



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:45 am BST

PDB ID : 2J0M
Title : Crystal structure a two-chain complex between the FERM and kinase domains of focal adhesion kinase.
Authors : Lietha, D.; Cai, X.; Li, Y.; Schaller, M.D.; Eck, M.J.
Deposited on : 2006-08-03
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

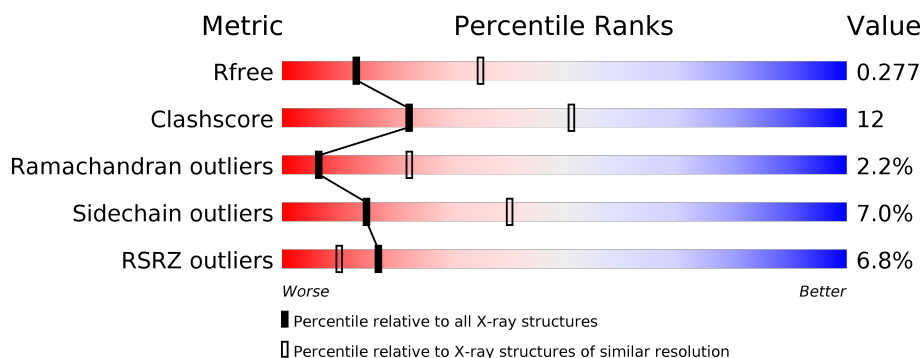
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	371	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>• •</div> <div>11%</div> </div> </div>
2	B	276	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	30	0	0
			2659	1697	457	493	12			

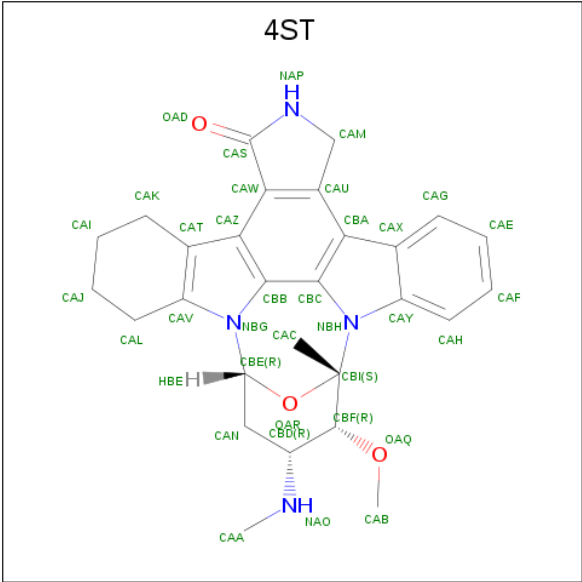
- Molecule 2 is a protein called FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	7	0	0
			2061	1318	356	370	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	449	LEU	MET	conflict	UNP Q00944
B	516	TYR	PHE	conflict	UNP Q00944
B	556	SER	ALA	conflict	UNP Q00944
B	557	ASN	THR	conflict	UNP Q00944

- Molecule 3 is 1,2,3,4-TETRAHYDROGEN-STAUROSPORINE (three-letter code: 4ST) (formula: C₂₈H₃₀N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			35	28	4	3		

