



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 10:07 PM JST

PDB ID : 9KOZ / pdb_00009koz
Title : Crystal structure of Arabidopsis thaliana HPPD complexed with iptriazopyrid
Authors : Nishio, T.; Nishijima, N.; Kubota, T.; Furuhata, Y.; Kato, Y.
Deposited on : 2024-11-22
Resolution : 2.15 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 Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

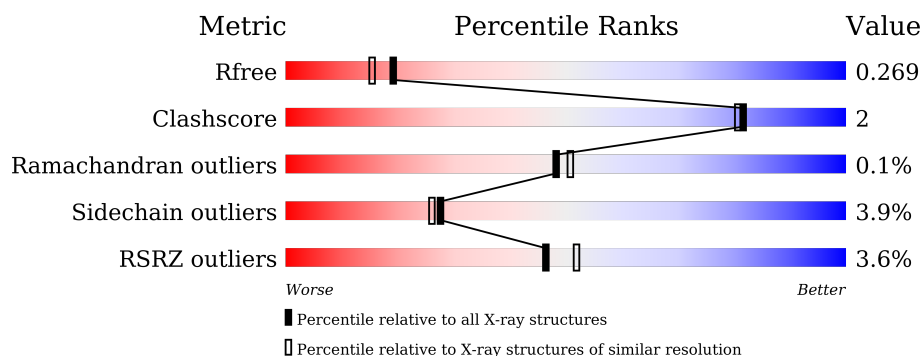
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	444	 3% 79% 10% 10%
1	B	444	 3% 80% 10% 10%
1	C	444	 2% 80% 8% 12%
1	D	444	 4% 82% 7% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12858 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.

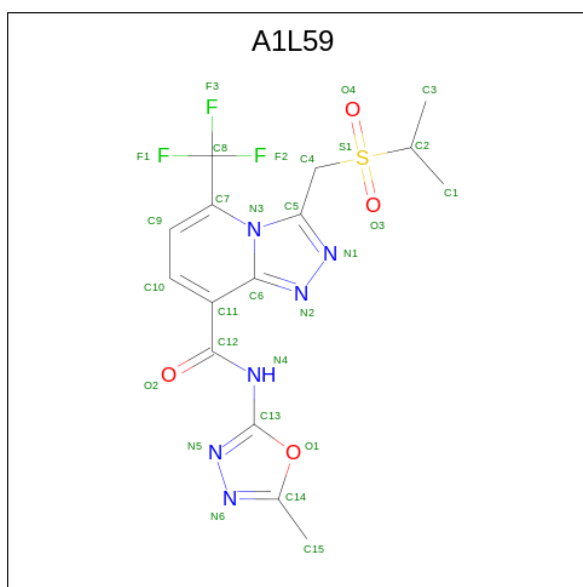
- Molecule 1 is a protein called 4-hydroxyphenylpyruvate dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3098	1969	527	589	13			
1	B	398	Total	C	N	O	S	0	0	0
			3102	1972	527	590	13			
1	C	392	Total	C	N	O	S	0	0	0
			3056	1941	521	581	13			
1	D	397	Total	C	N	O	S	0	0	0
			3094	1965	526	590	13			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		
2	C	1	Total	Co	0	0
			1	1		
2	D	1	Total	Co	0	0
			1	1		

- 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
3	C	1	Total 29	C 15	F 3	N 6	O 4	S 1	0	0
3	D	1	Total 29	C 15	F 3	N 6	O 4	S 1	0	0

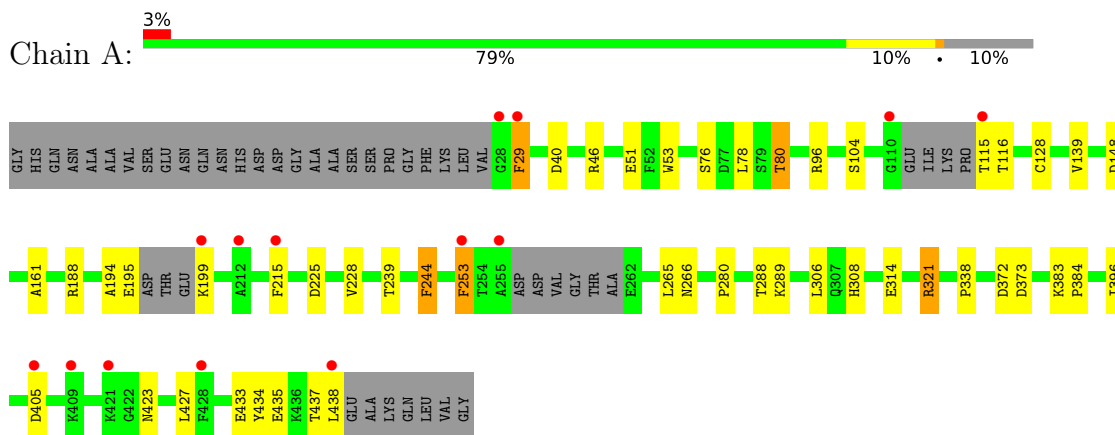
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	86	Total	O	0	0
			86	86		
4	C	96	Total	O	0	0
			96	96		
4	D	101	Total	O	0	0
			101	101		

