



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2021 – 10:04 AM EST

PDB ID : 6VNL
Title : JAK2 JH1 in complex with SG3-179
Authors : Davis, R.R.; Schonbrunn, E.
Deposited on : 2020-01-29
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17
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) : 2.17

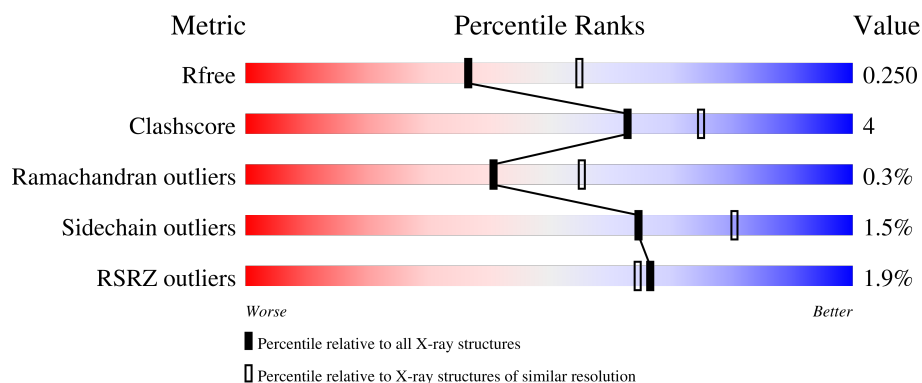
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	308	 84% 12% ..
1	B	308	 85% 11% ..
1	C	308	 81% 12% • 6%
1	D	308	 82% 11% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10106 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 Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	289	Total	C	N	O	P	S	0	0	0
			2395	1521	417	442	1	14			
1	B	298	Total	C	N	O	P	S	0	0	0
			2465	1567	427	456	1	14			
1	C	290	Total	C	N	O	P	S	0	0	0
			2402	1525	418	444	1	14			
1	A	298	Total	C	N	O	P	S	0	0	0
			2465	1567	427	456	1	14			

There are 60 discrepancies between the modelled and reference sequences:

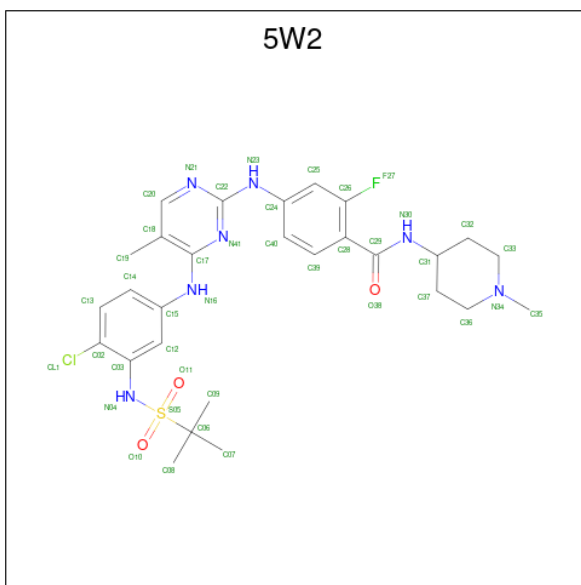
Chain	Residue	Modelled	Actual	Comment	Reference
D	825	HIS	-	expression tag	UNP O60674
D	826	HIS	-	expression tag	UNP O60674
D	827	HIS	-	expression tag	UNP O60674
D	828	HIS	-	expression tag	UNP O60674
D	829	HIS	-	expression tag	UNP O60674
D	830	HIS	-	expression tag	UNP O60674
D	831	HIS	-	expression tag	UNP O60674
D	832	HIS	-	expression tag	UNP O60674
D	833	GLU	-	expression tag	UNP O60674
D	834	ASN	-	expression tag	UNP O60674
D	835	LEU	-	expression tag	UNP O60674
D	836	TYR	-	expression tag	UNP O60674
D	837	PHE	-	expression tag	UNP O60674
D	838	GLN	-	expression tag	UNP O60674
D	839	GLY	-	expression tag	UNP O60674
B	825	HIS	-	expression tag	UNP O60674
B	826	HIS	-	expression tag	UNP O60674
B	827	HIS	-	expression tag	UNP O60674
B	828	HIS	-	expression tag	UNP O60674
B	829	HIS	-	expression tag	UNP O60674
B	830	HIS	-	expression tag	UNP O60674

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	831	HIS	-	expression tag	UNP O60674
B	832	HIS	-	expression tag	UNP O60674
B	833	GLU	-	expression tag	UNP O60674
B	834	ASN	-	expression tag	UNP O60674
B	835	LEU	-	expression tag	UNP O60674
B	836	TYR	-	expression tag	UNP O60674
B	837	PHE	-	expression tag	UNP O60674
B	838	GLN	-	expression tag	UNP O60674
B	839	GLY	-	expression tag	UNP O60674
C	825	HIS	-	expression tag	UNP O60674
C	826	HIS	-	expression tag	UNP O60674
C	827	HIS	-	expression tag	UNP O60674
C	828	HIS	-	expression tag	UNP O60674
C	829	HIS	-	expression tag	UNP O60674
C	830	HIS	-	expression tag	UNP O60674
C	831	HIS	-	expression tag	UNP O60674
C	832	HIS	-	expression tag	UNP O60674
C	833	GLU	-	expression tag	UNP O60674
C	834	ASN	-	expression tag	UNP O60674
C	835	LEU	-	expression tag	UNP O60674
C	836	TYR	-	expression tag	UNP O60674
C	837	PHE	-	expression tag	UNP O60674
C	838	GLN	-	expression tag	UNP O60674
C	839	GLY	-	expression tag	UNP O60674
A	825	HIS	-	expression tag	UNP O60674
A	826	HIS	-	expression tag	UNP O60674
A	827	HIS	-	expression tag	UNP O60674
A	828	HIS	-	expression tag	UNP O60674
A	829	HIS	-	expression tag	UNP O60674
A	830	HIS	-	expression tag	UNP O60674
A	831	HIS	-	expression tag	UNP O60674
A	832	HIS	-	expression tag	UNP O60674
A	833	GLU	-	expression tag	UNP O60674
A	834	ASN	-	expression tag	UNP O60674
A	835	LEU	-	expression tag	UNP O60674
A	836	TYR	-	expression tag	UNP O60674
A	837	PHE	-	expression tag	UNP O60674
A	838	GLN	-	expression tag	UNP O60674
A	839	GLY	-	expression tag	UNP O60674

- Molecule 2 is 4-[[4-[[3-(tert-butylsulfonylamino)-4-chloranyl-phenyl]amino]-5-methyl-pyrimidin-2-yl]amino]-2-fluoranyl- N-(1-methylpiperidin-4-yl)benzamide (three-letter code: 5W2) (formula: C₂₈H₃₅ClFN₇O₃S) (labeled as "Ligand of Interest" by depositor).



