



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:28 PM UTC

PDB ID : 5WNF / pdb_00005wnf
Title : X-RAY CO-STRUCTURE OF RHO-ASSOCIATED PROTEIN KINASE (ROCK1) WITH A HIGHLY SELECTIVE INHIBITOR
Authors : Li, X.
Deposited on : 2017-07-31
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

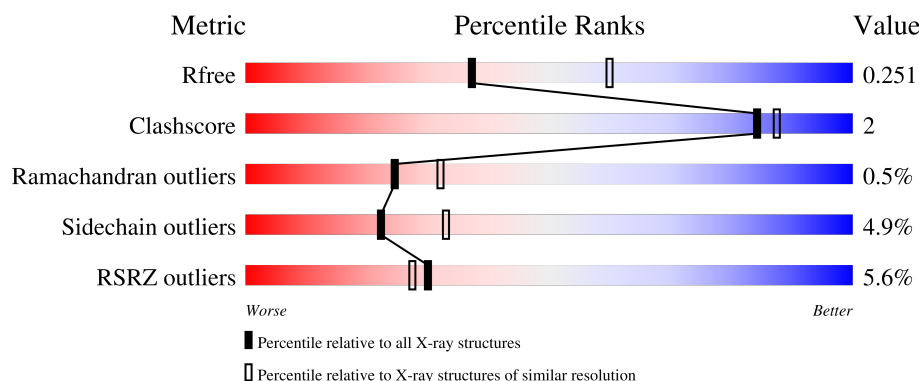
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	415	2% 86% 9% 5%
1	B	415	8% 76% 9% 14%
1	C	415	7% 81% 12% 7%
1	D	415	3% 83% 12% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12844 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.

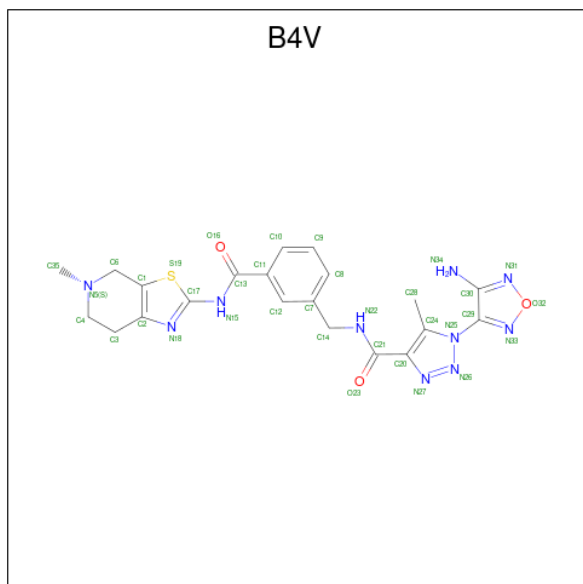
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3214	2055	530	608	21			
1	B	358	Total	C	N	O	S	0	0	0
			2934	1895	478	540	21			
1	C	386	Total	C	N	O	S	0	0	0
			3152	2022	520	588	22			
1	D	396	Total	C	N	O	S	0	1	0
			3230	2063	534	612	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q13464
A	2	SER	-	expression tag	UNP Q13464
A	3	LEU	-	expression tag	UNP Q13464
A	4	HIS	-	expression tag	UNP Q13464
A	5	MET	-	expression tag	UNP Q13464
B	1	GLY	-	expression tag	UNP Q13464
B	2	SER	-	expression tag	UNP Q13464
B	3	LEU	-	expression tag	UNP Q13464
B	4	HIS	-	expression tag	UNP Q13464
B	5	MET	-	expression tag	UNP Q13464
C	1	GLY	-	expression tag	UNP Q13464
C	2	SER	-	expression tag	UNP Q13464
C	3	LEU	-	expression tag	UNP Q13464
C	4	HIS	-	expression tag	UNP Q13464
C	5	MET	-	expression tag	UNP Q13464
D	1	GLY	-	expression tag	UNP Q13464
D	2	SER	-	expression tag	UNP Q13464
D	3	LEU	-	expression tag	UNP Q13464
D	4	HIS	-	expression tag	UNP Q13464
D	5	MET	-	expression tag	UNP Q13464

- Molecule 2 is 1-(4-amino-1,2,5-oxadiazol-3-yl)-5-methyl-N-({3-[(5-methyl-4,5,6,7-tetrahydro [1,3]thiazolo[5,4-c]pyridin-2-yl)carbamoyl]phenyl}methyl)-1H-1,2,3-triazole-4-carboxamide (CCD ID: B4V) (formula: $C_{21}H_{22}N_{10}O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	21	10	3	1		
2	B	1	Total	C	N	O	S	0	0
			35	21	10	3	1		
2	C	1	Total	C	N	O	S	0	0
			35	21	10	3	1		
2	D	1	Total	C	N	O	S	0	0
			35	21	10	3	1		

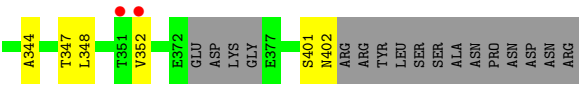
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



