Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2022 – 03:59 PM EDT

PDB ID	:	7S26
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 (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:

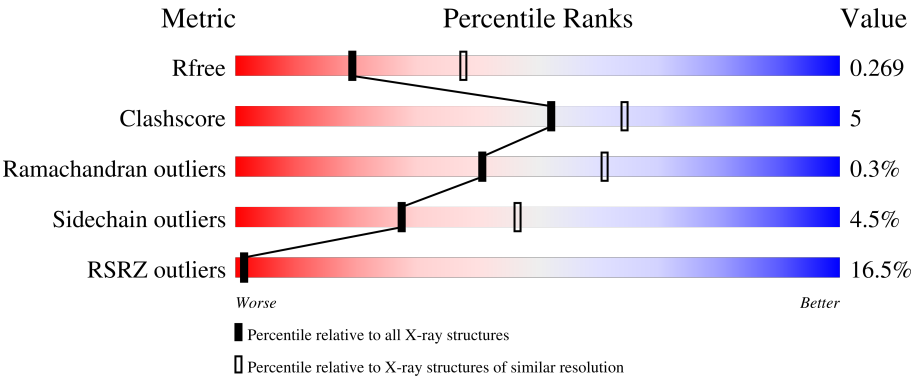
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 <=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	7% 80% 16%
1	B	398	12% 80% 13% 7%
1	C	398	11% 76% 15% 9%
1	D	398	29% 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.

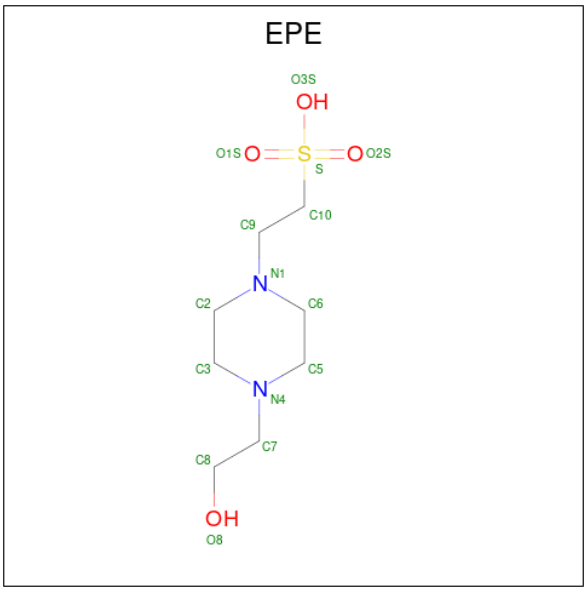
- Molecule 1 is a protein called Rho-associated protein kinase 1.

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:

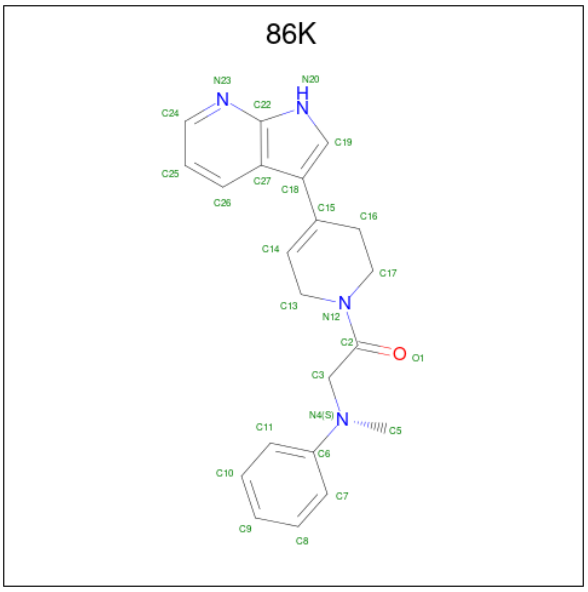
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP Q13464
B	5	ALA	-	expression tag	UNP Q13464
C	5	ALA	-	expression tag	UNP Q13464
D	5	ALA	-	expression tag	UNP Q13464

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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 (three-letter code: 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		

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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.

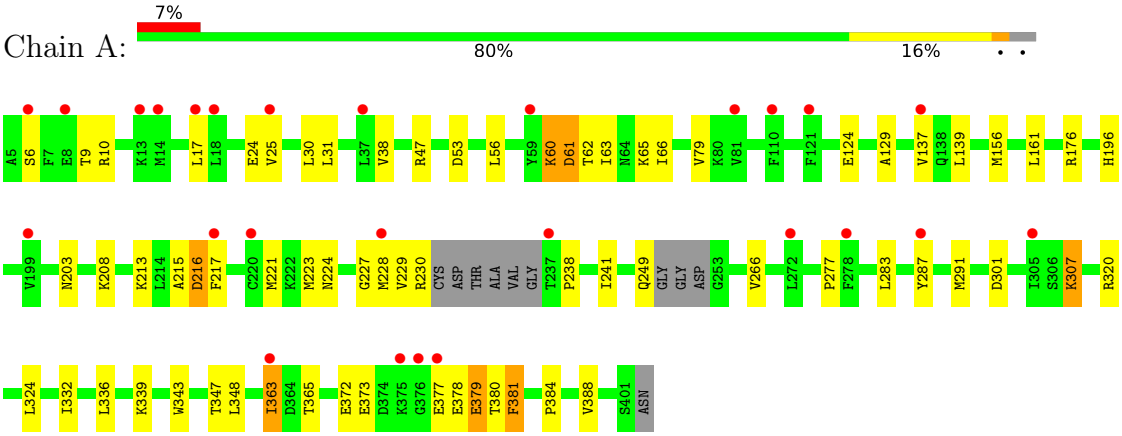
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	6	Total	O	0	0
			6	6		
4	C	20	Total	O	0	0
			20	20		
4	D	2	Total	O	0	0
			2	2		

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.

