



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:51 PM UTC

PDB ID : 8A66 / pdb_00008a66
Title : Crystal structure of MST2 in complex with XMU-MP-1
Authors : Nawrotek, A.; Vuillard, L.; Miallau, L.; Weber, C.
Deposited on : 2022-06-16
Resolution : 1.90 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

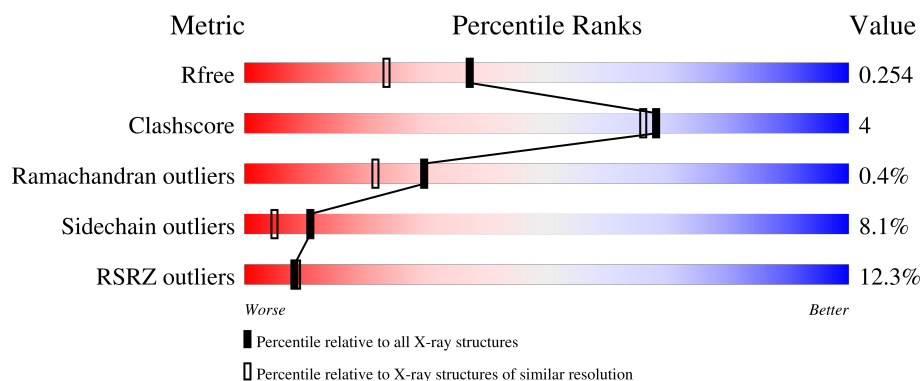
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	298	9% 75% 13% • 8%
2	B	298	14% 82% 12% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4757 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 Serine/threonine-protein kinase 3 36kDa subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	P	S	0	3	0
			2204	1418	368	405	1	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	expression tag	UNP Q13188

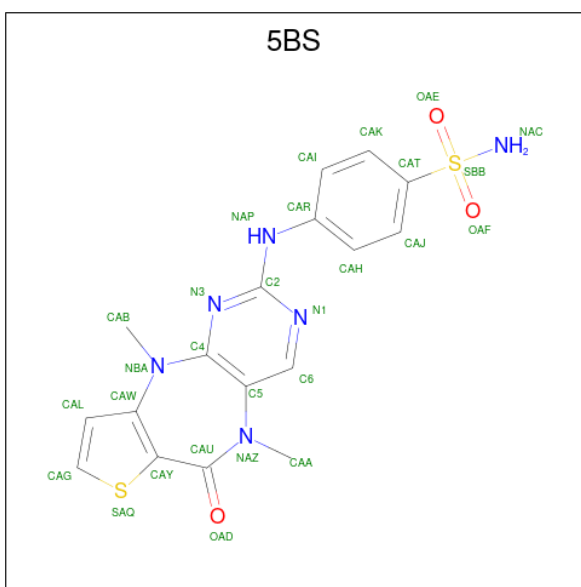
- Molecule 2 is a protein called Serine/threonine-protein kinase 3 36kDa subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	P	S	0	6	0
			2280	1463	376	424	3	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	GLY	-	expression tag	UNP Q13188

- Molecule 3 is 4-[(5,10-dimethyl-6-oxo-6,10-dihydro-5H-pyrimido[5,4-b]thieno[3,2-e][1,4]diazepin-2-yl)amino]benzenesulfonamide (CCD ID: 5BS) (formula: C₁₇H₁₆N₆O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 17	N 6	O 3	S 2	0	0
3	B	1	Total 28	C 17	N 6	O 3	S 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0

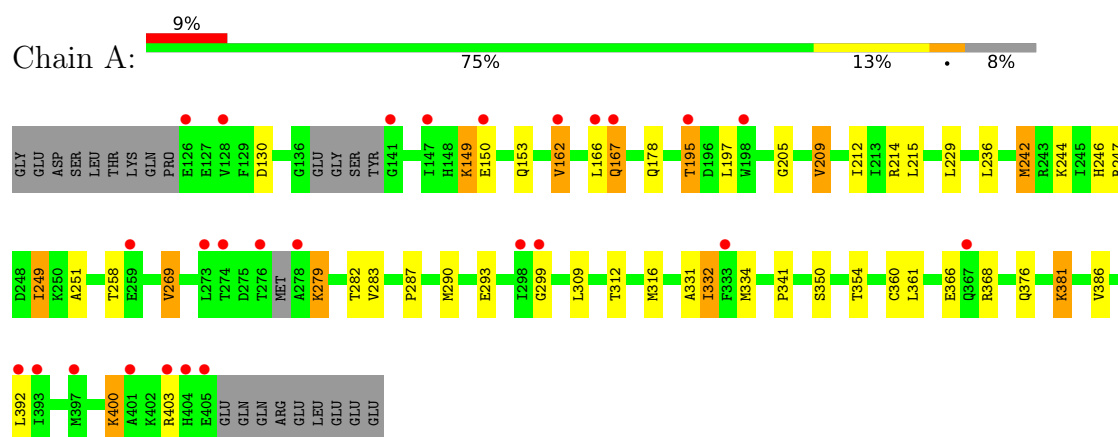
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	96	Total O 96 96	0	0
5	B	119	Total O 119 119	0	0

