



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 07:27 am GMT

PDB ID : 2J0K
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 : 3.00 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 : 4.02b-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

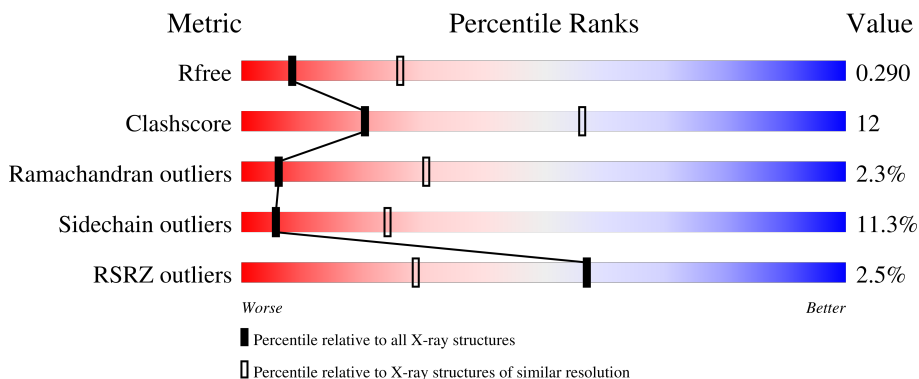
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	656	
1	B	656	

2 Entry composition i

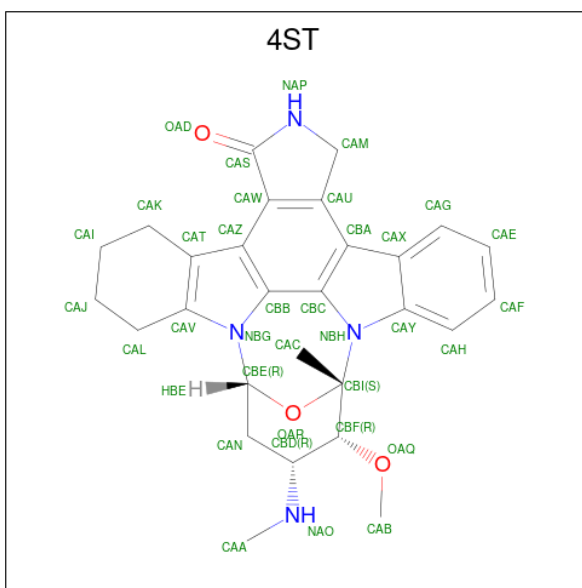
There are 3 unique types of molecules in this entry. The entry contains 9902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	598	Total 4836	3088	831	889	28	23	0	0
1	B	612	Total 4946	3152	852	913	29	12	0	0

- 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
			Total	C	N	O		
2	A	1	Total 35	28	4	3	0	0
2	B	1	Total 35	28	4	3	0	0

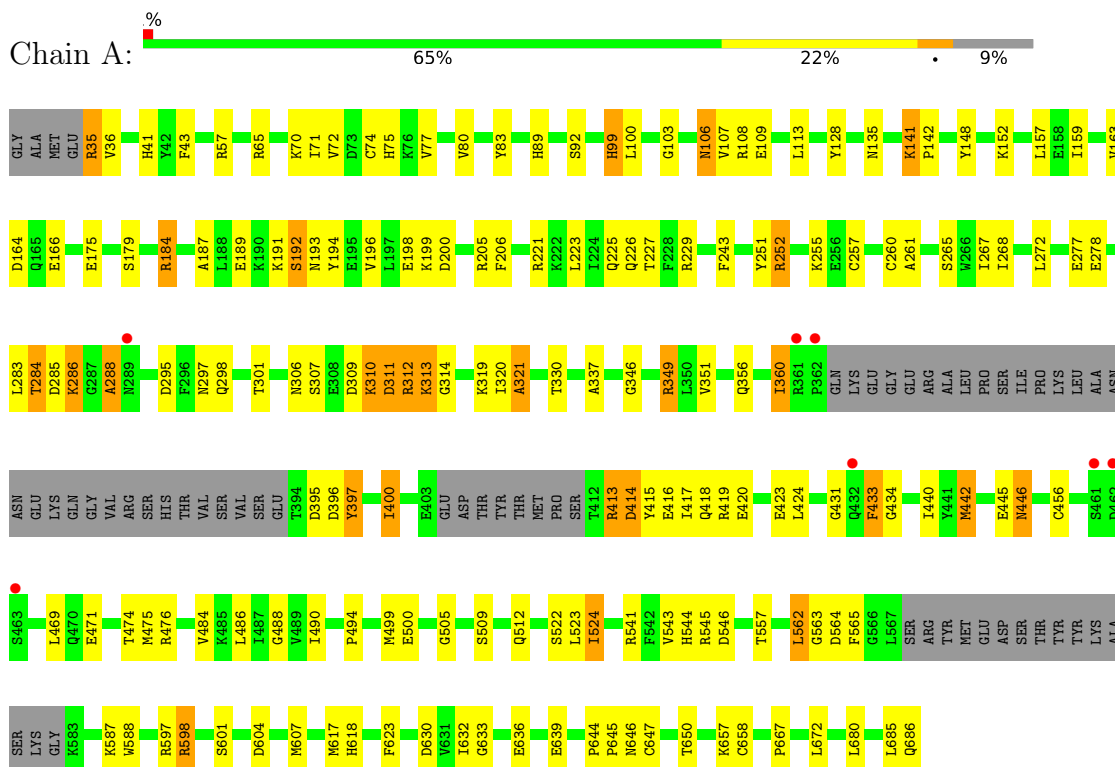
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	21	Total O 21 21	0	0

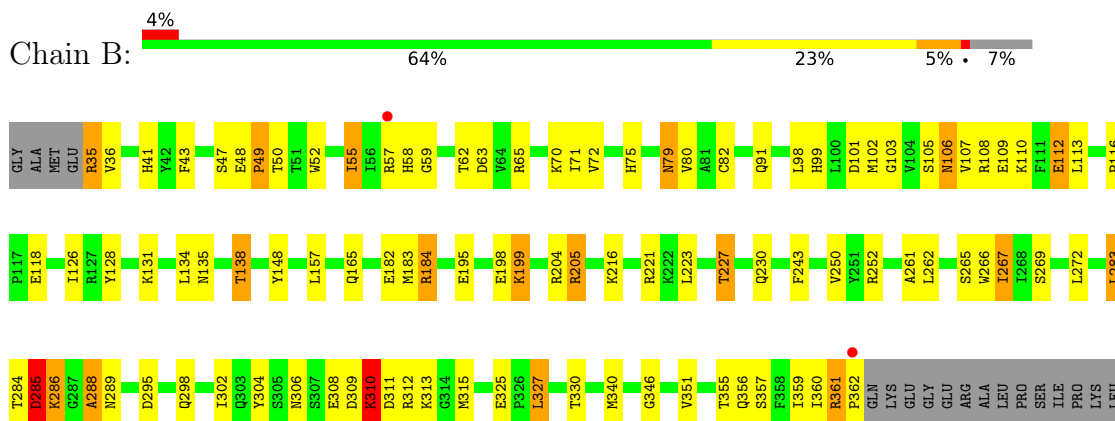
3 Residue-property plots [i](#)

