Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8ATL
Title	:	Discovery of IRAK4 Inhibitor 23
Authors	:	Schafer, M.; Bothe, U.; Schmidt, N.; Gunther, J.; Nubbemeyer, R.; Siebeneicher, H.; Ring, S.; Boemer, U.; Peters, M.; Denner, K.; Himmel, H.; Sutter, A.; Terebesi, I.; Lange, M.; Wenger, A.M.; Guimond, N.; Thaler, T.; Platzek, J.; Eberspaecher, U.; Steuber, H.; Steinmeyer, A.; Zollner, T.M.
Deposited on	:	2022-08-23
Resolution	:	2.46 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 (1)) were used in the production of this report:

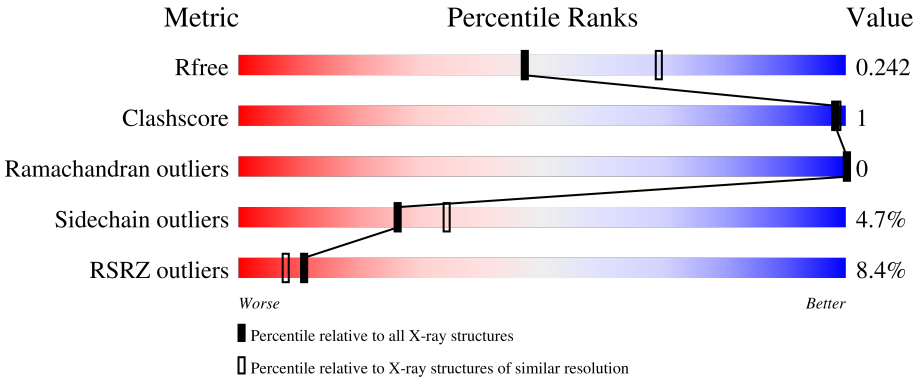
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	AAA	298	4% 89% 6% 5%
2	BBB	298	11% 86% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4517 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	AAA	282	Total	C	N	O	P	S	0	2	0
			2229	1402	375	435	2	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	163	GLY	-	expression tag	UNP Q9NWZ3
AAA	164	SER	-	expression tag	UNP Q9NWZ3
AAA	400	ALA	LYS	engineered mutation	UNP Q9NWZ3
AAA	401	ALA	GLU	engineered mutation	UNP Q9NWZ3
AAA	402	ALA	GLU	engineered mutation	UNP Q9NWZ3

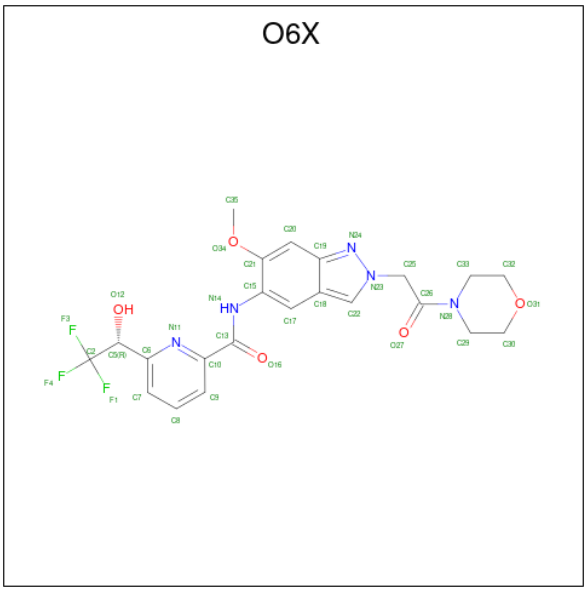
- Molecule 2 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	BBB	271	Total	C	N	O	P	S	0	1	0
			2148	1352	364	416	2	14			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	163	GLY	-	expression tag	UNP Q9NWZ3
BBB	164	SER	-	expression tag	UNP Q9NWZ3
BBB	400	ALA	LYS	engineered mutation	UNP Q9NWZ3
BBB	401	ALA	GLU	engineered mutation	UNP Q9NWZ3
BBB	402	ALA	GLU	engineered mutation	UNP Q9NWZ3

