Full wwPDB X-ray Structure Validation Report (i)

Apr 19, 2026 – 07:36 AM UTC

PDB ID	:	8A2J / pdb_00008a2j
Title	:	human STING in complex with 2'-3'-cyclic-GMP-7-deaza(4-biphenylyl)-AMP
Authors	:	Vavrina, Z.; Brynda, J.; Rezacova, P.
Deposited on	:	2022-06-03
Resolution	:	2.32 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:

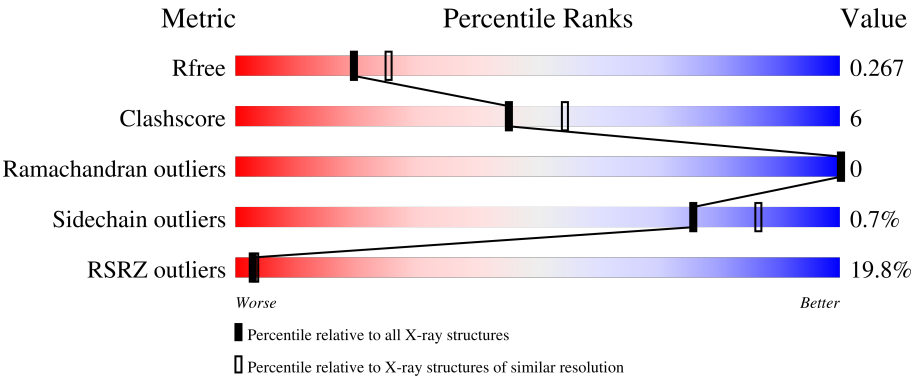
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	241	10% 68% 9% 23%
1	B	241	20% 65% 9% 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2933 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.

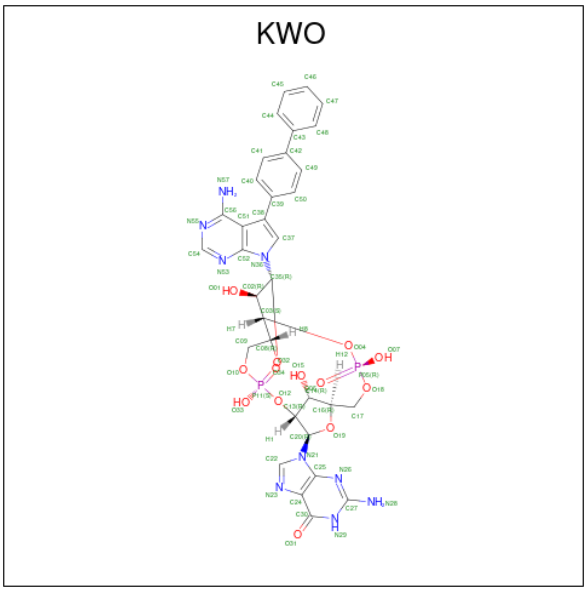
- Molecule 1 is a protein called Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	1	0
			1436	908	258	265	5			
1	B	179	Total	C	N	O	S	0	1	0
			1348	852	231	260	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	SER	-	expression tag	UNP Q86WV6
A	232	ARG	HIS	variant	UNP Q86WV6
B	139	SER	-	expression tag	UNP Q86WV6
B	232	ARG	HIS	variant	UNP Q86WV6

- Molecule 2 is 2-azanyl-9-[(1 {R},6 {R},8 {R},9 {R},10 {S},15 {R},17 {R},18 {R})-8-[4-azanyl-5-(4-phenylphenyl)pyrrolo[2,3-d]pyrimidin-7-yl]-3,9,12,18-tetrakis(oxidanyl)-3,12-bis(oxidanylidene)-2,4,7,11,13,16-hexaoxa-3$l^{5},12$l^{5}-diphosphatricyclo[13.2.1.0^{6,10}]octadecan-17-yl]-1 {H}-purin-6-one (CCD ID: KWO) (formula: $C_{33}H_{33}N_9O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			57	33	9	13	2		

- Molecule 3 is water.