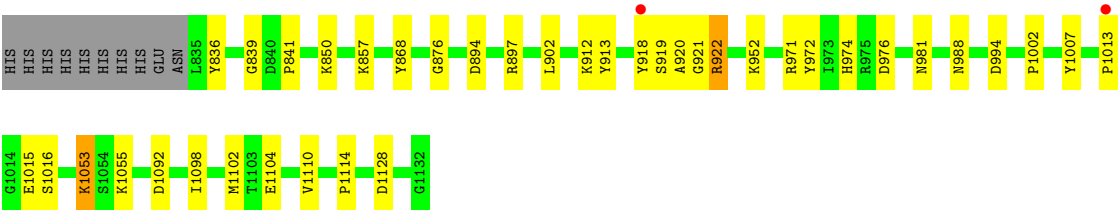
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	D	1	Total	C	Cl	F	N	O	S	0	0
			41	28	1	1	7	3	1		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			41	28	1	1	7	3	1		
2	C	1	Total	C	Cl	F	N	O	S	0	0
			41	28	1	1	7	3	1		
2	A	1	Total	C	Cl	F	N	O	S	0	0
			41	28	1	1	7	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	45	Total	O	0	0
			45	45		
3	B	49	Total	O	0	0
			49	49		
3	C	56	Total	O	0	0
			56	56		
3	A	65	Total	O	0	0
			65	65		

- Molecule 1: Tyrosine-protein kinase JAK2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.76Å 70.75Å 112.86Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	41.12 – 2.40 44.12 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.12-2.40) 99.8 (44.12-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14-3260_3260	Depositor
R, R_{free}	0.217 , 0.257 0.210 , 0.250	Depositor DCC
R_{free} test set	1600 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.110 for l,k,-h 0.018 for h,-k,-l 0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10106	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5W2, PTR

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	0.25	0/2502	0.46	1/3367 (0.0%)
1	B	0.26	0/2502	0.47	0/3367
1	C	0.26	0/2436	0.44	0/3277
1	D	0.26	0/2429	0.44	0/3267
All	All	0.26	0/9869	0.45	1/13278 (0.0%)

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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	839	GLY	C-N-CA	6.15	137.07	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1012	GLU	Peptide
1	B	840	ASP	Peptide

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	2465	0	2438	21	0
1	B	2465	0	2437	21	0
1	C	2402	0	2384	25	1
1	D	2395	0	2377	19	1
2	A	41	0	0	1	0
2	B	41	0	0	1	0
2	C	41	0	0	1	0
2	D	41	0	0	1	0
3	A	65	0	0	3	0
3	B	49	0	0	2	0
3	C	56	0	0	9	0
3	D	45	0	0	3	0
All	All	10106	0	9636	83	2

