Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 06:47 AM EDT

PDB ID	:	5D10
Title	:	Kinase domain of cSrc in complex with RL236
Authors	:	Becker, C.; Mayer-Wrangowski, S.C.; Julian, E.; Rauh, D.
Deposited on	:	2015-08-03
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

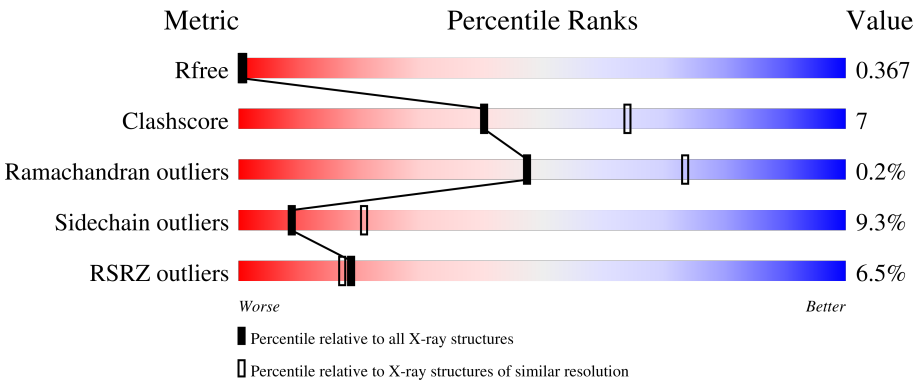
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	286	4% 70% 13% • • 13%
1	B	286	7% 70% 15% • 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4139 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.

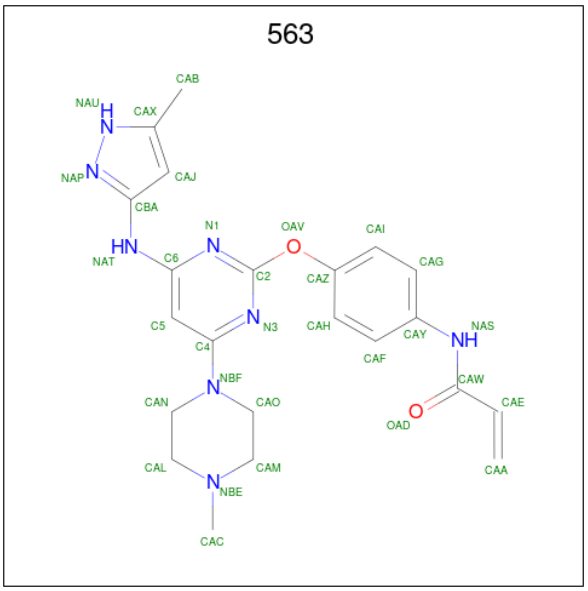
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	1993	1276	332	366	19	0	4	0
1	B	247	1982	1274	329	361	18	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	338	MET	THR	engineered mutation	UNP P00523
A	345	CYS	SER	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523
B	338	MET	THR	engineered mutation	UNP P00523
B	345	CYS	SER	engineered mutation	UNP P00523

- Molecule 2 is N-[4-({4-(4-methylpiperazin-1-yl)-6-[(5-methyl-1H-pyrazol-3-yl)amino]pyrimidin-2-yl}oxy)phenyl]prop-2-enamide (three-letter code: 563) (formula: $C_{22}H_{26}N_8O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	22	8	2	0	0
			Total	C	N	O		
2	B	1	32	22	8	2	0	0

- Molecule 3 is water.

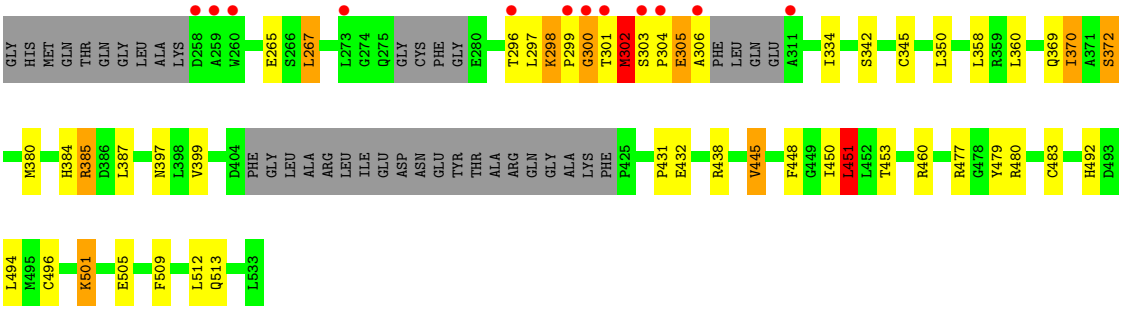
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	60	60	60	0	0
			Total	O		
3	B	40	40	40	0	0

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.