- Molecule 3 is {N}-[6-methoxy-2-(2-morpholin-4-yl-2-oxidanylidene-ethyl)indazol-5-yl]-6-[(1{R})-2,2,2-tris(fluoranyl)-1-oxidanyl-ethyl]pyridine-2-carboxamide (three-letter code: O6X) (formula: $C_{22}H_{22}F_3N_5O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C F N O 35 22 3 5 5	0	0
3	BBB	1	Total C F N O 35 22 3 5 5	0	0

- Molecule 4 is water.

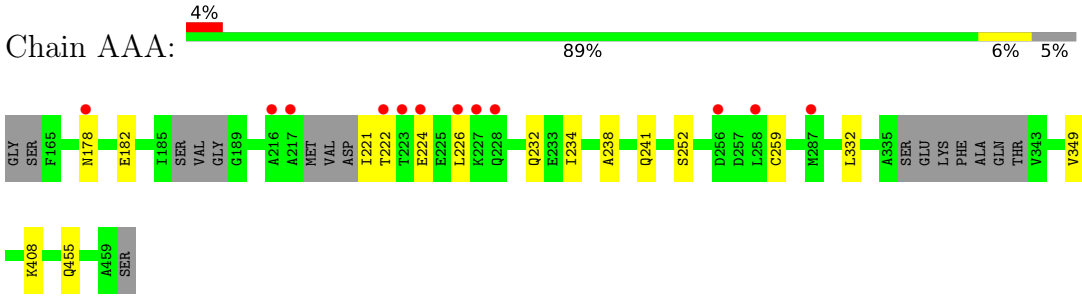
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	27	Total O 27 27	0	0
4	BBB	43	Total O 43 43	0	0

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.

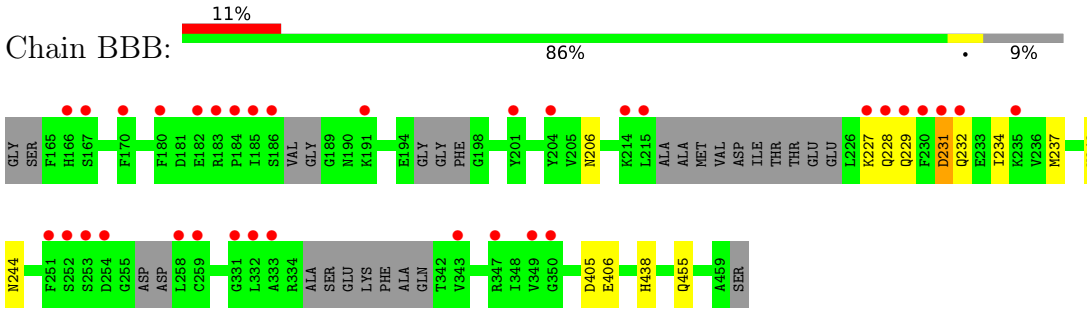
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain AAA:



• Molecule 2: Interleukin-1 receptor-associated kinase 4

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.86Å 118.79Å 138.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.35 – 2.46 46.35 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.35-2.46) 99.4 (46.35-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.243 0.206 , 0.242	Depositor DCC
R_{free} test set	1316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	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	0.95	EDS
Total number of atoms	4517	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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: CSO, TPO, O6X, 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	AAA	0.65	0/2241	0.71	0/3017
2	BBB	0.66	0/2160	0.71	0/2907
All	All	0.65	0/4401	0.71	0/5924

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2229	0	2204	3	0
2	BBB	2148	0	2124	2	0
3	AAA	35	0	0	0	0
3	BBB	35	0	0	0	0
4	AAA	27	0	0	0	0
4	BBB	43	0	0	0	0
All	All	4517	0	4328	5	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 1.