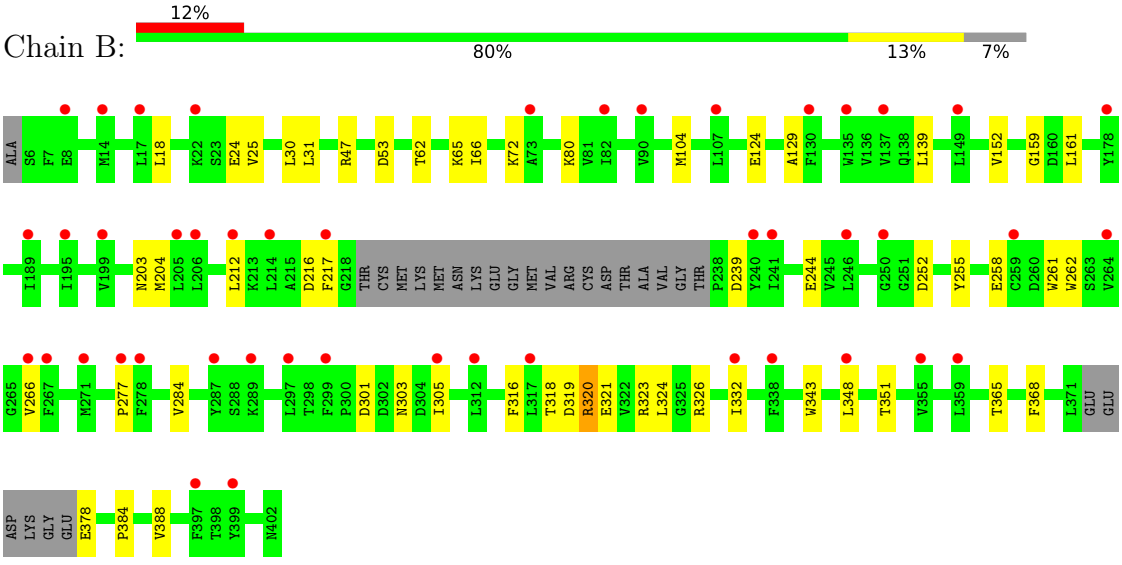
• Molecule 1: Rho-associated protein kinase 1

Chain A:



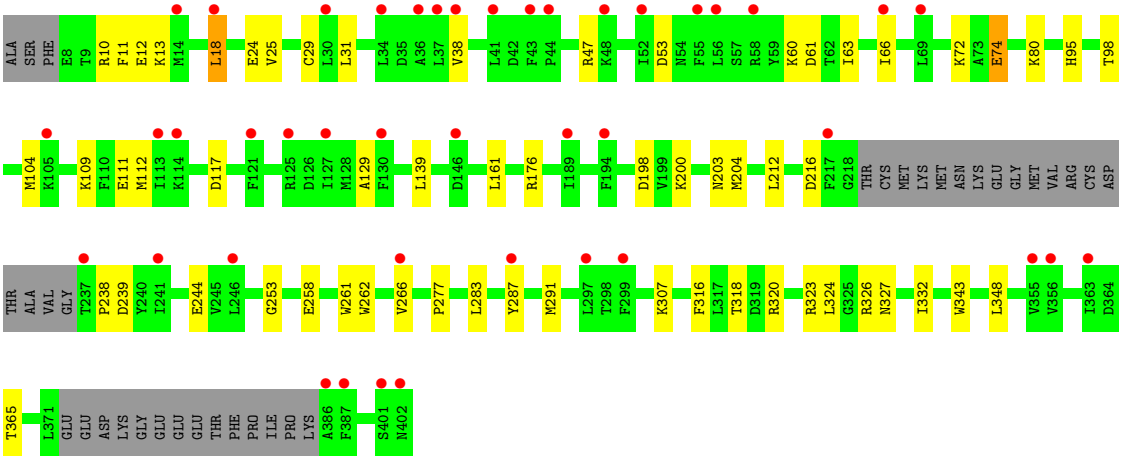
• Molecule 1: Rho-associated protein kinase 1

Chain B:



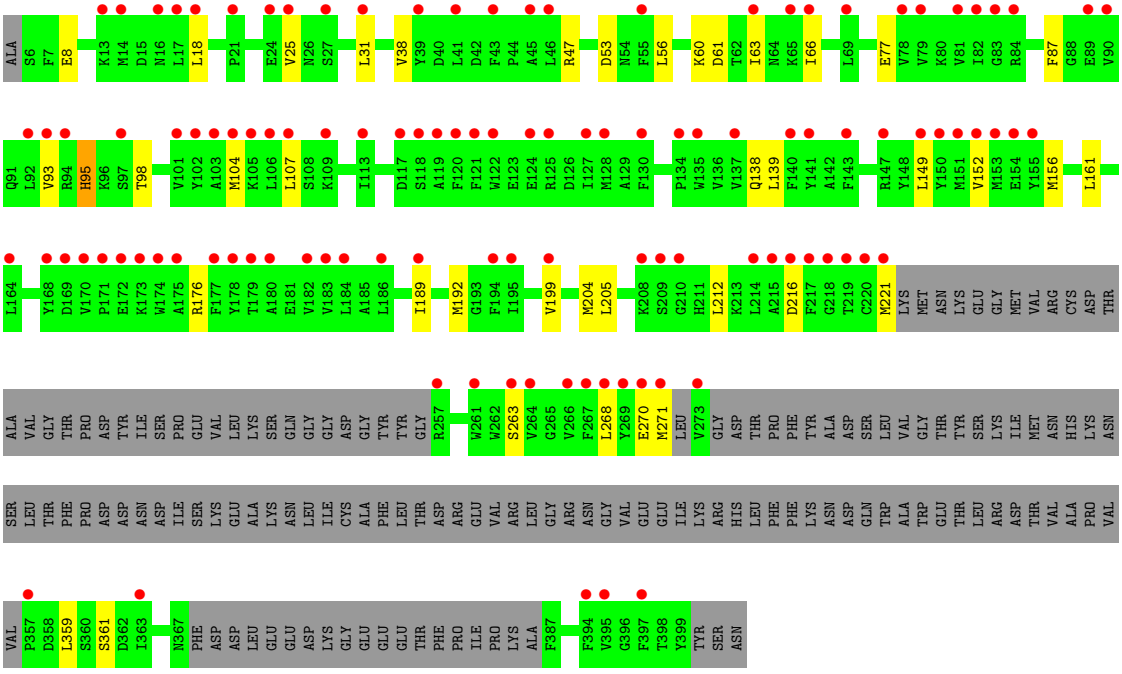
• Molecule 1: Rho-associated protein kinase 1

