



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:15 PM UTC

PDB ID : 5D11 / pdb_00005d11
Title : Kinase domain of cSrc in complex with RL235
Authors : Becker, C.; Gruetter, C.; Engel, J.; Rauh, D.
Deposited on : 2015-08-03
Resolution : 2.30 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

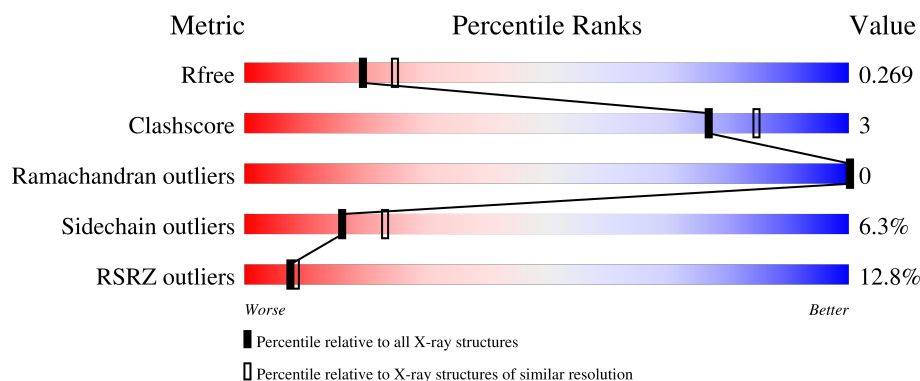
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	286	12% 74% 13% • 11%
1	B	286	11% 81% 7% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4253 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
1	A	254	Total	C	N	O	S	0	3	0
			2016	1291	336	371	18			
1	B	255	Total	C	N	O	S	0	3	0
			2063	1329	340	376	18			

There are 10 discrepancies between the modelled and reference sequences:

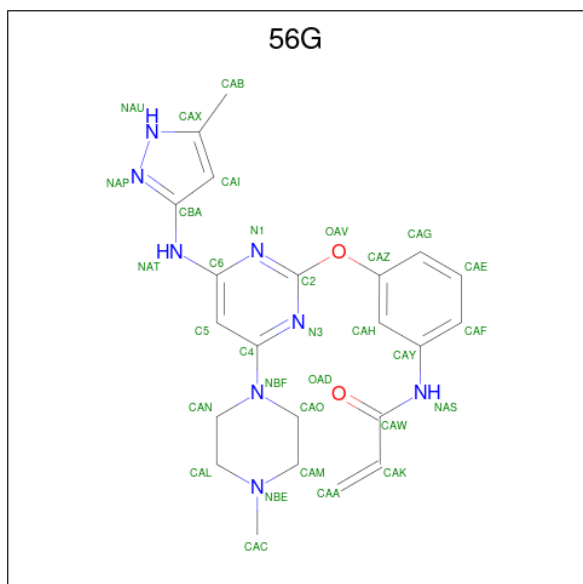
Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
A	338	MET	THR	engineered mutation	UNP P00523
A	345	CYS	SER	engineered mutation	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is N-[3-({4-(4-methylpiperazin-1-yl)-6-[(5-methyl-1H-pyrazol-3-yl)amino]pyrimidin-2-yl}oxy)phenyl]prop-2-enamide (CCD ID: 56G) (formula: C₂₂H₂₆N₈O₂).