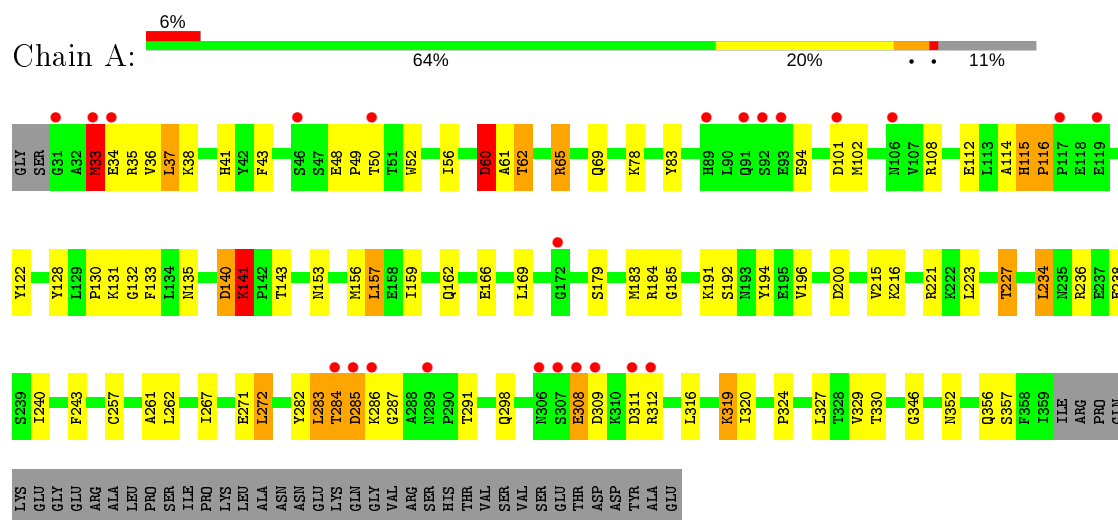
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	32	Total	O	0	0
			32	32		

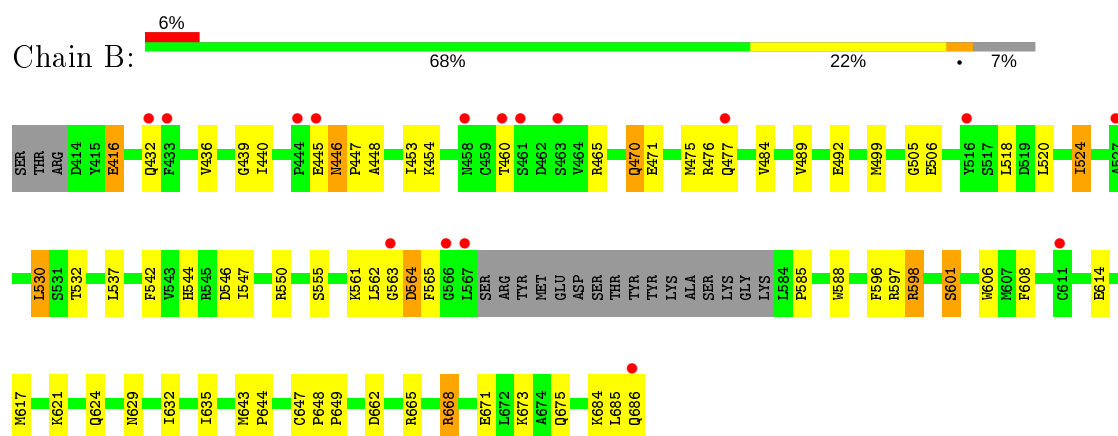
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: FOCAL ADHESION KINASE 1



• Molecule 2: FOCAL ADHESION KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	67.49 Å 90.60 Å 242.61 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.39 – 2.80 26.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.39-2.80) 93.2 (26.88-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.282 0.213 , 0.277	Depositor DCC
R_{free} test set	874 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4808	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: 4ST

