WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 10:26 pm GMT

PDB ID	:	2J0J
Title	:	Crystal structure of a fragment of focal adhesion kinase containing the FERM and kinase domains.
Authors	:	Lietha, D.; Cai, X.; Li, Y.; Schaller, M.D.; Eck, M.J.
Deposited on	:	2006-08-03
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

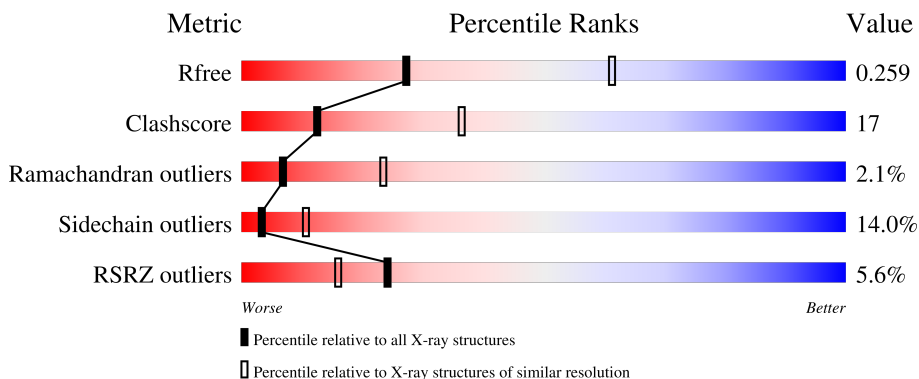|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.259
Clashscore		17
Ramachandran outliers		2.1%
Sidechain outliers		14.0%
RSRZ outliers		5.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 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	656	5% · 59% · 28% · 6% · 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4993 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.
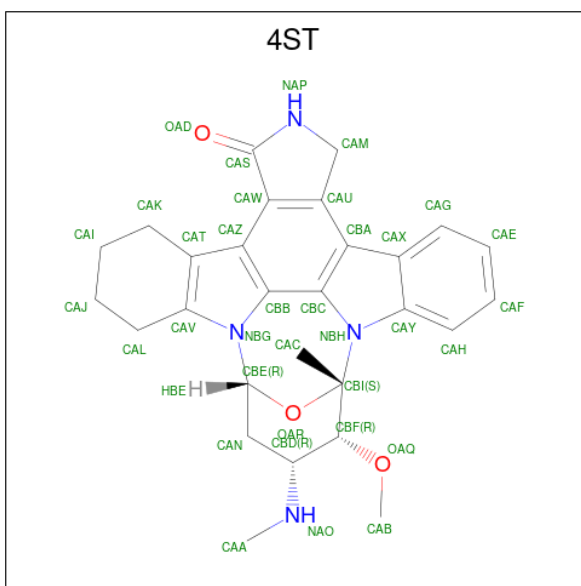
- Molecule 1 is a protein called FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total 4936	C 3148	N 845	O 913	S 30	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	SER	ALA	conflict	UNP Q00944
A	557	ASN	THR	conflict	UNP Q00944

- Molecule 2 is 1,2,3,4-TETRAHYDROGEN-STAUROSPORINE (three-letter code: 4ST) (formula: $C_{28}H_{30}N_4O_3$).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0

3 Residue-property plots ⓘ

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: FOCAL ADHESION KINASE 1

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	67.53Å 91.28Å 250.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.55 – 2.80 45.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (45.55-2.80) 91.2 (45.53-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.94 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.274 0.215 , 0.259	Depositor DCC
R_{free} test set	913 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 83.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4993	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (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	0.47	0/5043	0.66	1/6814 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	VAL	N-CA-C	5.64	126.22	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ARG	Peptide
1	A	36	VAL	Peptide
1	A	411	SER	Peptide
1	A	571	MET	Peptide

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	4936	0	4911	162	0
2	A	35	0	30	6	0
3	A	22	0	0	2	0
All	All	4993	0	4941	166	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 17.