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 (83) 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:859:ASN:ND2	1:B:1015:GLU:OE2	2.17	0.78
1:C:943:LYS:NZ	3:C:1305:HOH:O	2.16	0.78
1:C:869:ASP:OD1	3:C:1301:HOH:O	2.02	0.77
1:B:869:ASP:OD1	3:B:1301:HOH:O	2.04	0.73
1:D:993:GLY:O	3:D:1301:HOH:O	2.07	0.73
1:C:976:ASP:O	1:C:981:ASN:ND2	2.21	0.73
1:A:972:TYR:O	3:A:1301:HOH:O	2.06	0.72
1:B:1015:GLU:HB2	1:A:836:TYR:HB3	1.75	0.69
1:B:1013:PRO:HD2	1:A:841:PRO:HD3	1.75	0.69
1:C:847:ARG:NH1	3:C:1307:HOH:O	2.26	0.67
1:B:974:HIS:NE2	1:B:994:ASP:O	2.27	0.67
1:C:842:THR:O	3:C:1303:HOH:O	2.11	0.67
1:C:949:ASP:OD2	3:C:1304:HOH:O	2.12	0.67
1:C:868:TYR:O	1:C:876:GLY:HA3	1.95	0.66
2:A:1201:5W2:N04	3:A:1306:HOH:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:868:TYR:O	1:D:876:GLY:HA3	1.98	0.63
1:B:868:TYR:O	1:B:876:GLY:HA3	2.00	0.61
1:C:1006:GLU:OE1	1:A:857:LYS:NZ	2.34	0.60
1:B:952:LYS:NZ	1:B:988:ASN:OD1	2.36	0.59
1:A:974:HIS:NE2	1:A:994:ASP:O	2.36	0.58
1:A:894:ASP:OD1	1:A:897:ARG:NH2	2.38	0.57
1:A:868:TYR:O	1:A:876:GLY:HA3	2.06	0.56
1:C:842:THR:O	1:C:842:THR:OG1	2.24	0.54
1:B:1013:PRO:HD2	1:A:841:PRO:CD	2.38	0.53
1:B:976:ASP:O	1:B:981:ASN:ND2	2.43	0.52
1:C:1015:GLU:OE2	3:C:1306:HOH:O	2.19	0.52
1:A:976:ASP:O	1:A:981:ASN:ND2	2.41	0.51
1:A:1053:LYS:HZ3	1:A:1053:LYS:HA	1.75	0.51
1:C:932:LEU:HD12	1:C:983:LEU:HB2	1.93	0.51
1:D:856:GLY:HA3	2:D:1201:5W2:CL1	2.48	0.50
1:C:989:ARG:NH1	3:C:1311:HOH:O	2.44	0.49
1:D:848:HIS:CG	1:D:870:PRO:HA	2.48	0.49
1:C:843:GLN:HA	3:C:1303:HOH:O	2.12	0.49
1:C:965:GLU:O	1:C:969:THR:HG23	2.13	0.49
1:C:923:ARG:HG2	1:C:924:ASN:H	1.78	0.48
1:A:902:LEU:HG	1:A:913:TYR:HB2	1.96	0.48
1:A:1104:GLU:HG2	1:A:1114:PRO:HD3	1.97	0.47
1:B:902:LEU:HG	1:B:913:TYR:HB2	1.96	0.46
1:B:977:LEU:HD23	1:B:977:LEU:HA	1.80	0.46
1:C:856:GLY:HA3	2:C:1201:5W2:CL1	2.52	0.46
1:D:989:ARG:NH1	3:D:1308:HOH:O	2.44	0.46
1:B:869:ASP:HA	3:B:1301:HOH:O	2.16	0.46
1:C:1045:TYR:OH	1:C:1060:GLU:HG3	2.16	0.46
1:A:850:LYS:NZ	3:A:1307:HOH:O	2.32	0.46
1:C:977:LEU:HG	1:C:1043:VAL:HG21	1.98	0.45
1:B:838:GLN:HB3	1:B:839:GLY:HA3	1.99	0.45
1:A:1013:PRO:HB2	1:A:1016:SER:OG	2.17	0.45
1:B:841:PRO:HB2	1:B:842:THR:H	1.56	0.45
1:B:1045:TYR:OH	1:B:1060:GLU:HG3	2.17	0.45
1:B:856:GLY:HA3	2:B:1201:5W2:CL1	2.54	0.45
1:B:965:GLU:O	1:B:969:THR:HG23	2.17	0.45
1:B:923:ARG:HA	1:B:923:ARG:HD2	1.53	0.44
1:D:977:LEU:HG	1:D:1043:VAL:HG21	1.98	0.44
1:D:918:TYR:O	1:D:919:SER:HB3	2.17	0.44
1:D:902:LEU:HG	1:D:913:TYR:HB2	1.98	0.44
1:B:852:LEU:HD11	1:B:867:ARG:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:850:LYS:HA	1:C:850:LYS:HD3	1.75	0.43
1:D:850:LYS:HA	1:D:850:LYS:HD3	1.82	0.43
1:C:974:HIS:NE2	1:C:994:ASP:O	2.49	0.43
1:D:843:GLN:NE2	3:D:1311:HOH:O	2.52	0.43
1:D:932:LEU:HD12	1:D:983:LEU:HB2	1.99	0.43
1:C:1098:ILE:HG22	1:C:1102:MET:HE3	2.00	0.43
1:A:971:ARG:NH2	1:A:1002:PRO:O	2.47	0.43
1:C:989:ARG:NH1	3:C:1314:HOH:O	2.52	0.43
1:A:1055:LYS:NZ	1:A:1092:ASP:OD2	2.52	0.43
1:A:952:LYS:NZ	1:A:988:ASN:OD1	2.52	0.42
1:D:1009:LYS:HA	1:D:1029:SER:O	2.20	0.42
1:D:1045:TYR:OH	1:D:1060:GLU:HG3	2.19	0.42
1:B:1069:LYS:HD2	1:B:1069:LYS:N	2.34	0.42
1:C:1009:LYS:HA	1:C:1029:SER:O	2.20	0.42
1:C:844:PHE:HB2	1:C:917:CYS:HB2	2.02	0.41
1:D:937:LEU:N	1:D:982:ILE:O	2.35	0.41
1:B:954:LEU:HD21	1:B:1098:ILE:HD12	2.02	0.41
1:A:922:ARG:HA	1:A:922:ARG:HD2	1.80	0.41
1:C:857:LYS:HG2	1:C:862:SER:HB2	2.02	0.41
1:D:975:ARG:NH1	1:D:997:LEU:O	2.54	0.41
1:D:919:SER:OG	1:D:920:ALA:N	2.54	0.41
1:D:965:GLU:O	1:D:969:THR:HG23	2.21	0.41
1:D:1010:VAL:O	1:D:1029:SER:HB3	2.21	0.41
1:A:1098:ILE:HG22	1:A:1102:MET:HE3	2.03	0.41
1:D:1016:SER:O	1:D:1018:ILE:HG23	2.21	0.40
1:A:918:TYR:HB2	1:A:919:SER:H	1.67	0.40
1:A:920:ALA:HA	1:A:921:GLY:HA2	1.77	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:883:LYS:NZ	1:D:1007:PTR:O2P[2_546]	1.30	0.90
1:C:883:LYS:NZ	1:C:1007:PTR:O1P[2_645]	1.30	0.90

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	295/308 (96%)	287 (97%)	8 (3%)	0	100	100
1	B	295/308 (96%)	283 (96%)	8 (3%)	4 (1%)	11	15
1	C	287/308 (93%)	283 (99%)	4 (1%)	0	100	100
1	D	286/308 (93%)	279 (98%)	7 (2%)	0	100	100
All	All	1163/1232 (94%)	1132 (97%)	27 (2%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	841	PRO
1	B	1012	GLU
1	B	1014	GLY
1	B	839	GLY

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	270/280 (96%)	264 (98%)	6 (2%)	52	71
1	B	270/280 (96%)	266 (98%)	4 (2%)	65	80
1	C	264/280 (94%)	261 (99%)	3 (1%)	73	87
1	D	263/280 (94%)	260 (99%)	3 (1%)	73	87
All	All	1067/1120 (95%)	1051 (98%)	16 (2%)	65	80

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

Mol	Chain	Res	Type
1	D	847	ARG
1	D	922	ARG
1	D	1128	ASP
1	B	923	ARG
1	B	1011	LYS
1	B	1063	ARG
1	B	1128	ASP
1	C	842	THR
1	C	872	GLN
1	C	1128	ASP
1	A	912	LYS
1	A	922	ARG
1	A	1015	GLU
1	A	1053	LYS
1	A	1110	VAL
1	A	1128	ASP

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

Mol	Chain	Res	Type
1	A	843	GLN

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
1	PTR	D	1007	1	15,16,17	1.37	1 (6%)	19,22,24	0.54	0
1	PTR	C	1007	1	15,16,17	1.26	1 (6%)	19,22,24	0.60	0
1	PTR	B	1007	1	15,16,17	1.28	1 (6%)	19,22,24	0.70	0
1	PTR	A	1007	1	15,16,17	1.38	1 (6%)	19,22,24	0.52	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
1	PTR	D	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1007	PTR	OH-CZ	-4.50	1.30	1.40
1	C	1007	PTR	OH-CZ	-4.46	1.30	1.40
1	B	1007	PTR	OH-CZ	-4.44	1.30	1.40
1	A	1007	PTR	OH-CZ	-4.30	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	1007	PTR	0	1
1	C	1007	PTR	0	1