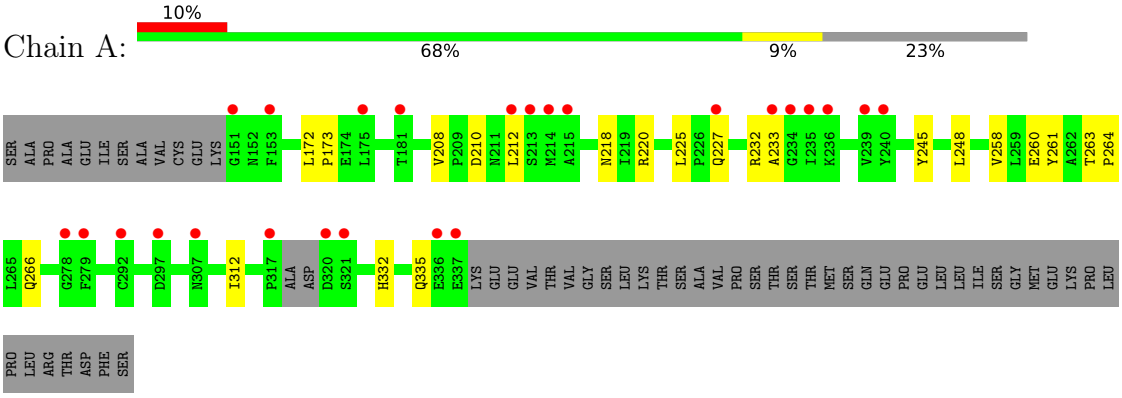
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		
3	B	35	Total	O	0	0
			35	35		

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.

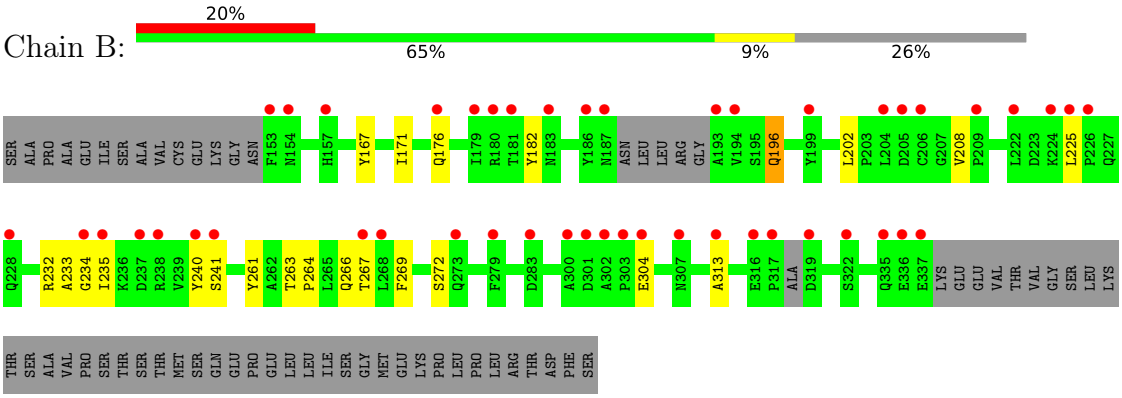
• Molecule 1: Stimulator of interferon genes protein

Chain A:



• Molecule 1: Stimulator of interferon genes protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.29Å 116.91Å 35.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.02 – 2.32 36.02 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.02-2.32) 99.0 (36.02-2.32)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.225 , 0.264 0.225 , 0.267	Depositor DCC
R_{free} test set	888 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2933	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: KWO

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	1.00	0/1464	1.35	0/1991
1	B	1.02	0/1372	1.36	0/1870
All	All	1.01	0/2836	1.35	0/3861

