501	618	C8-N7-C5	4.15	129.78	121.17
3	B	501	618	O15-C9-N10	-4.05	117.21	121.69
3	A	501	618	C34-C35-C30	-3.30	119.38	121.25
3	A	501	618	O15-C9-N10	-3.24	118.10	121.69
3	B	501	618	C8-N7-C5	3.02	127.43	121.17
3	B	501	618	C12-C11-S16	-2.98	106.18	112.57
3	A	501	618	C20-C17-C19	-2.84	106.15	110.78
3	B	501	618	C26-N27-N28	2.82	108.93	105.66
3	B	501	618	C20-C17-C19	-2.60	106.55	110.78
3	A	501	618	C12-C11-S16	-2.57	107.05	112.57
3	B	501	618	C19-C17-C18	2.40	116.90	111.57
3	A	501	618	C26-N27-N28	2.33	108.36	105.66
3	B	501	618	C17-C18-C21	2.25	117.92	113.28
3	A	501	618	C18-C17-S16	-2.23	100.31	104.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	618	C14-C8-N7-C5
3	B	501	618	C14-C8-N7-C5
5	B	301	BTB	O1-C1-C2-C3
5	B	301	BTB	O1-C1-C2-C4
5	B	301	BTB	O1-C1-C2-N
3	A	501	618	O6-C5-N7-C8
3	A	501	618	C3-C5-N7-C8
3	B	501	618	O6-C5-N7-C8
3	B	501	618	C3-C5-N7-C8
6	B	201	EDO	O1-C1-C2-O2
5	B	301	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
6	B	202	EDO	O1-C1-C2-O2
5	B	301	BTB	C3-C2-N-C7
5	B	301	BTB	C4-C2-N-C7
3	A	501	618	C4-C3-C5-N7
3	A	501	618	C4-C3-C5-O6
3	A	501	618	N2-C3-C5-N7
3	A	501	618	N2-C3-C5-O6

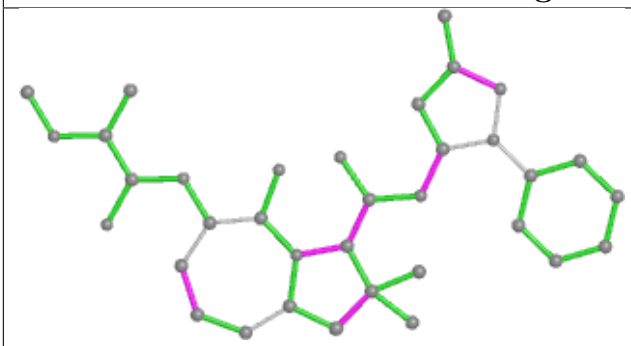
There are no ring outliers.

1 monomer is involved in 2 short contacts:

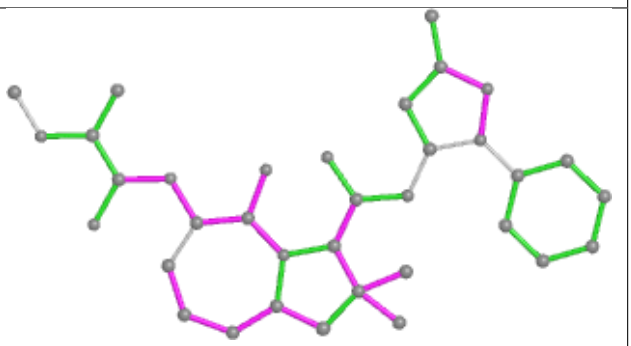
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	618	2	0

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 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.