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	5W2	A	1201	-	44,44,44	2.83	14 (31%)	63,65,65	2.37	17 (26%)
2	5W2	D	1201	-	44,44,44	2.88	14 (31%)	63,65,65	2.50	18 (28%)
2	5W2	B	1201	-	44,44,44	2.84	13 (29%)	63,65,65	2.37	20 (31%)
2	5W2	C	1201	-	44,44,44	2.84	13 (29%)	63,65,65	2.42	18 (28%)

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	5W2	A	1201	-	-	0/30/40/40	0/4/4/4
2	5W2	D	1201	-	-	11/30/40/40	0/4/4/4
2	5W2	B	1201	-	-	9/30/40/40	0/4/4/4
2	5W2	C	1201	-	-	11/30/40/40	0/4/4/4

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	5W2	C35-N34	-10.91	1.21	1.46
2	B	1201	5W2	C35-N34	-10.91	1.21	1.46
2	D	1201	5W2	C35-N34	-10.89	1.21	1.46
2	A	1201	5W2	C35-N34	-10.88	1.21	1.46
2	A	1201	5W2	S05-N04	9.09	1.72	1.59
2	B	1201	5W2	S05-N04	8.96	1.71	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	5W2	S05-N04	8.96	1.71	1.59
2	D	1201	5W2	S05-N04	8.89	1.71	1.59
2	D	1201	5W2	C17-N16	5.85	1.47	1.36
2	C	1201	5W2	C17-N16	5.76	1.46	1.36
2	A	1201	5W2	C17-N16	5.68	1.46	1.36
2	B	1201	5W2	C17-N16	5.68	1.46	1.36
2	D	1201	5W2	C29-N30	5.43	1.46	1.34
2	B	1201	5W2	C29-N30	5.30	1.45	1.34
2	C	1201	5W2	C29-N30	5.28	1.45	1.34
2	A	1201	5W2	C29-N30	5.23	1.45	1.34
2	D	1201	5W2	C22-N23	5.15	1.47	1.36
2	B	1201	5W2	C22-N23	5.06	1.46	1.36
2	C	1201	5W2	C22-N23	5.00	1.46	1.36
2	A	1201	5W2	C22-N23	4.79	1.46	1.36
2	D	1201	5W2	C32-C31	-3.37	1.44	1.52
2	D	1201	5W2	C37-C31	-3.21	1.44	1.52
2	C	1201	5W2	C32-C31	-3.07	1.44	1.52
2	B	1201	5W2	C32-C31	-3.05	1.44	1.52
2	C	1201	5W2	C37-C31	-2.98	1.45	1.52
2	B	1201	5W2	C37-C31	-2.92	1.45	1.52
2	A	1201	5W2	C32-C31	-2.81	1.45	1.52
2	D	1201	5W2	C24-N23	2.79	1.46	1.40
2	C	1201	5W2	C24-N23	2.73	1.46	1.40
2	A	1201	5W2	C37-C31	-2.72	1.45	1.52
2	B	1201	5W2	C24-N23	2.68	1.46	1.40
2	D	1201	5W2	C15-N16	2.60	1.46	1.40
2	C	1201	5W2	C15-N16	2.59	1.46	1.40
2	A	1201	5W2	C15-N16	2.54	1.46	1.40
2	A	1201	5W2	C24-N23	2.53	1.46	1.40
2	B	1201	5W2	C15-N16	2.48	1.46	1.40
2	B	1201	5W2	O38-C29	-2.23	1.18	1.23
2	C	1201	5W2	O38-C29	-2.18	1.18	1.23
2	A	1201	5W2	O38-C29	-2.17	1.18	1.23
2	D	1201	5W2	O38-C29	-2.17	1.18	1.23
2	D	1201	5W2	C02-CL1	2.16	1.78	1.73
2	B	1201	5W2	C02-CL1	2.12	1.78	1.73
2	C	1201	5W2	C02-CL1	2.12	1.78	1.73
2	D	1201	5W2	C06-S05	2.12	1.83	1.81
2	A	1201	5W2	C03-N04	2.11	1.46	1.42
2	D	1201	5W2	C03-N04	2.09	1.46	1.42
2	A	1201	5W2	C02-CL1	2.08	1.78	1.73
2	B	1201	5W2	C03-N04	2.07	1.46	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	5W2	O11-S05	2.06	1.47	1.43
2	A	1201	5W2	O10-S05	2.05	1.47	1.43
2	C	1201	5W2	C03-N04	2.04	1.46	1.42
2	C	1201	5W2	O11-S05	2.04	1.47	1.43
2	B	1201	5W2	O10-S05	2.03	1.47	1.43
2	A	1201	5W2	O11-S05	2.02	1.47	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1201	5W2	O11-S05-O10	-9.96	100.34	120.57
2	D	1201	5W2	O11-S05-O10	-9.80	100.68	120.57
2	B	1201	5W2	O11-S05-O10	-9.44	101.40	120.57
2	A	1201	5W2	O11-S05-O10	-9.34	101.62	120.57
2	B	1201	5W2	C18-C20-N21	-6.86	118.09	125.11
2	A	1201	5W2	C18-C20-N21	-6.85	118.11	125.11
2	C	1201	5W2	C18-C20-N21	-6.84	118.12	125.11
