



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 AM UTC

PDB ID : 2J4Z / pdb_00002j4z
Title : Structure of Aurora-2 in complex with PHA-680626
Authors : Cameron, A.D.; Izzo, G.; Storici, P.; Rusconi, L.; Fancelli, D.; Varasi, M.;
Berta, D.; Bindi, S.; Forte, B.; Severino, D.; Tonani, R.; Vianello, P.
Deposited on : 2006-09-08
Resolution : 2.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

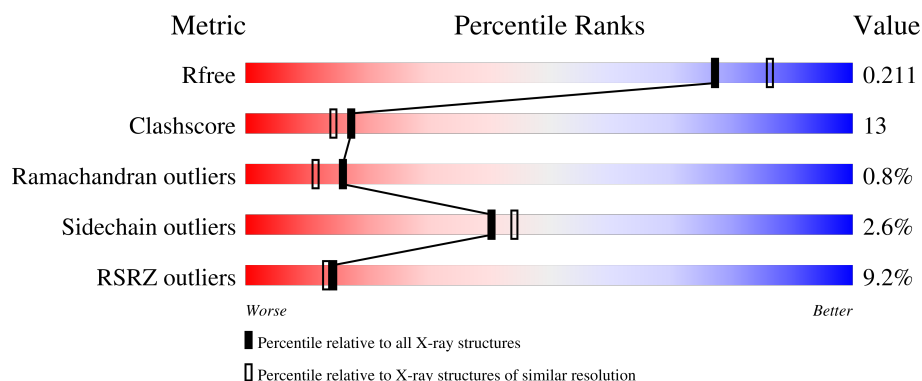
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	306	8% 66% 18% • 14%
1	B	306	8% 64% 21% • 12%

2 Entry composition [i](#)

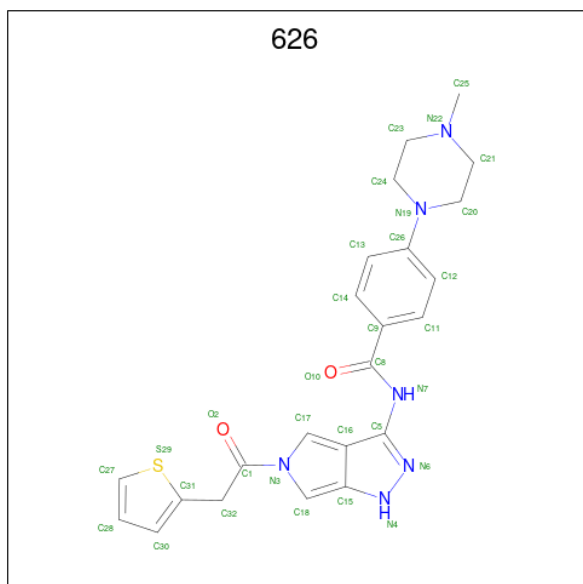
There are 4 unique types of molecules in this entry. The entry contains 4626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERINE THREONINE-PROTEIN KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	1
			2160	1386	383	385	6			
1	B	270	Total	C	N	O	S	0	0	1
			2205	1412	392	394	7			

- Molecule 2 is 4-(4-METHYLPIPERAZIN-1-YL)-N-[5-(2-THIENYLACETYL)-1,5-DIHYDROPYRROLO[3,4-C]PYRAZOL-3-YL]BENZAMIDE (CCD ID: 626) (formula: C₂₃H₂₄N₆O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	23	6	2	1		
2	B	1	Total	C	N	O	S	0	0
			32	23	6	2	1		

- Molecule 3 is ARSENIC (CCD ID: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	As 2	0	0
3	B	1	Total 1	As 1	0	0

