Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 09:38 AM EDT

PDB ID	:	3OCB
Title	:	Akt1 kinase domain with pyrrolopyrimidine inhibitor
Authors	:	Morales, T.H.; Vigers, G.P.A.; Brandhuber, B.J.
Deposited on	:	2010-08-09
Resolution	:	2.70 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:

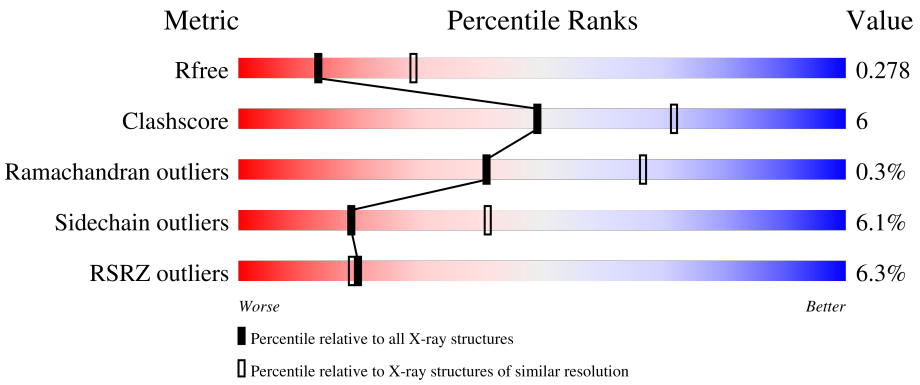
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	341	6%, 80%, 11%, • 7%
1	B	341	6%, 77%, 16%, • 6%
2	C	10	100%
2	D	10	80%, 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5519 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 v-akt murine thymoma viral oncogene homolog 1 (AKT1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	316	2589	1662	436	475	1	15	0	0	0
1	B	320	2619	1682	440	481	1	15	0	0	0

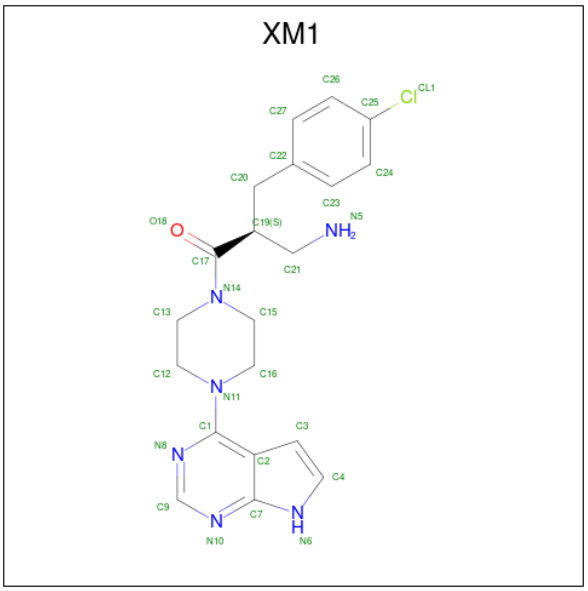
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	GLY	-	EXPRESSION TAG	UNP B2RAM5
A	141	ALA	-	EXPRESSION TAG	UNP B2RAM5
A	142	MET	-	EXPRESSION TAG	UNP B2RAM5
A	143	ALA	-	EXPRESSION TAG	UNP B2RAM5
A	473	ASP	SER	ENGINEERED MUTATION	UNP B2RAM5
B	140	GLY	-	EXPRESSION TAG	UNP B2RAM5
B	141	ALA	-	EXPRESSION TAG	UNP B2RAM5
B	142	MET	-	EXPRESSION TAG	UNP B2RAM5
B	143	ALA	-	EXPRESSION TAG	UNP B2RAM5
B	473	ASP	SER	ENGINEERED MUTATION	UNP B2RAM5

- Molecule 2 is a protein called GSK 3 beta peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	78	47	16	15	0	0	0
2	D	10	78	47	16	15	0	0	0

- Molecule 3 is (2S)-2-(4-chlorobenzyl)-3-oxo-3-[4-(7H-pyrrolo[2,3-d]pyrimidin-4-yl)piperazin-1-yl]propan-1-amine (three-letter code: XM1) (formula: $C_{20}H_{23}ClN_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	28	20	1	6	1	0	0
3	B	1	28	20	1	6	1	0	0

- Molecule 4 is water.