2	D	1201	5W2	C18-C20-N21	-6.67	118.29	125.11
2	D	1201	5W2	N21-C22-N41	-6.45	120.44	126.55
2	B	1201	5W2	N21-C22-N41	-6.29	120.59	126.55
2	C	1201	5W2	N21-C22-N41	-6.04	120.83	126.55
2	A	1201	5W2	N21-C22-N41	-5.99	120.87	126.55
2	D	1201	5W2	O10-S05-C06	5.40	111.94	107.60
2	C	1201	5W2	O10-S05-C06	4.94	111.56	107.60
2	A	1201	5W2	C37-C31-C32	4.48	118.59	110.82
2	D	1201	5W2	O11-S05-C06	4.30	111.05	107.60
2	A	1201	5W2	C20-N21-C22	4.26	122.31	115.88
2	B	1201	5W2	C20-N21-C22	4.26	122.30	115.88
2	D	1201	5W2	C18-C17-N41	-4.25	118.51	123.37
2	D	1201	5W2	C36-N34-C33	4.25	115.46	109.52
2	D	1201	5W2	C20-N21-C22	4.21	122.23	115.88
2	C	1201	5W2	C18-C17-N41	-4.18	118.60	123.37
2	C	1201	5W2	C20-N21-C22	4.17	122.17	115.88
2	B	1201	5W2	C18-C17-N41	-4.07	118.72	123.37
2	A	1201	5W2	C18-C17-N41	-3.94	118.87	123.37
2	A	1201	5W2	C36-C37-C31	3.93	117.40	110.50
2	B	1201	5W2	O10-S05-C06	3.90	110.73	107.60
2	D	1201	5W2	C37-C36-N34	3.80	116.32	111.22
2	B	1201	5W2	C31-N30-C29	-3.72	117.40	122.55
2	C	1201	5W2	C06-S05-N04	3.59	113.92	107.08
2	A	1201	5W2	C33-C32-C31	3.55	116.73	110.50
2	A	1201	5W2	O10-S05-C06	3.54	110.44	107.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	5W2	C28-C29-N30	3.24	122.80	116.80
2	C	1201	5W2	C25-C26-C28	-3.23	120.08	123.53
2	C	1201	5W2	O11-S05-C06	3.23	110.19	107.60
2	A	1201	5W2	C25-C26-C28	-3.18	120.13	123.53
2	B	1201	5W2	O11-S05-C06	3.15	110.13	107.60
2	D	1201	5W2	C15-N16-C17	-3.09	121.61	129.39
2	C	1201	5W2	C31-N30-C29	-3.08	118.28	122.55
2	D	1201	5W2	C06-S05-N04	3.06	112.92	107.08
2	B	1201	5W2	C25-C26-C28	-3.03	120.30	123.53
2	B	1201	5W2	N16-C17-N41	3.00	123.59	119.12
2	C	1201	5W2	C39-C28-C26	2.92	119.98	116.67
2	A	1201	5W2	C39-C28-C26	2.91	119.97	116.67
2	D	1201	5W2	C25-C26-C28	-2.88	120.46	123.53
2	C	1201	5W2	C02-C03-N04	-2.73	118.20	120.74
2	A	1201	5W2	C31-N30-C29	-2.58	118.97	122.55
2	A	1201	5W2	O11-S05-C06	2.54	109.64	107.60
2	C	1201	5W2	C15-N16-C17	-2.52	123.05	129.39
2	D	1201	5W2	C39-C28-C26	2.51	119.52	116.67
2	B	1201	5W2	C39-C28-C26	2.50	119.51	116.67
2	D	1201	5W2	C02-C03-N04	-2.48	118.43	120.74
2	C	1201	5W2	C28-C29-N30	2.44	121.31	116.80
2	A	1201	5W2	C06-S05-N04	2.43	111.72	107.08
2	A	1201	5W2	N16-C17-N41	2.42	122.72	119.12
2	B	1201	5W2	C06-S05-N04	2.39	111.65	107.08
2	B	1201	5W2	C33-C32-C31	2.39	114.69	110.50
2	A	1201	5W2	C28-C29-N30	2.39	121.22	116.80
2	C	1201	5W2	C07-C06-S05	2.27	111.18	107.86
2	B	1201	5W2	C37-C31-C32	2.26	114.74	110.82
2	B	1201	5W2	C19-C18-C17	-2.26	120.00	121.97
2	D	1201	5W2	C36-C37-C31	2.22	114.39	110.50
2	D	1201	5W2	C22-N41-C17	2.20	121.43	116.39
2	A	1201	5W2	C15-N16-C17	-2.20	123.86	129.39
2	B	1201	5W2	O38-C29-N30	-2.19	118.42	122.45
2	C	1201	5W2	N16-C17-N41	2.16	122.34	119.12
2	D	1201	5W2	C28-C29-N30	2.13	120.74	116.80
2	B	1201	5W2	C36-C37-C31	2.07	114.13	110.50
2	B	1201	5W2	C22-N41-C17	2.07	121.12	116.39
2	B	1201	5W2	O10-S05-N04	2.07	113.16	109.42
2	D	1201	5W2	C12-C03-C02	2.06	120.31	118.17
2	C	1201	5W2	C22-N41-C17	2.06	121.10	116.39
2	C	1201	5W2	C12-C03-C02	2.00	120.25	118.17

