



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 03:26 PM UTC

PDB ID : 7S25 / pdb_00007s25
Title : ROCK1 IN COMPLEX WITH LIGAND G4998
Authors : Ganichkin, O.; Harris, S.F.; Steinbacher, S.
Deposited on : 2021-09-03
Resolution : 2.34 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

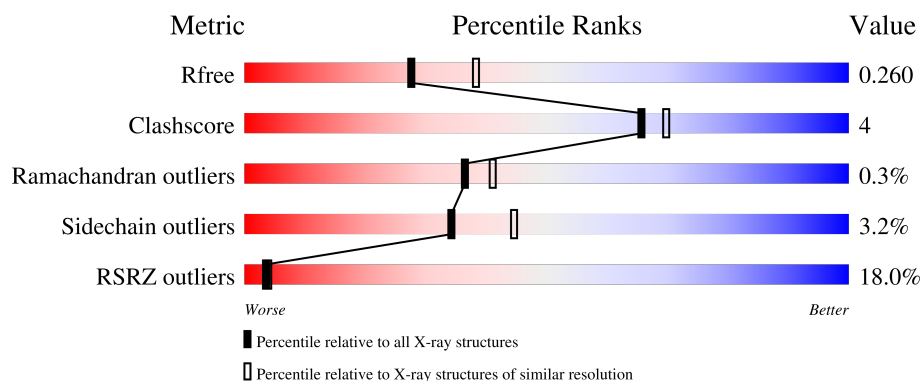
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	396	7% 83% 10% 6%
1	B	396	13% 81% 14% • •
1	C	396	16% 81% 9% • 9%
1	D	396	26% 58% 7% • 35%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11472 atoms, of which 54 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.

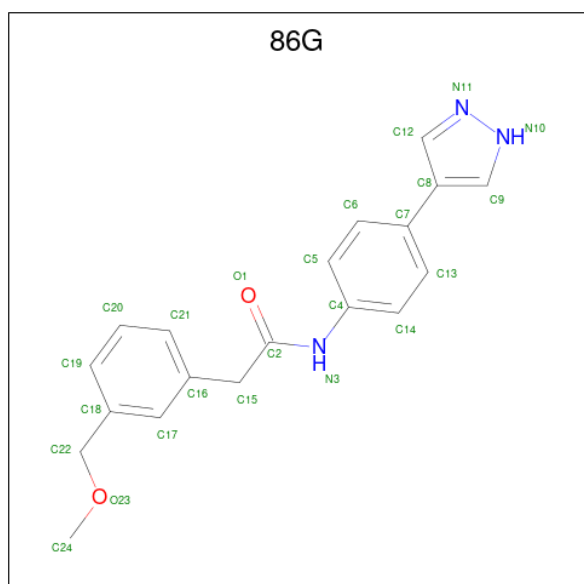
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	1	0
			3061	1965	502	578	16			
1	B	379	Total	C	N	O	S	0	0	0
			3088	1978	508	586	16			
1	C	361	Total	C	N	O	S	0	0	0
			2944	1890	486	552	16			
1	D	257	Total	C	N	O	S	0	0	0
			2122	1370	352	386	14			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cl	0	0
			3	3		

- Molecule 3 is 2-[3-(methoxymethyl)phenyl]-N-[4-(1H-pyrazol-4-yl)phenyl]acetamide (CCD ID: 86G) (formula: C₁₉H₁₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	18	0
			42	19	18	3	2		
3	B	1	Total	C	H	N	O	18	0
			42	19	18	3	2		
3	C	1	Total	C	H	N	O	18	0
			42	19	18	3	2		

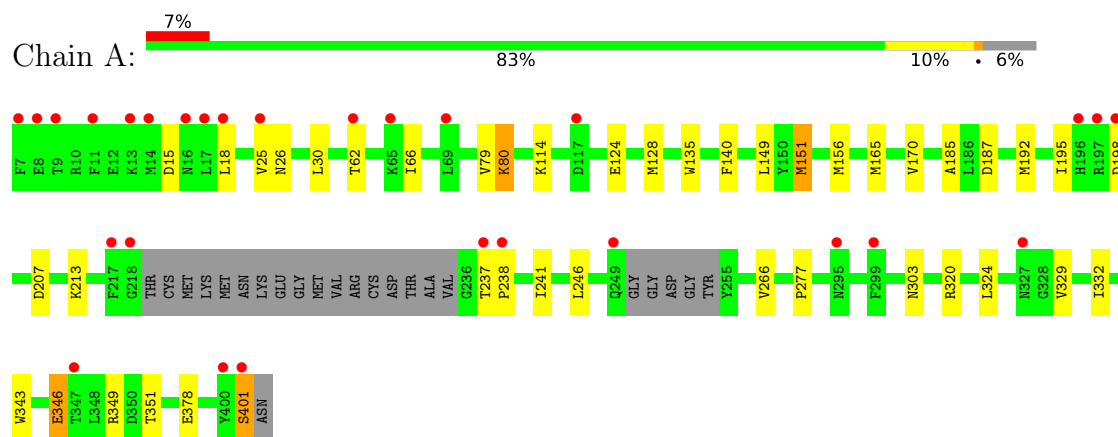
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	B	17	Total	O	0	0
			17	17		
4	C	23	Total	O	0	0
			23	23		

