



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:43 PM UTC

PDB ID : 5WNH / pdb_00005wnh
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 : 3.10 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

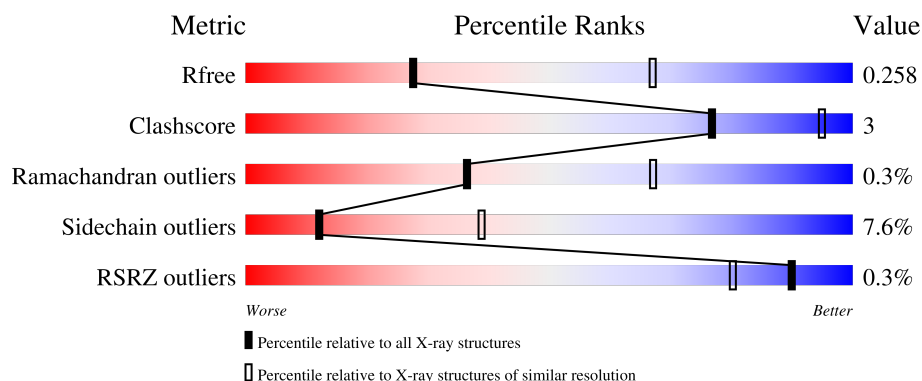
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

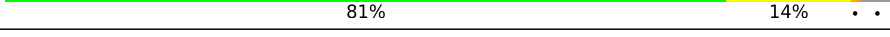
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	
1	B	415	
1	C	415	
1	D	415	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12783 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.

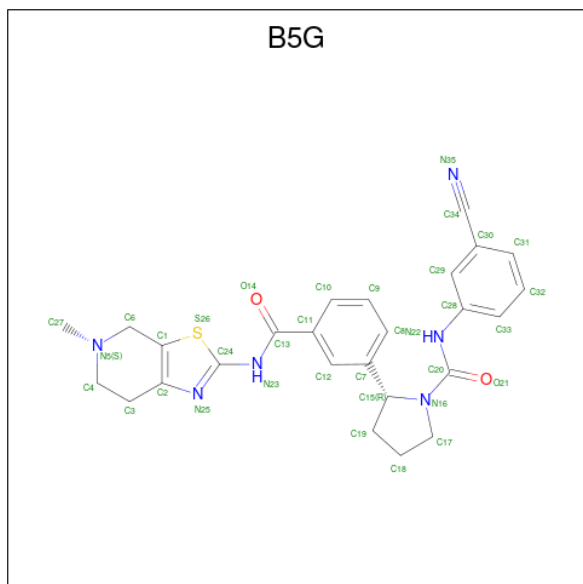
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3197	2045	525	606	21			
1	B	365	Total	C	N	O	S	0	0	0
			2977	1917	488	551	21			
1	C	388	Total	C	N	O	S	0	0	0
			3162	2028	522	590	22			
1	D	397	Total	C	N	O	S	0	0	0
			3228	2062	533	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 (2R)-N-(3-cyanophenyl)-2-{3-[(5-methyl-4,5,6,7-tetrahydro[1,3]thiazolo[5,4-c]pyridin-2-yl)carbamoyl]phenyl}pyrrolidine-1-carboxamide (CCD ID: B5G) (formula: C₂₆H₂₆N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	26	6	2	1		
2	B	1	Total	C	N	O	S	0	0
			35	26	6	2	1		
2	C	1	Total	C	N	O	S	0	0
			35	26	6	2	1		
2	D	1	Total	C	N	O	S	0	0
			35	26	6	2	1		

- Molecule 3 is water.

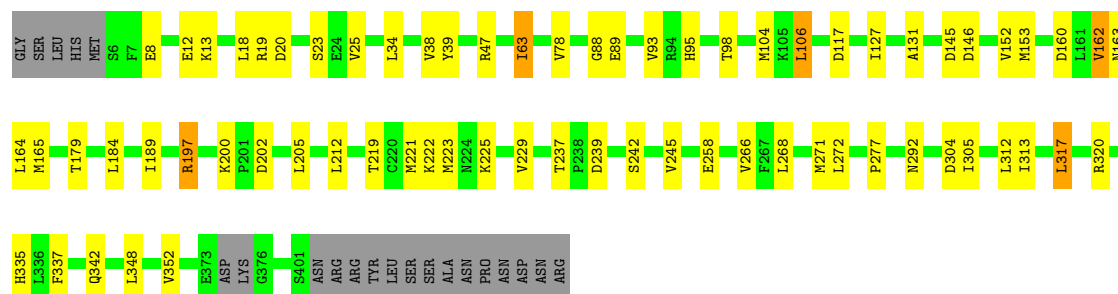
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		
3	D	27	Total	O	0	0
			27	27		

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.

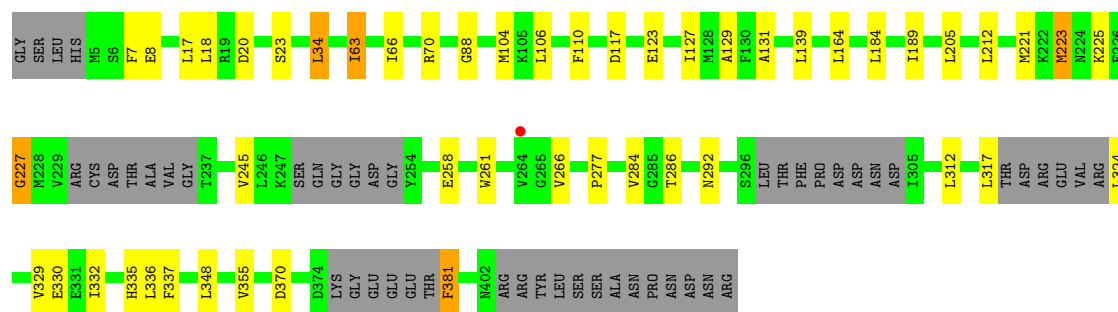
• Molecule 1: Rho-associated protein kinase 1