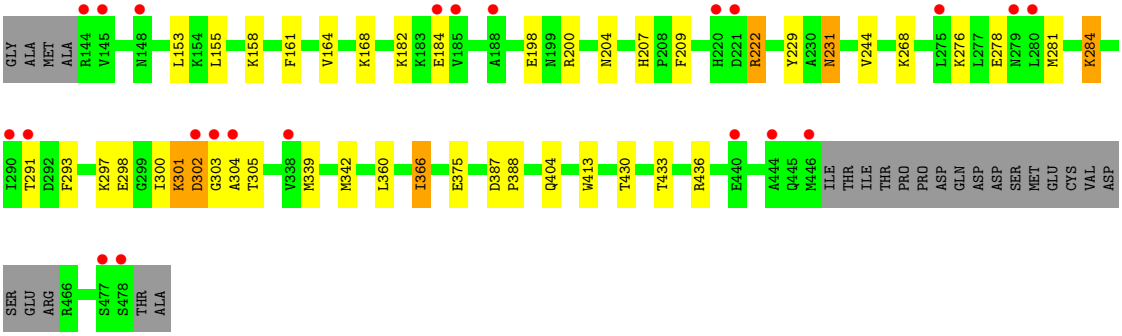
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	57	57	57	0	0
4	B	38	38	38	0	0
4	C	1	1	1	0	0
4	D	3	3	3	0	0

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.

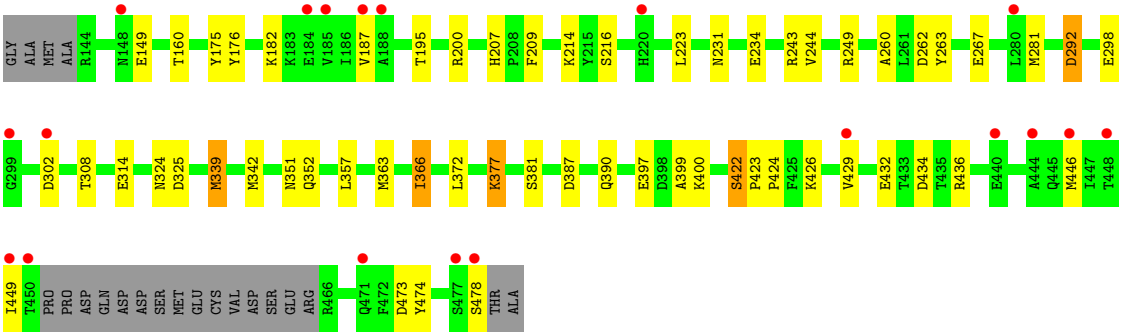
• Molecule 1: v-akt murine thymoma viral oncogene homolog 1 (AKT1)

Chain A:



• Molecule 1: v-akt murine thymoma viral oncogene homolog 1 (AKT1)

Chain B:



• Molecule 2: GSK 3 beta peptide

Chain C:

There are no outlier residues recorded for this chain.

• Molecule 2: GSK 3 beta peptide

Chain D:

G1
T6
E10

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.27Å 56.01Å 91.65Å 90.00° 104.27° 90.00°	Depositor
Resolution (Å)	29.72 – 2.70 29.72 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.72-2.70) 98.3 (29.72-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.282 0.212 , 0.278	Depositor DCC
R_{free} test set	1124 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5519	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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 47.38 % 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 1.0003e-04. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XM1, TPO

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	0.46	0/2639	0.58	0/3547
1	B	0.44	0/2669	0.59	0/3589
2	C	0.68	0/79	0.51	0/105
2	D	0.46	0/79	0.52	0/105
All	All	0.46	0/5466	0.58	0/7346

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 (i)

