Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 08:38 PM EDT

PDB ID	:	5WNH
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

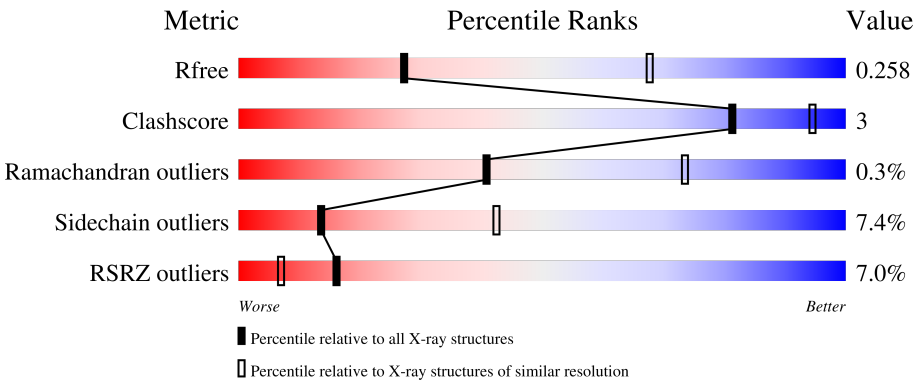
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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%, 80%, 14%, • 5%
1	B	415	13%, 77%, 10%, • 12%
1	C	415	10%, 81%, 13%, 7%
1	D	415	%, 81%, 13%, • •

2 Entry composition (i)

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.

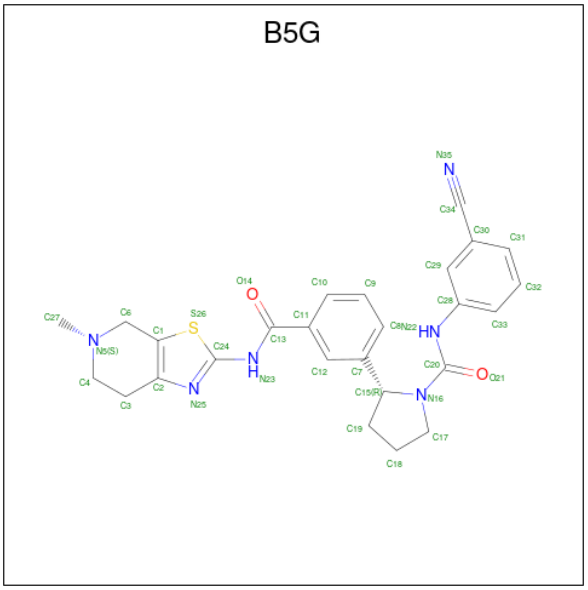
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3197	2045	525	606	21	0	0	0
1	B	365	2977	1917	488	551	21	0	0	0
1	C	388	3162	2028	522	590	22	0	0	0
1	D	397	3228	2062	533	612	21	0	0	0

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 (three-letter code: B5G) (formula: $C_{26}H_{26}N_6O_2S$).



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.

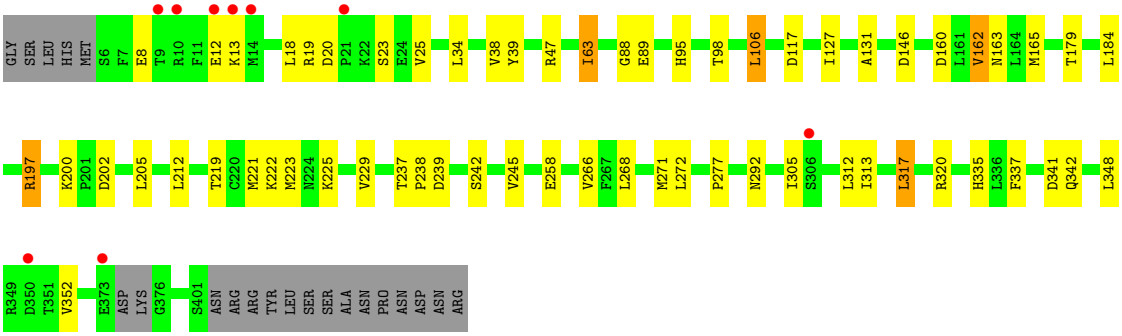
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		
3	D	27	Total	O	0	0
			27	27		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

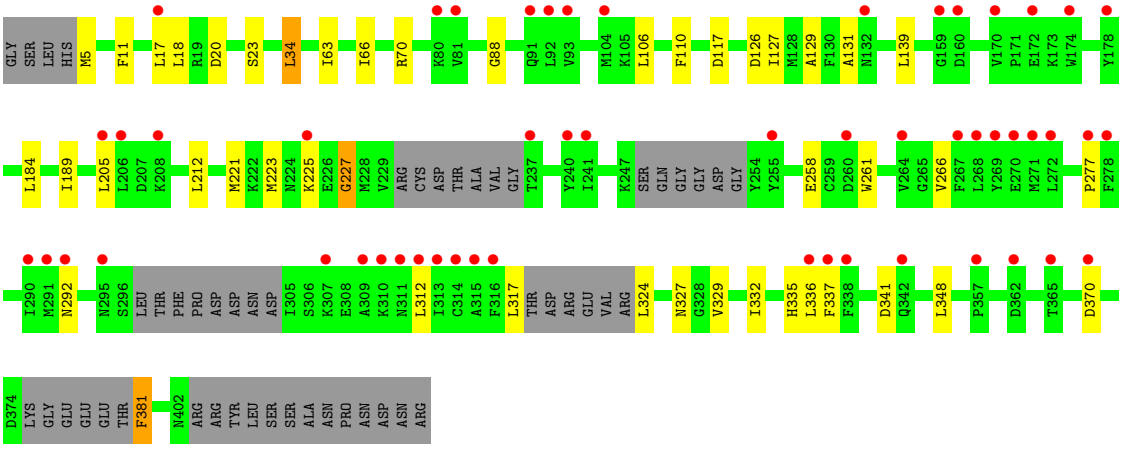
• Molecule 1: Rho-associated protein kinase 1