Chain A: 



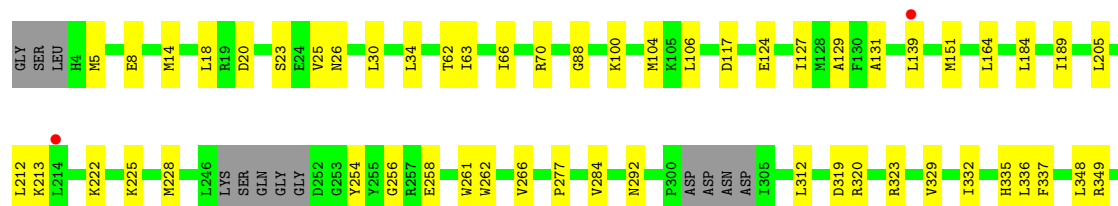
• Molecule 1: Rho-associated protein kinase 1

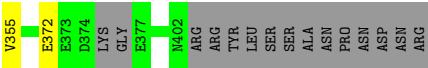
Chain B: 



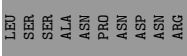
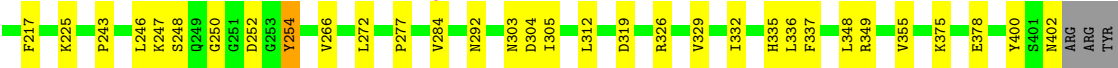
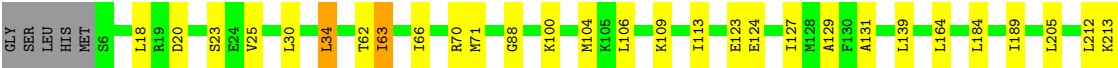
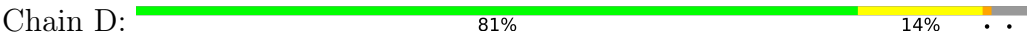
• Molecule 1: Rho-associated protein kinase 1

Chain C: 





● 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	162.92Å 81.97Å 167.48Å 90.00° 115.68° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10 40.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-3.10) 98.8 (40.00-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.227 , 0.234 0.243 , 0.258	Depositor DCC
R_{free} test set	1619 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 93.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: B5G

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	0.71	0/3273	1.27	4/4422 (0.1%)
1	B	0.70	0/3047	1.27	8/4110 (0.2%)
1	C	0.71	0/3237	1.25	2/4371 (0.0%)
1	D	0.70	0/3305	1.25	1/4465 (0.0%)
All	All	0.70	0/12862	1.26	15/17368 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304	ASP	N-CA-C	-6.15	105.94	113.50
1	B	7	PHE	CA-C-N	5.77	128.02	120.28
1	B	7	PHE	C-N-CA	5.77	128.02	120.28
1	A	304	ASP	N-CA-C	-5.77	106.40	113.50
1	B	286	THR	CA-C-N	5.57	127.75	120.28
1	B	286	THR	C-N-CA	5.57	127.75	120.28
1	C	5	MET	CA-C-N	5.49	132.03	121.54
1	C	5	MET	C-N-CA	5.49	132.03	121.54
1	A	145	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	330	GLU	CA-C-N	5.22	127.28	120.28
1	B	330	GLU	C-N-CA	5.22	127.28	120.28
1	B	245	VAL	CA-C-N	5.01	127.25	120.38
1	B	245	VAL	C-N-CA	5.01	127.25	120.38
1	A	153	MET	CA-C-N	5.00	127.95	120.95
1	A	153	MET	C-N-CA	5.00	127.95	120.95

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	3197	0	3090	23	0
1	B	2977	0	2888	14	0
1	C	3162	0	3066	18	0
1	D	3228	0	3125	20	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	33	0	0	0	0
3	B	10	0	0	0	0
3	C	9	0	0	0	0
3	D	27	0	0	0	0
All	All	12783	0	12169	71	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 3.

