Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2024 – 02:04 PM EDT

PDB ID	:	9CMZ
Title	:	Crystal Structure of Cdk-related protein kinase 6 (PK6) from Plasmodium falciparum in complex with inhibitor KG2-051
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2024-07-15
Resolution	:	2.45 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

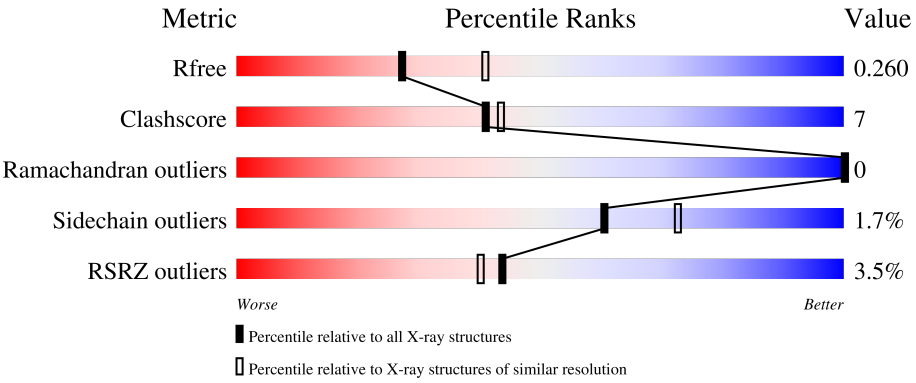
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.45 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	A	306	2% 77% 14% 9%
1	B	306	80% 12% • 7%
1	C	306	7% 73% 15% • 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6826 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 Protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2230	1459	356	405	10			
1	B	284	Total	C	N	O	S	0	0	0
			2284	1494	365	415	10			
1	C	271	Total	C	N	O	S	0	0	0
			2168	1416	344	398	10			

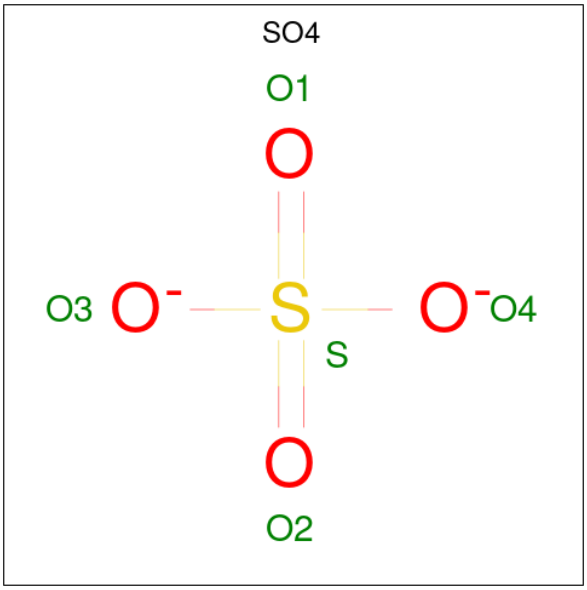
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8IDW1
A	0	SER	-	expression tag	UNP Q8IDW1
A	44	ASN	CYS	engineered mutation	UNP Q8IDW1
A	53	ARG	CYS	engineered mutation	UNP Q8IDW1
A	86	ALA	LYS	engineered mutation	UNP Q8IDW1
A	222	ASN	CYS	engineered mutation	UNP Q8IDW1
A	237	ALA	LYS	engineered mutation	UNP Q8IDW1
B	-1	GLY	-	expression tag	UNP Q8IDW1
B	0	SER	-	expression tag	UNP Q8IDW1
B	44	ASN	CYS	engineered mutation	UNP Q8IDW1
B	53	ARG	CYS	engineered mutation	UNP Q8IDW1
B	86	ALA	LYS	engineered mutation	UNP Q8IDW1
B	222	ASN	CYS	engineered mutation	UNP Q8IDW1
B	237	ALA	LYS	engineered mutation	UNP Q8IDW1
C	-1	GLY	-	expression tag	UNP Q8IDW1
C	0	SER	-	expression tag	UNP Q8IDW1
C	44	ASN	CYS	engineered mutation	UNP Q8IDW1
C	53	ARG	CYS	engineered mutation	UNP Q8IDW1
C	86	ALA	LYS	engineered mutation	UNP Q8IDW1
C	222	ASN	CYS	engineered mutation	UNP Q8IDW1
C	237	ALA	LYS	engineered mutation	UNP Q8IDW1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

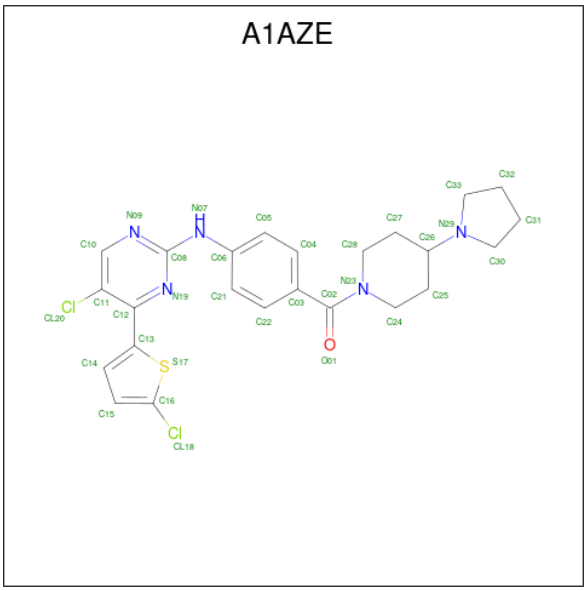
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cl 3 3	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is (4-{[5-chloro-4-(5-chlorothiophen-2-yl)pyrimidin-2-yl]amino}phenyl)[4-(pyrrolidin-1-yl)piperidin-1-yl]methanone (three-letter code: A1AZE) (formula: $C_{24}H_{25}Cl_2N_5OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N O S 33 24 2 5 1 1	0	0
4	B	1	Total C Cl N O S 33 24 2 5 1 1	0	0
4	C	1	Total C Cl N O S 33 24 2 5 1 1	0	0

- Molecule 5 is water.