Chain A:



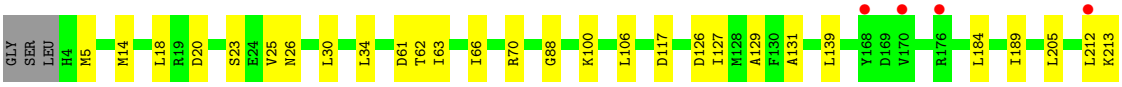
• Molecule 1: Rho-associated protein kinase 1

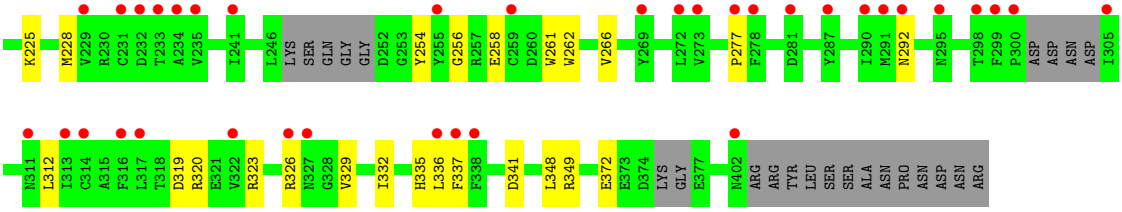
Chain B:



• Molecule 1: Rho-associated protein kinase 1

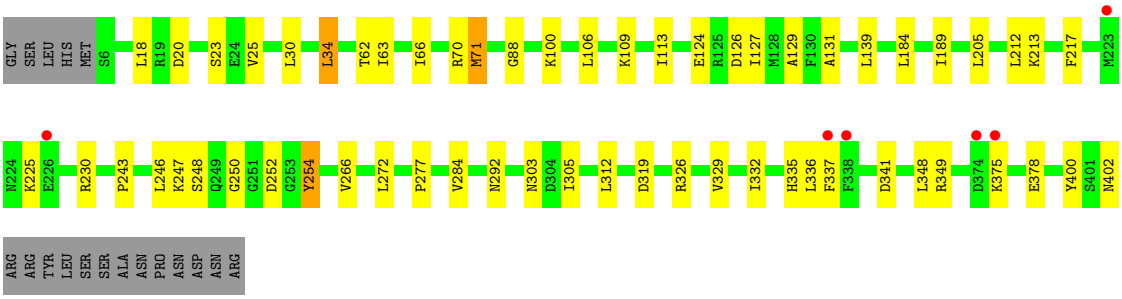
Chain C:





- Molecule 1: Rho-associated protein kinase 1

Chain D:



4 Data and refinement statistics (i)

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 47.19 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-3.10) 98.8 (47.19-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 93.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/3273	0.61	0/4422
1	B	0.38	0/3047	0.58	0/4110
1	C	0.38	0/3237	0.58	0/4371
1	D	0.38	0/3305	0.59	0/4465
All	All	0.38	0/12862	0.59	0/17368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3197	0	3090	21	0
1	B	2977	0	2888	13	0
1	C	3162	0	3066	16	0
1	D	3228	0	3125	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	65	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 (65) 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: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: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
1:B:127:ILE:O	1:B:131:ALA:HB2	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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 (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	390/415 (94%)	378 (97%)	12 (3%)	0	100	100
1	B	353/415 (85%)	343 (97%)	8 (2%)	2 (1%)	25	59
1	C	380/415 (92%)	368 (97%)	12 (3%)	0	100	100
1	D	395/415 (95%)	377 (95%)	16 (4%)	2 (0%)	29	64
All	All	1518/1660 (91%)	1466 (97%)	48 (3%)	4 (0%)	41	73

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/369 (95%)	318 (91%)	31 (9%)	9	34
1	B	324/369 (88%)	303 (94%)	21 (6%)	17	47
1	C	345/369 (94%)	321 (93%)	24 (7%)	15	45
1	D	353/369 (96%)	328 (93%)	25 (7%)	14	44
All	All	1371/1476 (93%)	1270 (93%)	101 (7%)	13	42

All (101) 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	89	GLU
1	A	106	LEU
1	A	117	ASP
1	A	162	VAL
1	A	163	ASN
1	A	165	MET
1	A	197	ARG
1	A	205	LEU
1	A	212	LEU
1	A	222	LYS
1	A	223	MET
1	A	225	LYS
1	A	229	VAL
1	A	237	THR
1	A	238	PRO
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	341	ASP
1	A	342	GLN
1	A	352	VAL
1	B	5	MET
1	B	11	PHE
1	B	17	LEU
1	B	18	LEU
1	B	34	LEU
1	B	70	ARG
1	B	117	ASP
1	B	126	ASP
1	B	189	ILE
1	B	205	LEU
1	B	212	LEU

