



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:01 PM UTC

PDB ID : 5WNE / pdb_00005wne
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 : 2.60 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

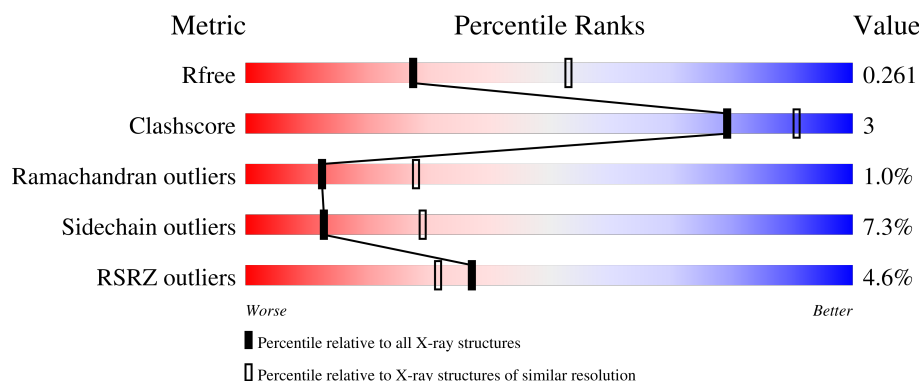
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 4 unique types of molecules in this entry. The entry contains 12536 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.

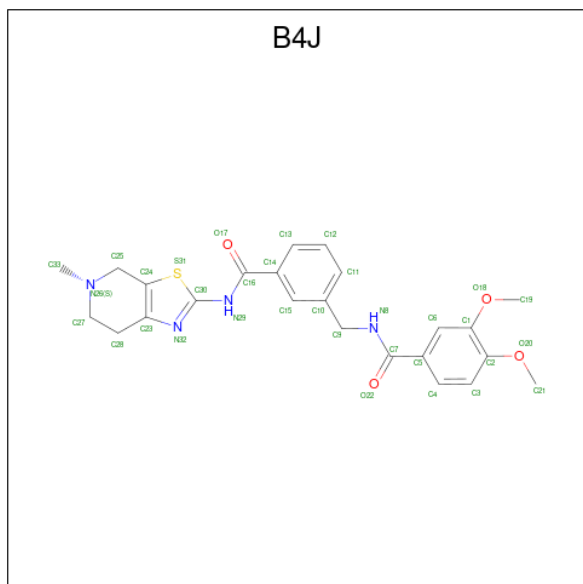
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3119	1995	514	589	21			
1	B	352	Total	C	N	O	S	0	0	0
			2885	1862	471	531	21			
1	C	384	Total	C	N	O	S	0	0	0
			3135	2011	518	584	22			
1	D	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	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 3,4-dimethoxy-N-({3-[(5-methyl-4,5,6,7-tetrahydro[1,3]thiazolo[5,4-c]pyridin-2-yl)carbamoyl]phenyl}methyl)benzamide (CCD ID: B4J) (formula: C₂₄H₂₆N₄O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	24	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			33	24	4	4	1		
2	C	1	Total	C	N	O	S	0	0
			33	24	4	4	1		
2	D	1	Total	C	N	O	S	0	0
			33	24	4	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

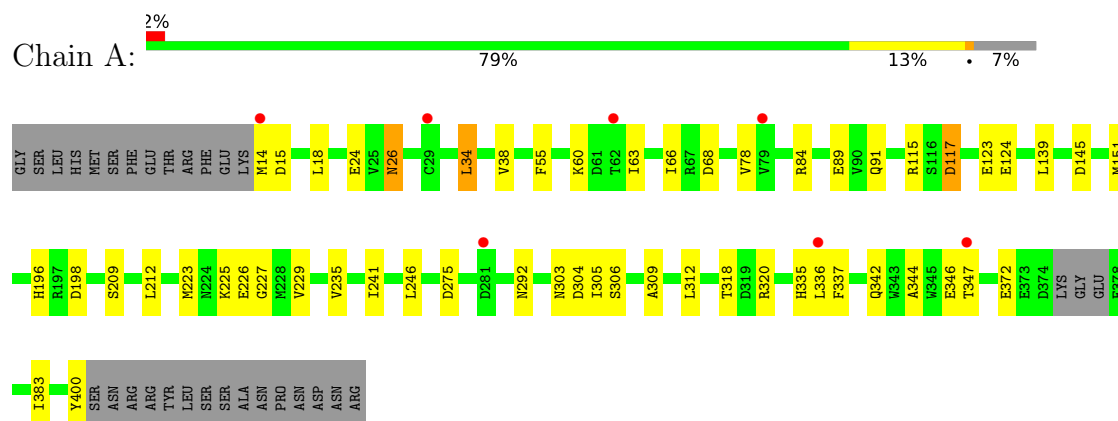
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	3	Total	O	0	0
			3	3		
4	C	8	Total	O	0	0
			8	8		
4	D	7	Total	O	0	0
			7	7		