Chain C:



• Molecule 1: Rho-associated protein kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	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 88.77 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.18-2.74) 99.8 (88.77-2.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (1.34%)	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)	0.32 , 88.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[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

5.1 Standard geometry

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

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	0.51	0/3247	0.64	0/4383
1	B	0.37	0/3117	0.57	0/4212
1	C	0.42	0/3036	0.59	0/4103
1	D	0.28	0/2152	0.49	0/2899
All	All	0.42	0/11552	0.58	0/15597

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

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	43	0
1	B	3042	0	2944	39	0
1	C	2965	0	2870	32	0
1	D	2104	0	2049	23	0
2	A	15	0	17	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	122	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 5.

All (122) 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:199:VAL:HB	1:D:263:SER:CB	2.06	0.85
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: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:307:LYS:NZ	4:A:601:HOH:O	2.22	0.71
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: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:A:156:MET:HE3	1:A:213:LYS:HD2	1.78	0.65
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:A:238:PRO:O	1:A:241:ILE:HG22	1.99	0.62
1:D:47:ARG:HH21	1:D:60:LYS:HZ3	1.48	0.61
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
1:B:318:THR:O	1:B:323:ARG:NH1	2.33	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:LYS:HG3	1:A:61:ASP:N	2.21	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:B:24:GLU:CD	1:B:24:GLU:H	2.11	0.54
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: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:B:129:ALA:HB2	1:B:139:LEU:HD23	1.94	0.50
1:D:93:VAL:HG21	1:D:104:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PHE:O	1:B:323:ARG:HD3	2.14	0.47
1:C:238:PRO:HG3	1:C:283:LEU:HD22	1.96	0.47
1:D:268:LEU:HA	1:D:271:MET:HE2	1.97	0.47
1:B:80:LYS:NZ	1:B:365:THR:HB	2.29	0.47
1:A:10:ARG:HH12	1:B:72:LYS:HZ3	1.62	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:D:189:ILE:HA	1:D:192:MET:CE	2.45	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:D:47:ARG:NH2	1:D:60:LYS:HZ2	2.13	0.46
1:B:343:TRP:CD2	1:B:348:LEU:HD13	2.51	0.45
1:D:47:ARG:O	1:D:53:ASP:HB2	2.17	0.45
1:C:316:PHE:O	1:C:323:ARG:HD3	2.17	0.45
1:A:223:MET:HB3	1:A:227:GLY:HA2	1.98	0.45
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:D:156:MET:HB2	1:D:205:LEU:HD22	1.99	0.44
1:D:47:ARG:NH2	1:D:60:LYS:HZ3	2.13	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:A:60:LYS:HZ1	1:A:61:ASP:CA	2.31	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: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:A:137:VAL:HG22	1:A:156:MET:HE3	2.02	0.41
1:C:112:MET:HB2	1:C:117:ASP:O	2.20	0.41
1:B:104:MET:CE	1:B:152:VAL:HG22	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:MET:HE2	1:C:104:MET:HB2	1.91	0.41
1:A:60:LYS:HZ1	1:A:61:ASP:HA	1.86	0.40
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:B:80:LYS:HZ1	1:B:365:THR:HB	1.87	0.40
1:B:244:GLU:H	1:B:244:GLU:CD	2.25	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

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%)	29	48
1	B	366/398 (92%)	354 (97%)	12 (3%)	0	100	100
1	C	357/398 (90%)	344 (96%)	12 (3%)	1 (0%)	41	61
1	D	248/398 (62%)	238 (96%)	9 (4%)	1 (0%)	34	55
All	All	1353/1592 (85%)	1303 (96%)	46 (3%)	4 (0%)	41	61

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 (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	347/353 (98%)	326 (94%)	21 (6%)	18 32
1	B	332/353 (94%)	325 (98%)	7 (2%)	53 72
1	C	323/353 (92%)	310 (96%)	13 (4%)	31 52
1	D	230/353 (65%)	215 (94%)	15 (6%)	17 30
All	All	1232/1412 (87%)	1176 (96%)	56 (4%)	27 47

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

Mol	Chain	Res	Type
1	A	60	LYS
1	A	61	ASP
1	A	65	LYS
1	A	161	LEU
1	A	208	LYS
1	A	221	MET
1	A	229	VAL
1	A	230	ARG
1	A	249	GLN
1	A	301	ASP
1	A	307	LYS
1	A	320	ARG
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	161	LEU
1	B	239	ASP
1	B	252	ASP

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Mol	Chain	Res	Type
1	B	284	VAL
1	B	301	ASP
1	B	320	ARG
1	B	378	GLU
1	C	10	ARG
1	C	11	PHE
1	C	12	GLU
1	C	13	LYS
1	C	18	LEU
1	C	60	LYS
1	C	61	ASP
1	C	74	GLU
1	C	111	GLU
1	C	161	LEU
1	C	239	ASP
1	C	307	LYS
1	C	320	ARG
1	D	8	GLU
1	D	61	ASP
1	D	77	GLU
1	D	87	PHE
1	D	95	HIS
1	D	138	GLN
1	D	139	LEU
1	D	161	LEU
1	D	176	ARG
1	D	204	MET
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	402	ASN
1	C	327	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 monosaccharides 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	$\#\|Z\| > 2$
2	EPE	B	501	-	15,15,15	1.07	1 (6%)	18,20,20	0.44	0
3	86K	B	502	-	27,29,29	1.49	3 (11%)	28,40,40	1.04	1 (3%)
3	86K	A	502	-	27,29,29	1.68	4 (14%)	28,40,40	1.12	1 (3%)
3	86K	C	501	-	27,29,29	1.66	4 (14%)	28,40,40	1.13	2 (7%)
2	EPE	A	501	-	15,15,15	1.26	1 (6%)	18,20,20	0.22	0