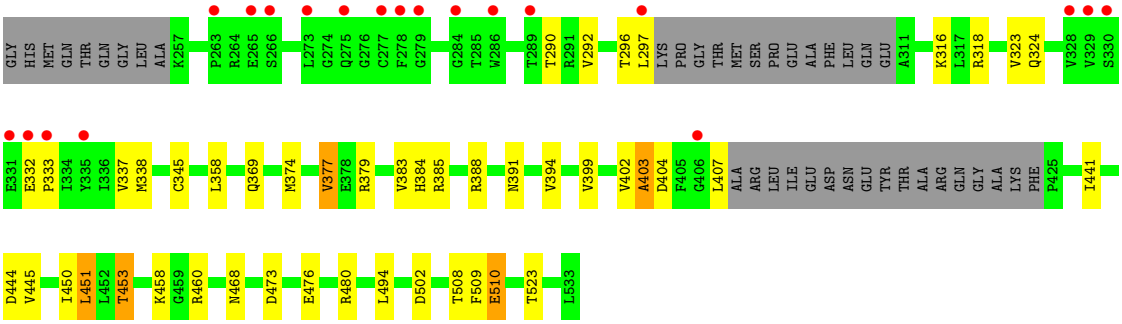
• Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain A:



• Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.90Å 63.50Å 76.60Å 79.20° 88.10° 90.10°	Depositor
Resolution (Å)	44.11 – 2.70 44.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	87.9 (44.11-2.70) 87.9 (44.11-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.269 , 0.359 0.274 , 0.367	Depositor DCC
R_{free} test set	750 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	4139	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 563

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	0.67	0/2051	0.90	4/2779 (0.1%)
1	B	0.68	0/2032	0.91	5/2750 (0.2%)
All	All	0.68	0/4083	0.90	9/5529 (0.2%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	451	LEU	CA-CB-CG	6.62	130.54	115.30
1	A	267	LEU	CA-CB-CG	6.25	129.66	115.30
1	B	460	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	460	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	451	LEU	CA-CB-CG	5.62	128.24	115.30
1	A	302	MET	C-N-CA	-5.62	107.66	121.70
1	B	379	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	473	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	480	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	PRO	Peptide
1	A	300	GLY	Peptide
1	A	302	MET	Peptide
1	B	403	ALA	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	1993	0	1965	41	1
1	B	1982	0	1960	17	0
2	A	32	0	26	0	0
2	B	32	0	26	0	0
3	A	60	0	0	3	0
3	B	40	0	0	1	0
All	All	4139	0	3977	58	1

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 7.