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	2589	0	2550	29	0
1	B	2619	0	2586	31	0
2	C	78	0	77	0	0
2	D	78	0	77	0	0
3	A	28	0	23	4	0
3	B	28	0	23	6	0
4	A	57	0	0	1	0
4	B	38	0	0	1	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3	0	0	0	0
All	All	5519	0	5336	63	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 6.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.06	1.08
1:A:222:ARG:HG3	1:A:222:ARG:NH1	1.85	0.84
3:A:1:XM1:H3	3:A:1:XM1:H16	1.59	0.83
3:B:2:XM1:H3	3:B:2:XM1:H16	1.65	0.77
1:A:413:TRP:H	1:B:352:GLN:NE2	1.82	0.77
1:A:413:TRP:H	1:B:352:GLN:HE22	1.35	0.74
1:A:229:TYR:CE2	1:A:231:ASN:HB3	2.24	0.73
1:A:231:ASN:HD21	1:A:284:LYS:HA	1.54	0.72
1:B:200:ARG:NH2	1:B:298:GLU:OE2	2.25	0.69
3:A:1:XM1:H16	3:A:1:XM1:C3	2.19	0.69
3:B:2:XM1:H16	3:B:2:XM1:C3	2.27	0.63
1:B:292:ASP:OD1	3:B:2:XM1:N5	2.34	0.60
1:B:429:VAL:HB	1:B:434:ASP:HB3	1.84	0.59
1:A:222:ARG:HH11	1:A:222:ARG:CG	1.97	0.57
1:A:231:ASN:HD21	1:A:284:LYS:CA	2.16	0.57
1:B:216:SER:HB2	1:B:474:TYR:HB3	1.85	0.57
1:B:281:MET:HE1	3:B:2:XM1:H12	1.87	0.56
1:B:234:GLU:HG2	1:B:281:MET:HE2	1.87	0.56
1:B:207:HIS:HD2	1:B:209:PHE:H	1.52	0.56
1:A:204:ASN:O	1:A:268:LYS:HD2	2.07	0.55
1:A:207:HIS:HD2	1:A:209:PHE:H	1.57	0.52
1:A:300:ILE:HD12	1:A:300:ILE:N	2.25	0.52
1:A:297:LYS:HG3	1:A:300:ILE:HD11	1.91	0.52
1:A:198:GLU:HG3	1:A:293:PHE:HB2	1.90	0.52
1:A:200:ARG:NH2	1:A:298:GLU:OE2	2.44	0.50
1:B:175:TYR:CD1	1:B:432:GLU:HG2	2.47	0.50
1:A:303:GLY:O	1:A:305:THR:HG23	2.12	0.50
1:B:249:ARG:HG3	1:B:424:PRO:HG2	1.93	0.49
1:A:276:LYS:HE3	1:A:278:GLU:HB2	1.94	0.48
1:A:281:MET:CE	1:A:291:THR:HG21	2.44	0.48
1:B:263:TYR:O	1:B:267:GLU:O	2.33	0.47
1:A:404:GLN:HE22	1:B:351:ASN:HD21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:MET:HA	1:A:342:MET:HE2	1.98	0.46
1:B:397:GLU:HB3	1:B:400:LYS:HB3	1.97	0.46
1:A:366:ILE:HG13	4:A:49:HOH:O	2.16	0.46
1:B:339:MET:HA	1:B:342:MET:HE2	1.98	0.46
1:B:366:ILE:HG13	4:B:25:HOH:O	2.14	0.45
1:B:207:HIS:CD2	1:B:209:PHE:H	2.32	0.45
1:B:231:ASN:ND2	1:B:429:VAL:HG21	2.31	0.45
1:B:176:TYR:OH	1:B:214:LYS:HD3	2.17	0.44
1:A:300:ILE:HG23	1:A:304:ALA:HB3	1.98	0.44
1:B:387:ASP:HB3	1:B:390:GLN:HE21	1.82	0.44
3:A:1:XM1:C3	3:A:1:XM1:C16	2.93	0.44
1:B:324:ASN:O	1:B:325:ASP:HB2	2.18	0.44
1:A:155:LEU:HD21	1:A:158:LYS:HG3	2.00	0.44
1:A:297:LYS:HG3	1:A:300:ILE:CD1	2.48	0.43
1:B:262:ASP:HB2	1:B:399:ALA:CB	2.48	0.43
1:B:249:ARG:HG3	1:B:424:PRO:CG	2.48	0.43
1:B:422:SER:HA	1:B:423:PRO:HD2	1.82	0.43
1:A:301:LYS:O	1:A:302:ASP:HB2	2.18	0.42
1:A:413:TRP:N	1:B:352:GLN:HE22	2.11	0.42
1:B:377:LYS:O	1:B:381:SER:HB2	2.20	0.41
3:B:2:XM1:H19	3:B:2:XM1:H15	1.79	0.41
1:B:234:GLU:HG2	1:B:281:MET:CE	2.50	0.41
1:A:153:LEU:HD11	1:A:168:LYS:HB2	2.02	0.41
1:B:234:GLU:CG	1:B:281:MET:HE2	2.50	0.41
1:A:164:VAL:HG21	3:A:1:XM1:H15A	2.03	0.41
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.90	0.41
1:B:260:ALA:O	1:B:263:TYR:HB3	2.21	0.41
3:B:2:XM1:C3	3:B:2:XM1:C16	2.97	0.41
1:B:195:THR:HG21	1:B:223:LEU:HD13	2.03	0.40
1:B:314:GLU:HA	1:B:357:LEU:HD21	2.04	0.40
1:A:387:ASP:HA	1:A:388:PRO:HD2	1.96	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	311/341 (91%)	291 (94%)	19 (6%)	1 (0%)	41	66
1	B	315/341 (92%)	297 (94%)	17 (5%)	1 (0%)	41	66
2	C	8/10 (80%)	8 (100%)	0	0	100	100
2	D	8/10 (80%)	8 (100%)	0	0	100	100
All	All	642/702 (92%)	604 (94%)	36 (6%)	2 (0%)	41	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASP
1	B	292	ASP

