



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:43 PM UTC

PDB ID : 5ZH4 / pdb_00005zh4
Title : CRYSTAL STRUCTURE OF PfkRS WITH INHIBITOR CLADO-7
Authors : Babbar, P.; Malhotra, N.; Sharma, M.; Harlos, K.; Reddy, D.S.; Manickam, Y.; Sharma, A.
Deposited on : 2018-03-11
Resolution : 2.60 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

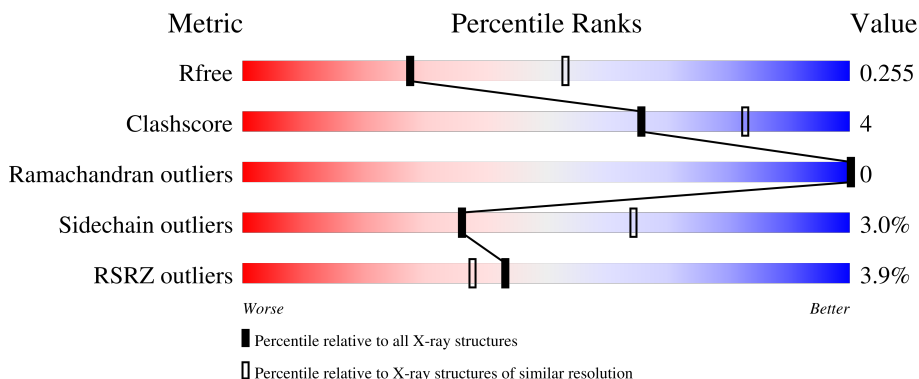
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	507	
1	B	507	

2 Entry composition [i](#)

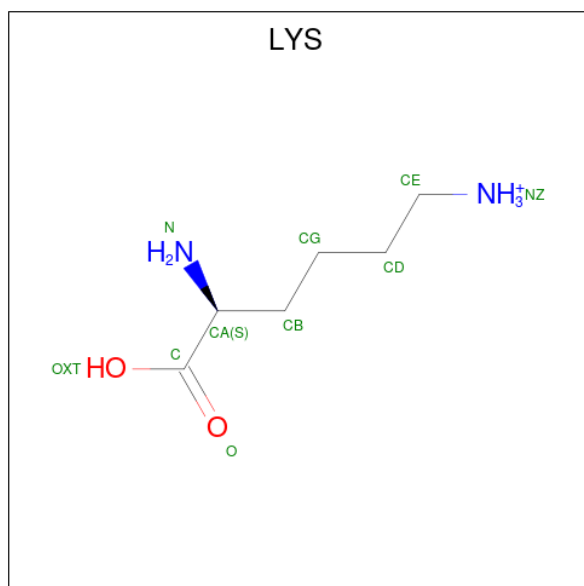
There are 4 unique types of molecules in this entry. The entry contains 7365 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lysine-tRNA ligase.

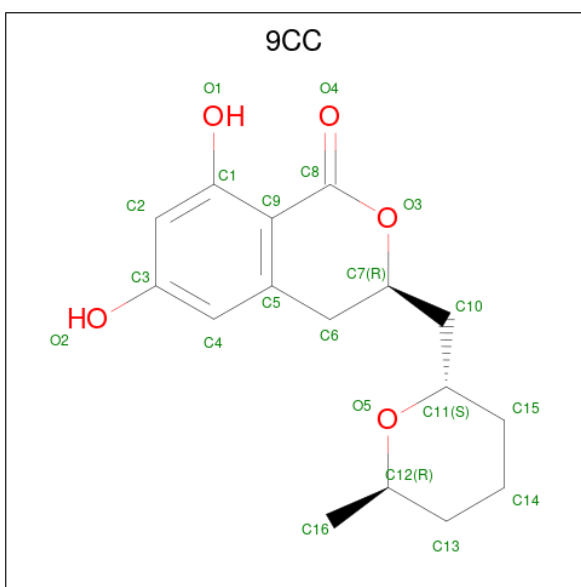
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3653	2361	615	662	15			
1	B	476	Total	C	N	O	S	0	0	0
			3645	2356	613	661	15			