All (58) 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:297:LEU:CB	1:A:334:ILE:HB	1.76	1.14
1:A:372:SER:HA	1:A:513:GLN:OE1	1.55	1.07
1:A:372:SER:CA	1:A:513:GLN:OE1	2.08	1.02
1:A:301:THR:O	1:A:303:SER:HA	1.69	0.92
1:A:297:LEU:CB	1:A:334:ILE:CB	2.51	0.88
1:A:302:MET:O	1:A:305:GLU:OE2	1.95	0.84
1:A:450:ILE:O	1:A:453:THR:HG22	1.79	0.82
1:A:300:GLY:HA3	1:A:303:SER:HB2	1.74	0.70
1:A:438[A]:ARG:NE	1:A:438[A]:ARG:HA	2.08	0.68
1:A:483[B]:CYS:SG	1:A:492:HIS:CG	2.88	0.65
1:A:298:LYS:HB3	1:A:301:THR:OG1	1.95	0.65
1:A:300:GLY:CA	1:A:303:SER:HB2	2.28	0.64
1:A:372:SER:CB	1:A:513:GLN:OE1	2.46	0.64
1:A:297:LEU:CB	1:A:334:ILE:CG1	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:N	1:A:303:SER:HB2	2.17	0.59
1:B:502:ASP:HB2	3:B:732:HOH:O	2.04	0.58
1:A:372:SER:N	1:A:513:GLN:OE1	2.39	0.55
1:A:369:GLN:HE22	1:A:399:VAL:HA	1.71	0.55
1:A:305:GLU:HB2	1:A:306:ALA:HB3	1.89	0.55
1:A:301:THR:O	1:A:303:SER:CA	2.51	0.54
1:A:480:ARG:NH1	1:A:496:CYS:O	2.40	0.54
1:B:383:VAL:HG12	1:B:385:ARG:HG3	1.91	0.53
1:B:391:ASN:O	1:B:403:ALA:O	2.27	0.52
1:B:374:MET:HE3	1:B:402:VAL:HG11	1.90	0.52
1:B:450:ILE:O	1:B:453:THR:HG22	2.10	0.51
1:A:483[B]:CYS:SG	1:A:492:HIS:CD2	3.04	0.51
1:A:303:SER:HB3	1:A:304:PRO:HD3	1.94	0.49
1:A:384:HIS:C	1:A:385:ARG:HG2	2.33	0.48
1:B:332:GLU:HG2	1:B:333:PRO:HA	1.95	0.47
1:A:380:MET:HE1	3:A:727:HOH:O	2.14	0.47
1:B:384:HIS:NE2	1:B:404:ASP:O	2.48	0.47
1:A:448:PHE:CE2	1:A:512:LEU:HD22	2.50	0.47
1:A:296:THR:OG1	1:A:297:LEU:N	2.49	0.46
1:A:445:VAL:HG12	1:A:509:PHE:CE2	2.51	0.46
1:B:292:VAL:HG11	1:B:337:VAL:HG13	1.98	0.45
1:B:384:HIS:O	1:B:385:ARG:HB2	2.17	0.45
1:A:298:LYS:C	1:A:300:GLY:HA2	2.37	0.45
1:A:370:ILE:CD1	1:A:451:LEU:HD21	2.47	0.45
1:B:508:THR:HG22	1:B:510:GLU:N	2.32	0.44
1:A:501[A]:LYS:HD3	1:A:501[A]:LYS:HA	1.79	0.43
1:B:374:MET:CE	1:B:402:VAL:HG11	2.48	0.43
1:A:431:PRO:O	1:A:432:GLU:C	2.57	0.43
1:B:441:ILE:O	1:B:444:ASP:HB2	2.18	0.43
1:A:298:LYS:HD2	1:A:298:LYS:HA	1.77	0.43
1:A:370:ILE:HD13	1:A:451:LEU:HD21	2.01	0.43
1:B:445:VAL:HG23	1:B:509:PHE:CE2	2.54	0.42
1:A:297:LEU:CB	1:A:334:ILE:HG13	2.49	0.42
1:A:384:HIS:C	1:A:385:ARG:CG	2.88	0.42
1:B:369:GLN:HE22	1:B:399:VAL:HA	1.83	0.42
1:A:298:LYS:O	1:A:300:GLY:CA	2.68	0.42
1:B:374:MET:HA	1:B:377:VAL:HG13	2.01	0.42
1:A:438[A]:ARG:NH2	3:A:702:HOH:O	2.52	0.42
1:A:298:LYS:O	1:A:300:GLY:HA3	2.20	0.41
1:A:448:PHE:O	1:A:451:LEU:N	2.53	0.41
1:A:479:TYR:HA	3:A:707:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:MET:HE3	1:B:402:VAL:HG21	2.03	0.41
1:B:323:VAL:HG12	1:B:338:MET:HE2	2.02	0.40
1:A:301:THR:C	1:A:302:MET:HG3	2.41	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASN:OD1	1:A:438[B]:ARG:NE[1_455]	2.08	0.12

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	244/286 (85%)	225 (92%)	19 (8%)	0	100	100
1	B	242/286 (85%)	226 (93%)	15 (6%)	1 (0%)	34	60
All	All	486/572 (85%)	451 (93%)	34 (7%)	1 (0%)	47	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	510	GLU

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	214/245 (87%)	193 (90%)	21 (10%)	8 18
1	B	212/245 (86%)	193 (91%)	19 (9%)	9 22
All	All	426/490 (87%)	386 (91%)	40 (9%)	9 20