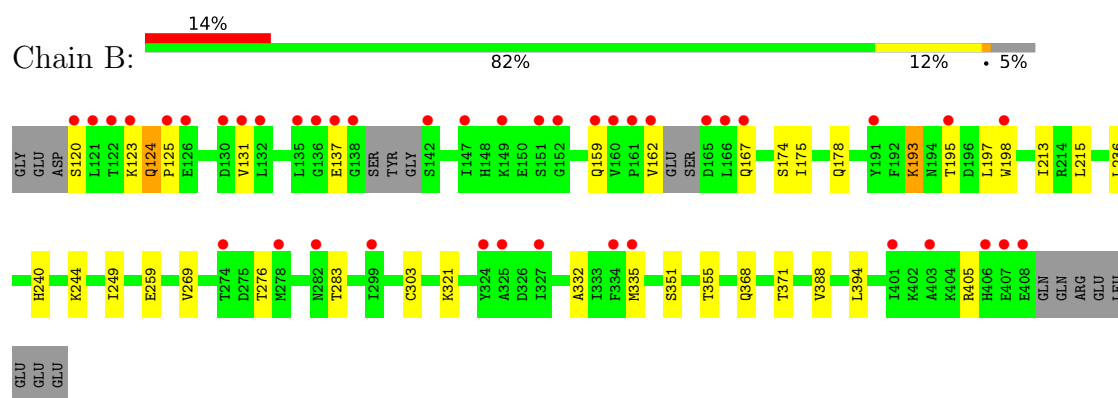
3 Residue-property plots [i](#)

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: Serine/threonine-protein kinase 3 36kDa subunit



- Molecule 2: Serine/threonine-protein kinase 3 36kDa subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	90.77Å 99.04Å 167.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.92 – 1.90 66.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	56.1 (66.92-1.90) 56.1 (66.92-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.218 , 0.258 0.212 , 0.254	Depositor DCC
R_{free} test set	1698 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4757	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NA, TPO, 5BS

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	0.75	0/2247	1.12	6/3038 (0.2%)
2	B	0.74	0/2309	1.07	2/3117 (0.1%)
All	All	0.74	0/4556	1.10	8/6155 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLY	N-CA-C	5.93	121.15	113.27
1	A	242	MET	CA-C-N	5.46	130.11	122.36
1	A	242	MET	C-N-CA	5.46	130.11	122.36
1	A	290	MET	CA-C-N	5.23	127.92	120.49
1	A	290	MET	C-N-CA	5.23	127.92	120.49
1	A	269	VAL	CB-CA-C	5.02	116.45	110.93
2	B	213	ILE	CA-C-N	5.01	126.95	120.44
2	B	213	ILE	C-N-CA	5.01	126.95	120.44

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	2204	0	2246	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2280	0	2320	11	0
3	A	28	0	0	1	0
3	B	28	0	0	0	0
4	A	2	0	0	0	0
5	A	96	0	0	0	0
5	B	119	0	0	0	0
All	All	4757	0	4566	33	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 4.