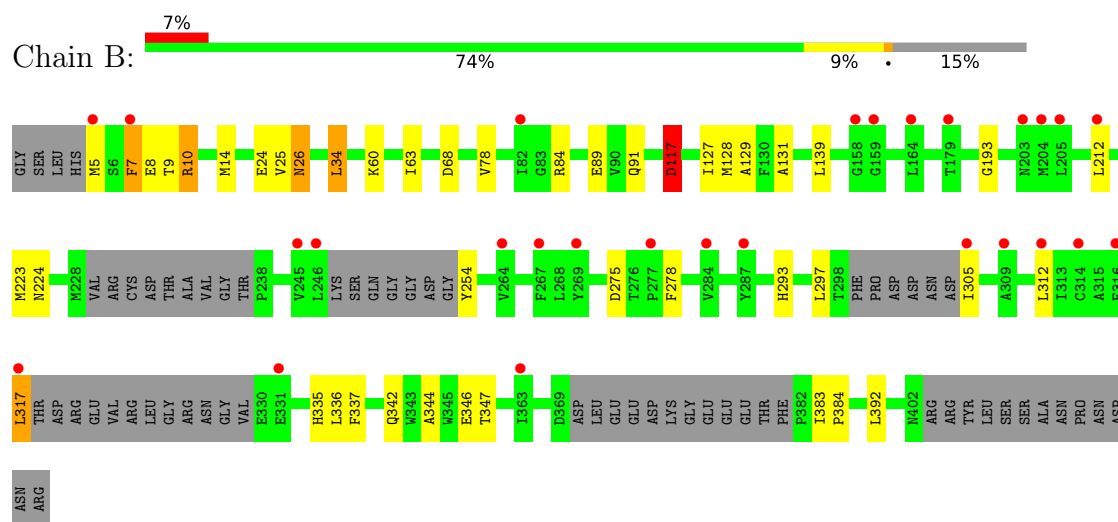
3 Residue-property plots [i](#)

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.

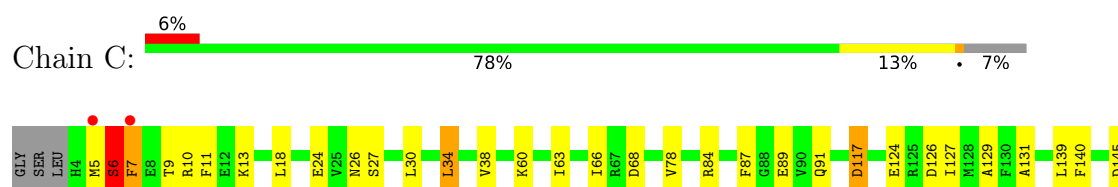
• Molecule 1: Rho-associated protein kinase 1

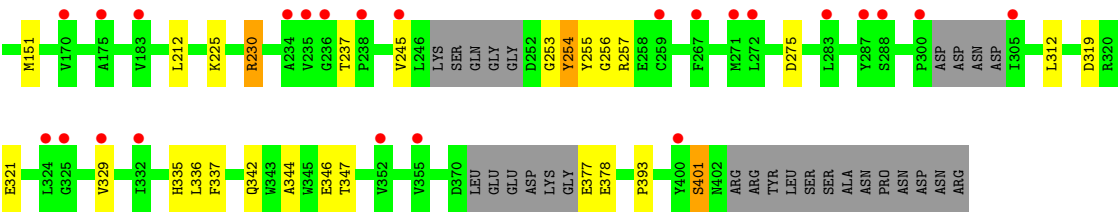


• Molecule 1: Rho-associated protein kinase 1

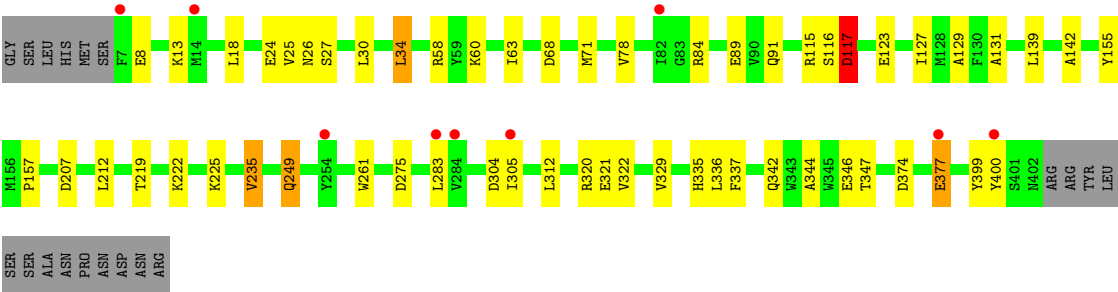
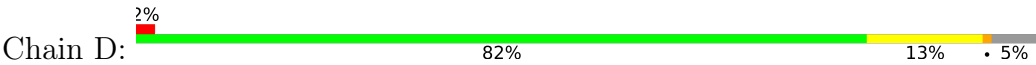


• Molecule 1: Rho-associated protein kinase 1





● 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	161.85Å 82.16Å 169.37Å 90.00° 115.05° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.60) 99.8 (40.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.228 , 0.246 0.244 , 0.261	Depositor DCC
R_{free} test set	3147 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12536	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: GOL, B4J