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	1.02	11/2715 (0.4%)	0.80	10/3664 (0.3%)
2	B	0.83	7/2107 (0.3%)	0.86	6/2850 (0.2%)
All	All	0.94	18/4822 (0.4%)	0.83	16/6514 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	MET	CG-SD	-28.42	1.07	1.81
1	A	308	GLU	CD-OE2	20.46	1.48	1.25
1	A	319	LYS	CG-CD	-16.69	0.95	1.52
1	A	69	GLN	CG-CD	-16.04	1.14	1.51
2	B	460	THR	CA-CB	16.03	1.95	1.53
2	B	445	GLU	CB-CG	13.14	1.77	1.52
2	B	465	ARG	CZ-NH1	10.62	1.46	1.33
1	A	308	GLU	CD-OE1	10.07	1.36	1.25
1	A	102	MET	CB-CG	-9.50	1.21	1.51
1	A	78	LYS	CD-CE	8.99	1.73	1.51
1	A	141	LYS	CE-NZ	8.79	1.71	1.49
2	B	476	ARG	CZ-NH1	8.30	1.43	1.33
2	B	492	GLU	CB-CG	6.93	1.65	1.52
1	A	140	ASP	CG-OD1	6.79	1.41	1.25
1	A	191	LYS	CG-CD	-6.65	1.29	1.52
2	B	476	ARG	CZ-NH2	6.42	1.41	1.33
2	B	477	GLN	CD-OE1	5.49	1.36	1.24
1	A	216	LYS	CB-CG	5.24	1.66	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	LYS	CB-CG-CD	17.71	157.65	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	MET	CA-CB-CG	16.80	141.85	113.30
2	B	460	THR	CA-CB-CG2	15.47	134.05	112.40
2	B	476	ARG	NE-CZ-NH2	-14.81	112.90	120.30
2	B	465	ARG	NE-CZ-NH2	-13.02	113.79	120.30
1	A	156	MET	CB-CG-SD	12.02	148.47	112.40
1	A	69	GLN	CB-CG-CD	10.44	138.75	111.60
2	B	460	THR	CB-CA-C	-10.39	83.56	111.60
1	A	48	GLU	CA-CB-CG	8.53	132.16	113.40
1	A	319	LYS	CG-CD-CE	7.88	135.54	111.90
2	B	465	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	B	460	THR	N-CA-CB	-5.79	99.29	110.30
1	A	69	GLN	CG-CD-OE1	5.35	132.30	121.60
1	A	69	GLN	CG-CD-NE2	-5.26	104.08	116.70
1	A	191	LYS	CB-CG-CD	5.21	125.16	111.60
1	A	140	ASP	CB-CG-OD1	-5.02	113.78	118.30