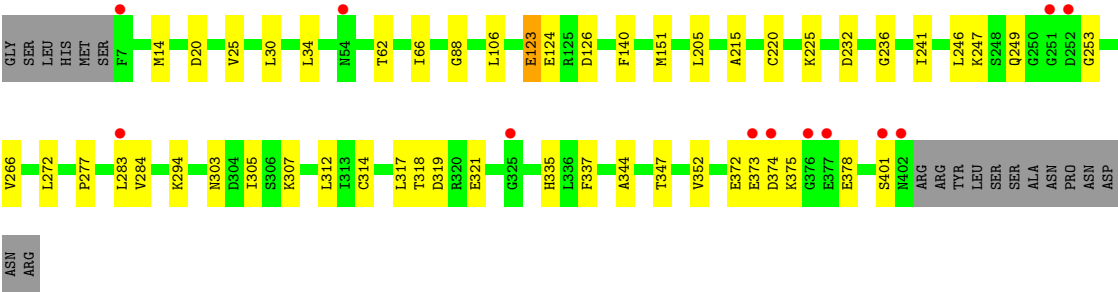
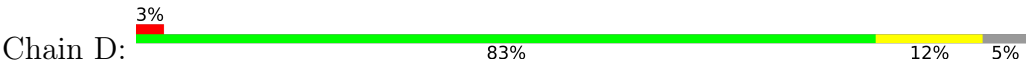
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	17	Total	O	0	0
			17	17		
4	C	25	Total	O	0	0
			25	25		
4	D	67	Total	O	0	0
			67	67		



● Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.91Å 82.29Å 169.74Å 90.00° 115.87° 90.00°	Depositor
Resolution (Å)	24.70 – 2.45 24.70 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.70-2.45) 99.4 (24.70-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.236 , 0.247 0.236 , 0.251	Depositor DCC
R_{free} test set	3641 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12844	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: B4V, GOL

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	0.73	0/3291	1.29	5/4446 (0.1%)
1	B	0.73	0/3004	1.30	5/4052 (0.1%)
1	C	0.73	0/3227	1.30	11/4357 (0.3%)
1	D	0.74	0/3307	1.29	5/4468 (0.1%)
All	All	0.73	0/12829	1.30	26/17323 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	236	GLY	N-CA-C	6.19	117.81	111.56
1	A	292	ASN	CA-CB-CG	6.11	118.71	112.60
1	D	319	ASP	CA-C-N	6.07	129.92	120.82
1	D	319	ASP	C-N-CA	6.07	129.92	120.82
1	C	306	SER	CA-C-N	5.82	128.07	120.28
1	C	306	SER	C-N-CA	5.82	128.07	120.28
1	C	401	SER	CA-C-N	5.69	131.95	121.70
1	C	401	SER	C-N-CA	5.69	131.95	121.70
1	C	236	GLY	CA-C-N	5.53	128.35	120.49
1	C	236	GLY	C-N-CA	5.53	128.35	120.49
1	A	232	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	195	ILE	N-CA-C	-5.51	100.48	108.36
1	C	145	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	113	ILE	CA-C-N	5.43	127.87	120.54
1	B	113	ILE	C-N-CA	5.43	127.87	120.54
1	A	145	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	16	ASN	CA-C-N	5.28	128.34	120.31
1	C	16	ASN	C-N-CA	5.28	128.34	120.31
1	C	13	LYS	CA-C-N	5.21	127.69	120.29
1	C	13	LYS	C-N-CA	5.21	127.69	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	208	LYS	CB-CG-CD	5.12	123.07	111.30
1	A	195	ILE	N-CA-CB	5.07	117.08	110.99
1	D	20	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	232	ASP	CA-CB-CG	5.02	117.62	112.60
1	B	20	ASP	CA-CB-CG	5.01	117.61	112.60

