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Full wwPDB X-ray Structure Validation Report (i)

Apr 14, 2025 – 11:33 am BST

PDB ID	:	8QSF / pdb_00008qsf
Title	:	Ternary structure of 14-3-3s, BRAF phosphopeptide (pS365) and compound 22 (1083853).
Authors	:	Konstantinidou, M.; Vickery, H.; Pennings, M.A.M.; Virta, J.; Visser, E.J.; Oetelaar, M.C.M.; Overmans, M.; Neitz, J.; Ottmann, C.; Brunsveld, L.; Arkin, M.R.
Deposited on	:	2023-10-10
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

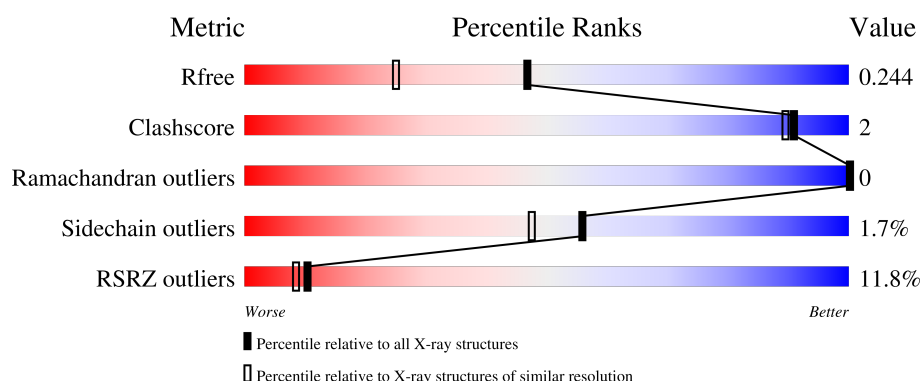|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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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 1.80 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.7%
RSRZ outliers		11.8%

Worse .... *Better*

■ Percentile relative to all X-ray structures
❒ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	236	10% / 96% / ..
1	J	236	12% / 96% / .
2	H	10	30% / 80% / 20%
2	S	10	30% / 90% / 10%

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2 Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 4327 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 14-3-3 protein sigma.

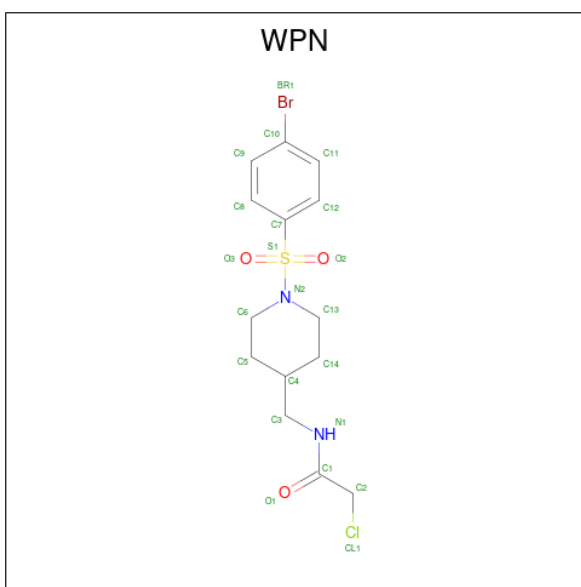| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1857	1156	314	376	11			
1	J	236	Total	C	N	O	S	0	1	0
			1865	1161	317	376	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P31947
A	-3	ALA	-	expression tag	UNP P31947
A	-2	MET	-	expression tag	UNP P31947
A	-1	GLY	-	expression tag	UNP P31947
A	0	SER	-	expression tag	UNP P31947
J	-4	GLY	-	expression tag	UNP P31947
J	-3	ALA	-	expression tag	UNP P31947
J	-2	MET	-	expression tag	UNP P31947
J	-1	GLY	-	expression tag	UNP P31947
J	0	SER	-	expression tag	UNP P31947

- Molecule 2 is a protein called BRAF peptide pS365.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	10	Total	C	N	O	P	0	0	0
			79	42	16	20	1			
2	S	10	Total	C	N	O	P	0	0	0
			79	42	16	20	1			

