



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:30 PM UTC

PDB ID : 7S26 / pdb_00007s26
Title : ROCK1 IN COMPLEX WITH LIGAND G5018
Authors : Ganichkin, O.; Harris, S.F.; Steinbacher, S.
Deposited on : 2021-09-03
Resolution : 2.74 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

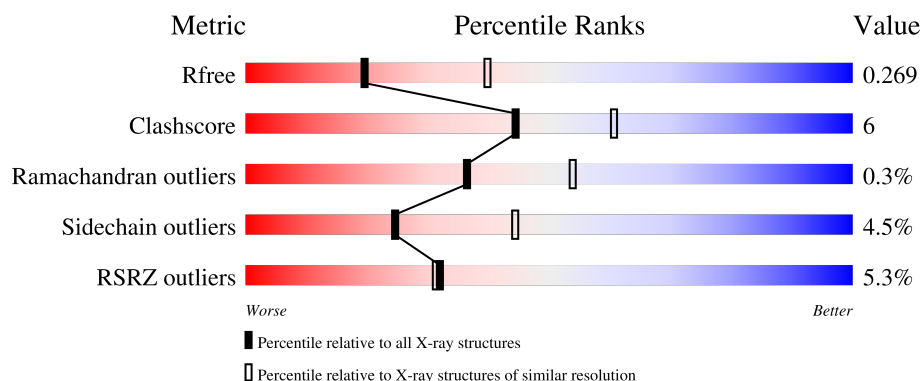
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	398	3% 78% 17% ...
1	B	398	6% 77% 15% 7%
1	C	398	4% 74% 17% 9%
1	D	398	6% 54% 10% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11523 atoms, of which 63 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	388	Total	C	N	O	S	0	0	0
			3172	2032	523	597	20			
1	B	372	Total	C	N	O	S	0	0	0
			3042	1954	501	571	16			
1	C	363	Total	C	N	O	S	0	0	0
			2965	1901	491	557	16			
1	D	256	Total	C	N	O	S	0	0	0
			2104	1354	347	387	16			

There are 4 discrepancies between the modelled and reference sequences:

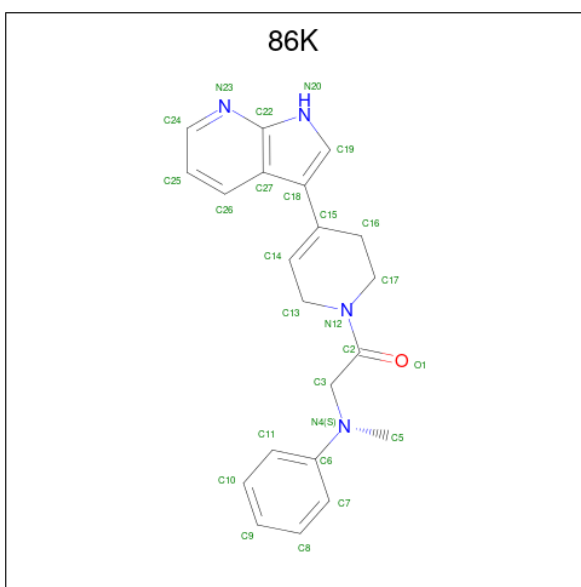
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP Q13464
B	5	ALA	-	expression tag	UNP Q13464
C	5	ALA	-	expression tag	UNP Q13464
D	5	ALA	-	expression tag	UNP Q13464

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is 2-[methyl(phenyl)amino]-1-[4-(1H-pyrrolo[2,3-b]pyridin-3-yl)-3,6-dihydropyridin-1(2H)-yl]ethan-1-one (CCD ID: 86K) (formula: $C_{21}H_{22}N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	21	0
			47	21	21	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	21	0
			47	21	21	4	1		
3	C	1	Total	C	H	N	O	21	0
			47	21	21	4	1		

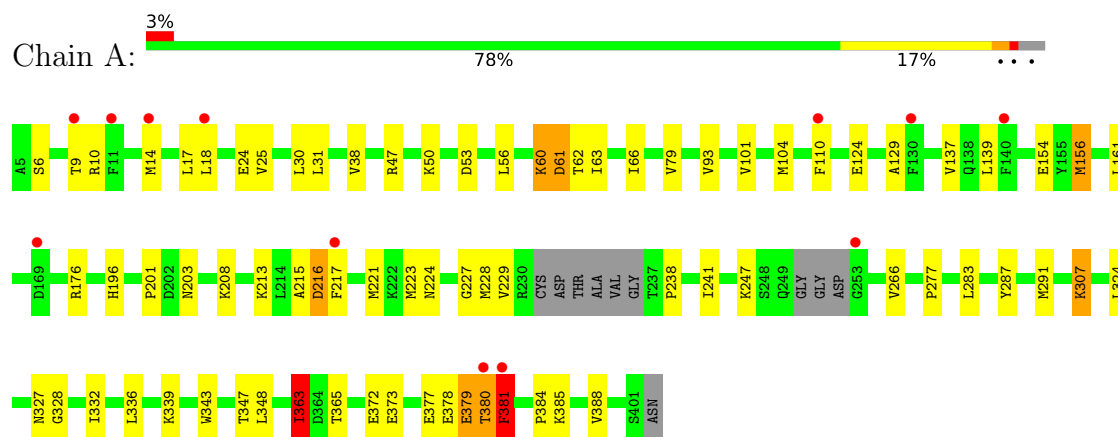
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	6	Total	O	0	0
			6	6		
4	C	20	Total	O	0	0
			20	20		
4	D	2	Total	O	0	0
			2	2		