All (166) 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:36:VAL:CG2	1:A:37:LEU:H	1.46	1.28
1:A:410:PRO:HA	1:A:411:SER:CB	1.75	1.13
1:A:36:VAL:HG22	1:A:37:LEU:H	0.97	1.08
1:A:349:ARG:HH11	1:A:349:ARG:HB3	1.23	1.04
1:A:410:PRO:CA	1:A:411:SER:HB3	1.87	1.03
1:A:35:ARG:HH11	1:A:35:ARG:HG2	1.20	1.03
1:A:36:VAL:CG2	1:A:37:LEU:N	2.18	1.03
1:A:524:ILE:HD11	1:A:680:LEU:HA	1.40	1.00
1:A:421:ARG:HG2	1:A:421:ARG:HH21	1.28	0.97
1:A:36:VAL:HG22	1:A:37:LEU:N	1.75	0.97
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.27	0.96
1:A:475:MET:SD	1:A:499:MET:HE1	2.14	0.86
1:A:410:PRO:HA	1:A:411:SER:HB3	0.91	0.85
2:A:1687:4ST:HAH	2:A:1687:4ST:HAC2	1.56	0.85
1:A:475:MET:SD	1:A:499:MET:CE	2.65	0.84
1:A:35:ARG:HG2	1:A:35:ARG:NH1	1.90	0.83
1:A:572:GLU:CD	1:A:573:ASP:H	1.82	0.83
1:A:307:SER:HB3	1:A:311:ASP:O	1.79	0.81
1:A:571:MET:H	1:A:572:GLU:HA	1.47	0.79
1:A:41:HIS:HD2	1:A:43:PHE:H	1.26	0.79
1:A:179:SER:O	1:A:597:ARG:NH2	2.17	0.78
1:A:36:VAL:HG23	1:A:37:LEU:H	1.48	0.76
1:A:571:MET:N	1:A:572:GLU:HA	2.00	0.76
1:A:184:ARG:HH11	1:A:184:ARG:HB3	1.50	0.75
1:A:587:LYS:HD3	1:A:623:PHE:HB2	1.68	0.75
1:A:394:THR:O	1:A:395:ASP:HB2	1.87	0.74
1:A:35:ARG:HH11	1:A:35:ARG:CG	1.98	0.73
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:GLY:HA2	2:A:1687:4ST:HAI2	1.71	0.71
1:A:94:GLU:OE2	1:A:96:HIS:HE1	1.72	0.71
1:A:445:GLU:O	1:A:446:ASN:CG	2.30	0.70
1:A:346:GLY:HA2	1:A:349:ARG:NH1	2.06	0.70
1:A:68:ILE:HD11	1:A:85:LEU:HB2	1.76	0.67
1:A:131:LYS:HD2	1:A:276:PRO:O	1.95	0.67
1:A:443:SER:OG	1:A:446:ASN:HB2	1.94	0.67
1:A:571:MET:N	1:A:571:MET:SD	2.69	0.66
1:A:72:VAL:HG21	1:A:80:VAL:HG13	1.78	0.65
1:A:421:ARG:HH21	1:A:421:ARG:CG	2.05	0.64
1:A:36:VAL:HG23	1:A:37:LEU:N	2.05	0.64
1:A:349:ARG:HB3	1:A:349:ARG:NH1	2.05	0.63
1:A:500:GLU:OE1	1:A:561:LYS:HD3	1.97	0.63
1:A:569:ARG:N	1:A:569:ARG:HD3	2.13	0.63
1:A:544:HIS:HD2	1:A:546:ASP:H	1.46	0.63
1:A:41:HIS:CD2	1:A:43:PHE:H	2.13	0.63
1:A:421:ARG:HG2	1:A:421:ARG:NH2	2.07	0.62
1:A:94:GLU:OE2	1:A:96:HIS:CE1	2.53	0.61
1:A:475:MET:SD	1:A:499:MET:HE3	2.40	0.61
1:A:613:TRP:CZ2	1:A:617:MET:HG3	2.35	0.61
1:A:613:TRP:CH2	1:A:617:MET:HG3	2.35	0.61
1:A:434:GLY:HA3	1:A:455:THR:O	2.00	0.60
1:A:572:GLU:CG	1:A:573:ASP:N	2.63	0.60
1:A:63:ASP:HA	1:A:103:GLY:HA2	1.83	0.60
1:A:164:ASP:O	1:A:167:ILE:HB	2.02	0.59
1:A:563:GLY:O	1:A:564:ASP:HB3	2.03	0.58
1:A:412:THR:O	1:A:414:ASP:N	2.37	0.57
1:A:303:GLN:HB3	1:A:317:GLN:HB2	1.85	0.57
1:A:677:SER:O	1:A:680:LEU:HB3	2.04	0.57