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	0.70	0/3193	1.25	4/4316 (0.1%)
1	B	0.69	0/2954	1.25	2/3982 (0.1%)
1	C	0.70	0/3210	1.27	11/4334 (0.3%)
1	D	0.70	0/3299	1.27	4/4457 (0.1%)
All	All	0.70	0/12656	1.26	21/17089 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	SER	N-CA-C	7.76	122.66	112.72
1	D	117	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	117	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	117	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	292	ASN	CA-CB-CG	6.28	118.88	112.60
1	B	117	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	11	PHE	CA-C-N	5.78	128.35	120.54
1	C	11	PHE	C-N-CA	5.78	128.35	120.54
1	D	304	ASP	N-CA-C	-5.69	106.01	113.12
1	A	26	ASN	CA-CB-CG	5.66	118.26	112.60
1	C	329	VAL	CA-C-N	5.65	128.42	120.28
1	C	329	VAL	C-N-CA	5.65	128.42	120.28
1	D	207	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	87	PHE	CA-CB-CG	5.22	119.02	113.80
1	D	322	VAL	N-CA-C	-5.21	108.76	113.71
1	C	237	THR	CB-CA-C	5.17	115.84	108.76
1	C	145	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	26	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	145	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	256	GLY	CA-C-N	5.02	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	GLY	C-N-CA	5.02	127.51	120.28

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	3119	0	3023	15	0
1	B	2885	0	2818	20	0
1	C	3135	0	3045	20	0
1	D	3222	0	3120	18	0
2	A	33	0	0	0	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	1	0
3	A	6	0	8	0	0
4	A	19	0	0	0	0
4	B	3	0	0	0	0
4	C	8	0	0	0	0
4	D	7	0	0	0	0
All	All	12536	0	12014	66	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 (66) 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:D:71:MET:H	1:D:400:TYR:HE1	1.42	0.65
1:C:6:SER:HB2	1:C:10:ARG:HG3	1.77	0.65
1:C:7:PHE:O	1:C:10:ARG:HB2	1.99	0.62
1:D:377:GLU:HA	1:D:377:GLU:OE2	2.01	0.60
1:B:297:LEU:HD22	1:B:317:LEU:HD22	1.83	0.60
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PHE:HZ	1:B:317:LEU:HD21	1.68	0.58
1:B:193:GLY:HA2	1:B:223:MET:HE2	1.85	0.58
1:B:335:HIS:HD2	1:B:337:PHE:H	1.54	0.56
1:B:7:PHE:HA	1:B:9:THR:N	2.21	0.56
1:A:335:HIS:HD2	1:A:337:PHE:H	1.54	0.55
1:B:129:ALA:HB2	1:B:139:LEU:HD23	1.89	0.55
1:C:124:GLU:HG2	1:C:151:MET:HE1	1.89	0.54
1:D:335:HIS:HD2	1:D:337:PHE:H	1.53	0.54
1:C:140:PHE:O	1:C:401:SER:HB2	2.06	0.54
1:C:335:HIS:HD2	1:C:337:PHE:H	1.54	0.54
1:C:230:ARG:HG2	1:C:254:TYR:HB3	1.89	0.53
1:A:124:GLU:HG2	1:A:151:MET:HE1	1.90	0.52
1:B:128:MET:HB3	1:B:139:LEU:HB2	1.91	0.52
1:A:344:ALA:HB3	1:A:347:THR:HG22	1.92	0.52
1:C:344:ALA:HB3	1:C:347:THR:HG22	1.92	0.51
1:B:344:ALA:HB3	1:B:347:THR:HG22	1.92	0.51