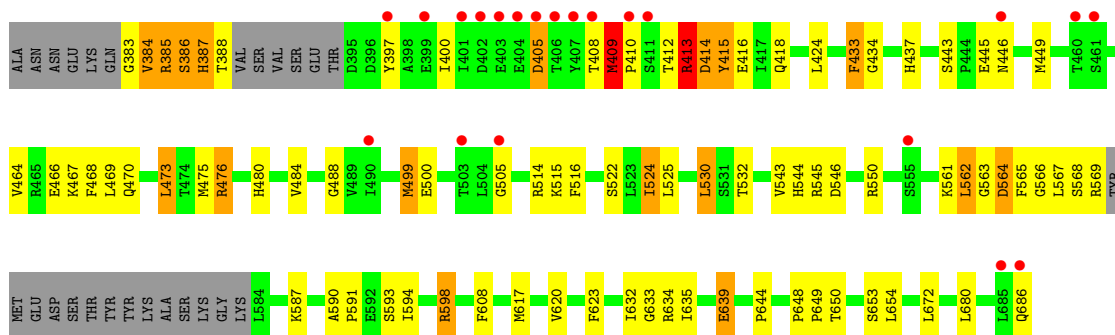
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FOCAL ADHESION KINASE 1



• Molecule 1: FOCAL ADHESION KINASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.02Å 106.21Å 240.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.49 – 3.00 38.48 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.49-3.00) 97.4 (38.48-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.299 0.221 , 0.290	Depositor DCC
R_{free} test set	1636 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9902	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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

5.1 Standard geometry

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	0.83	6/4939 (0.1%)	0.77	7/6670 (0.1%)
1	B	0.84	7/5052 (0.1%)	0.70	5/6824 (0.1%)
All	All	0.84	13/9991 (0.1%)	0.74	12/13494 (0.1%)