All (33) 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:214:ARG:HH11	1:A:403:ARG:NH1	1.85	0.74
1:A:312:THR:HG22	1:A:316:MET:HE3	1.72	0.72
1:A:212:ILE:HG21	1:A:392:LEU:HD13	1.72	0.72
1:A:214:ARG:HH11	1:A:403:ARG:HH12	1.40	0.69
1:A:209:VAL:HG22	1:A:251:ALA:HB1	1.78	0.66
1:A:287:PRO:HB3	1:A:332:ILE:HG12	1.80	0.64
2:B:175:ILE:HG23	2:B:244:LYS:HD3	1.79	0.64
1:A:360:CYS:O	1:A:368:ARG:HD2	2.02	0.59
1:A:350:SER:O	1:A:354:THR:HG23	2.06	0.56
1:A:341:PRO:HD2	1:A:361:LEU:HD13	1.92	0.52
1:A:279:LYS:HE2	1:A:299:GLY:HA3	1.92	0.51
2:B:178:GLN:HE21	2:B:244:LYS:NZ	2.08	0.51
1:A:376:GLN:HA	1:A:381:LYS:HG3	1.96	0.47
1:A:400:LYS:HG3	3:A:501:5BS:NAC	2.30	0.47
1:A:130:ASP:HB2	1:A:149:LYS:HD3	1.96	0.47
1:A:229:LEU:HD22	1:A:309:LEU:HD11	1.97	0.47
2:B:332:ALA:HA	2:B:335:MET:HE2	1.96	0.47
1:A:242:MET:HB3	1:A:244:LYS:NZ	2.30	0.47
2:B:124:GLN:HG3	2:B:125:PRO:HD2	1.96	0.47
2:B:174:SER:O	2:B:178:GLN:HG2	2.15	0.46
2:B:125:PRO:HG2	2:B:193:LYS:HB2	1.98	0.45
1:A:167:GLN:HE21	1:A:167:GLN:HB3	1.65	0.44
2:B:120:SER:HA	2:B:123:LYS:HG3	1.99	0.43
1:A:242:MET:HB3	1:A:244:LYS:HZ1	1.83	0.43
1:A:162:VAL:HG13	1:A:195:THR:O	2.20	0.42
2:B:123:LYS:O	2:B:124:GLN:CB	2.67	0.42
1:A:312:THR:CG2	1:A:316:MET:HE3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159[A]:GLN:NE2	2:B:198:TRP:CD1	2.88	0.41
1:A:331:ALA:HA	1:A:334:MET:HE2	2.01	0.41
1:A:246:HIS:HB3	1:A:249[A]:ILE:CD1	2.51	0.40
1:A:293:GLU:OE1	1:A:368:ARG:NH2	2.55	0.40
2:B:351:SER:O	2:B:355:THR:HG23	2.21	0.40
2:B:240:HIS:CG	2:B:303:CYS:HB3	2.56	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	271/298 (91%)	259 (96%)	12 (4%)	0	100	100
2	B	279/298 (94%)	265 (95%)	12 (4%)	2 (1%)	18	10
All	All	550/596 (92%)	524 (95%)	24 (4%)	2 (0%)	30	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	124	GLN
2	B	137	GLU

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	242/261 (93%)	218 (90%)	24 (10%)	7	3
2	B	249/259 (96%)	232 (93%)	17 (7%)	14	7
All	All	491/520 (94%)	450 (92%)	41 (8%)	11	4

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	150	GLU
1	A	153	GLN
1	A	162	VAL
1	A	166	LEU
1	A	167	GLN
1	A	178	GLN
1	A	195	THR
1	A	197	LEU
1	A	209	VAL
1	A	215	LEU
1	A	236	LEU
1	A	247	ARG
1	A	249[A]	ILE
1	A	249[B]	ILE
1	A	258	THR
1	A	269	VAL
1	A	279	LYS
1	A	283	VAL
1	A	332	ILE
1	A	366	GLU
1	A	381	LYS
1	A	386	VAL
1	A	400	LYS
2	B	131	VAL
2	B	162	VAL
2	B	167	GLN
2	B	193	LYS
2	B	195	THR
2	B	197	LEU
2	B	215	LEU
2	B	236	LEU
2	B	249[A]	ILE
2	B	249[B]	ILE
2	B	259	GLU

