Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 09:20 pm BST

PDB ID	:	4MAO
Title	:	RSK2 T493M C-Terminal Kinase Domain in Complex with RMM58
Authors	:	Miller, R.M.; Taunton, J.
Deposited on	:	2013-08-16
Resolution	:	2.60 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 following versions of software and data (see references (i)) were used in the production of this report:

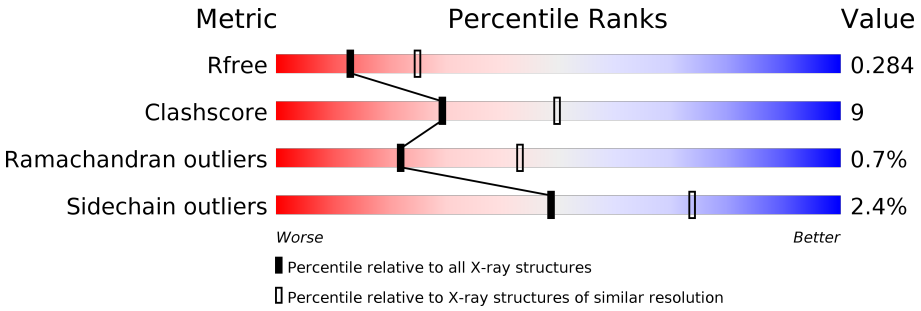
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Mol	Chain	Length	Quality of chain
1	A	355	66% 17% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4706 atoms, of which 2303 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.

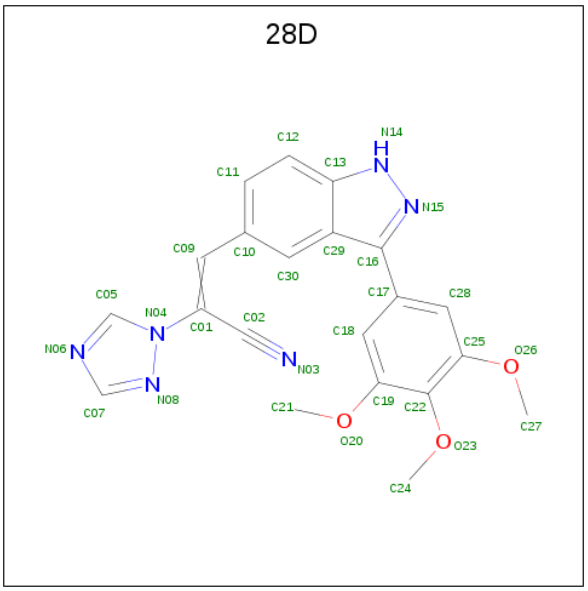
- Molecule 1 is a protein called Ribosomal protein S6 kinase alpha-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	H	N	O	S	0	0	0
			4616	1486	2285	393	440	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	ALA	-	EXPRESSION TAG	UNP P18654
A	387	HIS	-	EXPRESSION TAG	UNP P18654
A	388	HIS	-	EXPRESSION TAG	UNP P18654
A	389	HIS	-	EXPRESSION TAG	UNP P18654
A	390	HIS	-	EXPRESSION TAG	UNP P18654
A	391	HIS	-	EXPRESSION TAG	UNP P18654
A	392	HIS	-	EXPRESSION TAG	UNP P18654
A	393	VAL	-	EXPRESSION TAG	UNP P18654
A	394	ASP	-	EXPRESSION TAG	UNP P18654
A	395	ASP	-	EXPRESSION TAG	UNP P18654
A	396	ASP	-	EXPRESSION TAG	UNP P18654
A	397	ASP	-	EXPRESSION TAG	UNP P18654
A	398	LYS	-	EXPRESSION TAG	UNP P18654
A	493	MET	THR	ENGINEERED MUTATION	UNP P18654
A	591	GLU	LYS	ENGINEERED MUTATION	UNP P18654