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	1436	0	1364	14	0
1	B	1348	0	1242	21	0
2	B	57	0	0	7	0
3	A	57	0	0	4	0
3	B	35	0	0	3	0
All	All	2933	0	2606	32	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 (32) 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:235:ILE:HD12	2:B:401:KWO:C45	2.28	0.64
1:B:267:THR:OG1	3:B:501:HOH:O	2.14	0.63
1:B:235:ILE:HB	2:B:401:KWO:C45	2.29	0.63
1:A:227:GLN:OE1	3:A:401:HOH:O	2.16	0.61
1:B:241:SER:OG	3:B:502:HOH:O	2.16	0.60
1:A:312:ILE:HD12	1:A:332:HIS:CG	2.40	0.56
1:B:176:GLN:HG2	1:B:196:GLN:HB2	1.87	0.56
1:A:212:LEU:HD13	1:A:261:TYR:CE2	2.41	0.55
1:B:232:ARG:O	2:B:401:KWO:C46	2.57	0.53
2:B:401:KWO:N57	2:B:401:KWO:C40	2.74	0.51
1:B:263:THR:N	1:B:264:PRO:CD	2.75	0.50
1:B:240:TYR:CZ	2:B:401:KWO:C40	2.95	0.49
1:B:208:VAL:HB	1:B:266:GLN:HG3	1.95	0.48
1:A:245:TYR:OH	1:B:234:GLY:O	2.27	0.48
1:A:263:THR:N	1:A:264:PRO:CD	2.76	0.48
1:B:263:THR:HB	2:B:401:KWO:O01	2.13	0.48
1:A:220:ARG:CZ	1:A:248:LEU:HD11	2.43	0.48
1:B:304:GLU:OE2	3:B:503:HOH:O	2.20	0.46
1:A:172:LEU:N	1:A:173:PRO:CD	2.78	0.46
1:A:225:LEU:HD11	1:A:258:VAL:HG21	1.98	0.45
1:A:260:GLU:CD	1:B:235:ILE:HD11	2.42	0.45
1:A:208:VAL:HB	1:A:266:GLN:HG2	2.00	0.44
3:A:404:HOH:O	1:B:233:ALA:HB3	2.18	0.43
1:B:235:ILE:HB	2:B:401:KWO:C46	2.48	0.43
1:B:167:TYR:CZ	1:B:171:ILE:HD13	2.54	0.42
1:B:202:LEU:HB2	1:B:313:ALA:HA	2.02	0.42
1:A:210:ASP:HA	1:B:233:ALA:H	1.85	0.42
1:A:335:GLN:HG3	3:A:431:HOH:O	2.20	0.42
1:A:218:ASN:ND2	3:A:407:HOH:O	2.45	0.41
1:B:182:TYR:HB2	1:B:225:LEU:HD23	2.01	0.41
1:B:269:PHE:O	1:B:272:SER:OG	2.33	0.41
1:A:233:ALA:HB1	1:B:261:TYR:HB2	2.03	0.41

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	182/241 (76%)	176 (97%)	6 (3%)	0	100	100
1	B	174/241 (72%)	171 (98%)	3 (2%)	0	100	100
All	All	356/482 (74%)	347 (98%)	9 (2%)	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	144/210 (69%)	143 (99%)	1 (1%)	76	86
1	B	133/210 (63%)	132 (99%)	1 (1%)	73	85
All	All	277/420 (66%)	275 (99%)	2 (1%)	76	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	ARG
1	B	196	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	B	287	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	KWO	B	401	-	65,65,65	2.00	15 (23%)	94,100,100	2.21	24 (25%)

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	KWO	B	401	-	-	9/38/70/70	0/8/9/9