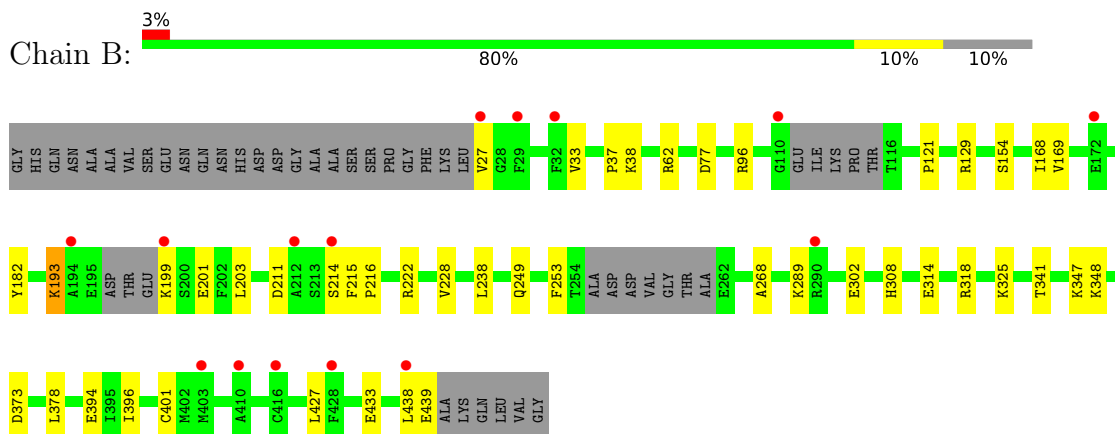
3 Residue-property plots [i](#)

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.

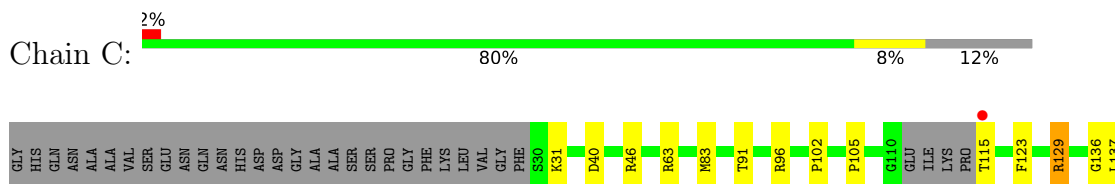
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

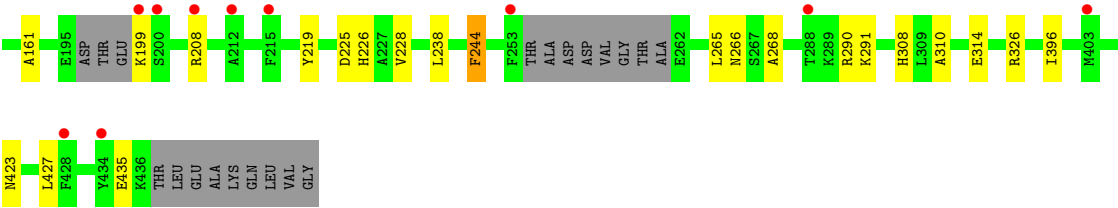


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

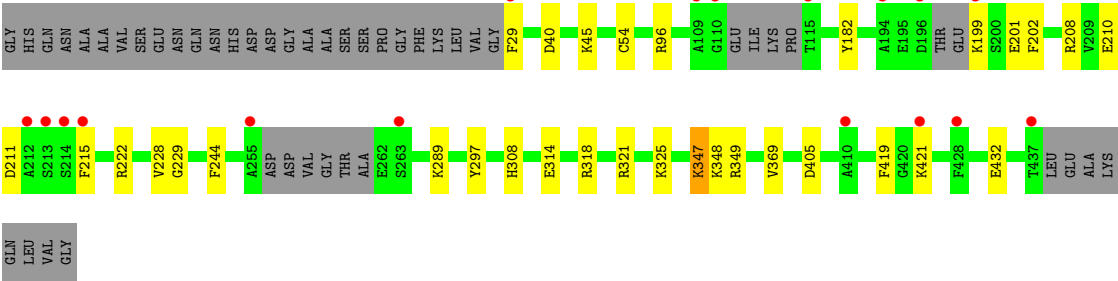
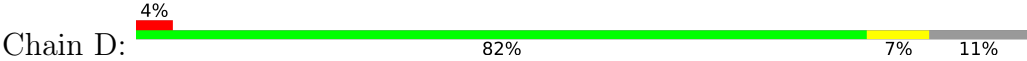


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





● Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.16Å 96.04Å 97.82Å 90.00° 92.81° 90.00°	Depositor
Resolution (Å)	48.02 – 2.15 48.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.02-2.15) 98.1 (48.02-2.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.211 , 0.266 0.218 , 0.269	Depositor DCC
R_{free} test set	4830 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.000 for -h,-l,-k 0.000 for -h,l,k 0.086 for k,h,-l 0.083 for -k,-h,-l 0.000 for l,h,k 0.000 for k,l,h 0.000 for -l,-h,k 0.000 for -k,-l,h 0.065 for h,-k,-l 0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12858	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: A1L59, CO

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	0/3167	0.96	7/4270 (0.2%)
1	B	0.54	0/3171	0.98	0/4275
1	C	0.54	0/3124	0.94	2/4211 (0.0%)
1	D	0.54	0/3163	0.98	7/4265 (0.2%)
All	All	0.54	0/12625	0.96	16/17021 (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	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	253	PHE	CA-CB-CG	5.93	119.73	113.80
1	D	244	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	29	PHE	CA-CB-CG	5.75	119.55	113.80
1	C	40	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	325	LYS	CB-CA-C	-5.64	101.09	110.68
1	C	244	PHE	CA-CB-CG	5.59	119.39	113.80
1	D	29	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	40	ASP	CA-CB-CG	5.50	118.10	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	405	ASP	CA-CB-CG	5.50	118.09	112.60
1	D	347	LYS	N-CA-CB	5.41	118.07	110.12
1	D	325	LYS	N-CA-CB	5.35	118.09	110.06
1	A	405	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	239	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	148	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	40	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ARG	Sidechain
1	A	96	ARG	Sidechain
1	B	62	ARG	Sidechain
1	B	96	ARG	Sidechain
1	D	96	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	3098	0	3028	19	0
1	B	3102	0	3031	17	0
1	C	3056	0	2986	12	0
1	D	3094	0	3018	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	29	0	0	1	0
3	B	29	0	0	0	0
3	C	29	0	0	0	0
3	D	29	0	0	1	0
4	A	105	0	0	1	0
4	B	86	0	0	3	0
4	C	96	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	101	0	0	2	0
All	All	12858	0	12063	58	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 2.