1:A:223:LEU:O	1:A:227:THR:HG23	2.05	0.57
1:A:252:ARG:HG2	1:A:252:ARG:NH1	2.06	0.57
1:A:346:GLY:HA2	1:A:349:ARG:CZ	2.36	0.56
1:A:449:MET:HE2	1:A:451:VAL:CG1	2.35	0.56
1:A:304:TYR:CE1	1:A:338:GLU:HG2	2.41	0.56
1:A:556:SER:HB3	1:A:559:CYS:HB3	1.87	0.56
1:A:184:ARG:HB3	1:A:184:ARG:NH1	2.21	0.55
1:A:68:ILE:HG12	1:A:124:LEU:CD1	2.37	0.55
1:A:417:ILE:O	1:A:490:ILE:HG12	2.07	0.55
1:A:613:TRP:CE2	1:A:641:LEU:HD22	2.42	0.55
1:A:519:ASP:OD1	1:A:522:SER:OG	2.25	0.55
1:A:426:ARG:HG2	1:A:427:CYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:CG	1:A:421:ARG:NH2	2.66	0.54
1:A:410:PRO:CA	1:A:411:SER:CB	2.66	0.53
1:A:111:PHE:C	1:A:113:LEU:H	2.11	0.53
1:A:258:PHE:O	1:A:271:GLU:HA	2.08	0.53
1:A:135:ASN:O	1:A:138:THR:HB	2.10	0.52
1:A:88:SER:HB2	1:A:95:VAL:HG23	1.90	0.52
1:A:159:ILE:HA	1:A:162:GLN:HE21	1.74	0.52
1:A:443:SER:HG	1:A:446:ASN:HB2	1.74	0.52
1:A:572:GLU:O	1:A:573:ASP:HB2	2.09	0.52
1:A:172:GLY:HA3	1:A:207:PHE:CE2	2.45	0.52
1:A:572:GLU:CG	1:A:573:ASP:H	2.23	0.52
1:A:572:GLU:HG2	1:A:573:ASP:N	2.25	0.51
1:A:572:GLU:OE1	1:A:573:ASP:C	2.49	0.51
2:A:1687:4ST:HAH	2:A:1687:4ST:CAC	2.35	0.51
1:A:35:ARG:HD3	1:A:36:VAL:O	2.11	0.51
1:A:55:ILE:HD13	1:A:402:ASP:HA	1.93	0.51
1:A:109:GLU:O	1:A:113:LEU:HB2	2.11	0.51
1:A:129:LEU:O	1:A:276:PRO:HB3	2.11	0.50
1:A:276:PRO:HG2	1:A:277:GLU:HG2	1.94	0.50
1:A:500:GLU:OE1	1:A:561:LYS:CD	2.59	0.50
1:A:613:TRP:NE1	1:A:641:LEU:HB3	2.26	0.50
1:A:194:TYR:CD2	1:A:221:ARG:HG3	2.46	0.50
1:A:46:SER:OG	1:A:571:MET:HB3	2.12	0.50
1:A:169:LEU:HD13	1:A:227:THR:HG21	1.94	0.50
1:A:35:ARG:HB3	1:A:58:HIS:HE1	1.77	0.49
1:A:60:ASP:O	1:A:105:SER:OG	2.30	0.49
1:A:270:VAL:HG11	1:A:282:TYR:CD1	2.47	0.49
1:A:606:TRP:CD1	1:A:606:TRP:C	2.86	0.49
1:A:295:ASP:HB2	1:A:298:GLN:HE21	1.77	0.49
1:A:572:GLU:CD	1:A:573:ASP:N	2.59	0.49
1:A:108:ARG:HG3	1:A:108:ARG:NH1	2.27	0.49
1:A:493:ASN:HB3	3:A:2009:HOH:O	2.13	0.49
1:A:48:GLU:OE1	1:A:205:ARG:NH2	2.45	0.48
1:A:49:PRO:HA	1:A:52:TRP:CE2	2.48	0.48
1:A:106:ASN:N	1:A:106:ASN:OD1	2.46	0.48
1:A:568:SER:C	1:A:569:ARG:HD3	2.33	0.48
1:A:419:ARG:NH2	1:A:494:PRO:O	2.47	0.48
1:A:632:ILE:HG13	1:A:633:GLY:N	2.28	0.48
1:A:598:ARG:HH21	1:A:598:ARG:HG3	1.78	0.48
1:A:198:GLU:HA	1:A:203:LEU:HG	1.95	0.48
1:A:349:ARG:HH11	1:A:349:ARG:CB	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:O	1:A:446:ASN:CB	2.62	0.48
1:A:461:SER:O	1:A:464:VAL:N	2.46	0.48
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.79	0.47
