



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 9KOY / pdb_00009koy
Title : Crystal structure of Oryza sativa HPPD complexed with iptriazopyrid
Authors : Nishio, T.; Nishijima, N.; Kubota, T.; Furuhashi, Y.; Kato, Y.
Deposited on : 2024-11-22
Resolution : 2.90 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

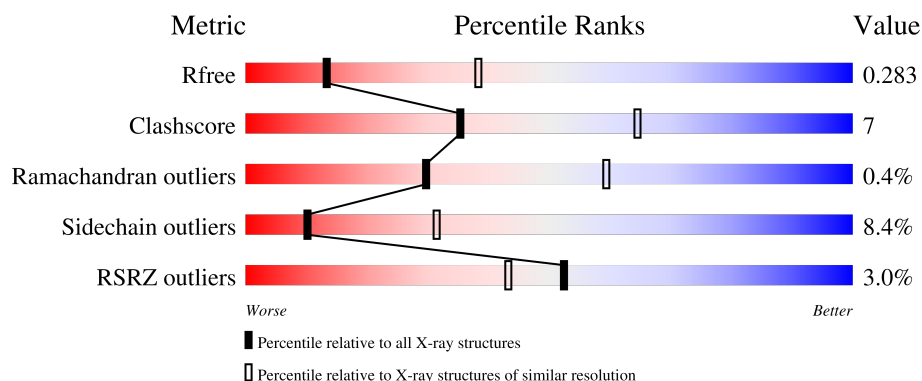
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	446	3% 70% 16% • 11%
1	B	446	2% 65% 19% • 15%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5948 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.

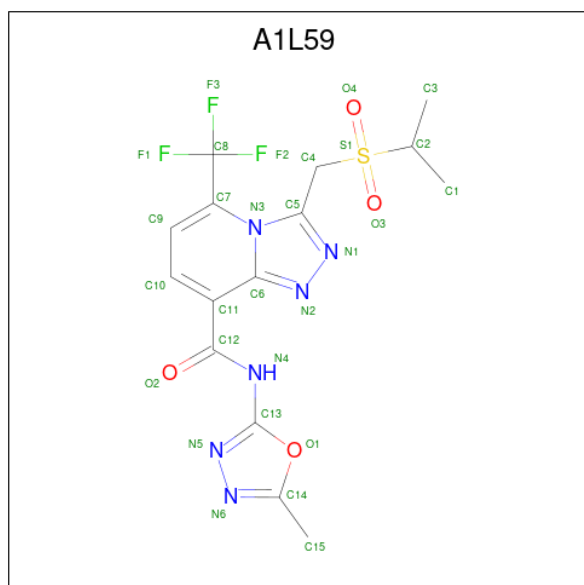
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	1	0
			2978	1879	526	564	9			
1	B	381	Total	C	N	O	S	0	1	0
			2875	1817	508	541	9			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	2	Total	Co	0	0
			2	2		

- Molecule 3 is iptriazopyrid (CCD ID: A1L59) (formula: C₁₅H₁₅F₃N₆O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 29	C 15	F 3	N 6	O 4	S 1	0	0
3	B	1	Total 29	C 15	F 3	N 6	O 4	S 1	0	0

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	I	0	0
			1	1		
4	B	1	Total	I	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	15	Total	O	0	0
			15	15		

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	158.61Å 158.61Å 84.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.65 – 2.90 46.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.65-2.90) 99.9 (46.65-2.90)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.203 , 0.285 0.211 , 0.283	Depositor DCC
R_{free} test set	1217 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: IOD, CO, A1L59

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	0.55	0/3052	1.13	7/4140 (0.2%)
1	B	0.54	0/2947	1.10	5/3996 (0.1%)
All	All	0.54	0/5999	1.11	12/8136 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	402	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	67	PHE	N-CA-CB	-6.95	99.87	110.16
1	B	250	PHE	CA-CB-CG	6.81	120.61	113.80
1	A	131	ARG	CB-CA-C	-6.24	100.82	110.81
1	A	254	ASP	CA-CB-CG	6.24	118.83	112.60
1	A	38	PRO	N-CA-C	5.53	120.43	114.68
1	B	215	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	370	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	131	ARG	N-CA-CB	5.17	117.65	109.94
1	B	367	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	78	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	ARG	Sidechain
1	A	346	ARG	Sidechain
1	B	368	ARG	Sidechain

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	2978	0	2854	37	0
1	B	2875	0	2759	49	0
2	A	2	0	0	1	0
2	B	2	0	0	0	0
3	A	29	0	0	2	0
3	B	29	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	0	2	0
5	B	15	0	0	0	0
All	All	5948	0	5613	85	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 7.