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:194:ALA:O	1:A:195:GLU:C	2.40	0.64
1:D:45:LYS:NZ	4:D:601:HOH:O	2.36	0.58
1:B:341:THR:HG21	1:B:433:GLU:HB3	1.86	0.58
1:A:76:SER:HA	1:A:80:THR:HG21	1.85	0.57
1:B:438:LEU:O	1:B:439:GLU:C	2.51	0.54
1:B:394:GLU:HG2	1:B:396:ILE:HG23	1.91	0.53
1:B:37:PRO:O	1:B:38:LYS:C	2.53	0.52
1:D:228:VAL:HG21	1:D:308:HIS:CE1	2.46	0.51
1:C:238:LEU:HD11	1:C:268:ALA:HB3	1.93	0.50
1:A:51:GLU:OE1	1:A:188:ARG:NH2	2.40	0.49
1:B:228:VAL:HG21	1:B:308:HIS:CE1	2.48	0.49
1:C:423:ASN:O	1:C:427:LEU:HB2	2.13	0.49
1:B:325:LYS:HE2	1:D:215:PHE:HB3	1.94	0.49
1:A:253:PHE:CD1	1:A:372:ASP:HA	2.48	0.48
1:A:139:VAL:HG11	1:A:306:LEU:HD13	1.95	0.48
1:A:228:VAL:HG21	1:A:308:HIS:CE1	2.48	0.48
1:A:423:ASN:O	1:A:427:LEU:HB2	2.14	0.48
1:B:222:ARG:NE	1:B:314:GLU:OE1	2.47	0.48
1:D:349:ARG:NH2	1:D:369:VAL:O	2.45	0.47
1:A:383:LYS:HB3	1:A:384:PRO:HD2	1.97	0.47
1:A:161:ALA:HB2	1:A:244:PHE:CG	2.50	0.46
1:A:433:GLU:O	1:A:437:THR:HG23	2.16	0.46
1:A:78:LEU:C	1:A:80:THR:H	2.24	0.45
1:C:225:ASP:CG	1:C:396:ILE:HD11	2.41	0.45
1:A:104:SER:OG	1:B:302:GLU:OE2	2.32	0.45
1:C:219:TYR:OH	1:C:326:ARG:NE	2.50	0.45
1:B:27:VAL:HG21	4:B:686:HOH:O	2.17	0.44
1:B:201:GLU:O	1:B:203:LEU:N	2.50	0.44
1:D:421:LYS:HD2	1:D:421:LYS:HA	1.81	0.43
1:B:238:LEU:HD11	1:B:268:ALA:HB3	1.99	0.43
1:D:348:LYS:HD3	4:D:631:HOH:O	2.19	0.43
1:C:105:PRO:HD3	1:C:129:ARG:HH12	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PRO:HB3	1:A:427:LEU:HD11	1.99	0.43
1:A:434:TYR:O	1:A:438:LEU:HG	2.18	0.43
1:D:201:GLU:O	1:D:202:PHE:HB3	2.19	0.43
4:B:623:HOH:O	1:D:321:ARG:HD3	2.18	0.43
1:C:91:THR:HG22	1:C:96:ARG:HG2	2.01	0.43
1:B:77:ASP:OD1	1:B:77:ASP:C	2.62	0.42
1:A:80:THR:CG2	4:A:617:HOH:O	2.68	0.42
1:A:427:LEU:HD12	1:A:427:LEU:HA	1.91	0.42
1:D:222:ARG:NE	1:D:314:GLU:OE1	2.53	0.42
1:D:297:TYR:CD1	1:D:297:TYR:C	2.98	0.42
1:C:63:ARG:C	1:C:63:ARG:HD3	2.45	0.42
1:B:216:PRO:HG2	4:B:623:HOH:O	2.20	0.41
1:B:121:PRO:HB2	1:B:168:ILE:HD13	2.01	0.41
1:A:53:TRP:CE3	1:A:128:CYS:HA	2.56	0.41
1:D:419:PHE:HB3	3:D:502:A1L59:C14	2.51	0.41
1:B:378:LEU:O	1:B:396:ILE:HA	2.20	0.41
1:C:228:VAL:HG21	1:C:308:HIS:CE1	2.55	0.41
1:C:226:HIS:CE1	1:C:310:ALA:CB	3.04	0.41
1:D:182:TYR:CZ	1:D:229:GLY:HA3	2.56	0.40
1:C:161:ALA:HB2	1:C:244:PHE:CG	2.56	0.40
1:A:225:ASP:CB	1:A:396:ILE:HD11	2.51	0.40
1:A:280:PRO:HB3	3:A:502:A1L59:C15	2.51	0.40
1:B:169:VAL:CG1	1:B:193:LYS:HE2	2.51	0.40
1:C:102:PRO:HB3	1:C:123:PHE:HZ	1.87	0.40
1:C:136:GLY:O	1:C:137:LEU:C	2.64	0.40
1:B:214:SER:O	1:B:215:PHE:HB2	2.21	0.40

There are no symmetry-related clashes.