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	1
1	B	1	3
All	All	1	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	GLU	CG-CD	-41.49	0.89	1.51
1	B	445	GLU	CD-OE2	33.59	1.62	1.25
1	B	445	GLU	CD-OE1	26.63	1.54	1.25
1	A	152	LYS	CD-CE	-14.87	1.14	1.51
1	A	442	MET	CG-SD	-14.79	1.42	1.81
1	B	405	ASP	CA-CB	13.06	1.82	1.53
1	B	413	ARG	CG-CD	8.95	1.74	1.51
1	A	319	LYS	CG-CD	-8.57	1.23	1.52
1	B	310	LYS	CB-CG	7.13	1.71	1.52
1	B	516	PHE	CE1-CZ	6.21	1.49	1.37
1	B	516	PHE	CG-CD1	5.77	1.47	1.38
1	A	310	LYS	CB-CG	-5.61	1.37	1.52
1	A	35	ARG	CZ-NH1	5.45	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLU	CG-CD-OE1	-18.73	80.83	118.30
1	A	166	GLU	CG-CD-OE2	17.49	153.29	118.30
1	A	442	MET	CG-SD-CE	12.99	120.98	100.20
1	A	166	GLU	CB-CG-CD	12.84	148.88	114.20
1	A	442	MET	CB-CG-SD	12.31	149.32	112.40
1	B	405	ASP	N-CA-CB	12.28	132.69	110.60
1	B	405	ASP	CA-CB-CG	-11.84	87.36	113.40
1	B	445	GLU	OE1-CD-OE2	9.00	134.09	123.30
1	B	414	ASP	N-CA-C	-6.70	92.92	111.00
1	B	445	GLU	CG-CD-OE2	-6.35	105.59	118.30
1	A	35	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	152	LYS	CG-CD-CE	5.05	127.06	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	405	ASP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	ARG	Peptide
1	B	288	ALA	Peptide
1	B	413	ARG	Peptide
1	B	414	ASP	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	4836	0	4838	97	0
1	B	4946	0	4934	138	0
2	A	35	0	30	5	0
2	B	35	0	30	6	0
3	A	29	0	0	1	0
3	B	21	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9902	0	9832	242	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 (242) 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)
2:A:1687:4ST:HAH	2:A:1687:4ST:HAC2	1.26	1.12
1:B:261:ALA:HB1	1:B:267:ILE:HG23	1.20	1.11
1:B:261:ALA:HB1	1:B:267:ILE:CG2	1.85	1.06
1:A:285:ASP:HB2	1:A:286:LYS:HA	1.07	1.05
1:B:361:ARG:HB3	1:B:362:PRO:HD3	1.36	1.04
1:A:285:ASP:CB	1:A:286:LYS:HA	1.91	1.01
1:B:475:MET:SD	1:B:499:MET:HE1	2.06	0.96
1:A:285:ASP:HB2	1:A:286:LYS:CA	1.96	0.95
1:B:288:ALA:HB3	1:B:289:ASN:HB3	1.51	0.90
1:B:285:ASP:HB2	1:B:286:LYS:HA	1.55	0.89
2:B:1687:4ST:HAC2	2:B:1687:4ST:HAH	1.55	0.88
1:B:412:THR:O	1:B:413:ARG:HB2	1.75	0.87
1:B:41:HIS:HD2	1:B:43:PHE:H	1.23	0.85
1:B:515:LYS:HE2	3:B:2018:HOH:O	1.75	0.84
1:B:475:MET:SD	1:B:499:MET:CE	2.65	0.84
1:B:385:ARG:HG3	1:B:386:SER:H	1.40	0.84
1:A:484:VAL:HG12	1:A:562:LEU:O	1.78	0.84
1:A:505:GLY:HA2	2:A:1687:4ST:HAJ2	1.60	0.82
1:B:415:TYR:HB2	1:B:488:GLY:HA2	1.63	0.81
1:A:41:HIS:HD2	1:A:43:PHE:H	1.26	0.81
1:A:598:ARG:HH21	1:A:598:ARG:HG3	1.45	0.80
1:B:385:ARG:HG3	1:B:386:SER:N	1.93	0.79
1:B:412:THR:HG23	1:B:413:ARG:H	1.48	0.79
1:B:36:VAL:O	1:B:108:ARG:NH2	2.16	0.78
1:B:385:ARG:CG	1:B:386:SER:H	1.97	0.77
1:B:285:ASP:HB2	1:B:286:LYS:CA	2.15	0.77
1:A:261:ALA:HB1	1:A:267:ILE:HG23	1.66	0.75
1:B:261:ALA:CB	1:B:267:ILE:HG23	2.09	0.74
1:A:349:ARG:HG3	1:A:349:ARG:HH11	1.52	0.74
1:B:598:ARG:HH21	1:B:598:ARG:HG3	1.55	0.72
1:A:285:ASP:O	1:A:288:ALA:HB3	1.88	0.72
1:A:475:MET:SD	1:A:499:MET:HE2	2.29	0.72
1:B:48:GLU:OE1	1:B:205:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1687:4ST:HAH	2:A:1687:4ST:CAC	2.14	0.71
1:B:35:ARG:HG3	1:B:36:VAL:H	1.55	0.71
1:A:685:LEU:O	1:A:686:GLN:HG2	1.91	0.70
1:B:524:ILE:HD11	1:B:680:LEU:HA	1.71	0.70
1:B:412:THR:HG21	1:B:416:GLU:HG3	1.72	0.69
2:A:1687:4ST:HAC2	2:A:1687:4ST:CAH	2.06	0.69
1:A:226:GLN:HA	1:A:229:ARG:HH11	1.57	0.69
1:B:598:ARG:HH21	1:B:598:ARG:CG	2.07	0.68
1:A:445:GLU:O	1:A:446:ASN:HB2	1.92	0.68
1:B:410:PRO:HG2	1:B:473:LEU:HD11	1.74	0.68
1:B:505:GLY:HA2	2:B:1687:4ST:HAI2	1.76	0.67
1:A:645:PRO:O	1:A:646:ASN:HB2	1.93	0.67
1:B:598:ARG:HG3	1:B:598:ARG:NH2	2.08	0.67
1:B:383:GLY:HA3	1:B:384:VAL:HG23	1.77	0.67
1:A:419:ARG:NH2	1:A:494:PRO:O	2.28	0.67
1:A:475:MET:SD	1:A:499:MET:CE	2.83	0.66
1:A:524:ILE:HD11	1:A:680:LEU:HA	1.76	0.66
1:B:311:ASP:O	1:B:313:LYS:N	2.29	0.66
1:A:184:ARG:HH12	1:A:636:GLU:HG2	1.62	0.65
1:B:261:ALA:CB	1:B:267:ILE:CG2	2.71	0.65
1:B:361:ARG:HB3	1:B:362:PRO:CD	2.22	0.64
1:B:544:HIS:HD2	1:B:546:ASP:H	1.43	0.64
1:B:106:ASN:OD1	1:B:106:ASN:N	2.29	0.64
1:B:288:ALA:HB3	1:B:289:ASN:CB	2.27	0.64
1:B:135:ASN:O	1:B:138:THR:HB	1.98	0.64
1:B:475:MET:CE	1:B:499:MET:HE1	2.27	0.63
1:B:41:HIS:CD2	1:B:43:PHE:H	2.10	0.63
1:B:449:MET:HE2	3:B:2017:HOH:O	1.99	0.63
1:B:409:MET:H	1:B:410:PRO:HD3	1.63	0.63
1:A:431:GLY:HA3	1:A:434:GLY:O	1.99	0.63
1:B:412:THR:HG23	1:B:413:ARG:N	2.14	0.62
1:B:564:ASP:C	1:B:566:GLY:H	2.02	0.62
1:B:71:ILE:O	1:B:75:HIS:HD2	1.83	0.61
1:B:128:TYR:CD2	1:B:346:GLY:HA3	2.36	0.61
1:A:414:ASP:O	1:A:416:GLU:N	2.33	0.61
1:A:523:LEU:HD11	1:A:618:HIS:CE1	2.34	0.61
1:A:311:ASP:OD1	1:A:313:LYS:HG2	2.00	0.61
1:B:65:ARG:NH2	1:B:355:THR:O	2.33	0.61
1:B:284:THR:O	1:B:286:LYS:HD2	2.00	0.61
1:A:36:VAL:HG12	1:A:57:ARG:HG2	1.82	0.60
1:B:484:VAL:HG12	1:B:562:LEU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ARG:HD2	1:B:112:GLU:OE2	2.01	0.60
1:B:295:ASP:HB2	1:B:298:GLN:HE21	1.66	0.60
1:B:385:ARG:CG	1:B:386:SER:N	2.60	0.60
1:B:361:ARG:CB	1:B:362:PRO:HD3	2.21	0.60
1:B:562:LEU:HD22	1:B:563:GLY:H	1.66	0.60
1:B:385:ARG:HE	1:B:386:SER:HB2	1.67	0.59
1:B:433:PHE:HD1	1:B:434:GLY:H	1.51	0.59
2:A:1687:4ST:CAC	2:A:1687:4ST:CAH	2.77	0.58
1:A:588:TRP:O	1:A:607:MET:HG2	2.04	0.58
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.18	0.57
1:B:272:LEU:HD12	1:B:340:MET:HE1	1.86	0.57
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.69	0.57
1:B:632:ILE:HG13	1:B:633:GLY:N	2.20	0.57
1:A:128:TYR:CE2	1:A:346:GLY:HA3	2.39	0.57
1:B:99:HIS:HE1	1:B:357:SER:OG	1.87	0.56
1:B:386:SER:O	1:B:387:HIS:CG	2.58	0.56
1:A:601:SER:O	1:A:604:ASP:HB2	2.06	0.56
1:A:179:SER:O	1:A:597:ARG:NH2	2.39	0.56
1:B:415:TYR:CE2	1:B:476:ARG:HG3	2.41	0.56
1:B:35:ARG:O	1:B:57:ARG:HA	2.07	0.55
1:B:433:PHE:N	1:B:433:PHE:CD1	2.75	0.55
1:B:522:SER:O	1:B:525:LEU:HB3	2.08	0.54
2:B:1687:4ST:HAH	2:B:1687:4ST:CAC	2.34	0.54
1:A:89:HIS:HB3	1:A:92:SER:HB3	1.90	0.54
1:B:59:GLY:HA3	1:B:397:TYR:CE1	2.43	0.54
1:A:423:GLU:HB2	1:A:440:ILE:HB	1.89	0.54
1:A:445:GLU:O	1:A:446:ASN:CB	2.55	0.54
1:B:128:TYR:CE2	1:B:346:GLY:HA3	2.43	0.54
1:A:314:GLY:HA3	1:A:337:ALA:HB2	1.90	0.53
1:B:544:HIS:CD2	1:B:546:ASP:H	2.25	0.53
1:B:412:THR:CG2	1:B:413:ARG:H	2.19	0.53
1:A:598:ARG:HH21	1:A:598:ARG:CG	2.16	0.53
1:A:658:CYS:SG	1:A:672:LEU:HD21	2.48	0.53
