Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	6F3E
Title	:	IRAK4 IN COMPLEX WITH inhibitor
Authors	:	Xue, Y.; Degorce, S.L.; Robb, G.R.; Ferguson, A.D.
Deposited on	:	2017-11-28
Resolution	:	2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

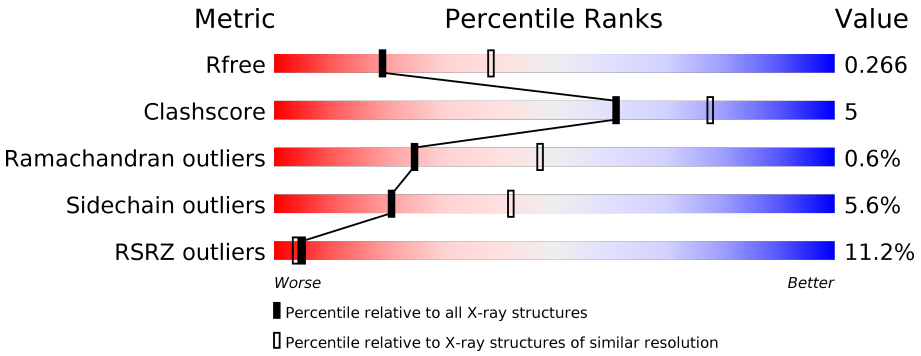
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	295	13% 80% 12% 8%
1	B	295	8% 79% 16%

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
1	TPO	A	342	-	-	-	X
1	TPO	B	342	-	-	-	X
1	TPO	B	345	-	-	-	X

2 Entry composition

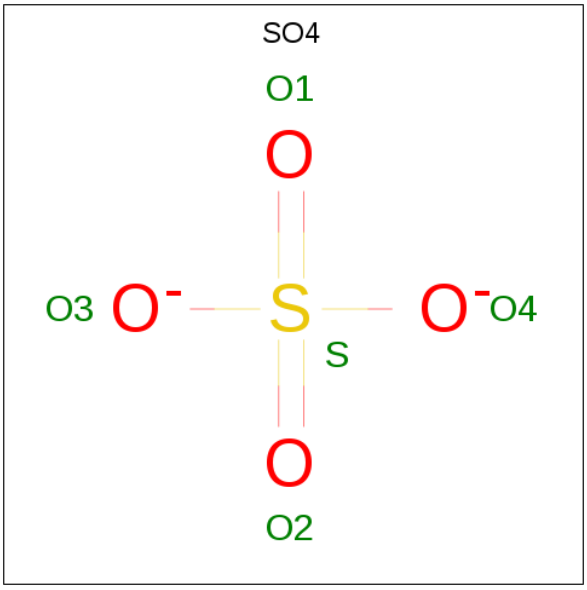
There are 4 unique types of molecules in this entry. The entry contains 4474 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

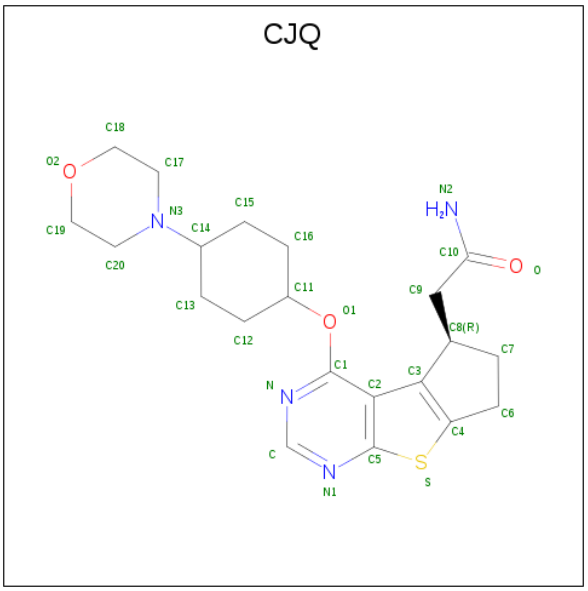
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	P	S	0	0	0
			2157	1361	363	417	2	14			
1	B	284	Total	C	N	O	P	S	0	0	0
			2245	1408	378	443	2	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 2-[(3 {R})-12-(4-morpholin-4-ylcyclohexyl)oxy-7-thia-9,11-diazatricyclo[6.4.0 .0^{2,6}]dodeca-1(8),2(6),9,11-tetraen-3-yl]ethanamide (three-letter code: CJQ) (formula: $C_{21}H_{28}N_4O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 29 21 4 3 1	0	0
3	B	1	Total C N O S 29 21 4 3 1	0	0

- Molecule 4 is water.