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Mol	Chain	Res	Type
2	B	269	VAL
2	B	321	LYS
2	B	368	GLN
2	B	388	VAL
2	B	394	LEU
2	B	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	159	GLN
1	A	167	GLN
1	A	178	GLN
1	A	261	HIS
1	A	272	GLN
1	A	281	ASN
1	A	296	GLN
2	B	148	HIS
2	B	167	GLN
2	B	177	GLN
2	B	178	GLN
2	B	194	ASN
2	B	217	ASN
2	B	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
2	TPO	B	371	2	8,10,11	1.82	2 (25%)	10,14,16	1.86	3 (30%)
1	TPO	A	282	1	8,10,11	0.86	0	10,14,16	1.77	4 (40%)
2	TPO	B	283	2	8,10,11	0.96	0	10,14,16	1.55	2 (20%)
2	TPO	B	276	2	8,10,11	1.26	1 (12%)	10,14,16	1.14	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
2	TPO	B	371	2	-	2/9/11/13	-
1	TPO	A	282	1	-	1/9/11/13	-
2	TPO	B	283	2	-	0/9/11/13	-
2	TPO	B	276	2	-	7/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	371	TPO	CG2-CB	3.38	1.59	1.51
2	B	371	TPO	P-OG1	2.97	1.64	1.59
2	B	276	TPO	CB-CA	2.65	1.59	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	TPO	CG2-CB-CA	-3.63	106.19	113.26
1	A	282	TPO	P-OG1-CB	-3.29	114.39	123.33
2	B	283	TPO	P-OG1-CB	-2.90	115.43	123.33
1	A	282	TPO	CG2-CB-CA	-2.82	107.77	113.26
2	B	371	TPO	O3P-P-OG1	2.40	115.19	105.85
1	A	282	TPO	O3P-P-OG1	2.36	115.03	105.85
2	B	276	TPO	O2P-P-OG1	2.34	114.96	105.85
2	B	283	TPO	O3P-P-O1P	-2.24	102.11	110.83
2	B	371	TPO	O-C-CA	-2.17	119.19	124.77
1	A	282	TPO	O-C-CA	-2.08	119.43	124.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	276	TPO	N-CA-CB-CG2
2	B	276	TPO	N-CA-CB-OG1
2	B	276	TPO	C-CA-CB-CG2
2	B	276	TPO	CA-CB-OG1-P
2	B	371	TPO	CB-OG1-P-O3P
1	A	282	TPO	CB-OG1-P-O3P
2	B	276	TPO	CB-OG1-P-O3P
2	B	276	TPO	O-C-CA-CB
2	B	371	TPO	O-C-CA-CB
2	B	276	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	5BS	B	501	-	28,31,31	0.34	0	35,47,47	2.54	3 (8%)
3	5BS	A	501	-	28,31,31	0.33	0	35,47,47	2.16	3 (8%)

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	5BS	B	501	-	-	2/10/10/10	0/3/4/4
3	5BS	A	501	-	-	4/10/10/10	0/3/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	5BS	C5-C4-NBA	14.23	129.30	120.14
3	A	501	5BS	C5-C4-NBA	11.89	127.79	120.14
3	B	501	5BS	C5-C4-N3	-2.96	118.62	123.32
3	A	501	5BS	C6-C5-NAZ	-2.54	114.85	118.99
3	A	501	5BS	C5-C4-N3	-2.38	119.54	123.32
3	B	501	5BS	C6-C5-NAZ	-2.08	115.60	118.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	5BS	CAJ-CAT-SBB-NAC
3	A	501	5BS	CAK-CAT-SBB-OAF
3	A	501	5BS	CAJ-CAT-SBB-OAF
3	A	501	5BS	CAK-CAT-SBB-NAC
3	B	501	5BS	CAJ-CAT-SBB-OAF
3	B	501	5BS	CAK-CAT-SBB-OAF