All (5) 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:AAA:234:ILE:O	1:AAA:238:ALA:HB2	2.11	0.51
2:BBB:231:ASP:HA	2:BBB:234:ILE:HB	1.94	0.48
2:BBB:242:HIS:CD2	2:BBB:244:ASN:H	2.35	0.45
1:AAA:252:SER:HB3	1:AAA:259:CYS:HB2	1.99	0.44
1:AAA:332:LEU:HD22	1:AAA:349:VAL:HG11	2.01	0.43

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	AAA	273/298 (92%)	266 (97%)	7 (3%)	0	100	100
2	BBB	258/298 (87%)	249 (96%)	9 (4%)	0	100	100
All	All	531/596 (89%)	515 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	241/252 (96%)	230 (95%)	11 (5%)	27	35
2	BBB	235/253 (93%)	224 (95%)	11 (5%)	26	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	476/505 (94%)	454 (95%)	22 (5%)	26 35

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	178	ASN
1	AAA	182	GLU
1	AAA	221	ILE
1	AAA	222	THR
1	AAA	224	GLU
1	AAA	226	LEU
1	AAA	232	GLN
1	AAA	241	GLN
1	AAA	365	THR
1	AAA	408	LYS
1	AAA	455	GLN
2	BBB	206	ASN
2	BBB	227	LYS
2	BBB	228	GLN
2	BBB	229	GLN
2	BBB	231	ASP
2	BBB	232	GLN
2	BBB	237	MET
2	BBB	405	ASP
2	BBB	406	GLU
2	BBB	438	HIS
2	BBB	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
2	SEP	BBB	346	2	8,9,10	0.60	0	8,12,14	0.65	0
1	SEP	AAA	346	1	8,9,10	0.61	0	8,12,14	0.64	0
1	CSO	AAA	240	1	3,6,7	0.84	0	0,6,8	-	-
2	TPO	BBB	345	2	8,10,11	0.83	0	10,14,16	0.78	0
1	TPO	AAA	345	1	8,10,11	0.83	0	10,14,16	0.79	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	SEP	BBB	346	2	-	1/5/8/10	-
1	SEP	AAA	346	1	-	4/5/8/10	-
1	CSO	AAA	240	1	-	1/1/5/7	-
2	TPO	BBB	345	2	-	3/9/11/13	-
1	TPO	AAA	345	1	-	2/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	345	TPO	N-CA-CB-OG1
1	AAA	346	SEP	CB-OG-P-O2P
1	AAA	346	SEP	CB-OG-P-O3P
2	BBB	345	TPO	N-CA-CB-OG1
2	BBB	345	TPO	O-C-CA-CB
2	BBB	346	SEP	N-CA-CB-OG
1	AAA	346	SEP	CB-OG-P-O1P
1	AAA	346	SEP	N-CA-CB-OG
1	AAA	240	CSO	N-CA-CB-SG
2	BBB	345	TPO	CB-OG1-P-O2P
1	AAA	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	O6X	AAA	1001	-	35,38,38	1.35	2 (5%)	48,55,55	1.80	12 (25%)
3	O6X	BBB	1001	-	35,38,38	1.49	2 (5%)	48,55,55	1.67	11 (22%)