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLU
1	A	267	LEU
1	A	298	LYS
1	A	302	MET
1	A	305	GLU
1	A	342	SER
1	A	345	CYS
1	A	350	LEU
1	A	358	LEU
1	A	360	LEU
1	A	370	ILE
1	A	372	SER
1	A	385	ARG
1	A	387	LEU
1	A	445	VAL
1	A	451	LEU
1	A	477	ARG
1	A	494	LEU
1	A	501[A]	LYS
1	A	501[B]	LYS
1	A	505	GLU
1	B	290	THR
1	B	296	THR
1	B	297	LEU
1	B	316	LYS
1	B	318	ARG
1	B	324	GLN
1	B	345	CYS
1	B	358	LEU
1	B	377	VAL
1	B	388	ARG
1	B	394	VAL
1	B	407	LEU
1	B	451	LEU
1	B	453	THR

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Mol	Chain	Res	Type
1	B	458	LYS
1	B	468	ASN
1	B	476	GLU
1	B	494	LEU
1	B	523	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	A	391	ASN
1	B	369	GLN
1	B	468	ASN
1	B	474	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	563	B	601	-	34,35,35	2.07	7 (20%)	42,48,48	2.76	16 (38%)
2	563	A	601	-	34,35,35	2.18	8 (23%)	42,48,48	2.60	16 (38%)

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	563	B	601	-	-	4/16/28/28	0/4/4/4
2	563	A	601	-	-	4/16/28/28	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	563	NAP-NAU	-7.02	1.23	1.37
2	B	601	563	NAP-NAU	-6.80	1.24	1.37
2	A	601	563	CAE-CAW	5.02	1.56	1.48
2	A	601	563	CAA-CAE	4.98	1.55	1.30
2	B	601	563	CAA-CAE	4.88	1.54	1.30
2	B	601	563	CAE-CAW	4.31	1.55	1.48
2	A	601	563	CAN-NBF	3.29	1.51	1.46
2	A	601	563	CAY-NAS	-3.09	1.35	1.41
2	B	601	563	CAL-CAN	-2.95	1.40	1.51
2	B	601	563	CAJ-CAX	-2.67	1.34	1.39
2	B	601	563	CAN-NBF	2.59	1.50	1.46
2	B	601	563	CAY-NAS	-2.51	1.36	1.41
2	A	601	563	CAX-NAU	-2.40	1.30	1.34
2	A	601	563	CAJ-CAX	-2.39	1.34	1.39
2	A	601	563	CAL-CAN	-2.14	1.43	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	563	CAE-CAW-NAS	11.55	121.45	113.84
2	A	601	563	CAE-CAW-NAS	9.59	120.16	113.84
2	B	601	563	C2-OAV-CAZ	4.69	130.85	118.78
2	A	601	563	CAO-NBF-CAN	4.19	120.76	111.52
2	A	601	563	CAJ-CBA-NAP	-4.08	104.63	110.47
2	B	601	563	CAO-NBF-CAN	3.95	120.25	111.52
2	B	601	563	C2-N3-C4	3.90	122.59	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	563	C2-N3-C4	3.76	122.28	114.06
2	A	601	563	CAO-CAM-NBE	-3.67	106.65	110.80
2	A	601	563	C2-OAV-CAZ	3.65	128.16	118.78
2	A	601	563	N3-C2-N1	-3.64	120.61	127.63
2	B	601	563	CAM-CAO-NBF	3.49	117.48	110.70
2	B	601	563	CAC-NBE-CAM	-3.48	105.45	110.66
2	B	601	563	N3-C2-N1	-3.43	121.03	127.63
2	A	601	563	C5-C6-N1	-3.43	116.15	123.41
2	A	601	563	CAN-CAL-NBE	3.25	114.48	110.80
2	A	601	563	C5-C4-N3	-3.19	116.94	123.15
2	B	601	563	C5-C4-N3	-3.07	117.17	123.15
2	A	601	563	NAT-C6-N1	2.99	125.40	116.95
2	A	601	563	CAL-CAN-NBF	2.91	116.36	110.70
2	B	601	563	OAD-CAW-CAE	-2.90	118.09	122.72
2	B	601	563	NAT-C6-N1	2.87	125.06	116.95
2	B	601	563	C5-C6-N1	-2.76	117.56	123.41
2	A	601	563	OAD-CAW-NAS	-2.72	119.93	123.05
2	B	601	563	OAV-C2-N1	2.72	125.56	116.10
2	B	601	563	CAJ-CBA-NAP	-2.63	106.71	110.47
2	A	601	563	OAV-C2-N1	2.52	124.85	116.10
2	B	601	563	CAB-CAX-NAU	2.51	125.07	120.07
2	A	601	563	CAC-NBE-CAM	-2.36	107.13	110.66
2	B	601	563	OAD-CAW-NAS	-2.26	120.46	123.05
2	B	601	563	CAX-CAJ-CBA	-2.04	105.13	107.23
2	A	601	563	CAY-NAS-CAW	-2.00	125.23	128.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

