



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 12:21 pm GMT

PDB ID : 8S0H
Title : A fragment-based inhibitor of SHP2
Authors : Cleasby, A.; Price, A.
Deposited on : 2024-02-14
Resolution : 1.99 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

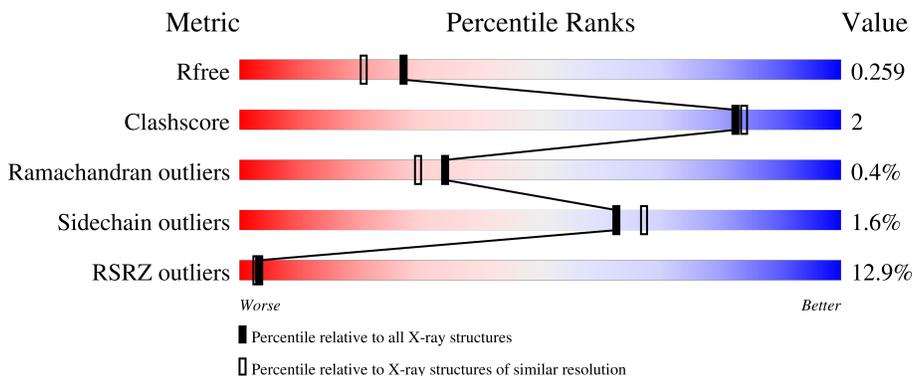
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	537	 12% 87% 7% 6%
1	B	537	 12% 85% 7% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 atoms, of which 40 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.

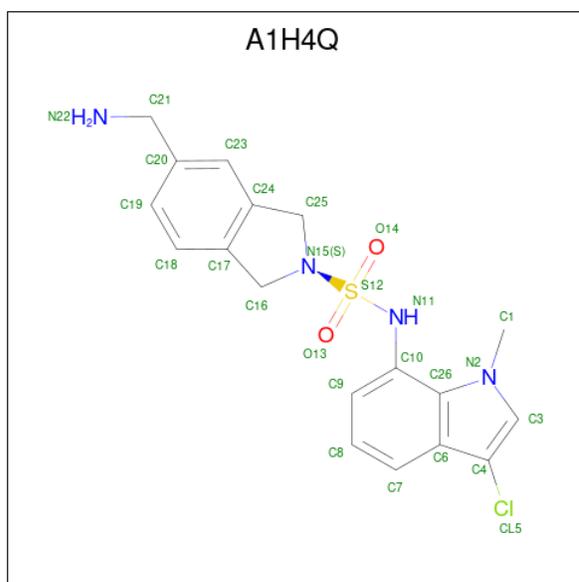
- Molecule 1 is a protein called Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	4098	2572	735	772	19	0	2	0
1	B	500	4055	2547	726	762	20	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q06124
A	529	LEU	-	expression tag	UNP Q06124
A	530	GLU	-	expression tag	UNP Q06124
A	531	HIS	-	expression tag	UNP Q06124
A	532	HIS	-	expression tag	UNP Q06124
A	533	HIS	-	expression tag	UNP Q06124
A	534	HIS	-	expression tag	UNP Q06124
A	535	HIS	-	expression tag	UNP Q06124
A	536	HIS	-	expression tag	UNP Q06124
B	0	HIS	-	expression tag	UNP Q06124
B	529	LEU	-	expression tag	UNP Q06124
B	530	GLU	-	expression tag	UNP Q06124
B	531	HIS	-	expression tag	UNP Q06124
B	532	HIS	-	expression tag	UNP Q06124
B	533	HIS	-	expression tag	UNP Q06124
B	534	HIS	-	expression tag	UNP Q06124
B	535	HIS	-	expression tag	UNP Q06124
B	536	HIS	-	expression tag	UNP Q06124

- Molecule 2 is 5-(aminomethyl)-N-(3-chloranyl-1-methyl-indol-7-yl)-1,3-dihydroisoindole-2-sulfonamide (three-letter code: A1H4Q) (formula: C₁₈H₁₉ClN₄O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	Cl	H	N	O			S
2	A	1	46	18	1	20	4	2	1	0	0
2	B	1	46	18	1	20	4	2	1	0	0