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	2659	0	2651	55	0
2	B	2061	0	2069	52	0
3	B	35	0	30	8	0
4	A	21	0	0	1	0
4	B	32	0	0	0	0
All	All	4808	0	4750	109	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 12.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:CE	1:A:141:LYS:NZ	1.71	1.48
2:B:446:ASN:HB3	2:B:447:PRO:HD3	1.23	1.11
1:A:284:THR:HA	1:A:285:ASP:HB2	1.16	1.11
1:A:33:MET:HB2	1:A:34:GLU:HA	1.35	1.07
2:B:564:ASP:HB3	2:B:565:PHE:HA	1.33	1.05
2:B:564:ASP:CB	2:B:565:PHE:HA	1.91	1.00
2:B:446:ASN:HB3	2:B:447:PRO:CD	1.96	0.94
1:A:284:THR:HA	1:A:285:ASP:CB	1.99	0.92
2:B:668:ARG:HA	2:B:668:ARG:HE	1.33	0.91
3:B:1687:4ST:HAC2	3:B:1687:4ST:HAH	1.54	0.88
1:A:33:MET:HB2	1:A:34:GLU:CA	2.02	0.88
2:B:564:ASP:HB3	2:B:565:PHE:CA	2.03	0.87
2:B:563:GLY:O	2:B:564:ASP:HB2	1.79	0.82
1:A:284:THR:CA	1:A:285:ASP:HB2	2.05	0.80
1:A:33:MET:CB	1:A:34:GLU:HA	2.11	0.77
2:B:520:LEU:O	2:B:524:ILE:HG12	1.87	0.74
2:B:505:GLY:HA2	3:B:1687:4ST:HA12	1.74	0.70
2:B:564:ASP:CG	2:B:565:PHE:HA	2.12	0.69
2:B:564:ASP:CB	2:B:565:PHE:CA	2.69	0.69
1:A:286:LYS:HB3	1:A:287:GLY:HA2	1.75	0.67
2:B:446:ASN:CB	2:B:447:PRO:HD3	2.13	0.67
2:B:684:LYS:C	2:B:686:GLN:H	2.00	0.64
1:A:308:GLU:HA	1:A:309:ASP:C	2.17	0.64
1:A:316:LEU:HB3	1:A:329:VAL:HB	1.81	0.60
1:A:130:PRO:HD2	1:A:133:PHE:HB3	1.83	0.60
3:B:1687:4ST:HAH	3:B:1687:4ST:CAC	2.31	0.59
2:B:475:MET:SD	2:B:499:MET:CE	2.91	0.59
2:B:544:HIS:HB3	2:B:547:ILE:HD11	1.85	0.58
2:B:432:GLN:HA	2:B:432:GLN:OE1	2.03	0.57
2:B:617:MET:SD	2:B:644:PRO:HB3	2.45	0.56
1:A:308:GLU:HG3	1:A:309:ASP:O	2.06	0.56
1:A:37:LEU:HD22	1:A:56:ILE:HD11	1.88	0.56
1:A:261:ALA:HB1	1:A:267:ILE:HG23	1.88	0.55
2:B:606:TRP:HZ2	2:B:635:ILE:HD13	1.72	0.55
1:A:41:HIS:HD2	1:A:43:PHE:H	1.54	0.54
1:A:141:LYS:CD	1:A:141:LYS:NZ	2.65	0.54
2:B:668:ARG:CA	2:B:668:ARG:HE	2.12	0.54
2:B:550:ARG:HH22	2:B:585:PRO:HB3	1.72	0.54
1:A:83:TYR:OH	1:A:143:THR:HG23	2.08	0.53
1:A:140:ASP:OD1	1:A:143:THR:OG1	2.22	0.53
1:A:286:LYS:CB	1:A:287:GLY:HA2	2.37	0.53
2:B:684:LYS:O	2:B:686:GLN:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:O	1:A:112:GLU:HB3	2.09	0.52
2:B:475:MET:SD	2:B:499:MET:HE3	2.50	0.52
1:A:196:VAL:HA	1:A:200:ASP:OD2	2.10	0.51
2:B:537:LEU:HD22	2:B:542:PHE:CD1	2.46	0.51
1:A:262:LEU:HD22	1:A:327:LEU:HD11	1.92	0.51
2:B:629:ASN:O	2:B:632:ILE:HG12	2.11	0.51
2:B:601:SER:HB3	2:B:668:ARG:HH22	1.75	0.51
2:B:671:GLU:O	2:B:675:GLN:HG2	2.11	0.50
1:A:261:ALA:HB3	1:A:330:THR:HB	1.94	0.50
3:B:1687:4ST:HAC2	3:B:1687:4ST:CAH	2.34	0.50
1:A:65:ARG:HD3	4:A:2021:HOH:O	2.12	0.50
2:B:564:ASP:HB3	2:B:565:PHE:CG	2.47	0.49
2:B:475:MET:SD	2:B:499:MET:HE1	2.53	0.49
1:A:49:PRO:HA	1:A:52:TRP:CD2	2.47	0.49
1:A:283:LEU:HD23	1:A:286:LYS:HE3	1.95	0.48
2:B:544:HIS:HD2	2:B:546:ASP:H	1.60	0.48