All (71) 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:179:THR:HG21	1:A:268:LEU:HD12	1.69	0.75
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.72	0.71
1:C:66:ILE:HD11	1:D:25:VAL:HG21	1.75	0.69
1:A:95:HIS:HD2	1:A:98:THR:H	1.42	0.67
1:A:197:ARG:HH11	1:A:197:ARG:HG3	1.62	0.65
1:A:93:VAL:HG21	1:A:104:MET:HE3	1.80	0.64
1:C:320:ARG:HA	1:C:323:ARG:HD2	1.84	0.60
1:A:200:LYS:HE2	1:A:202:ASP:HB2	1.84	0.59
1:A:38:VAL:HG11	1:A:63:ILE:HG21	1.85	0.59
1:D:127:ILE:O	1:D:131:ALA:HB2	2.05	0.57
1:A:313:ILE:HG23	1:A:317:LEU:HD23	1.87	0.56
1:D:104:MET:HE3	1:D:106:LEU:HD11	1.88	0.56
1:B:104:MET:HE3	1:B:106:LEU:HD11	1.88	0.56
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.86	0.55
1:C:127:ILE:O	1:C:131:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:131:ALA:HB2	2.07	0.54
1:C:104:MET:HE3	1:C:106:LEU:HD11	1.90	0.54
1:C:262:TRP:HB2	1:C:323:ARG:NH2	2.22	0.54
1:A:197:ARG:NH1	1:A:221:MET:HB2	2.23	0.53
1:D:272:LEU:HB3	1:D:305:ILE:HD12	1.89	0.53
1:B:129:ALA:HB2	1:B:139:LEU:HD23	1.92	0.52
1:A:335:HIS:HD2	1:A:337:PHE:H	1.58	0.51
1:D:71:MET:HG3	1:D:400:TYR:HE1	1.75	0.51
1:D:129:ALA:HB2	1:D:139:LEU:HD23	1.93	0.51
1:A:8:GLU:O	1:A:12:GLU:HG2	2.11	0.51
1:C:129:ALA:HB2	1:C:139:LEU:HD23	1.94	0.50
1:B:335:HIS:HD2	1:B:337:PHE:H	1.60	0.50
1:C:124:GLU:HG2	1:C:151:MET:HE1	1.93	0.49
1:B:258:GLU:HA	1:B:261:TRP:HD1	1.77	0.48
1:C:335:HIS:HD2	1:C:337:PHE:H	1.60	0.48
1:C:25:VAL:HG21	1:D:66:ILE:HD11	1.95	0.47
1:D:335:HIS:HD2	1:D:337:PHE:H	1.60	0.47
1:A:127:ILE:O	1:A:131:ALA:HB2	2.15	0.46
1:A:179:THR:CG2	1:A:268:LEU:HD12	2.44	0.46
1:A:242:SER:HB3	1:A:245:VAL:HG22	1.98	0.46
1:C:20:ASP:HB3	1:C:23:SER:HB2	1.98	0.46
1:B:88:GLY:HA3	1:B:106:LEU:O	2.17	0.45
1:A:88:GLY:HA3	1:A:106:LEU:O	2.17	0.45
1:B:110:PHE:CD1	1:B:381:PHE:HB2	2.52	0.45
1:D:88:GLY:HA3	1:D:106:LEU:O	2.17	0.45
1:C:88:GLY:HA3	1:C:106:LEU:O	2.18	0.44
1:B:329:VAL:HA	1:B:332:ILE:HD12	1.99	0.44
1:D:243:PRO:O	1:D:247:LYS:HB2	2.18	0.44
1:A:160:ASP:OD2	1:A:162:VAL:HG12	2.17	0.44
1:A:197:ARG:HB2	1:A:219:THR:HG22	2.00	0.44
1:D:184:LEU:HD12	1:D:348:LEU:HD23	2.00	0.43
1:A:104:MET:HE2	1:A:152:VAL:HG22	2.00	0.43
1:C:329:VAL:HA	1:C:332:ILE:HD12	2.00	0.43
1:B:223:MET:HG2	1:B:227:GLY:HA2	2.01	0.43
1:D:266:VAL:HG13	1:D:277:PRO:HD2	2.00	0.43
1:B:184:LEU:HD12	1:B:348:LEU:HD23	2.02	0.42
1:C:266:VAL:HG13	1:C:277:PRO:HD2	2.01	0.42
1:C:184:LEU:HD12	1:C:348:LEU:HD23	2.01	0.42
1:C:258:GLU:HA	1:C:261:TRP:HD1	1.85	0.42
1:D:109:LYS:O	1:D:113:ILE:HG12	2.19	0.42
1:A:184:LEU:HD12	1:A:348:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:VAL:HG13	1:A:277:PRO:HD2	2.02	0.42
1:D:248:SER:HA	1:D:252:ASP:HB3	2.01	0.42
1:C:213:LYS:HE2	1:C:349:ARG:HH22	1.85	0.41
1:B:34:LEU:HD12	1:B:63:ILE:HD13	2.03	0.41
1:D:124:GLU:HA	1:D:217:PHE:HB2	2.02	0.41
1:B:20:ASP:HB3	1:B:23:SER:HB2	2.02	0.41
1:D:20:ASP:HB3	1:D:23:SER:HB2	2.03	0.41
1:D:34:LEU:HD12	1:D:63:ILE:HD13	2.02	0.41
1:D:329:VAL:HA	1:D:332:ILE:HD12	2.02	0.41
1:A:39:TYR:CE1	1:A:146:ASP:HB3	2.56	0.41
1:A:272:LEU:HB3	1:A:305:ILE:CG2	2.51	0.41
1:C:228:MET:HA	1:C:256:GLY:HA2	2.02	0.41
1:A:20:ASP:HB3	1:A:23:SER:HB2	2.03	0.41
1:B:266:VAL:HG13	1:B:277:PRO:HD2	2.02	0.41
1:D:213:LYS:HE2	1:D:349:ARG:HH22	1.85	0.41

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	390/415 (94%)	378 (97%)	12 (3%)	0	100	100
1	B	353/415 (85%)	343 (97%)	8 (2%)	2 (1%)	21	52
1	C	380/415 (92%)	368 (97%)	12 (3%)	0	100	100
1	D	395/415 (95%)	377 (95%)	16 (4%)	2 (0%)	24	57
All	All	1518/1660 (91%)	1466 (97%)	48 (3%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	254	TYR
1	B	225	LYS
1	D	250	GLY
1	B	227	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	349/369 (95%)	317 (91%)	32 (9%)	8	31
1	B	324/369 (88%)	301 (93%)	23 (7%)	13	41
1	C	345/369 (94%)	321 (93%)	24 (7%)	14	41
1	D	353/369 (96%)	328 (93%)	25 (7%)	13	41
All	All	1371/1476 (93%)	1267 (92%)	104 (8%)	12	39