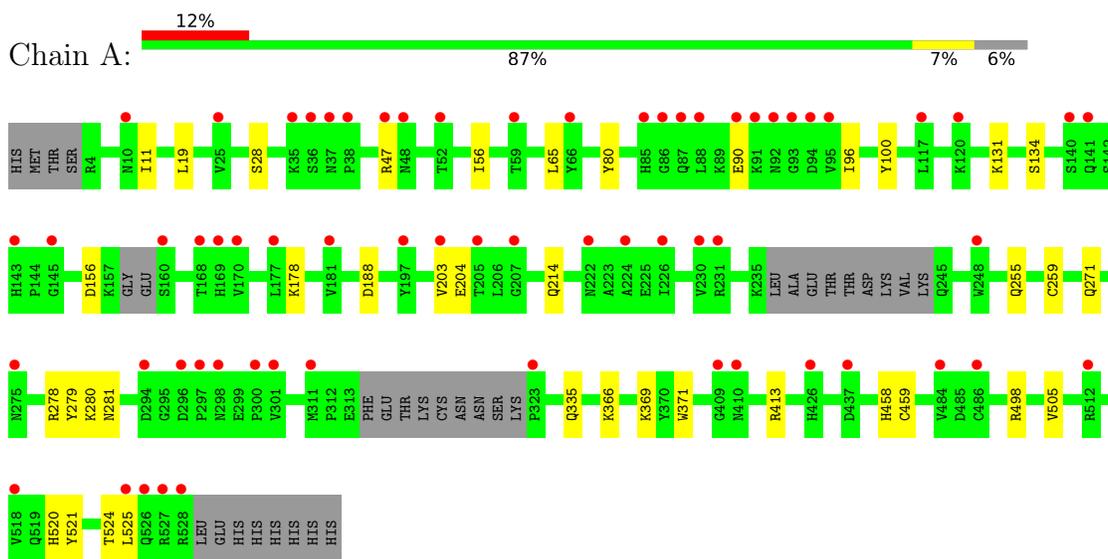
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	403	403	403	0	0
3	B	382	382	382	0	0

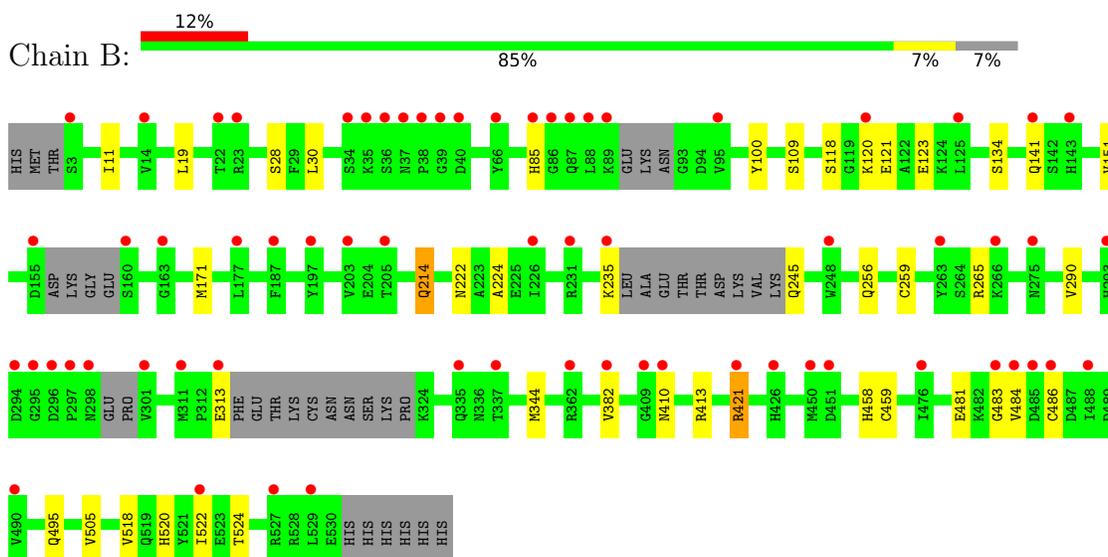
3 Residue-property plots [i](#)

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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 1: Tyrosine-protein phosphatase non-receptor type 11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.10Å 215.84Å 56.51Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	107.92 – 1.99 107.92 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (107.92-1.99) 99.7 (107.92-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.00Å)	Xtrriage
Refinement program		Depositor
R, R_{free}	0.204 , 0.254 0.212 , 0.259	Depositor DCC
R_{free} test set	3751 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.485	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.62% 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: A1H4Q