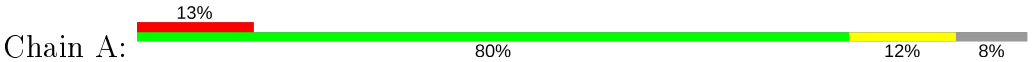
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	B	4	Total O 4 4	0	0

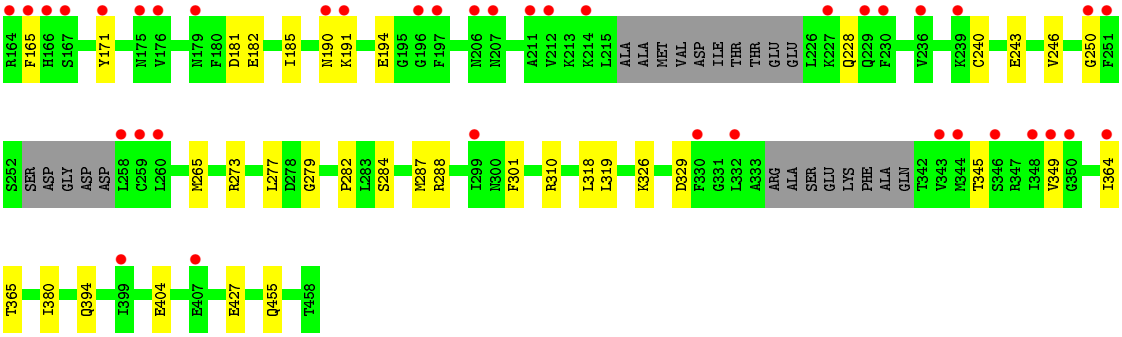
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

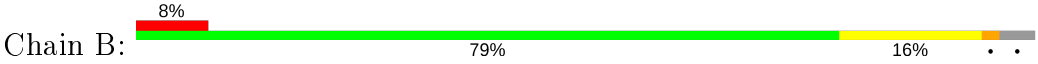
Chain A:

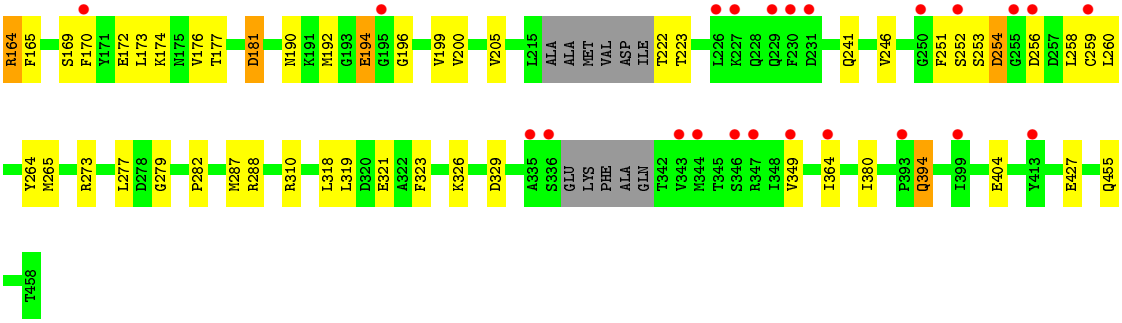




- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	87.18Å 109.37Å 141.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.17 – 2.67 54.69 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.5 (68.17-2.67) 99.9 (54.69-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.5 PACIOREK	Depositor
R, R_{free}	0.199 , 0.254 0.211 , 0.266	Depositor DCC
R_{free} test set	998 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4474	wwPDB-VP
Average B, all atoms (Å^2)	85.0	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 22.38 % 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 5.7641e-03. 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: TPO, CJQ, SO4

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	0.49	0/2170	0.67	0/2920
1	B	0.53	0/2259	0.71	0/3042
All	All	0.51	0/4429	0.69	0/5962

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	A	2157	0	2142	14	0
1	B	2245	0	2212	28	0
2	A	5	0	0	0	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
All	All	4474	0	4354	40	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 5.