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Mol	Chain	Res	Type
1	B	221	MET
1	B	292	ASN
1	B	312	LEU
1	B	317	LEU
1	B	324	LEU
1	B	327	ASN
1	B	336	LEU
1	B	341	ASP
1	B	370	ASP
1	B	381	PHE
1	C	5	MET
1	C	14	MET
1	C	18	LEU
1	C	26	ASN
1	C	34	LEU
1	C	61	ASP
1	C	62	THR
1	C	63	ILE
1	C	70	ARG
1	C	100	LYS
1	C	117	ASP
1	C	126	ASP
1	C	189	ILE
1	C	205	LEU
1	C	212	LEU
1	C	225	LYS
1	C	254	TYR
1	C	292	ASN
1	C	312	LEU
1	C	319	ASP
1	C	326	ARG
1	C	336	LEU
1	C	341	ASP
1	C	372	GLU
1	D	18	LEU
1	D	34	LEU
1	D	62	THR
1	D	70	ARG
1	D	71	MET
1	D	100	LYS
1	D	126	ASP
1	D	189	ILE

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Mol	Chain	Res	Type
1	D	205	LEU
1	D	212	LEU
1	D	225	LYS
1	D	230	ARG
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	341	ASP
1	D	375	LYS
1	D	378	GLU
1	D	402	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	335	HIS
1	A	342	GLN
1	B	16	ASN
1	B	335	HIS
1	C	16	ASN
1	C	335	HIS
1	D	16	ASN
1	D	190	HIS
1	D	335	HIS

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 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	B5G	D	900	-	36,39,39	0.98	1 (2%)	42,55,55	2.11	5 (11%)
2	B5G	A	900	-	36,39,39	1.01	2 (5%)	42,55,55	2.11	5 (11%)
2	B5G	C	900	-	36,39,39	1.01	2 (5%)	42,55,55	2.20	5 (11%)
2	B5G	B	900	-	36,39,39	1.04	1 (2%)	42,55,55	2.31	6 (14%)

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	D	900	-	-	0/20/41/41	0/5/5/5
2	B5G	A	900	-	-	0/20/41/41	0/5/5/5
2	B5G	C	900	-	-	0/20/41/41	0/5/5/5
2	B5G	B	900	-	-	0/20/41/41	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	B5G	C2-C1	-4.10	1.34	1.42
2	A	900	B5G	C2-C1	-3.74	1.35	1.42
2	C	900	B5G	C2-C1	-3.72	1.35	1.42
2	D	900	B5G	C2-C1	-3.66	1.35	1.42
2	A	900	B5G	C24-N23	2.06	1.40	1.36
2	C	900	B5G	C24-N23	2.04	1.40	1.36

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	B5G	C6-N5-C4	11.19	119.47	109.74
2	D	900	B5G	C3-C4-N5	8.36	118.25	110.60
2	C	900	B5G	C3-C4-N5	8.28	118.17	110.60
2	A	900	B5G	C6-N5-C4	8.28	116.93	109.74
2	C	900	B5G	C6-N5-C4	8.24	116.91	109.74
2	D	900	B5G	C6-N5-C4	8.08	116.77	109.74
2	A	900	B5G	C3-C4-N5	7.82	117.75	110.60
2	B	900	B5G	C3-C4-N5	5.54	115.67	110.60
2	B	900	B5G	C19-C15-N16	4.46	107.06	101.94
2	C	900	B5G	C19-C15-N16	4.15	106.70	101.94
2	D	900	B5G	C19-C15-N16	4.10	106.65	101.94
2	C	900	B5G	C17-N16-C15	-3.99	107.20	111.83
2	A	900	B5G	C19-C15-N16	3.89	106.41	101.94
2	B	900	B5G	C17-N16-C15	-3.52	107.74	111.83
2	A	900	B5G	C17-N16-C15	-3.38	107.90	111.83
2	D	900	B5G	C17-N16-C15	-3.38	107.91	111.83
2	B	900	B5G	C4-C3-C2	-2.82	107.80	113.00
2	C	900	B5G	C18-C17-N16	2.75	108.07	103.25
2	B	900	B5G	C18-C17-N16	2.72	108.03	103.25
2	A	900	B5G	C18-C17-N16	2.40	107.47	103.25
2	D	900	B5G	C18-C17-N16	2.27	107.24	103.25

There are no chirality outliers.