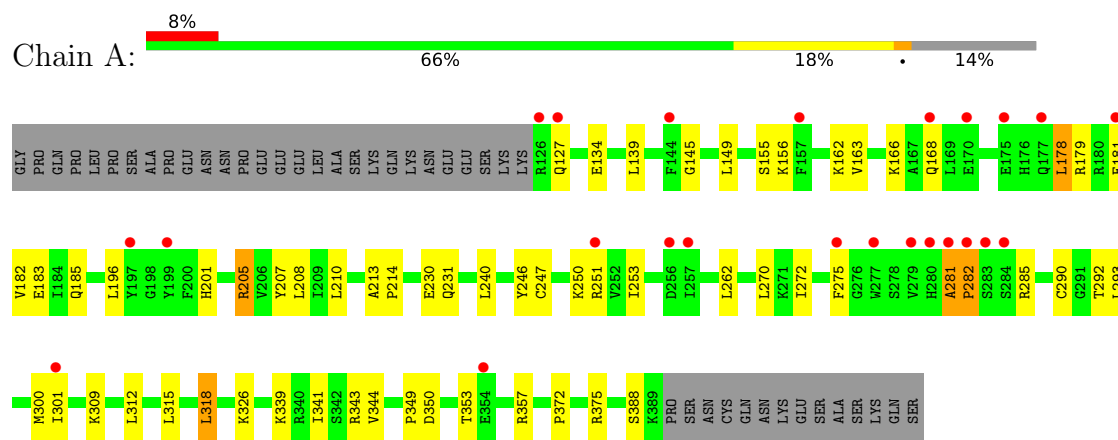
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total 110	O 110	0	0
4	B	84	Total 84	O 84	0	0

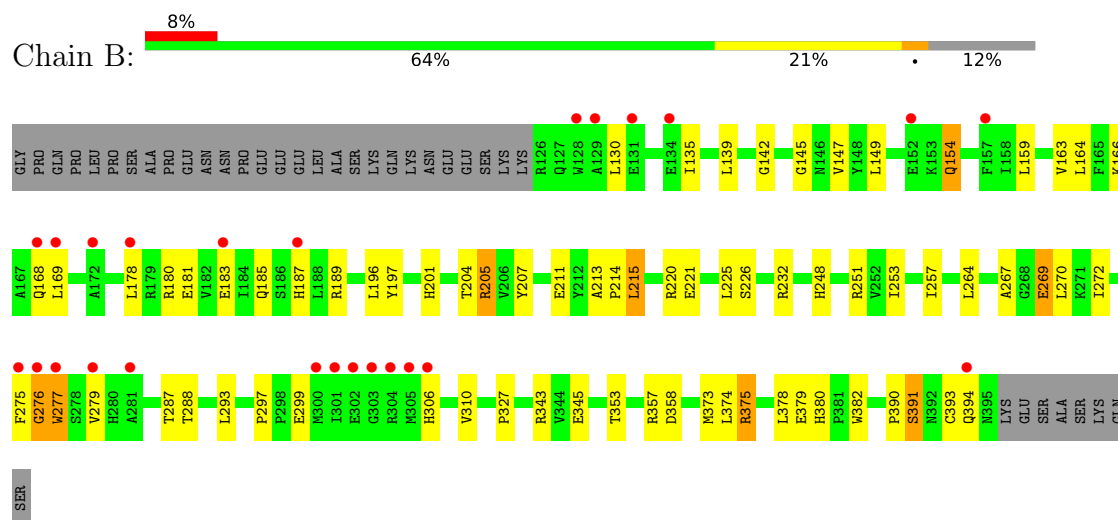
3 Residue-property plots [i](#)

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: SERINE THREONINE-PROTEIN KINASE 6



• Molecule 1: SERINE THREONINE-PROTEIN KINASE 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.13Å 89.44Å 94.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.00 29.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.58-2.00) 99.9 (29.58-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.00Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.214 , 0.249 0.213 , 0.211	Depositor DCC
R_{free} test set	2086 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4626	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: ARS, 626