- Molecule 2 is (2Z)-2-(1H-1,2,4-triazol-1-yl)-3-[3-(3,4,5-trimethoxyphenyl)-1H-indazol-5-yl]prop-2-enenitrile (three-letter code: 28D) (formula: $C_{21}H_{18}N_6O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			48	21	18	6	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

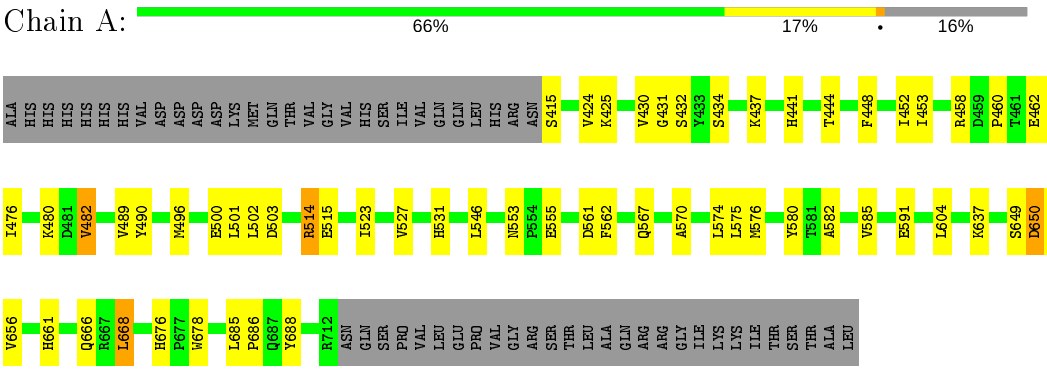
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		

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. 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. 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: Ribosomal protein S6 kinase alpha-3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	47.50Å 47.50Å 288.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.12 – 2.60 46.87 – 1.81	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.12-2.60) 67.9 (46.87-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.85 (at 1.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.235 , 0.292 0.232 , 0.284	Depositor DCC
R_{free} test set	1383 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4706	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: NA, 28D

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	0.37	0/2384	0.51	0/3238

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	2331	2285	2273	44	0
2	A	30	18	17	1	0
3	A	1	0	0	0	0
4	A	41	0	0	10	0
All	All	2403	2303	2290	44	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 9.