1:A:15:ASP:HB2	1:A:18:LEU:HD12	1.92	0.51
1:D:344:ALA:HB3	1:D:347:THR:HG22	1.92	0.50
1:C:27:SER:HB2	1:D:18:LEU:HD13	1.93	0.49
1:B:293:HIS:HB2	1:B:317:LEU:HD21	1.95	0.47
1:A:34:LEU:HD23	1:A:63:ILE:HD11	1.97	0.47
1:C:66:ILE:HD11	1:D:25:VAL:HG21	1.97	0.46
1:A:66:ILE:HD12	1:B:14:MET:HE1	1.97	0.46
1:C:34:LEU:HD23	1:C:63:ILE:HD11	1.97	0.45
1:D:127:ILE:O	1:D:131:ALA:HB2	2.16	0.45
1:B:7:PHE:HB3	1:B:10:ARG:HD2	1.99	0.45
1:D:142:ALA:HB3	1:D:399:TYR:HB3	1.99	0.44
1:B:34:LEU:HD23	1:B:63:ILE:HD11	1.99	0.44
1:A:196:HIS:HD2	1:A:198:ASP:H	1.65	0.44
1:C:245:VAL:HG22	1:C:255:TYR:CZ	2.53	0.44
1:D:261:TRP:CZ2	1:D:329:VAL:HG12	2.52	0.44
1:C:6:SER:HB3	1:C:9:THR:HB	2.00	0.43
1:B:293:HIS:HB2	1:B:317:LEU:CD2	2.48	0.43
1:C:129:ALA:HB2	1:C:139:LEU:HD23	2.01	0.43
2:D:900:B4J:O17	2:D:900:B4J:S31	2.77	0.43
1:D:84:ARG:HD3	1:D:89:GLU:HB3	1.99	0.43
1:A:305:ILE:O	1:A:309:ALA:HB3	2.19	0.43
1:B:84:ARG:HD3	1:B:89:GLU:HB3	2.00	0.42
1:C:18:LEU:HD13	1:D:27:SER:HB2	2.01	0.42
1:C:335:HIS:CD2	1:C:337:PHE:H	2.36	0.42
1:A:223:MET:HB3	1:A:227:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HD3	1:A:89:GLU:HB3	2.00	0.42
1:A:55:PHE:HB2	1:B:392:LEU:HB3	2.02	0.42
1:A:38:VAL:HG21	1:A:63:ILE:HG13	2.02	0.42
1:A:335:HIS:CD2	1:A:337:PHE:H	2.36	0.42
1:C:84:ARG:HD3	1:C:89:GLU:HB3	2.01	0.41
1:A:66:ILE:HD11	1:B:25:VAL:HG21	2.01	0.41
1:C:38:VAL:HG21	1:C:63:ILE:HG13	2.02	0.41
1:B:335:HIS:CD2	1:B:337:PHE:H	2.36	0.41
1:C:393:PRO:HA	1:D:58:ARG:NH2	2.36	0.41
1:D:155:TYR:O	1:D:157:PRO:HD3	2.21	0.41
1:D:34:LEU:HD23	1:D:63:ILE:HD11	2.01	0.41
1:C:127:ILE:O	1:C:131:ALA:HB2	2.21	0.41
1:B:383:ILE:HA	1:B:384:PRO:HD3	1.93	0.41
1:D:129:ALA:HB2	1:D:139:LEU:HD23	2.03	0.41
1:D:335:HIS:CD2	1:D:337:PHE:H	2.36	0.40
1:A:241:ILE:HG21	1:A:246:LEU:HD13	2.02	0.40
1:B:127:ILE:O	1:B:131:ALA:HB2	2.21	0.40
1:B:7:PHE:HA	1:B:9:THR:H	1.85	0.40
1:D:219:THR:HB	1:D:235:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/415 (92%)	359 (94%)	17 (4%)	4 (1%)	11	25
1	B	340/415 (82%)	325 (96%)	12 (4%)	3 (1%)	14	30
1	C	376/415 (91%)	357 (95%)	16 (4%)	3 (1%)	16	34
1	D	394/415 (95%)	373 (95%)	16 (4%)	5 (1%)	9	21
All	All	1490/1660 (90%)	1414 (95%)	61 (4%)	15 (1%)	12	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	224	ASN
1	C	60	LYS
1	D	249	GLN
1	A	60	LYS
1	A	303	ASN
1	A	304	ASP
1	B	60	LYS
1	D	60	LYS
1	D	117	ASP
1	D	374	ASP
1	A	306	SER
1	D	116	SER
1	B	117	ASP
1	C	7	PHE
1	C	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	341/369 (92%)	314 (92%)	27 (8%)	11	26
1	B	316/369 (86%)	296 (94%)	20 (6%)	16	36
1	C	343/369 (93%)	317 (92%)	26 (8%)	12	27
1	D	352/369 (95%)	326 (93%)	26 (7%)	13	29
All	All	1352/1476 (92%)	1253 (93%)	99 (7%)	13	29