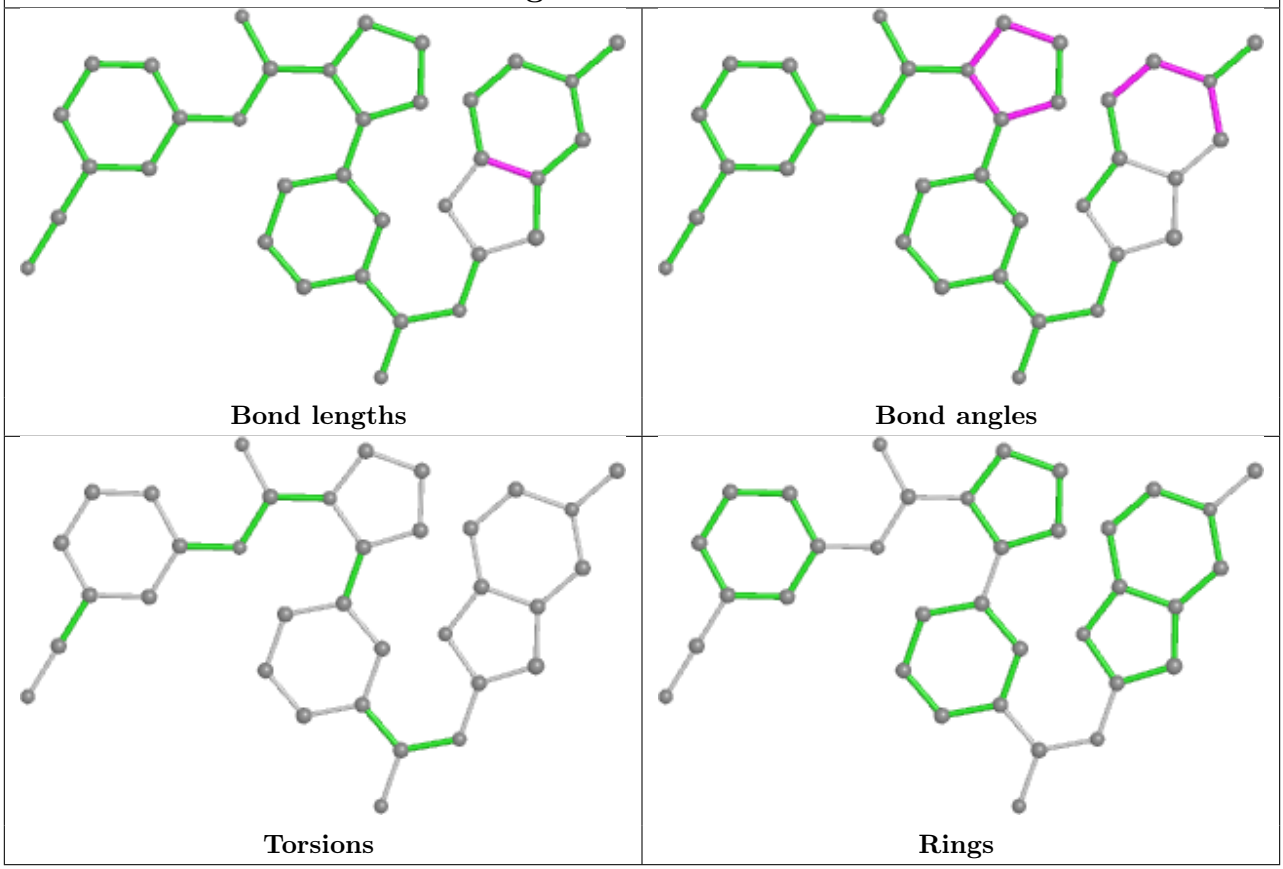
There are no torsion outliers.

There are no ring outliers.

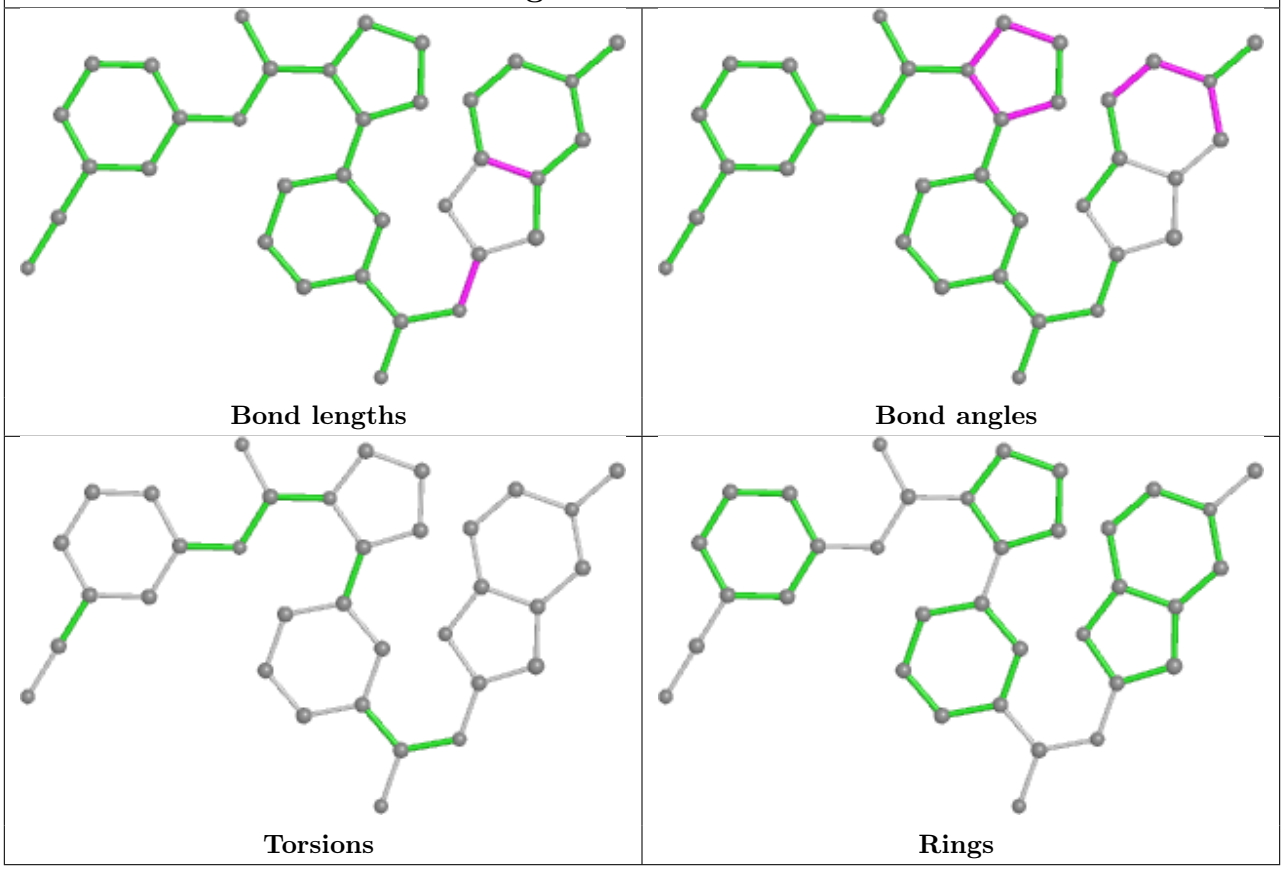
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