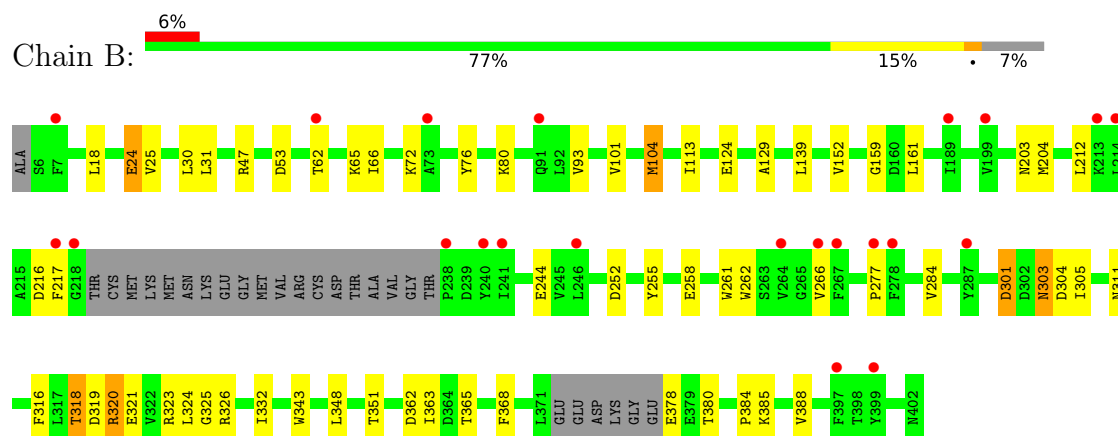
3 Residue-property plots [i](#)

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.

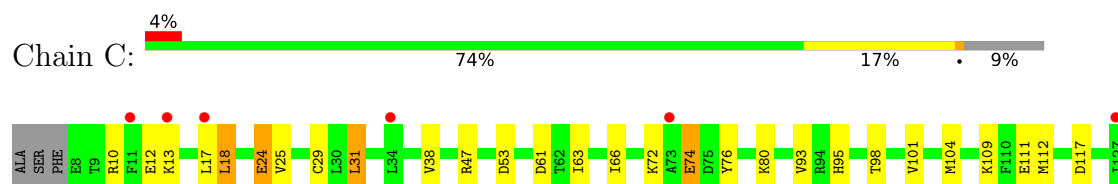
- Molecule 1: Rho-associated protein kinase 1



- Molecule 1: Rho-associated protein kinase 1



- Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.14Å 101.60Å 182.66Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	49.18 – 2.74 49.18 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.18-2.74) 99.8 (49.18-2.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.247 , 0.269 0.239 , 0.269	Depositor DCC
R_{free} test set	733 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11523	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, 86K

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	0.86	2/3247 (0.1%)	1.14	14/4383 (0.3%)
1	B	0.69	2/3117 (0.1%)	1.08	12/4212 (0.3%)
1	C	0.73	1/3036 (0.0%)	1.08	4/4103 (0.1%)
1	D	0.60	1/2152 (0.0%)	1.00	5/2899 (0.2%)
All	All	0.74	6/11552 (0.1%)	1.08	35/15597 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	SD-CE	-11.75	1.50	1.79
1	B	113	ILE	CG1-CD1	-7.06	1.24	1.51
1	D	192	MET	SD-CE	-6.23	1.64	1.79
1	B	104	MET	SD-CE	-5.61	1.65	1.79
1	A	381	PHE	CA-C	5.47	1.59	1.53
1	C	165	MET	SD-CE	-5.33	1.66	1.79

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	GLY	CA-C-N	7.14	129.73	120.44
1	C	325	GLY	C-N-CA	7.14	129.73	120.44
1	A	381	PHE	N-CA-C	-6.94	101.02	109.83
1	B	301	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	363	ILE	N-CA-CB	-6.50	104.79	112.39
1	A	381	PHE	CA-CB-CG	6.37	120.17	113.80
1	C	311	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	380	THR	CA-C-N	5.94	128.93	120.49
1	A	380	THR	C-N-CA	5.94	128.93	120.49
1	A	61	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	363	ILE	N-CA-CB	-5.90	104.64	112.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ASP	CA-C-N	5.77	129.12	120.69
1	B	304	ASP	C-N-CA	5.77	129.12	120.69
1	A	110	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	385	LYS	CA-C-N	5.63	131.37	122.36
1	A	385	LYS	C-N-CA	5.63	131.37	122.36
1	A	327	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	328	GLY	N-CA-C	5.45	118.93	112.33
1	C	303	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	325	GLY	CA-C-N	5.37	127.42	120.44
1	B	325	GLY	C-N-CA	5.37	127.42	120.44
1	B	303	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	311	ASN	CA-CB-CG	5.30	117.90	112.60
1	A	110	PHE	N-CA-CB	5.19	117.60	110.07
1	D	109	LYS	CA-C-N	5.18	127.54	120.54
1	D	109	LYS	C-N-CA	5.18	127.54	120.54
1	B	385	LYS	CA-C-N	5.17	130.63	122.36
1	B	385	LYS	C-N-CA	5.17	130.63	122.36
1	B	362	ASP	CA-C-N	5.14	128.64	122.26
1	B	362	ASP	C-N-CA	5.14	128.64	122.26
1	D	270	GLU	CB-CG-CD	5.12	121.31	112.60
1	D	59	TYR	CA-C-N	5.05	127.01	120.44
1	D	59	TYR	C-N-CA	5.05	127.01	120.44
1	A	201	PRO	CA-C-N	5.01	127.49	120.28
1	A	201	PRO	C-N-CA	5.01	127.49	120.28