All (85) 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:313:VAL:HB	1:B:394:GLN:HB2	1.70	0.72
1:A:177:LEU:HD11	1:A:189:ARG:HD3	1.73	0.70
2:A:504:CO:CO	5:A:605:HOH:O	1.41	0.68
1:A:198:ASP:O	1:A:199:ALA:C	2.39	0.65
1:B:225:VAL:HG21	1:B:305:HIS:CE1	2.34	0.63
1:A:252:ALA:HB2	1:A:262:LEU:O	1.98	0.62
1:A:409:GLN:N	5:A:602:HOH:O	2.32	0.62
1:A:368:ARG:HH11	1:A:368:ARG:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:MET:HE1	1:A:392:MET:HE3	1.83	0.59
1:B:371:GLN:O	1:B:398:CYS:SG	2.62	0.58
1:B:317:LEU:HD22	1:B:321:ARG:HD3	1.86	0.57
1:B:79:LEU:HD22	1:B:104:TYR:CZ	2.39	0.56
1:B:149:ASP:O	1:B:150:ALA:HB3	2.04	0.56
1:B:250:PHE:CE2	1:B:418:LYS:HB3	2.41	0.56
1:A:250:PHE:HD2	1:A:255:VAL:HG11	1.70	0.56
1:B:228:VAL:HB	1:B:229:PRO:HD2	1.87	0.55
1:A:251:THR:O	1:A:255:VAL:HB	2.06	0.55
1:B:380:LYS:O	1:B:381:PRO:C	2.47	0.55
1:B:361:GLU:HG2	1:B:362:LEU:HD23	1.88	0.54
1:B:370:ASP:OD1	1:B:371:GLN:N	2.41	0.54
1:A:54:TRP:CE3	1:A:129:ALA:HA	2.42	0.54
1:A:400:GLU:O	1:A:407:GLU:HA	2.08	0.54
1:B:135:ASP:O	1:B:385:ARG:NH2	2.44	0.51
1:B:163:ARG:HD2	1:B:181:GLU:OE1	2.10	0.51
1:A:317:LEU:HD21	1:A:377:ILE:HG21	1.92	0.51
1:B:277:PRO:HB3	3:B:502:A1L59:C15	2.41	0.51
1:B:88:SER:O	1:B:89:LEU:HD23	2.12	0.49
1:B:399:MET:HA	1:B:408:TYR:O	2.12	0.49
1:A:67:PHE:HB2	1:B:67:PHE:CZ	2.47	0.49
1:A:307:ALA:HA	1:A:391:GLU:O	2.12	0.49
1:A:361:GLU:HG3	1:A:362:LEU:HG	1.95	0.49
1:A:250:PHE:CD2	1:A:255:VAL:HG11	2.48	0.48
1:B:43:PHE:CE2	1:B:242:THR:HA	2.48	0.48
1:A:154:PHE:O	1:A:157:SER:N	2.48	0.47
1:B:198:ASP:O	1:B:199:ALA:C	2.58	0.47
1:B:232:ALA:N	1:B:233:PRO:HD2	2.29	0.47
1:A:397:GLY:O	1:A:398:CYS:C	2.58	0.47
1:B:369:ASP:O	1:B:370:ASP:C	2.58	0.46
1:B:223:HIS:CE1	1:B:307:ALA:CB	2.97	0.46
1:B:376:GLN:NE2	1:B:416:PHE:O	2.49	0.46
1:B:175:PHE:CD1	1:B:203:PRO:HG3	2.51	0.46
1:B:175:PHE:CE2	1:B:193:HIS:HB3	2.51	0.46
1:B:282:VAL:O	1:B:285:THR:HB	2.16	0.46
1:B:78:ASP:HB2	1:B:104:TYR:OH	2.16	0.45
1:A:88:SER:HB3	1:A:99:LEU:HD11	1.97	0.45