- Molecule 3 is {N}-[[1-(4-bromophenyl)sulfonylpiperidin-4-yl]methyl]-2-chloranyl-ethanamide (CCD ID: WPN) (formula: $C_{14}H_{18}BrClN_2O_3S$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 21	Br 1	C 14	N 2	O 3	S 1	0	0
3	J	1	Total 21	Br 1	C 14	N 2	O 3	S 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Mg 3	0	0
4	J	4	Total 4	Mg 4	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	J	1	Total 1	Cl 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	225	Total 225	O 225	0	0

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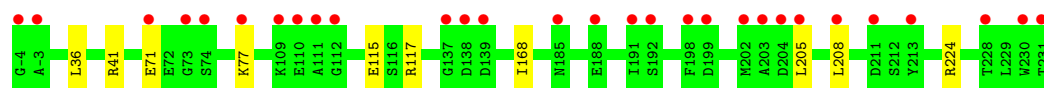| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	12	Total 12	O 12	0	0
6	J	150	Total 150	O 150	0	0
6	S	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

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.
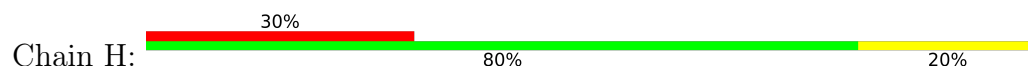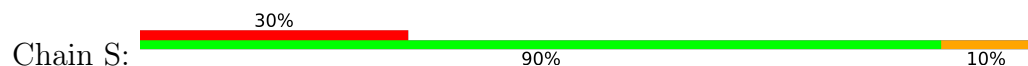
- Molecule 1: 14-3-3 protein sigma
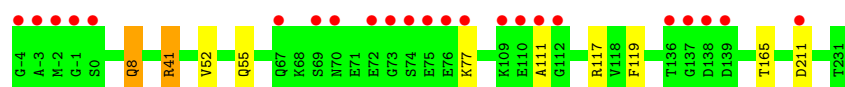
Chain A:

- Molecule 1: 14-3-3 protein sigma

Chain J:

- Molecule 2: BRAF peptide pS365

Chain H:

- Molecule 2: BRAF peptide pS365

Chain S:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.00Å 88.19Å 118.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.00 – 1.80 61.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.00-1.80) 99.5 (61.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.80Å)	Xtriage
Refinement program	PDB-REDO	Depositor
R, R_{free}	0.179 , 0.203 0.222 , 0.244	Depositor DCC
R_{free} test set	2959 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.2	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4327	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CL, MG, WPN, SEP

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	0.39	0/1883	0.56	0/2530
1	J	0.36	0/1894	0.55	0/2544
2	H	0.35	0/69	0.64	0/90
2	S	0.30	0/69	0.60	0/90
All	All	0.37	0/3915	0.56	0/5254

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	A	0	2
1	J	0	3
2	S	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	41	ARG	Sidechain
1	J	117[A]	ARG	Sidechain
1	J	117[B]	ARG	Sidechain
1	J	224	ARG	Sidechain
2	S	362	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	1857	0	1830	6	0
1	J	1865	0	1843	4	0
2	H	79	0	63	1	0
2	S	79	0	63	1	0
3	A	21	0	0	1	0
3	J	21	0	0	0	0
4	A	3	0	0	0	0
4	J	4	0	0	0	0
5	A	1	0	0	0	0
5	J	1	0	0	0	0
6	A	225	0	0	3	0
6	H	12	0	0	0	0
6	J	150	0	0	0	0
6	S	9	0	0	1	0
All	All	4327	0	3799	12	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 (12) 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:111:ALA:CB	6:A:405:HOH:O	2.40	0.70
1:A:111:ALA:HB3	6:A:405:HOH:O	1.95	0.65
3:A:301:WPN:BR1	2:H:369:VAL:HG11	2.59	0.56
1:A:8:GLN:HE21	1:A:8:GLN:HA	1.71	0.54
1:J:205:LEU:O	1:J:205:LEU:HD13	2.10	0.50
1:A:111:ALA:HB2	6:A:405:HOH:O	2.05	0.50
1:A:41:ARG:HD2	1:A:119:PHE:CD2	2.49	0.48
1:J:205:LEU:HD22	1:J:208:LEU:HD12	1.98	0.44
1:J:115:GLU:CG	1:J:168:ILE:HD12	2.50	0.41
1:A:52:VAL:HA	1:A:55:GLN:HE21	1.86	0.41
2:S:362:ARG:NH2	6:S:402:HOH:O	2.53	0.40
1:J:36:LEU:O	1:J:41:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	234/236 (99%)	231 (99%)	3 (1%)	0	100	100
1	J	235/236 (100%)	233 (99%)	2 (1%)	0	100	100
2	H	7/10 (70%)	7 (100%)	0	0	100	100
2	S	7/10 (70%)	7 (100%)	0	0	100	100
All	All	483/492 (98%)	478 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	198/198 (100%)	194 (98%)	4 (2%)	50	40
1	J	199/198 (100%)	197 (99%)	2 (1%)	73	68
2	H	8/8 (100%)	7 (88%)	1 (12%)	3	1
2	S	8/8 (100%)	8 (100%)	0	100	100
All	All	413/412 (100%)	406 (98%)	7 (2%)	56	47