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

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

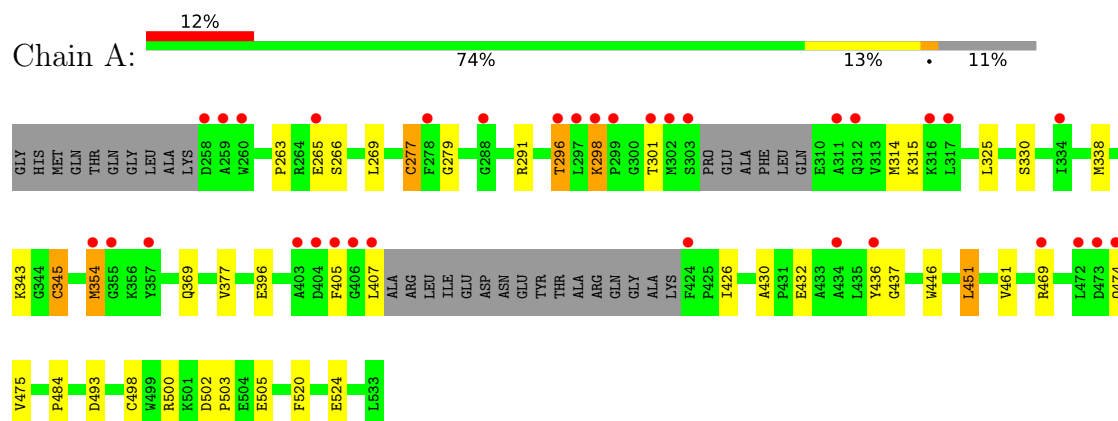
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	46	Total	O	0	0
			46	46		

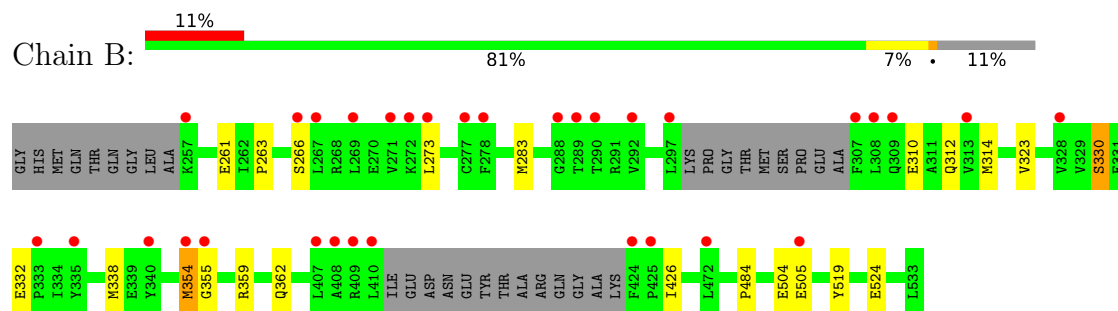
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.12Å 63.43Å 75.35Å 78.65° 89.55° 90.29°	Depositor
Resolution (Å)	43.54 – 2.30 43.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.54-2.30) 97.1 (43.54-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.214 , 0.269 0.220 , 0.269	Depositor DCC
R_{free} test set	991 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4253	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.19% 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: GOL, 56G

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.27	5/2072 (0.2%)	1.18	3/2808 (0.1%)
1	B	1.20	2/2121 (0.1%)	1.17	4/2870 (0.1%)
All	All	1.24	7/4193 (0.2%)	1.18	7/5678 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	PRO	CA-C	11.24	1.58	1.51
1	B	484	PRO	CA-C	7.95	1.56	1.51
1	A	369	GLN	CA-C	-7.43	1.43	1.52
1	B	505	GLU	CA-C	5.38	1.60	1.52
1	A	461	VAL	CA-C	-5.15	1.48	1.53
1	A	498	CYS	C-O	-5.04	1.17	1.24
1	A	461	VAL	C-O	-5.00	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	TYR	N-CA-C	6.59	118.12	111.07
1	A	430	ALA	CA-C-N	5.74	125.21	119.24
1	A	430	ALA	C-N-CA	5.74	125.21	119.24
1	A	345	CYS	CB-CA-C	-5.45	102.14	109.71
1	B	484	PRO	N-CA-C	5.41	115.66	110.47
1	B	283	MET	N-CA-C	-5.32	102.60	110.48
1	B	355	GLY	N-CA-C	5.09	120.51	113.99

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	2016	0	1966	15	3
1	B	2063	0	2040	9	0
2	A	6	0	8	0	0
2	B	6	0	8	2	0
3	A	32	0	25	0	0
3	B	32	0	25	0	0
4	A	52	0	0	1	0
4	B	46	0	0	0	0
All	All	4253	0	4072	24	3

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 3.