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	3172	0	3079	47	0
1	B	3042	0	2944	42	0
1	C	2965	0	2870	37	0
1	D	2104	0	2049	26	0
2	A	15	0	17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	17	0	0
3	A	26	21	0	0	0
3	B	26	21	0	0	0
3	C	26	21	0	0	0
4	A	41	0	0	1	0
4	B	6	0	0	0	0
4	C	20	0	0	0	0
4	D	2	0	0	0	0
All	All	11460	63	10976	135	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 6.

All (135) 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:104:MET:HE2	1:B:152:VAL:HG22	1.54	0.88
1:D:199:VAL:HB	1:D:263:SER:CB	2.06	0.85
1:C:104:MET:HE2	1:C:152:VAL:HG22	1.60	0.82
1:A:381:PHE:H	1:A:381:PHE:HD2	1.26	0.82
1:D:199:VAL:HB	1:D:263:SER:HB3	1.61	0.81
1:A:38:VAL:HG11	1:A:63:ILE:HG21	1.62	0.79
1:A:93:VAL:HG11	1:A:104:MET:HE2	1.65	0.77
1:C:38:VAL:HG11	1:C:63:ILE:HG21	1.68	0.76
1:D:38:VAL:HG11	1:D:63:ILE:HG21	1.69	0.74
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.69	0.73
1:A:137:VAL:HG22	1:A:156:MET:HE3	1.70	0.73
1:A:307:LYS:NZ	4:A:601:HOH:O	2.22	0.71
1:C:93:VAL:HG21	1:C:104:MET:HE3	1.73	0.69
1:A:6:SER:HB3	1:A:9:THR:HB	1.76	0.68
1:B:262:TRP:HE3	1:B:323:ARG:NH1	1.92	0.68
1:B:93:VAL:HG21	1:B:104:MET:HE3	1.77	0.67
1:B:343:TRP:HB3	1:B:351:THR:HG21	1.77	0.67
1:C:66:ILE:HD11	1:D:25:VAL:HG21	1.78	0.66
1:C:318:THR:O	1:C:323:ARG:NH1	2.31	0.64
1:D:47:ARG:HH21	1:D:60:LYS:NZ	1.96	0.63
1:A:79:VAL:HG11	1:A:363:ILE:HG13	1.79	0.63
1:D:47:ARG:HH21	1:D:60:LYS:HZ3	1.47	0.62
1:A:238:PRO:O	1:A:241:ILE:HG22	1.99	0.62
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.80	0.61
1:C:262:TRP:HE3	1:C:323:ARG:NH1	1.98	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:THR:O	1:B:323:ARG:NH1	2.33	0.61
1:A:14:MET:HE1	1:B:66:ILE:HG12	1.84	0.60
1:D:189:ILE:HA	1:D:192:MET:HE3	1.83	0.60
1:A:365:THR:HG22	1:A:365:THR:O	2.02	0.60
1:C:72:LYS:HG3	1:C:74:GLU:HG2	1.83	0.59
1:B:24:GLU:CD	1:B:24:GLU:H	2.11	0.59
1:C:80:LYS:HD2	1:C:365:THR:HG21	1.85	0.58
1:D:47:ARG:NH2	1:D:60:LYS:NZ	2.52	0.58
1:C:365:THR:O	1:C:365:THR:HG22	2.03	0.58
1:A:60:LYS:NZ	1:A:61:ASP:HA	2.19	0.58
1:D:199:VAL:HB	1:D:263:SER:HB2	1.86	0.57
1:B:365:THR:HG22	1:B:365:THR:O	2.05	0.57
1:C:25:VAL:HG21	1:D:66:ILE:HD11	1.87	0.56
1:C:326:ARG:HG2	1:C:327:ASN:ND2	2.19	0.56
1:B:203:ASN:HD22	1:B:216:ASP:HB3	1.71	0.56
1:C:266:VAL:HG13	1:C:277:PRO:HD2	1.88	0.56
1:A:79:VAL:HG11	1:A:363:ILE:CG1	2.36	0.56
1:A:47:ARG:O	1:A:53:ASP:HB2	2.06	0.55
1:A:247:LYS:HE3	1:A:291:MET:HE1	1.89	0.55
1:D:93:VAL:HG11	1:D:104:MET:HE3	1.87	0.55
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.89	0.55
1:C:31:LEU:HD11	1:D:18:LEU:HD11	1.87	0.54
1:A:24:GLU:HG3	1:B:62:THR:HG21	1.90	0.54
1:A:60:LYS:HG3	1:A:61:ASP:N	2.21	0.53
1:B:80:LYS:HD2	1:B:365:THR:HG21	1.90	0.53
1:A:124:GLU:HA	1:A:217:PHE:HB2	1.91	0.52
1:C:47:ARG:O	1:C:53:ASP:HB2	2.09	0.52
1:B:384:PRO:HB3	1:B:388:VAL:HG23	1.90	0.52
1:A:56:LEU:O	1:A:60:LYS:HB3	2.10	0.52
1:A:10:ARG:HH12	1:B:72:LYS:HZ3	1.56	0.52
1:A:196:HIS:CE1	1:A:203:ASN:ND2	2.78	0.52
1:D:95:HIS:CD2	1:D:98:THR:HG23	2.45	0.51
1:B:255:TYR:HA	1:B:320:ARG:HH12	1.76	0.51
1:C:203:ASN:HD22	1:C:216:ASP:HB3	1.76	0.51
1:A:30:LEU:HB3	1:B:30:LEU:HB3	1.94	0.50
1:C:24:GLU:O	1:C:29:CYS:SG	2.68	0.50
1:A:60:LYS:HZ1	1:A:61:ASP:CA	2.24	0.50
1:D:124:GLU:HG2	1:D:128:MET:HE2	1.92	0.50
1:B:129:ALA:HB2	1:B:139:LEU:HD23	1.94	0.50
1:B:124:GLU:HA	1:B:217:PHE:HB2	1.92	0.50
1:C:244:GLU:OE2	1:C:323:ARG:NH2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LEU:HA	1:D:271:MET:HE2	1.94	0.49