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	EPE	B	501	-	-	0/9/19/19	0/1/1/1
3	86K	B	502	-	-	7/12/26/26	0/4/4/4
3	86K	A	502	-	-	9/12/26/26	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	86K	C	501	-	-	7/12/26/26	0/4/4/4
2	EPE	A	501	-	-	0/9/19/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	86K	C16-C15	-5.48	1.31	1.49
3	A	502	86K	C16-C15	-5.37	1.31	1.49
3	B	502	86K	C16-C15	-5.33	1.31	1.49
2	A	501	EPE	C10-S	-4.81	1.70	1.77
2	B	501	EPE	C10-S	-3.96	1.71	1.77
3	A	502	86K	C6-N4	3.93	1.50	1.39
3	C	501	86K	C14-C15	3.07	1.50	1.36
3	B	502	86K	C14-C15	3.06	1.50	1.36
3	C	501	86K	C6-N4	3.05	1.47	1.39
3	A	502	86K	C14-C15	2.88	1.49	1.36
3	C	501	86K	C18-C27	2.87	1.45	1.42
3	B	502	86K	C18-C27	2.74	1.44	1.42
3	A	502	86K	C18-C27	2.55	1.44	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	86K	C13-C14-C15	-4.13	110.61	123.77
3	A	502	86K	C17-C16-C15	3.61	123.44	112.14
3	B	502	86K	C13-C14-C15	-3.39	112.99	123.77
3	C	501	86K	C13-N12-C2	2.03	126.21	121.03

There are no chirality outliers.

All (23) 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	N12-C2-C3-N4

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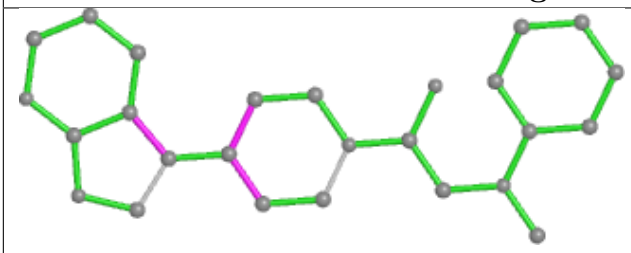
Mol	Chain	Res	Type	Atoms
3	A	502	86K	C7-C6-N4-C3
3	B	502	86K	C2-C3-N4-C5
3	C	501	86K	C2-C3-N4-C5
3	B	502	86K	N12-C2-C3-N4
3	C	501	86K	N12-C2-C3-N4
3	A	502	86K	O1-C2-C3-N4
3	B	502	86K	C11-C6-N4-C3
3	B	502	86K	O1-C2-C3-N4
3	C	501	86K	O1-C2-C3-N4
3	B	502	86K	C7-C6-N4-C3
3	C	501	86K	C7-C6-N4-C3
3	A	502	86K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

There are no ring outliers.

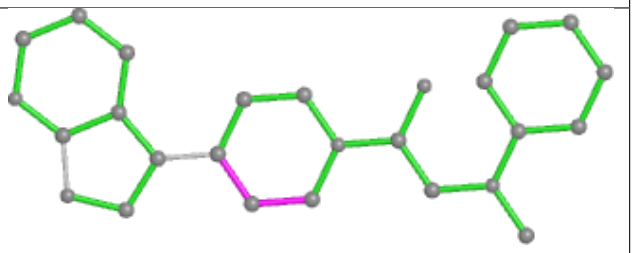
No monomer is involved in short contacts.

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.