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	0.50	0/4186	0.64	0/5645
1	B	0.50	0/4139	0.65	0/5578
All	All	0.50	0/8325	0.64	0/11223

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	265	ARG	Sidechain

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	4098	0	4025	19	0
1	B	4055	0	3985	21	0
2	A	26	20	0	0	0
2	B	26	20	0	1	0
3	A	403	0	0	3	0
3	B	382	0	0	3	0
All	All	8990	40	8010	40	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171[A]:MET:HE3	1:B:171[A]:MET:HA	1.76	0.65
1:A:520:HIS:O	1:A:524:THR:HG23	2.09	0.52
1:A:366:LYS:HE3	3:A:945:HOH:O	2.11	0.51
1:B:483:GLY:O	1:B:486:CYS:SG	2.63	0.51
1:B:171[A]:MET:HA	1:B:171[A]:MET:CE	2.42	0.50
1:B:518:VAL:O	1:B:522:ILE:HG12	2.11	0.50
1:A:131:LYS:HB2	1:A:156:ASP:OD2	2.12	0.49
1:A:11:ILE:HD11	1:A:19:LEU:HD12	1.95	0.49
1:A:134:SER:HA	1:A:214:GLN:O	2.13	0.49
1:A:271:GLN:NE2	3:A:703:HOH:O	2.34	0.49
1:B:382:VAL:HG12	3:B:1071:HOH:O	2.12	0.48
1:B:222:ASN:ND2	1:B:484:VAL:O	2.45	0.48
1:A:278:ARG:HD3	1:A:279:TYR:CE2	2.49	0.48
1:B:28:SER:HA	1:B:100:TYR:O	2.14	0.47
1:B:118:SER:OG	1:B:141:GLN:OE1	2.33	0.47
1:A:255:GLN:OE1	1:A:498:ARG:NH1	2.48	0.47
1:B:520:HIS:O	1:B:524:THR:HG23	2.16	0.46
1:A:521:TYR:O	1:A:525:LEU:HD13	2.16	0.45
1:A:280:LYS:HG3	1:A:281:ASN:OD1	2.16	0.45
1:B:495:GLN:HG2	2:B:601:A1H4Q:CL5	2.54	0.45
1:B:222:ASN:HD22	1:B:224:ALA:H	1.65	0.44
1:B:120:LYS:HA	1:B:123:GLU:HB2	1.99	0.44
1:B:134:SER:HA	1:B:214:GLN:O	2.18	0.44
1:A:369:LYS:HE2	1:A:371:TRP:NE1	2.33	0.44
1:A:524:THR:HG22	3:A:806:HOH:O	2.17	0.44
1:B:421:ARG:NH2	3:B:738:HOH:O	2.51	0.43
1:B:235:LYS:O	1:B:245:GLN:N	2.52	0.43
1:A:80:TYR:OH	1:A:280:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:A:96:ILE:HD11	2.01	0.42
1:B:410:ASN:ND2	3:B:729:HOH:O	2.48	0.42
1:B:109:SER:HB2	1:B:256:GLN:HG3	2.01	0.42
1:A:28:SER:HA	1:A:100:TYR:O	2.20	0.42
1:B:11:ILE:CD1	1:B:19:LEU:HD12	2.50	0.41
1:A:178:LYS:HE2	1:A:188:ASP:OD1	2.20	0.41
1:A:56:ILE:HG12	1:A:65:LEU:HD13	2.01	0.41
1:B:118:SER:HB2	1:B:121:GLU:OE1	2.21	0.41
1:B:30:LEU:HD12	1:B:30:LEU:C	2.41	0.41
1:A:80:TYR:CD1	1:A:281:ASN:ND2	2.89	0.40
1:A:203:VAL:HG12	1:A:204:GLU:O	2.22	0.40
1:B:290:VAL:HG11	1:B:344:MET:HG3	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	499/537 (93%)	485 (97%)	12 (2%)	2 (0%)	34	30
1	B	490/537 (91%)	476 (97%)	12 (2%)	2 (0%)	34	30
All	All	989/1074 (92%)	961 (97%)	24 (2%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	CYS
1	B	459	CYS
1	A	505	VAL
1	B	505	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	451/479 (94%)	445 (99%)	6 (1%)	69	74
1	B	446/479 (93%)	436 (98%)	10 (2%)	52	55
All	All	897/958 (94%)	881 (98%)	16 (2%)	62	63