All (44) 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:591:GLU:O	4:A:935:HOH:O	2.02	0.77
1:A:500:GLU:HG2	4:A:921:HOH:O	1.85	0.74
1:A:531:HIS:ND1	4:A:901:HOH:O	2.26	0.68
1:A:668:LEU:O	4:A:916:HOH:O	2.12	0.67
1:A:500:GLU:CG	4:A:921:HOH:O	2.41	0.65
1:A:502:LEU:HB3	4:A:921:HOH:O	1.97	0.65
1:A:661:HIS:CE1	1:A:666:GLN:HB2	2.34	0.62
1:A:415:SER:N	4:A:917:HOH:O	2.33	0.62
1:A:523:ILE:O	1:A:527:VAL:HG23	2.02	0.59
1:A:441:HIS:ND1	1:A:444:THR:HG22	2.17	0.59
1:A:432:SER:N	4:A:926:HOH:O	2.37	0.57
1:A:431:GLY:HA3	1:A:434:SER:O	2.06	0.55
1:A:570:ALA:HA	1:A:585:VAL:HG22	1.88	0.55
1:A:651:THR:HG23	1:A:678:TRP:HD1	1.71	0.55
1:A:553:ASN:HB3	1:A:555:GLU:OE2	2.08	0.54
1:A:500:GLU:HA	1:A:546:LEU:HG	1.90	0.53
1:A:650:ASP:N	4:A:925:HOH:O	2.39	0.53
1:A:561:ASP:O	1:A:562:PHE:HB2	2.10	0.52
1:A:652:ALA:O	1:A:656:VAL:HG23	2.09	0.52
1:A:448:PHE:CD1	1:A:480:LYS:HG3	2.46	0.51
1:A:424:VAL:HG12	1:A:425:LYS:N	2.26	0.51
1:A:561:ASP:HA	4:A:915:HOH:O	2.10	0.50
1:A:431:GLY:CA	1:A:434:SER:O	2.60	0.50
1:A:452:ILE:HG12	1:A:490:TYR:CD2	2.48	0.49
1:A:501:LEU:HD23	1:A:502:LEU:N	2.28	0.49
1:A:473:HIS:CB	1:A:476:ILE:HD12	2.43	0.48
1:A:434:SER:HB3	1:A:453:ILE:HA	1.94	0.48
1:A:462:GLU:O	1:A:462:GLU:HG3	2.13	0.47
1:A:460:PRO:HG2	1:A:489:VAL:HG21	1.97	0.46
1:A:473:HIS:HB3	1:A:476:ILE:HD12	1.99	0.44
1:A:514:ARG:HG3	1:A:685:LEU:HB2	1.98	0.44
1:A:574:LEU:O	1:A:576:MET:HG2	2.17	0.44
1:A:649:SER:OG	1:A:651:THR:HG22	2.18	0.43
1:A:580:TYR:CZ	1:A:582:ALA:HB3	2.53	0.43
1:A:567:GLN:HG2	1:A:575:LEU:CD1	2.49	0.42
1:A:448:PHE:CE1	1:A:480:LYS:HG3	2.54	0.42
1:A:567:GLN:HG2	1:A:575:LEU:HD11	2.02	0.41
1:A:424:VAL:HG11	1:A:437:LYS:HD2	2.03	0.41
1:A:655:LEU:HB2	1:A:676:HIS:CE1	2.56	0.41
1:A:482:VAL:HA	1:A:490:TYR:O	2.21	0.41
1:A:458:ARG:NH1	1:A:463:GLU:OE1	2.53	0.40
1:A:496:MET:HG2	2:A:801:28D:N15	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:VAL:HG21	1:A:604:LEU:HD11	2.03	0.40
1:A:686:PRO:HB3	1:A:688:TYR:CE1	2.57	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	296/355 (83%)	278 (94%)	16 (5%)	2 (1%)	22 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	637	LYS
1	A	430	VAL

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	249/308 (81%)	243 (98%)	6 (2%)	49 74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	VAL
1	A	503	ASP
1	A	514	ARG
1	A	515	GLU
1	A	650	ASP
1	A	668	LEU

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

Mol	Chain	Res	Type
1	A	666	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
2	28D	A	801	1	28,33,33	2.94	7 (25%)	33,46,46	3.50	13 (39%)

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	28D	A	801	1	-	7/14/20/20	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	28D	C09-C01	8.82	1.51	1.34
2	A	801	28D	C28-C25	7.12	1.51	1.38
2	A	801	28D	C18-C17	5.87	1.49	1.39
2	A	801	28D	C19-C22	5.03	1.51	1.41
2	A	801	28D	C02-C01	3.33	1.49	1.43
2	A	801	28D	N14-N15	-2.95	1.32	1.37
2	A	801	28D	N08-N04	-2.86	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	28D	C10-C09-C01	-14.05	105.41	130.46
2	A	801	28D	C01-N04-N08	5.70	125.55	119.03
2	A	801	28D	C07-N08-N04	4.83	106.67	102.85
2	A	801	28D	N06-C05-N04	-4.79	107.07	113.30
2	A	801	28D	C05-N06-C07	4.59	107.51	102.34
2	A	801	28D	O26-C25-C22	4.25	122.62	115.16
2	A	801	28D	C09-C01-N04	-4.18	111.19	120.21
2	A	801	28D	O26-C25-C28	-3.85	117.50	124.12
2	A	801	28D	O20-C19-C22	3.48	121.27	115.16
2	A	801	28D	O20-C19-C18	-3.36	118.33	124.12
2	A	801	28D	C17-C16-N15	2.63	125.29	120.78
2	A	801	28D	C11-C10-C30	2.37	121.73	118.58
2	A	801	28D	C30-C29-C13	2.20	121.27	118.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	28D	N04-C01-C09-C10
2	A	801	28D	C22-C25-O26-C27
2	A	801	28D	C28-C25-O26-C27