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	0.40	1/2214 (0.0%)	0.89	11/2994 (0.4%)
1	B	0.40	1/2260 (0.0%)	0.88	8/3056 (0.3%)
All	All	0.40	2/4474 (0.0%)	0.88	19/6050 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	394	GLN	C-N	-5.63	1.25	1.33
1	A	388	SER	C-N	-5.52	1.25	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	N-CA-C	-7.14	100.43	110.50
1	A	139	LEU	N-CA-C	-6.49	105.66	113.97
1	B	213	ALA	CA-C-N	6.08	126.25	119.32
1	B	213	ALA	C-N-CA	6.08	126.25	119.32
1	A	326	LYS	CA-C-N	6.07	124.03	119.66
1	A	326	LYS	C-N-CA	6.07	124.03	119.66
1	A	214	PRO	N-CA-C	5.92	121.54	113.84
1	B	276	GLY	N-CA-C	5.83	127.00	113.18
1	B	205	ARG	N-CA-C	5.83	117.11	108.60
1	B	139	LEU	N-CA-C	-5.72	106.17	114.12
1	B	215	LEU	N-CA-C	5.60	119.82	113.15
1	A	230	GLU	N-CA-C	5.58	117.37	111.28
1	B	149	LEU	N-CA-C	-5.48	101.05	109.76
1	A	213	ALA	CA-C-N	5.43	125.10	119.56
1	A	213	ALA	C-N-CA	5.43	125.10	119.56
1	A	253	ILE	N-CA-C	5.37	115.08	108.53
1	A	349	PRO	N-CA-C	-5.27	102.88	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	SER	N-CA-C	-5.27	103.07	110.50
1	A	134	GLU	N-CA-C	-5.01	101.24	109.40

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	2160	0	2165	46	0
1	B	2205	0	2208	63	0
2	A	32	0	24	0	0
2	B	32	0	24	1	0
3	A	2	0	0	2	0
3	B	1	0	0	0	0
4	A	110	0	0	1	0
4	B	84	0	0	3	0
All	All	4626	0	4421	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 13.