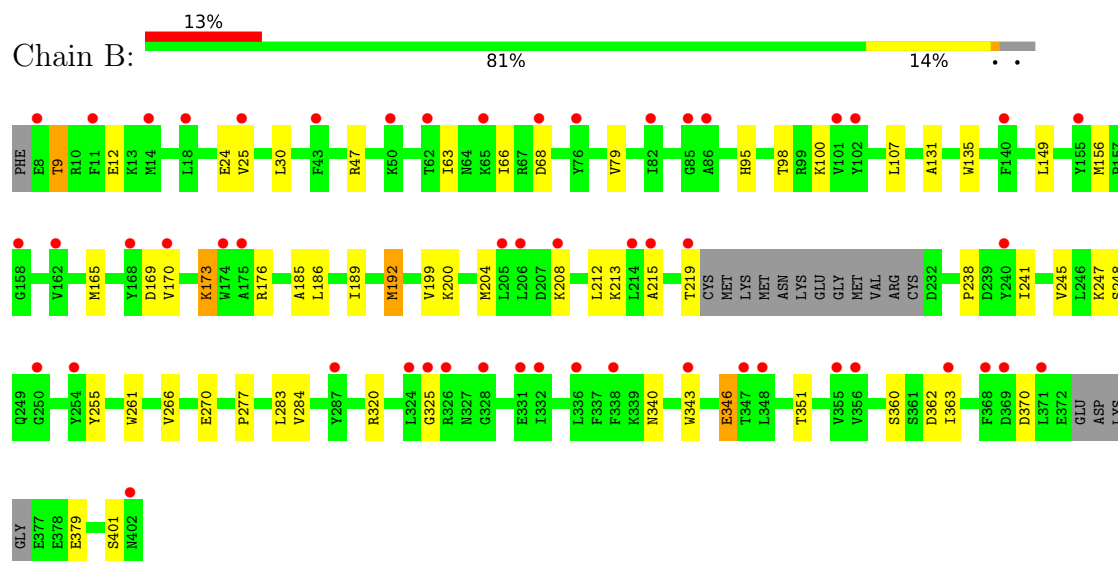
3 Residue-property plots [i](#)

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.

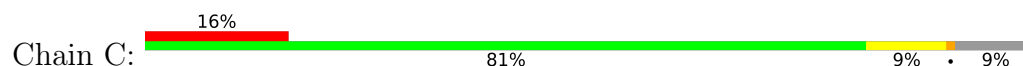
- Molecule 1: Rho-associated protein kinase 1

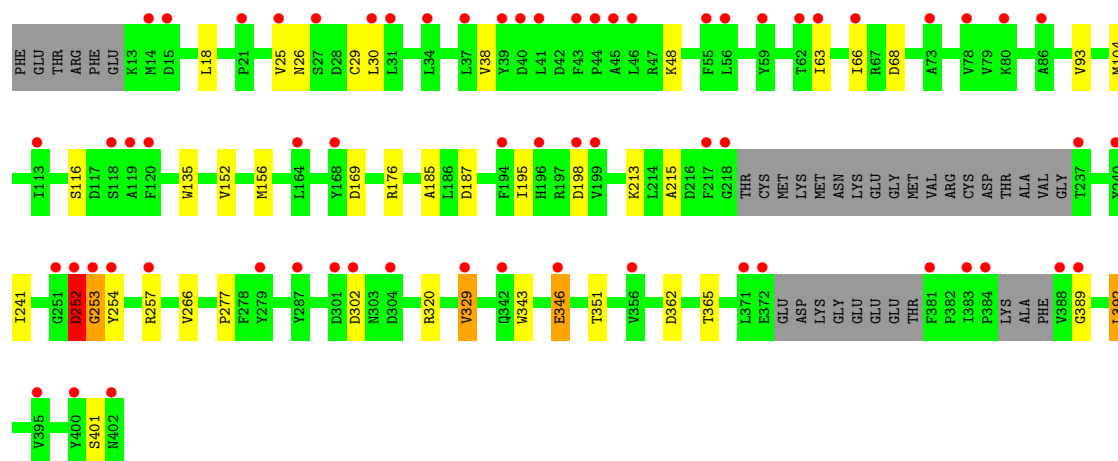


- Molecule 1: Rho-associated protein kinase 1

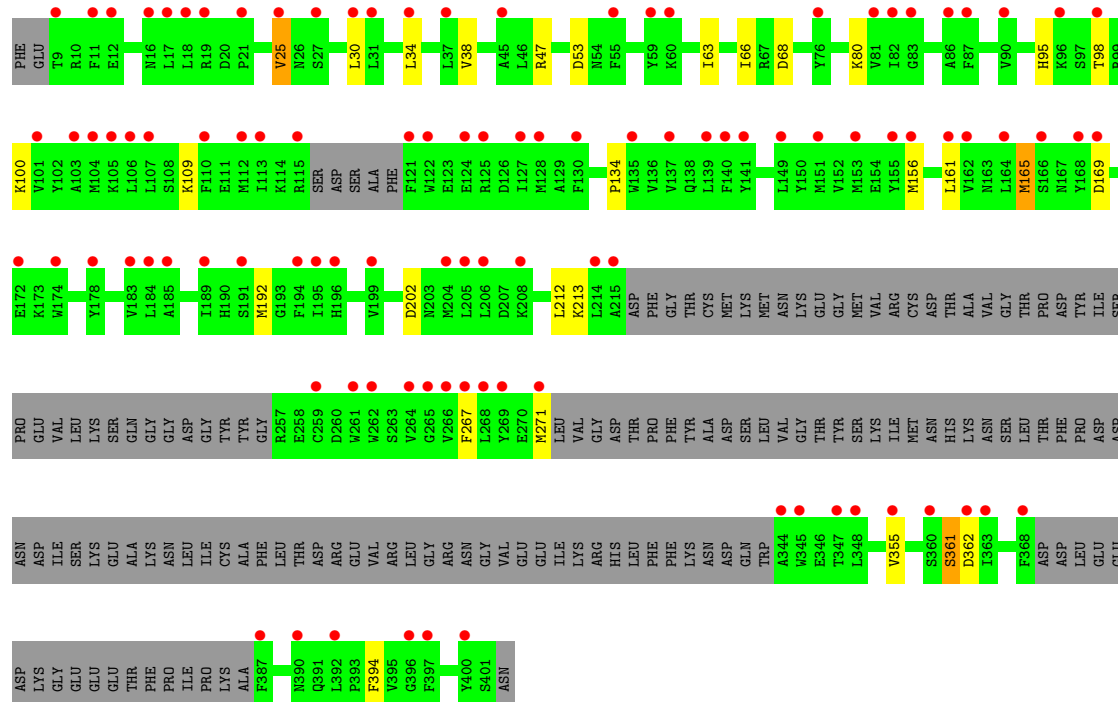


- Molecule 1: Rho-associated protein kinase 1





• Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 100.95Å 176.22Å 90.00° 90.84° 90.00°	Depositor
Resolution (Å)	176.20 – 2.34 176.20 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.3 (176.20-2.34) 98.3 (176.20-2.34)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.239 , 0.271 0.232 , 0.260	Depositor DCC
R_{free} test set	1238 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: 86G, CL