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Mol	Chain	Res	Type	Atoms
2	A	801	28D	C18-C19-O20-C21
2	A	801	28D	C22-C19-O20-C21
2	A	801	28D	C01-C09-C10-C30
2	A	801	28D	C01-C09-C10-C11

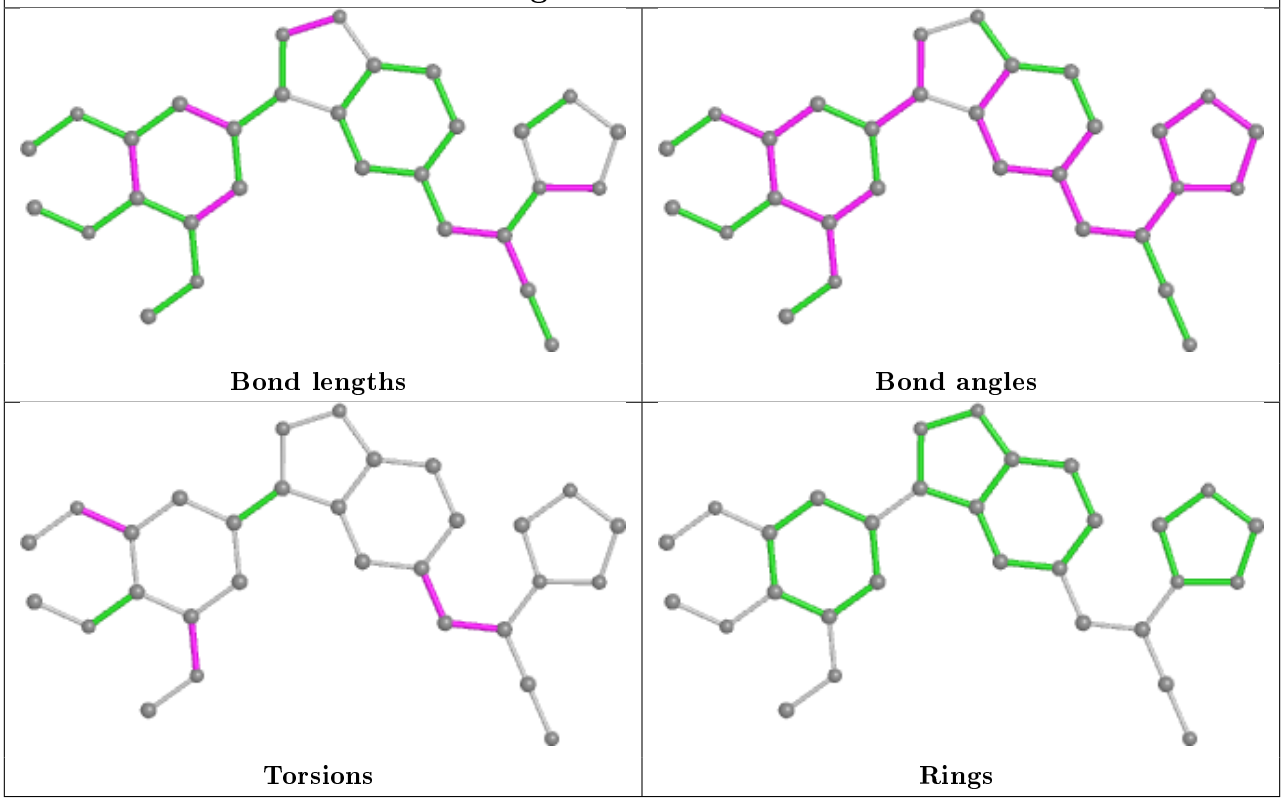
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	28D	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 28D A 801



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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