1:A:384:PRO:HB3	1:A:388:VAL:HG23	1.93	0.49
1:C:198:ASP:OD2	1:C:200:LYS:HE3	2.12	0.49
1:C:287:TYR:O	1:C:291:MET:HG2	2.13	0.49
1:B:262:TRP:CE3	1:B:323:ARG:NH1	2.78	0.49
1:D:156:MET:HG3	1:D:205:LEU:HD13	1.94	0.49
1:A:287:TYR:O	1:A:291:MET:HG2	2.12	0.49
1:C:204:MET:HB3	1:C:212:LEU:HD11	1.95	0.48
1:A:10:ARG:HH12	1:B:72:LYS:NZ	2.11	0.48
1:A:324:LEU:HG	1:A:332:ILE:HG12	1.95	0.48
1:A:129:ALA:HB2	1:A:139:LEU:HD23	1.95	0.48
1:C:129:ALA:HB2	1:C:139:LEU:HD23	1.95	0.48
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.95	0.48
1:C:18:LEU:HD21	1:D:31:LEU:HD11	1.96	0.48
1:A:6:SER:HB3	1:A:9:THR:CB	2.44	0.47
1:A:238:PRO:HG3	1:A:283:LEU:HD22	1.95	0.47
1:B:316:PHE:O	1:B:323:ARG:HD3	2.14	0.47
1:A:156:MET:HE1	1:A:213:LYS:HD2	1.94	0.47
1:A:154:GLU:HG3	1:A:156:MET:HE2	1.96	0.47
1:C:238:PRO:HG3	1:C:283:LEU:HD22	1.96	0.47
1:B:80:LYS:NZ	1:B:365:THR:HB	2.29	0.47
1:C:343:TRP:CD2	1:C:348:LEU:HD13	2.50	0.47
1:C:262:TRP:CE3	1:C:323:ARG:NH1	2.82	0.46
1:A:62:THR:HG21	1:B:24:GLU:CG	2.45	0.46
1:A:60:LYS:NZ	1:A:61:ASP:CA	2.78	0.46
1:A:66:ILE:HD11	1:B:25:VAL:HG11	1.98	0.46
1:B:47:ARG:O	1:B:53:ASP:HB2	2.15	0.46
1:B:80:LYS:HZ2	1:B:365:THR:HB	1.81	0.46
1:B:343:TRP:CD2	1:B:348:LEU:HD13	2.51	0.45
1:B:244:GLU:H	1:B:244:GLU:CD	2.25	0.45
1:D:47:ARG:O	1:D:53:ASP:HB2	2.17	0.45
1:D:47:ARG:NH2	1:D:60:LYS:HZ3	2.12	0.45
1:B:76:TYR:CD1	1:B:104:MET:HE1	2.52	0.45
1:C:316:PHE:O	1:C:323:ARG:HD3	2.17	0.45
1:D:47:ARG:NH2	1:D:60:LYS:HZ2	2.14	0.45
1:A:223:MET:HB3	1:A:227:GLY:HA2	1.98	0.45
1:A:60:LYS:HZ1	1:A:61:ASP:HA	1.82	0.44
1:B:204:MET:HB3	1:B:212:LEU:HD11	1.99	0.44
1:B:31:LEU:HD22	1:B:66:ILE:HG21	1.99	0.44
1:C:76:TYR:CD2	1:C:104:MET:HE1	2.52	0.44
1:C:154:GLU:HG3	1:C:156:MET:HE3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:MET:HB2	1:D:205:LEU:HD22	1.99	0.44
1:D:189:ILE:HA	1:D:192:MET:CE	2.45	0.44
1:A:17:LEU:HD11	1:B:65:LYS:HE2	1.99	0.44
1:C:109:LYS:HA	1:C:112:MET:HG2	1.99	0.43
1:D:107:LEU:HB2	1:D:149:LEU:HB2	2.00	0.43
1:A:31:LEU:HD11	1:B:18:LEU:HD11	2.00	0.42
1:A:336:LEU:HD23	1:A:339:LYS:HD3	2.01	0.42
1:A:66:ILE:CD1	1:B:25:VAL:HG11	2.49	0.42
1:B:321:GLU:HA	1:B:326:ARG:HH21	1.84	0.42
1:C:324:LEU:HG	1:C:332:ILE:HG12	2.02	0.42
1:B:303:ASN:HB2	1:B:305:ILE:HD12	2.01	0.42
1:C:17:LEU:HD21	1:D:65:LYS:HZ3	1.85	0.42
1:C:95:HIS:ND1	1:C:98:THR:HG23	2.35	0.42
1:A:176:ARG:HG2	1:A:343:TRP:HZ2	1.85	0.42
1:B:319:ASP:OD2	1:B:321:GLU:HG2	2.19	0.42
1:B:258:GLU:HA	1:B:261:TRP:HD1	1.85	0.42
1:B:324:LEU:HG	1:B:332:ILE:HG12	2.02	0.42
1:C:112:MET:HB2	1:C:117:ASP:O	2.20	0.41
1:D:56:LEU:O	1:D:60:LYS:HB2	2.21	0.41
1:D:104:MET:HG3	1:D:152:VAL:HG22	2.02	0.41
1:A:343:TRP:CD2	1:A:348:LEU:HD13	2.56	0.40
1:A:215:ALA:O	1:A:216:ASP:HB3	2.22	0.40
1:A:224:ASN:HD21	1:A:228:MET:HB2	1.87	0.40
1:C:176:ARG:HG2	1:C:343:TRP:HZ2	1.86	0.40
1:C:258:GLU:HA	1:C:261:TRP:HD1	1.86	0.40
1:B:159:GLY:HA2	1:B:368:PHE:CZ	2.57	0.40
1:C:80:LYS:NZ	1:C:365:THR:HB	2.36	0.40
1:C:104:MET:HE3	1:C:104:MET:HB2	1.96	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	382/398 (96%)	367 (96%)	13 (3%)	2 (0%)	24	40
1	B	366/398 (92%)	354 (97%)	12 (3%)	0	100	100
1	C	357/398 (90%)	344 (96%)	12 (3%)	1 (0%)	36	54
1	D	248/398 (62%)	238 (96%)	9 (4%)	1 (0%)	30	47
All	All	1353/1592 (85%)	1303 (96%)	46 (3%)	4 (0%)	36	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	GLY
1	A	379	GLU
1	D	216	ASP
1	A	216	ASP