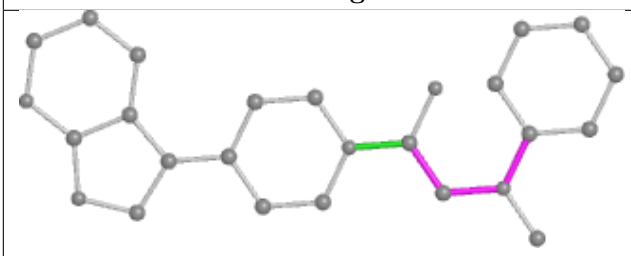
Ligand 86K B 502



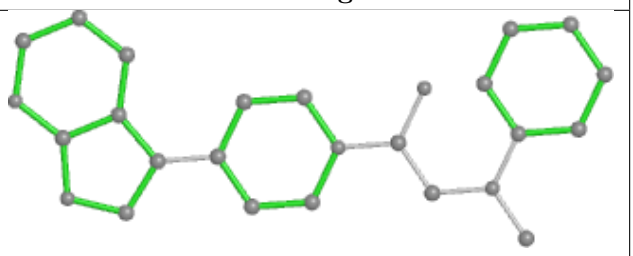
Bond lengths



Bond angles

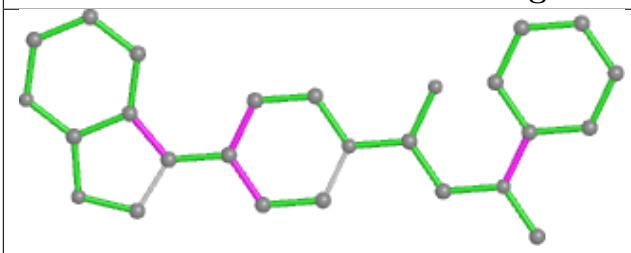


Torsions

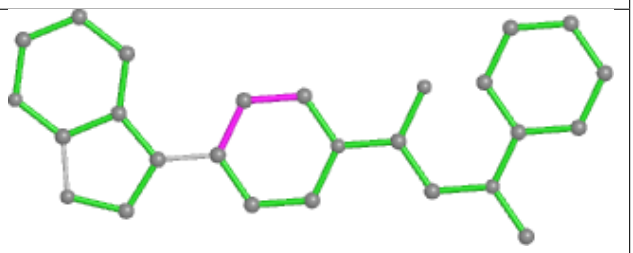


Rings

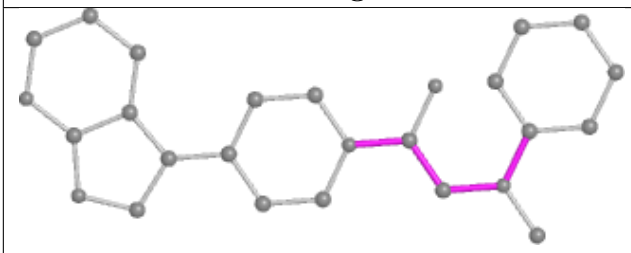
Ligand 86K A 502



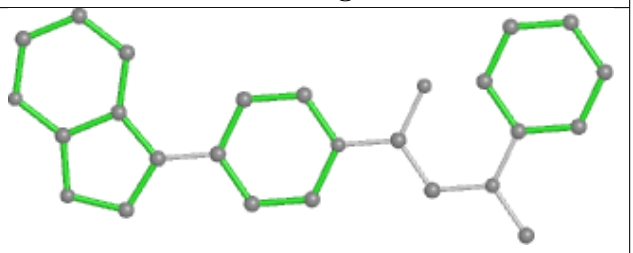
Bond lengths



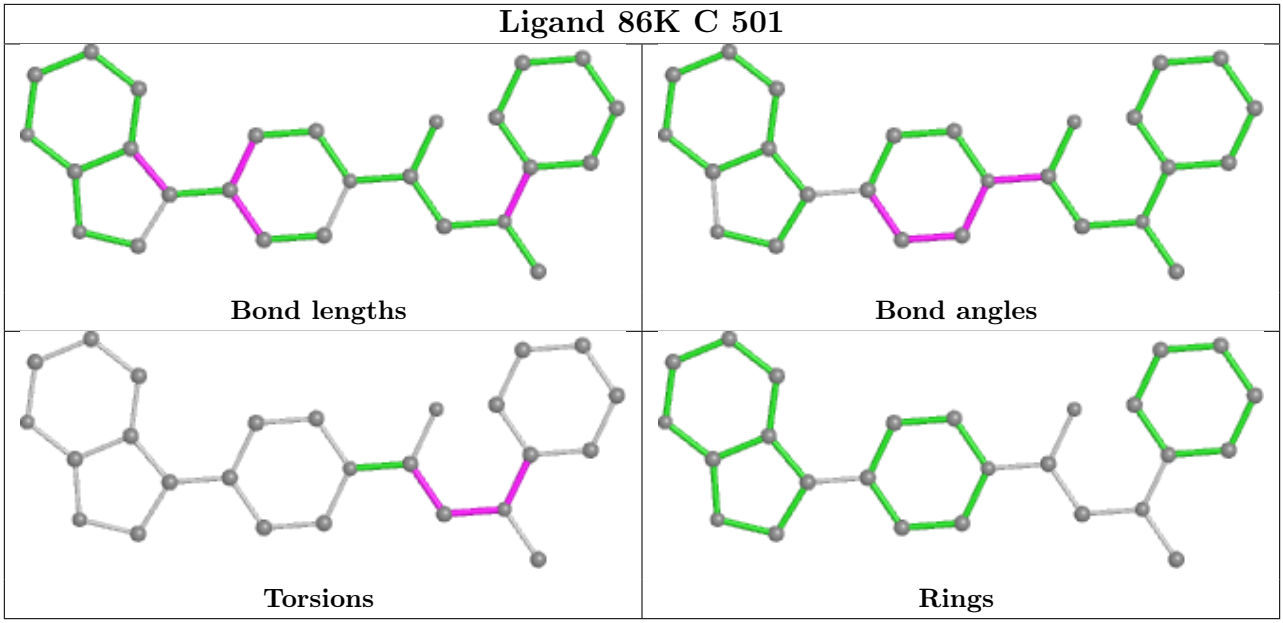
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.76	26 (6%) 17 20	66, 93, 137, 173	0
1	B	372/398 (93%)	0.80	46 (12%) 4 4	93, 121, 149, 156	0
1	C	363/398 (91%)	0.85	42 (11%) 4 4	68, 110, 169, 185	0
1	D	256/398 (64%)	2.01	114 (44%) 0 0	145, 184, 205, 209	0
All	All	1379/1592 (86%)	1.03	228 (16%) 1 1	66, 118, 194, 209	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	VAL	12.3
1	D	215	ALA	8.9
1	D	79	VAL	8.3
1	D	169	ASP	8.1
1	D	168	TYR	7.6
1	D	175	ALA	7.6
1	D	217	PHE	7.6
1	D	271	MET	7.3
1	D	104	MET	7.0
1	D	122	TRP	6.5
1	D	118	SER	6.4
1	C	287	TYR	6.2
1	D	106	LEU	6.1
1	D	164	LEU	6.1
1	D	267	PHE	6.0
1	D	130	PHE	6.0
1	D	155	TYR	5.9
1	D	94	ARG	5.8
1	D	183	VAL	5.8
1	D	153	MET	5.8
1	D	105	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	34	LEU	5.7
1	C	121	PHE	5.5
1	B	287	TYR	5.5
1	D	182	VAL	5.5
1	D	152	VAL	5.4
1	C	194	PHE	5.4
1	D	121	PHE	5.4
1	D	210	GLY	5.3
1	C	113	ILE	5.3
1	D	264	VAL	5.2
1	D	93	VAL	5.1
1	D	18	LEU	5.1
1	A	6	SER	5.0
1	D	107	LEU	4.9
1	C	43	PHE	4.9
1	C	44	PRO	4.8
1	D	17	LEU	4.8
1	D	266	VAL	4.7
1	D	178	TYR	4.7
1	B	359	LEU	4.7
1	B	297	LEU	4.5
1	D	214	LEU	4.4
1	D	151	MET	4.4
1	D	219	THR	4.4
1	C	237	THR	4.3
1	B	206	LEU	4.3
1	D	174	TRP	4.3
1	A	14	MET	4.3
1	B	397	PHE	4.2
1	B	82	ILE	4.1
1	D	89	GLU	4.1
1	D	140	PHE	4.1
1	D	82	ILE	4.0
1	D	273	VAL	4.0
1	B	246	LEU	4.0
1	D	180	ALA	3.9
1	C	402	ASN	3.9
1	D	43	PHE	3.9
1	D	90	VAL	3.8
1	B	277	PRO	3.8
1	D	119	ALA	3.8
1	C	48	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	102	TYR	3.8
1	A	377	GLU	3.8
1	D	179	THR	3.8
1	D	65	LYS	3.7
1	D	186	LEU	3.7
1	D	269	TYR	3.6
1	D	184	LEU	3.6
1	D	141	TYR	3.6
1	D	220	CYS	3.5
1	A	110	PHE	3.5
1	B	189	ILE	3.5
1	A	18	LEU	3.5
1	D	199	VAL	3.4
1	B	217	PHE	3.4
1	B	348	LEU	3.4
1	D	270	GLU	3.3
1	C	114	LYS	3.3
1	B	266	VAL	3.3
1	D	135	TRP	3.3
1	C	127	ILE	3.3
1	D	218	GLY	3.3
1	A	287	TYR	3.2
1	B	278	PHE	3.2
1	B	399	TYR	3.2
1	D	120	PHE	3.2
1	D	261	TRP	3.2
1	D	55	PHE	3.2
1	D	127	ILE	3.2
1	D	128	MET	3.1