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:B:375:ARG:H	1:B:375:ARG:HD2	0.90	1.03
1:B:375:ARG:HD2	1:B:375:ARG:N	1.75	1.00
1:A:281:ALA:HB3	1:A:282:PRO:HA	1.45	0.97
1:B:375:ARG:H	1:B:375:ARG:CD	1.75	0.96
1:A:162:LYS:HD3	1:A:208:LEU:HD12	1.54	0.89
1:A:281:ALA:CB	1:A:282:PRO:HA	2.11	0.80
1:A:205:ARG:HB2	1:A:205:ARG:HH11	1.46	0.80
1:B:373:MET:HB3	1:B:375:ARG:HH11	1.53	0.71
1:B:299:GLU:HG3	1:B:306:HIS:HB3	1.71	0.71
1:B:380:HIS:HD2	1:B:382:TRP:H	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HG3	1:A:275:PHE:CD1	2.27	0.70
1:B:297:PRO:HG3	1:B:310:VAL:HG13	1.77	0.67
1:B:375:ARG:O	1:B:379:GLU:HG3	1.96	0.66
1:B:204:THR:HB	1:B:205:ARG:NH1	2.10	0.66
1:B:374:LEU:H	1:B:375:ARG:NH1	1.93	0.65
1:B:380:HIS:CD2	1:B:382:TRP:H	2.15	0.64
1:B:204:THR:HB	1:B:205:ARG:HH11	1.63	0.63
1:A:281:ALA:HB3	1:A:282:PRO:CA	2.26	0.63
1:B:375:ARG:HG3	1:B:393:CYS:SG	2.39	0.63
1:A:281:ALA:CB	1:A:282:PRO:CA	2.76	0.63
1:B:358:ASP:OD1	1:B:380:HIS:HE1	1.85	0.60
1:A:166:LYS:NZ	1:A:201:HIS:HB2	2.17	0.60
1:A:290:CYS:HB3	1:A:300:MET:HE2	1.84	0.59
1:A:353:THR:O	1:A:357:ARG:HG3	2.04	0.58
1:B:373:MET:HB3	1:B:375:ARG:HD3	1.85	0.57
1:A:262:LEU:HB3	1:A:270:LEU:HD11	1.86	0.57
1:B:166:LYS:HG3	1:B:205:ARG:HA	1.87	0.56
1:B:180:ARG:O	1:B:183:GLU:HG2	2.06	0.56
1:A:181:GLU:HG2	1:A:275:PHE:CE1	2.41	0.55
1:B:225:LEU:O	1:B:226:SER:HB3	2.06	0.55
1:A:240:LEU:HD12	1:A:272:ILE:HD11	1.88	0.55
1:A:166:LYS:HZ1	1:A:201:HIS:HB2	1.72	0.54
1:A:344:VAL:O	1:A:344:VAL:HG12	2.06	0.54
1:A:162:LYS:HB3	1:A:208:LEU:HB2	1.89	0.54
1:B:164:LEU:O	1:B:205:ARG:HB2	2.08	0.54
1:B:220:ARG:HG2	1:B:220:ARG:HH11	1.73	0.53
1:B:178:LEU:C	1:B:178:LEU:HD23	2.34	0.52
1:B:327:PRO:HB2	4:B:2039:HOH:O	2.09	0.52
1:B:187:HIS:HA	1:B:189:ARG:NH1	2.25	0.52
1:B:135:ILE:HD12	1:B:135:ILE:N	2.23	0.52
1:B:205:ARG:HH11	1:B:205:ARG:HG2	1.74	0.51
1:B:185:GLN:HB2	1:B:275:PHE:CD2	2.46	0.51
1:B:248:HIS:CD2	1:B:253:ILE:HG22	2.47	0.50
1:B:343:ARG:HH22	1:B:345:GLU:CD	2.18	0.50
1:B:306:HIS:HB2	1:B:310:VAL:CG2	2.41	0.50
1:A:185:GLN:HG3	1:A:275:PHE:HD1	1.77	0.50
1:A:375:ARG:NH1	1:A:375:ARG:HB3	2.27	0.49
1:B:306:HIS:HB2	1:B:310:VAL:HG21	1.94	0.49
1:A:339:LYS:HB3	1:A:343:ARG:NH1	2.27	0.49
1:A:339:LYS:HB3	1:A:343:ARG:HH12	1.78	0.49
1:A:309:LYS:CD	1:A:312:LEU:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLY:HA3	1:A:163:VAL:O	2.13	0.49
1:A:178:LEU:O	1:A:182:VAL:HG23	2.13	0.48
1:A:155:SER:O	1:A:156:LYS:HB2	2.14	0.48
1:B:390:PRO:HD3	4:B:2078:HOH:O	2.12	0.48
1:B:374:LEU:H	1:B:375:ARG:HH11	1.59	0.48
1:B:142:GLY:HA3	1:B:279:VAL:HA	1.95	0.48