- Molecule 2 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is (3R)-6,8-dihydroxy-3-{[(2S,6R)-6-methyloxan-2-yl]methyl}-3,4-dihydro-1H-2-benzopyran-1-one (CCD ID: 9CC) (formula: $C_{16}H_{20}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	3	Total	Cl	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.62Å 126.04Å 181.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 2.60 40.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.93-2.60) 99.9 (40.93-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.216 , 0.264 0.216 , 0.255	Depositor DCC
R_{free} test set	1912 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7365	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: CL, 9CC

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	0.88	0/3745	0.93	7/5085 (0.1%)
1	B	0.89	0/3738	0.94	9/5087 (0.2%)
All	All	0.88	0/7483	0.94	16/10172 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LYS	N-CA-C	-12.80	98.16	114.04
1	B	457	ILE	CB-CA-C	-6.82	104.98	111.05
1	A	104	HIS	N-CA-C	6.78	119.68	111.82
1	A	471	HIS	CA-C-N	6.50	126.53	119.90
1	A	471	HIS	C-N-CA	6.50	126.53	119.90
1	B	275	THR	CA-C-N	-6.47	113.31	119.85
1	B	275	THR	C-N-CA	-6.47	113.31	119.85
1	A	457	ILE	CB-CA-C	-6.07	105.65	111.05
1	B	471	HIS	CA-C-N	5.51	125.52	119.90
1	B	471	HIS	C-N-CA	5.51	125.52	119.90
1	B	557	ILE	N-CA-C	5.49	115.69	110.42
1	B	205	SER	N-CA-C	5.33	117.17	109.07
1	A	205	SER	N-CA-C	5.32	117.28	109.24
1	B	308	GLU	N-CA-C	5.16	117.30	111.11
1	A	244	ASN	N-CA-C	5.12	116.96	108.20
1	B	209	LYS	N-CA-C	-5.09	107.20	113.41

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	3653	0	3459	29	0
1	B	3645	0	3393	27	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
3	A	21	0	0	0	0
3	B	21	0	0	0	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
All	All	7365	0	6876	54	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 4.