1	B	178	TYR	3.1
1	C	363	ILE	3.1
1	D	268	LEU	3.1
1	A	228	MET	3.1
1	D	221	MET	3.1
1	D	125	ARG	3.1
1	B	14	MET	3.0
1	D	84	ARG	3.0
1	B	267	PHE	3.0
1	B	299	PHE	3.0
1	D	25	VAL	3.0
1	D	83	GLY	3.0
1	C	355	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	386	ALA	2.9
1	D	150	TYR	2.9
1	D	45	ALA	2.9
1	B	241	ILE	2.9
1	D	394	PHE	2.9
1	D	66	ILE	2.9
1	C	52	ILE	2.9
1	C	401	SER	2.9
1	D	209	SER	2.9
1	B	199	VAL	2.9
1	D	69	LEU	2.8
1	A	237	THR	2.8
1	C	38	VAL	2.8
1	D	171	PRO	2.8
1	C	14	MET	2.8
1	D	16	ASN	2.8
1	B	271	MET	2.8
1	D	124	GLU	2.8
1	C	69	LEU	2.8
1	A	13	LYS	2.8
1	B	195	ILE	2.7
1	D	13	LYS	2.7
1	D	101	VAL	2.7
1	A	375	LYS	2.7
1	D	397	PHE	2.7
1	D	177	PHE	2.7
1	A	220	CYS	2.6
1	A	363	ILE	2.6
1	B	264	VAL	2.6
1	D	81	VAL	2.6
1	C	299	PHE	2.6
1	D	208	LYS	2.6
1	C	58	ARG	2.6
1	A	217	PHE	2.6
1	D	21	PRO	2.6
1	B	338	PHE	2.5
1	A	376	GLY	2.5
1	B	305	ILE	2.5
1	D	117	ASP	2.5
1	D	97	SER	2.5
1	D	113	ILE	2.5
1	D	137	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	250	GLY	2.5
1	C	217	PHE	2.5
1	C	105	LYS	2.5
1	C	146	ASP	2.5
1	B	214	LEU	2.4
1	D	357	PRO	2.4
1	A	199	VAL	2.4
1	D	173	LYS	2.4
1	C	18	LEU	2.4
1	D	194	PHE	2.4
1	A	17	LEU	2.4
1	D	147	ARG	2.4
1	D	172	GLU	2.4
1	D	149	LEU	2.4
1	D	78	VAL	2.4
1	B	240	TYR	2.3
1	D	14	MET	2.3
1	D	134	PRO	2.3
1	B	289	LYS	2.3
1	D	27	SER	2.3
1	D	92	LEU	2.3
1	D	395	VAL	2.3
1	B	317	LEU	2.3
1	C	387	PHE	2.3
1	C	55	PHE	2.3
1	D	189	ILE	2.3
1	D	41	LEU	2.3
1	D	31	LEU	2.3
1	B	73	ALA	2.3
1	A	278	PHE	2.3
1	D	263	SER	2.2
1	B	332	ILE	2.2
1	C	241	ILE	2.2
1	B	22	LYS	2.2
1	D	257	ARG	2.2
1	C	37	LEU	2.2
1	A	25	VAL	2.2
1	C	246	LEU	2.2
1	A	272	LEU	2.2
1	B	149	LEU	2.2
1	B	135	TRP	2.2
1	D	109	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	66	ILE	2.2
1	C	41	LEU	2.2
1	A	81	VAL	2.2
1	A	305	ILE	2.2
1	C	189	ILE	2.2
1	C	266	VAL	2.2
1	B	8	GLU	2.1
1	B	107	LEU	2.1
1	C	56	LEU	2.1
1	C	297	LEU	2.1
1	C	36	ALA	2.1
1	B	259	CYS	2.1
1	A	137	VAL	2.1
1	D	46	LEU	2.1
1	D	363	ILE	2.1
1	B	355	VAL	2.1
1	B	130	PHE	2.1
1	C	125	ARG	2.1
1	B	17	LEU	2.1
1	B	137	VAL	2.1
1	B	205	LEU	2.1
1	C	30	LEU	2.1
1	D	39	TYR	2.1
1	D	63	ILE	2.1
1	D	24	GLU	2.1
1	B	90	VAL	2.1
1	B	212	LEU	2.1
1	B	312	LEU	2.1
1	D	143	PHE	2.1
1	A	8	GLU	2.1
1	D	216	ASP	2.1
1	D	154	GLU	2.1
1	A	37	LEU	2.0
1	D	103	ALA	2.0
1	D	195	ILE	2.0
1	A	59	TYR	2.0
1	C	356	VAL	2.0
1	A	121	PHE	2.0
1	C	130	PHE	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)