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	3214	0	3114	16	0
1	B	2934	0	2867	20	0
1	C	3152	0	3062	16	0
1	D	3230	0	3125	16	0
2	A	35	0	0	0	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	A	12	0	16	0	0
4	A	53	0	0	0	0
4	B	17	0	0	0	0
4	C	25	0	0	0	0
4	D	67	0	0	0	0
All	All	12844	0	12184	58	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 (58) 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:223:MET:HB3	1:B:227:GLY:HA2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:MET:HE1	1:D:66:ILE:HG12	1.70	0.72
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.76	0.66
1:B:297:LEU:HD22	1:B:317:LEU:HD22	1.76	0.66
1:B:278:PHE:HZ	1:B:317:LEU:HD21	1.61	0.66
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.78	0.64
1:D:335:HIS:HD2	1:D:337:PHE:H	1.49	0.60
1:A:335:HIS:HD2	1:A:337:PHE:H	1.50	0.59
1:A:272:LEU:HB3	1:A:305:ILE:HG21	1.83	0.59
1:C:66:ILE:HD11	1:D:25:VAL:HG21	1.85	0.59
1:C:335:HIS:HD2	1:C:337:PHE:H	1.52	0.58
1:A:205:LEU:HD12	1:A:215:ALA:HB2	1.86	0.58
1:C:205:LEU:HD12	1:C:215:ALA:HB2	1.86	0.57
1:B:335:HIS:HD2	1:B:337:PHE:H	1.52	0.56
1:D:140:PHE:O	1:D:401:SER:HB2	2.05	0.55
1:C:66:ILE:HG12	1:D:14:MET:HE1	1.88	0.55
1:B:205:LEU:HD12	1:B:215:ALA:HB2	1.91	0.53
1:D:272:LEU:HB3	1:D:305:ILE:HD12	1.93	0.49
1:D:205:LEU:HD12	1:D:215:ALA:HB2	1.95	0.49
1:A:124:GLU:HG2	1:A:151:MET:HE1	1.95	0.49
1:C:61:ASP:O	1:C:65:LYS:HG2	2.12	0.48
1:B:124:GLU:HG2	1:B:151:MET:HE1	1.96	0.48
1:D:124:GLU:HG2	1:D:151:MET:HE1	1.96	0.48
1:A:344:ALA:HB3	1:A:347:THR:HG22	1.97	0.47
1:C:124:GLU:HG2	1:C:151:MET:HE1	1.96	0.46
1:A:196:HIS:HD2	1:A:198:ASP:H	1.64	0.46
1:A:66:ILE:HD11	1:B:25:VAL:HG11	1.98	0.46
1:A:66:ILE:HG12	1:B:14:MET:HE1	1.98	0.46
1:B:344:ALA:HB3	1:B:347:THR:HG22	1.98	0.45
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.99	0.45
1:A:66:ILE:CD1	1:B:25:VAL:HG11	2.47	0.45
1:D:241:ILE:HD13	1:D:246:LEU:HD13	1.98	0.45
1:A:272:LEU:HB3	1:A:305:ILE:CG2	2.46	0.45
1:C:344:ALA:HB3	1:C:347:THR:HG22	1.98	0.45
1:D:344:ALA:HB3	1:D:347:THR:HG22	1.98	0.45
1:D:123:GLU:HG3	1:D:220:CYS:O	2.18	0.44
1:C:266:VAL:HG13	1:C:277:PRO:HD2	1.99	0.43
1:A:205:LEU:HD12	1:A:215:ALA:CB	2.49	0.43
1:A:266:VAL:HG13	1:A:277:PRO:HD2	2.00	0.43
1:D:314:CYS:O	1:D:318:THR:HG23	2.19	0.43
1:D:266:VAL:HG13	1:D:277:PRO:HD2	2.00	0.43
1:B:266:VAL:HG13	1:B:277:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:HE2	1:C:154:GLU:HB3	1.85	0.42
1:B:193:GLY:HA2	1:B:223:MET:HE2	2.01	0.42
1:D:205:LEU:HD12	1:D:215:ALA:CB	2.49	0.42
1:C:205:LEU:HD12	1:C:215:ALA:CB	2.49	0.42
1:B:7:PHE:HA	1:B:8:GLU:HA	1.75	0.41
1:A:241:ILE:HD11	1:A:245:VAL:HG22	2.02	0.41
1:D:88:GLY:HA3	1:D:106:LEU:O	2.20	0.41
1:B:205:LEU:HD12	1:B:215:ALA:CB	2.50	0.41
1:B:223:MET:HA	1:B:229:VAL:HG22	2.01	0.41
1:C:129:ALA:HB2	1:C:139:LEU:HD23	2.03	0.41
1:C:184:LEU:HD12	1:C:348:LEU:HD23	2.03	0.41
1:B:129:ALA:HB2	1:B:139:LEU:HD23	2.03	0.40
1:C:38:VAL:HG21	1:C:63:ILE:HG13	2.03	0.40
1:C:225:LYS:H	1:C:225:LYS:HG2	1.52	0.40
1:A:14:MET:HE1	1:B:66:ILE:HG12	2.04	0.40
1:B:88:GLY:HA3	1:B:106:LEU:O	2.22	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	393/415 (95%)	384 (98%)	8 (2%)	1 (0%)	36	45
1	B	346/415 (83%)	337 (97%)	6 (2%)	3 (1%)	14	17
1	C	378/415 (91%)	371 (98%)	7 (2%)	0	100	100
1	D	395/415 (95%)	382 (97%)	9 (2%)	4 (1%)	12	14
All	All	1512/1660 (91%)	1474 (98%)	30 (2%)	8 (0%)	24	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	ASN
1	B	223	MET
1	B	227	GLY
1	D	373	GLU
1	D	249	GLN
1	D	372	GLU
1	A	378	GLU
1	D	253	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	351/369 (95%)	335 (95%)	16 (5%)	24	36
1	B	322/369 (87%)	309 (96%)	13 (4%)	28	41
1	C	345/369 (94%)	325 (94%)	20 (6%)	18	27
1	D	353/369 (96%)	335 (95%)	18 (5%)	21	31
All	All	1371/1476 (93%)	1304 (95%)	67 (5%)	22	33

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	48	LYS
1	A	62	THR
1	A	126	ASP
1	A	225	LYS
1	A	229	VAL
1	A	245	VAL
1	A	294	LYS
1	A	303	ASN
1	A	307	LYS
1	A	312	LEU
1	A	320	ARG
1	A	352	VAL
1	A	372	GLU