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	KWO	C25-N26	6.12	1.48	1.34
2	B	401	KWO	C27-N26	4.78	1.44	1.33
2	B	401	KWO	C27-N28	4.77	1.45	1.34
2	B	401	KWO	C56-N57	4.36	1.45	1.34
2	B	401	KWO	C14-C13	-4.09	1.44	1.53
2	B	401	KWO	C37-N36	-4.00	1.31	1.38
2	B	401	KWO	C02-C03	-3.19	1.46	1.53
2	B	401	KWO	C27-N29	3.04	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	KWO	C51-C38	-2.79	1.39	1.46
2	B	401	KWO	C24-N23	-2.56	1.33	1.39
2	B	401	KWO	C51-C52	-2.49	1.37	1.40
2	B	401	KWO	P05-O04	2.42	1.66	1.59
2	B	401	KWO	C25-N21	-2.31	1.32	1.38
2	B	401	KWO	C50-C39	-2.08	1.36	1.39
2	B	401	KWO	O31-C30	-2.03	1.19	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	KWO	C51-C52-N53	-8.74	117.70	126.97
2	B	401	KWO	C56-C51-C52	5.30	119.71	115.74
2	B	401	KWO	C38-C37-N36	-5.18	108.37	110.54
2	B	401	KWO	C51-C38-C37	5.12	109.03	106.03
2	B	401	KWO	C50-C39-C38	-4.94	114.79	120.98
2	B	401	KWO	C24-C25-N26	-4.09	121.87	128.39
2	B	401	KWO	N55-C54-N53	-3.79	122.84	128.58
2	B	401	KWO	C54-N53-C52	3.62	120.68	111.83
2	B	401	KWO	C27-N26-C25	3.54	118.40	112.30
2	B	401	KWO	C40-C41-C42	-3.46	116.68	121.12
2	B	401	KWO	N28-C27-N29	3.42	123.98	116.76
2	B	401	KWO	N53-C52-N36	3.37	132.90	127.17
2	B	401	KWO	C49-C42-C41	3.36	123.68	117.68
2	B	401	KWO	C45-C44-C43	-3.30	116.78	120.54
2	B	401	KWO	O34-C35-N36	3.15	114.14	108.09
2	B	401	KWO	C35-N36-C37	-3.06	122.26	125.72
2	B	401	KWO	C48-C43-C44	3.03	123.09	117.68
2	B	401	KWO	O33-P11-O12	-2.97	94.60	106.70
2	B	401	KWO	C13-C20-N21	-2.96	108.61	114.24
2	B	401	KWO	C49-C42-C43	-2.90	116.26	121.25
2	B	401	KWO	N21-C22-N23	-2.60	108.59	113.40
2	B	401	KWO	O31-C30-C24	-2.53	119.85	126.53
2	B	401	KWO	C40-C39-C38	2.50	124.11	120.98
2	B	401	KWO	C14-C13-C20	2.20	107.01	102.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	KWO	C09-O10-P11-O12
2	B	401	KWO	C09-O10-P11-O32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401	KWO	C13-O12-P11-O10
2	B	401	KWO	C14-C13-O12-P11
2	B	401	KWO	C20-C13-O12-P11
2	B	401	KWO	O34-C35-N36-C37
2	B	401	KWO	C09-O10-P11-O33
2	B	401	KWO	C17-O18-P05-O06
2	B	401	KWO	C13-O12-P11-O32

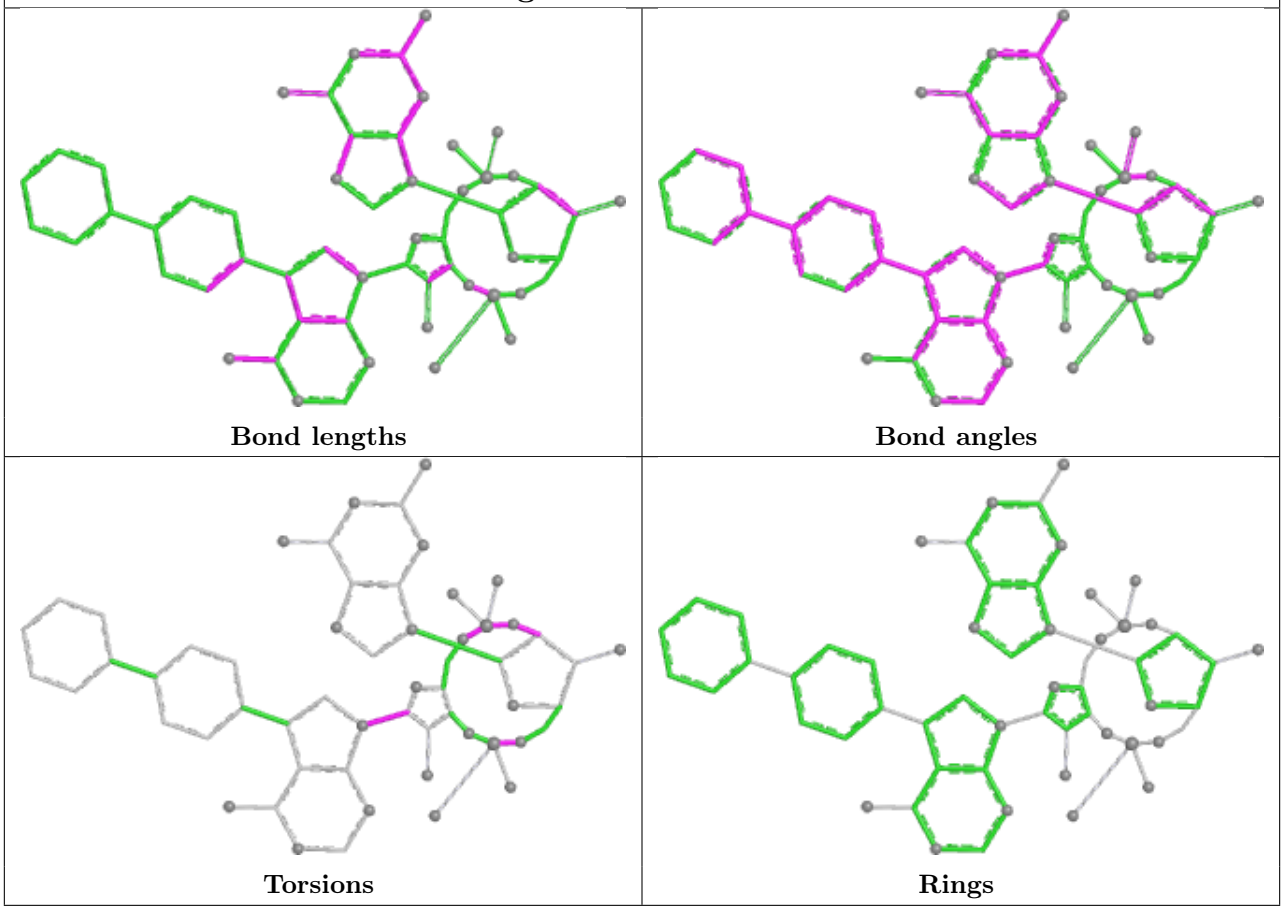
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	KWO	7	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 KWO B 401