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	MET
1	A	24	GLU
1	A	26	ASN
1	A	34	LEU
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	78	VAL
1	A	91	GLN
1	A	115	ARG
1	A	117	ASP
1	A	123	GLU
1	A	139	LEU
1	A	209	SER
1	A	212	LEU
1	A	225	LYS
1	A	226	GLU
1	A	229	VAL
1	A	235	VAL
1	A	275	ASP
1	A	312	LEU
1	A	318	THR
1	A	320	ARG
1	A	336	LEU
1	A	342	GLN
1	A	346	GLU
1	A	372	GLU
1	A	383	ILE
1	A	400	TYR
1	B	5	MET
1	B	7	PHE
1	B	8	GLU
1	B	10	ARG
1	B	24	GLU
1	B	26	ASN
1	B	34	LEU
1	B	68	ASP
1	B	78	VAL
1	B	91	GLN
1	B	117	ASP
1	B	212	LEU
1	B	254	TYR
1	B	275	ASP
1	B	305	ILE
1	B	312	LEU
1	B	317	LEU
1	B	336	LEU
1	B	342	GLN
1	B	346	GLU

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Mol	Chain	Res	Type
1	C	5	MET
1	C	6	SER
1	C	13	LYS
1	C	24	GLU
1	C	26	ASN
1	C	34	LEU
1	C	68	ASP
1	C	78	VAL
1	C	91	GLN
1	C	117	ASP
1	C	126	ASP
1	C	212	LEU
1	C	225	LYS
1	C	230	ARG
1	C	254	TYR
1	C	257	ARG
1	C	275	ASP
1	C	312	LEU
1	C	319	ASP
1	C	321	GLU
1	C	336	LEU
1	C	342	GLN
1	C	346	GLU
1	C	377	GLU
1	C	378	GLU
1	C	401	SER
1	D	8	GLU
1	D	13	LYS
1	D	24	GLU
1	D	26	ASN
1	D	34	LEU
1	D	68	ASP
1	D	78	VAL
1	D	91	GLN
1	D	115	ARG
1	D	117	ASP
1	D	123	GLU
1	D	212	LEU
1	D	222	LYS
1	D	225	LYS
1	D	235	VAL
1	D	249	GLN

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Mol	Chain	Res	Type
1	D	275	ASP
1	D	283	LEU
1	D	305	ILE
1	D	312	LEU
1	D	320	ARG
1	D	321	GLU
1	D	336	LEU
1	D	342	GLN
1	D	346	GLU
1	D	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	138	GLN
1	A	190	HIS
1	A	196	HIS
1	A	211	HIS
1	A	292	ASN
1	A	311	ASN
1	A	335	HIS
1	B	54	ASN
1	B	138	GLN
1	B	292	ASN
1	B	311	ASN
1	B	335	HIS
1	C	4	HIS
1	C	54	ASN
1	C	138	GLN
1	C	292	ASN
1	C	311	ASN
1	C	335	HIS
1	C	402	ASN
1	D	54	ASN
1	D	138	GLN
1	D	190	HIS
1	D	211	HIS
1	D	292	ASN
1	D	303	ASN
1	D	311	ASN
1	D	335	HIS

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 ⓘ

5 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	B4J	C	900	-	35,36,36	1.00	1 (2%)	46,50,50	2.43	12 (26%)
2	B4J	B	900	-	35,36,36	1.07	3 (8%)	46,50,50	2.71	12 (26%)
3	GOL	A	502	-	5,5,5	0.06	0	5,5,5	0.11	0
2	B4J	D	900	-	35,36,36	1.10	4 (11%)	46,50,50	2.35	9 (19%)
2	B4J	A	501	-	35,36,36	1.06	3 (8%)	46,50,50	2.52	11 (23%)

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	B4J	C	900	-	-	0/21/30/30	0/4/4/4
2	B4J	B	900	-	-	4/21/30/30	0/4/4/4
3	GOL	A	502	-	-	0/4/4/4	-
2	B4J	D	900	-	-	0/21/30/30	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B4J	A	501	-	-	0/21/30/30	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	B4J	C23-N32	-2.91	1.32	1.38
2	D	900	B4J	C25-N26	2.84	1.48	1.46
2	D	900	B4J	C23-N32	-2.68	1.32	1.38
2	A	501	B4J	C23-N32	-2.64	1.32	1.38
2	B	900	B4J	C25-C24	2.60	1.52	1.50
2	B	900	B4J	C23-N32	-2.59	1.32	1.38
2	D	900	B4J	C25-C24	2.51	1.52	1.50
2	B	900	B4J	C25-N26	2.22	1.48	1.46
2	A	501	B4J	C28-C23	2.18	1.54	1.50
2	A	501	B4J	C25-N26	2.07	1.47	1.46
2	D	900	B4J	C28-C23	2.00	1.53	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	B4J	C28-C27-N26	10.75	120.81	110.71
2	C	900	B4J	C28-C27-N26	10.17	120.26	110.71
2	B	900	B4J	C28-C27-N26	10.12	120.22	110.71
2	D	900	B4J	C28-C27-N26	9.86	119.97	110.71
2	B	900	B4J	S31-C30-N32	-8.05	108.58	115.78
2	C	900	B4J	S31-C30-N32	-6.92	109.59	115.78
2	A	501	B4J	S31-C30-N32	-6.72	109.77	115.78
2	D	900	B4J	S31-C30-N32	-6.37	110.08	115.78
2	B	900	B4J	C30-N32-C23	6.20	118.97	110.09
2	C	900	B4J	C30-N32-C23	5.99	118.67	110.09
2	B	900	B4J	C24-S31-C30	5.97	91.72	88.76
2	D	900	B4J	C30-N32-C23	5.70	118.25	110.09
2	A	501	B4J	C30-N32-C23	5.65	118.18	110.09
2	A	501	B4J	C25-C24-S31	4.86	126.30	121.91
2	B	900	B4J	C25-C24-S31	4.06	125.58	121.91
2	D	900	B4J	C25-C24-S31	4.05	125.57	121.91
2	D	900	B4J	C24-S31-C30	3.80	90.65	88.76
2	A	501	B4J	C24-S31-C30	3.73	90.61	88.76
2	B	900	B4J	O18-C1-C2	3.65	120.36	115.40
2	C	900	B4J	C24-S31-C30	3.49	90.50	88.76
2	C	900	B4J	C25-C24-S31	3.22	124.82	121.91
2	C	900	B4J	S31-C30-N29	3.14	127.93	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	B4J	C19-O18-C1	3.10	122.06	117.51
2	C	900	B4J	C19-O18-C1	3.09	122.04	117.51
2	B	900	B4J	C14-C16-N29	2.97	120.53	116.25
2	A	501	B4J	C19-O18-C1	2.95	121.83	117.51
2	A	501	B4J	O20-C2-C1	2.86	119.29	115.40
2	B	900	B4J	S31-C30-N29	2.77	127.43	123.72
2	B	900	B4J	C21-O20-C2	2.77	121.57	117.51
2	C	900	B4J	C21-O20-C2	2.69	121.46	117.51
2	B	900	B4J	O20-C2-C1	2.67	119.03	115.40
2	D	900	B4J	O20-C2-C1	2.60	118.94	115.40
2	A	501	B4J	C24-C25-N26	-2.48	107.61	109.49
2	B	900	B4J	O18-C1-C6	-2.44	119.87	124.08
2	A	501	B4J	O18-C1-C2	2.37	118.61	115.40
2	C	900	B4J	C30-N29-C16	2.31	127.50	123.67
2	D	900	B4J	O18-C1-C2	2.18	118.37	115.40
2	A	501	B4J	O20-C2-C3	-2.18	120.62	124.30
2	C	900	B4J	O20-C2-C1	2.17	118.35	115.40
2	D	900	B4J	C21-O20-C2	2.13	120.63	117.51
2	A	501	B4J	C14-C16-N29	2.12	119.31	116.25
2	B	900	B4J	C24-C25-N26	2.09	111.07	109.49
2	C	900	B4J	O18-C1-C2	2.07	118.21	115.40
2	C	900	B4J	C14-C16-N29	2.06	119.21	116.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	B4J	C2-C1-O18-C19
2	B	900	B4J	C1-C2-O20-C21
2	B	900	B4J	C6-C1-O18-C19
2	B	900	B4J	C3-C2-O20-C21