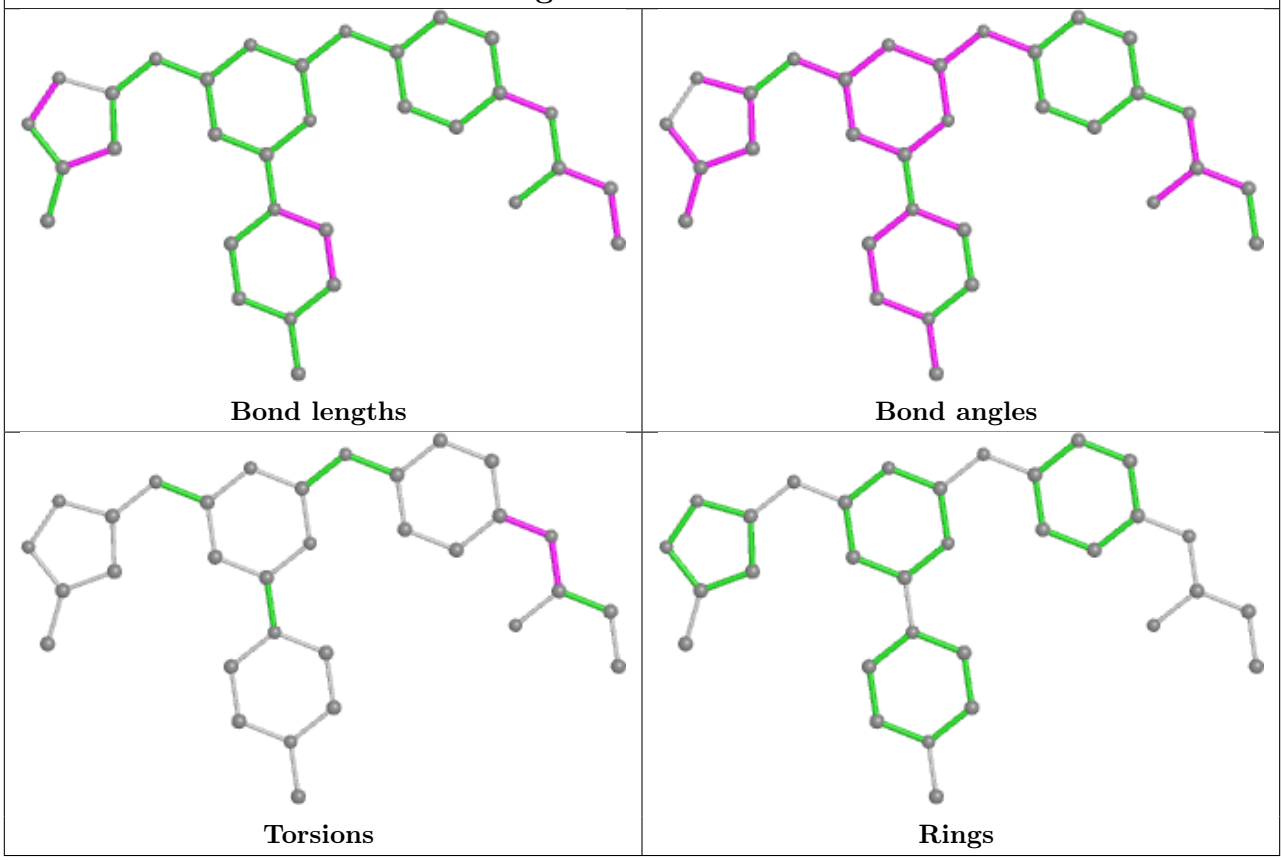
Mol	Chain	Res	Type	Atoms
2	A	601	563	OAD-CAW-NAS-CAY
2	A	601	563	CAE-CAW-NAS-CAY
2	B	601	563	OAD-CAW-NAS-CAY
2	B	601	563	CAE-CAW-NAS-CAY
2	A	601	563	CAG-CAY-NAS-CAW
2	A	601	563	CAF-CAY-NAS-CAW
2	B	601	563	CAG-CAY-NAS-CAW
2	B	601	563	CAF-CAY-NAS-CAW

There are no ring outliers.