All (54) 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:81:ARG:O	1:B:85:GLU:HG3	1.90	0.71
1:A:425:ILE:O	1:A:429:ILE:HG13	1.94	0.68
1:A:429:ILE:HG23	1:A:439:LEU:HD11	1.78	0.66
1:A:182:ASP:O	1:A:185:ARG:NH1	2.27	0.65
1:B:515:LYS:O	1:B:518:PHE:C	2.41	0.64
1:A:81:ARG:HG2	1:A:85:GLU:OE1	1.98	0.63
1:B:182:ASP:O	1:B:185:ARG:NH1	2.32	0.61
1:B:81:ARG:NH2	1:B:85:GLU:OE2	2.35	0.60
1:B:493:GLU:OE2	1:B:500:GLU:OE2	2.21	0.58
1:A:514:GLN:O	1:A:515:LYS:C	2.47	0.57
1:A:576:PHE:HB2	1:B:276:PRO:HG3	1.87	0.57
1:B:547:LEU:HD12	1:B:548:PRO:HD2	1.92	0.52
1:A:342:PHE:HB2	1:A:558:ASP:OD1	2.10	0.52
1:A:508:LEU:C	1:A:508:LEU:HD23	2.35	0.51
1:B:580:ARG:H	1:B:580:ARG:CD	2.23	0.51
1:B:580:ARG:H	1:B:580:ARG:HD3	1.76	0.51
1:B:504:ALA:HB2	1:B:553:LEU:HG	1.93	0.50
1:A:514:GLN:O	1:A:514:GLN:NE2	2.45	0.49
1:A:547:LEU:HD12	1:A:548:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LEU:C	1:B:508:LEU:HD23	2.37	0.49
1:B:536:ASP:HB3	1:B:539:PHE:H	1.79	0.48
1:B:411:THR:O	1:B:413:THR:HG23	2.14	0.47
1:B:514:GLN:O	1:B:515:LYS:C	2.57	0.47
1:A:312:LYS:NZ	1:A:507:GLU:OE1	2.36	0.47
1:A:553:LEU:C	1:A:553:LEU:HD23	2.39	0.47
1:A:504:ALA:HB2	1:A:553:LEU:HG	1.98	0.46
1:B:403:ILE:HD11	1:B:453:ALA:HB2	1.96	0.46
1:A:411:THR:O	1:A:413:THR:HG23	2.15	0.46
1:B:449:LEU:HD12	1:B:474:ILE:HD11	1.97	0.46
1:B:312:LYS:NZ	1:B:507:GLU:OE1	2.40	0.46
1:B:518:PHE:CB	1:B:535:LEU:HD22	2.47	0.45
1:B:553:LEU:HD23	1:B:553:LEU:C	2.41	0.45
1:A:369:VAL:HG12	1:A:375:THR:O	2.17	0.44
1:B:369:VAL:HG12	1:B:375:THR:O	2.18	0.44
1:B:536:ASP:HB2	1:B:539:PHE:HB3	1.99	0.44
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.51	0.43
1:B:476:SER:HB2	1:B:489:THR:HG21	2.01	0.43
1:A:432:ILE:HG23	1:A:437:ILE:HG13	2.01	0.43
1:A:507:GLU:OE2	1:A:552:GLY:HA3	2.19	0.43
1:A:104:HIS:CD2	1:B:480:LYS:HD3	2.54	0.42
1:A:468:ILE:HD12	1:A:495:PHE:CE1	2.54	0.42
1:B:478:LEU:HD23	1:B:514:GLN:OE1	2.18	0.42
1:A:432:ILE:HD13	1:A:439:LEU:HD12	2.02	0.42
1:A:145:SER:O	1:A:145:SER:OG	2.35	0.42
1:B:507:GLU:OE2	1:B:552:GLY:HA3	2.20	0.42
1:A:346:GLU:HA	1:A:553:LEU:O	2.19	0.41
1:A:476:SER:HB2	1:A:489:THR:HG21	2.03	0.41
1:A:87:ARG:NH1	1:A:188:ASP:OD1	2.39	0.41
1:A:410:VAL:HG21	1:A:456:PHE:HB3	2.03	0.41
1:A:353:ASP:OD1	1:A:353:ASP:C	2.63	0.41
1:A:461:TYR:C	1:A:462:ASN:HD22	2.28	0.41
1:A:164:LEU:C	1:A:164:LEU:HD23	2.46	0.40
1:B:353:ASP:OD1	1:B:353:ASP:C	2.64	0.40
1:A:417:GLN:HA	1:A:418:PRO:C	2.47	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	464/507 (92%)	452 (97%)	12 (3%)	0	100	100
1	B	466/507 (92%)	454 (97%)	12 (3%)	0	100	100
All	All	930/1014 (92%)	906 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	373/457 (82%)	363 (97%)	10 (3%)	39	67
1	B	365/457 (80%)	353 (97%)	12 (3%)	33	61
All	All	738/914 (81%)	716 (97%)	22 (3%)	36	64

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	87	ARG
1	A	143	SER
1	A	147	GLN
1	A	149	LEU
1	A	155	VAL
1	A	303	LEU
1	A	429	ILE