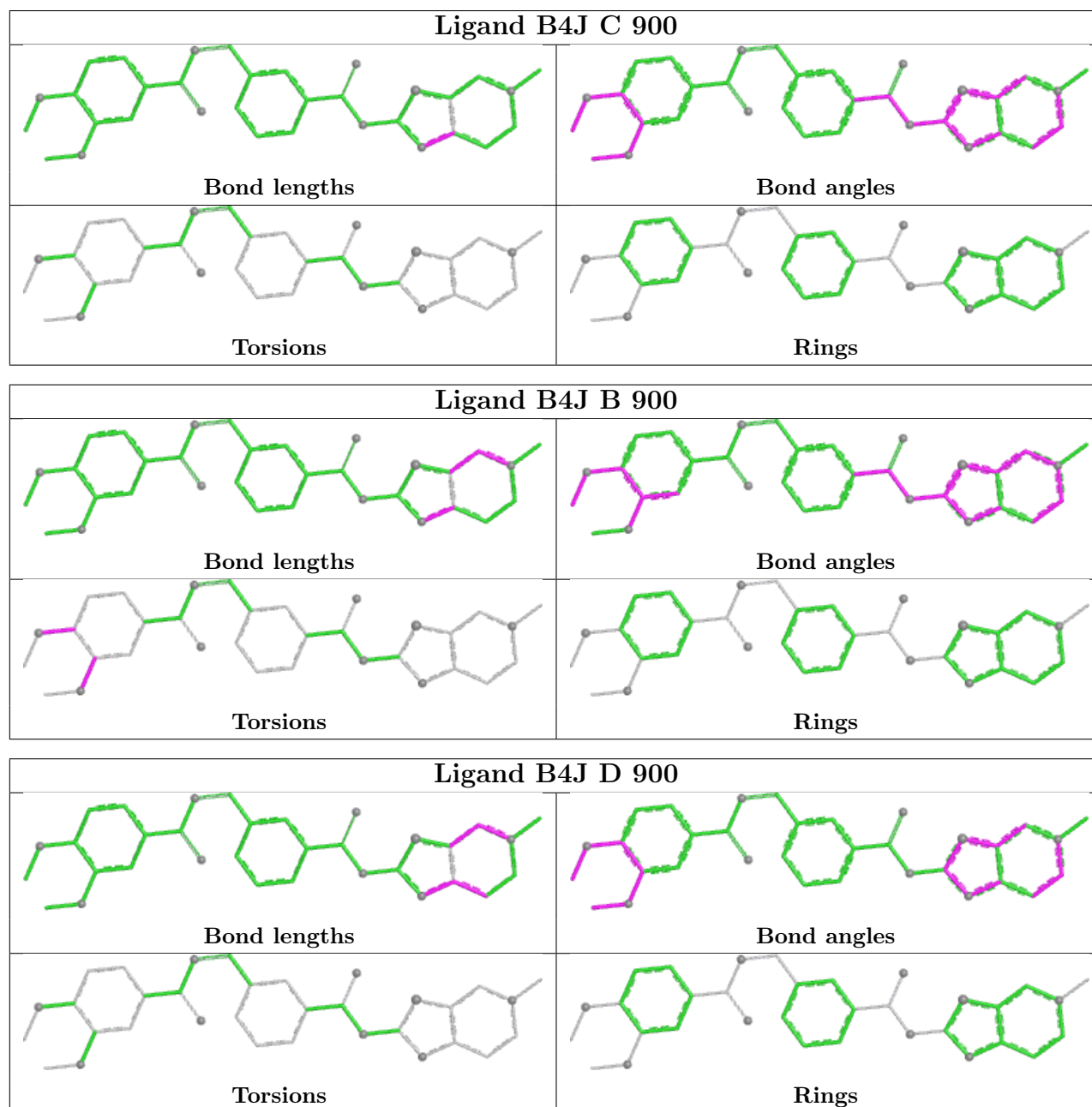
There are no ring outliers.