1:A:240:LEU:HD23	1:A:315:LEU:CD1	2.43	0.47
1:A:309:LYS:HD2	1:A:312:LEU:HD12	1.96	0.47
1:B:288:THR:HB	4:B:2036:HOH:O	2.14	0.46
1:B:353:THR:O	1:B:357:ARG:HG3	2.15	0.46
1:A:179:ARG:NH1	1:A:183:GLU:HB2	2.29	0.46
1:A:350:ASP:HB2	4:A:2092:HOH:O	2.14	0.46
1:B:197:TYR:HE1	1:B:211:GLU:HA	1.80	0.46
1:B:185:GLN:OE1	1:B:196:LEU:HD12	2.16	0.45
1:B:373:MET:HB3	1:B:375:ARG:NH1	2.26	0.45
1:B:185:GLN:HB2	1:B:275:PHE:CE2	2.52	0.45
1:A:375:ARG:HB3	1:A:375:ARG:CZ	2.46	0.45
1:A:205:ARG:HH11	1:A:205:ARG:CB	2.25	0.45
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.82	0.44
1:A:181:GLU:HG2	1:A:275:PHE:HE1	1.81	0.44
1:A:205:ARG:NH1	1:A:207:TYR:OH	2.51	0.44
1:A:231:GLN:H	1:A:231:GLN:CD	2.26	0.44
1:A:247:CYS:CB	3:A:1390:ARS:AS	3.26	0.44
1:B:130:LEU:HD13	1:B:207:TYR:CE2	2.52	0.44
1:B:373:MET:CB	1:B:375:ARG:HH11	2.28	0.44
1:B:205:ARG:NH1	1:B:205:ARG:HG2	2.32	0.43
1:B:378:LEU:HB3	1:B:391:SER:HB3	1.99	0.43
1:A:179:ARG:HH12	1:A:183:GLU:HB2	1.84	0.43
1:A:196:LEU:HA	1:A:210:LEU:HD23	1.99	0.43
1:B:159:LEU:HD12	1:B:159:LEU:C	2.44	0.43
1:B:214:PRO:O	2:B:1395:626:H12	2.18	0.43
1:A:301:ILE:HD12	1:A:341:ILE:HB	2.01	0.42
1:A:285:ARG:HD2	1:A:292:THR:HG21	2.01	0.42
1:B:178:LEU:HA	1:B:277:TRP:CZ3	2.54	0.42
1:A:312:LEU:HD13	1:A:372:PRO:O	2.20	0.42
1:B:375:ARG:N	1:B:375:ARG:CD	2.54	0.42
1:A:301:ILE:HD12	1:A:341:ILE:CG2	2.49	0.42
1:B:373:MET:HE2	1:B:375:ARG:HD3	2.01	0.42
1:A:231:GLN:CD	1:A:231:GLN:N	2.77	0.42
1:B:267:ALA:N	1:B:269:GLU:OE2	2.50	0.42
1:A:250:LYS:O	1:A:251:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LEU:C	1:A:293:LEU:HD23	2.45	0.42
1:B:169:LEU:HD13	1:B:178:LEU:HD12	2.01	0.42
1:B:287:THR:CG2	1:B:288:THR:N	2.83	0.42
1:B:221:GLU:HG2	1:B:232:ARG:NH2	2.35	0.41
1:B:257:ILE:HG22	1:B:272:ILE:HD12	2.03	0.41
1:A:240:LEU:HD22	1:A:318:LEU:HD12	2.01	0.41
1:B:154:GLN:OE1	1:B:154:GLN:HA	2.21	0.41
1:B:166:LYS:NZ	1:B:201:HIS:HD2	2.19	0.41
1:B:374:LEU:N	1:B:375:ARG:HH11	2.18	0.41
1:B:145:GLY:HA3	1:B:163:VAL:O	2.21	0.41
1:B:373:MET:HB3	1:B:375:ARG:CD	2.48	0.41
1:A:290:CYS:SG	3:A:1391:ARS:AS	3.39	0.41
1:B:270:LEU:C	1:B:270:LEU:HD23	2.46	0.41
1:A:246:TYR:O	1:A:250:LYS:HG2	2.21	0.41
1:B:163:VAL:CG1	1:B:205:ARG:HD2	2.51	0.40
1:B:215:LEU:HB2	1:B:264:LEU:HB2	2.04	0.40
1:B:196:LEU:C	1:B:196:LEU:HD23	2.46	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	262/306 (86%)	249 (95%)	12 (5%)	1 (0%)	30	27
1	B	268/306 (88%)	255 (95%)	10 (4%)	3 (1%)	11	7
All	All	530/612 (87%)	504 (95%)	22 (4%)	4 (1%)	16	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA