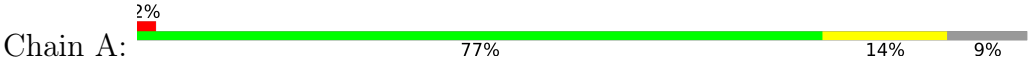
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	11	Total O 11 11	0	0
5	C	5	Total O 5 5	0	0

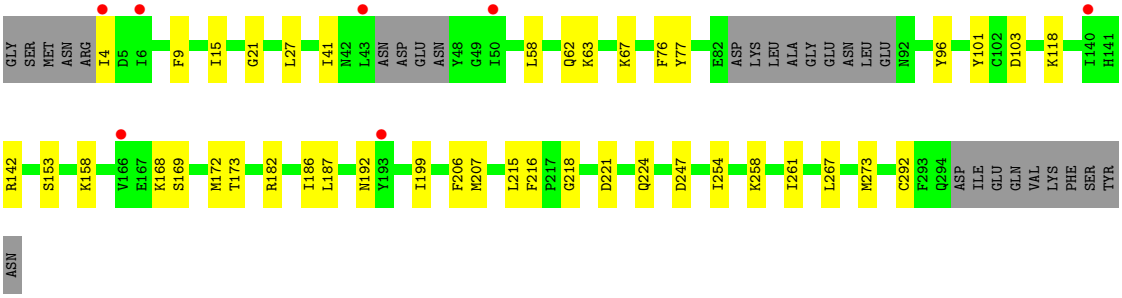
3 Residue-property plots (i)

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: Protein kinase 6

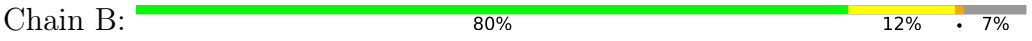
Chain A:

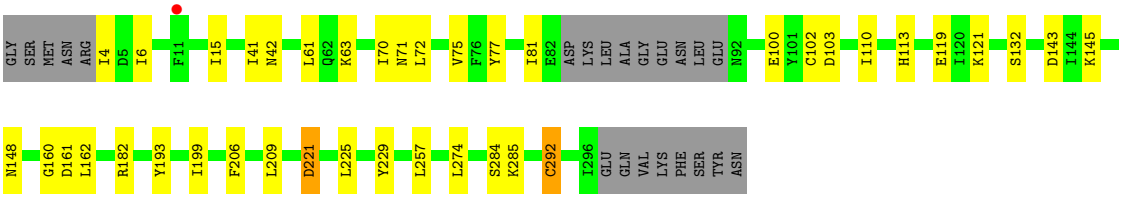




• Molecule 1: Protein kinase 6

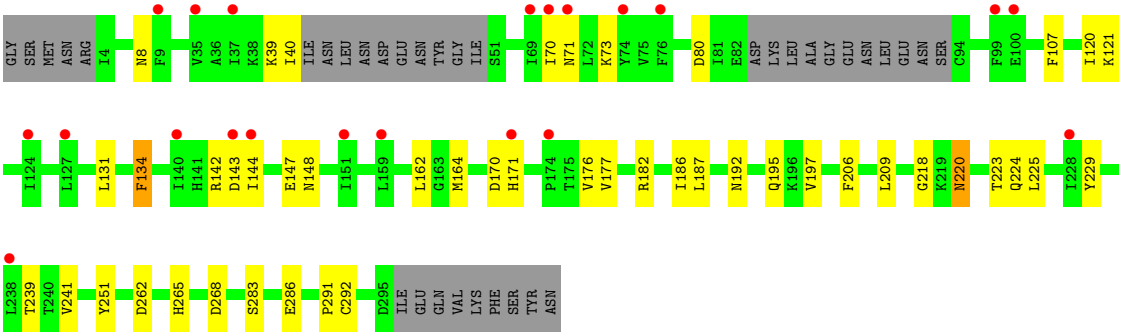
Chain B:





• Molecule 1: Protein kinase 6

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.54Å 99.43Å 78.15Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	34.66 – 2.45 44.40 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.66-2.45) 97.1 (44.40-2.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.45Å)	Xtriage
Refinement program	PHENIX dev_5383	Depositor
R, R_{free}	0.220 , 0.255 0.223 , 0.260	Depositor DCC
R_{free} test set	2095 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.095 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: SO4, A1AZE, CL

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	0.44	0/2275	0.62	0/3075
1	B	0.47	0/2331	0.62	0/3151
1	C	0.38	0/2211	0.56	0/2990
All	All	0.43	0/6817	0.60	0/9216

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	2230	0	2229	34	0
1	B	2284	0	2282	28	0
1	C	2168	0	2147	34	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	33	0	0	0	0
4	B	33	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	33	0	0	0	0
5	A	10	0	0	1	0
5	B	11	0	0	1	0
5	C	5	0	0	0	0
All	All	6826	0	6658	95	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 7.