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	77	LYS
1	A	165	THR
1	A	211	ASP
2	H	370	HIS
1	J	71	GLU
1	J	77	LYS

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	8	GLN
1	A	55	GLN
1	A	185	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\#|Z| > 2$
2	SEP	H	365	2	8,9,10	0.79	0	8,12,14	1.15	0
2	SEP	S	365	2	8,9,10	0.80	0	8,12,14	0.81	0

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	SEP	H	365	2	-	0/5/8/10	-
2	SEP	S	365	2	-	0/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 9 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	WPN	J	301	1	22,22,23	0.41	0	31,31,32	1.27	4 (12%)
3	WPN	A	301	1	22,22,23	0.53	0	31,31,32	1.44	7 (22%)

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	WPN	J	301	1	-	2/17/27/29	0/2/2/2
3	WPN	A	301	1	-	2/17/27/29	0/2/2/2

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There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	301	WPN	C14-C4-C5	3.65	118.25	109.33
3	A	301	WPN	C4-C3-N1	3.39	119.12	112.73
3	A	301	WPN	O1-C1-C2	-2.98	116.52	122.06
3	A	301	WPN	C14-C4-C5	2.95	116.55	109.33
3	J	301	WPN	C4-C3-N1	2.90	118.20	112.73
3	A	301	WPN	C5-C6-N2	2.55	112.90	109.43
3	A	301	WPN	C7-S1-N2	-2.35	104.51	107.30
3	A	301	WPN	C2-C1-N1	2.29	120.14	116.09
3	J	301	WPN	O1-C1-C2	-2.24	117.89	122.06
3	A	301	WPN	C14-C13-N2	2.05	112.22	109.43
3	J	301	WPN	C5-C6-N2	2.01	112.17	109.43