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	4/3138 (0.1%)	1.06	5/4240 (0.1%)
1	B	0.68	1/3162 (0.0%)	1.07	6/4276 (0.1%)
1	C	0.70	0/3015	1.04	5/4076 (0.1%)
1	D	0.61	1/2171 (0.0%)	1.01	5/2929 (0.2%)
All	All	0.73	6/11486 (0.1%)	1.05	21/15521 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	MET	SD-CE	-8.70	1.57	1.79
1	D	165	MET	SD-CE	-7.38	1.61	1.79
1	A	165	MET	SD-CE	-7.08	1.61	1.79
1	B	192	MET	SD-CE	-5.71	1.65	1.79
1	A	192	MET	SD-CE	-5.36	1.66	1.79
1	A	128	MET	SD-CE	-5.27	1.66	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	170	VAL	N-CA-C	6.06	113.07	107.56
1	A	170	VAL	N-CA-C	6.04	113.06	107.56
1	D	361	SER	CA-C-N	5.88	128.96	120.38
1	D	361	SER	C-N-CA	5.88	128.96	120.38
1	B	215	ALA	N-CA-C	-5.80	101.88	110.46
1	B	47	ARG	CB-CG-CD	-5.67	98.25	111.30
1	C	252	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	362	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	215	ALA	N-CA-C	-5.48	102.36	110.46
1	B	169	ASP	N-CA-C	-5.34	100.48	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	212	LEU	N-CA-C	5.32	118.29	109.46
1	D	169	ASP	N-CA-C	-5.31	101.12	109.25
1	B	362	ASP	CA-C-N	5.19	129.66	122.28
1	B	362	ASP	C-N-CA	5.19	129.66	122.28
1	A	378	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	195	ILE	CA-C-N	5.14	127.42	120.38
1	A	195	ILE	C-N-CA	5.14	127.42	120.38
1	C	362	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	169	ASP	N-CA-C	-5.05	100.93	108.96
1	A	149	LEU	N-CA-C	-5.03	102.08	110.17

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	3061	0	2964	18	0
1	B	3088	0	2983	40	0
1	C	2944	0	2854	18	0
1	D	2122	0	2079	18	0
2	A	3	0	0	0	0
3	A	24	18	0	0	0
3	B	24	18	0	0	0
3	C	24	18	0	0	0
4	A	88	0	0	0	0
4	B	17	0	0	0	0
4	C	23	0	0	0	0
All	All	11418	54	10880	85	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 4.