All (24) 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:362:GLN:HG3	2:B:601:GOL:H32	1.62	0.79
1:B:354:MET:HA	1:B:354:MET:HE2	1.87	0.56
1:A:354:MET:HA	1:A:354:MET:HE3	1.90	0.54
1:A:343:LYS:HE3	1:A:396[B]:GLU:OE1	2.09	0.53
1:A:377:VAL:HG21	1:A:405:PHE:HZ	1.75	0.52
1:B:263:PRO:O	1:B:266:SER:OG	2.29	0.51
1:B:314:MET:HE3	1:B:323:VAL:O	2.10	0.50
1:A:263:PRO:O	1:A:266:SER:OG	2.31	0.48
1:A:396[B]:GLU:OE1	1:A:396[B]:GLU:HA	2.13	0.48
1:B:314:MET:HE1	1:B:338:MET:SD	2.52	0.47
1:B:359:ARG:H	1:B:362:GLN:HE21	1.62	0.47
1:A:500:ARG:NH1	1:A:505:GLU:O	2.48	0.44
1:B:362:GLN:HG3	2:B:601:GOL:C3	2.42	0.43
1:A:279:GLY:HA3	1:A:296:THR:O	2.19	0.43
1:A:314:MET:SD	1:A:338:MET:HE2	2.59	0.42
1:A:315:LYS:HG3	1:A:325:LEU:HD23	2.01	0.42
1:B:261:GLU:OE1	1:B:330:SER:OG	2.36	0.42
1:A:502:ASP:O	1:A:503:PRO:C	2.61	0.42
1:A:354:MET:HA	1:A:354:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:O	1:B:314:MET:HB2	2.20	0.41
1:A:277:CYS:O	1:A:298:LYS:NZ	2.52	0.40
1:A:446:TRP:CD1	1:A:446:TRP:C	2.99	0.40
1:A:520:PHE:HB3	4:A:745:HOH:O	2.20	0.40
1:A:451:LEU:O	1:A:451:LEU:HD12	2.21	0.40

All (3) 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:396[B]:GLU:OE2	1:A:436:TYR:C[1_455]	1.77	0.43
1:A:396[B]:GLU:OE2	1:A:436:TYR:O[1_455]	1.98	0.22
1:A:396[B]:GLU:OE2	1:A:437:GLY:N[1_455]	2.14	0.06

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	251/286 (88%)	236 (94%)	15 (6%)	0	100	100
1	B	252/286 (88%)	241 (96%)	11 (4%)	0	100	100
All	All	503/572 (88%)	477 (95%)	26 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	212/245 (86%)	192 (91%)	20 (9%)	8	11
1	B	221/245 (90%)	213 (96%)	8 (4%)	31	47
All	All	433/490 (88%)	405 (94%)	28 (6%)	16	22

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	GLU
1	A	269	LEU
1	A	277	CYS
1	A	291	ARG
1	A	296	THR
1	A	298	LYS
1	A	301	THR
1	A	330	SER
1	A	345	CYS
1	A	354	MET
1	A	407	LEU
1	A	426	ILE
1	A	432	GLU
1	A	451	LEU
1	A	469	ARG
1	A	474	GLN
1	A	475	VAL
1	A	493[A]	ASP
1	A	493[B]	ASP
1	A	524	GLU
1	B	273	LEU
1	B	312	GLN
1	B	330	SER
1	B	332	GLU
1	B	354	MET
1	B	426	ILE
1	B	504	GLU
1	B	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	ASN
1	A	468	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GOL	A	601	-	5,5,5	0.49	0	5,5,5	0.62	0
3	56G	A	602	1	35,35,35	1.94	8 (22%)	45,48,48	3.45	21 (46%)
3	56G	B	602	1	35,35,35	1.63	8 (22%)	45,48,48	3.55	19 (42%)
2	GOL	B	601	-	5,5,5	0.38	0	5,5,5	1.14	1 (20%)