There are no chirality outliers.
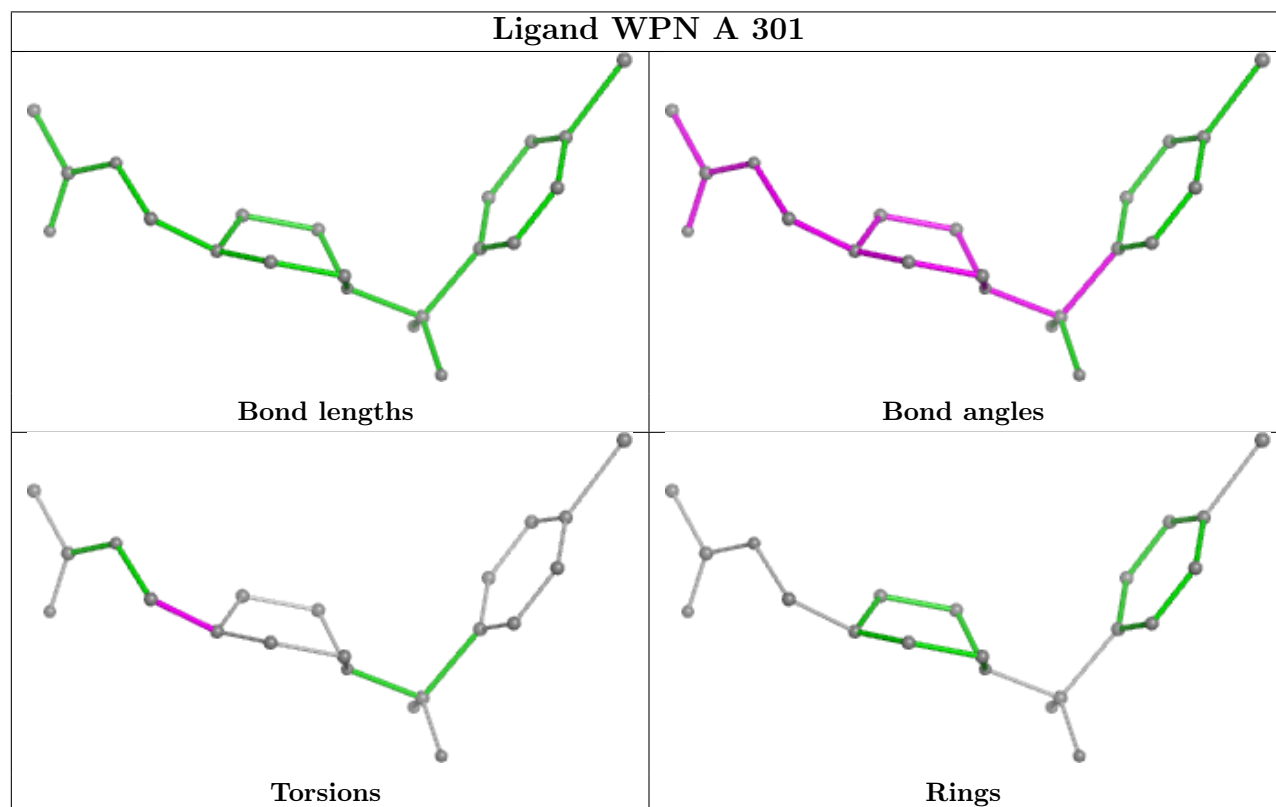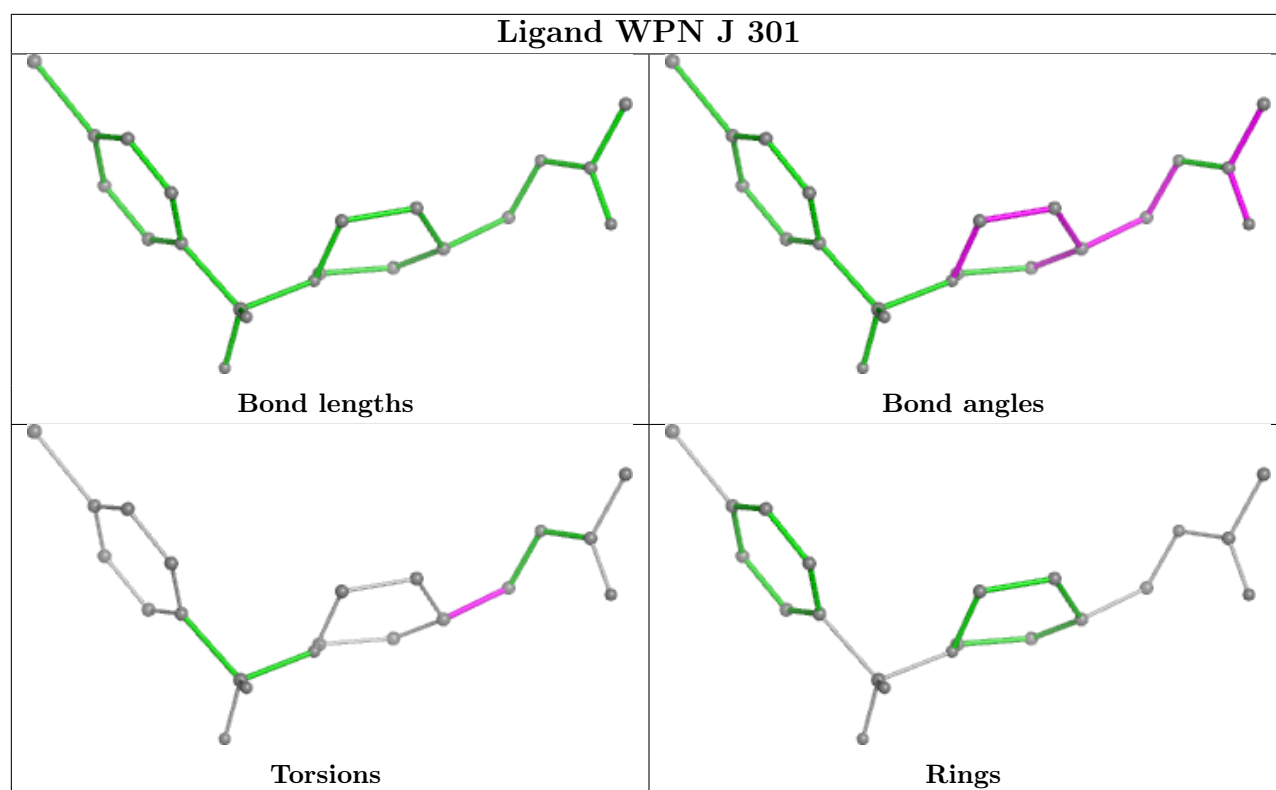
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	WPN	N1-C3-C4-C5
3	A	301	WPN	N1-C3-C4-C14
3	J	301	WPN	N1-C3-C4-C5
3	J	301	WPN	N1-C3-C4-C14