All (95) 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:C:239:THR:HG23	1:C:241:VAL:HG22	1.59	0.82
1:C:142:ARG:HD2	1:C:176:VAL:HG11	1.69	0.75
1:C:182:ARG:HD2	1:C:187:LEU:HD23	1.69	0.74
1:A:168:LYS:HA	1:A:172:MET:HE1	1.71	0.72
1:A:182:ARG:HD2	1:A:187:LEU:HD23	1.76	0.67
1:B:6:ILE:HD11	1:B:81:ILE:HD11	1.76	0.67
1:C:239:THR:CG2	1:C:241:VAL:HG22	2.25	0.66
1:A:15:ILE:HD11	1:A:101:TYR:HE1	1.61	0.65
1:B:225:LEU:HD11	1:B:229:TYR:CE2	2.33	0.63
1:C:220:ASN:OD1	1:C:223:THR:HG22	1.99	0.63
1:A:76:PHE:CE2	1:A:96:TYR:HB2	2.33	0.62
1:B:41:ILE:HD12	1:B:42:ASN:N	2.14	0.62
1:A:67:LYS:O	1:A:158:LYS:NZ	2.31	0.61
1:C:8:ASN:O	1:C:8:ASN:OD1	2.19	0.59
1:A:207:MET:HA	1:A:207:MET:HE2	1.84	0.59
1:A:173:THR:OG1	3:A:404:SO4:O4	2.17	0.59
1:B:257:LEU:HD11	1:B:274:LEU:HD12	1.84	0.59
1:B:4:ILE:HD12	1:B:4:ILE:C	2.24	0.57
1:B:63:LYS:O	1:B:63:LYS:HD2	2.04	0.57
1:C:131:LEU:HD21	1:C:144:ILE:HD11	1.86	0.57
1:A:168:LYS:HA	1:A:172:MET:CE	2.35	0.55
1:A:169:SER:H	1:A:172:MET:HE3	1.69	0.55
1:C:170:ASP:O	1:C:171:HIS:ND1	2.39	0.55
1:B:182:ARG:NH1	1:B:221:ASP:OD2	2.39	0.55
1:B:110:ILE:HD11	1:B:209:LEU:CD2	2.37	0.54
1:B:61:LEU:CD2	1:B:162:LEU:HD12	2.37	0.54
1:C:39:LYS:NZ	1:C:80:ASP:OD1	2.37	0.54
1:A:15:ILE:HD11	1:A:101:TYR:CE1	2.41	0.54
1:B:61:LEU:HD23	1:B:162:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LEU:HD11	1:B:229:TYR:CZ	2.44	0.53
1:C:164:MET:HE2	1:C:176:VAL:HG23	1.89	0.53
1:A:254:ILE:HA	1:A:258:LYS:HG3	1.90	0.53
1:A:182:ARG:CG	1:A:186:ILE:HG13	2.40	0.51
1:C:265:HIS:HB3	1:C:292:CYS:HB3	1.92	0.51
1:A:169:SER:N	1:A:172:MET:HE3	2.26	0.51
1:C:71:ASN:ND2	1:C:73:LYS:HE2	2.26	0.50
1:C:225:LEU:HD11	1:C:229:TYR:CZ	2.46	0.50
1:A:182:ARG:HG2	1:A:186:ILE:HG13	1.93	0.50
1:C:265:HIS:CE1	1:C:291:PRO:HB2	2.47	0.50
1:B:221:ASP:OD1	1:B:221:ASP:N	2.46	0.49
1:B:121:LYS:HE2	1:B:292:CYS:SG	2.54	0.48
1:C:107:PHE:HB2	1:C:147:GLU:HG3	1.95	0.48
1:A:4:ILE:HD11	1:A:76:PHE:HD1	1.79	0.47
1:A:77:TYR:CE1	1:B:77:TYR:CD1	3.02	0.47
1:A:207:MET:HE3	1:A:261:ILE:HD11	1.96	0.47
1:B:110:ILE:HD11	1:B:209:LEU:HD23	1.97	0.47
1:C:195:GLN:OE1	1:C:195:GLN:N	2.41	0.47
1:B:193:TYR:HA	5:B:511:HOH:O	2.14	0.47
1:B:70:ILE:HD11	1:B:161:ASP:HA	1.96	0.47
1:C:120:ILE:CD1	1:C:209:LEU:HB3	2.45	0.46
1:C:192:ASN:OD1	1:C:192:ASN:O	2.33	0.46
1:C:121:LYS:HE3	1:C:292:CYS:O	2.16	0.46
1:A:21:GLY:HA2	1:A:41:ILE:HG23	1.98	0.46
1:C:70:ILE:HD12	1:C:70:ILE:O	2.17	0.45
1:A:58:LEU:O	1:A:62:GLN:HG2	2.16	0.45
1:C:251:TYR:OH	1:C:268:ASP:OD1	2.23	0.45