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	GOL	A	601	-	-	2/4/4/4	-
3	56G	A	602	1	-	3/18/28/28	0/4/4/4
3	56G	B	602	1	-	2/18/28/28	0/4/4/4
2	GOL	B	601	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	56G	NAU-NAP	-4.74	1.26	1.36
3	B	602	56G	CAA-CAK	4.66	1.52	1.30
3	A	602	56G	CAA-CAK	4.41	1.51	1.30
3	A	602	56G	CAL-CAN	-3.95	1.37	1.51
3	A	602	56G	CAO-NBF	3.75	1.53	1.46
3	B	602	56G	CAI-CBA	-3.11	1.35	1.40
3	A	602	56G	CAY-NAS	-2.85	1.35	1.41
3	B	602	56G	CAY-NAS	-2.84	1.35	1.41
3	A	602	56G	CAI-CBA	-2.68	1.35	1.40
3	B	602	56G	CAL-CAN	-2.63	1.41	1.51
3	B	602	56G	CAK-CAW	2.58	1.52	1.48
3	B	602	56G	NAU-NAP	-2.29	1.31	1.36
3	B	602	56G	CAB-CAX	2.28	1.54	1.49
3	B	602	56G	CAX-NAU	-2.26	1.31	1.34
3	A	602	56G	CAX-NAU	-2.21	1.31	1.34
3	A	602	56G	CAH-CAY	2.16	1.43	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	56G	CAA-CAK-CAW	-12.94	108.00	122.22
3	A	602	56G	CBA-NAP-NAU	11.09	111.78	103.71
3	A	602	56G	CAI-CBA-NAP	-10.18	104.86	112.14
3	B	602	56G	CBA-NAP-NAU	9.65	110.73	103.71
3	A	602	56G	CAA-CAK-CAW	-9.60	111.67	122.22
3	B	602	56G	CAI-CBA-NAP	-8.82	105.83	112.14
3	A	602	56G	C6-C5-C4	5.93	121.39	116.64
3	B	602	56G	CAC-NBE-CAL	5.31	120.74	110.63
3	B	602	56G	C6-C5-C4	5.22	120.82	116.64
3	A	602	56G	N3-C2-N1	-4.94	118.67	127.65
3	B	602	56G	N3-C2-N1	-4.36	119.74	127.65
3	A	602	56G	CAM-NBE-CAL	4.28	116.35	109.54
3	A	602	56G	NAT-C6-N1	3.88	122.71	113.33
3	B	602	56G	CAK-CAW-NAS	3.79	116.41	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	56G	NAT-C6-N1	3.66	122.18	113.33
3	B	602	56G	C5-C4-N3	-3.64	116.33	123.34
3	A	602	56G	C5-C6-N1	-3.64	115.81	123.35
3	B	602	56G	CAN-CAL-NBE	3.61	116.65	110.86
3	B	602	56G	C5-C6-N1	-3.20	116.71	123.35
3	B	602	56G	CAX-NAU-NAP	-3.19	106.94	112.47
3	A	602	56G	C2-OAV-CAZ	-3.13	110.91	118.72
3	A	602	56G	OAV-C2-N3	3.06	126.58	116.09
3	A	602	56G	C5-C4-N3	-3.02	117.53	123.34
3	A	602	56G	CAX-NAU-NAP	-2.97	107.32	112.47
3	B	602	56G	CAX-CAI-CBA	2.96	106.85	104.78
3	A	602	56G	CAH-CAY-NAS	2.75	129.06	120.13
3	B	602	56G	CAO-CAM-NBE	2.75	115.27	110.86
3	B	602	56G	CAM-NBE-CAL	2.73	113.89	109.54
3	A	602	56G	CAB-CAX-CAI	-2.66	127.76	131.96
3	A	602	56G	CAO-NBF-CAN	2.64	117.51	111.57
3	A	602	56G	CAI-CAX-NAU	2.62	109.97	106.38
3	A	602	56G	CAY-NAS-CAW	-2.51	123.35	128.07
3	A	602	56G	CAF-CAY-NAS	-2.43	112.25	120.41
3	A	602	56G	CAM-CAO-NBF	2.39	115.82	110.78
3	B	602	56G	CAI-CAX-NAU	2.38	109.64	106.38
2	B	601	GOL	O3-C3-C2	2.37	121.05	110.38
3	B	602	56G	OAV-C2-N3	2.27	123.88	116.09
3	A	602	56G	N3-C4-NBF	2.25	119.40	116.56
3	B	602	56G	OAD-CAW-CAK	-2.21	119.38	122.70
3	A	602	56G	NAT-CBA-NAP	2.19	122.80	117.81
3	B	602	56G	C5-C4-NBF	2.14	124.94	122.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