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Mol	Chain	Res	Type
1	B	276	GLY
1	B	154	GLN
1	B	277	TRP

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	232/271 (86%)	226 (97%)	6 (3%)	40	44
1	B	238/271 (88%)	232 (98%)	6 (2%)	42	45
All	All	470/542 (87%)	458 (97%)	12 (3%)	40	44

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	168	GLN
1	A	178	LEU
1	A	205	ARG
1	A	282	PRO
1	A	318	LEU
1	B	147	VAL
1	B	168	GLN
1	B	181	GLU
1	B	269	GLU
1	B	293	LEU
1	B	375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	254	HIS
1	B	201	HIS

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Mol	Chain	Res	Type
1	B	380	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	626	A	1389	-	36,36,36	3.50	16 (44%)	42,51,51	2.67	12 (28%)
2	626	B	1395	-	36,36,36	3.48	19 (52%)	42,51,51	2.60	8 (19%)

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	626	A	1389	-	-	1/20/30/30	0/5/5/5
2	626	B	1395	-	-	1/20/30/30	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1389	626	C18-C15	9.76	1.50	1.36
2	B	1395	626	C18-C15	9.69	1.50	1.36
2	A	1389	626	C18-N3	7.85	1.50	1.37
2	B	1395	626	C17-N3	7.76	1.50	1.37
2	A	1389	626	C17-N3	7.73	1.50	1.37
2	B	1395	626	C18-N3	7.48	1.49	1.37
2	A	1389	626	C17-C16	7.14	1.49	1.38
2	A	1389	626	C16-C5	-6.68	1.33	1.45
2	B	1395	626	C17-C16	6.64	1.48	1.38
2	B	1395	626	C16-C5	-6.31	1.34	1.45
2	B	1395	626	C26-N19	4.58	1.51	1.38
2	A	1389	626	C26-N19	4.34	1.50	1.38
2	A	1389	626	C5-N7	3.93	1.46	1.38
2	A	1389	626	C20-N19	3.80	1.53	1.46
2	A	1389	626	C24-N19	3.73	1.53	1.46
2	B	1395	626	C20-N19	3.73	1.53	1.46
2	B	1395	626	C5-N7	3.47	1.45	1.38
2	B	1395	626	C24-N19	3.46	1.52	1.46
2	B	1395	626	C15-N4	3.29	1.39	1.35
2	B	1395	626	C5-N6	-3.22	1.28	1.32
2	B	1395	626	C14-C9	2.80	1.43	1.39
2	A	1389	626	C15-N4	2.78	1.38	1.35
2	A	1389	626	C5-N6	-2.62	1.28	1.32
2	A	1389	626	C14-C9	2.61	1.43	1.39
2	A	1389	626	C11-C9	2.54	1.43	1.39
2	B	1395	626	C11-C9	2.50	1.43	1.39
2	B	1395	626	C12-C26	2.50	1.44	1.39
2	A	1389	626	C12-C26	2.41	1.43	1.39
2	A	1389	626	C32-C31	2.38	1.55	1.50
2	B	1395	626	C13-C26	2.24	1.43	1.39
2	B	1395	626	C23-N22	2.24	1.51	1.46
2	A	1389	626	C13-C26	2.20	1.43	1.39
2	B	1395	626	C21-N22	2.18	1.51	1.46
2	B	1395	626	C16-C15	-2.18	1.41	1.45
2	B	1395	626	C32-C31	2.15	1.54	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1395	626	C5-N6-N4	11.95	112.48	103.32
2	A	1389	626	C5-N6-N4	11.81	112.38	103.32
2	B	1395	626	C15-N4-N6	-6.62	101.03	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1389	626	C15-N4-N6	-6.56	101.12	112.34
2	A	1389	626	C17-C16-C5	4.19	150.89	138.76
2	B	1395	626	C17-C16-C5	4.13	150.73	138.76
2	A	1389	626	C18-N3-C17	4.11	113.31	108.92
2	B	1395	626	C18-N3-C17	4.01	113.21	108.92
2	B	1395	626	C23-N22-C21	3.63	115.32	109.54
2	A	1389	626	C23-N22-C21	3.60	115.27	109.54
2	A	1389	626	C21-C20-N19	2.73	116.53	110.78
2	A	1389	626	C16-C17-N3	-2.70	104.58	108.73
2	B	1395	626	C16-C17-N3	-2.67	104.62	108.73
2	A	1389	626	C24-N19-C20	2.62	117.46	111.57
2	A	1389	626	C9-C8-N7	2.57	119.96	116.25
2	A	1389	626	C24-C23-N22	2.54	114.93	110.86
2	A	1389	626	C23-C24-N19	2.23	115.48	110.78
2	A	1389	626	C16-C15-N4	2.11	111.85	106.66
2	B	1395	626	C16-C15-N4	2.07	111.74	106.66
2	B	1395	626	C9-C8-N7	2.06	119.22	116.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1389	626	C16-C5-N7-C8
2	B	1395	626	C16-C5-N7-C8