1:C:182:ARG:HD2	1:C:187:LEU:CD2	2.42	0.45
1:C:120:ILE:HD13	1:C:209:LEU:HB3	1.98	0.44
1:A:199:ILE:HG23	1:A:273:MET:HG2	2.00	0.44
1:B:143:ASP:OD1	1:B:145:LYS:HE2	2.17	0.44
1:C:186:ILE:HD13	1:C:197:VAL:HG11	1.99	0.44
1:A:63:LYS:O	1:A:63:LYS:HG3	2.17	0.44
1:B:102:CYS:O	4:B:403:A1AZE:N07	2.51	0.44
1:C:40:ILE:HD12	1:C:40:ILE:N	2.32	0.44
1:A:261:ILE:HD12	1:A:267:LEU:CD1	2.49	0.43
1:C:176:VAL:HG13	1:C:177:VAL:HG23	2.01	0.43
1:A:192:ASN:N	1:A:192:ASN:OD1	2.51	0.43
1:A:4:ILE:C	1:A:4:ILE:HD12	2.39	0.43
1:A:247:ASP:HA	5:A:508:HOH:O	2.18	0.43
1:C:265:HIS:CD2	1:C:291:PRO:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:HD2	1:B:63:LYS:C	2.40	0.43
1:B:15:ILE:HD13	1:B:15:ILE:HG21	1.84	0.42
1:C:120:ILE:HD13	1:C:209:LEU:CB	2.48	0.42
1:B:72:LEU:HD21	1:B:75:VAL:CG2	2.49	0.42
1:C:143:ASP:OD2	1:C:148:ASN:ND2	2.53	0.42
1:A:221:ASP:N	1:A:221:ASP:OD1	2.53	0.42
1:C:265:HIS:NE2	1:C:291:PRO:HB2	2.35	0.42
1:C:218:GLY:HA3	1:C:224:GLN:OE1	2.20	0.41
1:A:4:ILE:CD1	1:A:76:PHE:HD1	2.33	0.41
1:A:9:PHE:HA	1:A:27:LEU:O	2.20	0.41
1:B:71:ASN:HB3	1:B:100:GLU:HG3	2.02	0.41
1:C:283:SER:OG	1:C:286:GLU:HG3	2.20	0.41
1:C:134:PHE:CZ	1:C:162:LEU:HD22	2.55	0.41
1:A:218:GLY:HA3	1:A:224:GLN:OE1	2.21	0.41
1:A:207:MET:HA	1:A:207:MET:CE	2.51	0.41
1:A:103:ASP:OD2	1:A:153:SER:HB3	2.20	0.41
1:B:113:HIS:HE1	1:B:119:GLU:OE1	2.02	0.41
1:B:285:LYS:HD3	1:B:285:LYS:HA	1.90	0.40
1:A:215:LEU:HD23	1:A:216:PHE:CE2	2.57	0.40
1:C:220:ASN:OD1	1:C:223:THR:CG2	2.69	0.40
1:A:76:PHE:CE2	1:A:96:TYR:CB	3.01	0.40
1:A:261:ILE:HD12	1:A:267:LEU:HD13	2.02	0.40
1:B:132:SER:OG	1:B:285:LYS:HE2	2.22	0.40
1:B:148:ASN:O	1:B:160:GLY:HA3	2.20	0.40
1:B:199:ILE:HD11	1:B:284:SER:HB3	2.04	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	272/306 (89%)	262 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	280/306 (92%)	269 (96%)	11 (4%)	0	100	100
1	C	265/306 (87%)	254 (96%)	11 (4%)	0	100	100
All	All	817/918 (89%)	785 (96%)	32 (4%)	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	A	242/283 (86%)	238 (98%)	4 (2%)	60	73
1	B	247/283 (87%)	243 (98%)	4 (2%)	62	74
1	C	234/283 (83%)	230 (98%)	4 (2%)	60	73
All	All	723/849 (85%)	711 (98%)	12 (2%)	60	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	142	ARG
1	A	206	PHE
1	A	292	CYS
1	B	103	ASP
1	B	206	PHE
1	B	221	ASP
1	B	292	CYS
1	C	134	PHE
1	C	206	PHE
1	C	220	ASN
1	C	262	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	71	ASN
1	A	113	HIS
1	B	108	ASN
1	B	113	HIS
1	B	138	ASN