All (40) 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:176:VAL:HG11	1:B:205:VAL:HG12	1.54	0.87
1:B:253:SER:HA	1:B:258:LEU:HD22	1.75	0.69
1:B:181:ASP:HB3	1:B:190:ASN:HB2	1.76	0.67
1:A:182:GLU:HA	1:A:191:LYS:HB2	1.81	0.62
1:B:265:MET:CE	1:B:326:LYS:HG3	2.31	0.61
1:B:265:MET:HE2	1:B:326:LYS:HG3	1.83	0.61
1:A:265:MET:HE2	1:A:326:LYS:HG3	1.82	0.60
1:A:265:MET:CE	1:A:326:LYS:HG3	2.31	0.60
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.87	0.56
1:B:172:GLU:O	1:B:176:VAL:HG13	2.06	0.56
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.89	0.55
1:B:273:ARG:HG3	1:B:319:LEU:HD12	1.88	0.54
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.89	0.54
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.90	0.54
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.91	0.52
1:A:273:ARG:HG3	1:A:319:LEU:HD12	1.91	0.52
1:B:192:MET:HE1	1:B:200:VAL:HG12	1.92	0.51
1:B:251:PHE:HB3	1:B:260:LEU:HD23	1.94	0.50
1:B:169:SER:HB3	1:B:172:GLU:HG3	1.93	0.50
1:B:310:ARG:HD3	1:B:364:ILE:HG23	1.95	0.49
1:A:310:ARG:HD3	1:A:364:ILE:HG23	1.95	0.49
1:B:321:GLU:CD	1:B:321:GLU:H	2.16	0.49
1:B:205:VAL:HG23	1:B:205:VAL:O	2.14	0.48
1:A:284:SER:H	1:A:287:MET:HE3	1.78	0.47
1:A:165:PHE:HB3	1:A:250:GLY:HA2	1.97	0.45
1:B:170:PHE:CE1	1:B:259:CYS:SG	3.10	0.44
1:B:222:THR:HG22	1:B:223:THR:H	1.82	0.43
1:A:240:CYS:HB3	1:A:301:PHE:HE2	1.83	0.43
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.01	0.43
1:B:287:MET:CE	1:B:323:PHE:HB3	2.48	0.42
1:A:282:PRO:HG2	1:B:279:GLY:HA2	2.02	0.41
1:A:345:TPO:HB	1:A:364:ILE:HD11	2.03	0.41
1:B:192:MET:SD	1:B:264:TYR:HE1	2.43	0.41
1:A:181:ASP:HB3	1:A:190:ASN:HB2	2.01	0.41
1:A:279:GLY:HA2	1:B:282:PRO:HG2	2.03	0.41
1:B:176:VAL:HG23	1:B:177:THR:HG23	2.03	0.41
1:B:194:GLU:H	1:B:194:GLU:CD	2.23	0.41
1:B:287:MET:HE2	1:B:323:PHE:HB3	2.03	0.40
1:B:394:GLN:HE21	1:B:394:GLN:HB3	1.71	0.40
1:B:164:ARG:HD2	1:B:165:PHE:H	1.85	0.40

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	263/295 (89%)	247 (94%)	16 (6%)	0	100	100
1	B	277/295 (94%)	260 (94%)	14 (5%)	3 (1%)	14	31
All	All	540/590 (92%)	507 (94%)	30 (6%)	3 (1%)	25	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	ASP
1	B	254	ASP
1	B	196	GLY