1:A:627:LYS:O	1:A:630:ASP:HB2	2.14	0.47
1:A:159:ILE:HA	1:A:162:GLN:NE2	2.29	0.47
1:A:333:SER:OG	1:A:336:ILE:HG13	2.15	0.46
1:A:567:LEU:HD23	1:A:569:ARG:HG2	1.98	0.46
1:A:361:ARG:HA	1:A:362:PRO:HD2	1.81	0.46
1:A:525:LEU:O	1:A:529:GLN:HG3	2.15	0.45
1:A:307:SER:C	1:A:309:ASP:H	2.19	0.45
1:A:572:GLU:O	1:A:573:ASP:CB	2.64	0.45
1:A:36:VAL:HB	1:A:57:ARG:HA	1.99	0.45
1:A:235:ASN:C	1:A:235:ASN:OD1	2.56	0.44
1:A:605:VAL:HG13	1:A:672:LEU:HD11	2.00	0.44
1:A:629:ASN:O	1:A:632:ILE:HG12	2.18	0.44
1:A:240:ILE:O	1:A:243:PHE:HB3	2.18	0.44
1:A:183:MET:O	1:A:183:MET:HG3	2.16	0.44
1:A:55:ILE:HD12	1:A:55:ILE:N	2.33	0.43
1:A:302:ILE:O	1:A:359:ILE:HA	2.18	0.43
1:A:70:LYS:HG3	1:A:398:ALA:O	2.19	0.43
1:A:475:MET:CE	1:A:499:MET:HE1	2.47	0.43
1:A:295:ASP:H	1:A:298:GLN:HE21	1.66	0.43
1:A:450:ALA:HB1	1:A:501:LEU:HD23	2.01	0.43
1:A:623:PHE:HB3	1:A:626:VAL:HB	2.00	0.43
1:A:544:HIS:O	1:A:545:ARG:HB2	2.17	0.43
1:A:352:ASN:C	1:A:354:ALA:H	2.21	0.43
2:A:1687:4ST:HAC2	2:A:1687:4ST:CAH	2.33	0.43
1:A:418:GLN:HB3	1:A:420:GLU:OE2	2.18	0.43
1:A:669:PHE:HA	1:A:672:LEU:HD12	2.00	0.43
1:A:266:TRP:HD1	3:A:2004:HOH:O	1.99	0.43
2:A:1687:4ST:CAC	2:A:1687:4ST:CAH	2.94	0.43
1:A:248:SER:N	1:A:249:PRO:CD	2.82	0.42
1:A:490:ILE:O	1:A:495:VAL:HA	2.19	0.42
1:A:45:ASN:OD1	1:A:571:MET:CE	2.67	0.42
1:A:402:ASP:HB2	1:A:403:GLU:HG3	2.00	0.42
1:A:506:GLU:H	1:A:506:GLU:HG2	1.60	0.42
1:A:650:THR:O	1:A:653:SER:HB3	2.19	0.42
1:A:499:MET:HB3	1:A:499:MET:HE2	1.63	0.42
1:A:349:ARG:O	1:A:349:ARG:HG2	2.20	0.42
1:A:400:ILE:H	1:A:400:ILE:HG13	1.56	0.42
1:A:352:ASN:O	1:A:354:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:HB2	1:A:212:LEU:HD21	2.02	0.41
1:A:309:ASP:HB2	1:A:310:LYS:H	1.72	0.41
1:A:415:TYR:CD1	1:A:489:VAL:HG22	2.55	0.41
1:A:48:GLU:HA	1:A:49:PRO:HD3	1.96	0.41
1:A:588:TRP:O	1:A:607:MET:HG2	2.20	0.41
1:A:682:GLU:O	1:A:686:GLN:N	2.51	0.41
1:A:569:ARG:HA	1:A:570:TYR:HA	1.88	0.41
1:A:461:SER:HB2	1:A:464:VAL:HB	2.02	0.41
1:A:466:GLU:HA	1:A:469:LEU:HD23	2.03	0.41
1:A:493:ASN:HA	1:A:494:PRO:HA	1.83	0.41
1:A:627:LYS:HB2	1:A:630:ASP:OD1	2.21	0.41
1:A:630:ASP:O	1:A:634:ARG:HG3	2.21	0.41
1:A:505:GLY:HA2	2:A:1687:4ST:CAI	2.47	0.40
1:A:644:PRO:HA	1:A:645:PRO:HD3	1.86	0.40
1:A:295:ASP:H	1:A:298:GLN:NE2	2.18	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	605/656 (92%)	533 (88%)	59 (10%)	13 (2%)	7	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	395	ASP
1	A	413	ARG
1	A	446	ASN
1	A	564	ASP
1	A	411	SER