1:B:184:ARG:HD3	1:B:632:ILE:HD11	1.91	0.53
1:A:295:ASP:H	1:A:298:GLN:HE21	1.55	0.53
1:A:35:ARG:HE	1:A:108:ARG:NE	2.07	0.53
1:B:49:PRO:HA	1:B:52:TRP:CE2	2.44	0.53
1:B:409:MET:N	1:B:410:PRO:CD	2.72	0.52
1:A:320:ILE:CG2	1:A:321:ALA:N	2.72	0.52
1:A:587:LYS:HD3	1:A:623:PHE:HB2	1.90	0.52
1:A:562:LEU:CD2	1:A:563:GLY:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ARG:CD	1:B:386:SER:H	2.21	0.52
1:B:409:MET:N	1:B:410:PRO:HD3	2.24	0.52
1:A:524:ILE:HD11	1:A:680:LEU:CA	2.39	0.52
1:B:285:ASP:HB2	1:B:286:LYS:CB	2.39	0.52
1:B:587:LYS:HD3	1:B:623:PHE:HB2	1.92	0.52
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.23	0.51
1:B:102:MET:SD	1:B:107:VAL:HG22	2.50	0.51
1:B:106:ASN:HA	1:B:109:GLU:HB2	1.91	0.51
1:B:227:THR:O	1:B:230:GLN:HG2	2.10	0.51
1:B:272:LEU:HD12	1:B:340:MET:CE	2.41	0.51
1:A:221:ARG:O	1:A:225:GLN:HG3	2.11	0.51
1:B:35:ARG:HA	1:B:35:ARG:NH1	2.26	0.51
1:B:530:LEU:HB3	1:B:608:PHE:HE2	1.76	0.50
1:B:108:ARG:O	1:B:112:GLU:HB2	2.12	0.50
1:B:360:ILE:O	1:B:361:ARG:HB2	2.12	0.50
1:A:159:ILE:HG12	1:A:251:TYR:CD1	2.47	0.50
1:B:35:ARG:HG3	1:B:36:VAL:N	2.24	0.50
1:B:443:SER:HB2	3:B:2016:HOH:O	2.12	0.50
1:A:41:HIS:CD2	1:A:43:PHE:H	2.18	0.49
1:B:415:TYR:CE2	1:B:476:ARG:CG	2.95	0.49
1:B:500:GLU:OE1	1:B:561:LYS:HD2	2.12	0.49
1:B:594:ILE:HG21	1:B:632:ILE:HG22	1.95	0.49
1:A:349:ARG:HH11	1:A:349:ARG:CG	2.23	0.49
1:B:415:TYR:CD2	1:B:415:TYR:N	2.79	0.49
1:B:63:ASP:HA	1:B:103:GLY:HA2	1.94	0.49
2:B:1687:4ST:HAC2	2:B:1687:4ST:CAH	2.34	0.49
1:A:200:ASP:HB3	1:A:598:ARG:NH2	2.28	0.49
1:A:509:SER:HA	1:A:512:GLN:OE1	2.13	0.49
1:B:311:ASP:N	3:B:2009:HOH:O	2.45	0.49
1:B:98:LEU:HD13	1:B:107:VAL:HG11	1.95	0.48
1:A:617:MET:SD	1:A:644:PRO:HB3	2.53	0.48
1:A:141:LYS:HD2	1:A:142:PRO:HD3	1.96	0.48
1:A:312:ARG:NH2	1:B:116:PRO:HG3	2.29	0.48
1:B:283:LEU:HD12	1:B:286:LYS:HG3	1.96	0.48
1:A:106:ASN:HA	1:A:109:GLU:CB	2.44	0.48
1:A:184:ARG:HH11	1:A:184:ARG:HB2	1.79	0.47
1:B:195:GLU:O	1:B:199:LYS:HB2	2.14	0.47
1:A:187:ALA:HB1	1:A:193:ASN:HD22	1.79	0.47
1:A:484:VAL:HG23	1:A:500:GLU:HG3	1.95	0.47
1:B:261:ALA:HB3	1:B:330:THR:HB	1.96	0.47
1:B:564:ASP:C	1:B:566:GLY:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:GLY:CA	1:B:384:VAL:HG23	2.44	0.47
1:A:360:ILE:HD11	3:A:2017:HOH:O	2.14	0.47
1:A:400:ILE:H	1:A:400:ILE:HG13	1.63	0.46
1:A:475:MET:SD	1:A:499:MET:HE1	2.54	0.46
1:B:415:TYR:HB2	1:B:488:GLY:CA	2.40	0.46
1:B:284:THR:HG21	3:B:2008:HOH:O	2.14	0.46
1:B:634:ARG:O	1:B:639:GLU:HB2	2.15	0.46
1:A:417:ILE:O	1:A:490:ILE:HG12	2.16	0.46
1:A:194:TYR:CZ	1:A:221:ARG:HA	2.51	0.46
1:A:65:ARG:HA	1:A:100:LEU:HD22	1.98	0.46
1:A:311:ASP:CG	1:A:312:ARG:N	2.69	0.46
1:A:349:ARG:HG3	1:A:349:ARG:NH1	2.26	0.46
1:A:71:ILE:O	1:A:75:HIS:HD2	1.99	0.46
1:B:103:GLY:O	1:B:107:VAL:HG23	2.15	0.46
1:B:262:LEU:HD22	1:B:327:LEU:HD11	1.98	0.46
1:A:252:ARG:HD2	1:A:255:LYS:HE3	1.98	0.46
1:B:55:ILE:HD12	1:B:55:ILE:N	2.31	0.46
1:B:286:LYS:HG2	1:B:286:LYS:O	2.15	0.46
1:B:562:LEU:CD2	1:B:563:GLY:H	2.28	0.46
1:A:106:ASN:HA	1:A:109:GLU:HB3	1.97	0.45
1:A:471:GLU:HG3	1:A:565:PHE:O	2.17	0.45
1:A:35:ARG:HG2	1:A:36:VAL:N	2.31	0.45
1:A:431:GLY:C	1:A:433:PHE:H	2.20	0.45
1:A:475:MET:HB3	1:A:486:LEU:HB2	1.97	0.45
1:A:285:ASP:CB	1:A:286:LYS:CA	2.67	0.45
1:B:41:HIS:CD2	1:B:43:PHE:HB2	2.52	0.45
1:B:543:VAL:HG12	1:B:545:ARG:HG3	1.98	0.45
1:A:100:LEU:HD12	1:A:349:ARG:CZ	2.47	0.45
1:B:302:ILE:O	1:B:359:ILE:HA	2.17	0.45
1:A:35:ARG:HG2	1:A:36:VAL:H	1.80	0.44
1:B:35:ARG:N	1:B:58:HIS:O	2.50	0.44
1:B:184:ARG:HH11	1:B:184:ARG:HB3	1.83	0.44
1:B:35:ARG:HG3	1:B:36:VAL:HG12	1.99	0.44
1:B:295:ASP:H	1:B:298:GLN:NE2	2.16	0.44
1:B:424:LEU:HD11	1:B:437:HIS:CG	2.52	0.44
1:A:349:ARG:CG	1:A:349:ARG:NH1	2.80	0.44
1:A:562:LEU:HD22	1:A:563:GLY:H	1.81	0.44
1:B:530:LEU:HD12	1:B:608:PHE:CE2	2.53	0.43
1:B:99:HIS:CE1	1:B:357:SER:OG	2.70	0.43
1:A:108:ARG:O	1:A:109:GLU:C	2.56	0.43
1:A:543:VAL:HG12	1:A:545:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:O	1:A:107:VAL:HG23	2.18	0.43
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.88	0.43
1:A:544:HIS:CD2	1:A:546:ASP:H	2.36	0.43
1:B:408:THR:HG22	1:B:408:THR:O	2.18	0.43
2:B:1687:4ST:CAC	2:B:1687:4ST:CAH	2.95	0.43
1:A:644:PRO:HG2	1:A:647:CYS:HB2	2.00	0.43
1:A:297:ASN:HB3	1:A:351:VAL:HG11	2.01	0.43
1:B:82:CYS:HB3	1:B:126:ILE:HG23	2.01	0.43
1:B:288:ALA:HB3	1:B:289:ASN:CA	2.49	0.43
1:A:417:ILE:HD12	1:A:488:GLY:HA3	2.01	0.42
1:B:590:ALA:O	1:B:593:SER:HB2	2.19	0.42
1:A:77:VAL:HG11	1:A:83:TYR:CE1	2.55	0.42
1:A:72:VAL:HG21	1:A:80:VAL:HG13	2.02	0.42
1:B:648:PRO:HA	1:B:649:PRO:HD3	1.98	0.42
1:B:654:LEU:HD11	1:B:672:LEU:HD23	2.01	0.42
1:B:408:THR:HG23	1:B:470:GLN:HE21	1.85	0.42
1:B:591:PRO:HG3	1:B:635:ILE:HG21	2.00	0.42
1:A:632:ILE:HG13	1:A:633:GLY:N	2.34	0.42
1:B:546:ASP:OD2	1:B:550:ARG:NH2	2.53	0.41
1:A:99:HIS:ND1	1:A:99:HIS:N	2.68	0.41
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.89	0.41
1:B:475:MET:SD	1:B:499:MET:HE2	2.58	0.41
1:B:464:VAL:O	1:B:468:PHE:HB2	2.20	0.41
1:B:285:ASP:CB	1:B:286:LYS:HA	2.40	0.41
1:B:505:GLY:HA2	2:B:1687:4ST:CAI	2.49	0.41
1:A:198:GLU:OE1	1:A:199:LYS:HE3	2.21	0.41
1:B:480:HIS:HE1	1:B:532:THR:OG1	2.03	0.41
1:A:257:CYS:HA	1:A:272:LEU:O	2.20	0.41
1:A:148:TYR:HE1	1:A:243:PHE:CG	2.38	0.41
1:A:657:LYS:O	1:A:667:PRO:HD3	2.20	0.41
1:A:598:ARG:CG	1:A:598:ARG:NH2	2.81	0.41
1:B:617:MET:SD	1:B:644:PRO:HB3	2.60	0.41
1:B:79:ASN:H	1:B:79:ASN:ND2	2.18	0.41
1:B:148:TYR:HE1	1:B:243:PHE:CG	2.39	0.41
1:B:304:TYR:HE2	1:B:359:ILE:HG21	1.86	0.41
1:B:99:HIS:CD2	1:B:101:ASP:H	2.39	0.40
1:B:617:MET:O	1:B:620:VAL:HG23	2.20	0.40
1:B:386:SER:O	1:B:387:HIS:CB	2.68	0.40
1:A:192:SER:O	1:A:196:VAL:HG23	2.21	0.40
1:A:260:CYS:HB2	1:A:330:THR:O	2.22	0.40
1:A:395:ASP:C	1:A:397:TYR:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:VAL:HG21	1:B:80:VAL:HG13	2.03	0.40
1:B:530:LEU:HD22	1:B:530:LEU:HA	1.85	0.40
1:A:175:GLU:HG3	1:A:206:PHE:HD2	1.85	0.40
1:A:223:LEU:O	1:A:227:THR:HG23	2.21	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	590/656 (90%)	519 (88%)	60 (10%)	11 (2%)	8	36
1	B	604/656 (92%)	540 (89%)	47 (8%)	17 (3%)	5	25
All	All	1194/1312 (91%)	1059 (89%)	107 (9%)	28 (2%)	6	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	GLU
1	A	311	ASP
1	A	414	ASP
1	A	415	TYR
1	A	446	ASN
1	B	285	ASP
1	B	310	LYS
1	B	312	ARG
1	B	361	ARG
1	B	386	SER
1	B	387	HIS
1	B	413	ARG
1	A	284	THR
1	A	307	SER