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	237/255 (93%)	224 (94%)	13 (6%)	21	43
1	B	247/255 (97%)	233 (94%)	14 (6%)	20	41
All	All	484/510 (95%)	457 (94%)	27 (6%)	21	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	TYR
1	A	185	ILE
1	A	194	GLU
1	A	228	GLN
1	A	243	GLU
1	A	277	LEU
1	A	329	ASP
1	A	349	VAL
1	A	365	THR
1	A	394	GLN
1	A	404	GLU
1	A	427	GLU
1	A	455	GLN
1	B	164	ARG
1	B	174	LYS
1	B	194	GLU
1	B	199	VAL
1	B	241	GLN
1	B	254	ASP
1	B	256	ASP
1	B	277	LEU
1	B	329	ASP
1	B	349	VAL
1	B	394	GLN
1	B	404	GLU
1	B	427	GLU
1	B	455	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	394	GLN
1	A	438	HIS
1	B	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	A	342	1	8,10,11	1.21	1 (12%)	10,14,16	1.30	2 (20%)
1	TPO	A	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.20	2 (20%)
1	TPO	B	345	1	8,10,11	1.22	0	10,14,16	1.14	1 (10%)
1	TPO	B	342	1	8,10,11	1.05	0	10,14,16	1.44	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	CB-CA	2.36	1.59	1.53
1	A	342	TPO	P-OG1	-2.24	1.55	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	342	TPO	P-OG1-CB	-2.86	114.57	123.21
1	A	342	TPO	P-OG1-CB	-2.45	115.79	123.21
1	A	345	TPO	O2P-P-OG1	2.19	115.81	105.99
1	B	345	TPO	O2P-P-OG1	2.19	115.79	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	342	TPO	CG2-CB-CA	2.09	117.29	113.16
1	A	345	TPO	CG2-CB-CA	2.08	117.27	113.16

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	342	TPO	N-CA-CB-OG1
1	B	342	TPO	C-CA-CB-CG2
1	B	342	TPO	O-C-CA-CB
1	A	342	TPO	C-CA-CB-CG2
1	A	342	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	CJQ	B	501	-	28,33,33	0.66	0	29,47,47	1.15	3 (10%)
2	SO4	A	501	-	4,4,4	0.24	0	6,6,6	0.29	0
3	CJQ	A	502	-	28,33,33	0.72	1 (3%)	29,47,47	1.16	4 (13%)

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	CJQ	B	501	-	-	5/12/39/39	0/5/5/5
3	CJQ	A	502	-	-	6/12/39/39	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	CJQ	C3-C2	2.11	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	CJQ	O1-C11-C16	-3.72	100.08	108.31
3	B	501	CJQ	C20-N3-C14	3.16	121.53	112.64
3	A	502	CJQ	C9-C8-C3	-2.83	106.80	113.89
3	A	502	CJQ	C20-N3-C14	2.44	119.50	112.64
3	A	502	CJQ	O1-C11-C12	-2.19	103.47	108.31
3	B	501	CJQ	O1-C11-C12	2.06	112.87	108.31
3	A	502	CJQ	C17-N3-C20	2.05	112.83	109.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	CJQ	C13-C14-N3-C17
3	A	502	CJQ	C13-C14-N3-C20
3	A	502	CJQ	C13-C14-N3-C17
3	A	502	CJQ	C15-C14-N3-C20
3	A	502	CJQ	C15-C14-N3-C17
3	B	501	CJQ	C13-C14-N3-C20
3	B	501	CJQ	C15-C14-N3-C17

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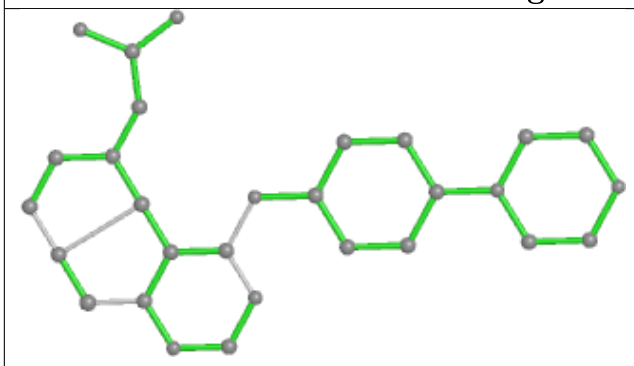
Mol	Chain	Res	Type	Atoms
3	B	501	CJQ	C7-C8-C9-C10
3	A	502	CJQ	O-C10-C9-C8
3	A	502	CJQ	N2-C10-C9-C8
3	B	501	CJQ	C15-C14-N3-C20

There are no ring outliers.