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	O6X	AAA	1001	-	-	9/27/36/36	0/4/4/4
3	O6X	BBB	1001	-	-	2/27/36/36	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	1001	O6X	C6-C5	-6.59	1.48	1.52
3	AAA	1001	O6X	C6-C5	-5.46	1.49	1.52
3	BBB	1001	O6X	C15-C21	3.85	1.48	1.40
3	AAA	1001	O6X	C15-C21	3.69	1.48	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	1001	O6X	C35-O34-C21	4.45	124.24	117.53
3	BBB	1001	O6X	C25-N23-C22	4.42	134.83	129.19
3	AAA	1001	O6X	C25-N23-C22	4.00	134.28	129.19
3	BBB	1001	O6X	O34-C21-C15	3.77	119.43	114.80
3	AAA	1001	O6X	C5-C6-N11	3.60	119.54	115.97
3	AAA	1001	O6X	C10-N11-C6	3.33	122.06	118.83
3	BBB	1001	O6X	O34-C21-C20	-3.30	120.97	125.24
3	AAA	1001	O6X	C22-C18-C17	-3.28	128.32	134.80
3	BBB	1001	O6X	C10-N11-C6	3.26	122.00	118.83
3	BBB	1001	O6X	C22-C18-C17	-3.05	128.76	134.80
3	AAA	1001	O6X	C9-C10-N11	-3.02	119.38	122.92
3	AAA	1001	O6X	C7-C6-N11	-2.85	119.50	122.45
3	BBB	1001	O6X	C35-O34-C21	2.78	121.73	117.53
3	AAA	1001	O6X	C22-C18-C19	2.55	110.06	104.66
3	BBB	1001	O6X	C9-C10-N11	-2.54	119.94	122.92
3	BBB	1001	O6X	C7-C6-N11	-2.49	119.87	122.45
3	BBB	1001	O6X	C5-C6-N11	2.44	118.39	115.97
3	AAA	1001	O6X	C25-C26-N28	2.35	120.01	117.07
3	BBB	1001	O6X	C22-C18-C19	2.26	109.44	104.66
3	AAA	1001	O6X	C26-C25-N23	-2.25	108.08	110.76
3	AAA	1001	O6X	O34-C21-C15	2.21	117.50	114.80
3	AAA	1001	O6X	C20-C19-N24	2.09	132.92	130.28
3	BBB	1001	O6X	F3-C2-C5	-2.02	107.64	112.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

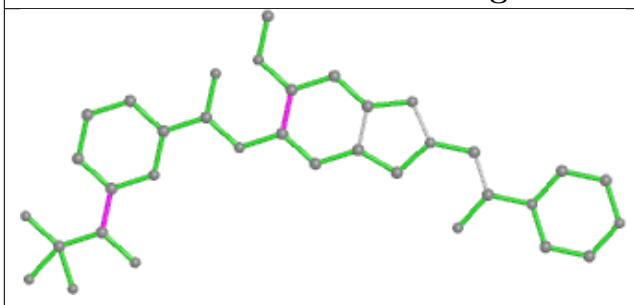
Mol	Chain	Res	Type	Atoms
3	AAA	1001	O6X	C25-C26-N28-C33
3	AAA	1001	O6X	C25-C26-N28-C29
3	BBB	1001	O6X	C15-C21-O34-C35
3	AAA	1001	O6X	O27-C26-N28-C29
3	BBB	1001	O6X	C20-C21-O34-C35
3	AAA	1001	O6X	O27-C26-N28-C33
3	AAA	1001	O6X	O12-C5-C6-N11
3	AAA	1001	O6X	O12-C5-C6-C7
3	AAA	1001	O6X	C2-C5-C6-C7
3	AAA	1001	O6X	C15-C21-O34-C35
3	AAA	1001	O6X	C20-C21-O34-C35

There are no ring outliers.

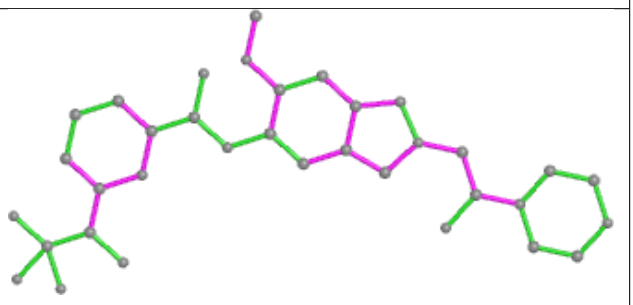
No monomer is involved in short contacts.

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.