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Mol	Chain	Res	Type
1	A	431	ILE
1	A	454	SER
1	B	142	VAL
1	B	143	SER
1	B	149	LEU
1	B	155	VAL
1	B	303	LEU
1	B	354	TYR
1	B	378	ILE
1	B	474	ILE
1	B	508	LEU
1	B	535	LEU
1	B	537	SER
1	B	580	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	263	ASN
1	A	294	HIS
1	A	295	ASN
1	A	435	HIS
1	A	462	ASN
1	B	162	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	LYS	A	601	-	8,9,9	0.75	0	7,10,10	0.56	0
3	9CC	B	602	-	23,23,23	1.92	5 (21%)	33,33,33	1.89	11 (33%)
2	LYS	B	601	-	8,9,9	1.08	1 (12%)	7,10,10	0.75	0
3	9CC	A	602	-	23,23,23	1.66	3 (13%)	33,33,33	1.30	5 (15%)

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	LYS	A	601	-	-	0/9/9/9	-
3	9CC	B	602	-	-	0/4/26/26	0/3/3/3
2	LYS	B	601	-	-	2/9/9/9	-
3	9CC	A	602	-	-	0/4/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	9CC	C6-C5	-5.57	1.41	1.51
3	A	602	9CC	C6-C5	-5.34	1.41	1.51
3	B	602	9CC	O5-C12	-4.34	1.36	1.44
3	B	602	9CC	C9-C8	-3.33	1.39	1.46
3	A	602	9CC	C15-C11	3.00	1.59	1.51
2	B	601	LYS	OXT-C	-2.85	1.21	1.30
3	A	602	9CC	C9-C8	-2.69	1.40	1.46
3	B	602	9CC	O5-C11	-2.50	1.40	1.44
3	B	602	9CC	C14-C15	-2.39	1.47	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	9CC	C14-C13-C12	-4.39	108.01	111.00
3	B	602	9CC	O3-C8-C9	-3.68	114.30	119.08
3	B	602	9CC	O3-C8-O4	3.33	121.17	117.53
3	B	602	9CC	C6-C5-C9	2.90	122.68	117.87
3	A	602	9CC	O3-C8-O4	2.89	120.69	117.53
3	B	602	9CC	C15-C14-C13	-2.86	104.95	113.00
3	A	602	9CC	C11-C10-C7	-2.47	110.69	114.43
3	A	602	9CC	O5-C11-C15	2.44	112.48	109.91
3	B	602	9CC	O5-C12-C13	2.37	111.70	109.91
3	B	602	9CC	O1-C1-C9	-2.31	116.87	121.14
3	B	602	9CC	O3-C7-C6	-2.30	107.33	110.16
3	B	602	9CC	C12-O5-C11	2.29	118.70	114.00
3	B	602	9CC	C7-O3-C8	-2.29	115.41	118.78
3	A	602	9CC	C1-C2-C3	2.23	121.73	119.67
3	B	602	9CC	C11-C10-C7	-2.22	111.08	114.43
3	A	602	9CC	C1-C9-C8	2.01	121.98	119.77

There are no chirality outliers.