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	390/444 (88%)	369 (95%)	21 (5%)	0	100	100
1	B	390/444 (88%)	374 (96%)	15 (4%)	1 (0%)	37	34
1	C	384/444 (86%)	366 (95%)	18 (5%)	0	100	100
1	D	389/444 (88%)	371 (95%)	18 (5%)	0	100	100
All	All	1553/1776 (87%)	1480 (95%)	72 (5%)	1 (0%)	48	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	LYS

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	335/370 (90%)	320 (96%)	15 (4%)	23	21
1	B	336/370 (91%)	321 (96%)	15 (4%)	23	21
1	C	331/370 (90%)	318 (96%)	13 (4%)	27	26
1	D	335/370 (90%)	326 (97%)	9 (3%)	40	42
All	All	1337/1480 (90%)	1285 (96%)	52 (4%)	27	26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	46	ARG
1	A	80	THR
1	A	115	THR
1	A	116	THR
1	A	199	LYS
1	A	215	PHE
1	A	265	LEU
1	A	266	ASN
1	A	288	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	289	LYS
1	A	314	GLU
1	A	321	ARG
1	A	373	ASP
1	A	435	GLU
1	B	33	VAL
1	B	129	ARG
1	B	154	SER
1	B	182	TYR
1	B	193	LYS
1	B	199	LYS
1	B	211	ASP
1	B	249	GLN
1	B	253	PHE
1	B	318	ARG
1	B	347	LYS
1	B	348	LYS
1	B	373	ASP
1	B	401	CYS
1	B	427	LEU
1	C	31	LYS
1	C	46	ARG
1	C	83	MET
1	C	115	THR
1	C	129	ARG
1	C	199	LYS
1	C	208	ARG
1	C	265	LEU
1	C	266	ASN
1	C	290	ARG
1	C	291	LYS
1	C	314	GLU
1	C	435	GLU
1	D	54	CYS
1	D	199	LYS
1	D	208	ARG
1	D	210	GLU
1	D	211	ASP
1	D	289	LYS
1	D	318	ARG
1	D	347	LYS
1	D	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	300	HIS
1	A	301	ASN
1	A	307	GLN
1	B	125	HIS
1	B	300	HIS
1	C	266	ASN
1	D	300	HIS
1	D	301	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](#)

Of 8 ligands modelled in this entry, 4 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	$\# Z > 2$
3	A1L59	B	502	2	24,31,31	0.82	1 (4%)	25,48,48	2.04	5 (20%)
3	A1L59	A	502	2	24,31,31	0.86	1 (4%)	25,48,48	1.89	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1L59	C	502	2	24,31,31	0.80	1 (4%)	25,48,48	1.98	5 (20%)
3	A1L59	D	502	2	24,31,31	0.88	1 (4%)	25,48,48	2.10	6 (24%)

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	B	502	2	-	0/21/25/25	0/3/3/3
3	A1L59	A	502	2	-	0/21/25/25	0/3/3/3
3	A1L59	C	502	2	-	0/21/25/25	0/3/3/3
3	A1L59	D	502	2	-	0/21/25/25	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	A1L59	C15-C14	-2.13	1.47	1.49
3	A	502	A1L59	C15-C14	-2.12	1.47	1.49
3	B	502	A1L59	C15-C14	-2.09	1.47	1.49
3	D	502	A1L59	C15-C14	-2.08	1.47	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	A1L59	C4-S1-C2	5.54	110.44	103.96
3	D	502	A1L59	C4-S1-C2	5.36	110.22	103.96
3	B	502	A1L59	C4-S1-C2	5.17	110.00	103.96
3	A	502	A1L59	C15-C14-N6	5.01	130.66	119.65
3	D	502	A1L59	C15-C14-N6	4.97	130.57	119.65
3	C	502	A1L59	C15-C14-N6	4.94	130.51	119.65
3	B	502	A1L59	C15-C14-N6	4.90	130.43	119.65
3	A	502	A1L59	C4-S1-C2	4.49	109.21	103.96
3	A	502	A1L59	O3-S1-C4	-4.31	104.68	108.63
3	B	502	A1L59	C11-C12-N4	4.15	121.00	114.79
3	D	502	A1L59	C10-C11-C12	3.58	124.42	118.52
3	D	502	A1L59	C11-C12-N4	3.50	120.02	114.79
3	D	502	A1L59	O4-S1-C4	-3.48	105.45	108.63
3	C	502	A1L59	O3-S1-C4	-3.28	105.62	108.63
3	C	502	A1L59	C10-C11-C12	3.25	123.86	118.52
3	A	502	A1L59	C10-C11-C12	2.98	123.42	118.52
3	C	502	A1L59	C11-C12-N4	2.94	119.19	114.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	A1L59	C10-C11-C12	2.87	123.25	118.52
3	B	502	A1L59	O3-S1-C4	-2.68	106.18	108.63
3	D	502	A1L59	C13-N4-C12	-2.47	120.52	126.64
3	A	502	A1L59	C11-C12-N4	2.06	117.86	114.79

There are no chirality outliers.

There are no torsion outliers.