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	259[A]	CYS
1	A	259[B]	CYS
1	A	335	GLN
1	A	413	ARG
1	A	458	HIS
1	B	85	HIS
1	B	151	VAL
1	B	214	GLN
1	B	259[A]	CYS
1	B	259[B]	CYS
1	B	313	GLU
1	B	413	ARG
1	B	421	ARG
1	B	458	HIS
1	B	481	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	B	141	GLN
1	B	408	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](#)

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](#)

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
2	A1H4Q	B	601	-	26,29,29	0.53	0	28,44,44	0.66	0
2	A1H4Q	A	601	-	26,29,29	0.54	0	28,44,44	0.69	1 (3%)

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	A1H4Q	B	601	-	-	1/11/21/21	0/4/4/4
2	A1H4Q	A	601	-	-	2/11/21/21	0/4/4/4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1H4Q	C7-C6-C26	2.34	121.10	116.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

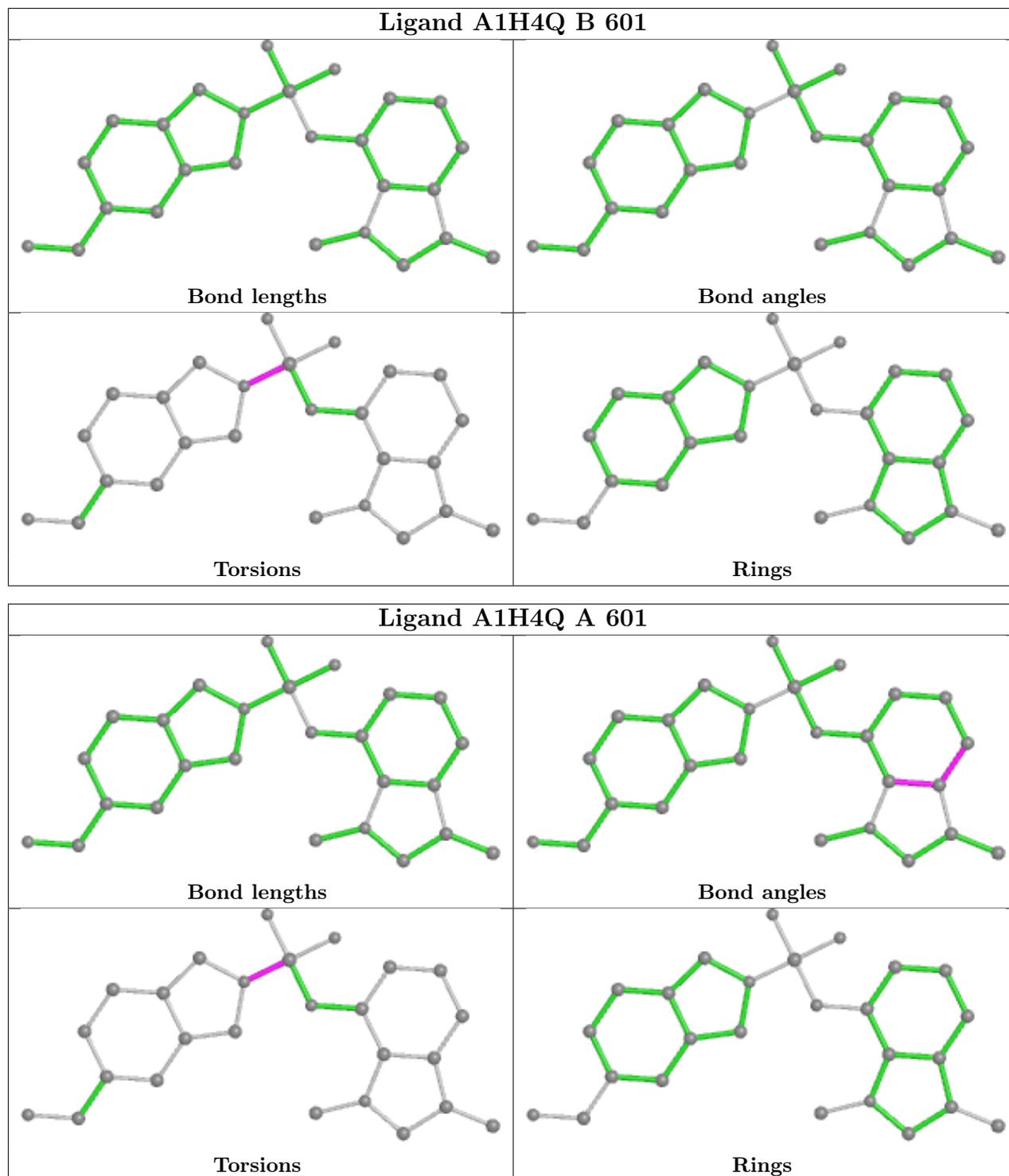
Mol	Chain	Res	Type	Atoms
2	A	601	A1H4Q	C25-N15-S12-O13
2	B	601	A1H4Q	C25-N15-S12-O13
2	A	601	A1H4Q	C16-N15-S12-O13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	A1H4Q	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