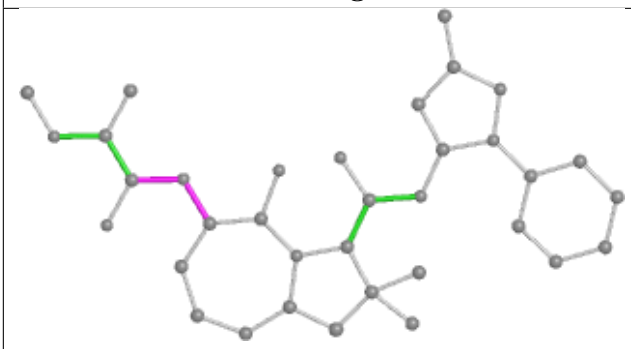
Ligand 618 B 501



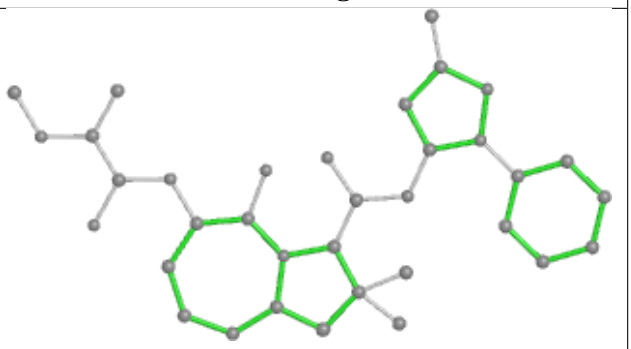
Bond lengths



Bond angles

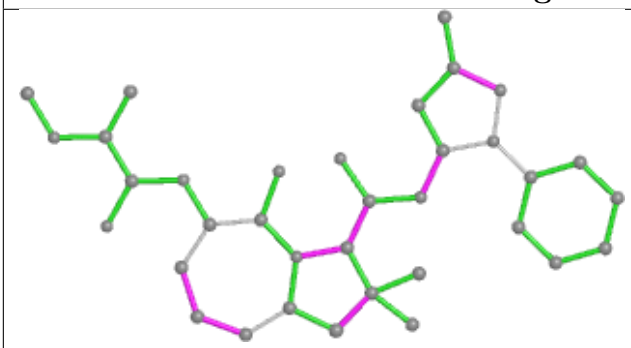


Torsions

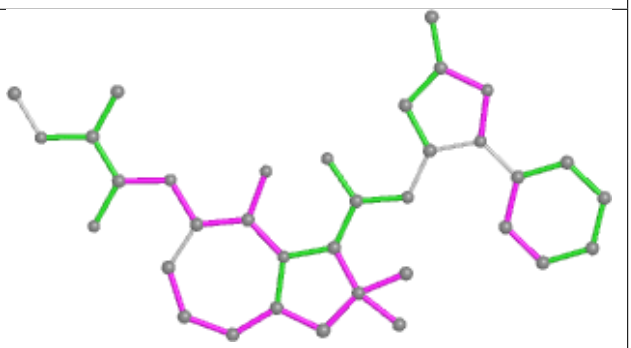


Rings

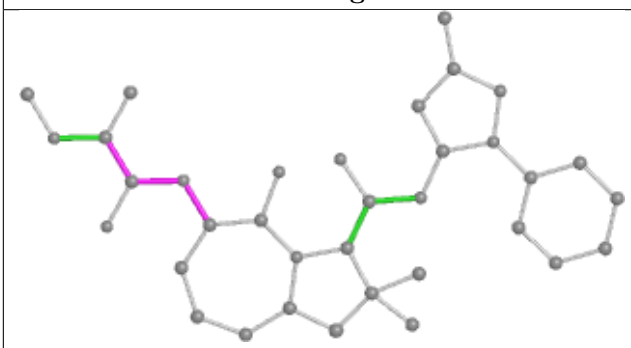
Ligand 618 A 501



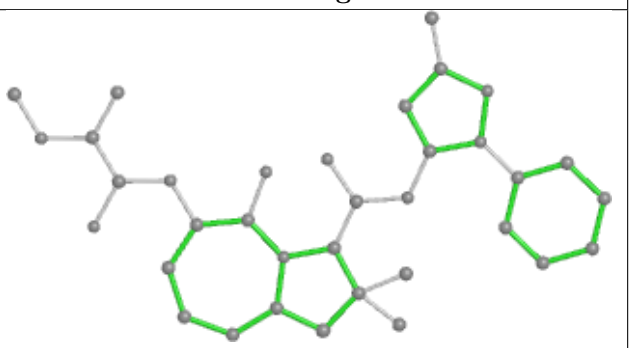
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	90/133 (67%)	0.40	8 (8%)	9	13	2, 2, 2, 3	0
1	B	95/133 (71%)	0.69	9 (9%)	8	11	2, 2, 2, 9	0
All	All	185/266 (69%)	0.55	17 (9%)	9	12	2, 2, 2, 9	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	8.4
1	B	170	HIS	5.5
1	B	171	SER	5.1
1	B	136	ARG	4.0
1	A	167	HIS	4.0
1	B	169	THR	3.9
1	A	165	ASN	3.8
1	A	118	HIS	3.3
1	A	119	GLN	3.0
1	A	154	LEU	2.4
1	A	164	ASN	2.2
1	B	119	GLN	2.2
1	A	163	ILE	2.1
1	B	163	ILE	2.1
1	A	159	GLY	2.1
1	B	161	GLU	2.0
1	B	168	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