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	347/353 (98%)	329 (95%)	18 (5%)	21	38
1	B	332/353 (94%)	322 (97%)	10 (3%)	36	58
1	C	323/353 (92%)	308 (95%)	15 (5%)	24	43
1	D	230/353 (65%)	217 (94%)	13 (6%)	18	34
All	All	1232/1412 (87%)	1176 (96%)	56 (4%)	24	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	50	LYS
1	A	60	LYS
1	A	101	VAL
1	A	161	LEU
1	A	208	LYS
1	A	221	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	VAL
1	A	307	LYS
1	A	347	THR
1	A	363	ILE
1	A	372	GLU
1	A	373	GLU
1	A	377	GLU
1	A	378	GLU
1	A	379	GLU
1	A	380	THR
1	A	381	PHE
1	B	24	GLU
1	B	101	VAL
1	B	161	LEU
1	B	252	ASP
1	B	284	VAL
1	B	301	ASP
1	B	318	THR
1	B	320	ARG
1	B	378	GLU
1	B	380	THR
1	C	10	ARG
1	C	12	GLU
1	C	13	LYS
1	C	18	LEU
1	C	24	GLU
1	C	31	LEU
1	C	61	ASP
1	C	74	GLU
1	C	101	VAL
1	C	111	GLU
1	C	161	LEU
1	C	301	ASP
1	C	307	LYS
1	C	320	ARG
1	C	363	ILE
1	D	8	GLU
1	D	77	GLU
1	D	87	PHE
1	D	138	GLN
1	D	139	LEU
1	D	156	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	161	LEU
1	D	173	LYS
1	D	212	LEU
1	D	221	MET
1	D	270	GLU
1	D	359	LEU
1	D	361	SER

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	163	ASN
1	A	203	ASN
1	A	295	ASN
1	B	163	ASN
1	B	295	ASN
1	C	163	ASN
1	C	249	GLN
1	C	295	ASN
1	C	327	ASN
1	D	390	ASN

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](#)

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	$\# Z > 2$
3	86K	B	502	-	28,29,29	2.30	2 (7%)	33,40,40	0.91	1 (3%)
2	EPE	A	501	-	15,15,15	1.29	1 (6%)	19,20,20	0.29	0
2	EPE	B	501	-	15,15,15	1.09	1 (6%)	19,20,20	0.38	0
3	86K	A	502	-	28,29,29	2.43	3 (10%)	33,40,40	1.06	2 (6%)
3	86K	C	501	-	28,29,29	2.43	3 (10%)	33,40,40	0.86	2 (6%)

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
3	86K	B	502	-	-	8/16/26/26	0/4/4/4
2	EPE	A	501	-	-	0/9/19/19	0/1/1/1
2	EPE	B	501	-	-	0/9/19/19	0/1/1/1
3	86K	A	502	-	-	9/16/26/26	0/4/4/4
3	86K	C	501	-	-	7/16/26/26	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	86K	C16-C15	-10.77	1.31	1.50
3	A	502	86K	C16-C15	-10.56	1.31	1.50
3	B	502	86K	C16-C15	-10.49	1.31	1.50
3	C	501	86K	C14-C15	5.77	1.50	1.34
3	B	502	86K	C14-C15	5.77	1.50	1.34
3	A	502	86K	C14-C15	5.46	1.49	1.34
2	A	501	EPE	C10-S	-4.94	1.70	1.77
3	A	502	86K	C6-N4	4.14	1.50	1.38
2	B	501	EPE	C10-S	-4.08	1.71	1.77
3	C	501	86K	C6-N4	3.21	1.47	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	86K	C17-C16-C15	3.77	123.44	112.24
3	B	502	86K	C16-C15-C18	2.94	122.41	117.09
3	A	502	86K	C16-C15-C18	2.44	121.50	117.09
3	C	501	86K	C16-C15-C18	2.28	121.21	117.09
3	C	501	86K	C13-N12-C2	2.03	126.21	121.03

There are no chirality outliers.