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Mol	Chain	Res	Type
1	A	312	ARG
1	A	321	ALA
1	B	50	THR
1	B	267	ILE
1	B	309	ASP
1	B	384	VAL
1	B	409	MET
1	B	565	PHE
1	B	568	SER
1	A	288	ALA
1	A	396	ASP
1	B	47	SER
1	B	223	LEU
1	B	49	PRO

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	531/582 (91%)	479 (90%)	52 (10%)	8 30
1	B	544/582 (94%)	475 (87%)	69 (13%)	4 19
All	All	1075/1164 (92%)	954 (89%)	121 (11%)	6 24

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	74	CYS
1	A	99	HIS
1	A	106	ASN
1	A	113	LEU
1	A	135	ASN
1	A	141	LYS
1	A	157	LEU
1	A	163	VAL

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Mol	Chain	Res	Type
1	A	164	ASP
1	A	184	ARG
1	A	189	GLU
1	A	191	LYS
1	A	192	SER
1	A	205	ARG
1	A	252	ARG
1	A	265	SER
1	A	268	ILE
1	A	277	GLU
1	A	283	LEU
1	A	284	THR
1	A	286	LYS
1	A	301	THR
1	A	306	ASN
1	A	309	ASP
1	A	310	LYS
1	A	313	LYS
1	A	349	ARG
1	A	356	GLN
1	A	360	ILE
1	A	397	TYR
1	A	400	ILE
1	A	413	ARG
1	A	418	GLN
1	A	420	GLU
1	A	424	LEU
1	A	433	PHE
1	A	442	MET
1	A	456	CYS
1	A	469	LEU
1	A	474	THR
1	A	476	ARG
1	A	522	SER
1	A	524	ILE
1	A	541	ARG
1	A	557	THR
1	A	562	LEU
1	A	564	ASP
1	A	598	ARG
1	A	630	ASP
1	A	639	GLU

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Mol	Chain	Res	Type
1	A	650	THR
1	B	35	ARG
1	B	55	ILE
1	B	62	THR
1	B	70	LYS
1	B	79	ASN
1	B	91	GLN
1	B	105	SER
1	B	106	ASN
1	B	110	LYS
1	B	112	GLU
1	B	113	LEU
1	B	118	GLU
1	B	131	LYS
1	B	138	THR
1	B	157	LEU
1	B	165	GLN
1	B	182	GLU
1	B	183	MET
1	B	184	ARG
1	B	198	GLU
1	B	199	LYS
1	B	204	ARG
1	B	205	ARG
1	B	216	LYS
1	B	221	ARG
1	B	227	THR
1	B	250	VAL
1	B	252	ARG
1	B	265	SER
1	B	266	TRP
1	B	269	SER
1	B	283	LEU
1	B	285	ASP
1	B	286	LYS
1	B	306	ASN
1	B	308	GLU
1	B	310	LYS
1	B	315	MET
1	B	325	GLU
1	B	327	LEU
1	B	351	VAL