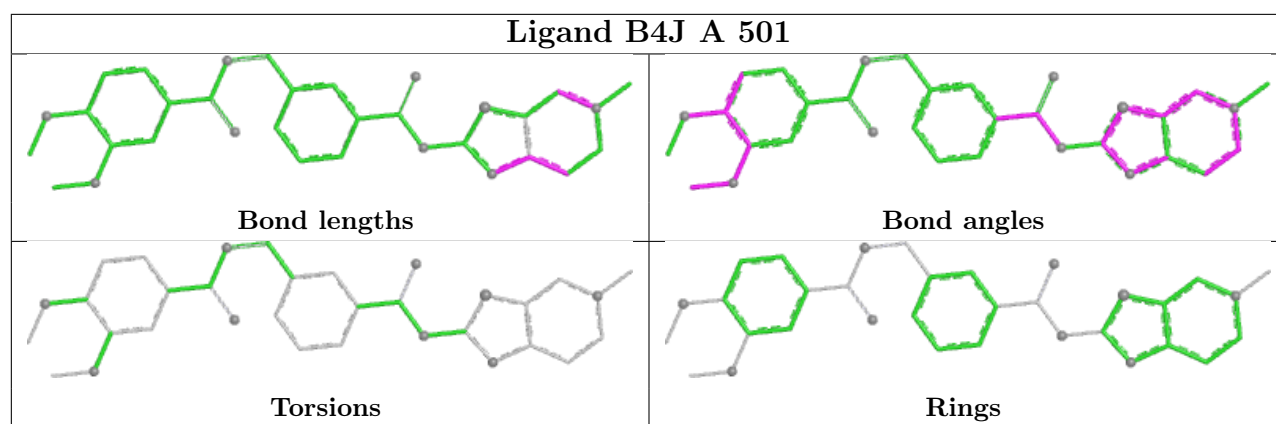
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	B4J	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	384/415 (92%)	0.13	7 (1%) 67 63	54, 81, 124, 169	0
1	B	352/415 (84%)	0.76	27 (7%) 19 15	89, 154, 216, 234	0
1	C	384/415 (92%)	0.55	26 (6%) 23 19	58, 119, 218, 244	0
1	D	396/415 (95%)	0.17	9 (2%) 61 55	51, 82, 125, 151	0
All	All	1516/1660 (91%)	0.39	69 (4%) 37 32	51, 100, 208, 244	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	TYR	4.8
1	C	235	VAL	4.4
1	C	329	VAL	4.1
1	B	309	ALA	3.8
1	C	287	TYR	3.7
1	D	377	GLU	3.5
1	B	305	ILE	3.5
1	B	314	CYS	3.5
1	C	305	ILE	3.5
1	C	5	MET	3.5
1	B	287	TYR	3.4
1	A	347	THR	3.4
1	B	312	LEU	3.2
1	B	205	LEU	3.2
1	B	204	MET	3.0
1	D	283	LEU	3.0
1	B	277	PRO	2.9
1	B	179	THR	2.9
1	C	300	PRO	2.9
1	C	267	PHE	2.9
1	C	355	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	14	MET	2.8
1	C	272	LEU	2.8
1	B	158	GLY	2.8
1	B	316	PHE	2.8
1	C	325	GLY	2.7
1	A	62	THR	2.7
1	B	245	VAL	2.7
1	B	203	ASN	2.7
1	C	245	VAL	2.7
1	A	281	ASP	2.7
1	B	331	GLU	2.6
1	B	264	VAL	2.6
1	C	288	SER	2.6
1	B	82	ILE	2.6
1	C	175	ALA	2.6
1	D	254	TYR	2.5
1	D	7	PHE	2.5
1	B	317	LEU	2.4
1	C	332	ILE	2.4
1	C	238	PRO	2.4
1	B	267	PHE	2.4
1	D	14	MET	2.4
1	B	269	TYR	2.4
1	C	352	VAL	2.4
1	B	7	PHE	2.4
1	B	246	LEU	2.3
1	C	236	GLY	2.3
1	D	82	ILE	2.3
1	C	7	PHE	2.3
1	A	29	CYS	2.2
1	B	164	LEU	2.2
1	B	284	VAL	2.2
1	C	259	CYS	2.2
1	C	170	VAL	2.2
1	C	234	ALA	2.2
1	B	5	MET	2.2
1	B	363	ILE	2.2
1	C	183	VAL	2.1
1	C	283	LEU	2.1
1	C	324	LEU	2.1
1	D	305	ILE	2.1
1	C	400	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	284	VAL	2.1
1	A	336	LEU	2.0
1	B	212	LEU	2.0
1	B	159	GLY	2.0
1	A	79	VAL	2.0
1	C	271	MET	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](#)