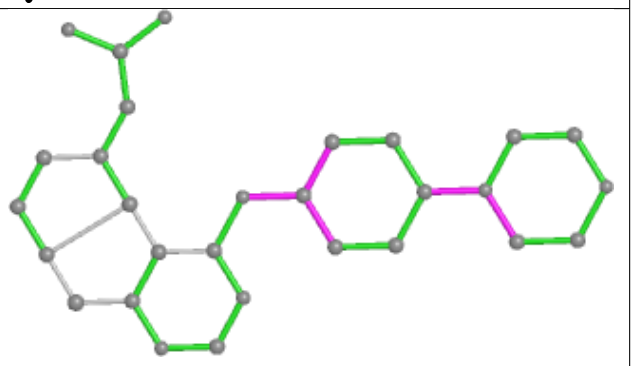
No monomer is involved in short contacts.

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.

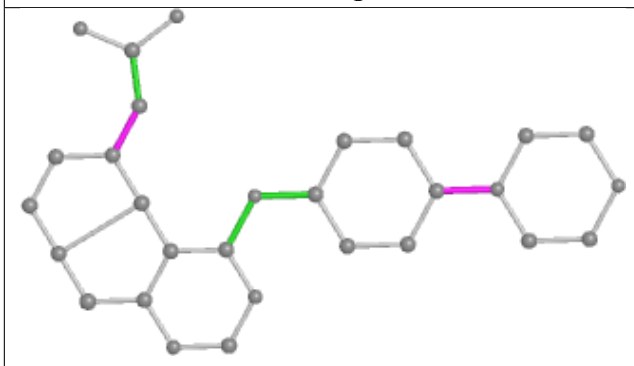
Ligand CJQ B 501



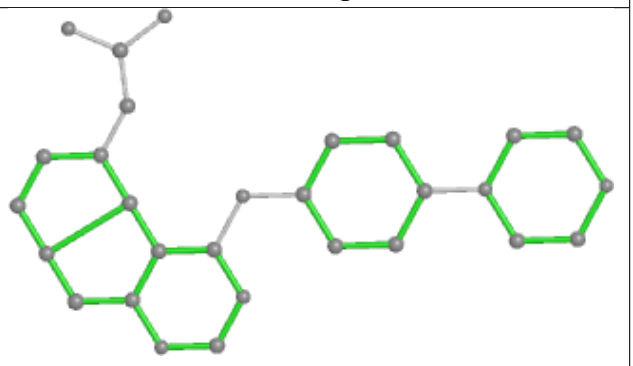
Bond lengths



Bond angles

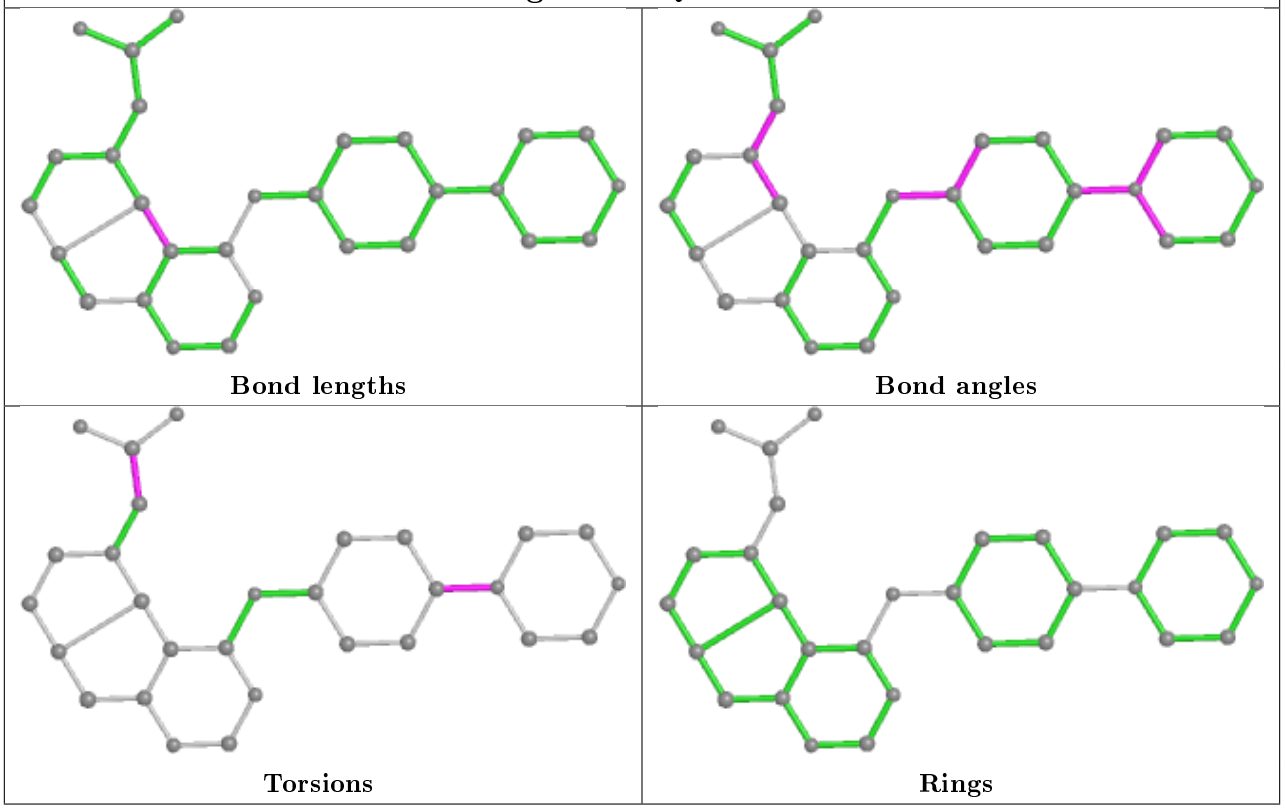


Torsions



Rings

Ligand CJQ A 502



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	270/295 (91%)	0.86	39 (14%)	2	1	42, 75, 158, 175	0
1	B	282/295 (95%)	0.69	23 (8%)	11	9	42, 76, 125, 171	0
All	All	552/590 (93%)	0.77	62 (11%)	5	4	42, 75, 154, 175	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	8.9
1	B	347	ARG	6.6
1	A	171	TYR	5.8
1	B	227	LYS	5.1
1	A	236	VAL	4.9
1	A	230	PHE	4.8
1	B	344	MET	4.8
1	A	346	SER	4.8
1	B	256	ASP	4.6
1	A	349	VAL	4.5
1	A	165	PHE	4.3
1	A	229	GLN	4.1
1	A	343	VAL	4.1
1	B	346	SER	3.9
1	B	413	TYR	3.9
1	A	196	GLY	3.8
1	B	335	ALA	3.8
1	B	226	LEU	3.7
1	B	364	ILE	3.6
1	B	349	VAL	3.5
1	A	179	ASN	3.5
1	A	350	GLY	3.5