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Mol	Chain	Res	Type
1	B	356	GLN
1	B	385	ARG
1	B	388	THR
1	B	400	ILE
1	B	405	ASP
1	B	409	MET
1	B	415	TYR
1	B	418	GLN
1	B	433	PHE
1	B	446	ASN
1	B	466	GLU
1	B	467	LYS
1	B	469	LEU
1	B	473	LEU
1	B	476	ARG
1	B	499	MET
1	B	514	ARG
1	B	524	ILE
1	B	530	LEU
1	B	562	LEU
1	B	564	ASP
1	B	567	LEU
1	B	569	ARG
1	B	598	ARG
1	B	639	GLU
1	B	650	THR
1	B	653	SER
1	B	686	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	75	HIS
1	A	79	ASN
1	A	135	ASN
1	A	136	GLN
1	A	298	GLN
1	A	544	HIS
1	A	618	HIS
1	B	41	HIS
1	B	45	ASN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	75	HIS
1	B	79	ASN
1	B	99	HIS
1	B	298	GLN
1	B	306	ASN
1	B	446	ASN
1	B	470	GLN
1	B	480	HIS
1	B	482	HIS
1	B	544	HIS
1	B	624	GLN
1	B	686	GLN

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](#)

2 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	4ST	B	1687	-	31,42,42	1.68	6 (19%)	28,68,68	2.35	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4ST	A	1687	-	31,42,42	2.01	8 (25%)	28,68,68	2.99	15 (53%)

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	B	1687	-	-	2/4/49/49	-
2	4ST	A	1687	-	-	2/4/49/49	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1687	4ST	CAW-CAS	-5.44	1.40	1.49
2	A	1687	4ST	OAQ-CBF	5.29	1.51	1.42
2	A	1687	4ST	CAS-NAP	4.50	1.38	1.35
2	A	1687	4ST	CAW-CAS	-3.68	1.43	1.49
2	B	1687	4ST	CBA-CBC	-2.87	1.39	1.42
2	A	1687	4ST	CAE-CAG	2.79	1.43	1.36
2	A	1687	4ST	CAI-CAJ	2.64	1.61	1.51
2	A	1687	4ST	CAN-CBD	2.57	1.57	1.53
2	B	1687	4ST	CAM-CAU	2.54	1.52	1.50
2	B	1687	4ST	CAL-CAV	2.44	1.55	1.50
2	B	1687	4ST	CAU-CBA	-2.25	1.39	1.42
2	A	1687	4ST	CAN-CBE	2.22	1.55	1.51
2	B	1687	4ST	OAQ-CBF	2.08	1.46	1.42
2	A	1687	4ST	OAQ-CAB	2.00	1.49	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	4ST	CAW-CAS-NAP	7.30	113.76	106.37
2	B	1687	4ST	CAW-CAS-NAP	6.78	113.23	106.37
2	A	1687	4ST	OAD-CAS-CAW	-6.26	121.89	129.32
2	B	1687	4ST	CAM-NAP-CAS	-5.32	108.73	113.85
2	A	1687	4ST	CAC-CBI-CBF	-4.67	103.56	112.64
2	A	1687	4ST	CAM-NAP-CAS	-4.56	109.47	113.85
2	B	1687	4ST	OAD-CAS-CAW	-4.45	124.03	129.32
2	A	1687	4ST	CAZ-CAW-CAS	4.34	136.25	129.76
2	A	1687	4ST	CAI-CAK-CAT	-4.15	106.19	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1687	4ST	CAT-CAV-NBG	3.76	109.05	106.66
2	A	1687	4ST	CAT-CAZ-CBB	-3.61	104.50	110.57
2	A	1687	4ST	CAT-CAV-NBG	3.58	108.93	106.66
2	A	1687	4ST	CAU-CAM-NAP	-3.21	98.50	101.76
2	B	1687	4ST	CAZ-CAW-CAS	3.13	134.44	129.76
2	B	1687	4ST	CAT-CAZ-CBB	-3.10	105.35	110.57
2	B	1687	4ST	CAC-CBI-CBF	-2.84	107.11	112.64
2	A	1687	4ST	CAW-CAU-CBA	-2.84	118.60	122.42
2	A	1687	4ST	OAR-CBE-CAN	-2.38	108.88	112.31
2	A	1687	4ST	CAE-CAF-CAH	-2.21	117.34	120.44
2	A	1687	4ST	CAF-CAH-CAY	2.21	123.68	119.44
2	B	1687	4ST	OAD-CAS-NAP	-2.19	122.71	125.27
2	A	1687	4ST	CAH-CAY-NBH	-2.17	129.67	132.29
2	A	1687	4ST	CAG-CAX-CAY	-2.00	116.86	119.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