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Mol	Chain	Res	Type
1	A	112	GLU
1	A	288	ALA
1	A	353	GLY
1	A	457	LYS
1	A	468	PHE
1	A	638	GLY
1	A	289	ASN

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	542/583 (93%)	466 (86%)	76 (14%)	3	11

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	36	VAL
1	A	37	LEU
1	A	54	SER
1	A	94	GLU
1	A	95	VAL
1	A	105	SER
1	A	106	ASN
1	A	108	ARG
1	A	113	LEU
1	A	118	GLU
1	A	119	GLU
1	A	128	TYR
1	A	131	LYS
1	A	135	ASN
1	A	141	LYS
1	A	144	LEU
1	A	157	LEU
1	A	161	ASP

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	166	GLU
1	A	183	MET
1	A	184	ARG
1	A	211	LEU
1	A	213	ASP
1	A	215	VAL
1	A	227	THR
1	A	248	SER
1	A	252	ARG
1	A	266	TRP
1	A	269	SER
1	A	272	LEU
1	A	284	THR
1	A	286	LYS
1	A	301	THR
1	A	304	TYR
1	A	309	ASP
1	A	312	ARG
1	A	315	MET
1	A	330	THR
1	A	334	LEU
1	A	335	THR
1	A	349	ARG
1	A	352	ASN
1	A	356	GLN
1	A	357	SER
1	A	400	ILE
1	A	402	ASP
1	A	420	GLU
1	A	438	GLN
1	A	449	MET
1	A	463	SER
1	A	470	GLN
1	A	476	ARG
1	A	484	VAL
1	A	499	MET
1	A	503	THR
1	A	506	GLU
1	A	512	GLN
1	A	514	ARG
1	A	522	SER