All (24) torsion outliers are listed below:

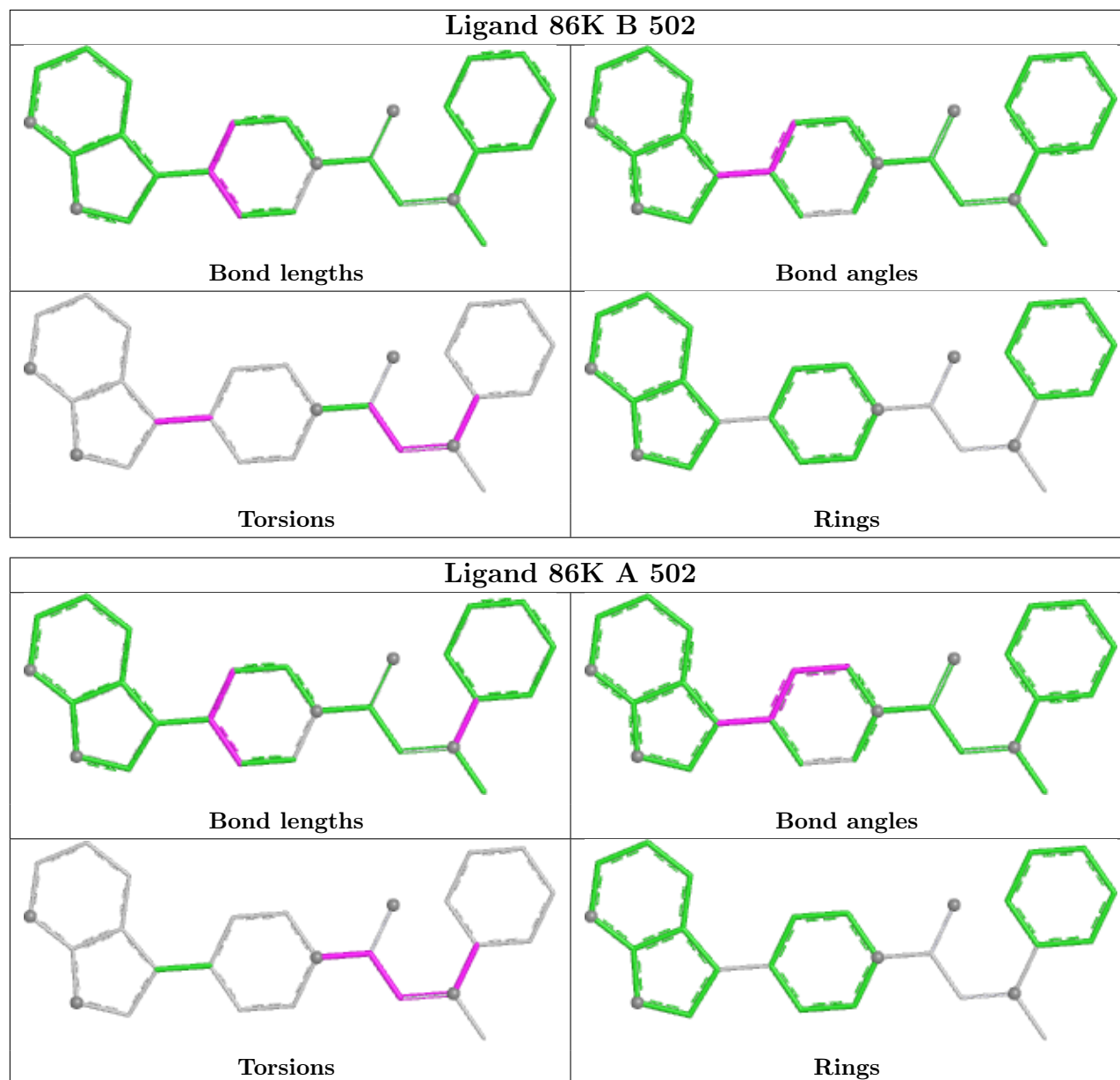
Mol	Chain	Res	Type	Atoms
3	A	502	86K	C3-C2-N12-C17
3	A	502	86K	C7-C6-N4-C5
3	A	502	86K	C11-C6-N4-C3
3	A	502	86K	C11-C6-N4-C5
3	B	502	86K	C7-C6-N4-C5
3	B	502	86K	C11-C6-N4-C5
3	C	501	86K	C7-C6-N4-C5
3	C	501	86K	C11-C6-N4-C5
3	A	502	86K	C7-C6-N4-C3
3	A	502	86K	N12-C2-C3-N4
3	B	502	86K	N12-C2-C3-N4
3	C	501	86K	N12-C2-C3-N4
3	A	502	86K	O1-C2-C3-N4
3	B	502	86K	C2-C3-N4-C5
3	C	501	86K	C2-C3-N4-C5
3	B	502	86K	C11-C6-N4-C3
3	B	502	86K	O1-C2-C3-N4
3	C	501	86K	O1-C2-C3-N4
3	A	502	86K	C2-C3-N4-C6
3	B	502	86K	C7-C6-N4-C3
3	C	501	86K	C7-C6-N4-C3
3	C	501	86K	C11-C6-N4-C3
3	A	502	86K	O1-C2-N12-C17
3	B	502	86K	C16-C15-C18-C19