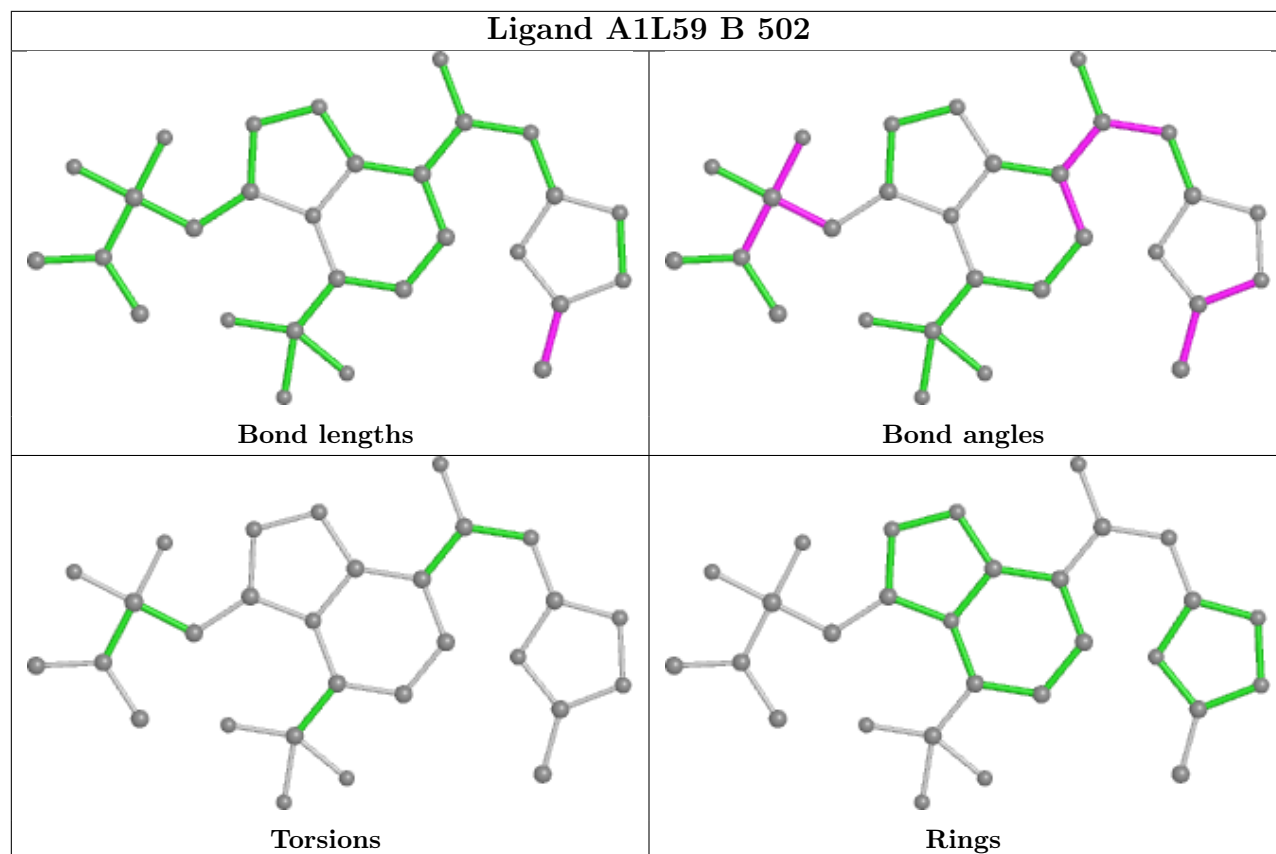
There are no ring outliers.

2 monomers are involved in 2 short contacts:

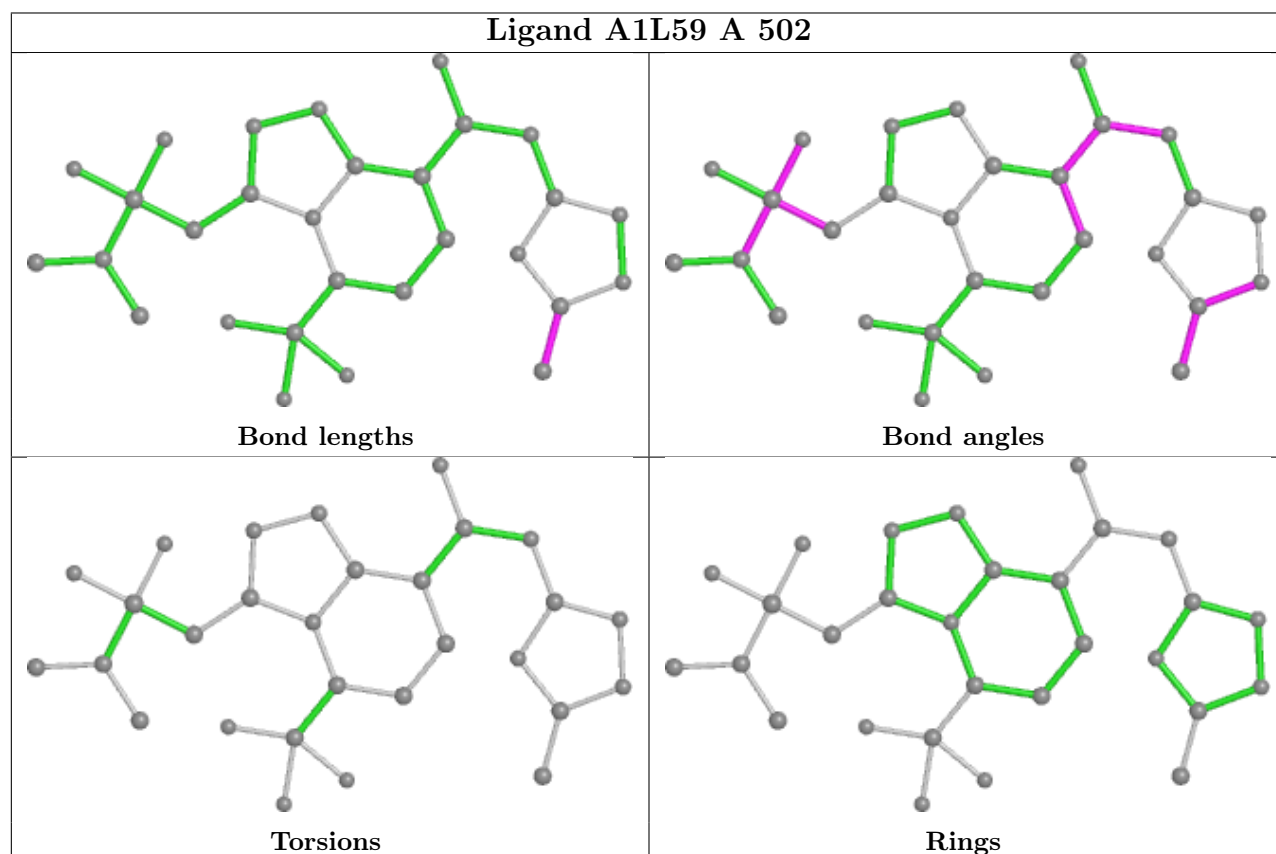
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	A1L59	1	0
3	D	502	A1L59	1	0