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SO4	B	402	-	4,4,4	0.62	0	6,6,6	0.51	0
4	A1AZE	A	405	-	34,37,37	2.25	14 (41%)	39,52,52	2.90	12 (30%)
4	A1AZE	C	402	-	34,37,37	2.37	17 (50%)	39,52,52	2.52	11 (28%)
4	A1AZE	B	403	-	34,37,37	2.47	14 (41%)	39,52,52	2.58	16 (41%)
3	SO4	C	401	-	4,4,4	0.60	0	6,6,6	0.28	0
3	SO4	A	404	-	4,4,4	0.64	0	6,6,6	0.39	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
4	A1AZE	C	402	-	-	0/16/37/37	0/5/5/5
4	A1AZE	A	405	-	-	1/16/37/37	0/5/5/5
4	A1AZE	B	403	-	-	4/16/37/37	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	A1AZE	C02-N23	7.31	1.51	1.34
4	C	402	A1AZE	C02-N23	5.86	1.47	1.34
4	A	405	A1AZE	C02-N23	5.17	1.46	1.34
4	A	405	A1AZE	C08-N07	4.84	1.46	1.36
4	A	405	A1AZE	C26-N29	3.88	1.59	1.48
4	B	403	A1AZE	C27-C28	3.86	1.63	1.52
4	C	402	A1AZE	C26-N29	3.83	1.58	1.48
4	B	403	A1AZE	C06-N07	3.79	1.49	1.40
4	B	403	A1AZE	C12-C13	3.71	1.57	1.49
4	A	405	A1AZE	C06-N07	3.60	1.48	1.40
4	C	402	A1AZE	C21-C06	3.58	1.45	1.39
4	C	402	A1AZE	C08-N09	3.48	1.39	1.34
4	B	403	A1AZE	C26-N29	3.38	1.57	1.48
4	C	402	A1AZE	C12-C13	3.33	1.56	1.49
4	C	402	A1AZE	C22-C21	3.27	1.44	1.38
4	A	405	A1AZE	C24-N23	3.14	1.52	1.47
4	B	403	A1AZE	C11-CL20	3.14	1.81	1.73
4	C	402	A1AZE	C06-N07	3.12	1.47	1.40
4	A	405	A1AZE	C25-C24	3.01	1.60	1.52
4	A	405	A1AZE	C08-N09	2.99	1.38	1.34
4	B	403	A1AZE	C08-N09	2.93	1.38	1.34
4	C	402	A1AZE	C03-C02	2.90	1.54	1.50
4	B	403	A1AZE	C21-C06	2.87	1.44	1.39
4	B	403	A1AZE	C03-C02	2.86	1.54	1.50
4	C	402	A1AZE	C25-C24	2.84	1.60	1.52
4	A	405	A1AZE	C21-C06	2.83	1.44	1.39
4	C	402	A1AZE	C25-C26	2.76	1.59	1.52
4	B	403	A1AZE	C08-N19	2.70	1.42	1.34
4	A	405	A1AZE	C33-N29	2.69	1.54	1.47
4	C	402	A1AZE	C08-N07	2.59	1.41	1.36
4	A	405	A1AZE	C22-C21	2.57	1.43	1.38
4	C	402	A1AZE	C33-N29	2.54	1.54	1.47
4	A	405	A1AZE	C08-N19	2.54	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	A1AZE	C25-C26	2.49	1.58	1.52
4	B	403	A1AZE	C33-N29	2.45	1.53	1.47
4	B	403	A1AZE	C08-N07	2.43	1.41	1.36
4	A	405	A1AZE	C15-C14	2.33	1.50	1.39
4	A	405	A1AZE	C11-CL20	2.31	1.79	1.73
4	C	402	A1AZE	C15-C14	2.28	1.50	1.39
4	C	402	A1AZE	C27-C28	2.28	1.58	1.52
4	B	403	A1AZE	C30-N29	2.18	1.53	1.47
4	C	402	A1AZE	C22-C03	2.09	1.42	1.39
4	C	402	A1AZE	C16-S17	2.06	1.76	1.72
4	C	402	A1AZE	C05-C06	2.06	1.42	1.39
4	A	405	A1AZE	C03-C02	2.03	1.53	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	405	A1AZE	N09-C08-N19	-9.14	117.89	126.55
4	A	405	A1AZE	C33-N29-C26	-8.94	105.47	114.12
4	C	402	A1AZE	N09-C08-N19	-8.18	118.80	126.55
4	B	403	A1AZE	N09-C08-N19	-7.56	119.39	126.55
4	C	402	A1AZE	C33-N29-C26	-6.61	107.72	114.12
4	A	405	A1AZE	C03-C02-N23	5.84	126.14	118.72
4	B	403	A1AZE	C33-N29-C26	-5.61	108.69	114.12
4	B	403	A1AZE	C25-C26-N29	-5.33	98.67	112.52
4	C	402	A1AZE	C25-C26-N29	-5.02	99.48	112.52
4	C	402	A1AZE	C03-C02-N23	4.69	124.67	118.72
4	B	403	A1AZE	C03-C02-N23	4.64	124.61	118.72
4	A	405	A1AZE	C30-N29-C26	4.55	118.52	114.12
4	A	405	A1AZE	C10-C11-C12	-4.36	118.25	120.39
4	B	403	A1AZE	C30-N29-C26	4.18	118.16	114.12
4	B	403	A1AZE	C25-C24-N23	3.96	116.85	110.82
4	B	403	A1AZE	C10-C11-C12	-3.87	118.49	120.39
4	A	405	A1AZE	C25-C26-N29	-3.59	103.19	112.52
4	C	402	A1AZE	C25-C24-N23	3.50	116.14	110.82
4	C	402	A1AZE	C32-C33-N29	-3.37	98.67	104.15
4	A	405	A1AZE	C10-N09-C08	3.29	120.84	115.88
4	A	405	A1AZE	C25-C24-N23	3.25	115.76	110.82
4	A	405	A1AZE	O01-C02-N23	-3.24	116.98	122.34
4	A	405	A1AZE	C32-C33-N29	-3.13	99.05	104.15
4	C	402	A1AZE	C10-N09-C08	3.10	120.56	115.88
4	C	402	A1AZE	C10-C11-C12	-3.04	118.90	120.39
4	B	403	A1AZE	C27-C28-N23	3.00	115.38	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	403	A1AZE	O01-C02-N23	-2.99	117.40	122.34
4	C	402	A1AZE	O01-C02-N23	-2.86	117.61	122.34
4	B	403	A1AZE	C10-N09-C08	2.75	120.03	115.88
4	B	403	A1AZE	C31-C30-N29	-2.65	99.83	104.15
4	C	402	A1AZE	C30-N29-C26	2.59	116.62	114.12
4	B	403	A1AZE	C32-C33-N29	-2.56	99.97	104.15
4	B	403	A1AZE	C27-C26-N29	2.53	119.10	112.52
4	B	403	A1AZE	C13-C12-N19	2.29	119.35	115.10
4	A	405	A1AZE	C05-C04-C03	2.27	123.42	120.78
4	A	405	A1AZE	N07-C08-N19	2.21	124.41	116.92
4	C	402	A1AZE	C05-C04-C03	2.14	123.26	120.78
4	B	403	A1AZE	N07-C08-N19	2.02	123.78	116.92
4	B	403	A1AZE	C05-C04-C03	2.00	123.11	120.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	A1AZE	C25-C26-N29-C30
4	B	403	A1AZE	C25-C26-N29-C33
4	B	403	A1AZE	C27-C26-N29-C30
4	B	403	A1AZE	C27-C26-N29-C33
4	A	405	A1AZE	C25-C26-N29-C33