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	276/297 (93%)	262 (95%)	14 (5%)	24	50
1	B	280/297 (94%)	261 (93%)	19 (7%)	16	36
2	C	8/8 (100%)	8 (100%)	0	100	100
2	D	8/8 (100%)	6 (75%)	2 (25%)	0	1
All	All	572/610 (94%)	537 (94%)	35 (6%)	18	41

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	PHE
1	A	182	LYS
1	A	184	GLU
1	A	222	ARG
1	A	231	ASN
1	A	244	VAL

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Mol	Chain	Res	Type
1	A	284	LYS
1	A	301	LYS
1	A	360	LEU
1	A	366	ILE
1	A	375	GLU
1	A	430	THR
1	A	433	THR
1	A	436	ARG
1	B	149	GLU
1	B	160	THR
1	B	182	LYS
1	B	187	VAL
1	B	243	ARG
1	B	244	VAL
1	B	302	ASP
1	B	339	MET
1	B	363	MET
1	B	366	ILE
1	B	372	LEU
1	B	377	LYS
1	B	422	SER
1	B	426	LYS
1	B	436	ARG
1	B	446	MET
1	B	449	ILE
1	B	473	ASP
1	B	478	SER
2	D	6	THR
2	D	10	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	HIS
1	A	231	ASN
1	A	324	ASN
1	A	404	GLN
1	B	148	ASN
1	B	207	HIS
1	B	352	GLN
1	B	390	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	308	1	8,10,11	0.68	0	10,14,16	1.13	0
1	TPO	B	308	1	8,10,11	0.67	0	10,14,16	1.58	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	308	1	-	1/9/11/13	-
1	TPO	B	308	1	-	4/9/11/13	-

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	308	TPO	P-OG1-CB	2.88	131.14	123.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	308	TPO	O-C-CA-CB
1	B	308	TPO	N-CA-CB-CG2
1	B	308	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
1	B	308	TPO	C-CA-CB-CG2
1	B	308	TPO	CG2-CB-OG1-P

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	XM1	A	1	-	28,31,31	1.34	4 (14%)	31,43,43	1.30	6 (19%)
3	XM1	B	2	-	28,31,31	1.32	3 (10%)	31,43,43	1.37	5 (16%)

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	XM1	A	1	-	-	1/18/28/28	0/4/4/4
3	XM1	B	2	-	-	4/18/28/28	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	XM1	C19-C17	2.70	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	XM1	C19-C17	2.62	1.55	1.51
3	A	1	XM1	C24-C25	2.22	1.42	1.38
3	B	2	XM1	C7-N10	-2.16	1.34	1.37
3	A	1	XM1	C26-C25	2.15	1.42	1.38
3	B	2	XM1	C24-C25	2.06	1.41	1.38
3	A	1	XM1	C7-N10	-2.04	1.34	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2	XM1	C13-C12-N11	3.28	117.69	110.78
3	B	2	XM1	O18-C17-C19	-3.18	116.19	120.86
3	A	1	XM1	C13-C12-N11	2.74	116.55	110.78
3	A	1	XM1	C15-C16-N11	2.42	115.88	110.78
3	B	2	XM1	C22-C20-C19	-2.41	109.15	113.74
3	B	2	XM1	C15-C16-N11	2.38	115.79	110.78
3	A	1	XM1	O18-C17-C19	-2.36	117.39	120.86
3	A	1	XM1	C22-C20-C19	-2.34	109.29	113.74
3	A	1	XM1	C19-C17-N14	2.30	120.97	118.80
3	B	2	XM1	C21-C19-C17	2.28	113.73	108.67
3	A	1	XM1	C3-C2-C7	2.07	111.19	105.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2	XM1	O18-C17-N14-C15
3	B	2	XM1	C17-C19-C21-N5
3	B	2	XM1	C20-C19-C21-N5
3	A	1	XM1	C17-C19-C21-N5
3	B	2	XM1	C2-C1-N11-C16

There are no ring outliers.