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Mol	Chain	Res	Type
1	A	375	LYS
1	A	380	THR
1	B	34	LEU
1	B	62	THR
1	B	126	ASP
1	B	208	LYS
1	B	221	MET
1	B	224	ASN
1	B	226	GLU
1	B	294	LYS
1	B	307	LYS
1	B	312	LEU
1	B	317	LEU
1	B	329	VAL
1	B	352	VAL
1	C	5	MET
1	C	8	GLU
1	C	34	LEU
1	C	48	LYS
1	C	62	THR
1	C	126	ASP
1	C	212	LEU
1	C	221	MET
1	C	225	LYS
1	C	229	VAL
1	C	230	ARG
1	C	246	LEU
1	C	254	TYR
1	C	294	LYS
1	C	299	PHE
1	C	305	ILE
1	C	307	LYS
1	C	312	LEU
1	C	352	VAL
1	C	402	ASN
1	D	34	LEU
1	D	62	THR
1	D	123	GLU
1	D	126	ASP
1	D	225	LYS
1	D	247	LYS
1	D	283	LEU

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Mol	Chain	Res	Type
1	D	284	VAL
1	D	294	LYS
1	D	303	ASN
1	D	307	LYS
1	D	312	LEU
1	D	317	LEU
1	D	321	GLU
1	D	352	VAL
1	D	374	ASP
1	D	375	LYS
1	D	378	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	91	GLN
1	A	196	HIS
1	A	292	ASN
1	A	295	ASN
1	A	303	ASN
1	A	335	HIS
1	A	342	GLN
1	B	91	GLN
1	B	190	HIS
1	B	335	HIS
1	B	342	GLN
1	C	4	HIS
1	C	91	GLN
1	C	190	HIS
1	C	196	HIS
1	C	335	HIS
1	C	342	GLN
1	D	91	GLN
1	D	190	HIS
1	D	196	HIS
1	D	211	HIS
1	D	303	ASN
1	D	335	HIS
1	D	342	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](#)

6 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	B4V	B	900	-	37,39,39	1.31	4 (10%)	47,56,56	2.75	17 (36%)
3	GOL	A	503	-	5,5,5	0.06	0	5,5,5	0.21	0
2	B4V	D	900	-	37,39,39	1.34	5 (13%)	47,56,56	2.65	16 (34%)
3	GOL	A	502	-	5,5,5	0.06	0	5,5,5	0.27	0
2	B4V	A	501	-	37,39,39	1.30	4 (10%)	47,56,56	2.68	13 (27%)
2	B4V	C	900	-	37,39,39	1.28	4 (10%)	47,56,56	2.79	15 (31%)

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	B4V	B	900	-	-	2/20/30/30	0/5/5/5
3	GOL	A	503	-	-	0/4/4/4	-
2	B4V	D	900	-	-	1/20/30/30	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	502	-	-	0/4/4/4	-
2	B4V	A	501	-	-	1/20/30/30	0/5/5/5
2	B4V	C	900	-	-	1/20/30/30	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	B4V	C6-N5	3.58	1.49	1.46
2	B	900	B4V	C6-N5	3.21	1.48	1.46
2	A	501	B4V	C6-N5	3.04	1.48	1.46
2	C	900	B4V	C6-N5	2.91	1.48	1.46
2	C	900	B4V	N25-N26	2.80	1.41	1.37
2	A	501	B4V	N25-N26	2.70	1.41	1.37
2	D	900	B4V	N25-N26	2.67	1.40	1.37
2	A	501	B4V	C2-N18	-2.59	1.32	1.38
2	B	900	B4V	N25-N26	2.57	1.40	1.37
2	B	900	B4V	C2-N18	-2.54	1.33	1.38
2	D	900	B4V	C2-N18	-2.47	1.33	1.38
2	C	900	B4V	C2-N18	-2.29	1.33	1.38
2	B	900	B4V	C30-N34	2.21	1.39	1.34
2	A	501	B4V	C30-N34	2.19	1.39	1.34
2	C	900	B4V	C30-N34	2.16	1.39	1.34
2	D	900	B4V	C30-N34	2.16	1.39	1.34
2	D	900	B4V	C17-S19	-2.13	1.70	1.73