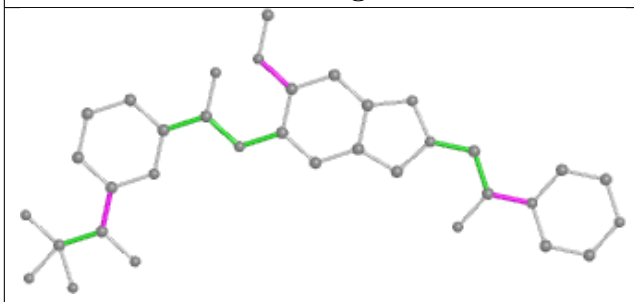
Ligand O6X AAA 1001



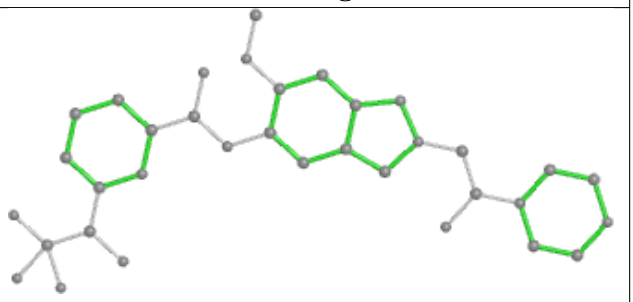
Bond lengths



Bond angles

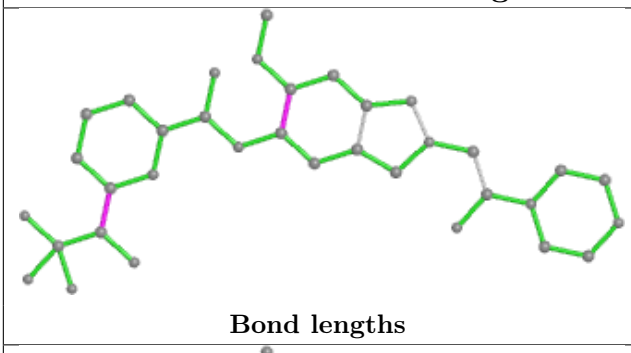


Torsions

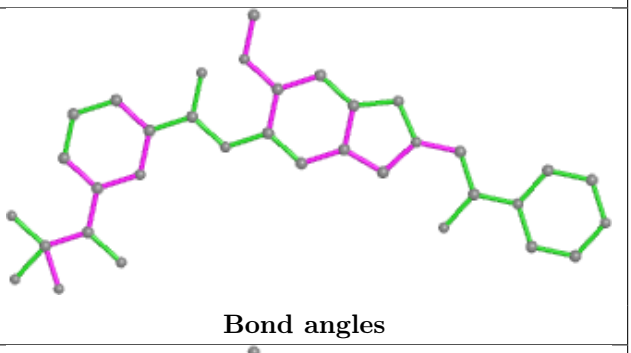


Rings

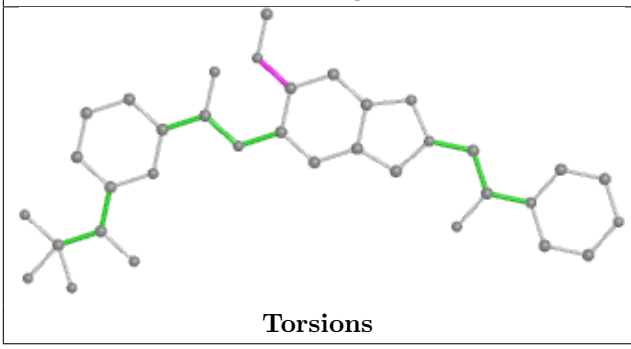
Ligand O6X BBB 1001



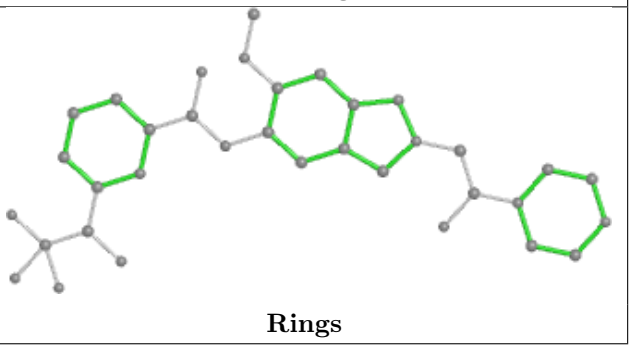
Bond lengths



Bond angles



Torsions



Rings

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

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	AAA	279/298 (93%)	0.24	12 (4%) 35 32	29, 51, 103, 135	0
2	BBB	269/298 (90%)	0.51	34 (12%) 3 2	31, 52, 118, 145	0
All	All	548/596 (91%)	0.37	46 (8%) 11 8	29, 52, 111, 145	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	343	VAL	5.6
1	AAA	222	THR	5.5
2	BBB	230	PHE	5.5
2	BBB	258	LEU	5.3
2	BBB	253	SER	4.9
1	AAA	226	LEU	4.9
2	BBB	350	GLY	4.8
2	BBB	227	LYS	4.7
2	BBB	252	SER	4.5
1	AAA	216	ALA	4.5
2	BBB	186	SER	4.4
1	AAA	256	ASP	4.3
2	BBB	254	ASP	3.9