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	18	LEU
1	A	19	ARG
1	A	34	LEU
1	A	47	ARG
1	A	63	ILE
1	A	78	VAL
1	A	89	GLU
1	A	106	LEU
1	A	117	ASP
1	A	162	VAL
1	A	163	ASN
1	A	164	LEU
1	A	165	MET
1	A	189	ILE
1	A	197	ARG
1	A	205	LEU
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	222	LYS
1	A	223	MET
1	A	225	LYS
1	A	229	VAL
1	A	237	THR
1	A	239	ASP
1	A	258	GLU
1	A	271	MET
1	A	292	ASN
1	A	312	LEU
1	A	317	LEU
1	A	320	ARG
1	A	342	GLN
1	A	352	VAL
1	B	8	GLU
1	B	17	LEU
1	B	18	LEU
1	B	34	LEU
1	B	63	ILE
1	B	70	ARG
1	B	117	ASP
1	B	123	GLU
1	B	164	LEU
1	B	189	ILE
1	B	205	LEU
1	B	212	LEU
1	B	221	MET
1	B	223	MET
1	B	284	VAL
1	B	292	ASN
1	B	312	LEU
1	B	317	LEU
1	B	324	LEU
1	B	336	LEU
1	B	355	VAL
1	B	370	ASP
1	B	381	PHE
1	C	8	GLU
1	C	14	MET
1	C	18	LEU
1	C	26	ASN
1	C	34	LEU

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Mol	Chain	Res	Type
1	C	62	THR
1	C	63	ILE
1	C	70	ARG
1	C	100	LYS
1	C	117	ASP
1	C	164	LEU
1	C	189	ILE
1	C	205	LEU
1	C	212	LEU
1	C	222	LYS
1	C	225	LYS
1	C	254	TYR
1	C	284	VAL
1	C	292	ASN
1	C	312	LEU
1	C	319	ASP
1	C	336	LEU
1	C	355	VAL
1	C	372	GLU
1	D	18	LEU
1	D	34	LEU
1	D	62	THR
1	D	63	ILE
1	D	70	ARG
1	D	100	LYS
1	D	123	GLU
1	D	164	LEU
1	D	189	ILE
1	D	205	LEU
1	D	212	LEU
1	D	225	LYS
1	D	246	LEU
1	D	254	TYR
1	D	284	VAL
1	D	292	ASN
1	D	303	ASN
1	D	312	LEU
1	D	319	ASP
1	D	326	ARG
1	D	336	LEU
1	D	355	VAL
1	D	375	LYS

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Mol	Chain	Res	Type
1	D	378	GLU
1	D	402	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	311	ASN
1	A	335	HIS
1	A	342	GLN
1	B	16	ASN
1	B	26	ASN
1	B	311	ASN
1	B	335	HIS
1	C	54	ASN
1	C	91	GLN
1	C	335	HIS
1	C	342	GLN
1	D	190	HIS
1	D	224	ASN
1	D	311	ASN
1	D	342	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B5G	C	900	-	38,39,39	1.01	3 (7%)	51,55,55	2.45	14 (27%)
2	B5G	D	900	-	38,39,39	1.01	2 (5%)	51,55,55	2.31	13 (25%)
2	B5G	A	900	-	38,39,39	1.00	2 (5%)	51,55,55	2.43	13 (25%)
2	B5G	B	900	-	38,39,39	1.08	2 (5%)	51,55,55	2.30	13 (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	B5G	C	900	-	-	0/22/41/41	0/5/5/5
2	B5G	D	900	-	-	0/22/41/41	0/5/5/5
2	B5G	A	900	-	-	0/22/41/41	0/5/5/5
2	B5G	B	900	-	-	2/22/41/41	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	B5G	C6-N5	3.87	1.49	1.46
2	D	900	B5G	C6-N5	2.91	1.48	1.46
2	A	900	B5G	C6-N5	2.90	1.48	1.46
2	C	900	B5G	C6-N5	2.65	1.48	1.46
2	B	900	B5G	C2-N25	-2.61	1.32	1.38
2	D	900	B5G	C2-N25	-2.54	1.33	1.38
2	C	900	B5G	C2-N25	-2.42	1.33	1.38
2	A	900	B5G	C2-N25	-2.30	1.33	1.38
2	C	900	B5G	C6-C1	2.15	1.52	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	B5G	C3-C4-N5	8.03	118.25	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	B5G	C3-C4-N5	7.94	118.17	110.71
2	A	900	B5G	S26-C24-N25	-7.60	108.98	115.78
2	A	900	B5G	C3-C4-N5	7.50	117.75	110.71
2	C	900	B5G	S26-C24-N25	-7.36	109.20	115.78
2	B	900	B5G	S26-C24-N25	-7.07	109.46	115.78
2	D	900	B5G	S26-C24-N25	-6.61	109.86	115.78
2	D	900	B5G	C6-C1-S26	5.95	127.29	121.91
2	A	900	B5G	C24-N25-C2	5.92	118.57	110.09
2	C	900	B5G	C24-N25-C2	5.81	118.40	110.09
2	B	900	B5G	C6-C1-S26	5.78	127.13	121.91
2	D	900	B5G	C24-N25-C2	5.59	118.09	110.09
2	A	900	B5G	C6-C1-S26	5.39	126.78	121.91
2	B	900	B5G	C24-N25-C2	5.39	117.81	110.09
2	B	900	B5G	C3-C4-N5	5.28	115.67	110.71
2	C	900	B5G	C6-C1-S26	5.18	126.59	121.91
2	B	900	B5G	C19-C15-N16	4.61	107.06	101.93
2	A	900	B5G	C1-S26-C24	4.58	91.03	88.76
2	C	900	B5G	C19-C15-N16	4.28	106.70	101.93
2	D	900	B5G	C19-C15-N16	4.24	106.65	101.93
2	C	900	B5G	C17-N16-C15	-4.16	107.20	111.88
2	C	900	B5G	C1-S26-C24	4.12	90.81	88.76
2	A	900	B5G	C19-C15-N16	4.02	106.41	101.93
2	B	900	B5G	C1-C6-N5	3.89	112.44	109.49
2	B	900	B5G	C1-S26-C24	3.71	90.60	88.76
2	B	900	B5G	C17-N16-C15	-3.68	107.74	111.88
2	A	900	B5G	C15-N16-C20	3.65	127.36	119.95
2	C	900	B5G	C15-N16-C20	3.57	127.18	119.95
2	A	900	B5G	C17-N16-C15	-3.54	107.90	111.88
2	D	900	B5G	C17-N16-C15	-3.53	107.91	111.88
2	B	900	B5G	C15-N16-C20	3.40	126.85	119.95
2	D	900	B5G	C15-N16-C20	3.27	126.57	119.95
2	B	900	B5G	N22-C20-N16	3.15	119.10	115.54
2	C	900	B5G	C1-C6-N5	2.96	111.73	109.49
2	D	900	B5G	C1-S26-C24	2.87	90.19	88.76
2	A	900	B5G	C1-C6-N5	2.81	111.62	109.49
2	C	900	B5G	C18-C17-N16	2.81	108.07	103.24
2	B	900	B5G	C18-C17-N16	2.78	108.03	103.24
2	C	900	B5G	N22-C20-N16	2.73	118.62	115.54
2	D	900	B5G	N22-C20-N16	2.68	118.57	115.54
2	A	900	B5G	N22-C20-N16	2.58	118.46	115.54
2	A	900	B5G	C11-C13-N23	2.55	119.92	116.25
2	B	900	B5G	C24-N23-C13	2.54	127.87	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	B5G	S26-C24-N23	2.48	127.03	123.72
2	A	900	B5G	C18-C17-N16	2.46	107.47	103.24
2	B	900	B5G	S26-C24-N23	2.34	126.85	123.72
2	D	900	B5G	C18-C17-N16	2.32	107.24	103.24
2	C	900	B5G	S26-C24-N23	2.25	126.73	123.72
2	D	900	B5G	C6-C1-C2	-2.23	123.71	125.23
2	A	900	B5G	S26-C24-N23	2.21	126.68	123.72
2	C	900	B5G	C11-C13-N23	2.18	119.39	116.25
2	C	900	B5G	C24-N23-C13	2.15	127.22	123.67
2	D	900	B5G	C24-N23-C13	2.10	127.15	123.67