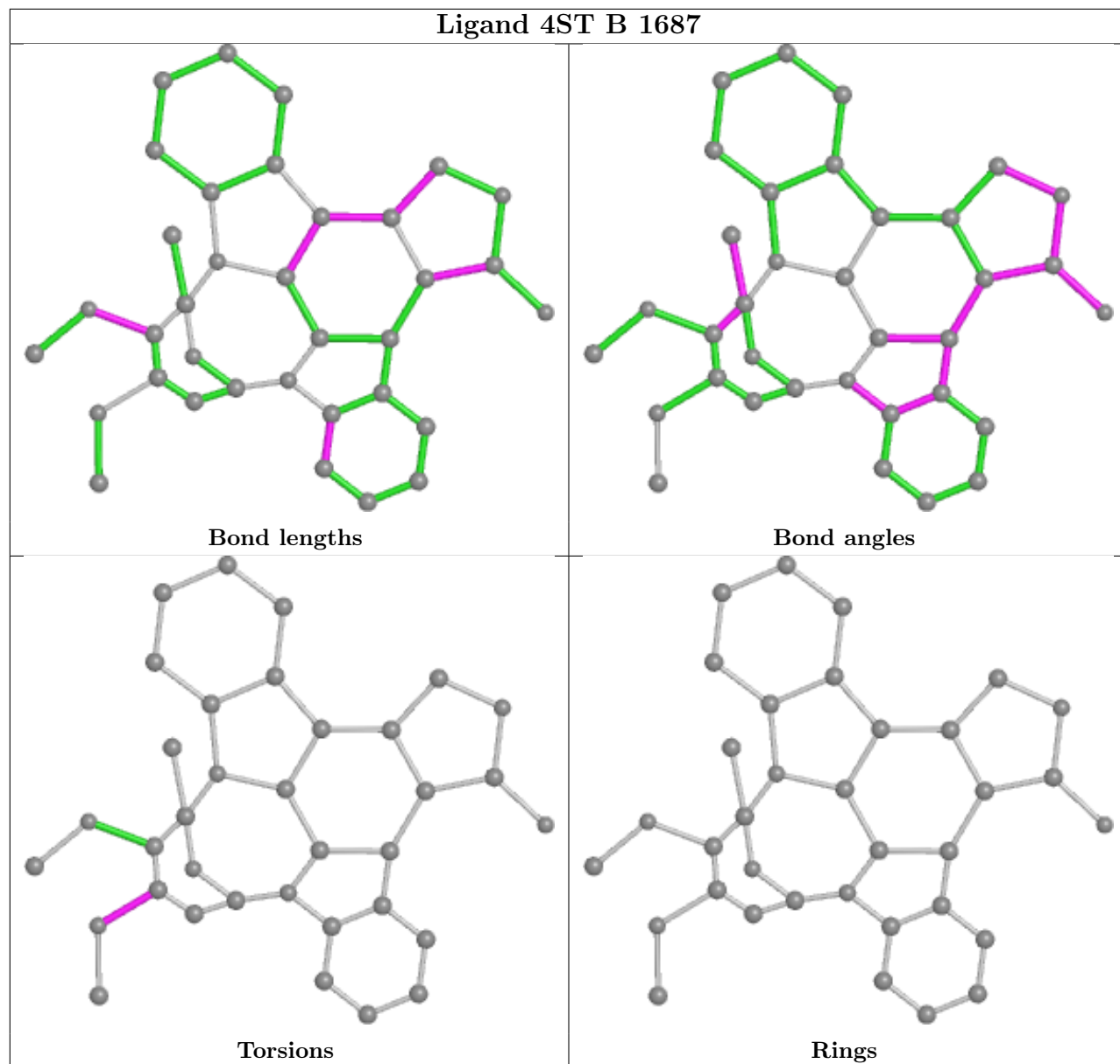
There are no ring outliers.

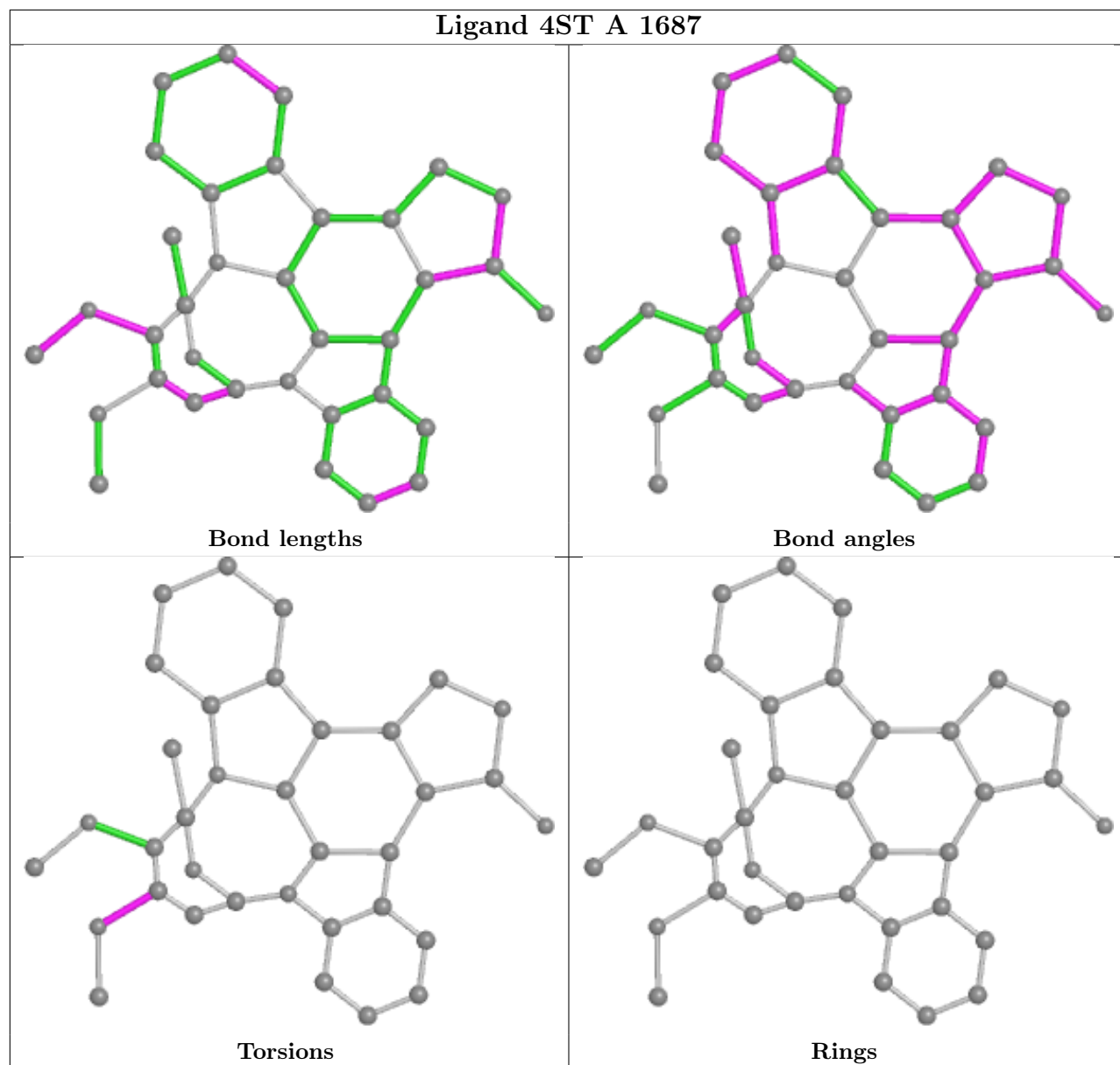
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1687	4ST	6	0
2	A	1687	4ST	5	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	598/656 (91%)	-0.04	7 (1%) 79 54	62, 81, 102, 139	8 (1%)
1	B	612/656 (93%)	0.06	23 (3%) 40 16	56, 80, 109, 139	3 (0%)
All	All	1210/1312 (92%)	0.01	30 (2%) 57 29	56, 81, 105, 139	11 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	ILE	4.7
1	B	460	THR	4.6
1	B	685	LEU	4.1
1	B	408	THR	3.7
1	B	406	THR	3.7
1	B	405	ASP	3.7
1	A	362	PRO	3.0
1	B	407	TYR	3.0
1	B	461	SER	2.9
1	B	399	GLU	2.8
1	A	289	ASN	2.7
1	A	463	SER	2.6
1	B	555	SER	2.6
1	B	404	GLU	2.6
1	B	410	PRO	2.6
1	A	432	GLN	2.5
1	A	361	ARG	2.4
1	A	462	ASP	2.3
1	B	505	GLY	2.3
1	B	490	ILE	2.3
1	B	403	GLU	2.2
1	B	503	THR	2.2
1	B	402	ASP	2.2
1	B	411	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	397	TYR	2.1
1	A	461	SER	2.1
1	B	686	GLN	2.0
1	B	57	ARG	2.0
1	B	362	PRO	2.0
1	B	446	ASN	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](#)