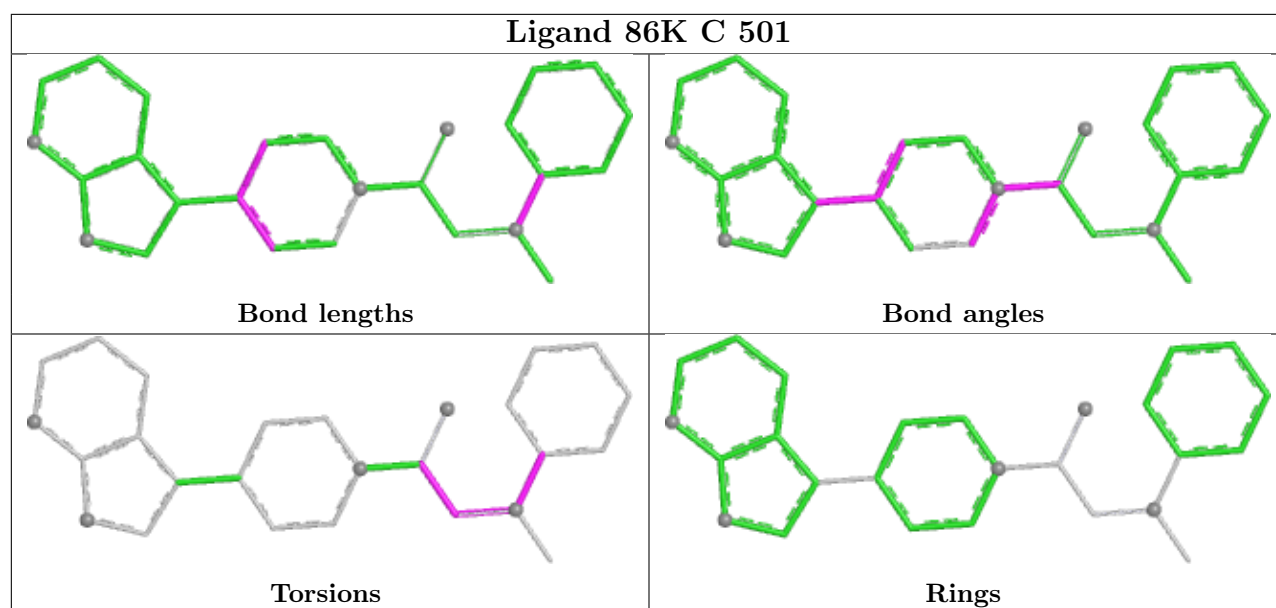
There are no ring outliers.

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	388/398 (97%)	0.27	12 (3%)	51 49	66, 93, 137, 173	0
1	B	372/398 (93%)	0.51	22 (5%)	28 28	93, 121, 149, 156	0
1	C	363/398 (91%)	0.37	16 (4%)	39 38	68, 110, 169, 185	0
1	D	256/398 (64%)	0.65	23 (8%)	15 15	145, 184, 205, 209	0
All	All	1379/1592 (86%)	0.43	73 (5%)	32 31	66, 118, 194, 209	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	194	PHE	6.1
1	C	287	TYR	4.9
1	C	34	LEU	4.3
1	D	169	ASP	3.9
1	B	287	TYR	3.9
1	B	277	PRO	3.8
1	A	381	PHE	3.8
1	B	91	GLN	3.5
1	D	168	TYR	3.5
1	B	397	PHE	3.5
1	D	365	THR	3.3
1	A	14	MET	3.3
1	B	266	VAL	3.3
1	B	238	PRO	3.2
1	D	215	ALA	3.2
1	C	127	ILE	3.1
1	D	268	LEU	3.1
1	D	175	ALA	2.9
1	B	217	PHE	2.9
1	D	105	LYS	2.7
1	A	9	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	PHE	2.7
1	C	237	THR	2.7
1	B	399	TYR	2.7
1	B	246	LEU	2.7
1	C	322	VAL	2.7
1	D	183	VAL	2.6
1	D	62	THR	2.6
1	D	106	LEU	2.6
1	B	214	LEU	2.6
1	D	87	PHE	2.6
1	B	73	ALA	2.5
1	D	130	PHE	2.5
1	C	11	PHE	2.5
1	C	130	PHE	2.4
1	A	380	THR	2.4
1	C	355	VAL	2.4
1	B	278	PHE	2.4
1	A	18	LEU	2.4
1	B	213	LYS	2.4
1	B	189	ILE	2.3
1	A	169	ASP	2.3
1	B	267	PHE	2.3
1	C	217	PHE	2.3
1	D	399	TYR	2.3
1	A	130	PHE	2.3
1	C	402	ASN	2.3
1	C	253	GLY	2.3
1	A	217	PHE	2.3
1	D	107	LEU	2.2
1	A	110	PHE	2.2
1	B	7	PHE	2.2
1	D	367	ASN	2.2
1	B	218	GLY	2.2
1	C	17	LEU	2.2
1	D	27	SER	2.2
1	D	170	VAL	2.2
1	B	241	ILE	2.2
1	B	240	TYR	2.2
1	D	164	LEU	2.2
1	D	151	MET	2.2
1	D	217	PHE	2.2
1	B	62	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	73	ALA	2.1
1	D	214	LEU	2.1
1	B	199	VAL	2.1
1	A	140	PHE	2.1
1	C	189	ILE	2.1
1	B	264	VAL	2.1
1	D	79	VAL	2.1
1	D	182	VAL	2.1
1	A	253	GLY	2.0
1	C	13	LYS	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](#)