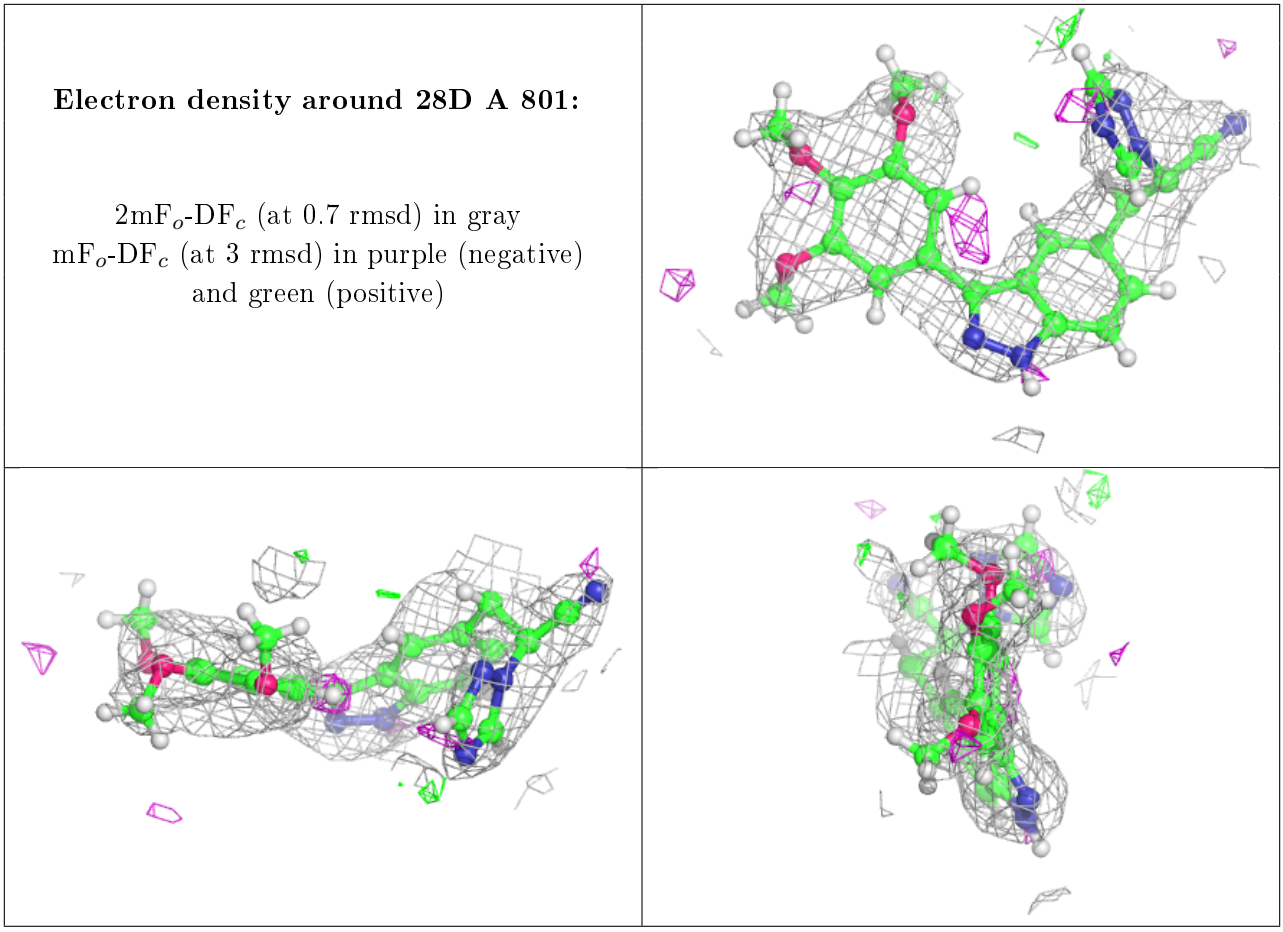
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 28D A 801:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.