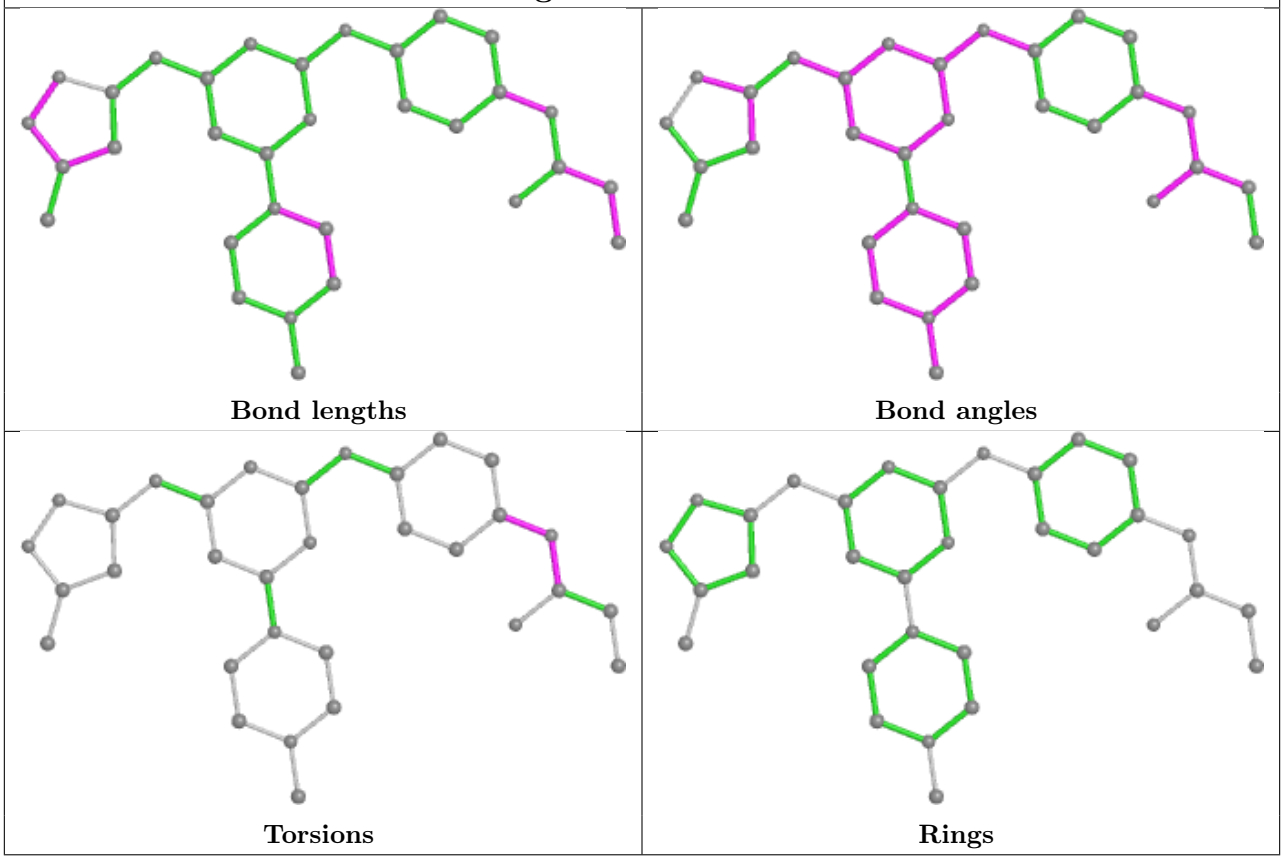
No monomer is involved in short contacts.