All (85) 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:C:104:MET:HE2	1:C:152:VAL:HG22	1.36	1.05
1:C:343:TRP:HB3	1:C:351:THR:HG21	1.55	0.87
1:B:173:LYS:HD3	1:B:176:ARG:HH12	1.41	0.84
1:B:95:HIS:CD2	1:B:98:THR:HG22	2.12	0.83
1:B:165:MET:HE1	1:B:270:GLU:HG2	1.59	0.83
1:A:343:TRP:HB3	1:A:351:THR:HG21	1.59	0.83
1:A:124:GLU:HG2	1:A:151:MET:HE1	1.63	0.80
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.64	0.79
1:B:189:ILE:HA	1:B:192:MET:HE3	1.65	0.79
1:B:343:TRP:HB3	1:B:351:THR:HG21	1.65	0.76
1:A:187:ASP:HB2	1:A:329:VAL:HG11	1.67	0.76
1:D:165:MET:CE	1:D:271:MET:HG3	2.17	0.75
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.70	0.73
1:B:360:SER:HB2	1:D:134:PRO:HB3	1.70	0.73
1:B:200:LYS:NZ	1:B:219:THR:H	1.85	0.73
1:B:79:VAL:HG11	1:B:363:ILE:HD12	1.71	0.72
1:B:200:LYS:HZ1	1:B:219:THR:N	1.88	0.72
1:B:9:THR:HA	1:B:12:GLU:HG2	1.70	0.72
1:D:95:HIS:ND1	1:D:98:THR:HG22	2.06	0.70
1:A:30:LEU:HB3	1:B:30:LEU:HB3	1.78	0.66
1:D:161:LEU:HD23	1:D:267:PHE:CZ	2.31	0.65
1:D:165:MET:HE3	1:D:271:MET:HG3	1.79	0.65
1:B:241:ILE:CG2	1:B:245:VAL:HG23	2.28	0.64
1:C:389:GLY:HA3	1:C:392:LEU:HD22	1.79	0.63
1:A:238:PRO:O	1:A:241:ILE:HG22	1.99	0.63
1:A:207:ASP:OD2	1:A:349:ARG:NH2	2.35	0.58
1:B:200:LYS:NZ	1:B:219:THR:N	2.50	0.57
1:B:238:PRO:HA	1:B:241:ILE:HG12	1.88	0.55
1:B:204:MET:HB3	1:B:212:LEU:HD11	1.88	0.55
1:B:95:HIS:HD2	1:B:98:THR:HG22	1.68	0.55
1:B:261:TRP:CD1	1:B:325:GLY:HA3	2.43	0.54
1:D:165:MET:HE2	1:D:271:MET:HG3	1.90	0.54
1:B:107:LEU:HB2	1:B:149:LEU:HB2	1.89	0.54
1:A:140:PHE:O	1:A:401:SER:HB2	2.07	0.53
1:C:25:VAL:HG11	1:D:66:ILE:HD11	1.90	0.53
1:B:189:ILE:HA	1:B:192:MET:CE	2.37	0.53
1:B:245:VAL:HG12	1:B:255:TYR:CG	2.45	0.52
1:C:187:ASP:HB2	1:C:329:VAL:HG11	1.93	0.51
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.92	0.50
1:A:62:THR:HG21	1:B:24:GLU:HB2	1.94	0.50
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.94	0.49
1:D:161:LEU:HD23	1:D:267:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HG23	1:B:245:VAL:CG2	2.43	0.49
1:C:252:ASP:O	1:C:253:GLY:O	2.31	0.49
1:C:266:VAL:HG13	1:C:277:PRO:HD2	1.95	0.49
1:A:324:LEU:HG	1:A:332:ILE:HG12	1.95	0.48
1:A:79:VAL:HG12	1:A:80:LYS:HD2	1.95	0.47
1:B:98:THR:HG23	1:B:100:LYS:H	1.79	0.47
1:B:135:TRP:HB3	1:B:185:ALA:HA	1.96	0.47
1:B:165:MET:HE1	1:B:270:GLU:CG	2.38	0.47
1:B:363:ILE:HG22	1:B:363:ILE:O	2.14	0.47
1:B:241:ILE:HG23	1:B:245:VAL:HG23	1.96	0.47
1:D:156:MET:HE2	1:D:213:LYS:HB2	1.96	0.47
1:A:18:LEU:HA	1:A:26:ASN:HA	1.96	0.47
1:B:241:ILE:CG2	1:B:245:VAL:CG2	2.93	0.47
1:B:346:GLU:H	1:B:346:GLU:CD	2.23	0.47
1:D:109:LYS:NZ	1:D:394:PHE:CG	2.80	0.46
1:C:346:GLU:H	1:C:346:GLU:CD	2.24	0.46
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.99	0.45
1:A:241:ILE:HG21	1:A:246:LEU:HD21	1.98	0.44
1:B:186:LEU:HD21	1:B:199:VAL:HG21	2.00	0.44
1:C:26:ASN:ND2	1:C:29:CYS:SG	2.90	0.44
1:B:241:ILE:HG22	1:B:245:VAL:HG23	1.97	0.44
1:B:360:SER:CB	1:D:134:PRO:HB3	2.44	0.44
1:A:135:TRP:HB3	1:A:185:ALA:HB2	2.00	0.43
1:C:66:ILE:HD11	1:D:25:VAL:HG21	2.01	0.43
1:D:98:THR:HG23	1:D:100:LYS:H	1.83	0.43
1:A:156:MET:HE2	1:A:213:LYS:HB2	2.01	0.42
1:B:156:MET:HE2	1:B:213:LYS:HB2	2.00	0.42
1:C:176:ARG:HG2	1:C:343:TRP:HZ2	1.84	0.42
1:C:254:TYR:CE2	1:C:320:ARG:NH2	2.88	0.42
1:C:38:VAL:HG11	1:C:63:ILE:HG21	2.02	0.42
1:D:161:LEU:HD23	1:D:267:PHE:HZ	1.80	0.42
1:B:363:ILE:O	1:B:363:ILE:CG2	2.68	0.41
1:C:156:MET:HE2	1:C:213:LYS:HB2	2.02	0.41
1:B:131:ALA:HA	1:B:192:MET:SD	2.59	0.41
1:D:192:MET:HE2	1:D:192:MET:HB2	1.91	0.41
1:A:346:GLU:CD	1:A:346:GLU:H	2.28	0.41
1:D:38:VAL:HG11	1:D:63:ILE:HG21	2.03	0.41
1:B:63:ILE:HD12	1:B:63:ILE:HA	1.99	0.40
1:C:93:VAL:HG21	1:C:104:MET:HE3	2.04	0.40
1:D:47:ARG:O	1:D:53:ASP:HB2	2.21	0.40
1:C:195:ILE:HD12	1:C:257:ARG:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:HIS:HD2	1:B:98:THR:CG2	2.35	0.40
1:C:135:TRP:HB3	1:C:185:ALA:HB2	2.04	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	368/396 (93%)	359 (98%)	9 (2%)	0	100	100
1	B	373/396 (94%)	365 (98%)	8 (2%)	0	100	100
1	C	353/396 (89%)	342 (97%)	8 (2%)	3 (1%)	16	16
1	D	247/396 (62%)	241 (98%)	5 (2%)	1 (0%)	30	32
All	All	1341/1584 (85%)	1307 (98%)	30 (2%)	4 (0%)	36	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	253	GLY
1	D	355	VAL
1	C	116	SER
1	C	252	ASP

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	335/352 (95%)	326 (97%)	9 (3%)	39	51
1	B	337/352 (96%)	323 (96%)	14 (4%)	26	34
1	C	322/352 (92%)	312 (97%)	10 (3%)	35	45
1	D	231/352 (66%)	225 (97%)	6 (3%)	40	53
All	All	1225/1408 (87%)	1186 (97%)	39 (3%)	34	44

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	80	LYS
1	A	114	LYS
1	A	198	ASP
1	A	237	THR
1	A	303	ASN
1	A	320	ARG
1	A	346	GLU
1	A	401	SER
1	B	9	THR
1	B	68	ASP
1	B	173	LYS
1	B	208	LYS
1	B	247	LYS
1	B	248	SER
1	B	283	LEU
1	B	284	VAL
1	B	320	ARG
1	B	340	ASN
1	B	346	GLU
1	B	370	ASP
1	B	379	GLU
1	B	401	SER
1	C	18	LEU
1	C	48	LYS
1	C	68	ASP
1	C	198	ASP
1	C	241	ILE
1	C	329	VAL
1	C	346	GLU
1	C	365	THR
1	C	392	LEU
1	C	401	SER

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Mol	Chain	Res	Type
1	D	25	VAL
1	D	34	LEU
1	D	68	ASP
1	D	80	LYS
1	D	202	ASP
1	D	361	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	B	295	ASN
1	B	402	ASN
1	C	26	ASN
1	C	342	GLN
1	D	26	ASN
1	D	91	GLN
1	D	163	ASN
1	D	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	86G	B	501	-	26,26,26	0.90	2 (7%)	34,34,34	0.85	0
3	86G	A	504	-	26,26,26	1.07	3 (11%)	34,34,34	0.98	1 (2%)
3	86G	C	501	-	26,26,26	1.05	3 (11%)	34,34,34	1.05	1 (2%)