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

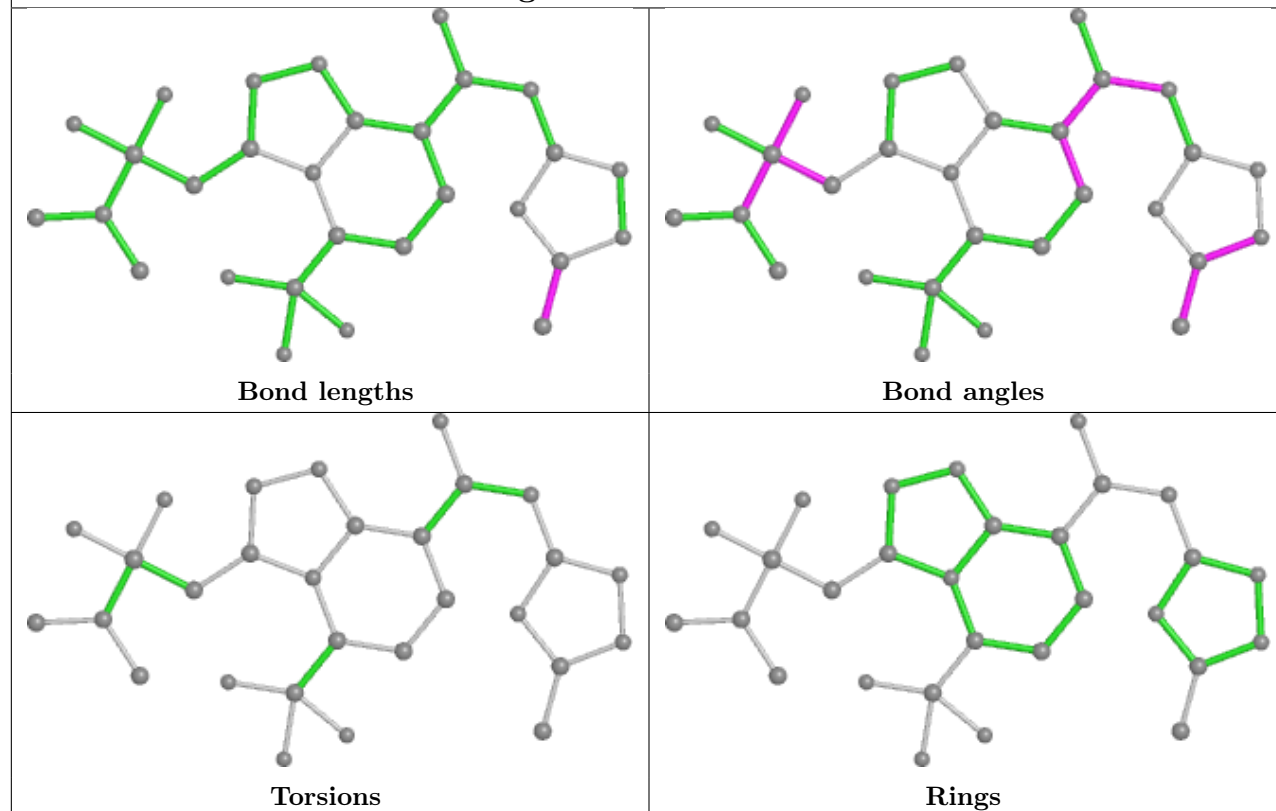
Ligand A1L59 B 502



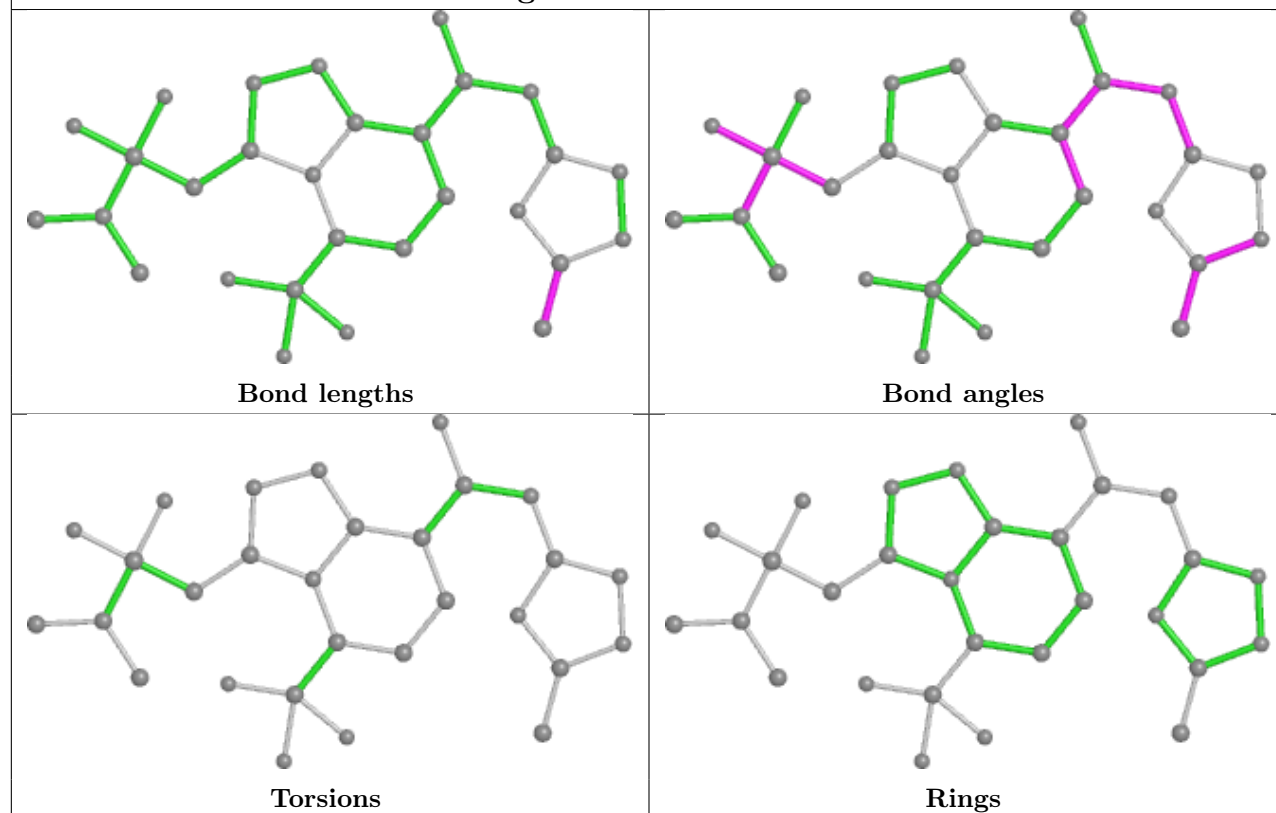
Ligand A1L59 A 502



Ligand A1L59 C 502



Ligand A1L59 D 502



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	398/444 (89%)	0.22	14 (3%) 47 53	30, 46, 90, 153	0
1	B	398/444 (89%)	0.21	15 (3%) 44 50	30, 47, 90, 116	0
1	C	392/444 (88%)	0.17	11 (2%) 55 60	30, 45, 86, 123	0
1	D	397/444 (89%)	0.29	17 (4%) 40 46	31, 48, 93, 129	0
All	All	1585/1776 (89%)	0.22	57 (3%) 46 52	30, 47, 90, 153	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	PHE	5.1
1	B	27	VAL	4.2
1	A	428	PHE	4.0
1	A	115	THR	3.8
1	A	199	LYS	3.8
1	D	115	THR	3.7
1	D	255	ALA	3.7
1	D	428	PHE	3.4
1	A	255	ALA	3.4
1	A	29	PHE	3.3
1	D	215	PHE	3.3
1	C	199	LYS	3.3
1	A	215	PHE	3.3
1	D	110	GLY	3.2
1	B	29	PHE	3.1
1	D	29	PHE	3.1
1	B	110	GLY	3.1
1	D	213	SER	3.0
1	B	194	ALA	3.0
1	B	410	ALA	3.0
1	A	110	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	199	LYS	3.0
1	B	199	LYS	2.9
1	B	438	LEU	2.9
1	C	200	SER	2.8
1	A	28	GLY	2.8
1	C	212	ALA	2.8
1	D	196	ASP	2.8