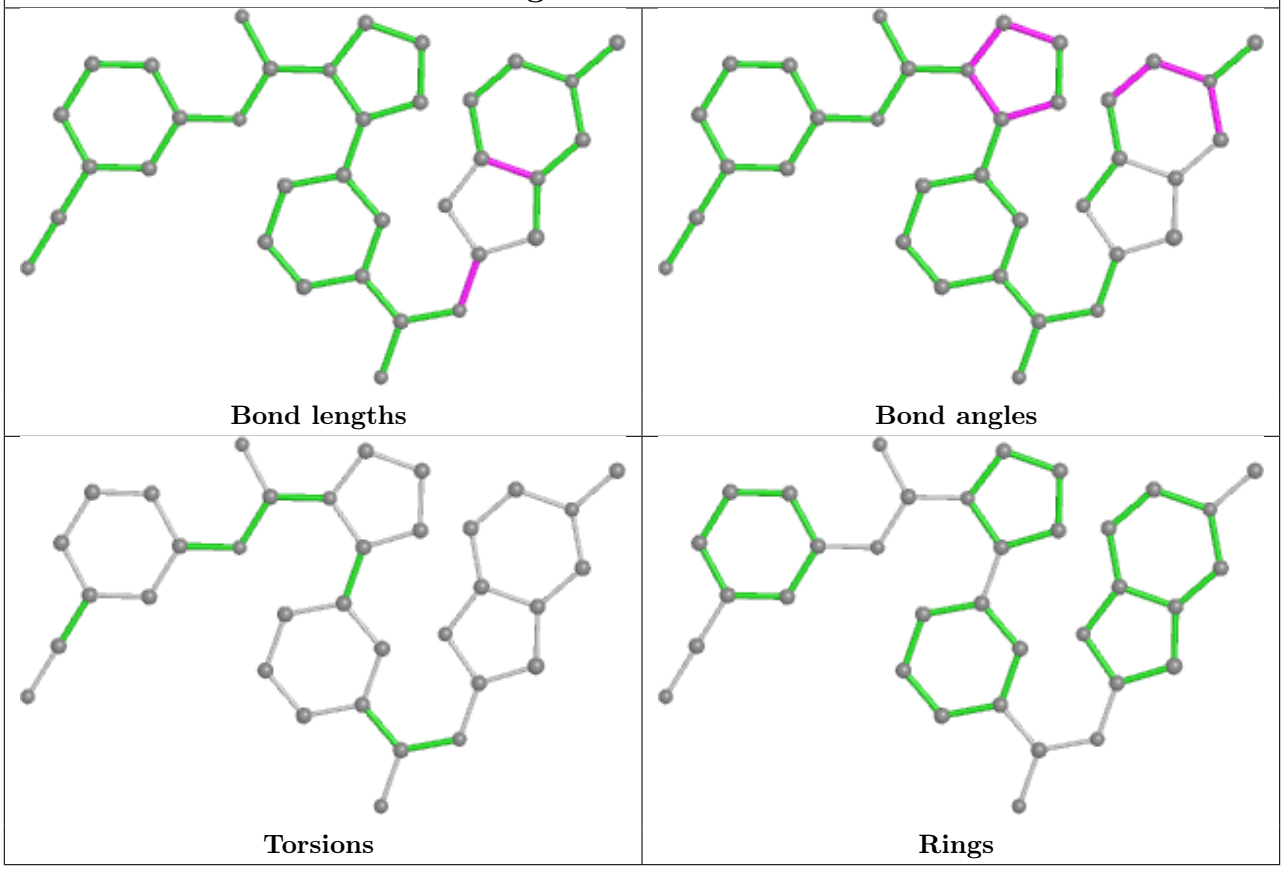
Ligand B5G D 900

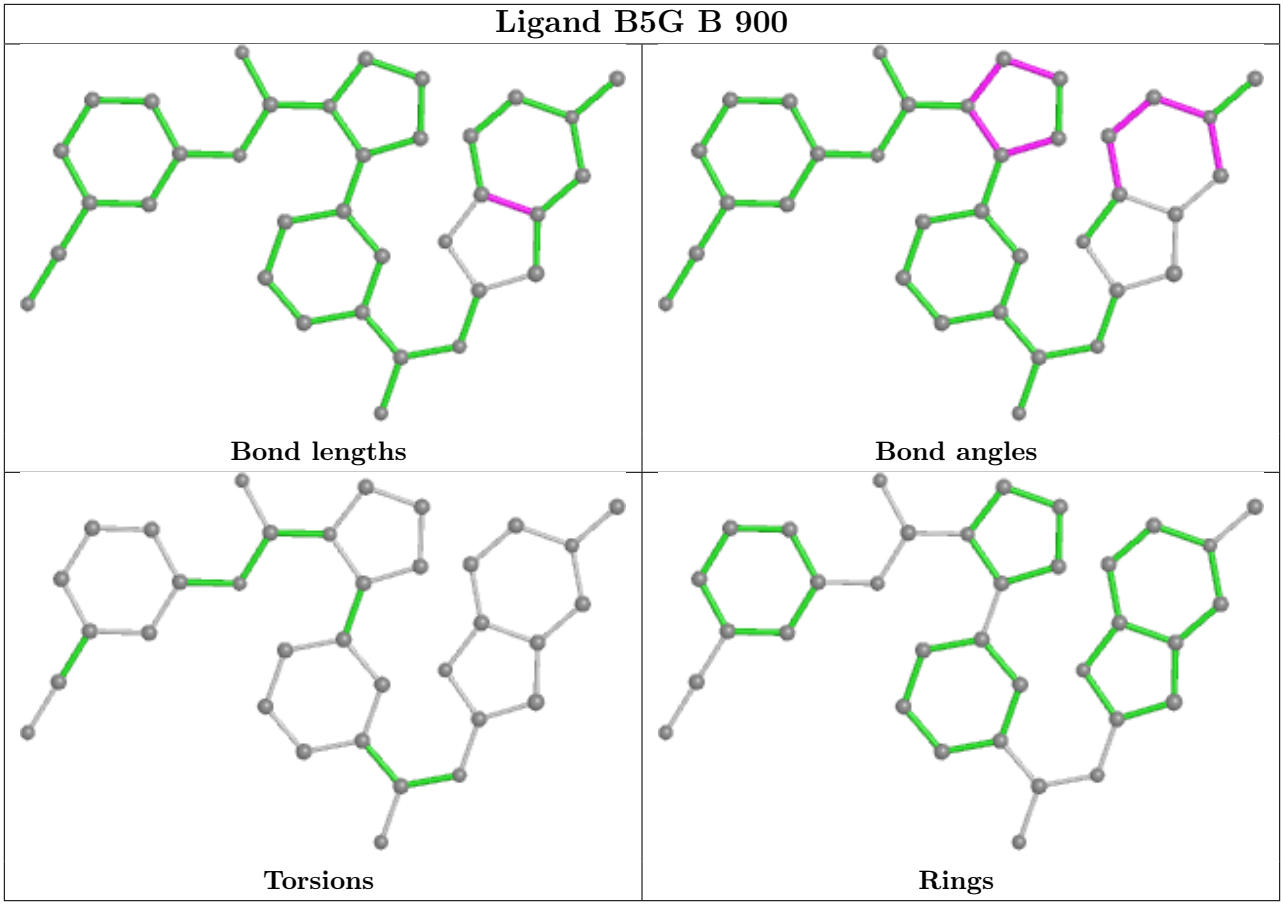


Ligand B5G A 900



Ligand B5G C 900





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%)	0.32	9 (2%) 60 39	82, 109, 155, 207	0
1	B	365/415 (87%)	0.94	53 (14%) 2 1	104, 151, 215, 241	0
1	C	388/415 (93%)	0.64	40 (10%) 6 2	81, 131, 202, 235	0
1	D	397/415 (95%)	0.27	6 (1%) 73 54	77, 107, 152, 166	0
All	All	1544/1660 (93%)	0.53	108 (6%) 16 7	77, 121, 198, 241	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	ALA	10.2
1	B	314	CYS	6.3
1	B	337	PHE	6.2
1	C	281	ASP	6.1
1	B	338	PHE	5.5
1	D	226	GLU	5.2
1	A	373	GLU	5.2
1	B	268	LEU	5.2
1	B	271	MET	4.9
1	B	312	LEU	4.7
1	C	338	PHE	4.4
1	B	92	LEU	4.3
1	B	278	PHE	4.2
1	C	232	ASP	4.2
1	C	287	TYR	4.2
1	C	305	ILE	4.2
1	B	160	ASP	4.2
1	C	241	ILE	4.2
1	C	231	CYS	4.2
1	B	336	LEU	4.1
1	B	311	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	272	LEU	4.0
1	C	291	MET	4.0