2:B:439:GLY:HA3	2:B:453:ILE:HD11	1.96	0.48
2:B:532:THR:HG22	2:B:673:LYS:HE3	1.95	0.48
2:B:555:SER:HB2	2:B:561:LYS:HD2	1.95	0.48
2:B:454:LYS:HZ2	3:B:1687:4ST:HAF	1.79	0.48
2:B:601:SER:HB3	2:B:668:ARG:NH2	2.29	0.48
1:A:159:ILE:HA	1:A:162:GLN:NE2	2.30	0.47
2:B:530:LEU:HB3	2:B:608:PHE:HE2	1.79	0.47
1:A:141:LYS:HZ2	1:A:141:LYS:HG3	1.80	0.46
1:A:286:LYS:CB	1:A:287:GLY:CA	2.94	0.46
1:A:128:TYR:CE2	1:A:346:GLY:HA3	2.51	0.46
1:A:194:TYR:CZ	1:A:221:ARG:HA	2.51	0.46
1:A:60:ASP:HA	1:A:61:ALA:HA	1.73	0.45
1:A:61:ALA:O	1:A:62:THR:HB	2.16	0.45
2:B:416:GLU:HA	2:B:489:VAL:O	2.16	0.45
3:B:1687:4ST:CAH	3:B:1687:4ST:CAC	2.91	0.45
2:B:648:PRO:HA	2:B:649:PRO:HD2	1.78	0.45
1:A:169:LEU:HD13	1:A:227:THR:HG21	1.98	0.45
2:B:662:ASP:OD2	2:B:662:ASP:C	2.54	0.45
1:A:179:SER:O	2:B:597:ARG:NH2	2.43	0.44
2:B:436:VAL:HG21	3:B:1687:4ST:HAC1	1.99	0.44
1:A:223:LEU:O	1:A:227:THR:HG23	2.17	0.44
1:A:282:TYR:CE2	1:A:291:THR:HB	2.53	0.44
2:B:440:ILE:CG2	2:B:448:ALA:HB1	2.48	0.43
2:B:598:ARG:HD2	2:B:598:ARG:HA	1.70	0.43
1:A:166:GLU:HA	1:A:169:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:CZ	1:A:185:GLY:H	2.31	0.43
2:B:518:LEU:HA	2:B:518:LEU:HD23	1.92	0.43
1:A:37:LEU:CD2	1:A:56:ILE:HD11	2.48	0.43
1:A:37:LEU:HD11	1:A:122:TYR:CZ	2.54	0.43
1:A:35:ARG:HB3	1:A:36:VAL:H	1.65	0.43
2:B:436:VAL:CG2	3:B:1687:4ST:HAC1	2.48	0.43
1:A:141:LYS:HG3	1:A:141:LYS:NZ	2.34	0.42
1:A:141:LYS:CG	1:A:141:LYS:NZ	2.81	0.42
1:A:257:CYS:HA	1:A:272:LEU:O	2.19	0.42
1:A:65:ARG:HG3	1:A:65:ARG:O	2.19	0.42
2:B:643:MET:HA	2:B:644:PRO:HD2	1.90	0.42
1:A:153:ASN:O	1:A:157:LEU:HB2	2.19	0.42
1:A:128:TYR:CD2	1:A:346:GLY:HA3	2.54	0.42
2:B:662:ASP:HB3	2:B:665:ARG:HD2	2.02	0.42
1:A:240:ILE:O	1:A:243:PHE:HB3	2.20	0.42
2:B:470:GLN:HE21	2:B:470:GLN:HB2	1.74	0.42
2:B:684:LYS:C	2:B:686:GLN:N	2.70	0.42
1:A:298:GLN:HB3	1:A:320:ILE:HG23	2.02	0.41
2:B:588:TRP:HE1	2:B:614:GLU:CD	2.23	0.41
1:A:115:HIS:O	1:A:116:PRO:C	2.59	0.41
1:A:183:MET:SD	2:B:596:PHE:CE1	3.14	0.41
2:B:621:LYS:HB2	2:B:624:GLN:HE21	1.85	0.41
2:B:470:GLN:O	2:B:471:GLU:C	2.59	0.41
1:A:284:THR:CA	1:A:285:ASP:CB	2.82	0.40
1:A:234:LEU:HG	1:A:238:GLU:HB3	2.03	0.40
1:A:271:GLU:HB3	1:A:283:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/371 (88%)	275 (84%)	42 (13%)	10 (3%)	4	14
2	B	253/276 (92%)	230 (91%)	20 (8%)	3 (1%)	13	39
All	All	580/647 (90%)	505 (87%)	62 (11%)	13 (2%)	6	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	62	THR
1	A	285	ASP
2	B	446	ASN
2	B	564	ASP
1	A	352	ASN
2	B	685	LEU
1	A	114	ALA
1	A	311	ASP
1	A	60	ASP
1	A	116	PRO
1	A	324	PRO
1	A	132	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/327 (89%)	265 (91%)	25 (9%)	10	30
2	B	227/246 (92%)	216 (95%)	11 (5%)	25	58
All	All	517/573 (90%)	481 (93%)	36 (7%)	15	40