There are no ring outliers.

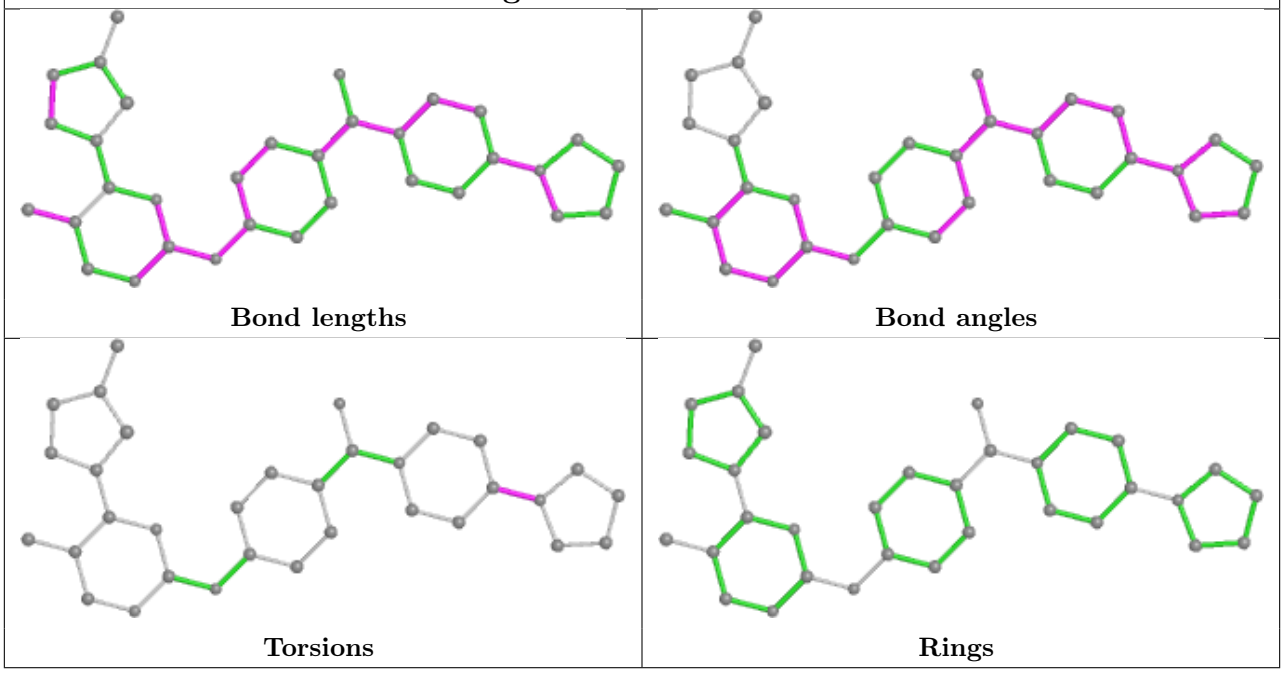
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	A1AZE	1	0
3	A	404	SO4	1	0

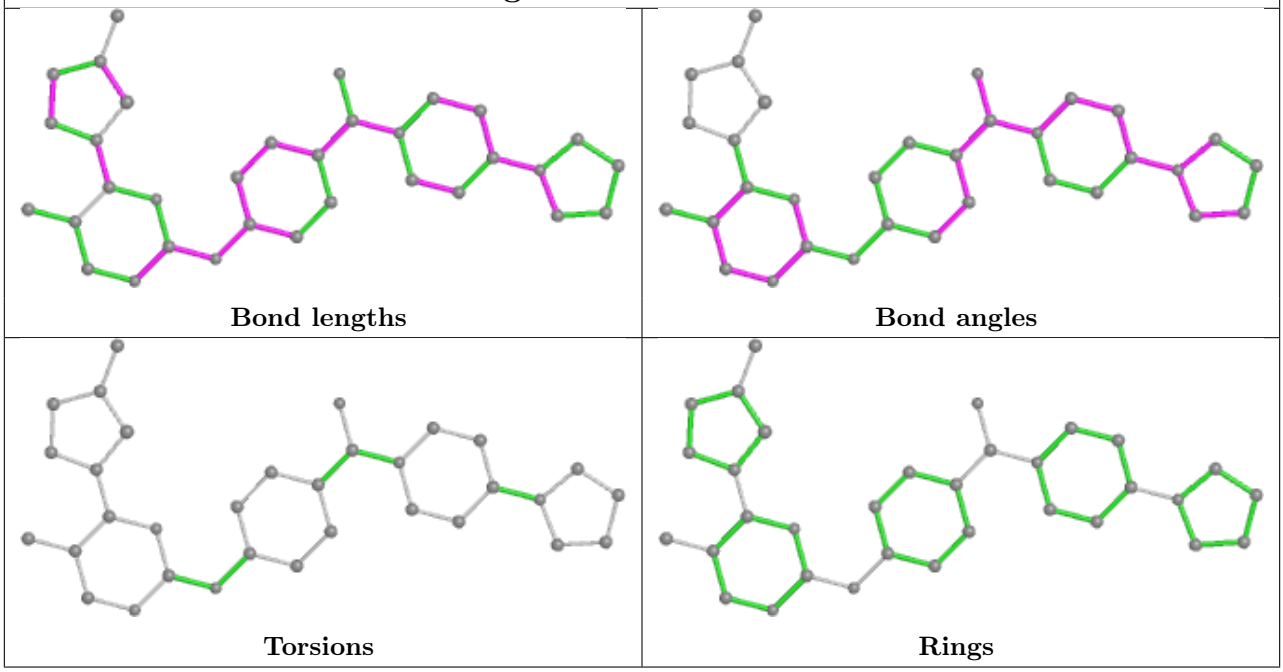
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