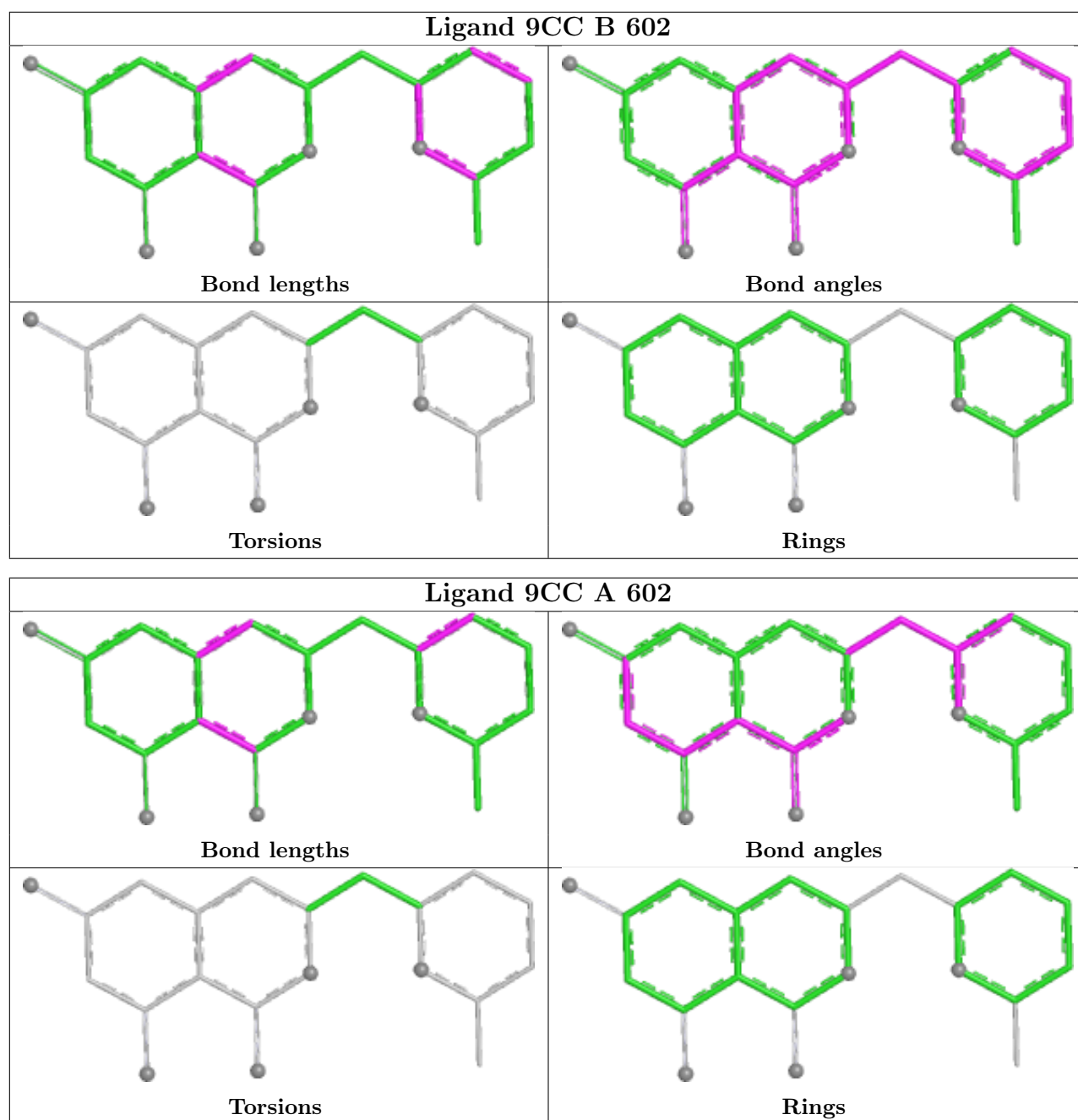
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	LYS	C-CA-CB-CG
2	B	601	LYS	N-CA-CB-CG

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 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	472/507 (93%)	0.20	16 (3%)	48	42	39, 68, 125, 146	1 (0%)
1	B	476/507 (93%)	0.15	21 (4%)	39	33	30, 66, 98, 129	2 (0%)
All	All	948/1014 (93%)	0.18	37 (3%)	43	38	30, 67, 110, 146	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	THR	4.5
1	A	279	ASN	4.4
1	B	125	GLY	3.9
1	B	231	GLU	3.8
1	B	279	ASN	3.5
1	A	515	LYS	3.4
1	A	496	ILE	3.0
1	B	171	ASN	3.0
1	B	534	GLN	2.9
1	A	463	ASP	2.8
1	A	263	ASN	2.8
1	B	122	LEU	2.7
1	A	464	LYS	2.7
1	B	199	SER	2.7
1	A	516	GLU	2.6
1	B	77	GLU	2.6
1	B	130	ASP	2.6
1	B	518	PHE	2.6
1	A	354	TYR	2.6
1	B	535	LEU	2.6
1	B	456	PHE	2.5
1	B	263	ASN	2.5
1	A	425	ILE	2.5
1	A	283	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	204	LEU	2.4
1	A	538	ALA	2.4
1	B	144	ALA	2.3
1	A	389	PRO	2.3
1	A	224	LYS	2.3
1	B	220	MET	2.2
1	B	179	GLU	2.2
1	A	412	ASN	2.2
1	B	98	GLY	2.1
1	B	354	TYR	2.1
1	B	517	CYS	2.1
1	A	474	ILE	2.0
1	B	387	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