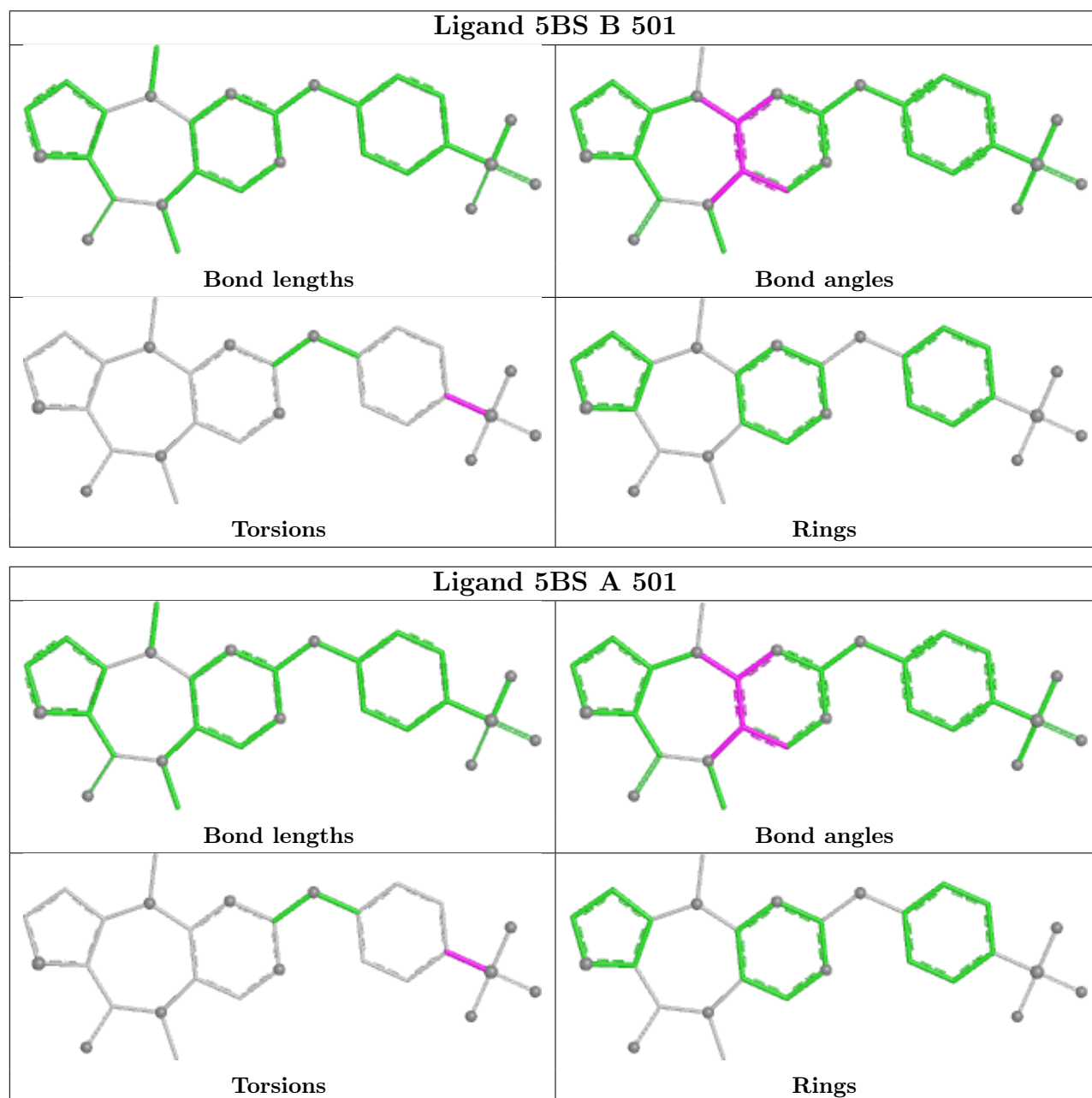
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	5BS	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 than 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.



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, 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	274/298 (91%)	0.75	26 (9%)	14 14	16, 39, 59, 90	3 (1%)
2	B	279/298 (93%)	0.75	42 (15%)	5 5	15, 36, 65, 99	6 (2%)
All	All	553/596 (92%)	0.75	68 (12%)	8 9	15, 37, 61, 99	9 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	162	VAL	5.3
2	B	166	LEU	5.3
2	B	278	MET	5.0
2	B	136	GLY	4.8
2	B	120	SER	4.5
2	B	122	THR	4.5
1	A	166	LEU	4.2
1	A	333	PHE	4.0
2	B	161	PRO	4.0
2	B	137	GLU	3.9
2	B	121	LEU	3.9
1	A	274	THR	3.8
1	A	276	THR	3.7
1	A	298	ILE	3.7
2	B	299	ILE	3.7
1	A	141	GLY	3.5
1	A	405	GLU	3.5
1	A	195	THR	3.4
2	B	191	TYR	3.4
2	B	198	TRP	3.3
2	B	159[A]	GLN	3.1
2	B	125	PRO	3.0
2	B	401	ILE	3.0
1	A	392	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	GLU	3.0
2	B	123	LYS	2.9
2	B	152	GLY	2.9
2	B	408	GLU	2.9
1	A	278	ALA	2.8
1	A	167	GLN	2.7
1	A	299	GLY	2.7
2	B	138	GLY	2.7
2	B	147	ILE	2.7
1	A	403	ARG	2.6
2	B	131	VAL	2.6
2	B	160	VAL	2.5
2	B	406	HIS	2.5
2	B	334	PHE	2.5
2	B	142	SER	2.5
2	B	403	ALA	2.4
2	B	324	TYR	2.4
1	A	162	VAL	2.4
1	A	404	HIS	2.4
2	B	135	LEU	2.3
2	B	407	GLU	2.3
1	A	367	GLN	2.3
1	A	393	ILE	2.3
2	B	130	ASP	2.3
2	B	132	LEU	2.3
2	B	126	GLU	2.2
2	B	151	SER	2.2
2	B	165	ASP	2.2
1	A	273	LEU	2.2
1	A	198	TRP	2.2
1	A	150	GLU	2.2
2	B	195	THR	2.2
2	B	335	MET	2.1
2	B	274	THR	2.1
2	B	167	GLN	2.1
2	B	327	ILE	2.1
1	A	128	VAL	2.1
1	A	397	MET	2.1
2	B	325	ALA	2.1
1	A	147	ILE	2.1
1	A	259	GLU	2.1
2	B	282	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	401	ALA	2.0
2	B	149	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, 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
2	TPO	B	276	11/12	0.84	0.13	56,59,76,79	0
2	TPO	B	371	11/12	0.87	0.14	23,26,29,29	5
2	TPO	B	283	11/12	0.96	0.07	30,33,35,35	0
1	TPO	A	282	11/12	0.96	0.07	36,40,52,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