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

Ligand 563 B 601



Ligand 563 A 601



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	248/286 (86%)	0.30	12 (4%)	30	28	8, 24, 66, 95	0
1	B	247/286 (86%)	0.34	20 (8%)	12	10	5, 22, 63, 82	0
All	All	495/572 (86%)	0.32	32 (6%)	18	17	5, 23, 65, 95	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	PHE	7.0
1	A	303	SER	4.4
1	B	297	LEU	4.1
1	A	259	ALA	3.8
1	B	277	CYS	3.7
1	B	279	GLY	3.4
1	B	265	GLU	3.3
1	B	330	SER	3.2
1	B	331	GLU	3.2
1	B	329	VAL	3.2
1	B	328	VAL	3.0
1	A	258	ASP	2.9
1	A	304	PRO	2.9
1	A	296	THR	2.8
1	A	311	ALA	2.8
1	A	260	TRP	2.7
1	A	301	THR	2.6
1	A	299	PRO	2.6
1	B	286	TRP	2.5
1	A	300	GLY	2.5
1	A	306	ALA	2.5
1	B	284	GLY	2.5
1	B	335	TYR	2.5
1	B	275	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	406	GLY	2.4
1	A	273	LEU	2.4
1	B	266	SER	2.2
1	B	333	PRO	2.1
1	B	263	PRO	2.1
1	B	289	THR	2.1
1	B	273	LEU	2.1
1	B	332	GLU	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)

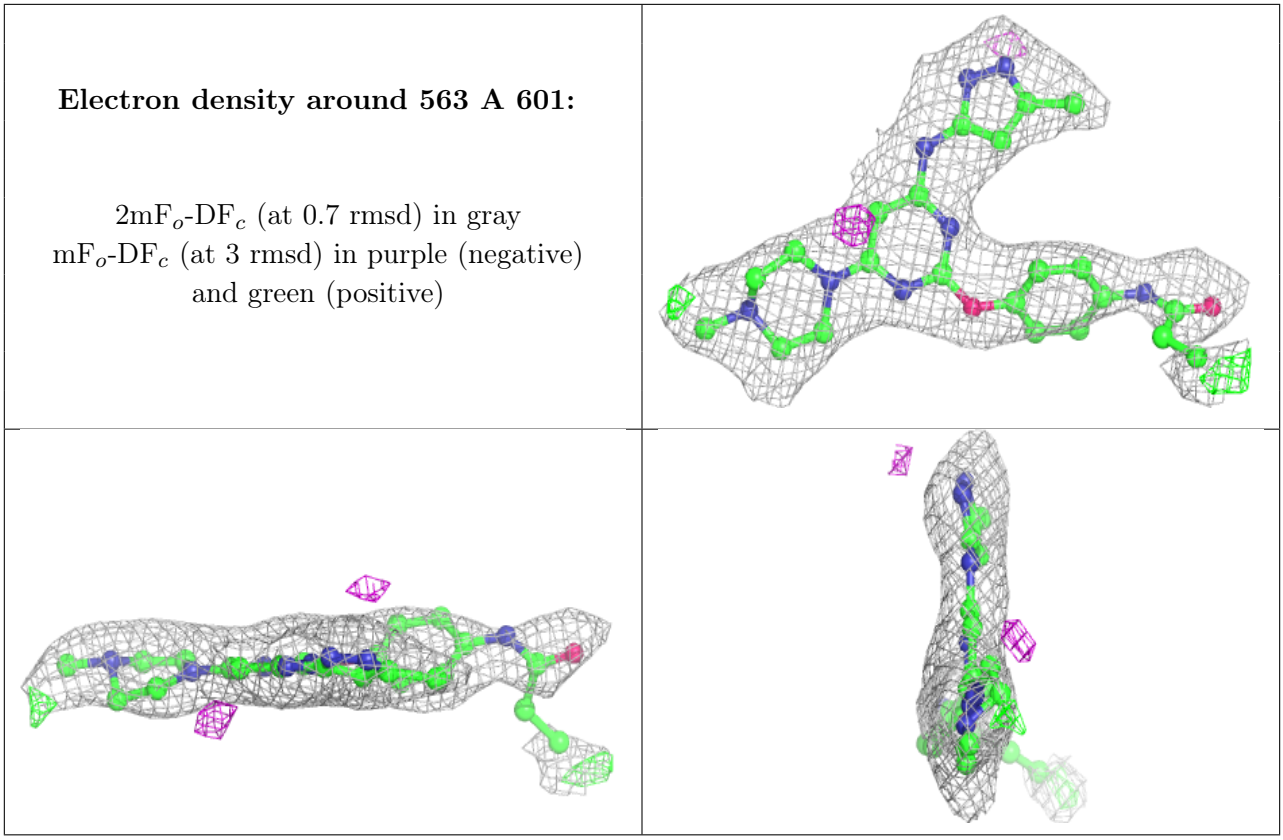
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	563	A	601	32/32	0.89	0.25	22,31,51,52	0
2	563	B	601	32/32	0.89	0.24	22,28,58,63	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.