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	86G	B	501	-	-	0/15/15/15	0/3/3/3
3	86G	A	504	-	-	0/15/15/15	0/3/3/3
3	86G	C	501	-	-	0/15/15/15	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	86G	C9-N10	-3.23	1.29	1.34
3	A	504	86G	C9-C8	2.50	1.42	1.38
3	B	501	86G	C9-N10	-2.44	1.30	1.34
3	A	504	86G	N10-N11	2.35	1.41	1.35
3	C	501	86G	N10-N11	2.25	1.40	1.35
3	A	504	86G	C12-N11	2.21	1.37	1.33
3	C	501	86G	C12-C8	-2.18	1.36	1.40
3	B	501	86G	N10-N11	2.04	1.40	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	86G	C15-C2-N3	2.58	119.55	114.73
3	A	504	86G	C15-C2-N3	2.09	118.64	114.73

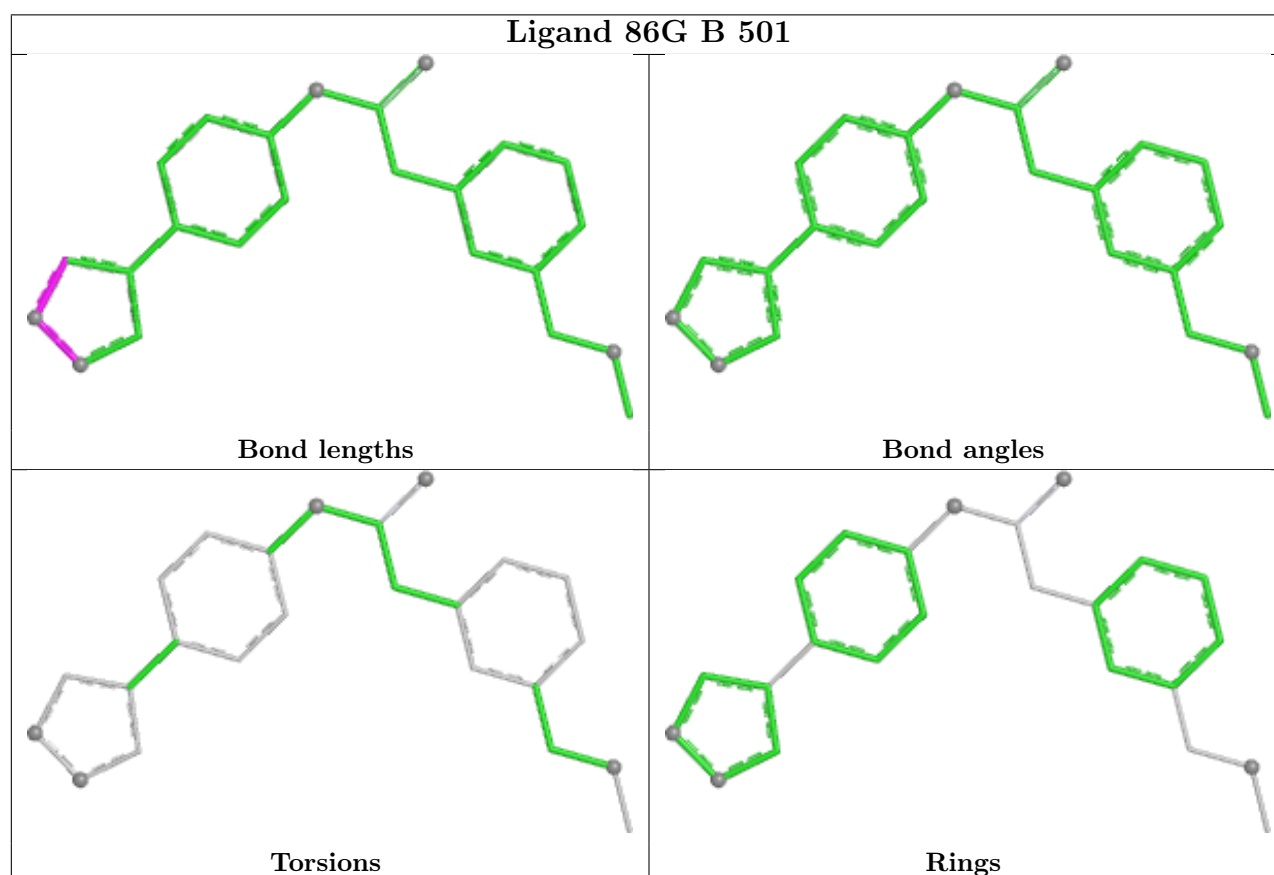
There are no chirality outliers.

There are no torsion outliers.

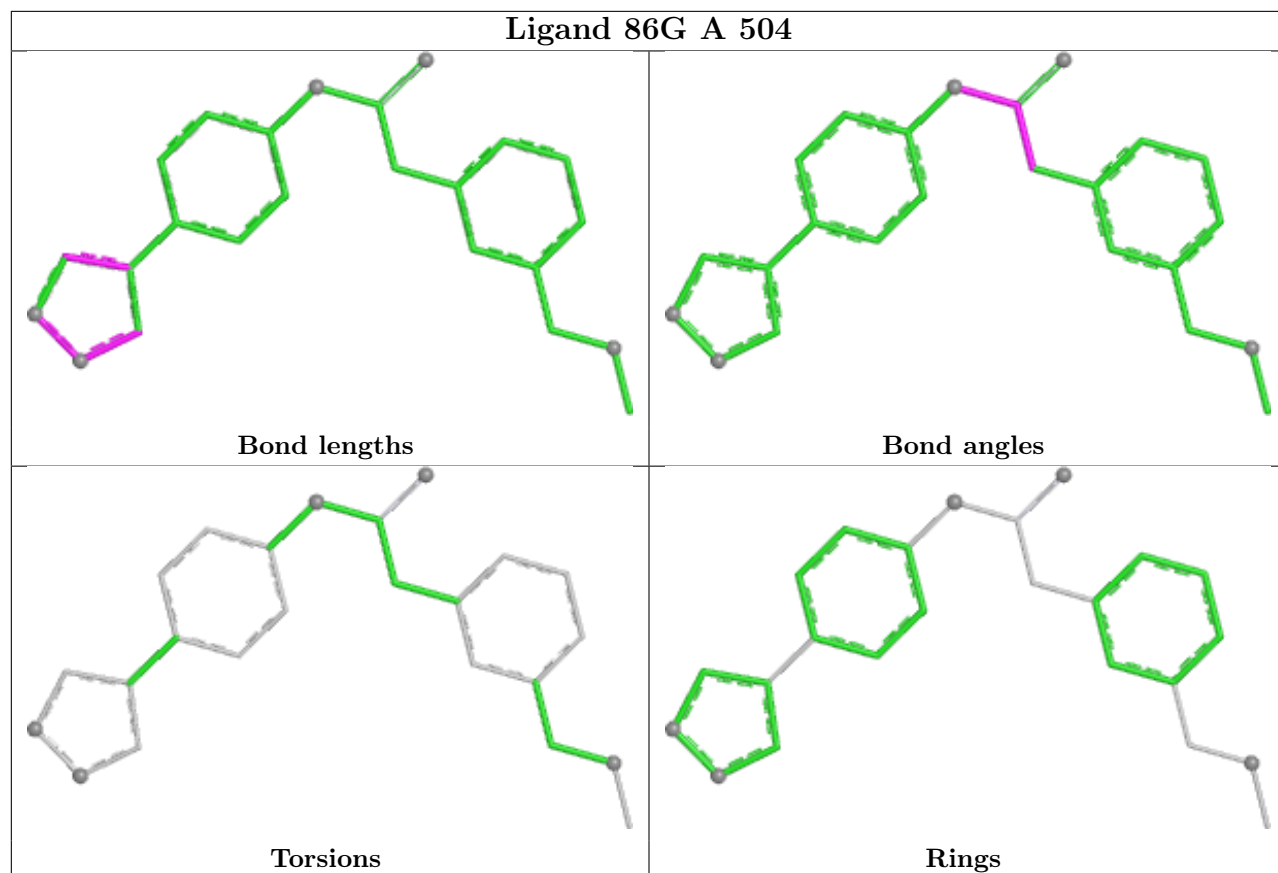
There are no ring outliers.