1	B	416	CYS	2.7
1	C	115	THR	2.7
1	D	194	ALA	2.7
1	C	428	PHE	2.7
1	A	212	ALA	2.6
1	A	253	PHE	2.5
1	D	212	ALA	2.4
1	B	428	PHE	2.4
1	A	438	LEU	2.4
1	B	212	ALA	2.4
1	B	32	PHE	2.4
1	B	403	MET	2.3
1	C	208	ARG	2.3
1	D	437	THR	2.3
1	D	421	LYS	2.2
1	C	253	PHE	2.2
1	D	109	ALA	2.1
1	D	410	ALA	2.1
1	A	405	ASP	2.1
1	B	214	SER	2.1
1	D	214	SER	2.1
1	A	409	LYS	2.1
1	A	421	LYS	2.1
1	B	290	ARG	2.1
1	C	288	THR	2.1
1	C	403	MET	2.1
1	D	263	SER	2.0
1	B	172	GLU	2.0
1	C	434	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

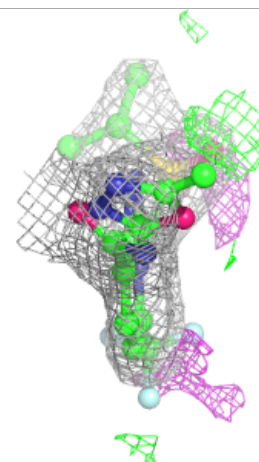
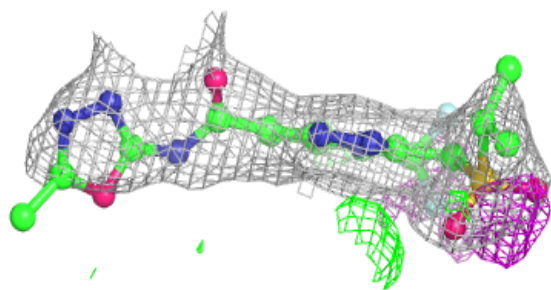
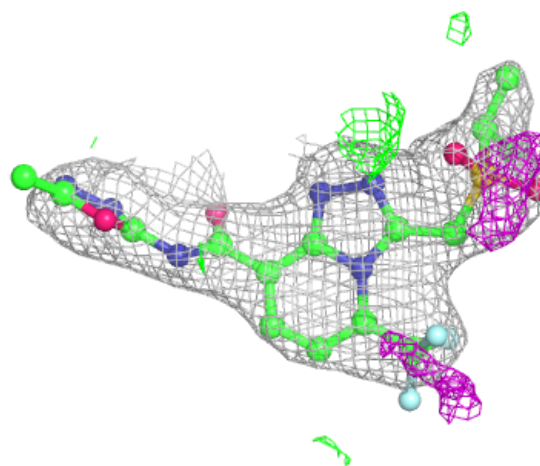
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1L59	A	502	29/29	0.82	0.16	69,85,102,102	0
3	A1L59	C	502	29/29	0.86	0.14	64,75,86,94	0
3	A1L59	D	502	29/29	0.86	0.14	61,72,88,96	0
3	A1L59	B	502	29/29	0.88	0.12	57,65,82,83	0
2	CO	C	501	1/1	0.99	0.07	53,53,53,53	0
2	CO	D	501	1/1	0.99	0.04	49,49,49,49	0
2	CO	A	501	1/1	0.99	0.04	54,54,54,54	0
2	CO	B	501	1/1	1.00	0.06	49,49,49,49	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.