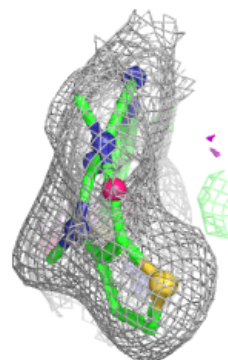
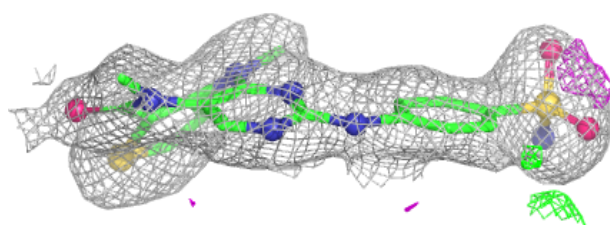
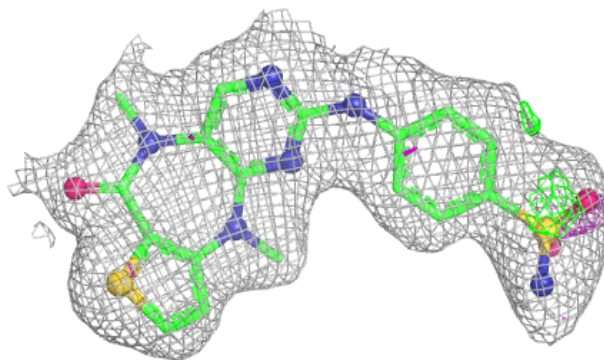
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	5BS	B	501	28/28	0.94	0.09	28,31,39,40	0
3	5BS	A	501	28/28	0.95	0.08	29,30,41,41	0
4	NA	A	502	1/1	0.96	0.07	35,35,35,35	0
4	NA	A	503	1/1	0.97	0.10	33,33,33,33	0

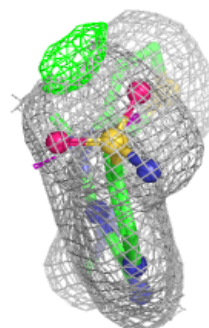
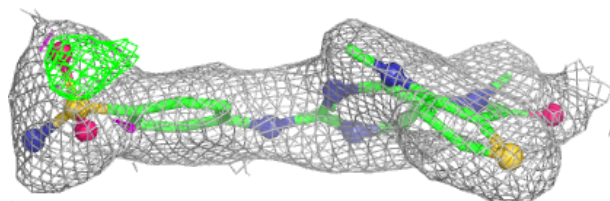
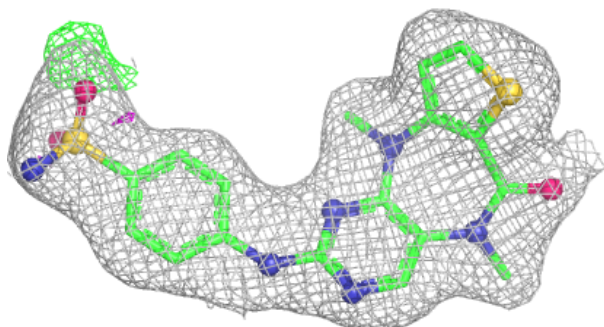
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5BS 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)

**Electron density around 5BS A 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.