No monomer is involved in short contacts.

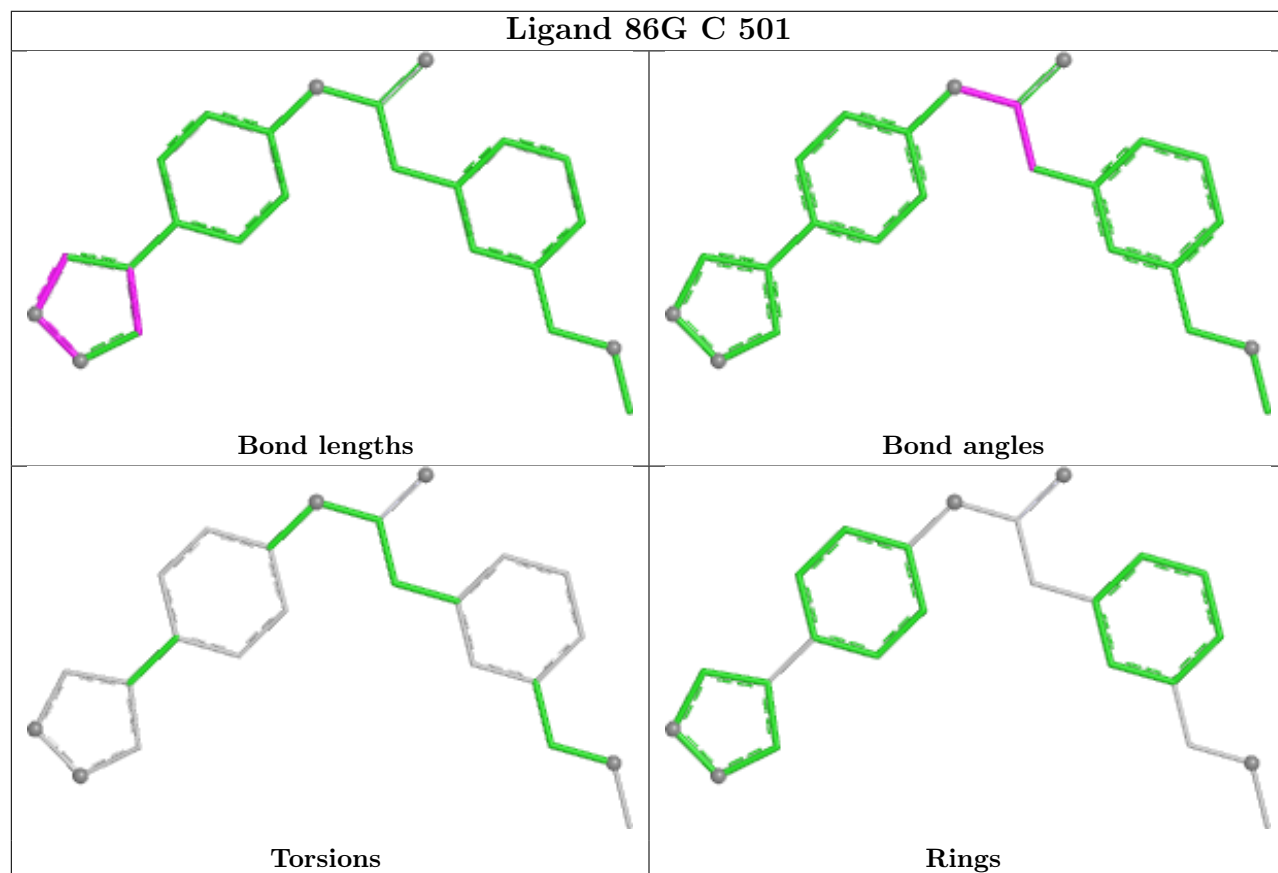
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



Ligand 86G A 504



Ligand 86G C 501



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	373/396 (94%)	0.61	28 (7%) 20 24	47, 63, 103, 130	1 (0%)
1	B	379/396 (95%)	1.13	52 (13%) 6 7	61, 89, 114, 126	0
1	C	361/396 (91%)	1.16	64 (17%) 4 4	55, 86, 143, 153	0
1	D	257/396 (64%)	1.88	103 (40%) 0 0	113, 142, 171, 175	0
All	All	1370/1584 (86%)	1.14	247 (18%) 3 4	47, 88, 157, 175	1 (0%)