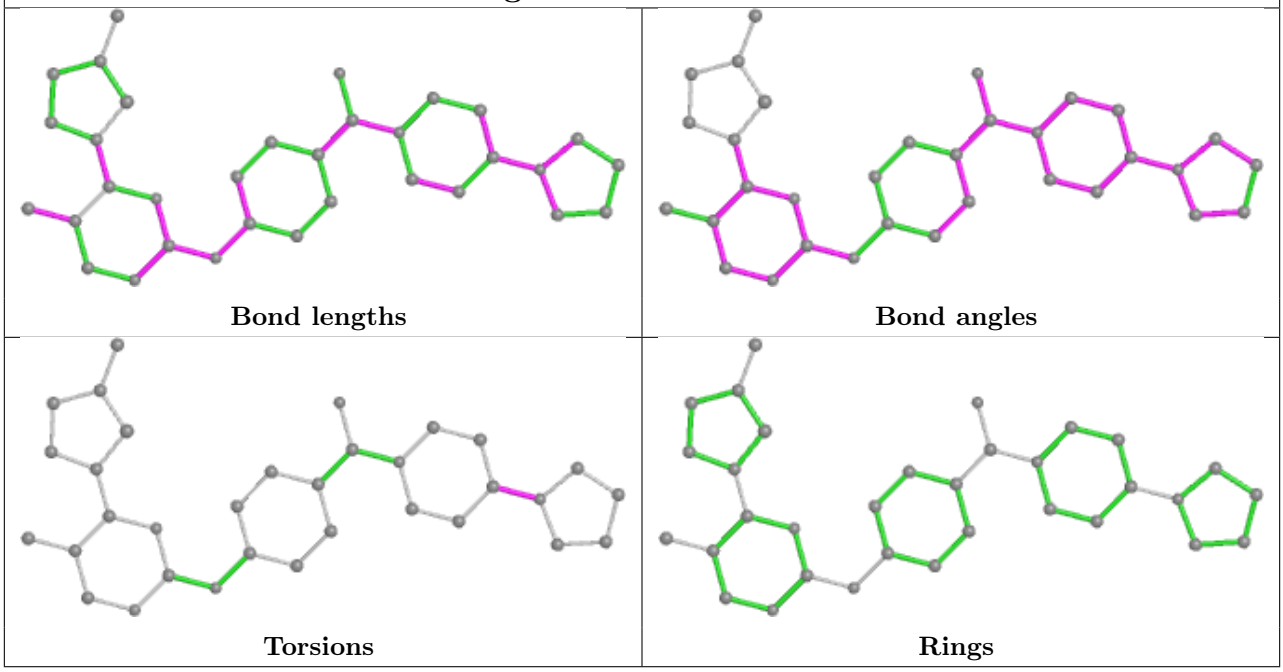
Ligand A1AZE A 405



Ligand A1AZE C 402



Ligand A1AZE B 403



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	278/306 (90%)	0.25	7 (2%)	57	53	44, 62, 93, 153	0
1	B	284/306 (92%)	0.25	1 (0%)	92	93	40, 58, 93, 135	0
1	C	271/306 (88%)	0.54	21 (7%)	13	10	53, 77, 109, 126	0
All	All	833/918 (90%)	0.34	29 (3%)	44	40	40, 66, 104, 153	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	5.0
1	A	50	ILE	4.8
1	C	143	ASP	4.5
1	C	238	LEU	4.3
1	C	74	TYR	3.9
1	C	76	PHE	3.4
1	B	11	PHE	3.4
1	C	124	ILE	3.4
1	C	174	PRO	3.2
1	A	43	LEU	3.2
1	A	166	VAL	2.9
1	C	37	ILE	2.9
1	C	35	VAL	2.8
1	C	70	ILE	2.7
1	C	9	PHE	2.7
1	C	144	ILE	2.4
1	C	100	GLU	2.4
1	A	6	ILE	2.4
1	A	140	ILE	2.3
1	C	71	ASN	2.3
1	C	159	LEU	2.3
1	C	127	LEU	2.2
1	C	228	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	193	TYR	2.1
1	C	99	PHE	2.1
1	C	171	HIS	2.1
1	C	69	ILE	2.1
1	C	151	ILE	2.0
1	C	140	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

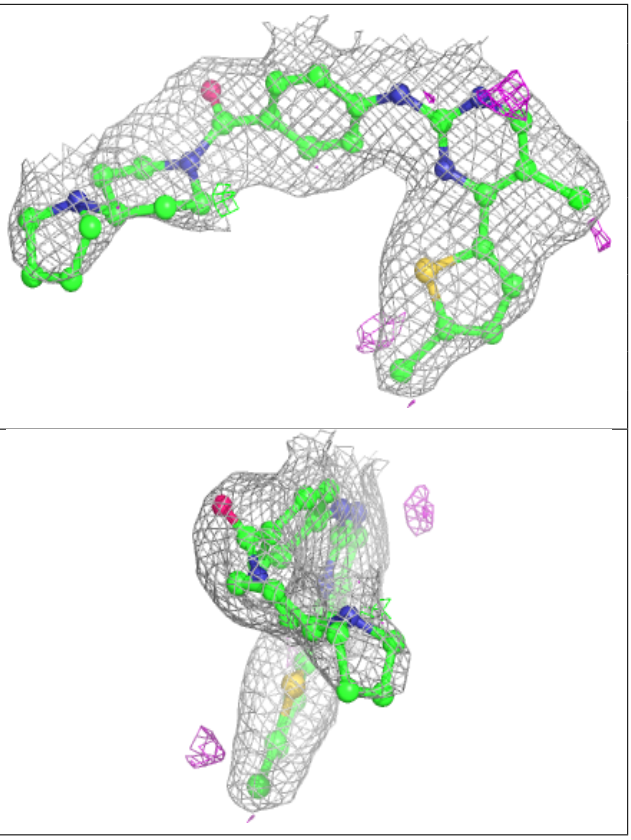
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CL	A	402	1/1	0.80	0.12	76,76,76,76	0
2	CL	A	403	1/1	0.83	0.10	78,78,78,78	0
2	CL	B	401	1/1	0.83	0.10	77,77,77,77	0
2	CL	A	401	1/1	0.86	0.13	81,81,81,81	0
4	A1AZE	C	402	33/33	0.93	0.24	58,68,85,90	0
3	SO4	C	401	5/5	0.95	0.19	80,83,92,105	0
3	SO4	A	404	5/5	0.95	0.11	69,77,84,86	0
4	A1AZE	A	405	33/33	0.96	0.17	36,51,61,65	0
4	A1AZE	B	403	33/33	0.96	0.19	42,53,69,78	0
3	SO4	B	402	5/5	0.96	0.15	51,60,68,69	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.