2	BBB	349	VAL	3.8
2	BBB	184	PRO	3.7
1	AAA	217	ALA	3.7
2	BBB	231	ASP	3.6
1	AAA	228	GLN	3.5
2	BBB	251	PHE	3.4
2	BBB	215	LEU	3.4
2	BBB	183	ARG	3.3
2	BBB	228	GLN	3.3
2	BBB	333	ALA	3.3
2	BBB	259	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	BBB	331	GLY	3.0
2	BBB	185	ILE	2.9
2	BBB	232	GLN	2.9
2	BBB	214	LYS	2.7
2	BBB	182	GLU	2.7
2	BBB	166	HIS	2.6
2	BBB	167	SER	2.4
1	AAA	287[A]	MET	2.4
2	BBB	170	PHE	2.4
1	AAA	178	ASN	2.4
2	BBB	235	LYS	2.3
2	BBB	229	GLN	2.2
2	BBB	347	ARG	2.2
1	AAA	224	GLU	2.2
2	BBB	180	PHE	2.2
1	AAA	223	THR	2.2
1	AAA	258	LEU	2.2
2	BBB	201	TYR	2.1
2	BBB	204	TYR	2.1
1	AAA	227	LYS	2.0
2	BBB	191	LYS	2.0
2	BBB	332	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	SEP	BBB	346	10/11	0.71	0.28	101,118,151,152	0
1	CSO	AAA	240	7/8	0.76	0.19	72,78,87,88	0
1	SEP	AAA	346	10/11	0.81	0.41	100,128,142,143	0
2	TPO	BBB	345	11/12	0.86	0.22	75,92,98,100	0
1	TPO	AAA	345	11/12	0.92	0.21	75,88,96,96	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