1	A	260	LEU	3.4
1	A	344	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	167	SER	3.2
1	A	239	LYS	3.2
1	B	230	PHE	3.1
1	A	212	VAL	3.1
1	A	211	ALA	3.0
1	A	251	PHE	2.9
1	A	364	ILE	2.9
1	A	197	PHE	2.9
1	A	176	VAL	2.9
1	A	190	ASN	2.8
1	B	252	SER	2.8
1	A	407	GLU	2.7
1	B	255	GLY	2.7
1	B	250	GLY	2.6
1	B	336	SER	2.6
1	B	170	PHE	2.6
1	A	207	ASN	2.5
1	A	348	ILE	2.5
1	A	164	ARG	2.4
1	A	206	ASN	2.4
1	A	259	CYS	2.4
1	B	259	CYS	2.4
1	B	195	GLY	2.3
1	A	399	ILE	2.3
1	B	393	PRO	2.3
1	A	166	HIS	2.3
1	A	175	ASN	2.3
1	A	258	LEU	2.3
1	A	214	LYS	2.3
1	A	250	GLY	2.2
1	B	229	GLN	2.2
1	B	399	ILE	2.2
1	A	191	LYS	2.1
1	B	231	ASP	2.1
1	A	332	LEU	2.1
1	A	330	PHE	2.1
1	A	299	ILE	2.0
1	A	227	LYS	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
1	TPO	B	345	11/12	0.54	0.45	159,165,171,174	0
1	TPO	A	342	11/12	0.57	0.52	151,153,157,159	0
1	TPO	B	342	11/12	0.63	0.41	167,175,183,187	0
1	TPO	A	345	11/12	0.78	0.30	142,149,153,157	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