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	B4V	C24-N25-N26	-8.86	106.21	111.10
2	D	900	B4V	C24-N25-N26	-8.86	106.21	111.10
2	A	501	B4V	C24-N25-N26	-8.82	106.24	111.10
2	B	900	B4V	C24-N25-N26	-8.74	106.28	111.10
2	C	900	B4V	C3-C4-N5	7.40	117.66	110.71
2	A	501	B4V	C3-C4-N5	7.00	117.28	110.71
2	B	900	B4V	S19-C17-N18	-6.91	109.59	115.78
2	C	900	B4V	S19-C17-N18	-6.74	109.75	115.78
2	A	501	B4V	S19-C17-N18	-6.58	109.89	115.78
2	B	900	B4V	C3-C4-N5	6.41	116.73	110.71
2	D	900	B4V	S19-C17-N18	-6.35	110.10	115.78
2	D	900	B4V	C3-C4-N5	5.71	116.07	110.71
2	B	900	B4V	C17-N18-C2	5.66	118.20	110.09
2	C	900	B4V	C17-N18-C2	5.54	118.03	110.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B4V	C17-N18-C2	5.42	117.84	110.09
2	C	900	B4V	C6-C1-S19	5.26	126.67	121.91
2	D	900	B4V	C17-N18-C2	5.05	117.32	110.09
2	B	900	B4V	C6-C1-S19	4.77	126.22	121.91
2	D	900	B4V	O32-N33-C29	4.64	109.01	104.61
2	A	501	B4V	C6-C1-S19	4.63	126.09	121.91
2	C	900	B4V	O32-N33-C29	4.43	108.81	104.61
2	B	900	B4V	O32-N33-C29	4.36	108.74	104.61
2	D	900	B4V	C6-C1-S19	4.18	125.68	121.91
2	A	501	B4V	O32-N33-C29	4.18	108.57	104.61
2	D	900	B4V	C1-S19-C17	4.01	90.75	88.76
2	B	900	B4V	C1-S19-C17	3.79	90.64	88.76
2	D	900	B4V	N33-O32-N31	-3.70	106.91	111.49
2	C	900	B4V	C20-C24-N25	3.58	106.64	103.76
2	B	900	B4V	N33-O32-N31	-3.54	107.10	111.49
2	D	900	B4V	C20-C24-N25	3.46	106.55	103.76
2	A	501	B4V	C1-S19-C17	3.46	90.48	88.76
2	C	900	B4V	N33-O32-N31	-3.43	107.23	111.49
2	B	900	B4V	C1-C6-N5	3.41	112.08	109.49
2	A	501	B4V	N33-O32-N31	-3.34	107.35	111.49
2	B	900	B4V	C20-C24-N25	3.28	106.40	103.76
2	C	900	B4V	C1-S19-C17	3.28	90.39	88.76
2	B	900	B4V	N25-C29-N33	3.24	126.53	119.80
2	D	900	B4V	N25-C29-N33	3.20	126.46	119.80
2	C	900	B4V	N25-C29-N33	3.11	126.26	119.80
2	A	501	B4V	C20-C24-N25	3.11	106.26	103.76
2	A	501	B4V	N25-C29-N33	3.10	126.25	119.80
2	D	900	B4V	O32-N31-C30	2.95	108.51	105.47
2	A	501	B4V	N25-N26-N27	2.94	109.24	106.63
2	D	900	B4V	C1-C6-N5	2.79	111.61	109.49
2	C	900	B4V	N25-N26-N27	2.75	109.07	106.63
2	B	900	B4V	N25-N26-N27	2.74	109.07	106.63
2	B	900	B4V	O32-N31-C30	2.74	108.29	105.47
2	D	900	B4V	N25-N26-N27	2.69	109.02	106.63
2	A	501	B4V	O32-N31-C30	2.61	108.16	105.47
2	C	900	B4V	O32-N31-C30	2.55	108.09	105.47
2	B	900	B4V	C17-N15-C13	2.44	127.72	123.67
2	D	900	B4V	C20-C21-N22	2.38	118.64	115.57
2	D	900	B4V	C24-C20-N27	-2.34	107.97	109.19
2	B	900	B4V	S19-C17-N15	2.32	126.83	123.72
2	C	900	B4V	C24-C20-N27	-2.32	107.98	109.19
2	B	900	B4V	C28-C24-N25	2.11	127.11	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	B4V	S19-C17-N15	2.10	126.53	123.72
2	A	501	B4V	C28-C24-N25	2.09	127.08	123.44
2	D	900	B4V	N15-C17-N18	2.07	124.76	121.18
2	C	900	B4V	C17-N15-C13	2.07	127.10	123.67
2	B	900	B4V	C20-C21-N22	2.03	118.19	115.57

There are no chirality outliers.