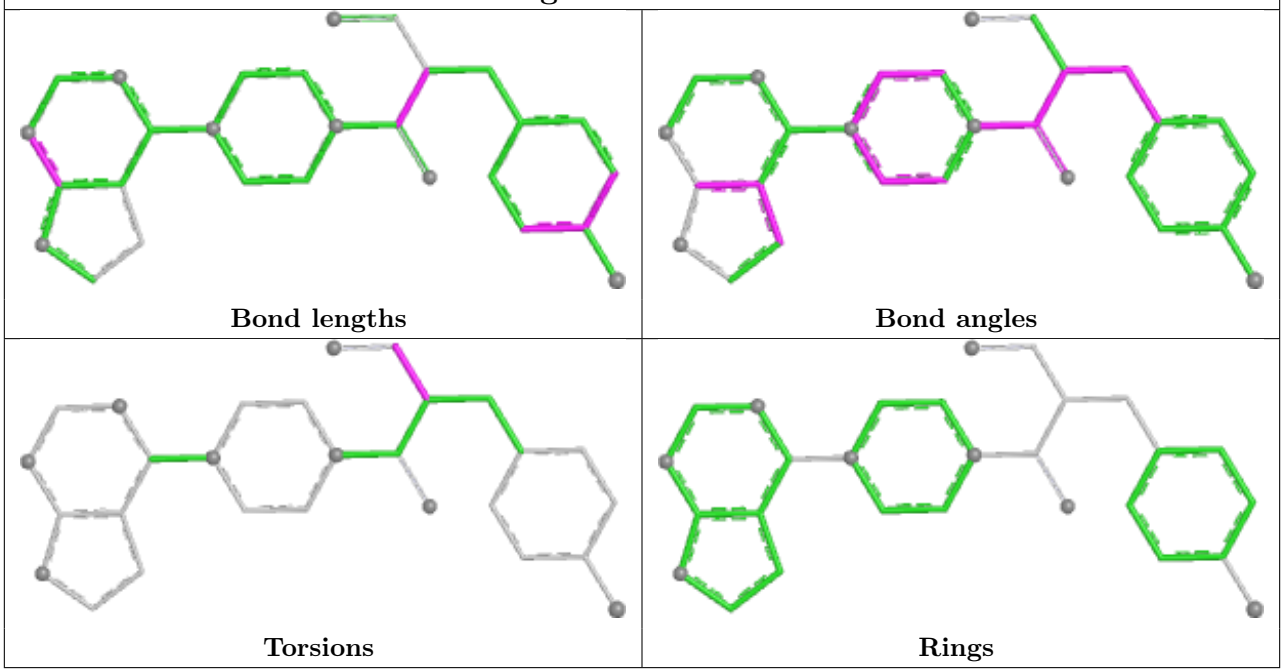
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	XM1	4	0
3	B	2	XM1	6	0