1	C	316	PHE	4.0
1	B	267	PHE	3.8
1	C	290	ILE	3.8
1	B	357	PRO	3.8
1	B	313	ILE	3.7
1	D	374	ASP	3.7
1	B	240	TYR	3.7
1	B	370	ASP	3.6
1	C	292	ASN	3.5
1	C	327	ASN	3.5
1	B	264	VAL	3.5
1	C	295	ASN	3.4
1	B	260	ASP	3.4
1	B	291	MET	3.4
1	B	315	ALA	3.4
1	C	311	ASN	3.4
1	B	310	LYS	3.3
1	B	277	PRO	3.2
1	C	322	VAL	3.2
1	C	176	ARG	3.2
1	C	233	THR	3.2
1	C	278	PHE	3.2
1	B	342	GLN	3.1
1	B	174	TRP	3.1
1	B	91	GLN	3.1
1	B	365	THR	3.1
1	A	13	LYS	3.1
1	B	178	TYR	3.0
1	B	172	GLU	3.0
1	C	269	TYR	3.0
1	A	9	THR	3.0
1	B	362	ASP	2.9
1	B	292	ASN	2.9
1	B	159	GLY	2.9
1	C	313	ILE	2.9
1	C	299	PHE	2.9
1	C	337	PHE	2.8
1	A	12	GLU	2.8
1	C	277	PRO	2.8
1	B	307	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	234	ALA	2.7
1	B	237	THR	2.7
1	B	269	TYR	2.7
1	C	259	CYS	2.6
1	C	326	ARG	2.6
1	C	235	VAL	2.6
1	D	223	MET	2.6
1	B	290	ILE	2.6
1	B	80	LYS	2.5
1	A	10	ARG	2.5
1	C	298	THR	2.5
1	C	314	CYS	2.5
1	B	208	LYS	2.5
1	B	170	VAL	2.5
1	B	206	LEU	2.4