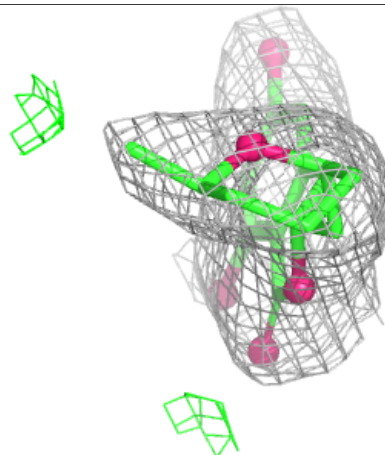
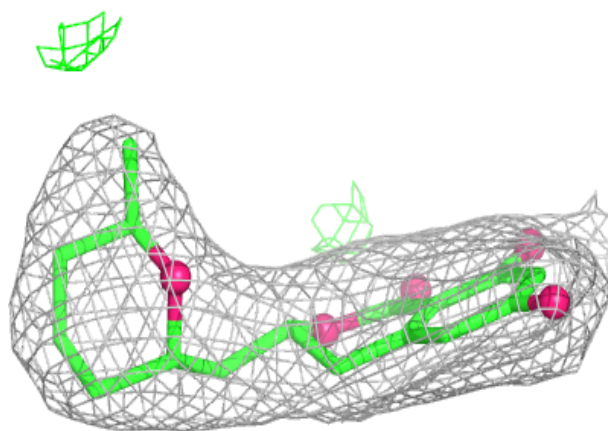
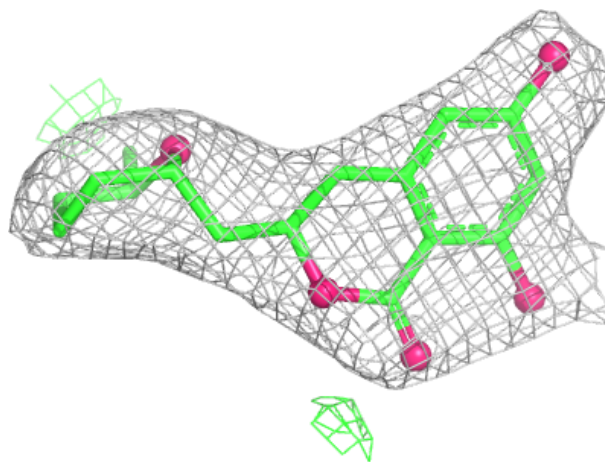
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