There are no chirality outliers.

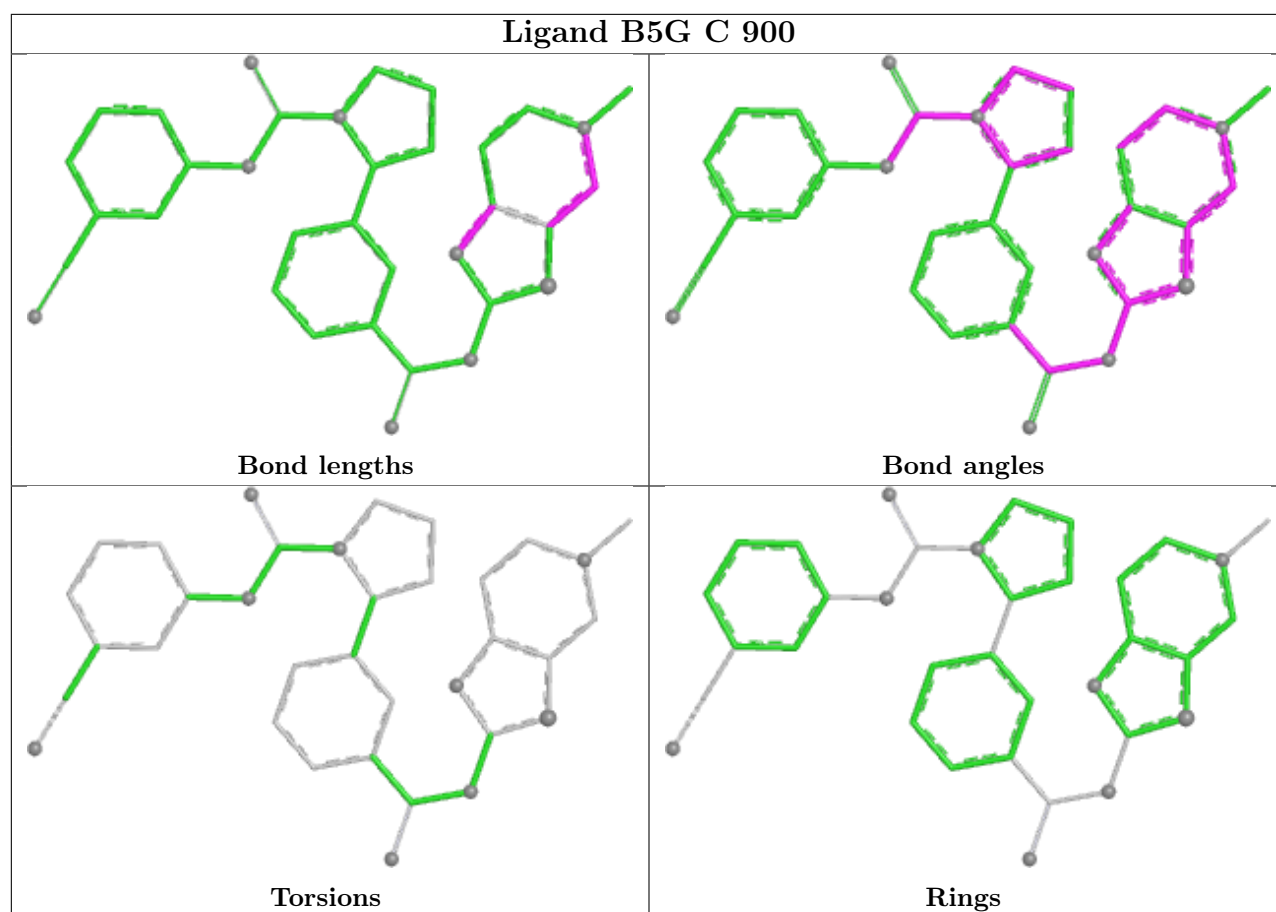
All (2) torsion outliers are listed below:

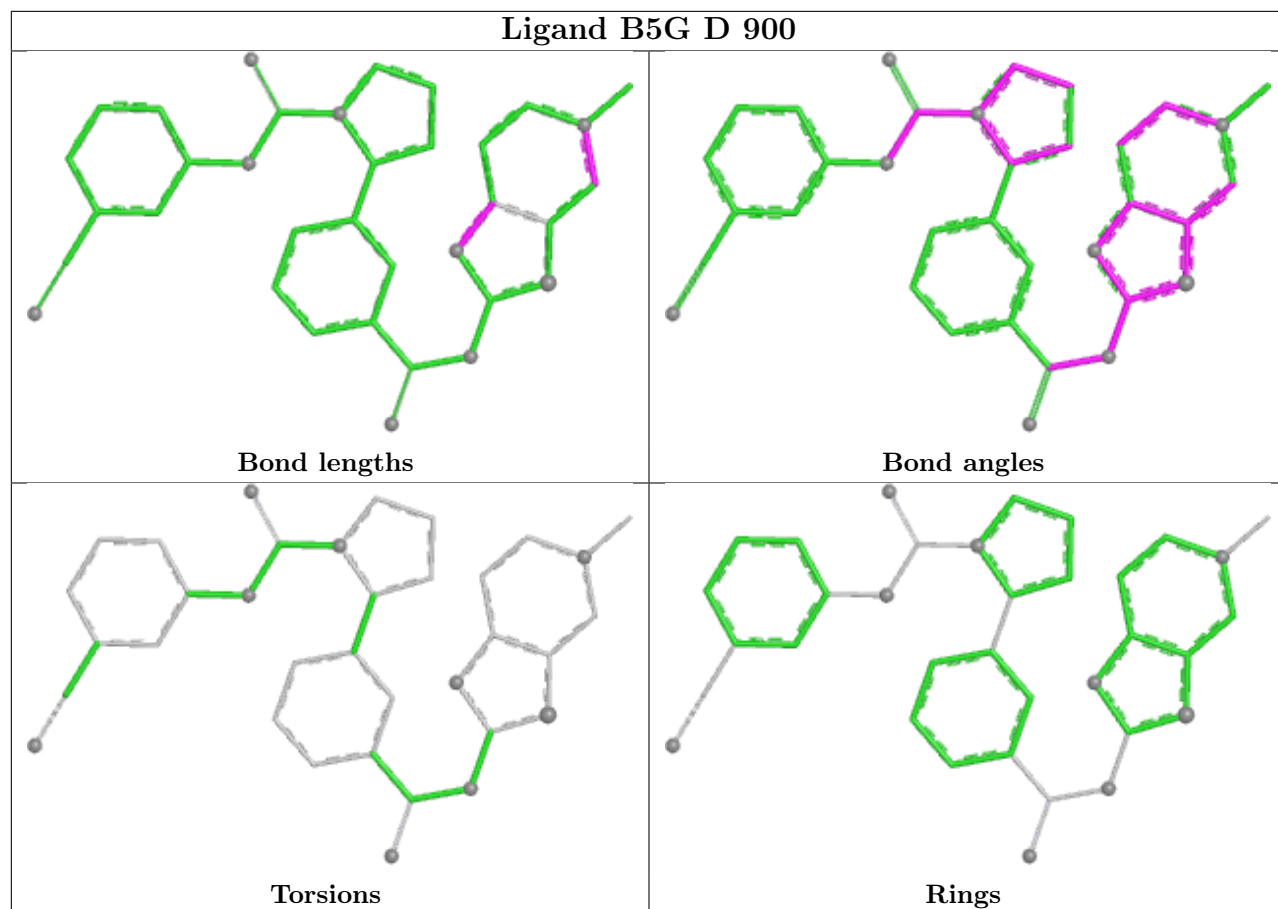
Mol	Chain	Res	Type	Atoms
2	B	900	B5G	S26-C24-N23-C13
2	B	900	B5G	N25-C24-N23-C13