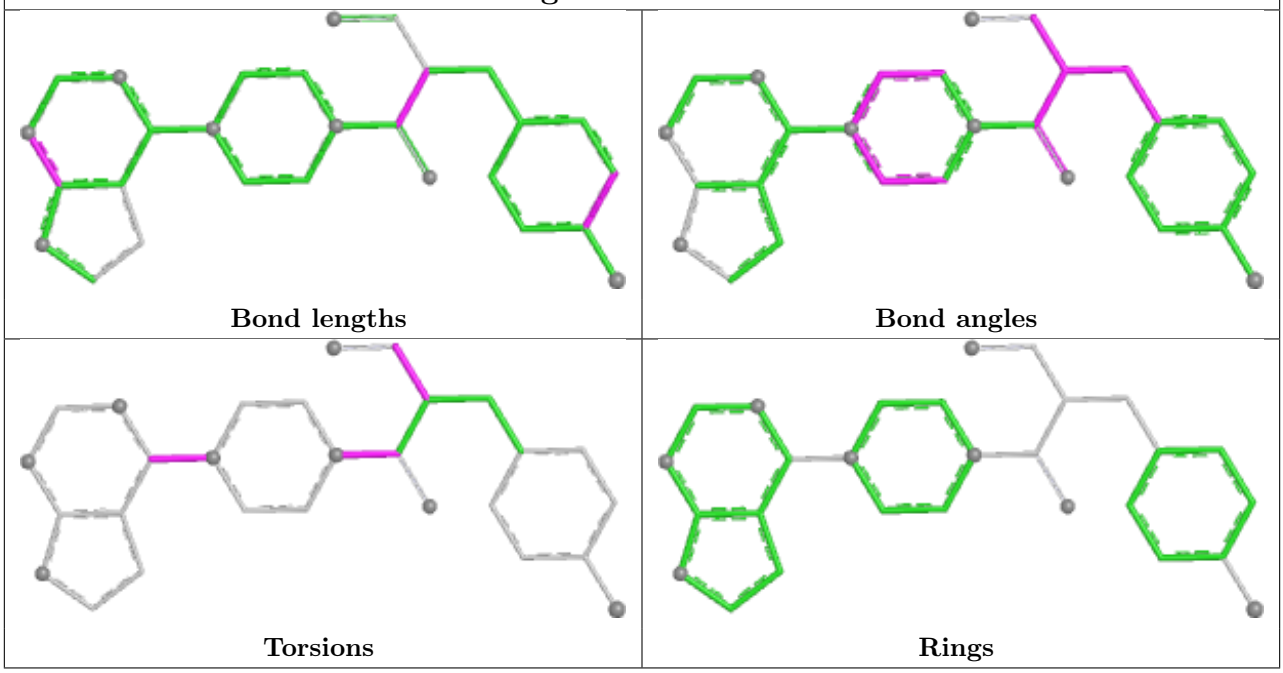
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 XM1 A 1



Ligand XM1 B 2



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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	315/341 (92%)	0.38	22 (6%)	16	14	30, 49, 76, 98	0
1	B	319/341 (93%)	0.34	19 (5%)	21	20	31, 51, 85, 104	0
2	C	10/10 (100%)	0.27	0	100	100	46, 50, 54, 58	0
2	D	10/10 (100%)	0.15	0	100	100	55, 57, 58, 60	0
All	All	654/702 (93%)	0.36	41 (6%)	20	19	30, 50, 83, 104	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	MET	6.2
1	B	448	THR	5.3
1	B	187	VAL	4.6
1	B	444	ALA	4.6
1	B	478	SER	4.4
1	A	478	SER	4.3
1	A	220	HIS	4.1
1	B	440	GLU	3.7
1	A	304	ALA	3.5
1	A	184	GLU	3.3
1	A	144	ARG	3.3
1	B	184	GLU	3.2
1	B	449	ILE	3.2
1	B	220	HIS	3.2
1	A	477	SER	3.1
1	B	446	MET	3.0
1	A	444	ALA	3.0
1	B	148	ASN	2.9
1	A	280	LEU	2.8
1	B	302	ASP	2.7
1	A	185	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	188	ALA	2.7
1	A	279	ASN	2.6
1	B	185	VAL	2.6
1	A	221	ASP	2.6
1	A	440	GLU	2.5
1	A	302	ASP	2.4
1	B	450	THR	2.4
1	A	145	VAL	2.4
1	B	429	VAL	2.4
1	A	338	VAL	2.3
1	A	148	ASN	2.3
1	B	477	SER	2.2
1	A	290	ILE	2.2
1	B	471	GLN	2.2
1	B	299	GLY	2.1
1	A	303	GLY	2.1
1	B	280	LEU	2.1
1	A	275	LEU	2.1
1	B	188	ALA	2.1
1	A	291	THR	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, 95th 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	308	11/12	0.94	0.14	45,46,50,53	0
1	TPO	A	308	11/12	0.98	0.11	43,45,48,48	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,