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	185/241 (76%)	1.11	25 (13%)	7	7	25, 52, 72, 92	1 (0%)
1	B	179/241 (74%)	1.40	47 (26%)	1	1	29, 54, 80, 90	1 (0%)
All	All	364/482 (75%)	1.26	72 (19%)	3	3	25, 52, 76, 92	2 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	PRO	4.6
1	B	181	THR	4.2
1	B	194	VAL	4.1
1	A	233	ALA	4.0
1	B	302	ALA	3.9
1	B	319	ASP	3.8
1	A	151	GLY	3.8
1	A	320	ASP	3.7
1	B	234	GLY	3.7
1	A	234	GLY	3.7
1	B	301	ASP	3.6
1	A	337	GLU	3.4
1	B	186	TYR	3.4
1	A	297	ASP	3.3
1	B	193	ALA	3.3
1	B	180	ARG	3.2
1	A	215	ALA	3.2
1	A	235	ILE	3.2
1	B	267	THR	3.1
1	A	240	TYR	3.1
1	A	278	GLY	3.1
1	B	279	PHE	3.1
1	A	239	VAL	3.1
1	B	300	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	153	PHE	3.0
1	A	279	PHE	3.0
1	B	187	ASN	2.9
1	B	237	ASP	2.9
1	B	307	ASN	2.9
1	B	154	ASN	2.8
1	B	240	TYR	2.8
1	B	337	GLU	2.8
1	A	236	LYS	2.8
1	B	225	LEU	2.8
1	B	153	PHE	2.8
1	A	212	LEU	2.7
1	B	179	ILE	2.7
1	A	175	LEU	2.7
1	B	336	GLU	2.6
1	A	317	PRO	2.6
1	B	176	GLN	2.6
1	B	205	ASP	2.6
1	B	199	TYR	2.5
1	B	322	SER	2.5
1	B	209	PRO	2.5
1	B	228	GLN	2.5
1	A	336	GLU	2.4
1	B	316	GLU	2.4
1	A	321	SER	2.4
1	B	226	PRO	2.4
1	A	213	SER	2.4
1	B	235	ILE	2.4
1	B	183	ASN	2.3
1	B	241	SER	2.3
1	B	157	HIS	2.3
1	B	273	GLN	2.3
1	B	303	PRO	2.3
1	B	204	LEU	2.2
1	B	222	LEU	2.2
1	B	313	ALA	2.2
1	B	238	ARG	2.2
1	B	268	LEU	2.1
1	B	206	CYS	2.1
1	B	224	LYS	2.1
1	A	227	GLN	2.1
1	A	181	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	MET	2.1
1	B	304	GLU	2.0
1	A	307	ASN	2.0
1	B	283	ASP	2.0
1	A	292	CYS	2.0
1	B	335	GLN	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 oligosaccharides in this entry.