1	C	170	VAL	2.4
1	A	350	ASP	2.4
1	B	93	VAL	2.4
1	A	306	SER	2.4
1	B	241	ILE	2.4
1	B	81	VAL	2.3
1	C	336	LEU	2.2
1	C	168	TYR	2.2
1	B	225	LYS	2.2
1	B	132	ASN	2.2
1	C	229	VAL	2.2
1	C	255	TYR	2.2
1	B	205	LEU	2.2
1	D	337	PHE	2.2
1	A	14	MET	2.2
1	B	295	ASN	2.1
1	C	273	VAL	2.1
1	A	21	PRO	2.1
1	B	104	MET	2.1
1	B	255	TYR	2.1
1	B	316	PHE	2.1
1	C	212	LEU	2.1
1	C	272	LEU	2.1
1	B	270	GLU	2.1
1	D	375	LYS	2.1
1	C	317	LEU	2.1
1	D	338	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	300	PRO	2.0
1	C	402	ASN	2.0
1	B	17	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 monosaccharides in this entry.

6.4 Ligands (i)

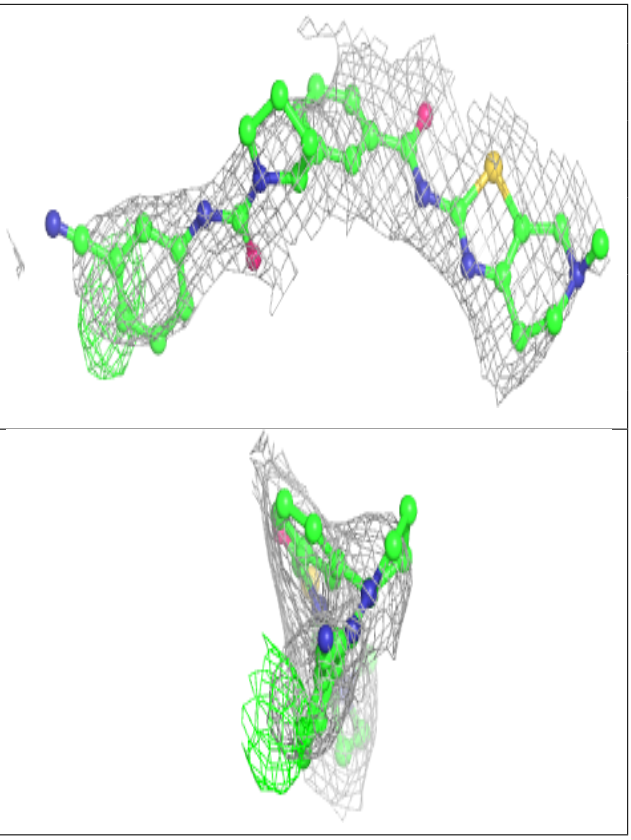
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B5G	B	900	35/35	0.83	0.32	137,143,148,150	0
2	B5G	D	900	35/35	0.88	0.32	93,101,103,104	0
2	B5G	A	900	35/35	0.91	0.29	102,103,107,113	0
2	B5G	C	900	35/35	0.93	0.22	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.