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Mol	Chain	Res	Type
1	A	524	ILE
1	A	530	LEU
1	A	555	SER
1	A	562	LEU
1	A	567	LEU
1	A	569	ARG
1	A	570	TYR
1	A	571	MET
1	A	572	GLU
1	A	598	ARG
1	A	635	ILE
1	A	639	GLU
1	A	641	LEU
1	A	650	THR
1	A	668	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	69	GLN
1	A	75	HIS
1	A	96	HIS
1	A	135	ASN
1	A	162	GLN
1	A	230	GLN
1	A	298	GLN
1	A	446	ASN
1	A	470	GLN
1	A	544	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
2	4ST	A	1687	-	31,42,42	1.69	4 (12%)	28,68,68	2.47	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
2	4ST	A	1687	-	-	1/4/49/49	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1687	4ST	CAW-CAS	-5.78	1.40	1.49
2	A	1687	4ST	OAQ-CBF	3.06	1.47	1.42
2	A	1687	4ST	CBA-CBC	-3.03	1.38	1.42
2	A	1687	4ST	CAU-CBA	-2.79	1.38	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	4ST	CAW-CAS-NAP	7.20	113.65	106.37
2	A	1687	4ST	CAM-NAP-CAS	-5.59	108.48	113.85
2	A	1687	4ST	OAD-CAS-CAW	-4.00	124.58	129.32
2	A	1687	4ST	CAT-CAV-NBG	3.73	109.03	106.66
2	A	1687	4ST	CAT-CAZ-CBB	-3.58	104.55	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1687	4ST	CAZ-CAW-CAS	3.54	135.06	129.76
2	A	1687	4ST	OAD-CAS-NAP	-3.08	121.67	125.27
2	A	1687	4ST	OAR-CBE-CAN	2.41	115.80	112.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