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	505/537 (94%)	0.95	64 (12%) 3 3	17, 40, 80, 108	0
1	B	500/537 (93%)	1.03	66 (13%) 3 2	19, 42, 79, 110	0
All	All	1005/1074 (93%)	0.99	130 (12%) 3 3	17, 41, 80, 110	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	SER	7.7
1	B	37	ASN	7.3
1	B	89	LYS	7.2
1	B	529	LEU	6.3
1	A	93	GLY	6.1
1	B	301	VAL	5.6
1	B	296	ASP	5.5
1	A	92	ASN	5.4
1	B	141	GLN	5.1
1	B	486	CYS	5.1
1	A	526	GLN	4.9
1	B	409	GLY	4.8
1	A	177	LEU	4.7
1	A	248	TRP	4.7
1	B	248	TRP	4.6
1	B	177	LEU	4.6
1	B	160	SER	4.5
1	B	35	LYS	4.3
1	B	38	PRO	4.3
1	A	117	LEU	4.2
1	B	294	ASP	3.9
1	A	86	GLY	3.9
1	A	224	ALA	3.9
1	B	85	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	91	LYS	3.8
1	A	36	SER	3.8
1	A	66	TYR	3.8
1	B	426	HIS	3.7
1	A	301	VAL	3.7
1	B	87	GLN	3.7
1	B	226	ILE	3.6
1	B	295	GLY	3.6
1	A	85	HIS	3.6
1	A	226	ILE	3.5
1	A	294	ASP	3.5
1	A	38	PRO	3.4
1	A	323	PRO	3.4
1	A	525	LEU	3.4
1	A	410	ASN	3.4
1	A	205	THR	3.3
1	A	35	LYS	3.3
1	B	484	VAL	3.3
1	B	298	ASN	3.3
1	A	222	ASN	3.2
1	B	231	ARG	3.2
1	A	140	SER	3.2
1	B	34	SER	3.2
1	B	163	GLY	3.1
1	A	528	ARG	3.0
1	A	300	PRO	3.0
1	A	296	ASP	3.0
1	A	48	ASN	3.0
1	B	483	GLY	3.0
1	A	59	THR	3.0
1	B	311	MET	3.0
1	A	120	LYS	3.0
1	A	527	ARG	2.9
1	B	293	HIS	2.9
1	A	10	ASN	2.9
1	B	275	ASN	2.8
1	A	207	GLY	2.7
1	A	181	VAL	2.7
1	B	3	SER	2.7
1	A	484	VAL	2.6
1	B	14	VAL	2.6
1	B	382	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	451	ASP	2.6
1	A	486	CYS	2.6
1	B	522	ILE	2.6
1	A	145	GLY	2.6
1	B	23	ARG	2.6
1	B	86	GLY	2.6
1	B	120	LYS	2.6
1	A	297	PRO	2.6
1	A	90	GLU	2.5
1	B	313	GLU	2.5
1	B	235	LYS	2.5
1	B	362	ARG	2.5
1	A	143	HIS	2.4
1	B	450	MET	2.4
1	A	95	VAL	2.4
1	A	275[A]	ASN	2.4
1	B	337	THR	2.4
1	A	52	THR	2.4
1	A	298	ASN	2.4
1	B	527	ARG	2.4
1	A	168	THR	2.4
1	B	203	VAL	2.4
1	B	155	ASP	2.4
1	A	409	GLY	2.4
1	B	485	ASP	2.4
1	A	426	HIS	2.4
1	B	263	TYR	2.4
1	B	40	ASP	2.4
1	B	488	ILE	2.4
1	A	512	ARG	2.3
1	B	95	VAL	2.3
1	B	39	GLY	2.3
1	A	88	LEU	2.3
1	A	311	MET	2.3
1	A	37	ASN	2.3
1	B	205	THR	2.2
1	A	160	SER	2.2
1	A	87	GLN	2.2
1	A	94	ASP	2.2
1	A	197	TYR	2.2
1	B	143	HIS	2.2
1	B	410	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	335	GLN	2.2
1	A	25	VAL	2.2
1	B	421	ARG	2.2
1	B	125	LEU	2.2
1	B	476	ILE	2.1
1	B	490	VAL	2.1
1	B	22	THR	2.1
1	B	66	TYR	2.1
1	B	197	TYR	2.1
1	A	169	HIS	2.1
1	A	47	ARG	2.1
1	A	170	VAL	2.1
1	A	230	VAL	2.1
1	B	266	LYS	2.1
1	A	437	ASP	2.0
1	A	203	VAL	2.0
1	B	297	PRO	2.0
1	B	88	LEU	2.0
1	A	141	GLN	2.0
1	A	518	VAL	2.0
1	B	187	PHE	2.0
1	A	231	ARG	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, 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.