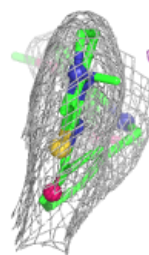
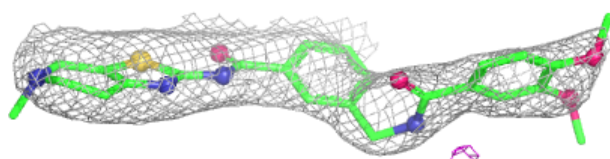
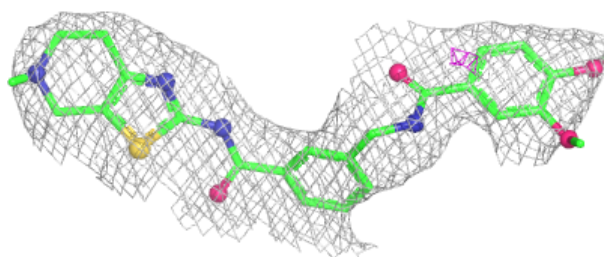
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	502	6/6	0.65	0.10	133,134,134,134	0
2	B4J	B	900	33/33	0.92	0.10	133,141,149,157	0
2	B4J	A	501	33/33	0.93	0.10	67,70,78,81	0
2	B4J	C	900	33/33	0.94	0.10	87,91,95,96	0
2	B4J	D	900	33/33	0.96	0.07	57,59,61,63	0

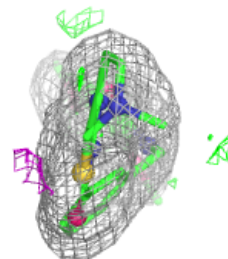
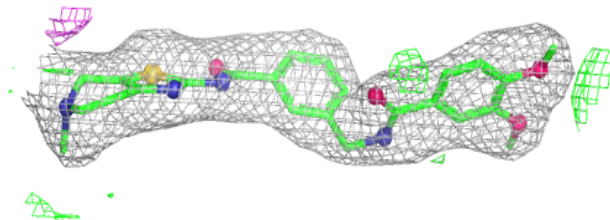
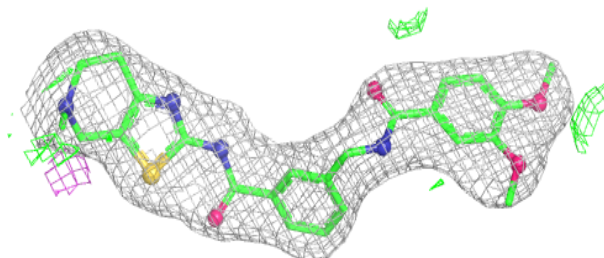
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B4J 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)

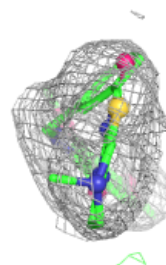
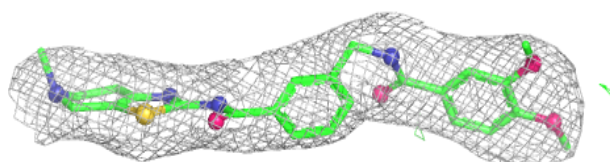
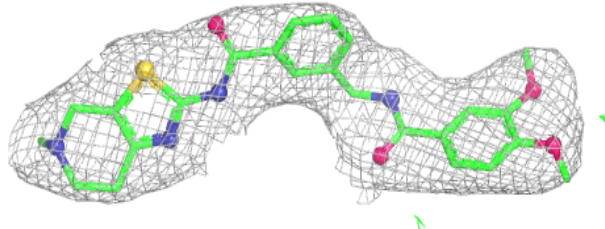
**Electron density around B4J A 501:**

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

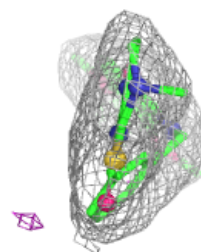
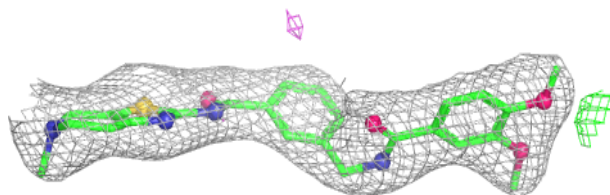
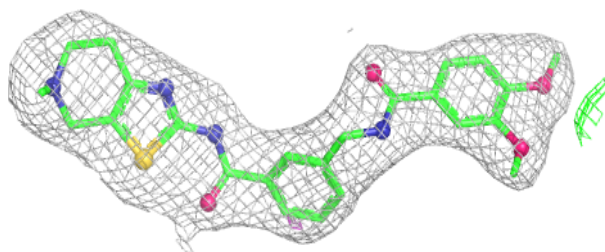


Electron density around B4J C 900:

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

**Electron density around B4J 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.