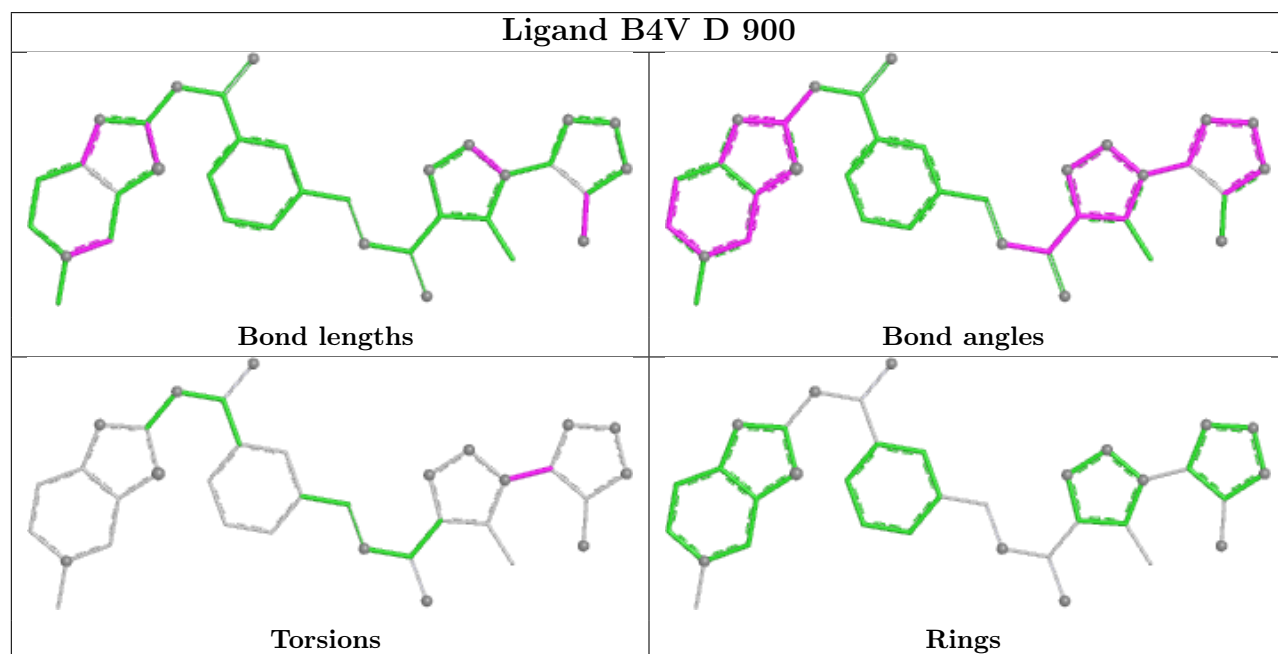
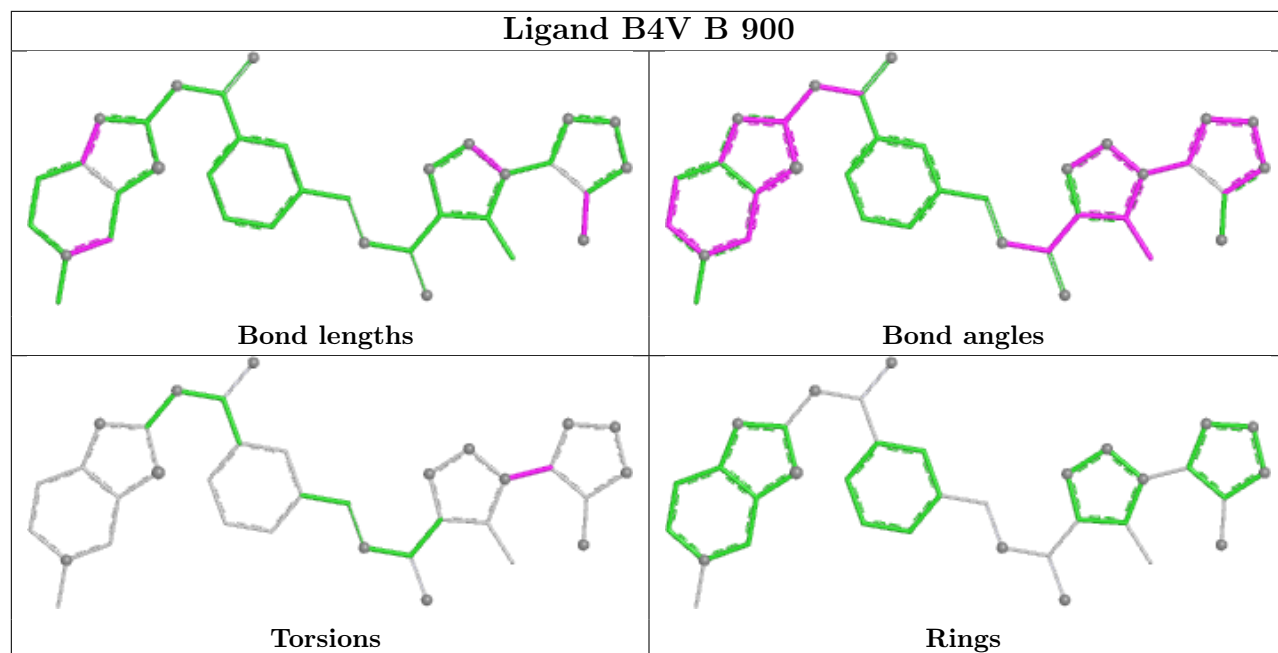
All (5) torsion outliers are listed below:

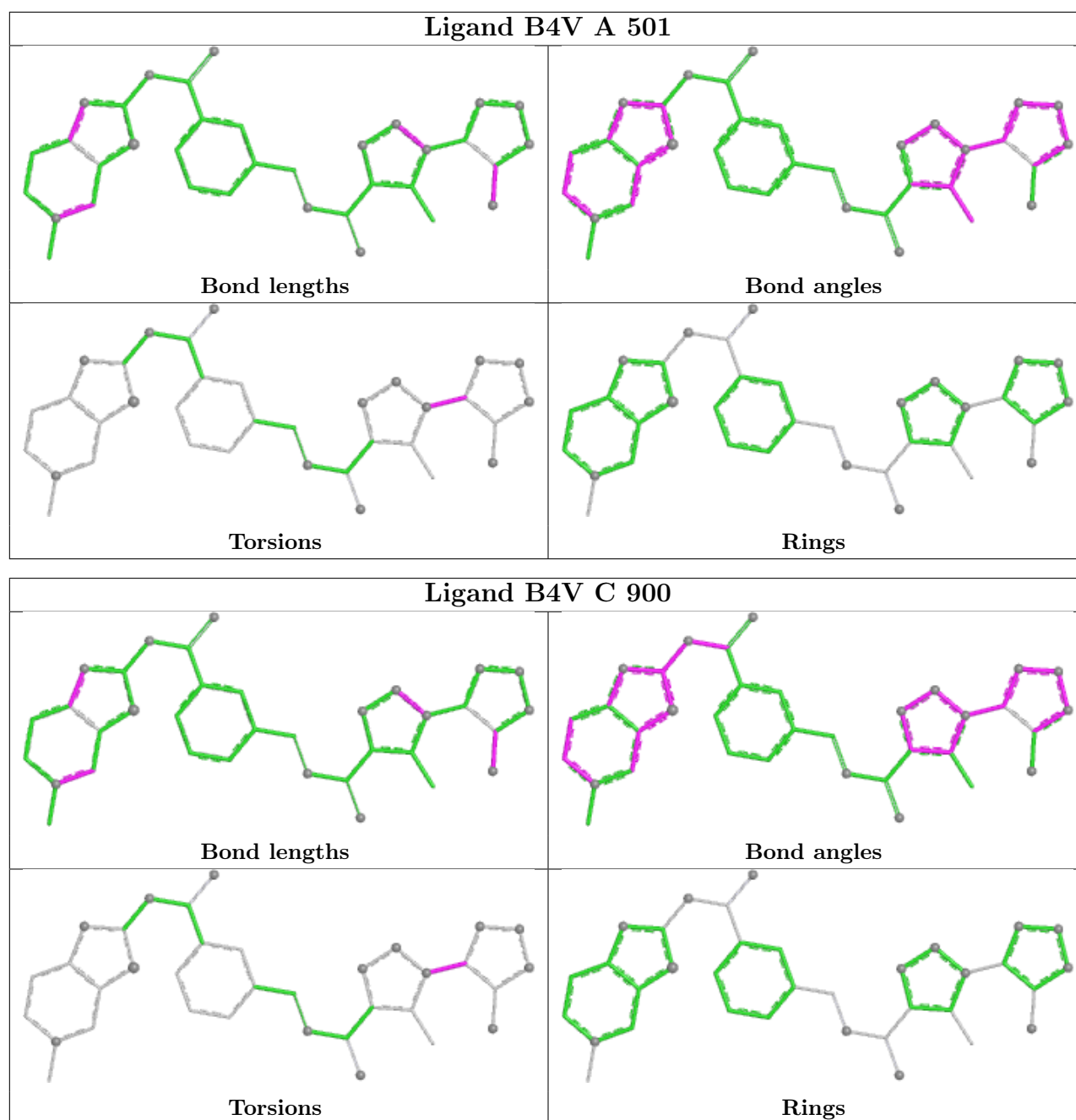
Mol	Chain	Res	Type	Atoms
2	A	501	B4V	C30-C29-N25-N26
2	B	900	B4V	C30-C29-N25-N26
2	C	900	B4V	C30-C29-N25-N26
2	D	900	B4V	C30-C29-N25-N26
2	B	900	B4V	N33-C29-N25-N26

There are no ring outliers.

No monomer is involved in short contacts.

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	395/415 (95%)	0.28	10 (2%) 58 61	52, 74, 124, 166	0
1	B	358/415 (86%)	0.97	35 (9%) 13 11	76, 129, 194, 211	0
1	C	386/415 (93%)	0.71	29 (7%) 20 17	54, 94, 166, 206	0
1	D	396/415 (95%)	0.23	12 (3%) 52 53	35, 72, 111, 133	1 (0%)
All	All	1535/1660 (92%)	0.54	86 (5%) 30 27	35, 86, 180, 211	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	HIS	6.1
1	B	329	VAL	5.1
1	C	5	MET	4.7
1	C	234	ALA	4.7
1	D	251	GLY	4.4
1	B	317	LEU	4.4
1	D	7	PHE	4.3
1	A	401	SER	4.3
1	D	376	GLY	4.2
1	C	245	VAL	3.9
1	A	400	TYR	3.8
1	B	287	TYR	3.8
1	B	290	ILE	3.7
1	C	290	ILE	3.5
1	B	381	PHE	3.4
1	B	245	VAL	3.3
1	C	183	VAL	3.3
1	B	305	ILE	3.3
1	A	375	LYS	3.3
1	C	175	ALA	3.3
1	B	247	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	254	TYR	3.3
1	B	170	VAL	3.2
1	B	266	VAL	3.2
1	D	283	LEU	3.2
1	C	291	MET	3.1
1	B	277	PRO	3.1
1	A	9	THR	3.0
1	C	351	THR	3.0
1	D	252	ASP	3.0
1	B	272	LEU	3.0
1	C	235	VAL	3.0
1	C	352	VAL	2.9
1	C	233	THR	2.8
1	C	300	PRO	2.8
1	B	298	THR	2.8
1	B	254	TYR	2.7
1	D	54[A]	ASN	2.7
1	C	170	VAL	2.7
1	B	274	GLY	2.6
1	A	347	THR	2.6
1	B	278	PHE	2.5
1	C	246	LEU	2.5
1	C	252	ASP	2.5
1	B	283	LEU	2.5
1	C	324	LEU	2.5
1	C	255	TYR	2.5
1	B	368	PHE	2.5
1	D	402	ASN	2.5
1	C	297	LEU	2.5
1	A	62	THR	2.5
1	B	5	MET	2.5
1	A	372	GLU	2.4
1	C	229	VAL	2.4
1	B	7	PHE	2.4
1	B	309	ALA	2.4
1	B	297	LEU	2.3
1	B	312	LEU	2.3
1	B	281	ASP	2.3
1	B	288	SER	2.3
1	A	11	PHE	2.3
1	B	273	VAL	2.3
1	B	164	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	305	ILE	2.2
1	C	332	ILE	2.2
1	A	373	GLU	2.2
1	B	224	ASN	2.2
1	B	269	TYR	2.2
1	C	228	MET	2.2
1	B	361	SER	2.2
1	C	19	ARG	2.2
1	B	359	LEU	2.1
1	B	339	LYS	2.1
1	A	7	PHE	2.1
1	D	401	SER	2.1
1	C	339	LYS	2.1
1	B	262	TRP	2.1
1	D	373	GLU	2.1
1	D	325	GLY	2.1
1	B	175	ALA	2.0
1	C	259	CYS	2.0
1	B	336	LEU	2.0
1	D	377	GLU	2.0
1	C	256	GLY	2.0
1	C	238	PRO	2.0
1	D	374	ASP	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.