6.4 Ligands (i)

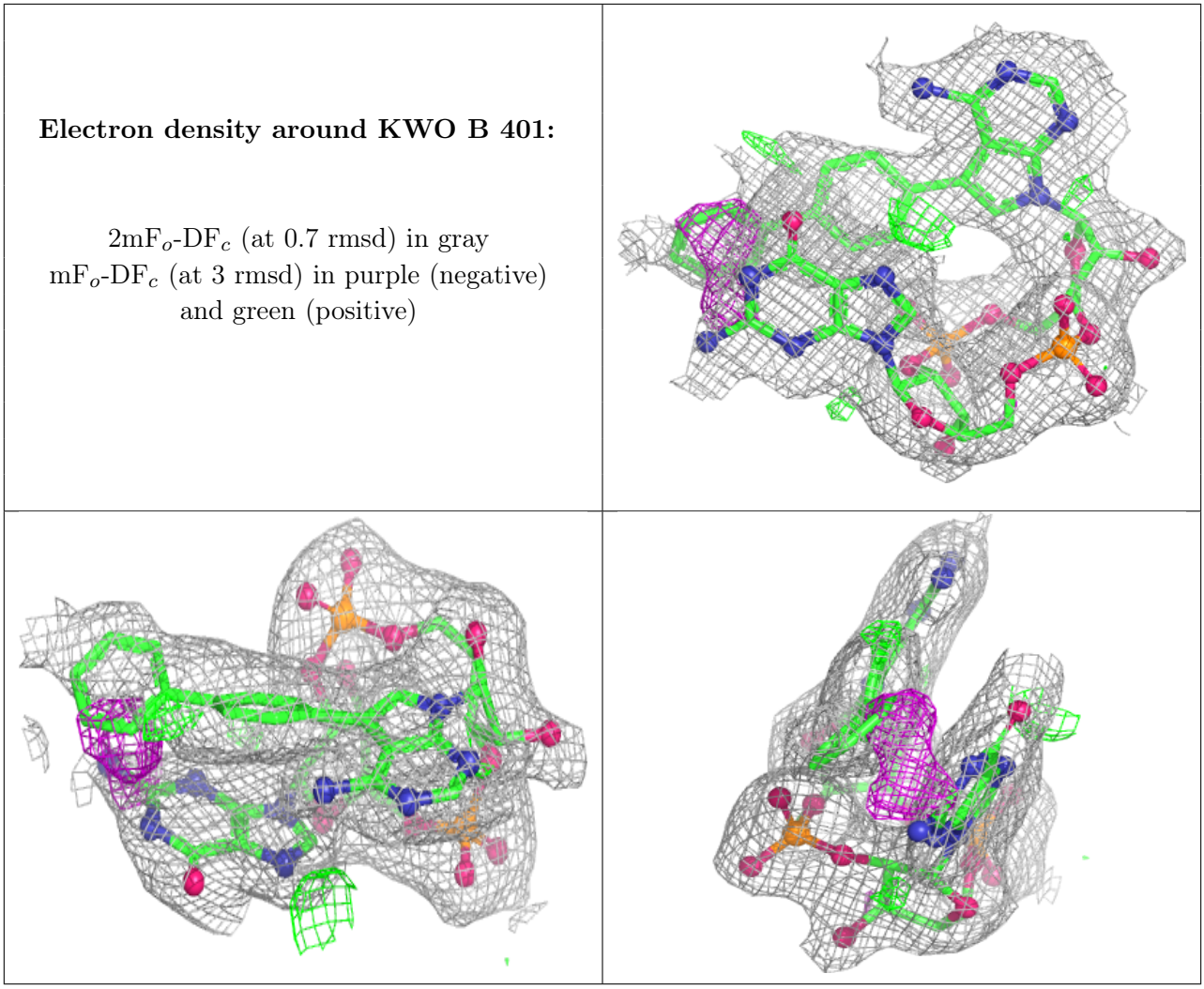
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KWO	B	401	57/57	0.93	0.13	38,49,70,80	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 KWO B 401:

$2mF_o$-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.