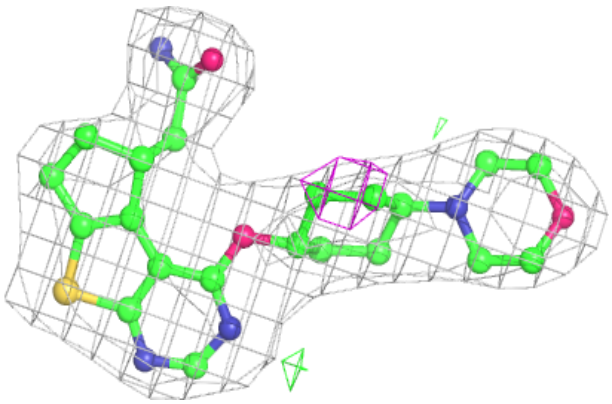
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

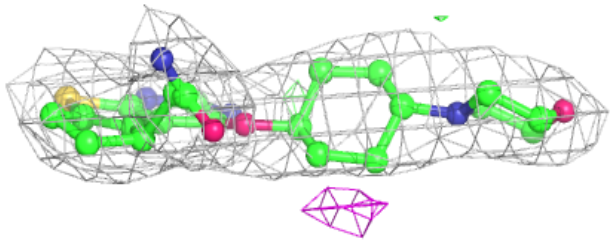
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	501	5/5	0.95	0.27	90,92,93,95	0
3	CJQ	A	502	29/29	0.96	0.19	50,61,66,67	0
3	CJQ	B	501	29/29	0.98	0.22	43,47,55,56	0

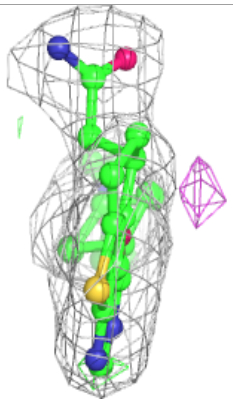
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CJQ A 502:

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

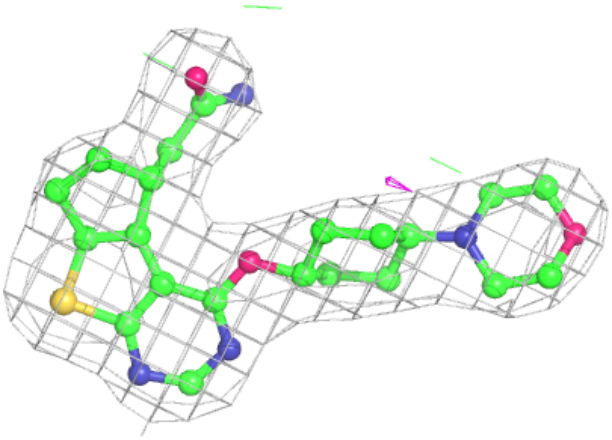


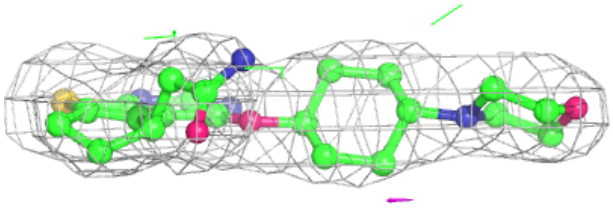


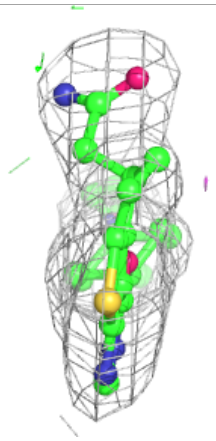


Electron density around CJQ B 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.