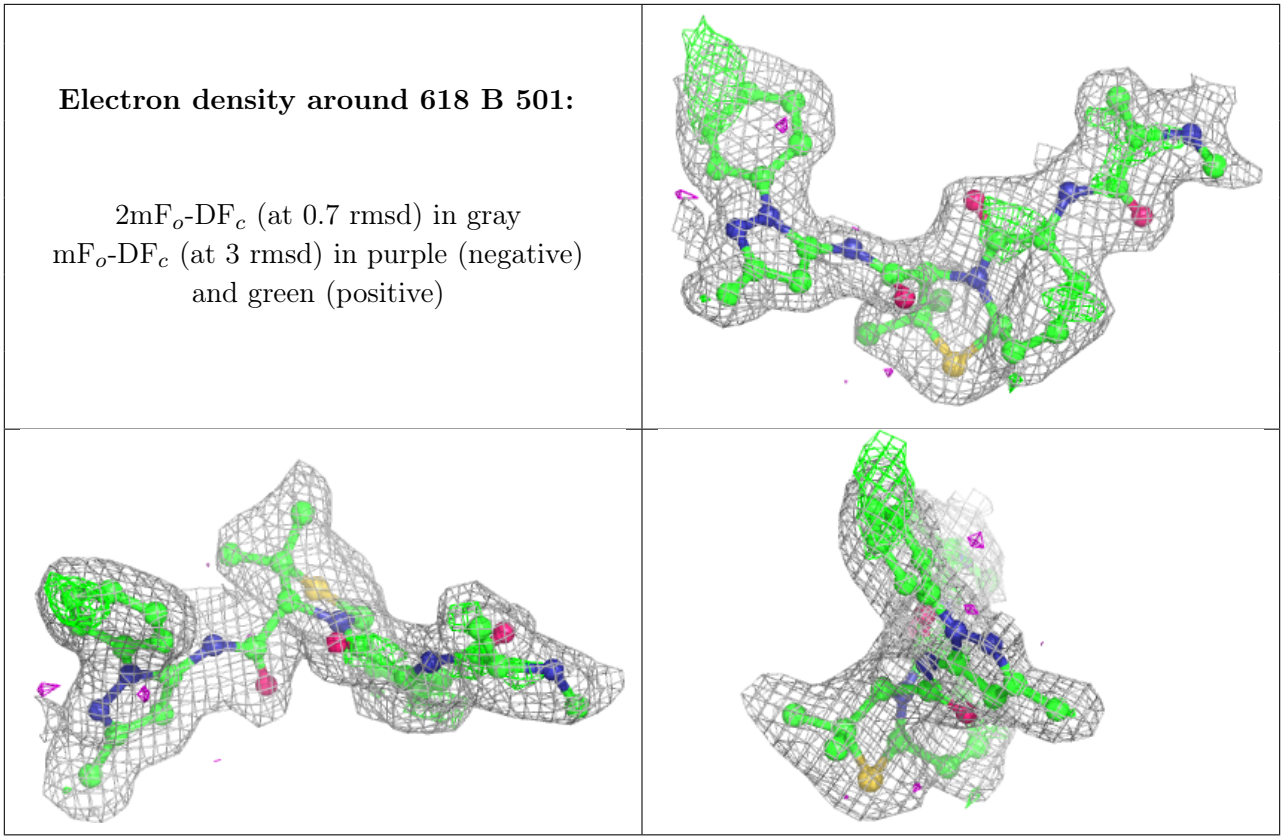
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	618	B	501	35/35	0.74	0.26	2,2,2,2	0
5	BTB	B	301	14/14	0.76	0.47	2,2,2,2	0
3	618	A	501	35/35	0.78	0.25	2,2,2,2	0
6	EDO	B	201	4/4	0.84	0.26	2,2,2,2	0
4	LI	B	1002	1/1	0.86	0.54	2,2,2,2	0
6	EDO	B	202	4/4	0.86	0.41	2,2,2,2	0
2	ZN	A	1001	1/1	0.99	0.03	2,2,2,2	0
2	ZN	B	1001	1/1	1.00	0.04	2,2,2,2	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.