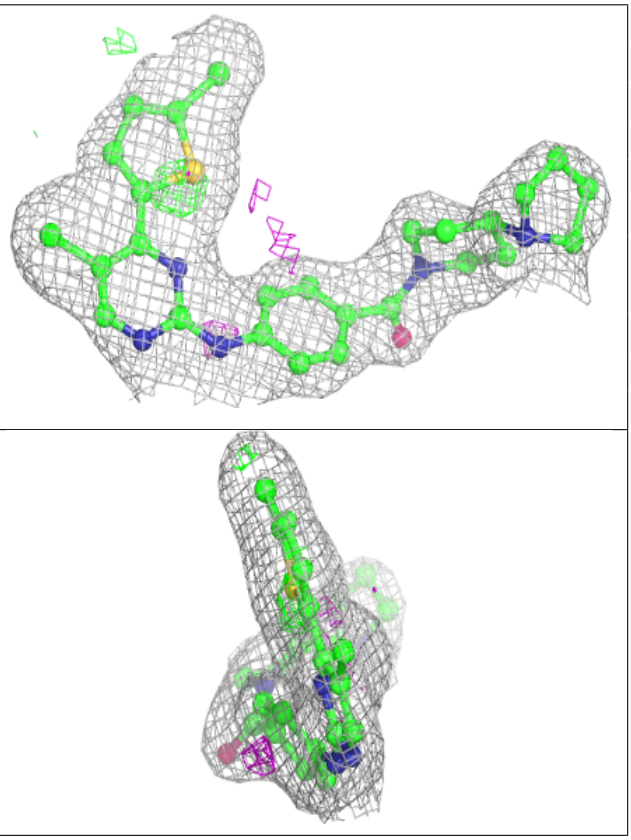
Electron density around A1AZE C 402:

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



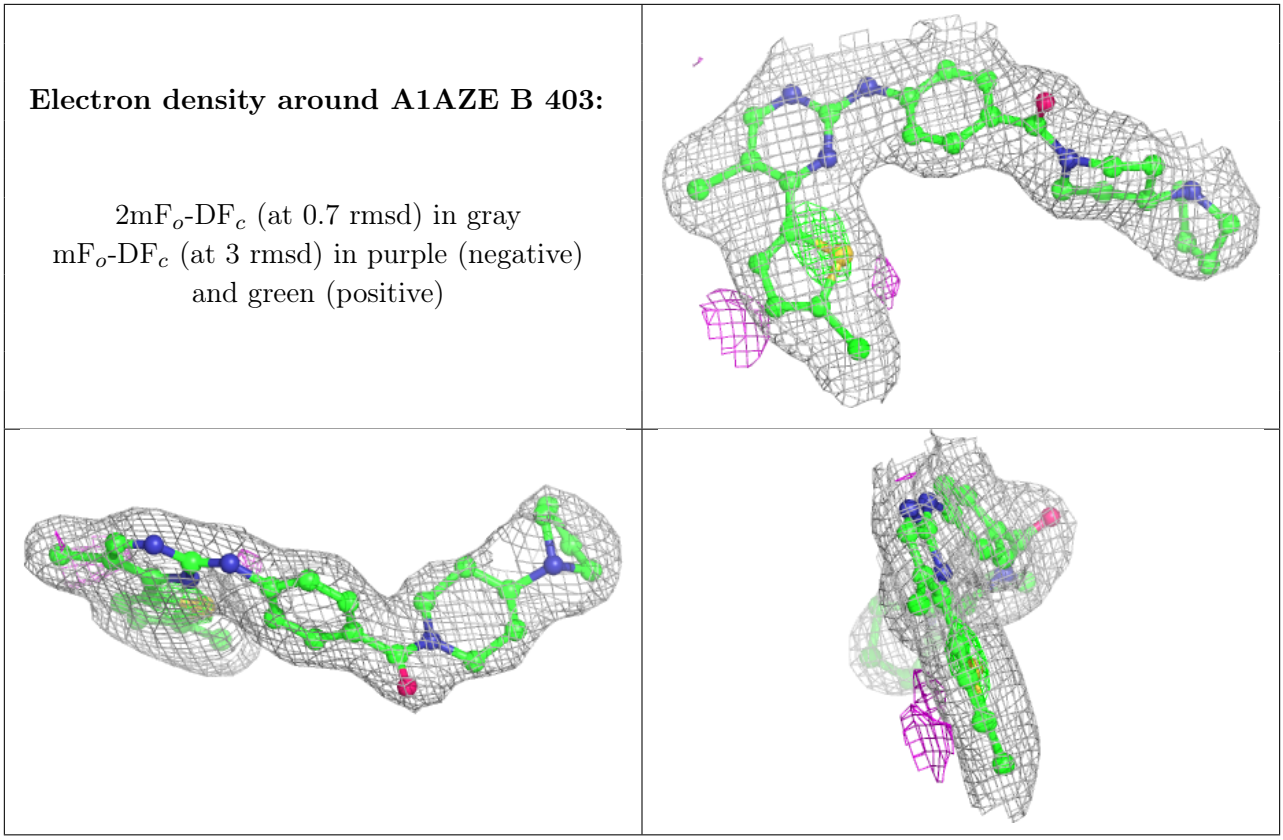
Electron density around A1AZE A 405:

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



Electron density around A1AZE B 403:

$2mF_o$-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.