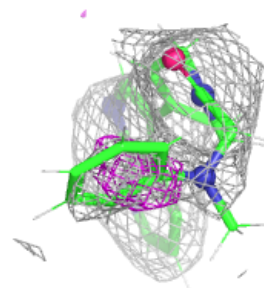
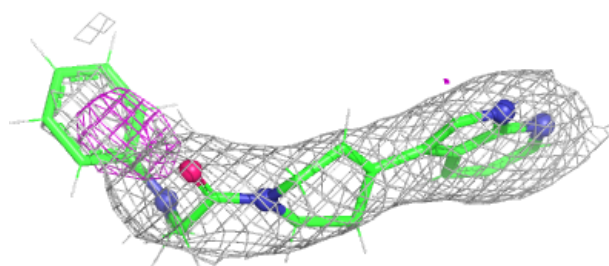
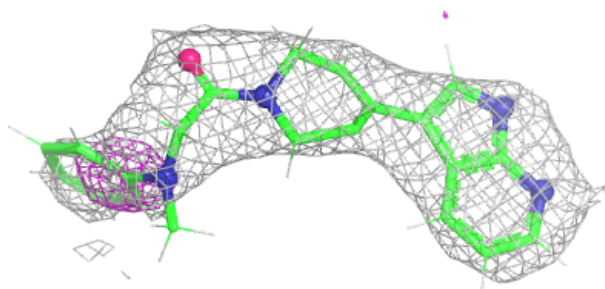
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EPE	B	501	15/15	0.79	0.15	166,166,166,166	0
3	86K	C	501	26/26	0.89	0.12	95,104,114,114	21
3	86K	B	502	26/26	0.91	0.15	128,129,130,130	21
2	EPE	A	501	15/15	0.91	0.09	144,145,147,147	0
3	86K	A	502	26/26	0.93	0.11	63,70,85,85	21

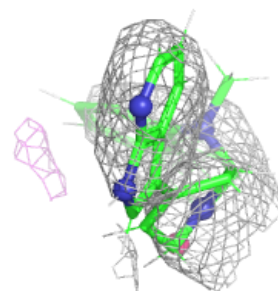
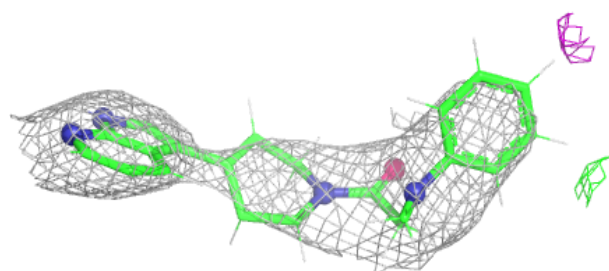
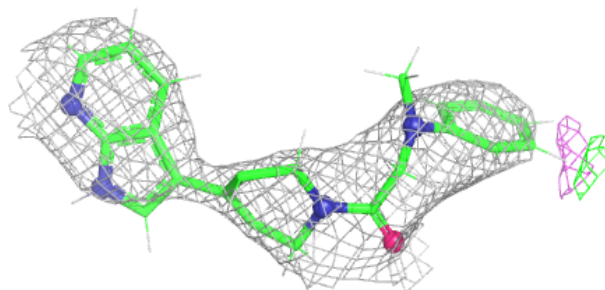
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 86K C 501:

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

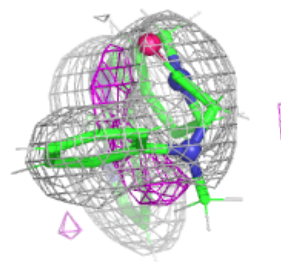
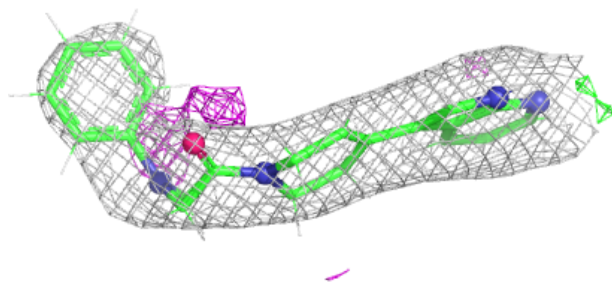
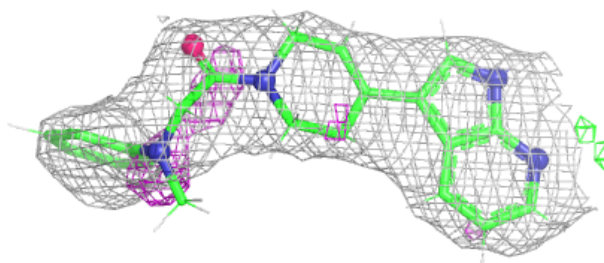
**Electron density around 86K B 502:**

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



Electron density around 86K A 502:

$2mF_o-DF_c$ (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.