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	264	VAL	6.0
1	A	218	GLY	5.9
1	D	214	LEU	5.7
1	C	73	ALA	5.5
1	D	19	ARG	5.4
1	C	384	PRO	5.1
1	D	268	LEU	5.0
1	B	348	LEU	5.0
1	D	368	PHE	5.0
1	D	169	ASP	4.6
1	A	7	PHE	4.6
1	D	267	PHE	4.4
1	D	396	GLY	4.4
1	A	237	THR	4.3
1	C	194	PHE	4.2
1	C	14	MET	4.1
1	D	215	ALA	4.1
1	D	124	GLU	4.1
1	D	107	LEU	4.0
1	D	127	ILE	4.0
1	A	11	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	27	SER	4.0
1	D	90	VAL	4.0
1	C	118	SER	4.0
1	D	21	PRO	3.9
1	C	381	PHE	3.9
1	D	55	PHE	3.8
1	D	87	PHE	3.8
1	A	400	TYR	3.7
1	D	121	PHE	3.7
1	D	140	PHE	3.7
1	A	14	MET	3.6
1	D	34	LEU	3.6
1	D	106	LEU	3.6
1	C	237	THR	3.6
1	D	151	MET	3.6
1	B	343	TRP	3.5
1	B	240	TYR	3.5
1	D	162	VAL	3.4
1	C	46	LEU	3.4
1	C	56	LEU	3.4
1	D	168	TYR	3.4
1	A	217	PHE	3.4
1	D	82	ILE	3.4
1	D	345	TRP	3.4
1	C	302	ASP	3.4
1	D	387	PHE	3.3
1	C	27	SER	3.3
1	C	15	ASP	3.3
1	B	324	LEU	3.3
1	D	205	LEU	3.3
1	C	402	ASN	3.3
1	D	37	LEU	3.3
1	D	105	LYS	3.3
1	C	34	LEU	3.3
1	C	346	GLU	3.3
1	A	9	THR	3.3
1	C	388	VAL	3.3
1	C	37	LEU	3.2
1	C	383	ILE	3.2
1	B	25	VAL	3.2
1	B	18	LEU	3.2
1	D	204	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	3.2
1	A	13	LYS	3.2
1	C	218	GLY	3.2
1	D	266	VAL	3.2
1	A	196	HIS	3.2
1	D	113	ILE	3.2
1	C	240	TYR	3.1
1	B	208	LYS	3.1
1	C	120	PHE	3.1
1	D	183	VAL	3.1
1	C	31	LEU	3.1
1	C	25	VAL	3.1
1	D	199	VAL	3.1
1	D	110	PHE	3.1
1	D	397	PHE	3.1
1	B	102	TYR	3.0
1	D	269	TYR	3.0
1	D	12	GLU	3.0
1	D	195	ILE	3.0
1	B	11	PHE	3.0
1	C	30	LEU	3.0
1	D	81	VAL	3.0
1	D	265	GLY	3.0
1	D	128	MET	3.0
1	D	155	TYR	3.0
1	D	16	ASN	3.0
1	D	189	ILE	3.0
1	B	371	LEU	2.9
1	D	348	LEU	2.9
1	C	199	VAL	2.9
1	B	355	VAL	2.9
1	C	78	VAL	2.9
1	C	62	THR	2.9
1	D	125	ARG	2.9
1	C	113	ILE	2.9
1	D	59	TYR	2.8
1	D	31	LEU	2.8
1	D	104	MET	2.8
1	B	254	TYR	2.8
1	D	178	TYR	2.8
1	D	400	TYR	2.8
1	C	395	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	355	VAL	2.8
1	B	219	THR	2.8
1	D	362	ASP	2.8
1	B	155	TYR	2.8
1	D	122	TRP	2.8
1	C	59	TYR	2.8
1	D	161	LEU	2.8
1	A	62	THR	2.7
1	D	262	TRP	2.7
1	B	14	MET	2.7
1	D	344	ALA	2.7
1	B	338	PHE	2.7
1	C	196	HIS	2.7
1	D	101	VAL	2.7
1	C	44	PRO	2.7
1	C	41	LEU	2.7
1	C	287	TYR	2.7
1	D	11	PHE	2.7
1	B	158	GLY	2.7
1	D	166	SER	2.7
1	C	342	GLN	2.6
1	B	76	TYR	2.6
1	A	401	SER	2.6
1	D	153	MET	2.6
1	D	45	ALA	2.6
1	B	331	GLU	2.6
1	A	249	GLN	2.6
1	B	336	LEU	2.6
1	B	86	ALA	2.6
1	A	117	ASP	2.6
1	C	304	ASP	2.6
1	D	130	PHE	2.6
1	D	164	LEU	2.6
1	D	112	MET	2.6
1	B	8	GLU	2.5
1	C	301	ASP	2.5
1	B	347	THR	2.5
1	B	205	LEU	2.5
1	B	206	LEU	2.5
1	D	17	LEU	2.5
1	C	80	LYS	2.5
1	D	137	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	326	ARG	2.5
1	C	254	TYR	2.5
1	D	103	ALA	2.5
1	A	238	PRO	2.5
1	C	251	GLY	2.5
1	B	356	VAL	2.5
1	D	261	TRP	2.5
1	B	287	TYR	2.5
1	C	168	TYR	2.5
1	D	206	LEU	2.5
1	D	86	ALA	2.5
1	C	55	PHE	2.4
1	D	360	SER	2.4
1	B	82	ILE	2.4
1	A	17	LEU	2.4
1	D	185	ALA	2.4
1	D	259	CYS	2.4
1	C	63	ILE	2.4
1	A	18	LEU	2.4
1	C	252	ASP	2.4
1	D	390	ASN	2.4
1	C	372	GLU	2.4
1	A	25	VAL	2.4
1	C	217	PHE	2.4
1	D	156	MET	2.4
1	B	215	ALA	2.4
1	D	208	LYS	2.4
1	B	363	ILE	2.4
1	C	43	PHE	2.4
1	C	371	LEU	2.4
1	D	196	HIS	2.4
1	A	327	ASN	2.3
1	B	101	VAL	2.3
1	D	194	PHE	2.3
1	D	30	LEU	2.3
1	C	40	ASP	2.3
1	C	39	TYR	2.3
1	C	279	TYR	2.3
1	B	250	GLY	2.3
1	D	363	ILE	2.3
1	A	8	GLU	2.3
1	C	45	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	172	GLU	2.3
1	D	60	LYS	2.3
1	D	115	ARG	2.3
1	B	368	PHE	2.2
1	D	184	LEU	2.2
1	D	392	LEU	2.2
1	A	197	ARG	2.2
1	B	62	THR	2.2
1	D	98	THR	2.2
1	D	141	TYR	2.2
1	B	332	ILE	2.2
1	B	162	VAL	2.2
1	D	271	MET	2.2
1	C	329	VAL	2.2
1	B	140	PHE	2.2
1	D	191	SER	2.2
1	D	135	TRP	2.2
1	D	139	LEU	2.2
1	B	68	ASP	2.2
1	B	402	ASN	2.2
1	C	198	ASP	2.2
1	C	356	VAL	2.2
1	D	25	VAL	2.2
1	B	65	LYS	2.2
1	B	168	TYR	2.1
1	D	174	TRP	2.1
1	C	21	PRO	2.1
1	B	325	GLY	2.1
1	B	328	GLY	2.1
1	D	9	THR	2.1
1	B	214	LEU	2.1
1	C	389	GLY	2.1
1	A	295	ASN	2.1
1	C	66	ILE	2.1
1	A	299	PHE	2.1
1	D	83	GLY	2.1
1	A	347	THR	2.1
1	D	347	THR	2.1
1	C	86	ALA	2.1
1	C	119	ALA	2.1
1	D	18	LEU	2.1
1	D	149	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	16	ASN	2.1
1	B	170	VAL	2.1
1	B	43	PHE	2.1
1	B	85	GLY	2.1
1	B	174	TRP	2.1
1	A	65	LYS	2.0
1	A	69	LEU	2.0
1	B	369	ASP	2.0
1	C	400	TYR	2.0
1	D	76	TYR	2.0
1	C	253	GLY	2.0
1	D	96	LYS	2.0
1	A	198	ASP	2.0
1	C	164	LEU	2.0
1	C	257	ARG	2.0
1	B	50	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](#)