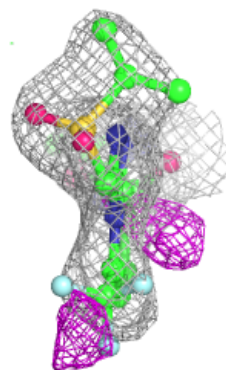
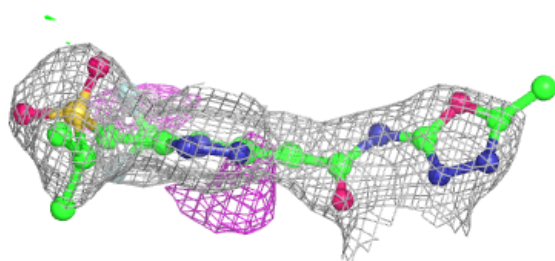
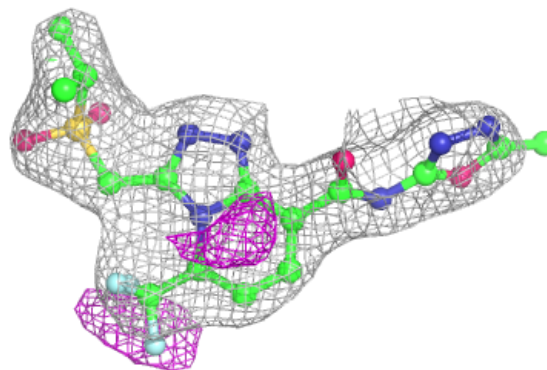
Electron density around A1L59 A 502:

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

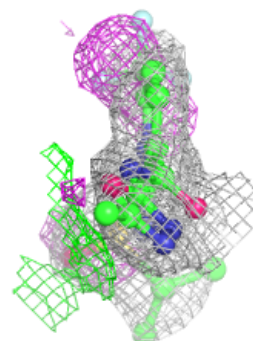
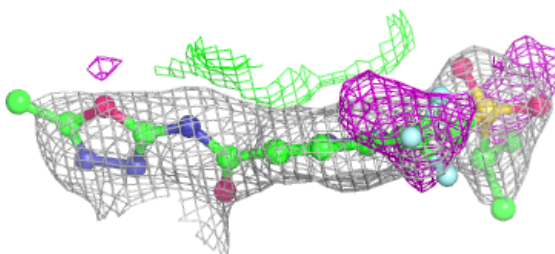
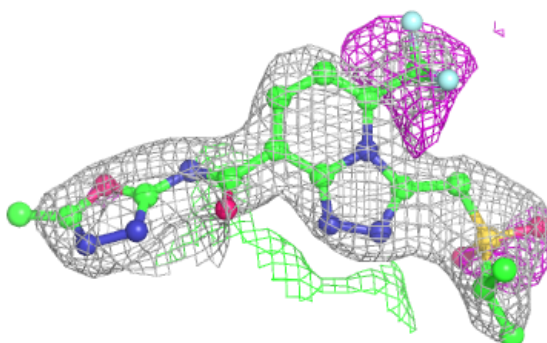


Electron density around A1L59 C 502:

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

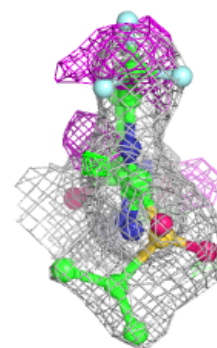
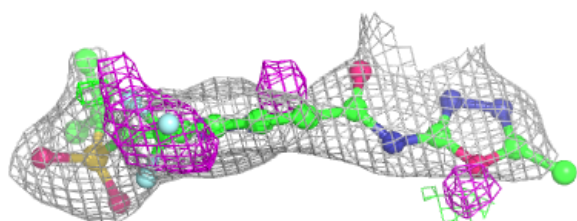
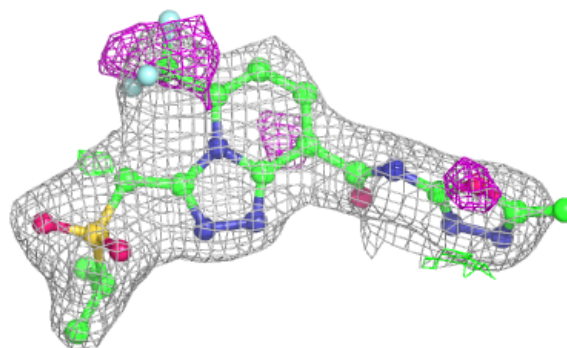
**Electron density around A1L59 D 502:**

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



Electron density around A1L59 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.