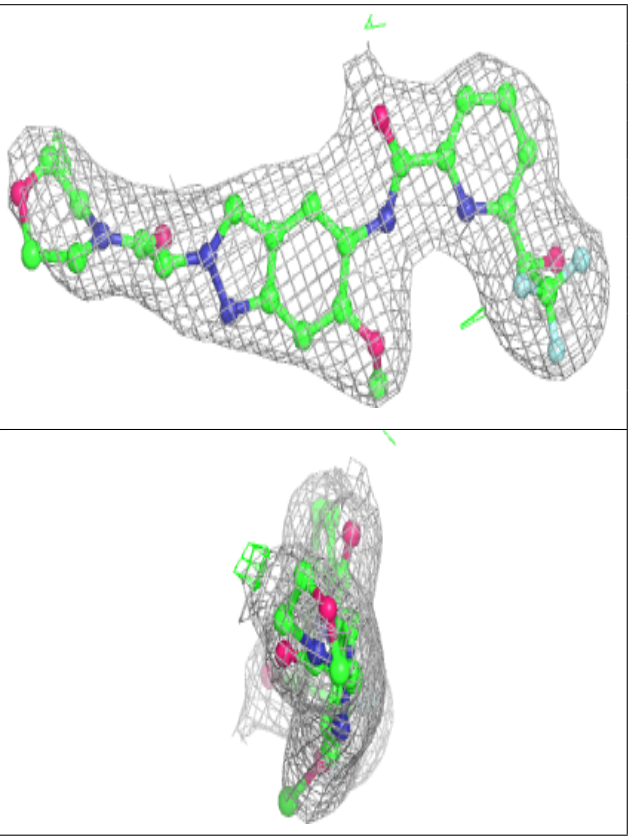
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	O6X	BBB	1001	35/35	0.92	0.17	40,48,87,94	0
3	O6X	AAA	1001	35/35	0.96	0.15	31,40,67,71	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.

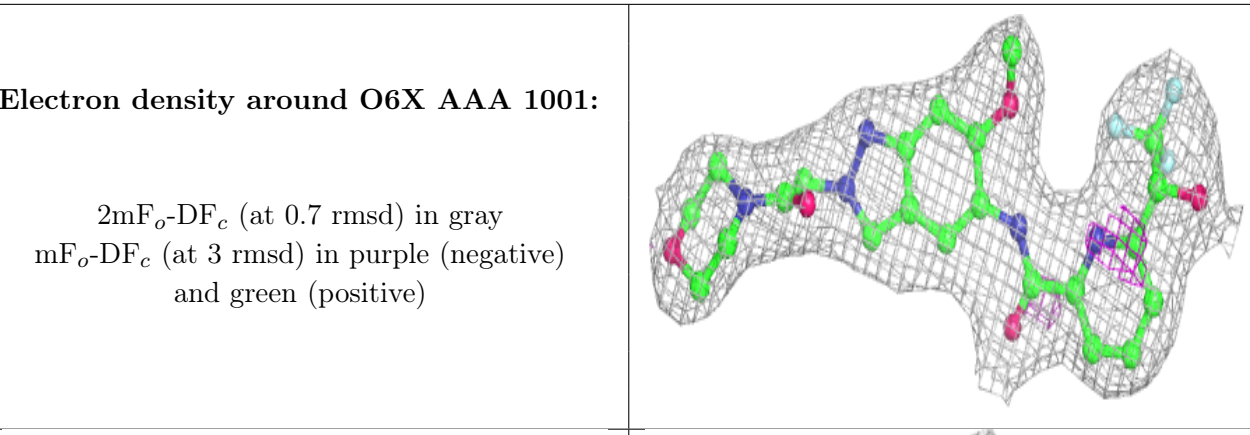
Electron density around O6X BBB 1001:

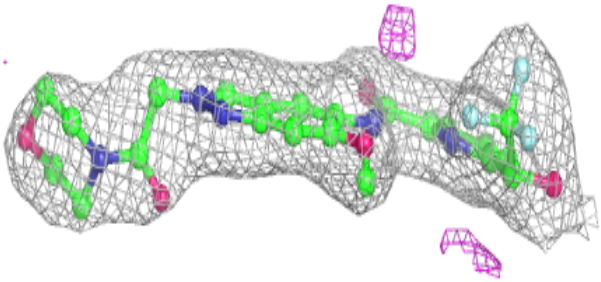
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

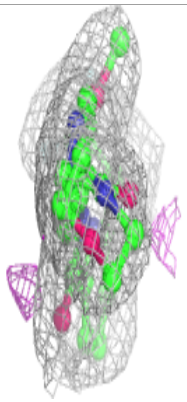


Electron density around O6X AAA 1001:

$2mF_o$-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.