1:A:346:ARG:CZ	1:A:346:ARG:CB	2.95	0.45
1:B:307:ALA:HA	1:B:391:GLU:HB3	1.99	0.45
1:B:123:SER:O	1:B:124:PHE:C	2.58	0.45
1:A:162:ALA:HB2	1:A:241:PHE:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CE2	1:A:323:ARG:HB3	2.52	0.44
1:A:64:ARG:HD2	1:B:63:GLY:HA3	1.98	0.44
1:A:175:PHE:CE2	1:A:193:HIS:HB3	2.53	0.44
1:A:326:MET:O	1:B:67:PHE:HB3	2.18	0.44
1:A:295:LEU:HD23	1:A:300:GLY:O	2.18	0.44
1:B:313:VAL:O	1:B:317:LEU:HB2	2.17	0.43
1:B:360:GLN:O	1:B:361:GLU:C	2.61	0.43
1:B:338:ASN:O	1:B:339:TYR:C	2.62	0.43
1:A:323:ARG:O	1:A:324:SER:C	2.62	0.43
1:B:401:LYS:HA	1:B:407:GLU:HA	2.00	0.43
1:A:174:GLY:O	1:A:194:PRO:HD3	2.19	0.42
3:B:502:A1L59:C4	3:B:502:A1L59:F1	2.57	0.42
1:B:365:LEU:HD22	1:B:424:LEU:HD21	2.01	0.42
1:B:88:SER:HA	1:B:100:PHE:O	2.19	0.42
1:B:363:GLY:O	1:B:377:ILE:HD13	2.19	0.42
1:A:340:TYR:CD2	1:A:360:GLN:HG3	2.54	0.42
1:B:152:ASP:OD1	1:B:155:ARG:NH2	2.53	0.42
1:B:149:ASP:O	1:B:150:ALA:CB	2.68	0.42
1:B:391:GLU:HG2	1:B:393:ILE:HG22	2.01	0.42
1:A:53:LEU:HD12	1:A:53:LEU:N	2.35	0.41
1:A:378:PHE:CZ	3:A:502:A1L59:C6	3.03	0.41
1:B:92:ARG:HD2	1:B:94:ALA:O	2.20	0.41
1:B:182:LEU:HD13	1:B:188:LEU:HB2	2.01	0.41
1:A:350:VAL:HG23	1:A:351:LEU:HD13	2.01	0.41
1:A:149:ASP:OD1	1:A:151:ALA:N	2.52	0.41
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.95	0.41
1:A:83:ASN:HA	1:A:118:THR:HB	2.02	0.41
1:A:225:VAL:HG21	1:A:305:HIS:CE1	2.56	0.41
1:A:369:ASP:OD1	1:A:372:GLY:N	2.54	0.41
1:B:38:PRO:O	1:B:39:ARG:HB2	2.20	0.41
1:A:67:PHE:CG	1:B:67:PHE:CE2	3.09	0.40
1:B:53:LEU:HD12	1:B:53:LEU:N	2.36	0.40
3:A:502:A1L59:F2	3:A:502:A1L59:C4	2.59	0.40
1:B:183:TYR:CZ	1:B:226:GLY:HA3	2.55	0.40
1:B:250:PHE:HD1	1:B:250:PHE:N	2.19	0.40
1:B:250:PHE:N	1:B:250:PHE:CD1	2.89	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	393/446 (88%)	353 (90%)	37 (9%)	3 (1%)	16	44
1	B	376/446 (84%)	343 (91%)	33 (9%)	0	100	100
All	All	769/892 (86%)	696 (90%)	70 (9%)	3 (0%)	30	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	CYS
1	A	258	ALA
1	A	381	PRO