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	37	LEU
1	A	38	LYS

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Mol	Chain	Res	Type
1	A	50	THR
1	A	60	ASP
1	A	65	ARG
1	A	94	GLU
1	A	101	ASP
1	A	115	HIS
1	A	131	LYS
1	A	135	ASN
1	A	141	LYS
1	A	157	LEU
1	A	192	SER
1	A	215	VAL
1	A	227	THR
1	A	234	LEU
1	A	236	ARG
1	A	272	LEU
1	A	283	LEU
1	A	284	THR
1	A	312	ARG
1	A	319	LYS
1	A	356	GLN
1	A	357	SER
2	B	416	GLU
2	B	470	GLN
2	B	484	VAL
2	B	506	GLU
2	B	524	ILE
2	B	530	LEU
2	B	562	LEU
2	B	598	ARG
2	B	601	SER
2	B	647	CYS
2	B	668	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	45	ASN
1	A	75	HIS
2	B	470	GLN
2	B	544	HIS

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Mol	Chain	Res	Type
2	B	557	ASN
2	B	624	GLN
2	B	637	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	4ST	B	1687	-	31,42,42	2.50	7 (22%)	28,68,68	2.43	8 (28%)

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	4ST	B	1687	-	-	0/4/49/49	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1687	4ST	CAM-CAU	10.26	1.58	1.50
3	B	1687	4ST	CAW-CAS	-3.81	1.43	1.49
3	B	1687	4ST	CAC-CBI	3.81	1.56	1.51
3	B	1687	4ST	CAM-NAP	3.37	1.49	1.45
3	B	1687	4ST	CBA-CBC	-2.76	1.39	1.42
3	B	1687	4ST	OAQ-CBF	2.57	1.46	1.42
3	B	1687	4ST	CAW-CAZ	2.36	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1687	4ST	CAW-CAS-NAP	6.44	112.89	106.37
3	B	1687	4ST	CAM-NAP-CAS	-5.12	108.93	113.85
3	B	1687	4ST	OAR-CBE-CAN	5.04	119.58	112.31
3	B	1687	4ST	OAD-CAS-NAP	-3.74	120.89	125.27
3	B	1687	4ST	CAT-CAV-NBG	3.72	109.03	106.66
3	B	1687	4ST	CAW-CAU-CBA	-2.93	118.48	122.42
3	B	1687	4ST	CAT-CAZ-CBB	-2.87	105.74	110.57
3	B	1687	4ST	OAD-CAS-CAW	-2.62	126.22	129.32

There are no chirality outliers.