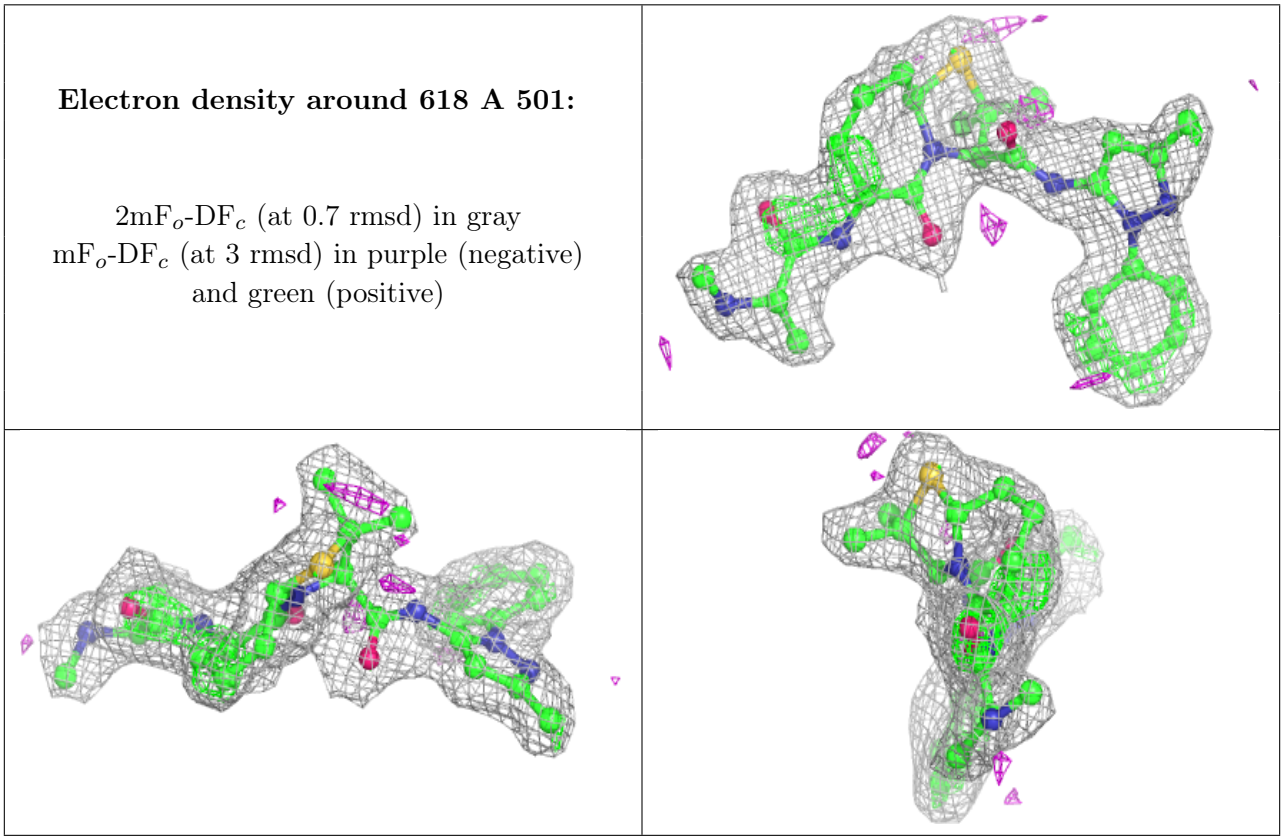
Electron density around 618 B 501:

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



Electron density around 618 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)



6.5 Other polymers (i)

There are no such residues in this entry.