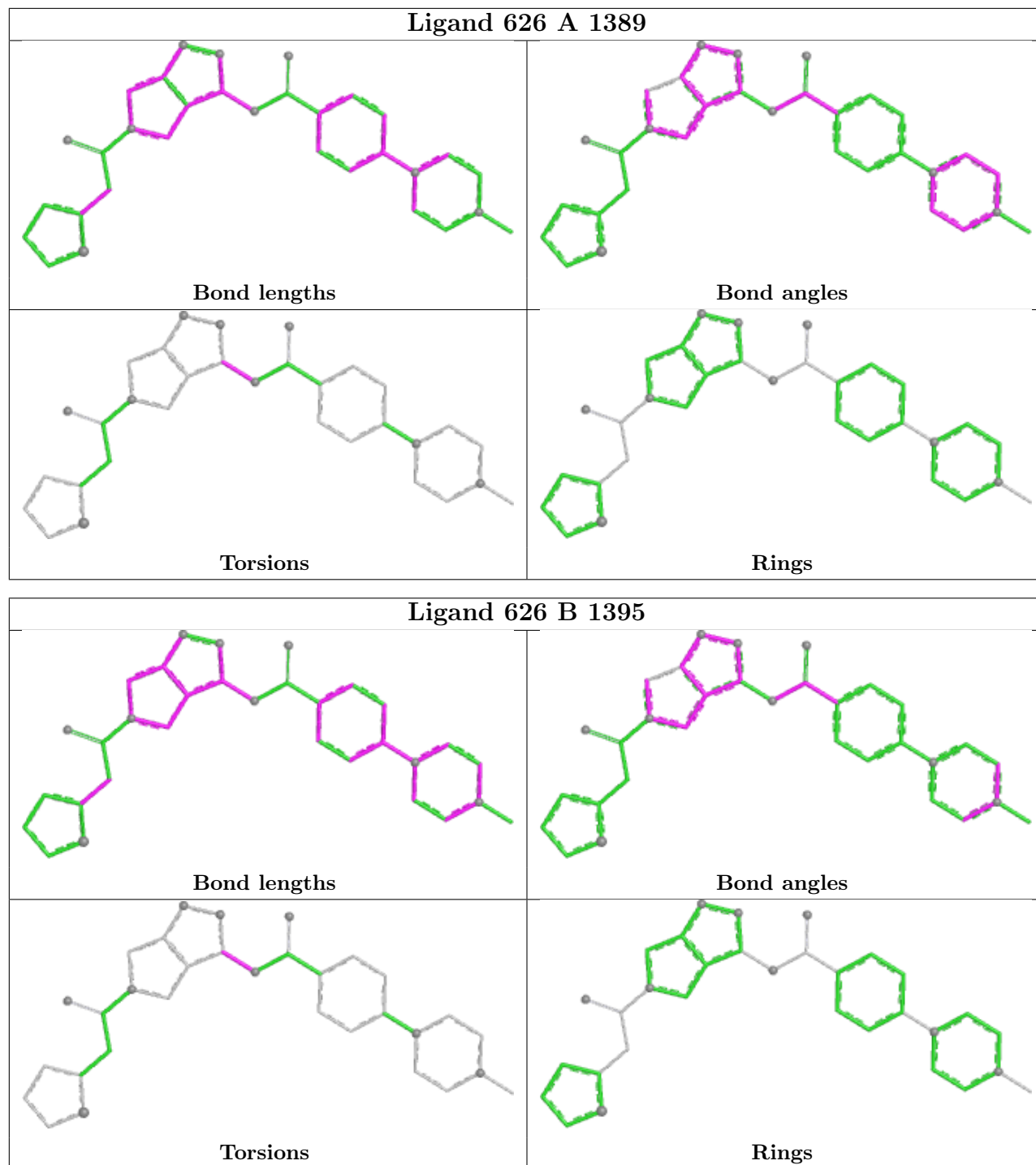
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1395	626	1	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 ⓘ