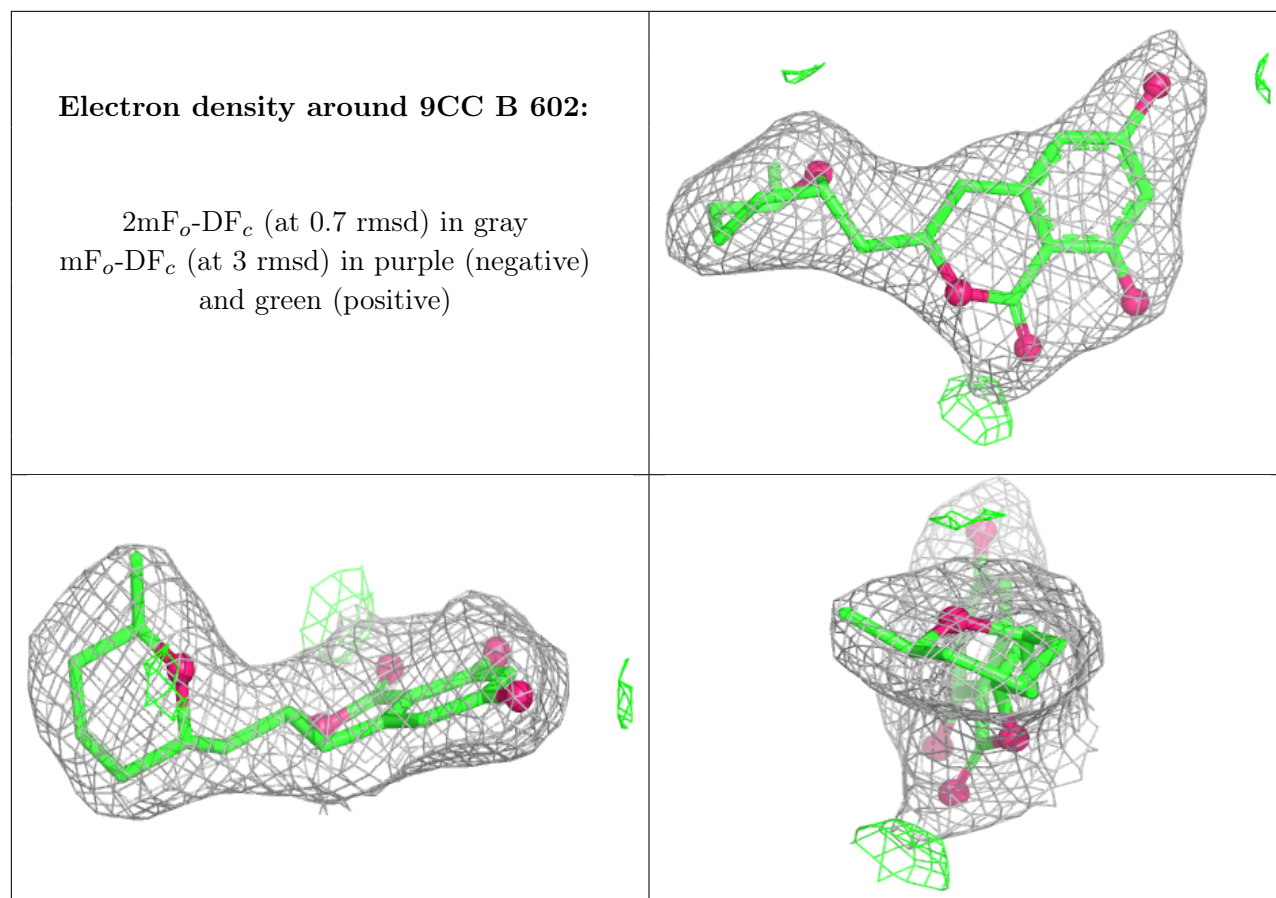
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	604	1/1	0.84	0.18	95,95,95,95	0
4	CL	B	605	1/1	0.84	0.23	88,88,88,88	0
4	CL	B	604	1/1	0.87	0.22	81,81,81,81	0
4	CL	A	603	1/1	0.89	0.19	90,90,90,90	0
2	LYS	A	601	10/10	0.92	0.15	57,58,61,61	10
2	LYS	B	601	10/10	0.92	0.22	45,47,51,51	10
3	9CC	A	602	21/21	0.94	0.08	54,63,67,69	0
3	9CC	B	602	21/21	0.95	0.07	45,51,54,59	0
4	CL	B	603	1/1	0.95	0.18	83,83,83,83	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 9CC 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.