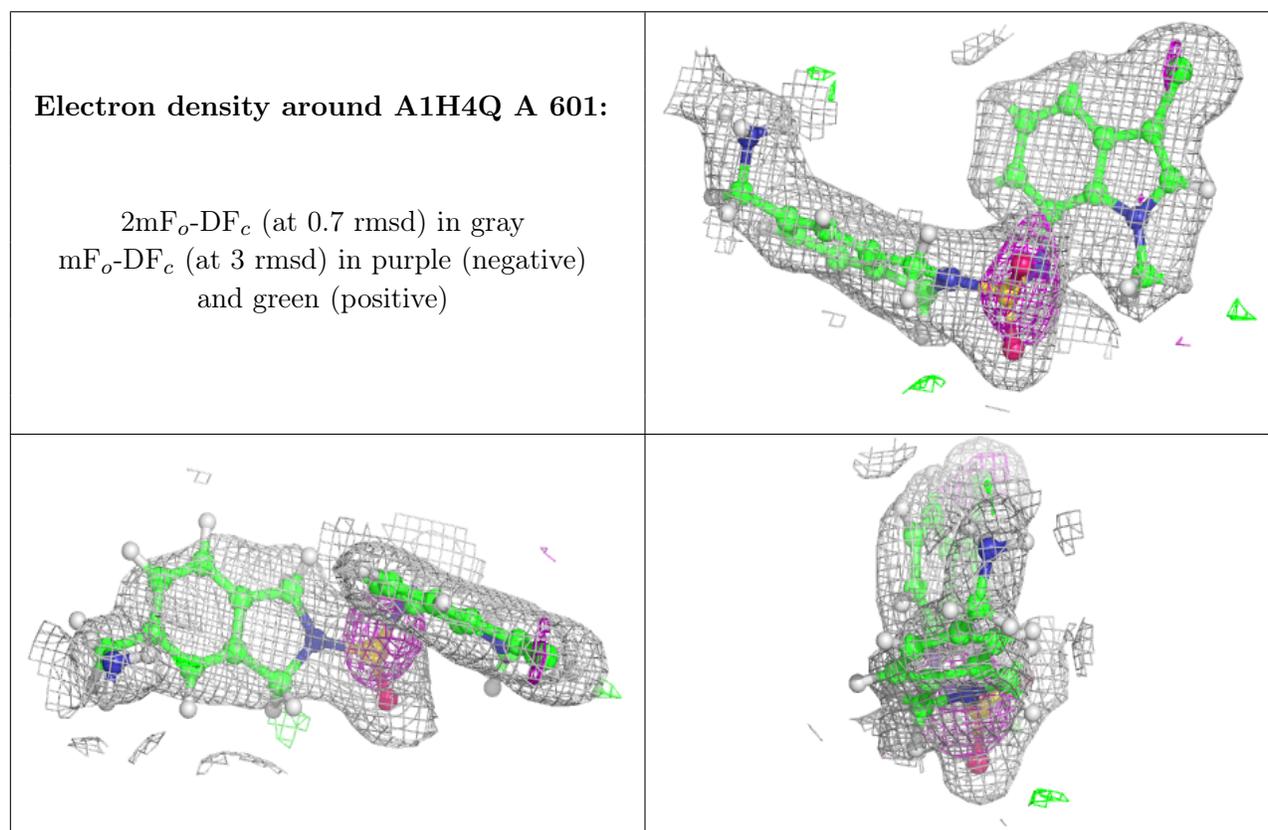
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1H4Q	A	601	26/26	0.92	0.12	23,31,36,38	0