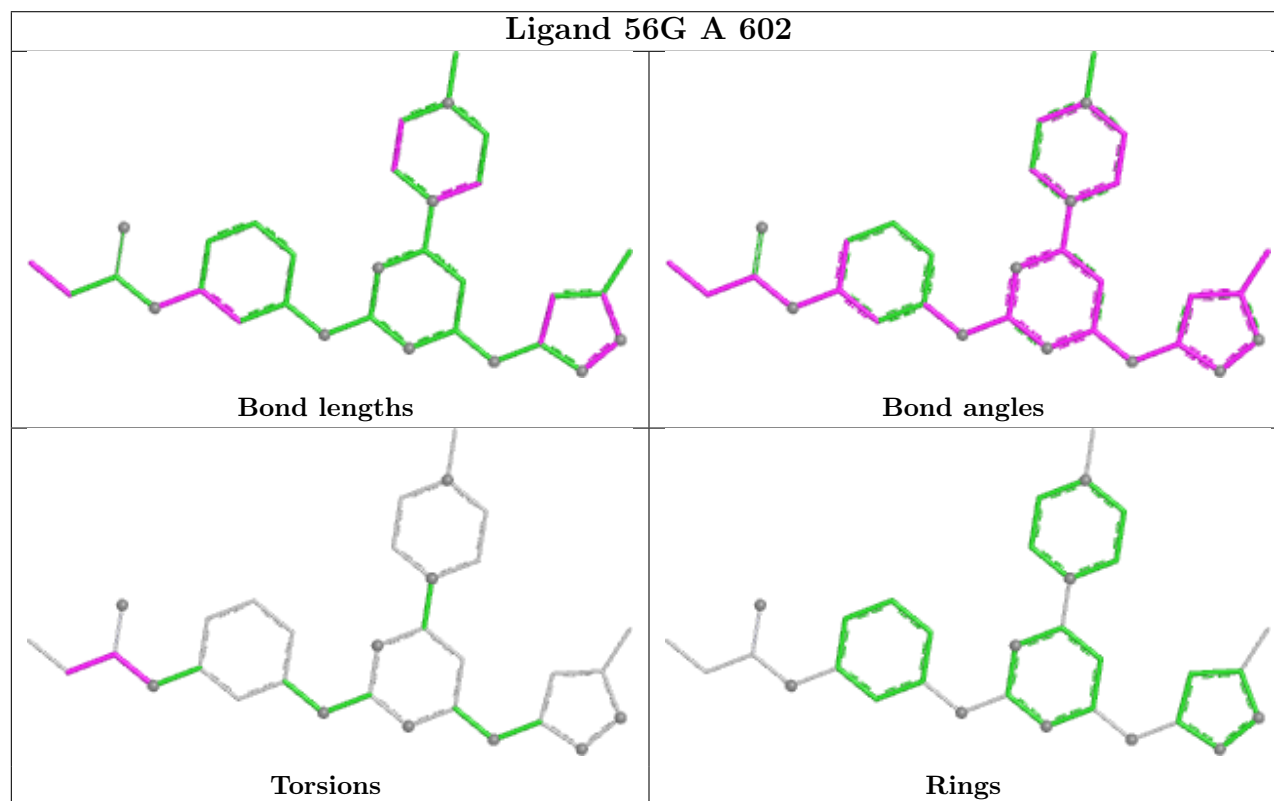
Mol	Chain	Res	Type	Atoms
2	A	601	GOL	C1-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3
3	A	602	56G	CAA-CAK-CAW-NAS
3	A	602	56G	CAA-CAK-CAW-OAD
3	B	602	56G	CAA-CAK-CAW-NAS
3	B	602	56G	CAA-CAK-CAW-OAD
2	A	601	GOL	O2-C2-C3-O3
3	A	602	56G	OAD-CAW-NAS-CAY