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	264/306 (86%)	0.54	24 (9%) 15 13	20, 34, 56, 73	0
1	B	270/306 (88%)	0.61	25 (9%) 14 13	20, 38, 62, 75	0
All	All	534/612 (87%)	0.57	49 (9%) 14 13	20, 36, 60, 75	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ALA	5.8
1	B	303	GLY	4.6
1	B	305	MET	4.5
1	A	199	TYR	3.9
1	A	251	ARG	3.5
1	B	302	GLU	3.3
1	A	275	PHE	3.2
1	A	282	PRO	3.1
1	B	178	LEU	3.0
1	B	301	ILE	3.0
1	A	170	GLU	2.8
1	A	277	TRP	2.8
1	A	283	SER	2.7
1	B	275	PHE	2.7
1	B	306	HIS	2.7
1	B	134	GLU	2.6
1	B	183	GLU	2.6
1	B	304	ARG	2.6
1	A	177	GLN	2.6
1	A	257	ILE	2.6
1	B	276	GLY	2.6
1	A	168	GLN	2.5
1	A	175	GLU	2.5
1	A	301	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	394	GLN	2.5
1	A	144	PHE	2.5
1	B	300	MET	2.5
1	A	256	ASP	2.4
1	B	157	PHE	2.4
1	A	127	GLN	2.4
1	A	280	HIS	2.4
1	B	281	ALA	2.4
1	B	128	TRP	2.4
1	B	152	GLU	2.3
1	A	126	ARG	2.3
1	A	197	TYR	2.3
1	A	354	GLU	2.2
1	A	279	VAL	2.2
1	B	131	GLU	2.2
1	B	129	ALA	2.2
1	B	168	GLN	2.2
1	B	277	TRP	2.2
1	A	181	GLU	2.1
1	B	172	ALA	2.1
1	A	157	PHE	2.1
1	B	169	LEU	2.1
1	B	279	VAL	2.1
1	B	187	HIS	2.0
1	A	284	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

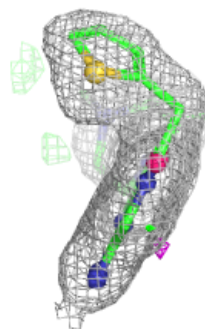
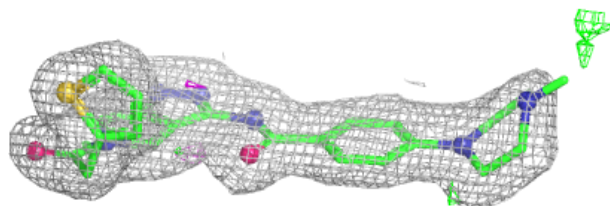
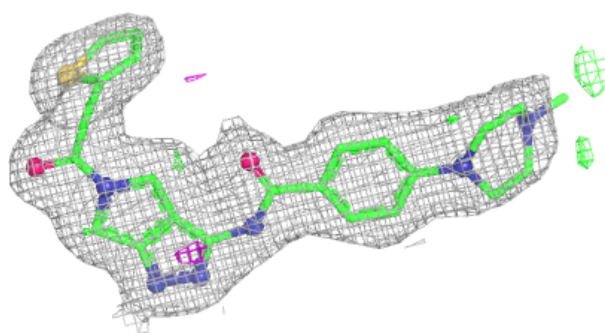
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	626	B	1395	32/32	0.92	0.10	25,36,52,55	0
2	626	A	1389	32/32	0.93	0.10	23,31,44,46	0
3	ARS	A	1391	1/1	0.95	0.07	106,106,106,106	0
3	ARS	A	1390	1/1	0.96	0.06	52,52,52,52	0
3	ARS	B	1396	1/1	0.96	0.06	43,43,43,43	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.

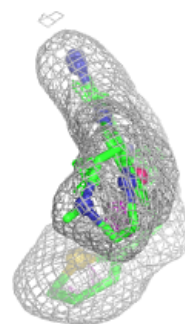
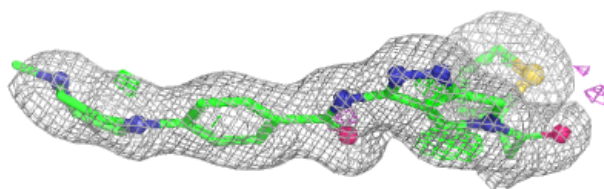
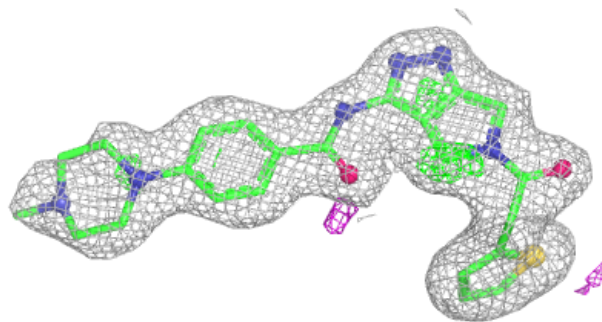
Electron density around 626 B 1395:

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 626 A 1389:

$2mF_o-DF_c$ (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.