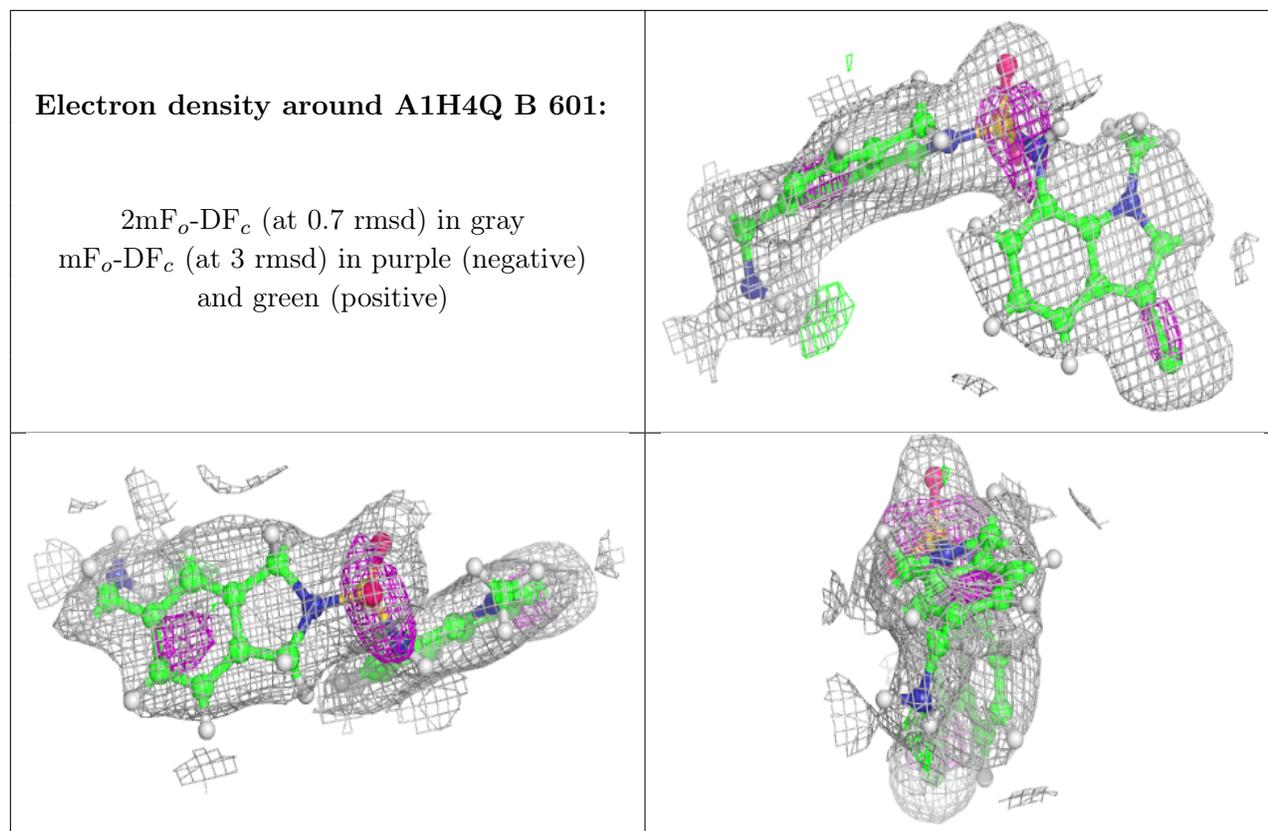
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1H4Q	B	601	26/26	0.92	0.14	25,32,38,40	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.