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	WPN	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 WPN J 301

Bond lengths

Bond angles

Torsions

Rings

Ligand WPN A 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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	236/236 (100%)	0.29	23 (9%)	15	12	8, 15, 55, 103	0
1	J	236/236 (100%)	0.62	29 (12%)	9	8	9, 16, 41, 67	1 (0%)
2	H	9/10 (90%)	1.09	3 (33%)	1	1	10, 11, 30, 37	0
2	S	9/10 (90%)	1.26	3 (33%)	1	1	10, 12, 29, 31	0
All	All	490/492 (99%)	0.48	58 (11%)	10	8	8, 15, 44, 103	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	ALA	6.6
1	A	-4	GLY	6.1
1	A	111	ALA	6.1
1	J	208	LEU	4.3
1	A	77	LYS	4.2
1	J	109	LYS	4.2
1	A	72	GLU	4.2
1	A	73	GLY	4.2
1	J	77	LYS	4.0
1	A	110	GLU	3.8
2	H	369	VAL	3.8
1	J	112	GLY	3.7
1	A	137	GLY	3.7
1	A	112	GLY	3.6
2	H	370	HIS	3.6
2	S	369	VAL	3.6
1	A	70	ASN	3.5
1	A	138	ASP	3.5
1	A	74	SER	3.4
1	J	-4	GLY	3.4
1	A	136	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	203	ALA	3.4
1	A	109	LYS	3.3
1	A	139	ASP	3.2
1	A	76	GLU	3.2
1	J	138	ASP	3.2
1	J	111	ALA	3.2
1	A	0	SER	3.1
1	A	69	SER	3.0
1	J	73	GLY	3.0
1	J	74	SER	3.0
1	J	205	LEU	2.9
1	J	-3	ALA	2.9
1	J	110	GLU	2.8
1	A	67	GLN	2.8
1	J	213	TYR	2.7
1	A	-1	GLY	2.7
1	A	-2	MET	2.7
2	S	361	ASP	2.6
2	S	370	HIS	2.5
1	J	231	THR	2.4
1	J	185	ASN	2.4
1	J	202	MET	2.4
1	J	211	ASP	2.4
1	A	75	GLU	2.4
1	J	71	GLU	2.3
1	A	211	ASP	2.3
1	J	137	GLY	2.3
1	J	228	THR	2.3
1	J	188	GLU	2.3
1	J	191	ILE	2.2
1	J	139	ASP	2.2
1	J	198	PHE	2.2
2	H	361	ASP	2.1
1	J	199	ASP	2.1
1	J	192	SER	2.1
1	J	204	ASP	2.0
1	J	230	TRP	2.0