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	298/328 (91%)	271 (91%)	27 (9%)	9	28
1	B	289/328 (88%)	266 (92%)	23 (8%)	11	34
All	All	587/656 (90%)	537 (92%)	50 (8%)	10	31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	131	ARG
1	A	215	ASP

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Mol	Chain	Res	Type
1	A	250	PHE
1	A	260	SER
1	A	262	LEU
1	A	272	GLU
1	A	283	HIS
1	A	286	LYS
1	A	288	ARG
1	A	304	GLN
1	A	319	GLU
1	A	338	ASN
1	A	343	VAL
1	A	345	ARG
1	A	361	GLU
1	A	368	ARG
1	A	381	PRO
1	A	382	VAL
1	A	390	LEU
1	A	400	GLU
1	A	401	LYS
1	A	403	GLU
1	A	409	GLN
1	A	418	LYS
1	A	422	SER
1	A	423	GLU
1	B	44	GLN
1	B	46	LEU
1	B	55[A]	CYS
1	B	55[B]	CYS
1	B	79	LEU
1	B	168	PRO
1	B	185	ASP
1	B	250	PHE
1	B	251	THR
1	B	286	LYS
1	B	287	ARG
1	B	288	ARG
1	B	290	GLN
1	B	313	VAL
1	B	317	LEU
1	B	338	ASN
1	B	343	VAL
1	B	368	ARG

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Mol	Chain	Res	Type
1	B	371	GLN
1	B	382	VAL
1	B	390	LEU
1	B	393	ILE
1	B	409	GLN

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	167	GLN
1	A	298	HIS
1	A	338	ASN
1	A	406	GLN
1	B	167	GLN
1	B	355	GLN
1	B	409	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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
3	A1L59	A	502	2	29,31,31	0.96	3 (10%)	34,48,48	2.03	8 (23%)
3	A1L59	B	502	2	29,31,31	0.94	2 (6%)	34,48,48	1.70	6 (17%)

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
3	A1L59	A	502	2	-	14/25/25/25	0/3/3/3
3	A1L59	B	502	2	-	18/25/25/25	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	A1L59	O1-C13	-2.50	1.32	1.36
3	B	502	A1L59	C2-S1	2.47	1.84	1.79
3	A	502	A1L59	C2-S1	2.24	1.83	1.79
3	A	502	A1L59	O1-C13	-2.23	1.33	1.36
3	A	502	A1L59	C11-C6	-2.09	1.40	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1L59	C10-C11-C12	7.26	123.47	117.94
3	B	502	A1L59	C10-C11-C12	5.31	121.99	117.94
3	B	502	A1L59	C4-C5-N3	4.62	130.93	124.19
3	A	502	A1L59	O3-S1-C2	4.18	112.20	108.49
3	A	502	A1L59	C4-C5-N3	3.99	130.01	124.19
3	B	502	A1L59	C4-C5-N1	-3.78	119.86	125.43
3	A	502	A1L59	O4-S1-C2	-3.06	105.78	108.49
3	B	502	A1L59	C15-C14-N6	2.85	130.63	129.21
3	A	502	A1L59	N3-C5-N1	-2.82	108.60	110.42
3	A	502	A1L59	C4-C5-N1	-2.75	121.37	125.43
3	A	502	A1L59	C15-C14-N6	2.62	130.52	129.21
3	B	502	A1L59	O4-S1-C2	2.42	110.64	108.49
3	A	502	A1L59	O1-C14-N6	-2.32	111.47	112.34
3	B	502	A1L59	O3-S1-C2	2.09	110.35	108.49

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	A1L59	C1-C2-S1-C4
3	A	502	A1L59	C1-C2-S1-O3
3	A	502	A1L59	C1-C2-S1-O4
3	A	502	A1L59	C3-C2-S1-C4
3	A	502	A1L59	C3-C2-S1-O3
3	A	502	A1L59	C3-C2-S1-O4
3	A	502	A1L59	S1-C4-C5-N1
3	A	502	A1L59	S1-C4-C5-N3
3	A	502	A1L59	C6-C11-C12-O2
3	A	502	A1L59	C10-C11-C12-N4
3	A	502	A1L59	C10-C11-C12-O2
3	B	502	A1L59	C1-C2-S1-C4
3	B	502	A1L59	C1-C2-S1-O3
3	B	502	A1L59	C1-C2-S1-O4
3	B	502	A1L59	C3-C2-S1-C4
3	B	502	A1L59	C3-C2-S1-O3
3	B	502	A1L59	C3-C2-S1-O4
3	B	502	A1L59	N3-C7-C8-F2
3	B	502	A1L59	C6-C11-C12-O2
3	B	502	A1L59	C10-C11-C12-N4
3	B	502	A1L59	C10-C11-C12-O2
3	B	502	A1L59	N5-C13-N4-C12
3	B	502	A1L59	O1-C13-N4-C12
3	B	502	A1L59	N3-C7-C8-F1
3	B	502	A1L59	N3-C7-C8-F3
3	B	502	A1L59	C9-C7-C8-F2
3	B	502	A1L59	C9-C7-C8-F3
3	A	502	A1L59	C6-C11-C12-N4
3	B	502	A1L59	C6-C11-C12-N4
3	B	502	A1L59	C9-C7-C8-F1
3	A	502	A1L59	N3-C7-C8-F1
3	A	502	A1L59	N3-C7-C8-F3