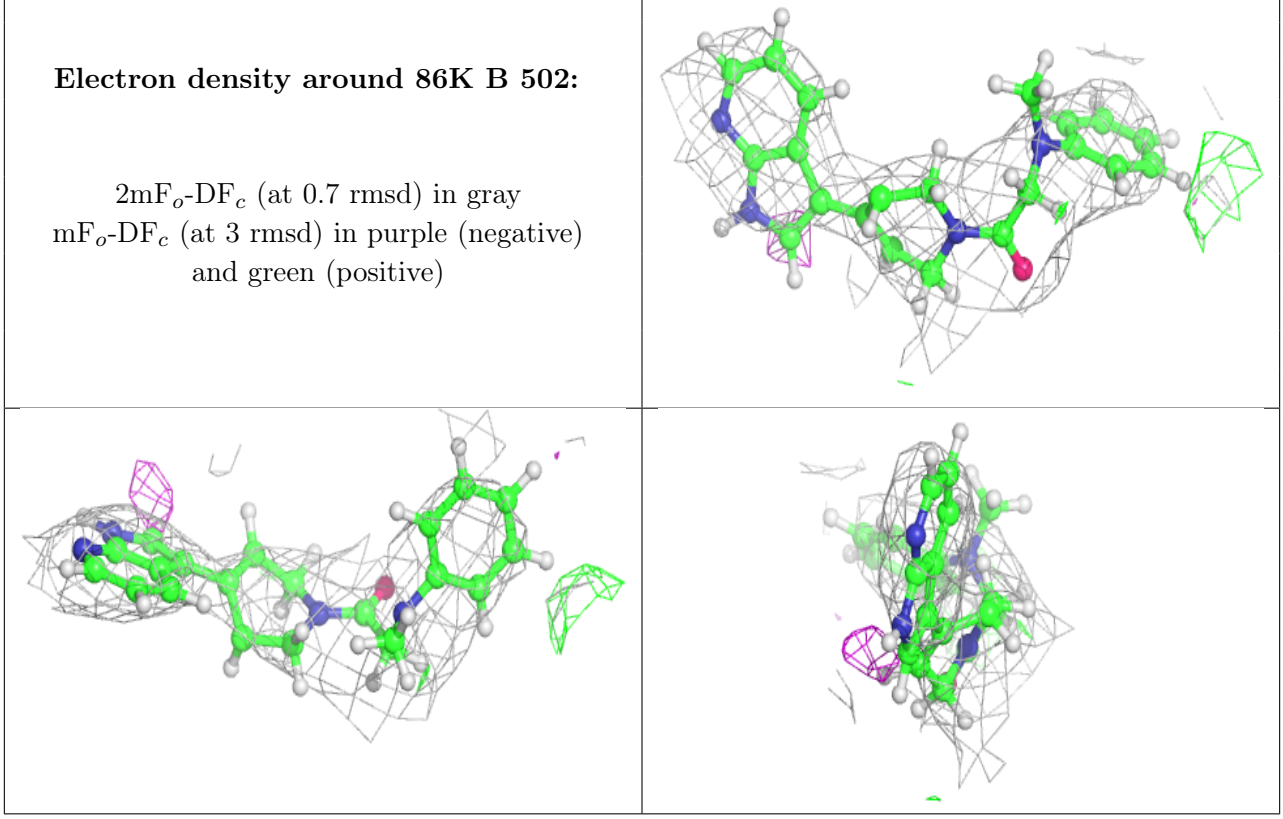
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EPE	B	501	15/15	0.75	0.34	166,166,166,166	0
3	86K	B	502	26/26	0.83	0.33	128,129,130,130	21
2	EPE	A	501	15/15	0.89	0.26	144,145,147,147	0
3	86K	C	501	26/26	0.91	0.34	95,104,114,114	21
3	86K	A	502	26/26	0.95	0.29	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.