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

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	SEP	S	365	10/11	0.98	0.06	5,7,9,10	0
2	SEP	H	365	10/11	0.99	0.06	7,9,10,11	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	MG	J	306	1/1	0.53	0.34	76,76,76,76	0
4	MG	A	303	1/1	0.69	0.22	68,68,68,68	0
4	MG	J	305	1/1	0.75	0.25	51,51,51,51	0
4	MG	J	304	1/1	0.77	0.14	25,25,25,25	0
4	MG	A	304	1/1	0.86	0.24	50,50,50,50	0
3	WPN	J	301	21/22	0.92	0.13	24,29,35,48	0
4	MG	A	302	1/1	0.96	0.07	32,32,32,32	0
3	WPN	A	301	21/22	0.96	0.10	21,26,32,35	0
4	MG	J	303	1/1	0.97	0.12	19,19,19,19	0
5	CL	A	305	1/1	0.99	0.07	23,23,23,23	0
5	CL	J	302	1/1	0.99	0.08	25,25,25,25	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 WPN J 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
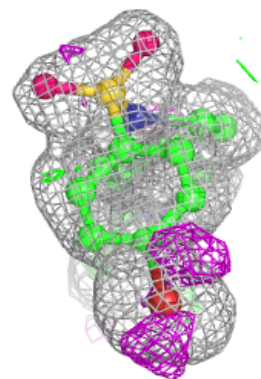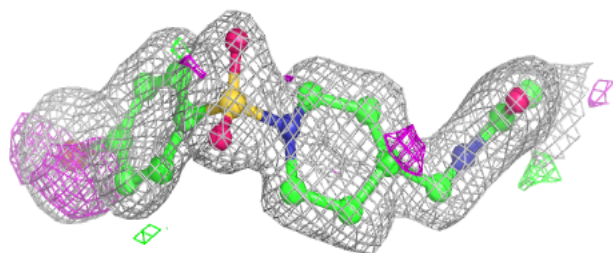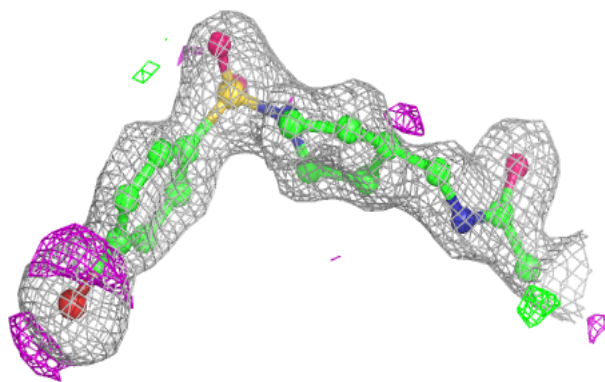
Electron density around WPN A 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
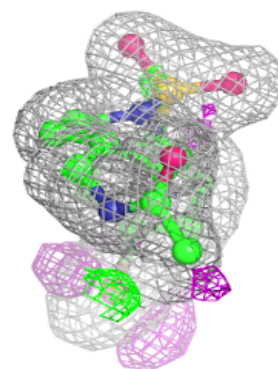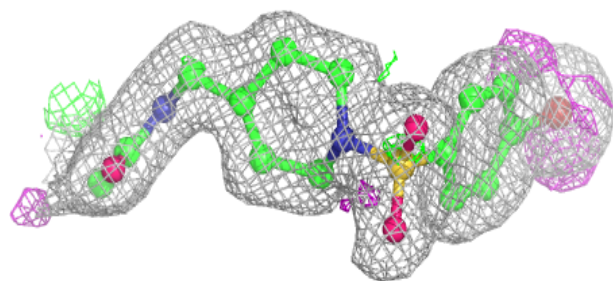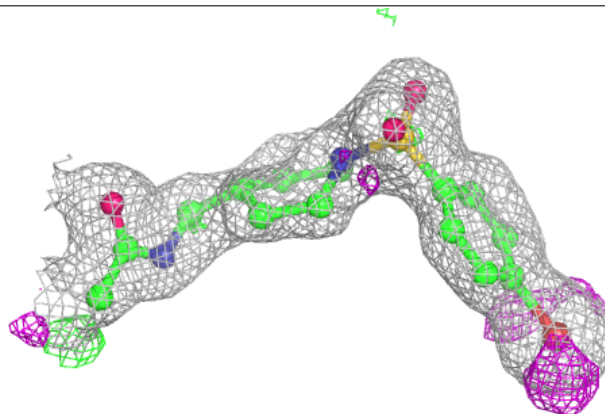
6.5 Other polymers (i)

There are no such residues in this entry.