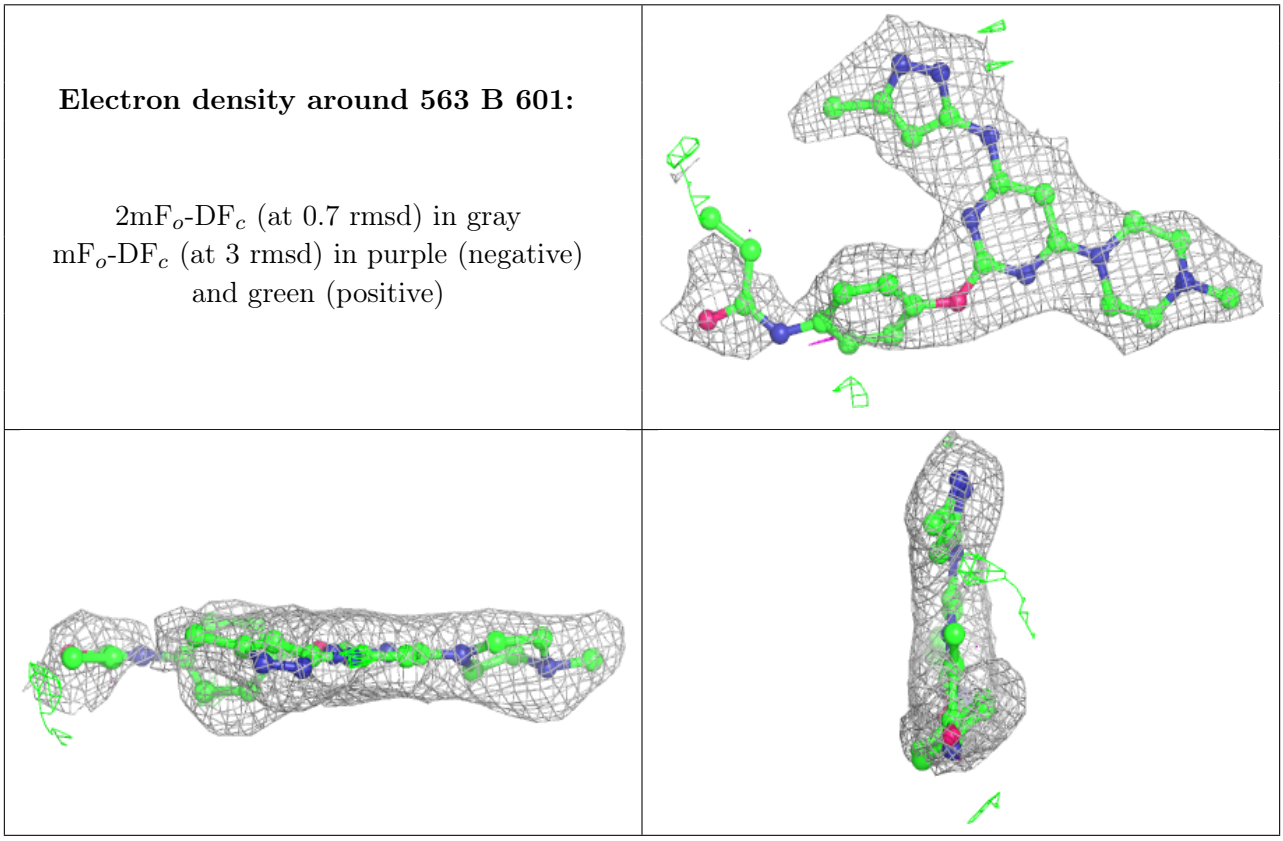
Electron density around 563 A 601:

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



Electron density around 563 B 601:

$2mF_o$-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.