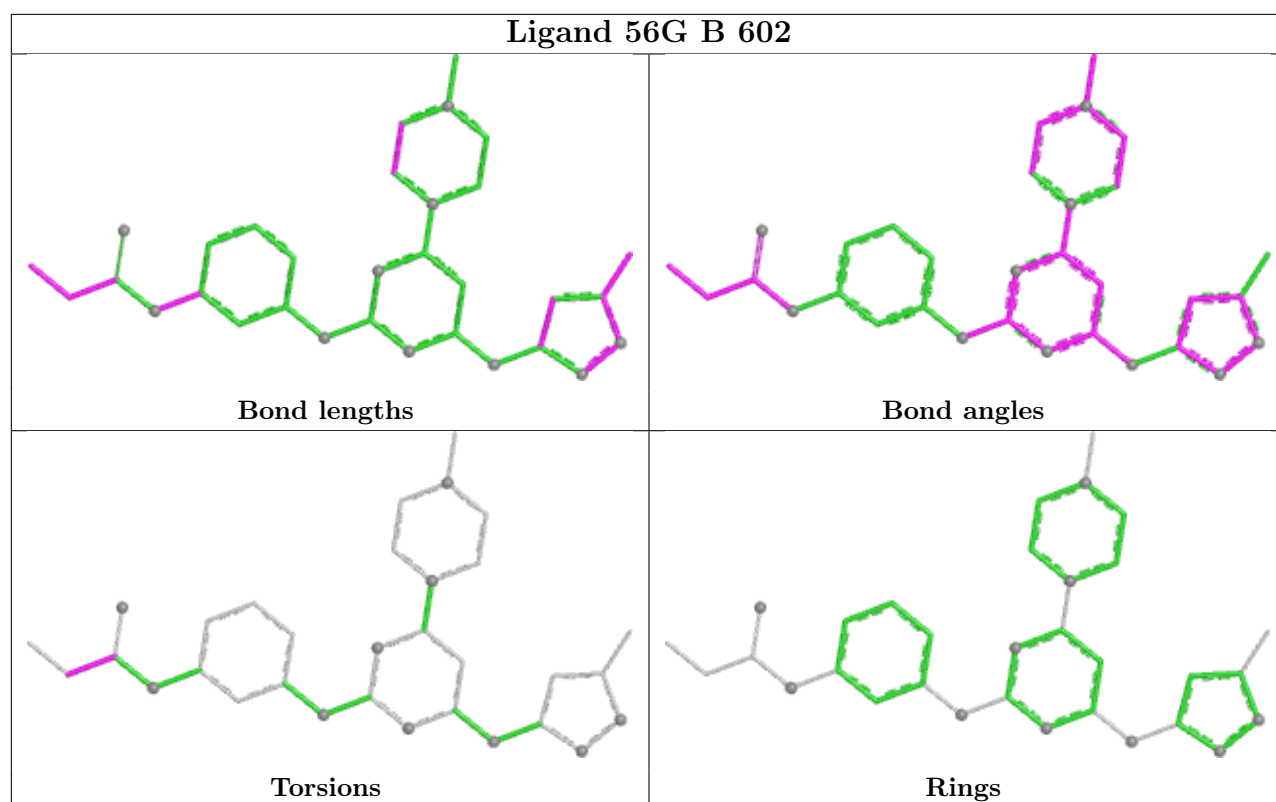
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GOL	2	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	254/286 (88%)	0.80	33 (12%) 7 8	16, 37, 79, 98	3 (1%)
1	B	255/286 (89%)	0.71	32 (12%) 8 9	18, 35, 80, 98	3 (1%)
All	All	509/572 (88%)	0.75	65 (12%) 7 8	16, 36, 80, 98	6 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	LEU	8.0
1	A	258	ASP	6.3
1	A	303	SER	6.2
1	A	424	PHE	5.9
1	B	408	ALA	5.6
1	A	406	GLY	5.5
1	A	405	PHE	5.1
1	B	297	LEU	5.0
1	B	407	LEU	4.9
1	B	410	LEU	4.6
1	A	260	TRP	4.5
1	B	424	PHE	4.2
1	A	302	MET	3.9
1	A	278	PHE	3.9
1	A	297	LEU	3.8
1	B	278	PHE	3.8
1	B	271	VAL	3.7
1	B	309	GLN	3.5
1	A	301	THR	3.3
1	A	259	ALA	3.3
1	B	257	LYS	3.2
1	B	425	PRO	3.2
1	B	354	MET	3.2
1	B	289	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	3.0
1	B	328	VAL	3.0
1	B	335	TYR	3.0
1	B	333	PRO	2.9
1	A	472	LEU	2.9
1	B	269	LEU	2.8
1	B	409	ARG	2.8
1	A	312	GLN	2.8
1	B	267	LEU	2.8
1	B	308	LEU	2.8
1	A	403	ALA	2.7
1	A	334	ILE	2.7
1	B	355	GLY	2.7
1	B	266	SER	2.7
1	A	404	ASP	2.6
1	B	277	CYS	2.6
1	A	288	GLY	2.6
1	A	317	LEU	2.5
1	A	354	MET	2.5
1	A	298	LYS	2.5
1	A	436	TYR	2.5
1	A	473	ASP	2.5
1	B	313	VAL	2.4
1	A	299	PRO	2.4
1	B	290	THR	2.4
1	A	265	GLU	2.4
1	B	273	LEU	2.3
1	A	296	THR	2.3
1	B	288	GLY	2.2
1	B	272	LYS	2.2
1	A	357	TYR	2.2
1	A	311	ALA	2.2
1	B	292	VAL	2.1
1	A	474	GLN	2.1
1	A	355	GLY	2.1
1	A	434	ALA	2.1
1	A	316	LYS	2.1
1	B	472	LEU	2.1
1	B	340	TYR	2.0
1	A	469	ARG	2.0
1	B	505	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