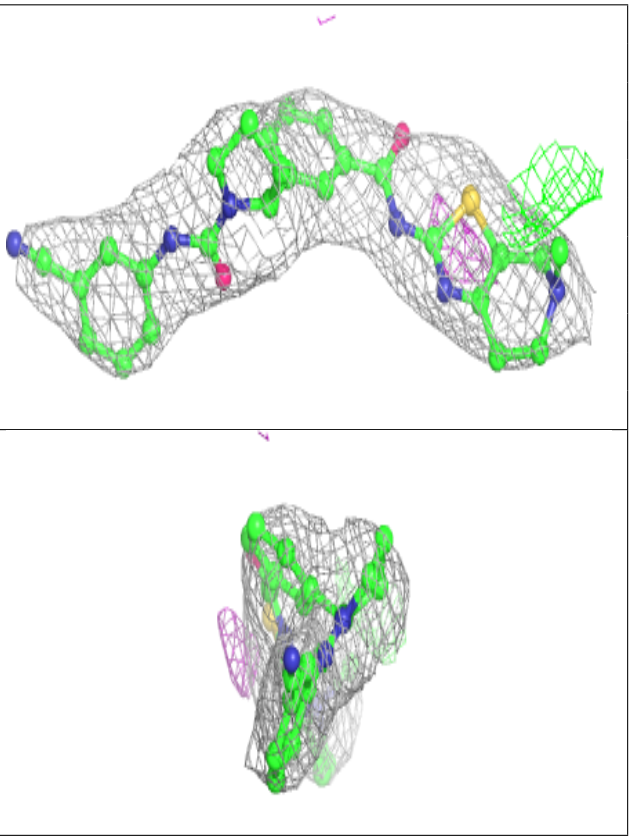
Electron density around B5G B 900:

$2mF_o$-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 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 A 900:

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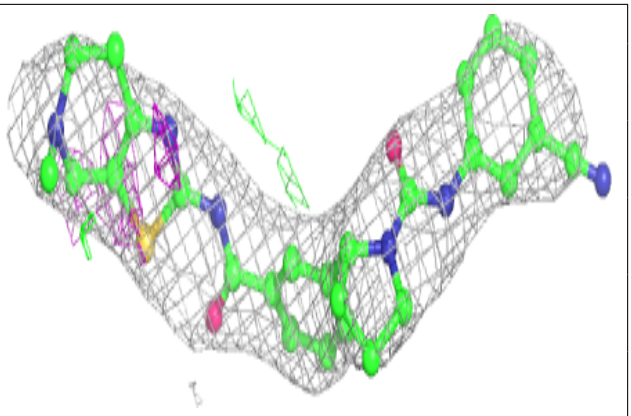
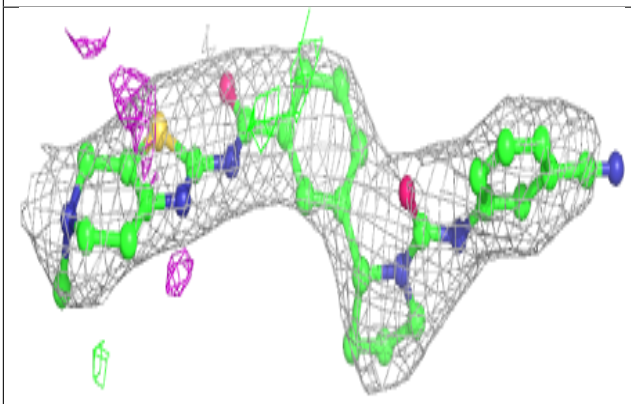
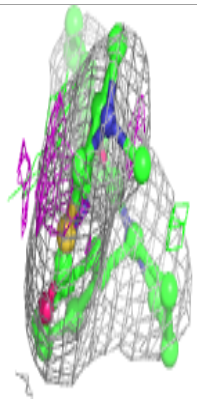
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

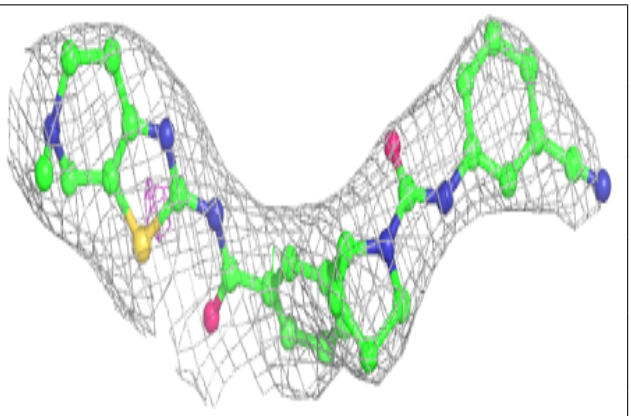


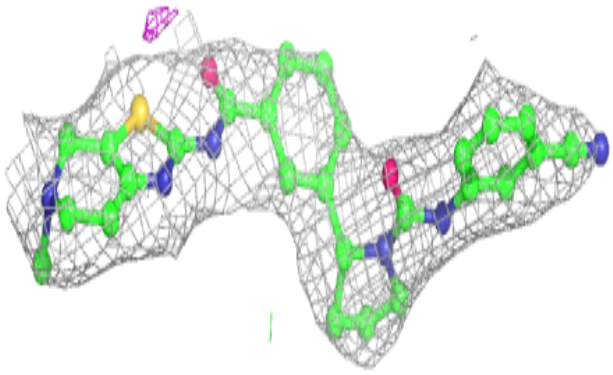


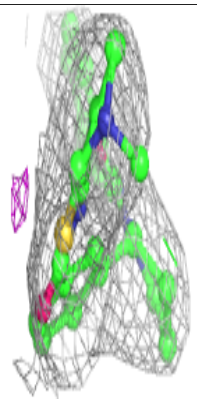


Electron density around B5G C 900:

$2mF_o$-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.