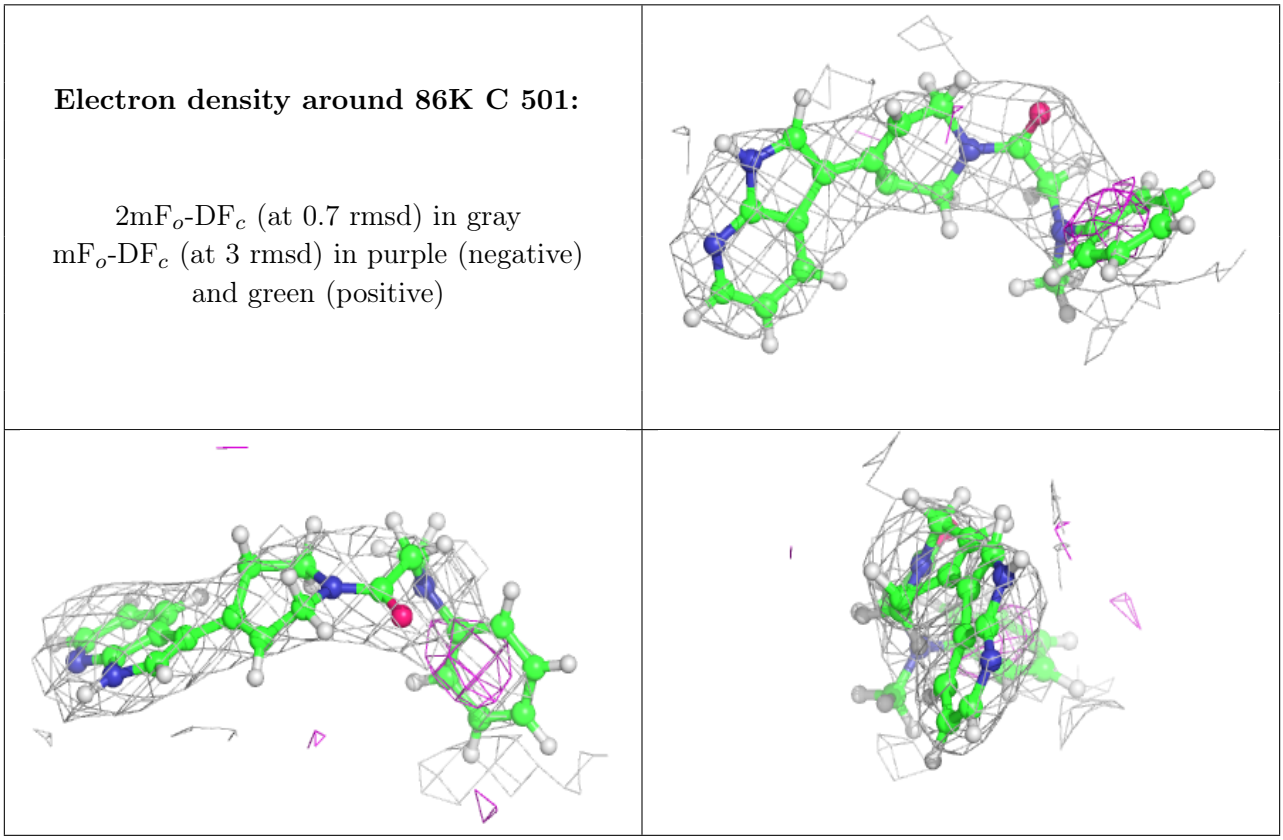
Electron density around 86K B 502:

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



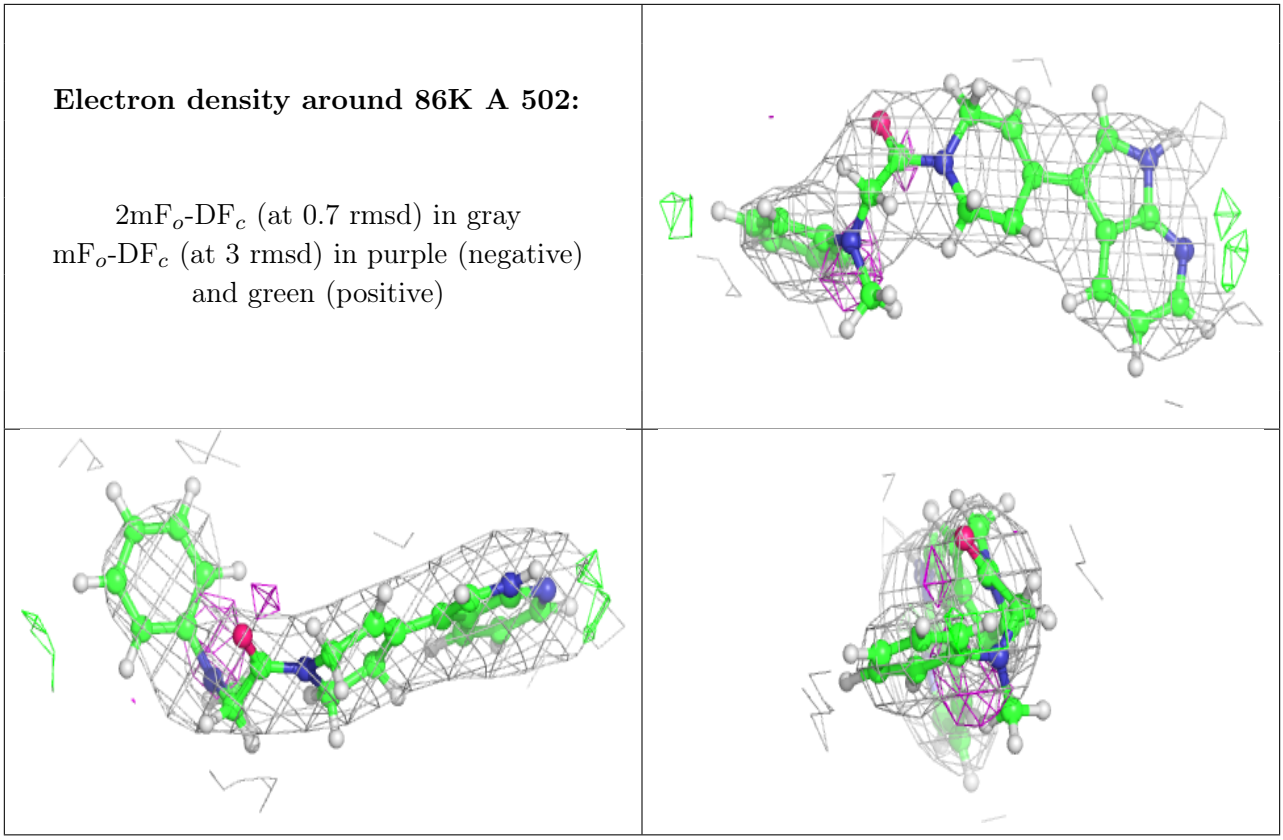
Electron density around 86K C 501:

$2mF_o$-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 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.