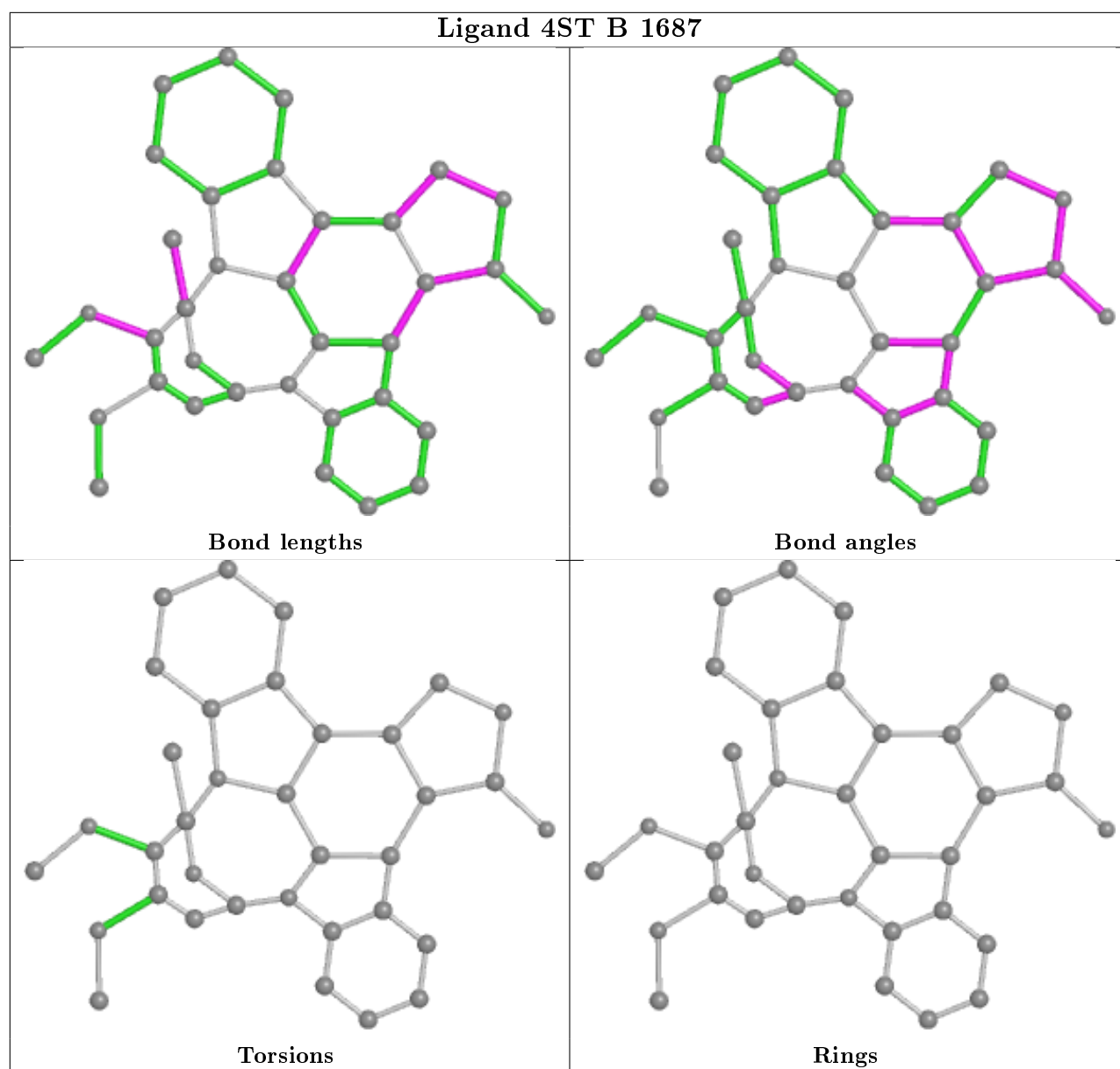
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1687	4ST	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/371 (88%)	0.37	24 (7%) 15 8	51, 62, 72, 80	9 (2%)
2	B	257/276 (93%)	0.21	16 (6%) 20 13	33, 58, 68, 77	2 (0%)
All	All	586/647 (90%)	0.30	40 (6%) 17 10	33, 60, 71, 80	11 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ARG	7.3
1	A	91	GLN	4.8
1	A	311	ASP	4.4
2	B	686	GLN	4.2
1	A	289	ASN	4.2
1	A	285	ASP	4.2
1	A	306	ASN	4.2
1	A	31	GLY	4.0
1	A	93	GLU	3.7
1	A	101	ASP	3.5
1	A	309	ASP	3.5
2	B	566	GLY	3.2
2	B	463	SER	3.1
1	A	308	GLU	3.1
1	A	307	SER	3.1
1	A	33	MET	3.0
1	A	284	THR	3.0
2	B	563	GLY	2.9
2	B	477	GLN	2.7
2	B	461	SER	2.6
1	A	117	PRO	2.6
2	B	433	PHE	2.5
1	A	92	SER	2.4
2	B	432	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	444	PRO	2.3
2	B	516	TYR	2.3
2	B	567	LEU	2.3
1	A	119	GLU	2.2
1	A	106	ASN	2.1
1	A	172	GLY	2.1
2	B	611	CYS	2.1
1	A	34	GLU	2.1
1	A	89	HIS	2.1
1	A	46	SER	2.1
2	B	460	THR	2.1
2	B	527	ALA	2.1
2	B	445	GLU	2.1
2	B	458	ASN	2.1
1	A	286	LYS	2.0
1	A	50	THR	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](#)