There are no chirality outliers.

All (31) torsion outliers are listed below:

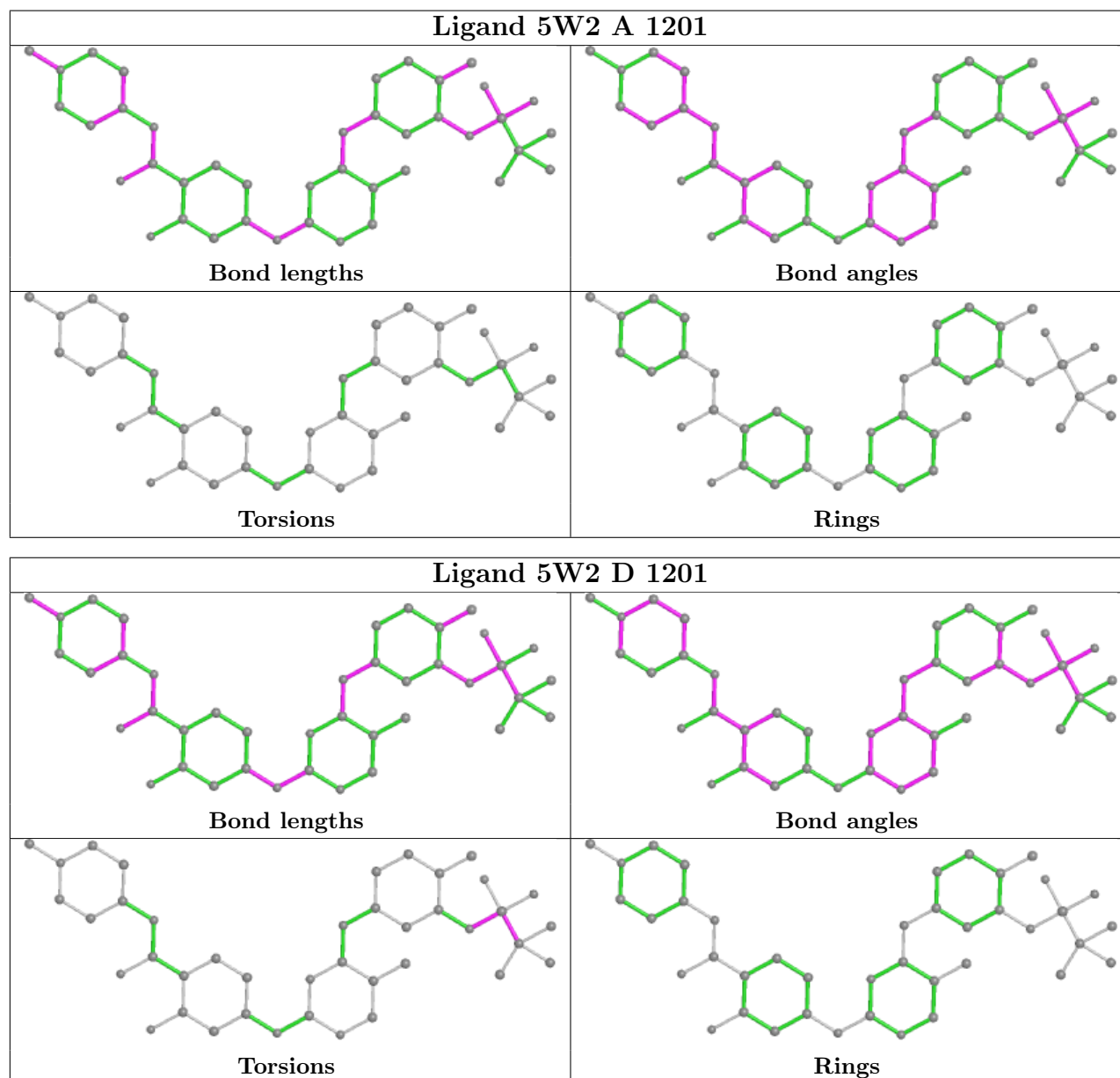
Mol	Chain	Res	Type	Atoms
2	D	1201	5W2	C03-N04-S05-C06
2	D	1201	5W2	C03-N04-S05-O10
2	D	1201	5W2	C07-C06-S05-N04
2	D	1201	5W2	C08-C06-S05-N04
2	D	1201	5W2	C09-C06-S05-N04
2	D	1201	5W2	C07-C06-S05-O11
2	C	1201	5W2	C03-N04-S05-C06
2	C	1201	5W2	C03-N04-S05-O10
2	C	1201	5W2	C07-C06-S05-N04
2	C	1201	5W2	C08-C06-S05-N04
2	C	1201	5W2	C09-C06-S05-N04
2	D	1201	5W2	C08-C06-S05-O11
2	D	1201	5W2	C09-C06-S05-O11
2	B	1201	5W2	C07-C06-S05-O10
2	B	1201	5W2	C08-C06-S05-O10
2	B	1201	5W2	C09-C06-S05-O10
2	C	1201	5W2	C07-C06-S05-O11
2	C	1201	5W2	C08-C06-S05-O11
2	C	1201	5W2	C09-C06-S05-O11
2	D	1201	5W2	C08-C06-S05-O10
2	D	1201	5W2	C09-C06-S05-O10
2	D	1201	5W2	C07-C06-S05-O10
2	B	1201	5W2	C09-C06-S05-N04
2	B	1201	5W2	C07-C06-S05-N04
2	B	1201	5W2	C08-C06-S05-N04
2	C	1201	5W2	C08-C06-S05-O10
2	B	1201	5W2	C08-C06-S05-O11
2	B	1201	5W2	C09-C06-S05-O11
2	C	1201	5W2	C07-C06-S05-O10
2	C	1201	5W2	C09-C06-S05-O10
2	B	1201	5W2	C07-C06-S05-O11