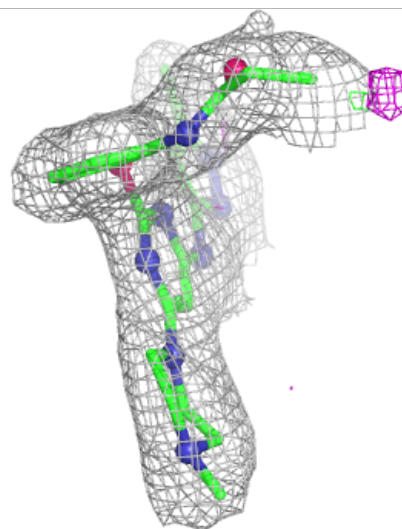
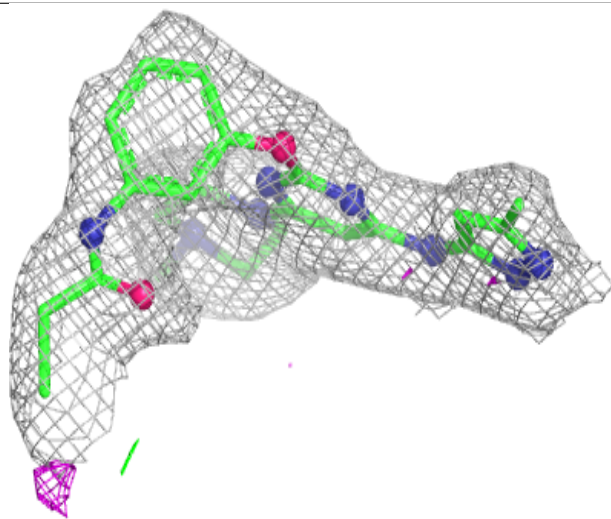
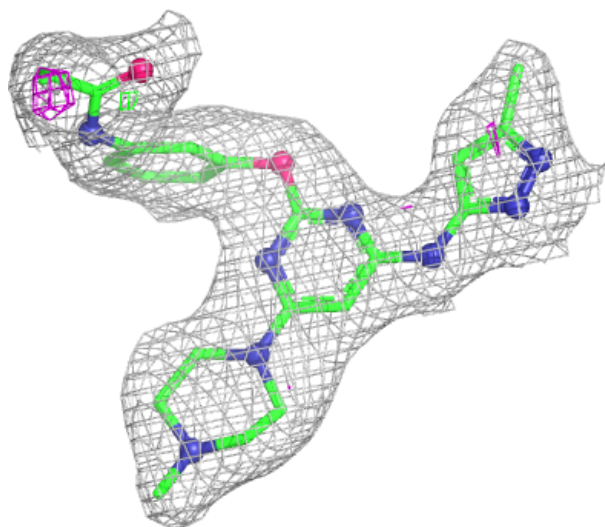
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	601	6/6	0.80	0.16	50,53,59,60	0
2	GOL	A	601	6/6	0.83	0.14	50,52,56,59	0
3	56G	A	602	32/32	0.94	0.09	25,32,46,52	0
3	56G	B	602	32/32	0.94	0.09	24,34,45,46	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.