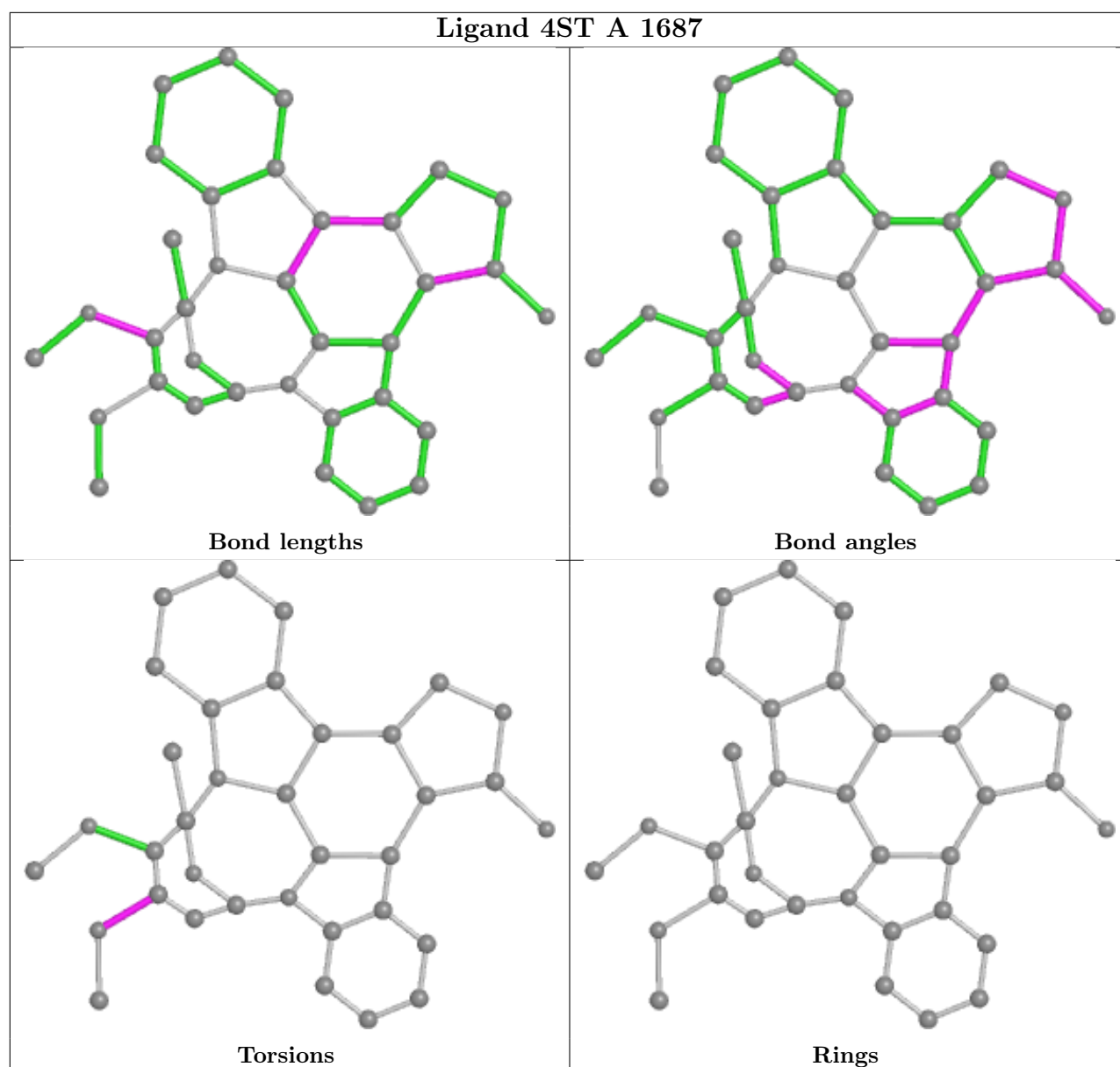| Mol	Chain	Res	Type	Atoms
2	A	1687	4ST	CAN-CBD-NAO-CAA

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1687	4ST	6	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 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 4ST A 1687

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, 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	611/656 (93%)	0.40	34 (5%)	24	16	48, 68, 85, 111	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ALA	5.6
1	A	287	GLY	5.4
1	A	394	THR	4.1
1	A	433	PHE	4.0
1	A	286	LYS	3.7
1	A	309	ASP	3.7
1	A	403	GLU	3.6
1	A	46	SER	3.6
1	A	285	ASP	3.5
1	A	107	VAL	3.5
1	A	315	MET	3.3
1	A	268	ILE	3.0
1	A	310	LYS	3.0
1	A	120	TRP	3.0
1	A	266	TRP	2.8
1	A	308	GLU	2.8
1	A	118	GLU	2.8
1	A	56	ILE	2.6
1	A	463	SER	2.6
1	A	289	ASN	2.5
1	A	412	THR	2.5
1	A	307	SER	2.5
1	A	396	ASP	2.5
1	A	284	THR	2.4
1	A	267	ILE	2.4
1	A	39	VAL	2.3
1	A	312	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	95	VAL	2.2
1	A	566	GLY	2.1
1	A	334	LEU	2.1
1	A	413	ARG	2.1
1	A	318	LEU	2.1
1	A	271	GLU	2.1
1	A	316	LEU	2.0