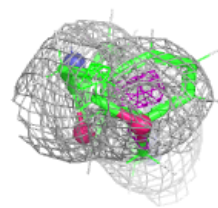
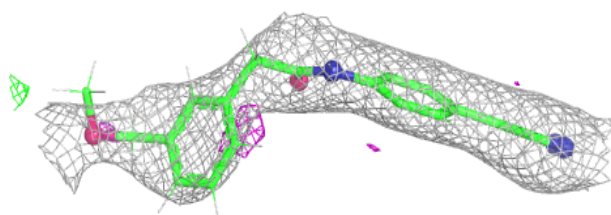
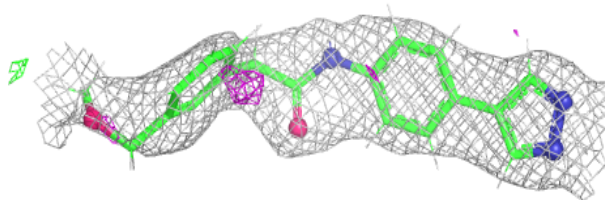
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	502	1/1	0.90	0.22	100,100,100,100	0
2	CL	A	503	1/1	0.90	0.14	106,106,106,106	0
3	86G	C	501	24/24	0.90	0.12	65,76,88,88	18
2	CL	A	501	1/1	0.91	0.22	109,109,109,109	0
3	86G	B	501	24/24	0.94	0.13	86,89,93,93	18
3	86G	A	504	24/24	0.95	0.09	48,58,70,70	18

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.

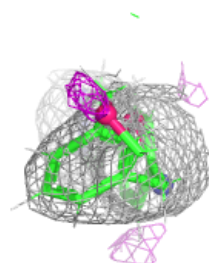
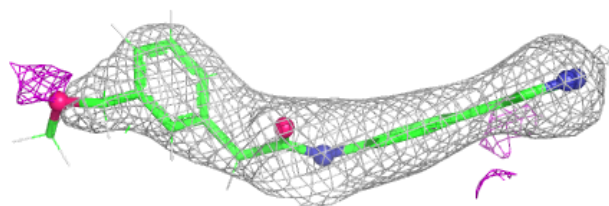
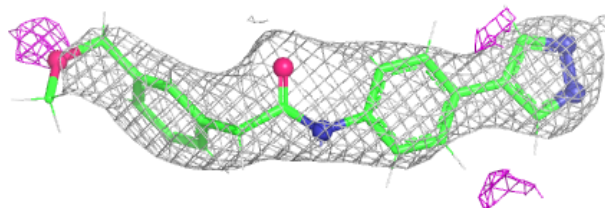
Electron density around 86G C 501:

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

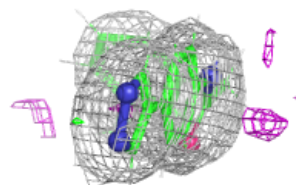
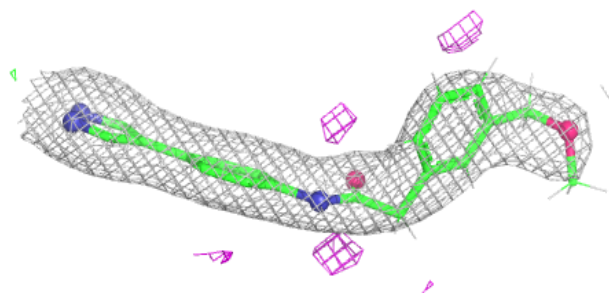
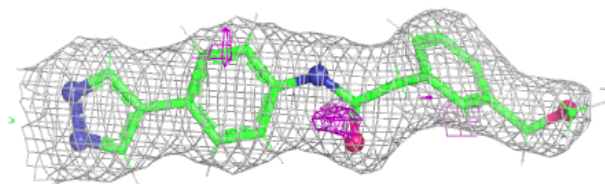


Electron density around 86G B 501:

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

**Electron density around 86G A 504:**

$2mF_o-DF_c$ (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.