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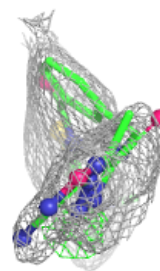
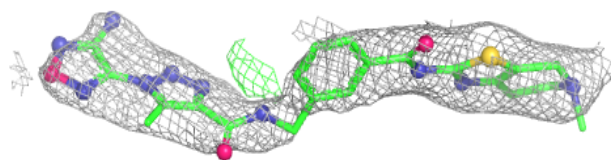
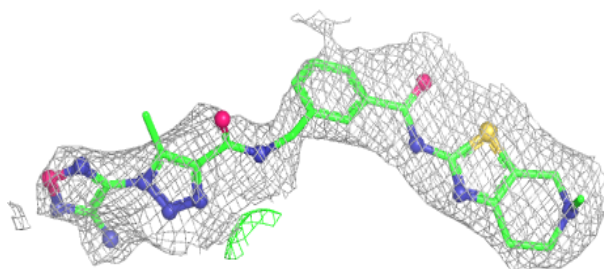
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	503	6/6	0.73	0.14	96,97,99,100	0
3	GOL	A	502	6/6	0.82	0.12	107,109,110,111	0
2	B4V	B	900	35/35	0.90	0.11	110,120,142,143	0
2	B4V	A	501	35/35	0.94	0.09	57,72,94,95	0
2	B4V	C	900	35/35	0.95	0.09	67,75,97,99	0
2	B4V	D	900	35/35	0.96	0.07	52,60,78,79	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.

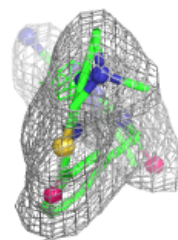
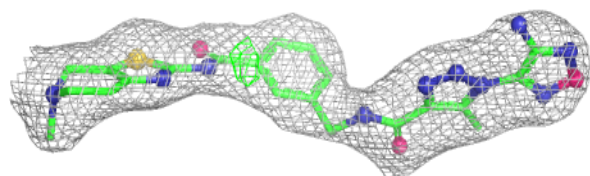
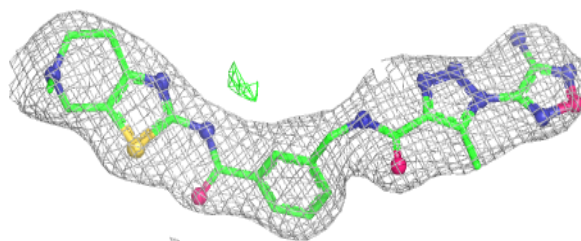
Electron density around B4V B 900:

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

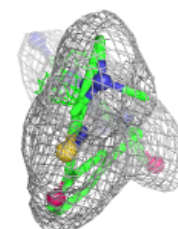
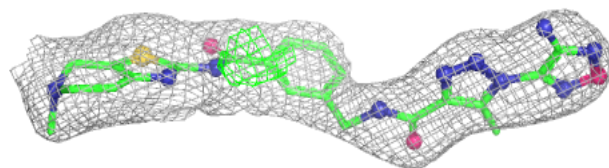
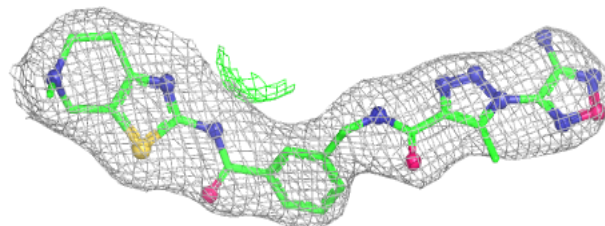


Electron density around B4V A 501:

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

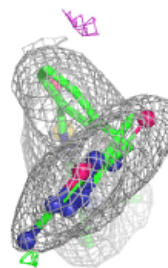
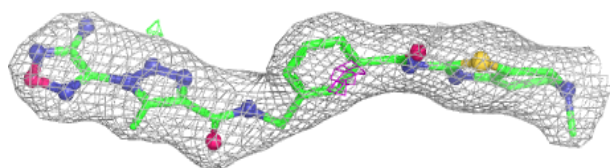
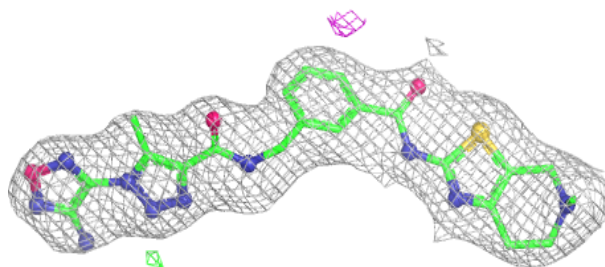
**Electron density around B4V C 900:**

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



Electron density around B4V D 900:

$2mF_o - DF_c$ (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.