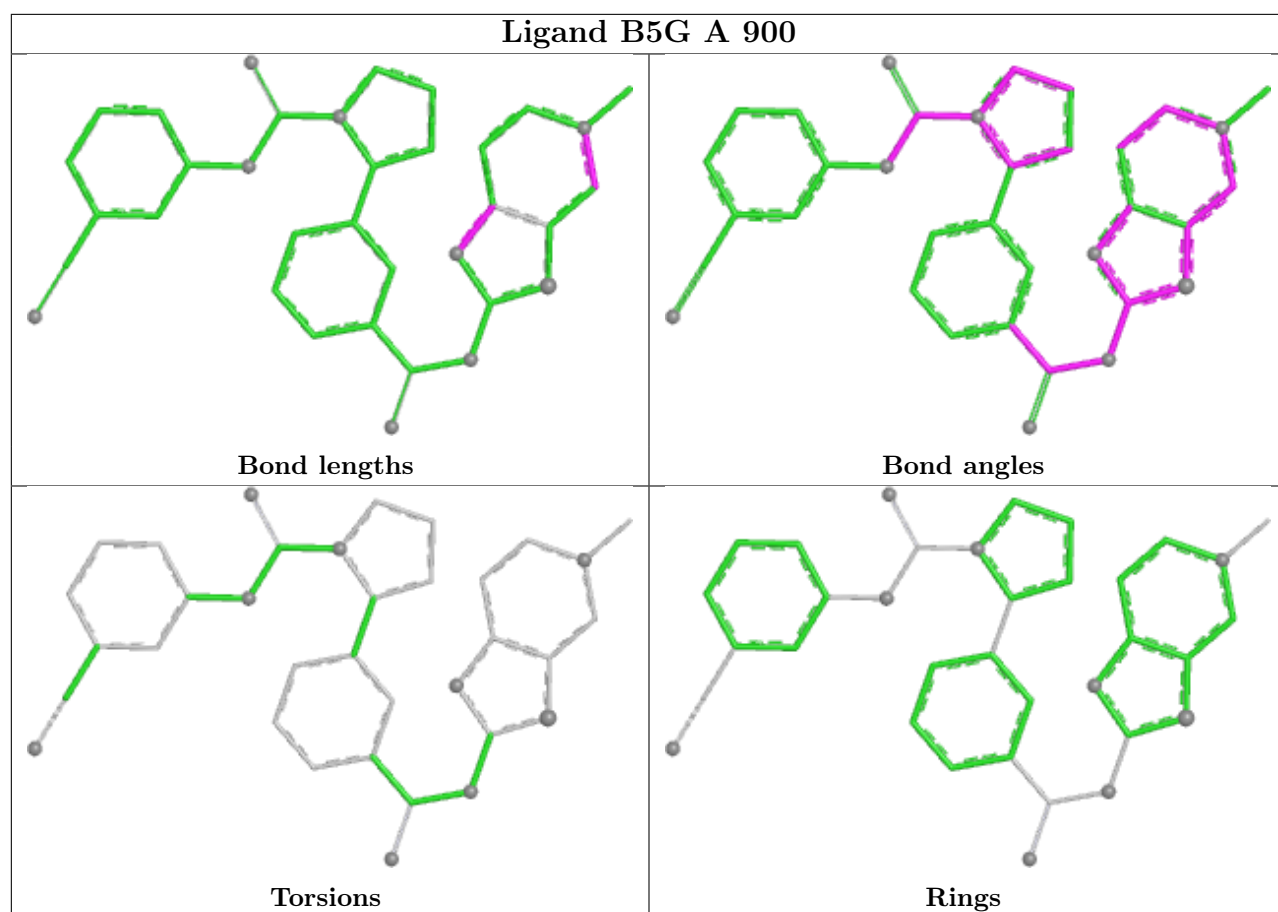
There are no ring outliers.

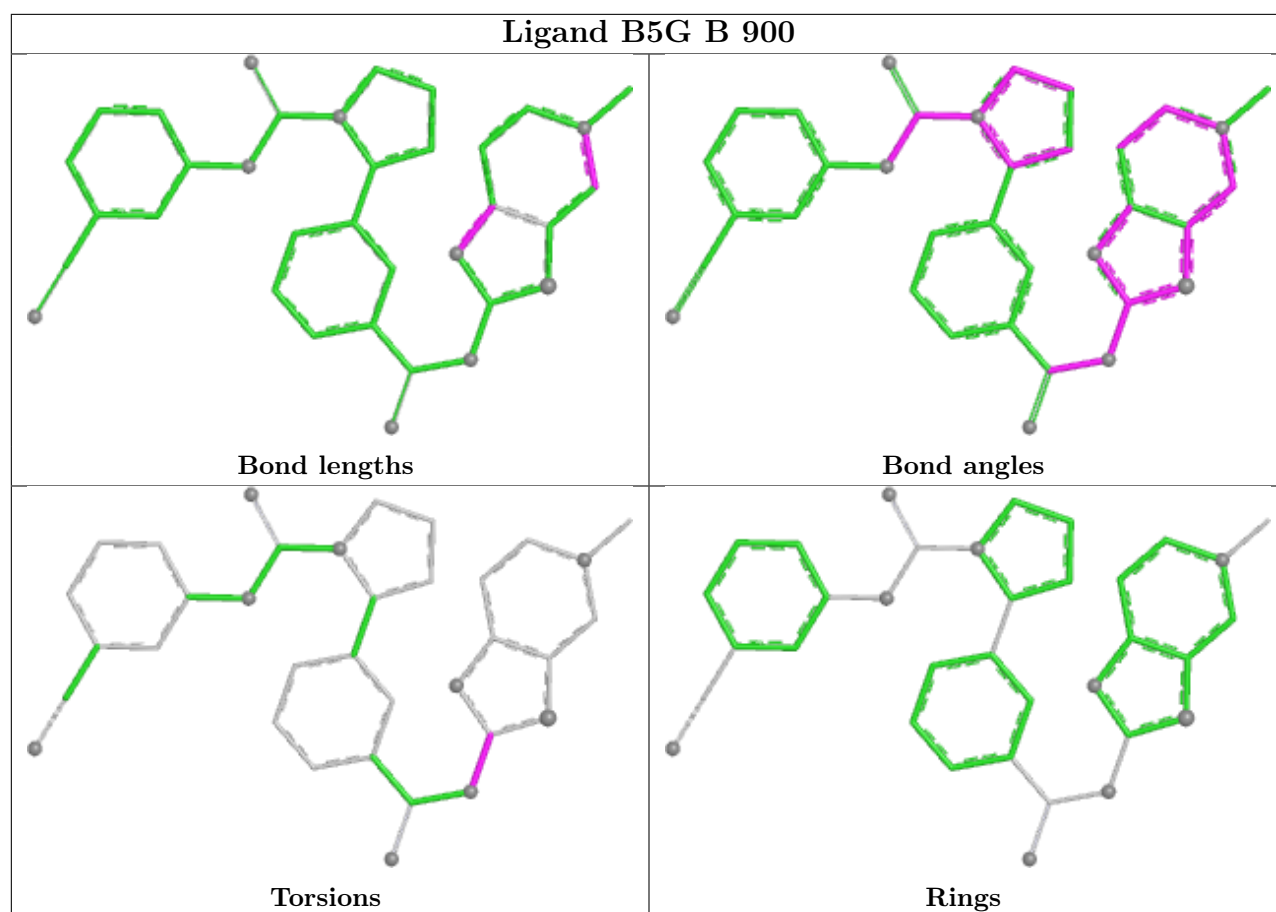
No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	394/415 (94%)	-0.26	0 100 100	82, 109, 155, 207	0
1	B	365/415 (87%)	-0.11	1 (0%) 90 80	104, 151, 215, 241	0
1	C	388/415 (93%)	-0.16	2 (0%) 87 73	81, 131, 202, 235	0
1	D	397/415 (95%)	-0.29	1 (0%) 90 80	77, 107, 152, 166	0
All	All	1544/1660 (93%)	-0.21	4 (0%) 90 80	77, 121, 198, 241	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	VAL	2.5
1	C	139	LEU	2.4
1	B	264	VAL	2.1
1	C	214	LEU	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](#)