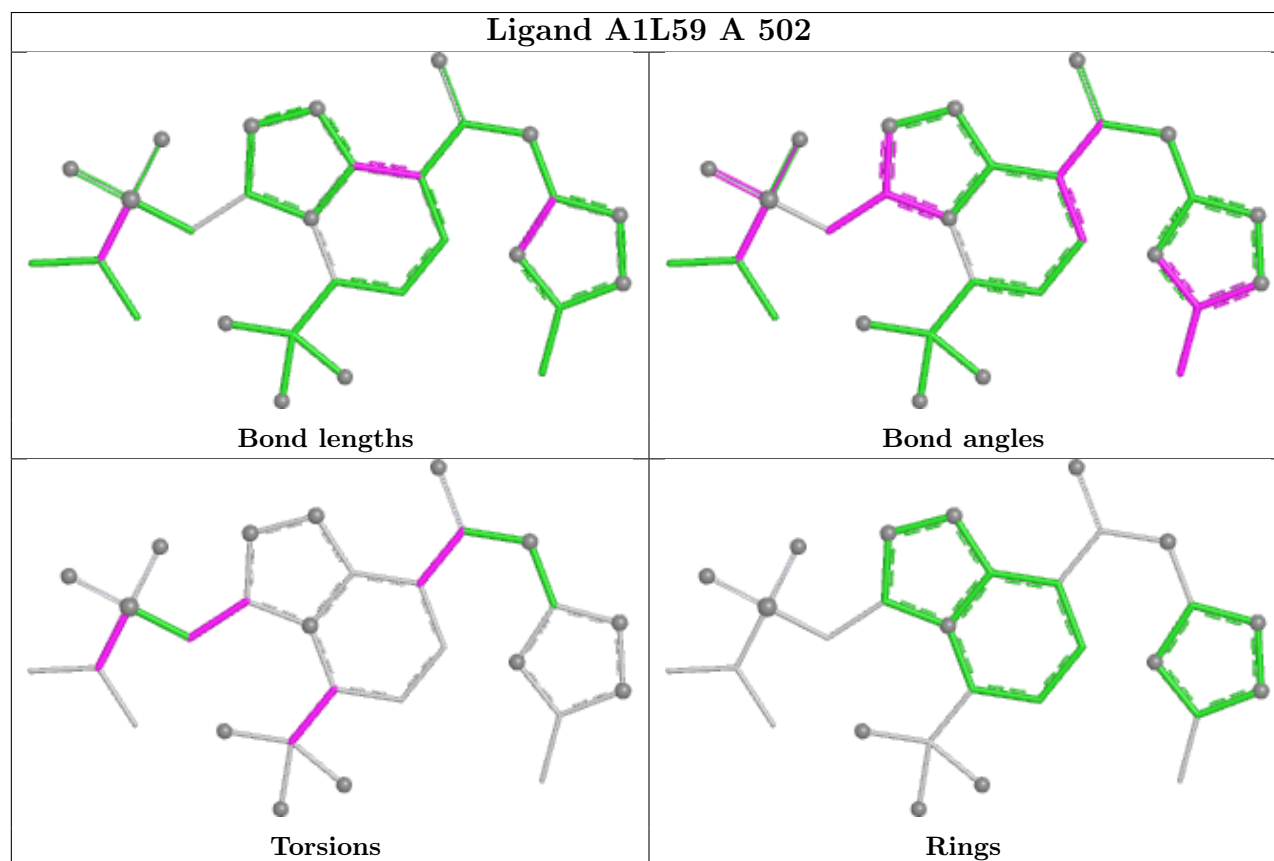
There are no ring outliers.