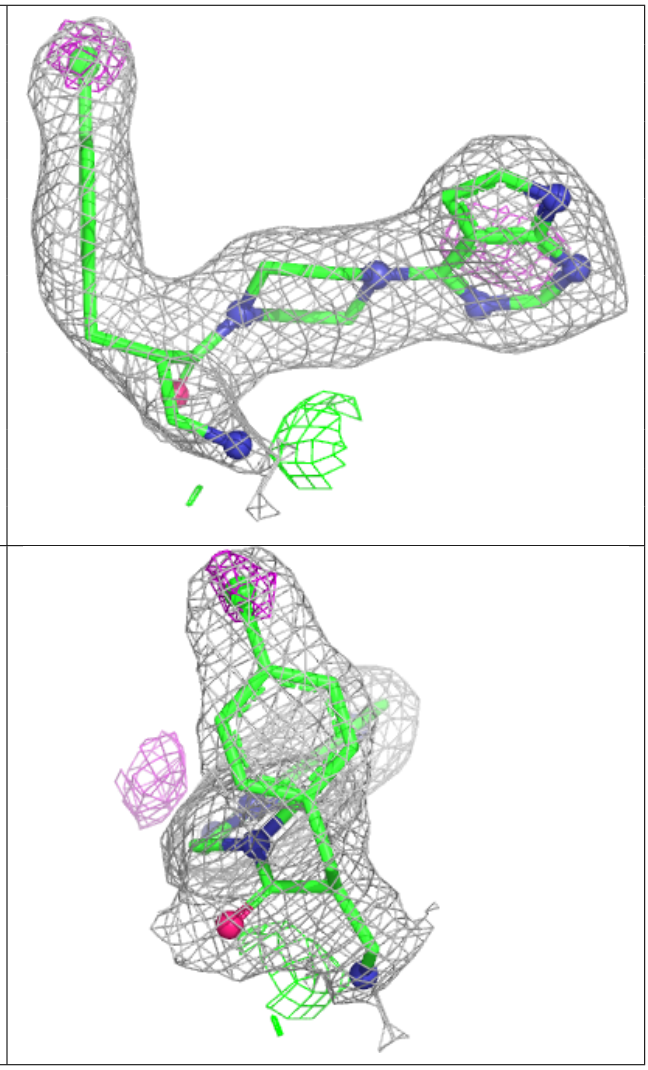
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XM1	A	1	28/28	0.92	0.23	45,49,60,64	0
3	XM1	B	2	28/28	0.92	0.25	52,59,66,68	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.

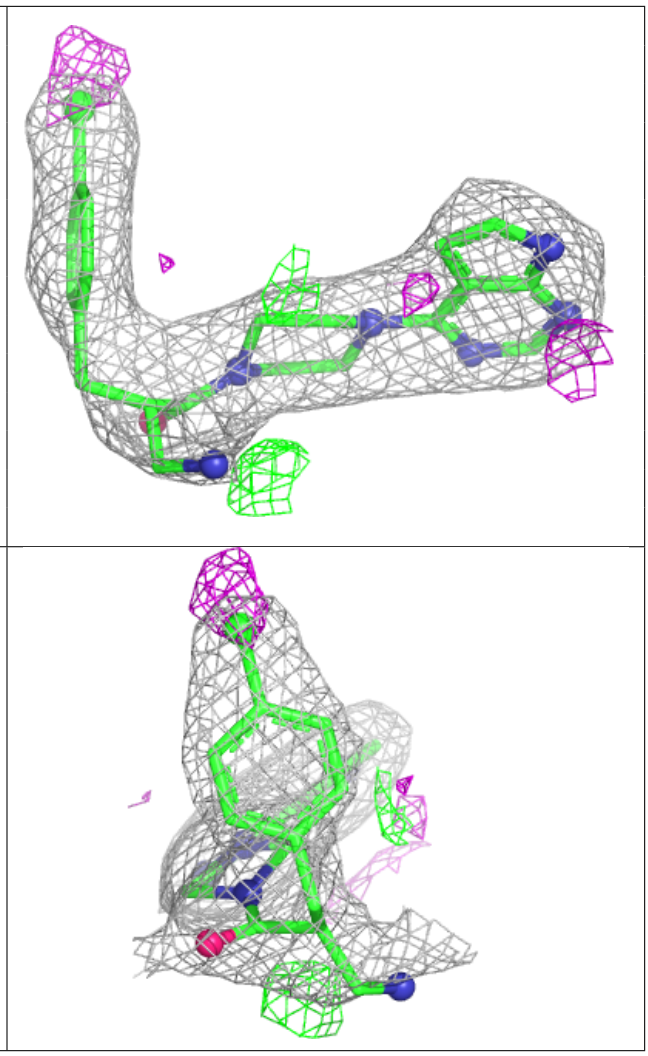
Electron density around XM1 A 1:

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 XM1 B 2:

$2mF_o$-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.