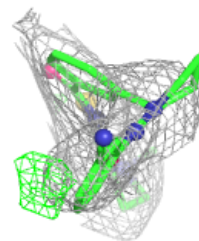
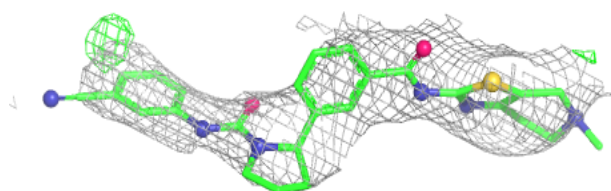
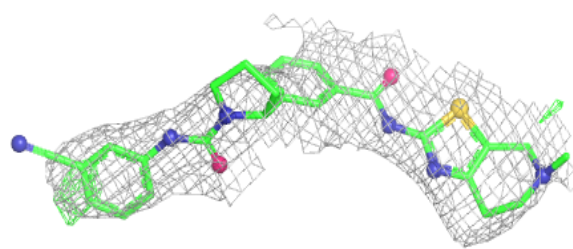
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B5G	B	900	35/35	0.86	0.10	137,143,148,150	0
2	B5G	A	900	35/35	0.92	0.10	102,103,107,113	0
2	B5G	D	900	35/35	0.92	0.10	93,101,103,104	0
2	B5G	C	900	35/35	0.93	0.08	99,102,104,105	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.

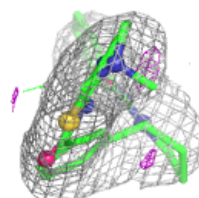
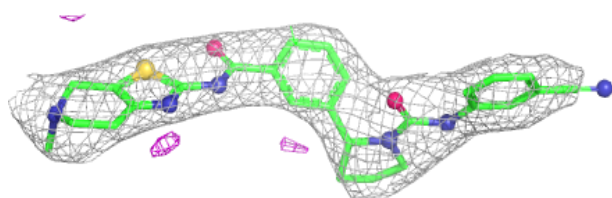
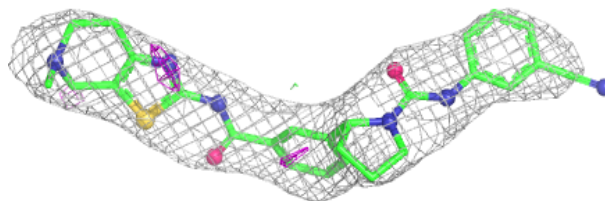
Electron density around B5G B 900:

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

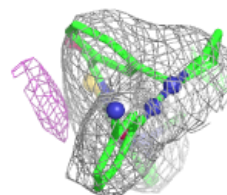
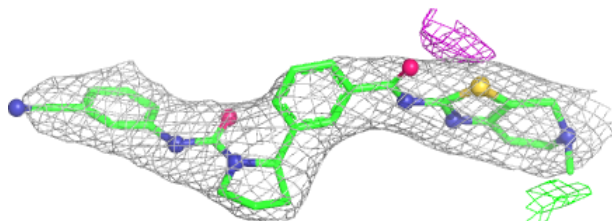
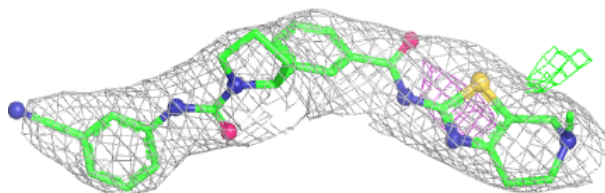


Electron density around B5G A 900:

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

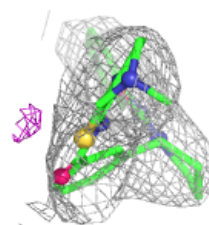
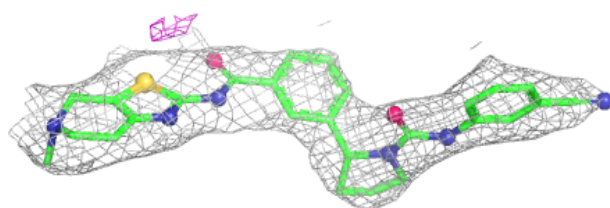
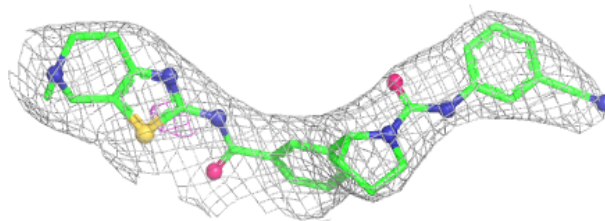
**Electron density around B5G D 900:**

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



Electron density around B5G 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.