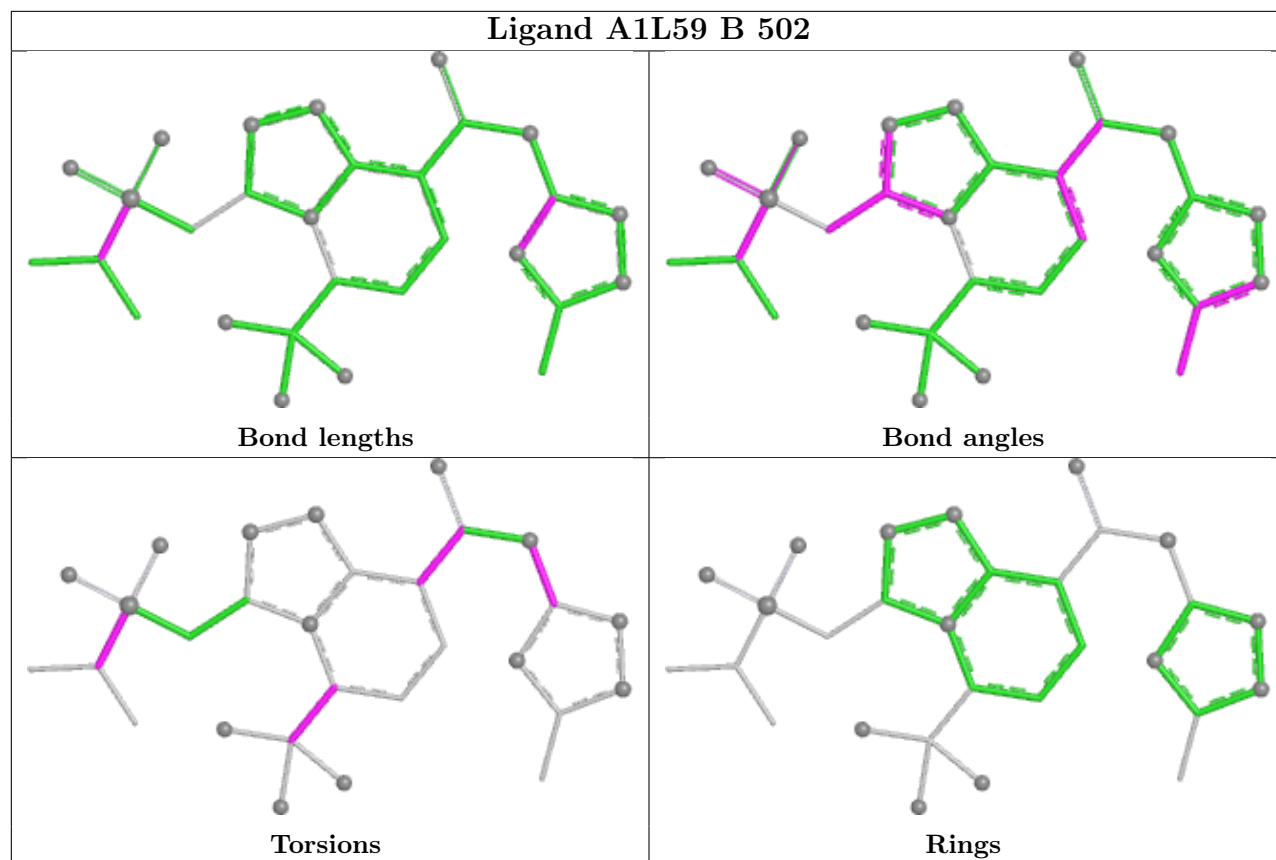
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	A1L59	2	0
3	B	502	A1L59	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	396/446 (88%)	0.14	13 (3%)	49 40	42, 74, 121, 167	1 (0%)
1	B	381/446 (85%)	0.00	10 (2%)	57 48	41, 73, 131, 176	1 (0%)
All	All	777/892 (87%)	0.07	23 (2%)	52 43	41, 73, 128, 176	2 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	ALA	4.8
1	B	405	GLY	4.2
1	B	200	PRO	3.9
1	A	251	THR	3.6
1	A	200	PRO	3.2
1	A	115	ALA	3.2
1	B	404	SER	3.0
1	A	33	PHE	2.9
1	A	257	THR	2.8
1	B	407	GLU	2.7
1	B	251	THR	2.5
1	B	402	ASP	2.5
1	B	250	PHE	2.4
1	A	408	TYR	2.4
1	A	399	MET	2.4
1	B	261	GLY	2.3
1	A	199	ALA	2.3
1	A	254	ASP	2.2
1	B	125	SER	2.2
1	A	255	VAL	2.1
1	A	36	ALA	2.1
1	A	289	SER	2.0
1	B	285	THR	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](#)