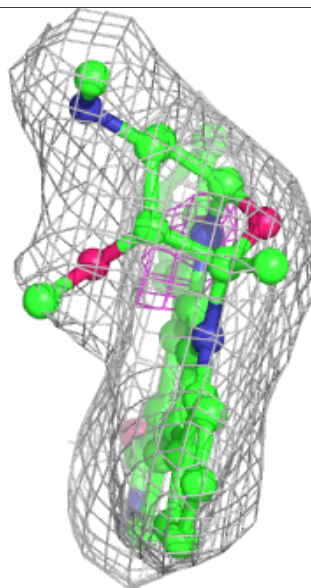
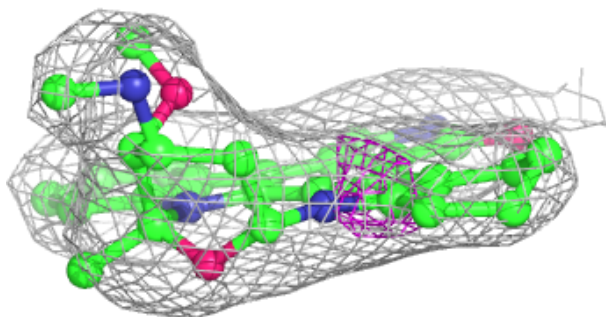
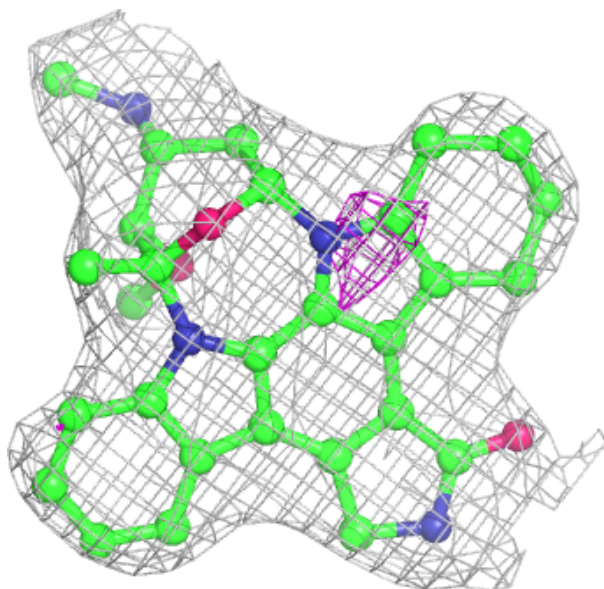
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

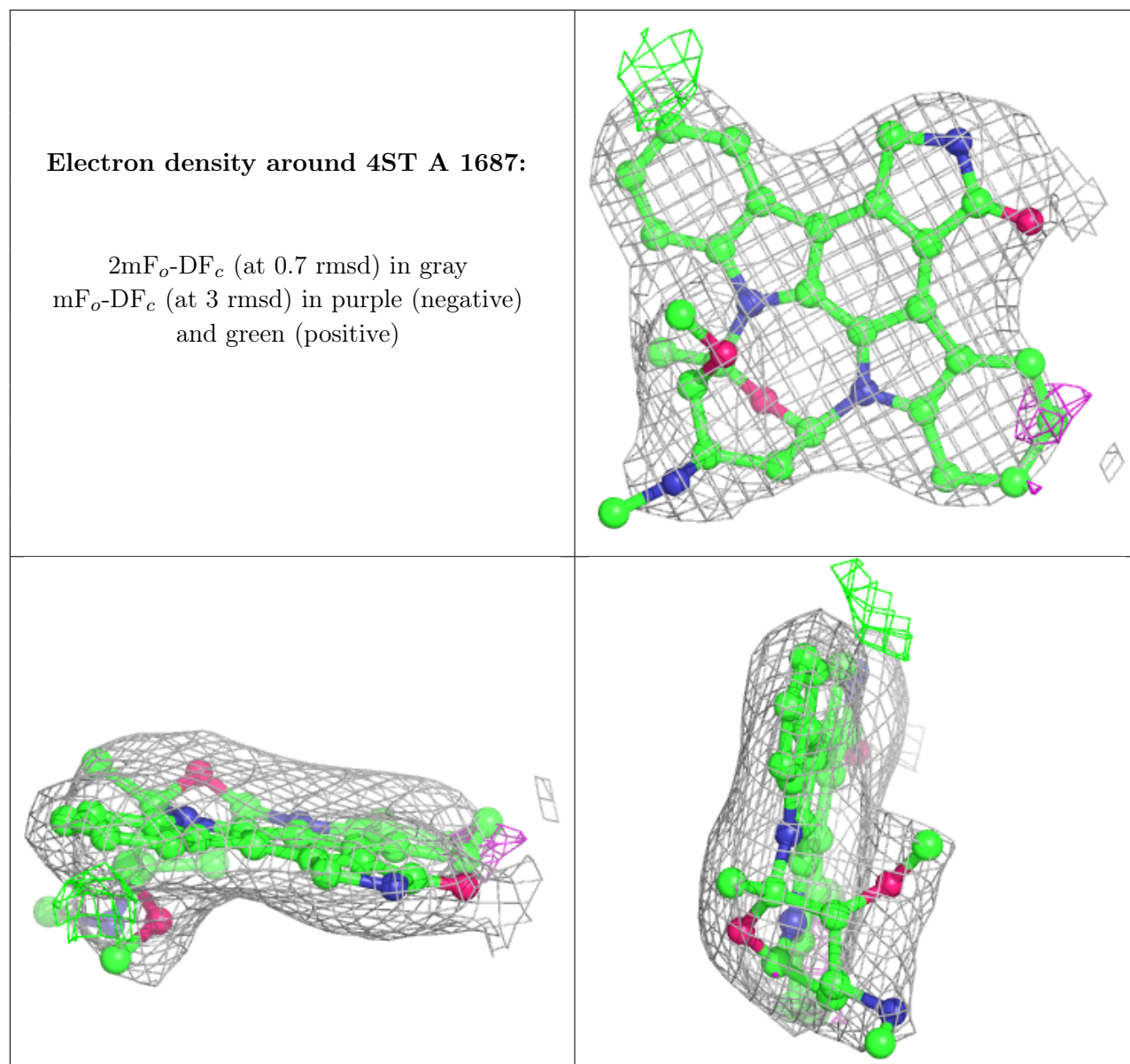
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4ST	B	1687	35/35	0.96	0.15	56,59,59,60	0
2	4ST	A	1687	35/35	0.98	0.15	54,55,61,62	0

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.

Electron density around 4ST B 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 [i](#)

There are no such residues in this entry.