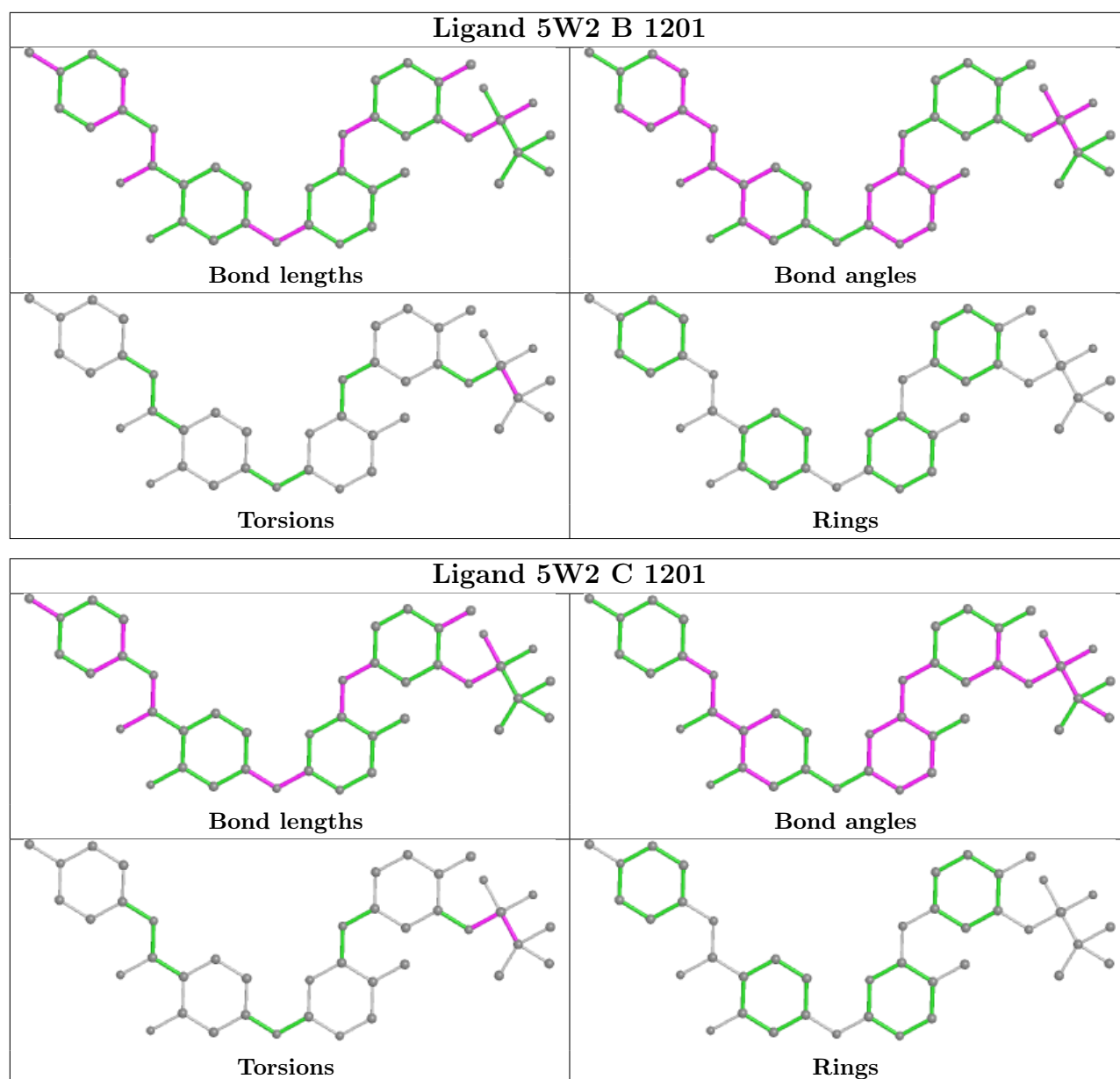
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	5W2	1	0
2	D	1201	5W2	1	0
2	B	1201	5W2	1	0
2	C	1201	5W2	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	297/308 (96%)	-0.06	2 (0%) 87 86	38, 57, 90, 118	0
1	B	297/308 (96%)	-0.05	4 (1%) 77 75	41, 57, 94, 120	0
1	C	289/308 (93%)	0.01	9 (3%) 49 47	36, 56, 99, 127	0
1	D	288/308 (93%)	0.02	7 (2%) 59 57	38, 55, 99, 127	0
All	All	1171/1232 (95%)	-0.02	22 (1%) 66 64	36, 56, 97, 127	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	920	ALA	8.3
1	B	836	TYR	5.2
1	D	920	ALA	5.1
1	D	921	GLY	4.6
1	D	922	ARG	4.4
1	B	835	LEU	4.1
1	B	1013	PRO	2.8
1	C	922	ARG	2.8
1	A	1013	PRO	2.7
1	C	886	HIS	2.7
1	B	921	GLY	2.5
1	A	918	TYR	2.5
1	C	921	GLY	2.5
1	C	859	ASN	2.5
1	C	1053	LYS	2.4
1	C	1074	ILE	2.4
1	D	1053	LYS	2.3
1	C	1072	GLN	2.1
1	D	918	TYR	2.1
1	C	1083	LYS	2.1
1	D	1070	GLN	2.0
1	D	860	PHE	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(\AA^2)	Q<0.9
1	PTR	A	1007	16/17	0.91	0.15	60,86,128,131	0
1	PTR	B	1007	16/17	0.94	0.14	57,77,114,122	0
1	PTR	C	1007	16/17	0.95	0.13	45,66,93,115	0
1	PTR	D	1007	16/17	0.97	0.13	37,64,88,119	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

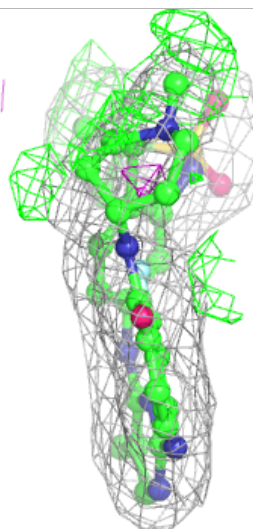
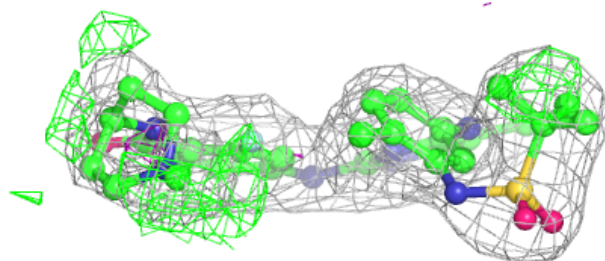
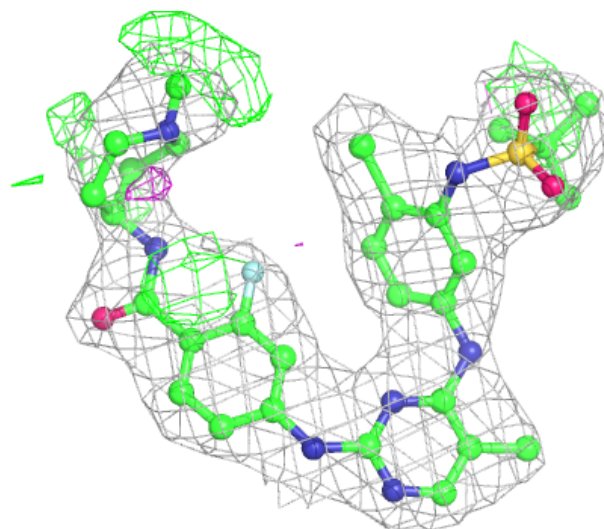
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	5W2	D	1201	41/41	0.94	0.15	44,63,91,107	0
2	5W2	B	1201	41/41	0.97	0.16	38,55,86,96	0
2	5W2	C	1201	41/41	0.97	0.16	40,60,104,115	0
2	5W2	A	1201	41/41	0.97	0.18	41,65,86,90	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.