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.
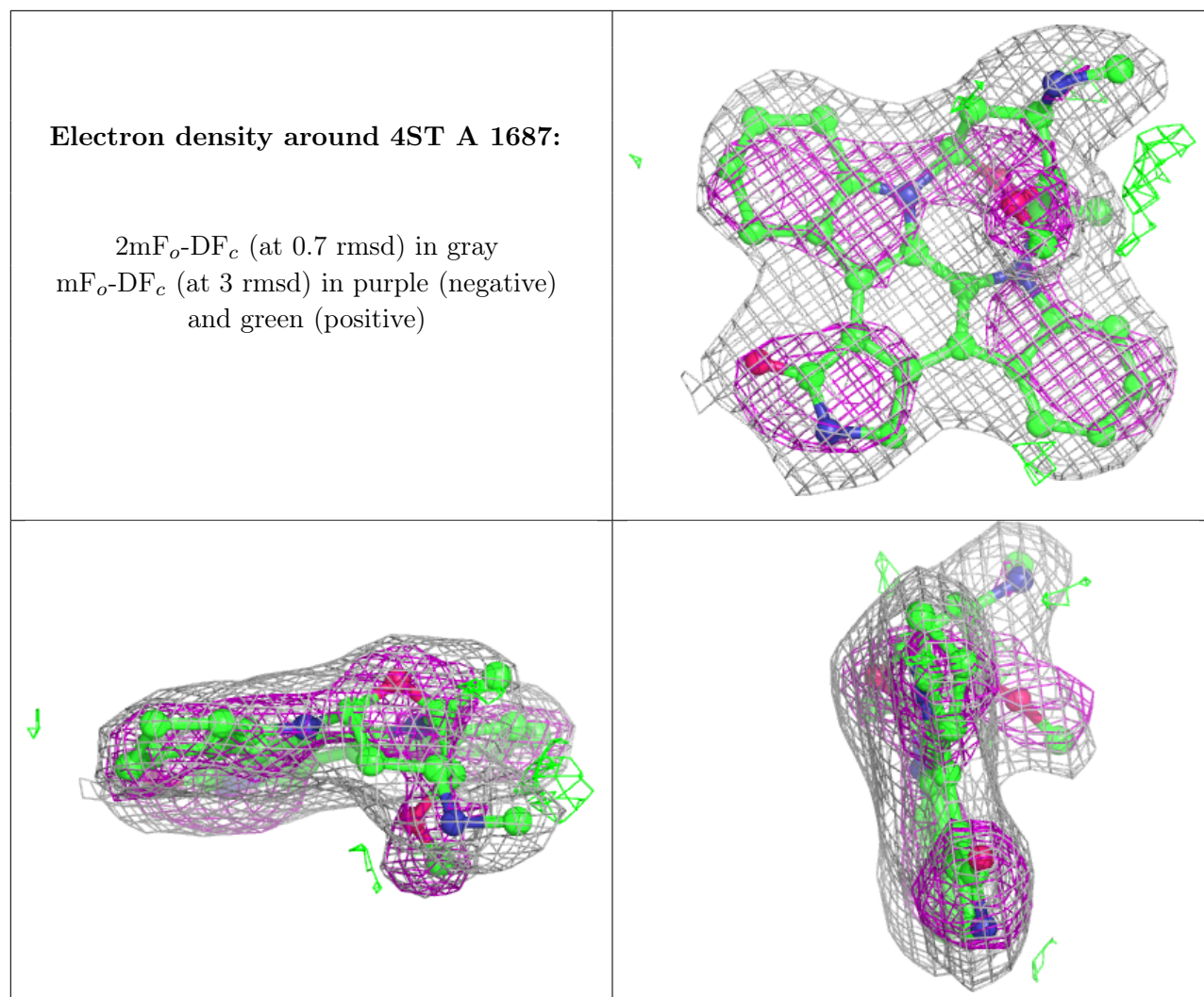
6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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	4ST	A	1687	35/35	0.97	0.14	42,45,54,56	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.

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PROTEIN DATA BANK

Electron density around 4ST A 1687:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.