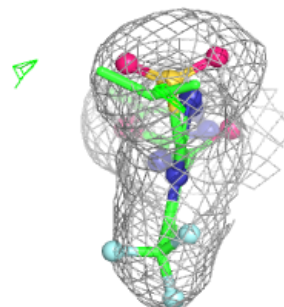
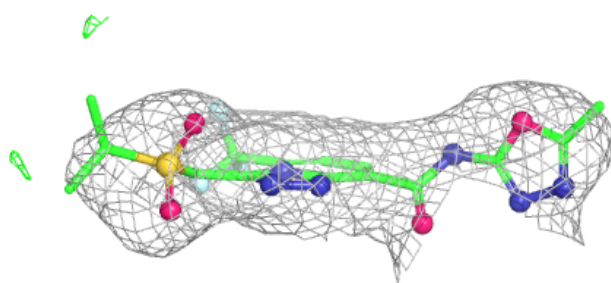
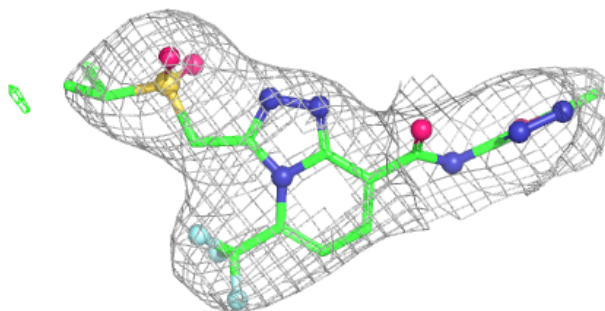
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	A1L59	B	502	29/29	0.93	0.09	57,71,99,112	0
3	A1L59	A	502	29/29	0.96	0.08	55,68,92,92	0
4	IOD	A	503	1/1	0.98	0.07	97,97,97,97	0
4	IOD	B	503	1/1	0.98	0.12	119,119,119,119	0
2	CO	B	504	1/1	0.99	0.08	52,52,52,52	0
2	CO	B	501	1/1	1.00	0.03	58,58,58,58	0
2	CO	A	501	1/1	1.00	0.03	61,61,61,61	0
2	CO	A	504	1/1	1.00	0.03	69,69,69,69	0

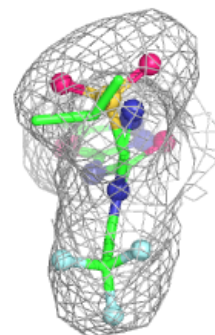
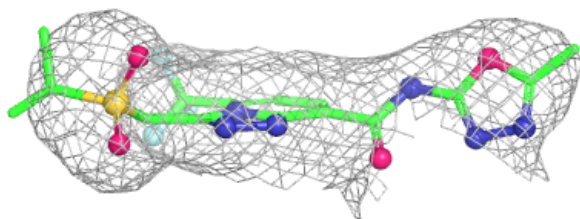
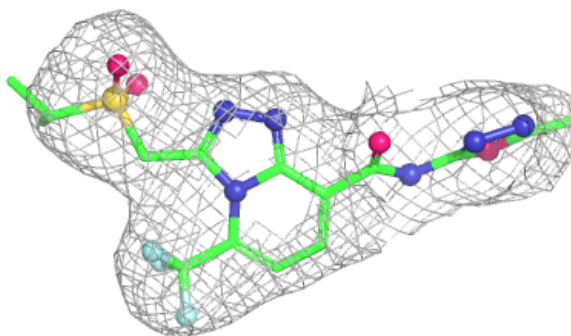
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around A1L59 B 502:

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

**Electron density around A1L59 A 502:**

$2mF_o-DF_c$ (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.