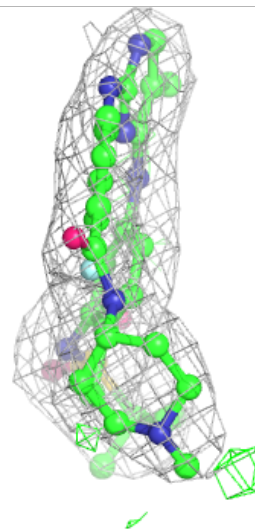
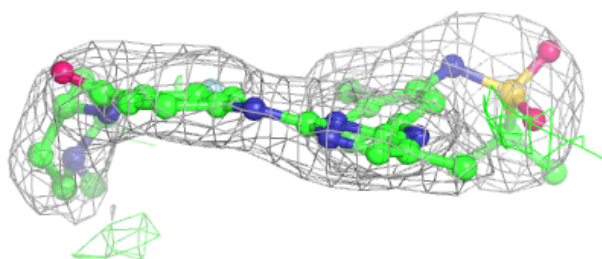
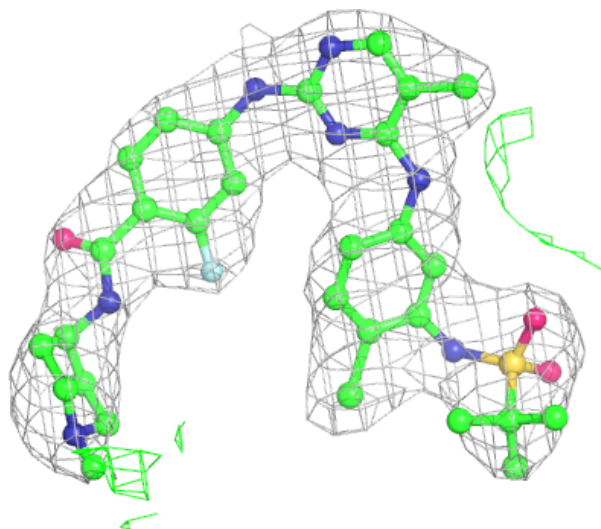
Electron density around 5W2 D 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



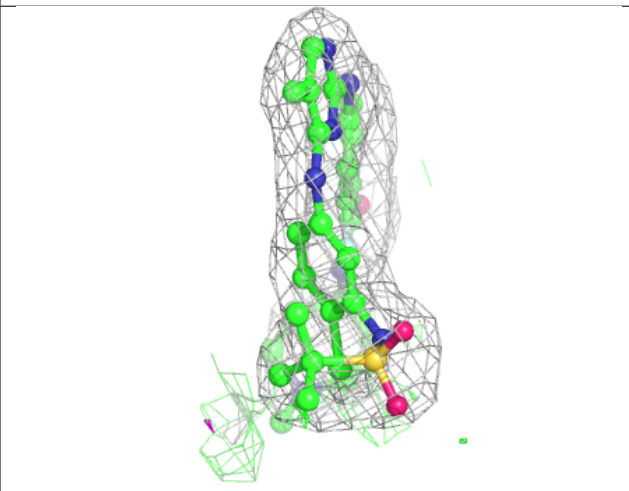
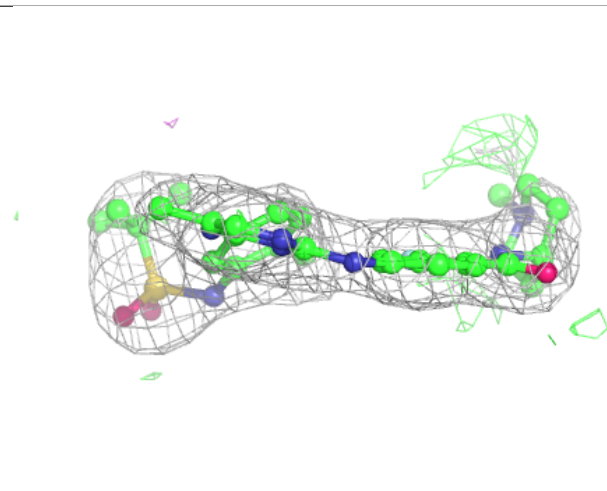
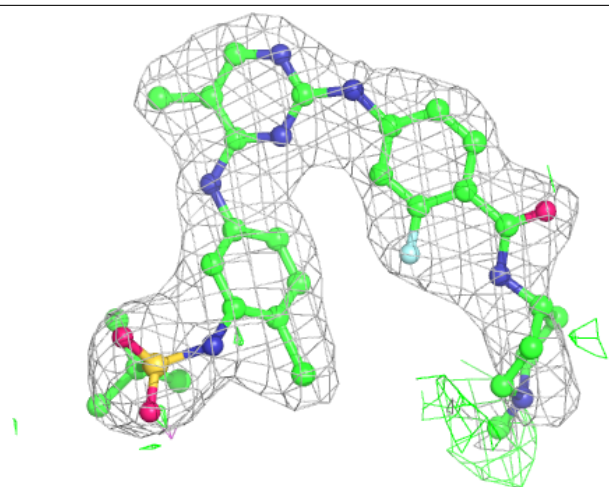
Electron density around 5W2 B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



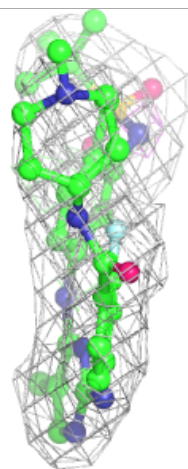
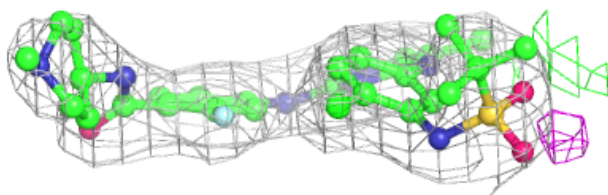
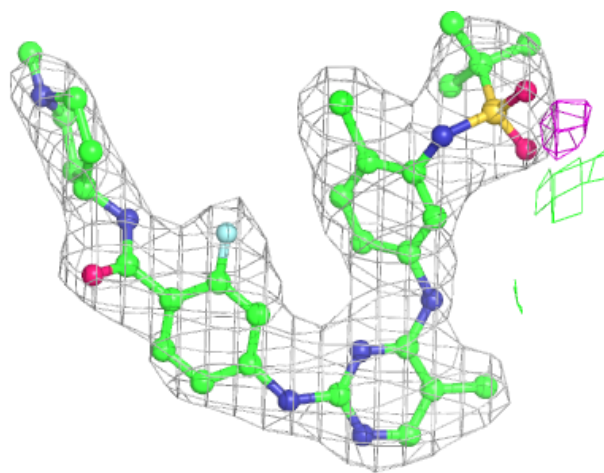
Electron density around 5W2 C 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5W2 A 1201:

$2mF_o-DF_c$ (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.