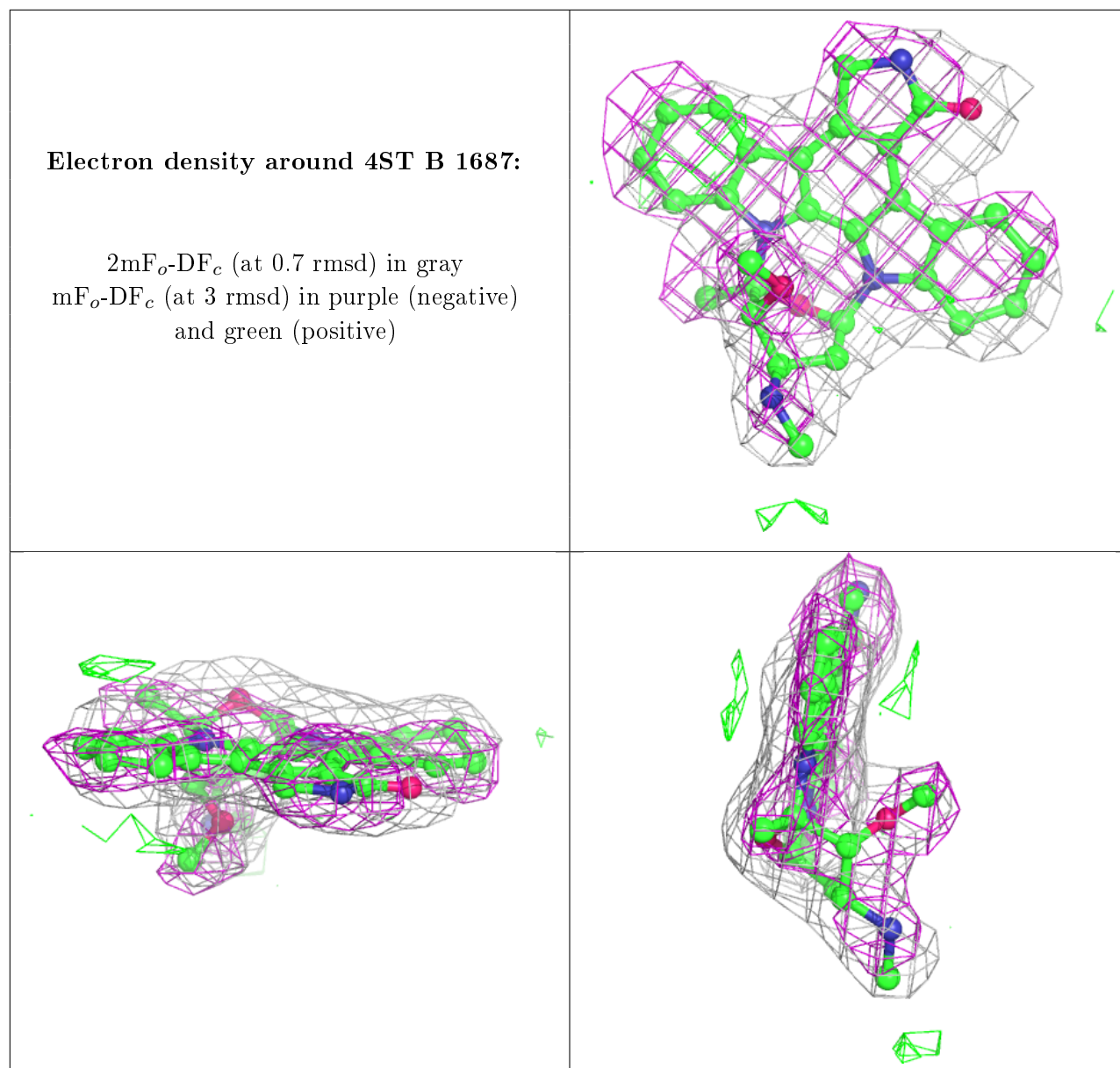
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
3	4ST	B	1687	35/35	0.97	0.13	36,37,39,40	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.