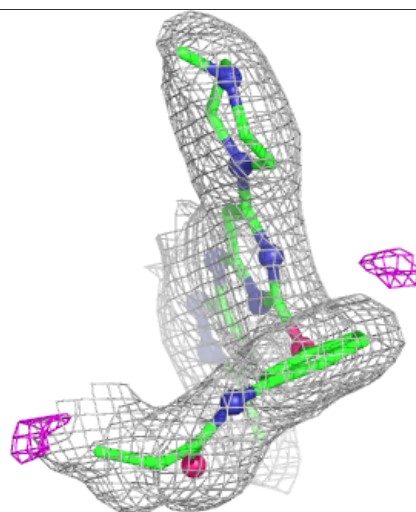
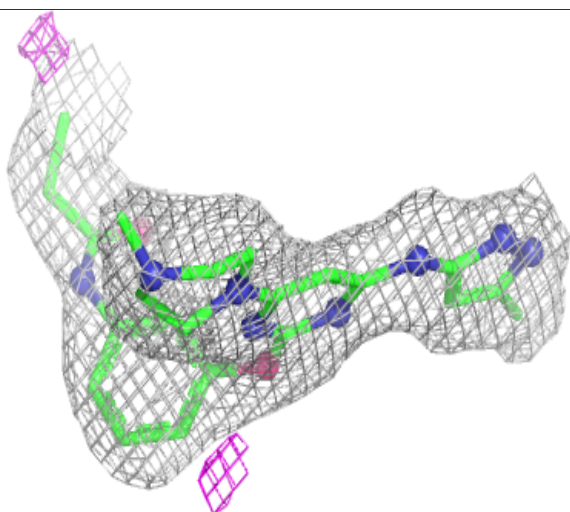
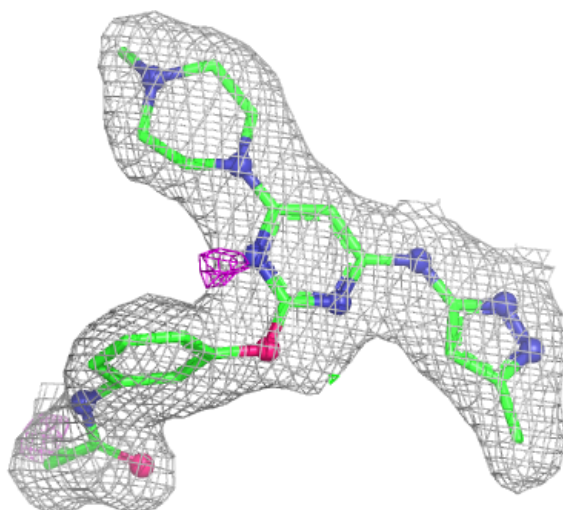
Electron density around 56G A 602:

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



Electron density around 56G B 602:

$2mF_o-DF_c$ (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.