



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 12:14 PM JST

PDB ID : 7X7L
Title : Crystal structure of ZmHPPD-Y13161 complex
Authors : Lin, H.-Y.; Dong, J.; Yang, G.-F.
Deposited on : 2022-03-09
Resolution : 1.89 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

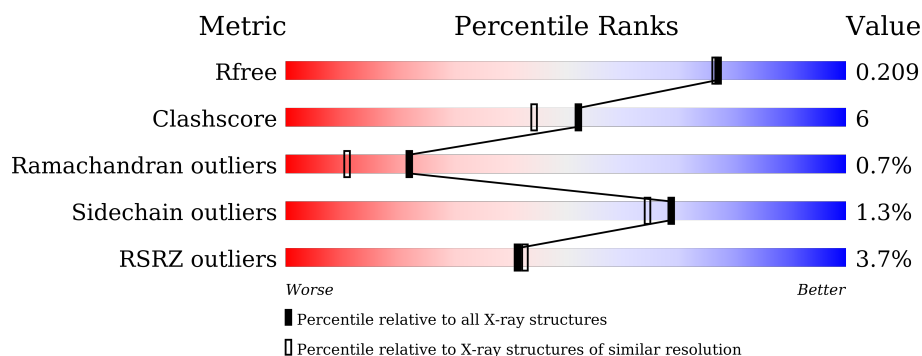
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>7%</div> <div>18%</div> </div> </div>
1	B	444	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>18%</div> </div> </div>
1	C	444	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>15%</div> </div> </div>
1	D	444	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>8%</div> <div>17%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12413 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	364	Total	C	N	O	S	0	0	0
			2695	1708	478	499	10			
1	B	363	Total	C	N	O	S	0	0	0
			2673	1692	473	498	10			
1	C	376	Total	C	N	O	S	0	0	0
			2758	1743	490	515	10			
1	D	367	Total	C	N	O	S	0	0	0
			2697	1705	478	504	10			

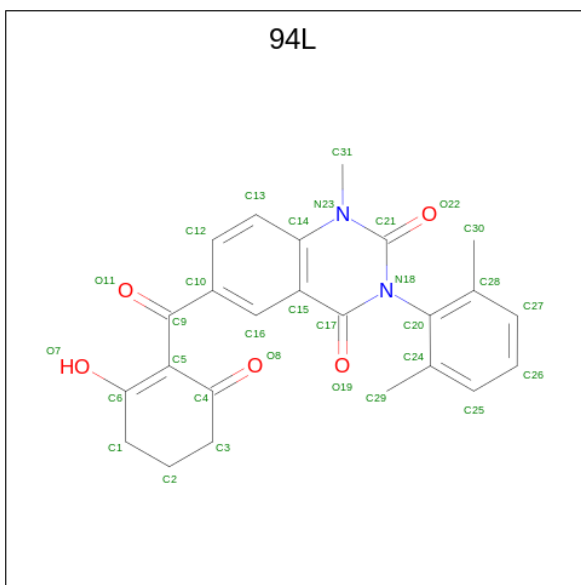
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	ARG	LYS	variant	UNP A0A1D6H1G0
B	397	ARG	LYS	variant	UNP A0A1D6H1G0
C	397	ARG	LYS	variant	UNP A0A1D6H1G0
D	397	ARG	LYS	variant	UNP A0A1D6H1G0

- Molecule 2 is COBALT (II) ION (three-letter code: 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 3-(2,6-dimethylphenyl)-1-methyl-6-(2-oxidanyl-6-oxidanylidene-cyclohexen-1-yl)carbonyl-quinazoline-2,4-dione (three-letter code: 94L) (formula: C₂₄H₂₂N₂O₅).

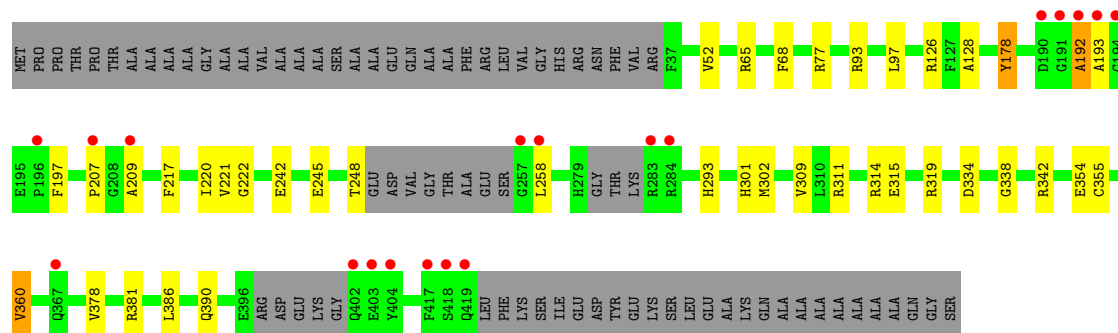
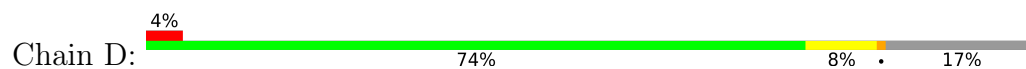


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	2	5		
3	B	1	Total	C	N	O	0	0
			31	24	2	5		
3	C	1	Total	C	N	O	0	0
			31	24	2	5		
3	D	1	Total	C	N	O	0	0
			31	24	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	360	Total	O	0	0
			360	360		
4	B	357	Total	O	0	0
			357	357		
4	C	367	Total	O	0	0
			367	367		
4	D	378	Total	O	0	0
			378	378		

- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.95Å 83.43Å 85.61Å 89.78° 97.46° 107.64°	Depositor
Resolution (Å)	45.62 – 1.89 46.53 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.62-1.89) 96.9 (46.53-1.89)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.173 , 0.207 0.174 , 0.209	Depositor DCC
R_{free} test set	5495 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -h,h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12413	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: CO, 94L

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	0.38	0/2760	0.58	1/3746 (0.0%)
1	B	0.37	0/2737	0.69	2/3717 (0.1%)
1	C	0.41	0/2825	0.65	4/3839 (0.1%)
1	D	0.37	0/2760	0.57	1/3749 (0.0%)
All	All	0.39	0/11082	0.63	8/15051 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	ARG	NE-CZ-NH2	-20.49	110.06	120.30
1	B	216	ARG	NE-CZ-NH1	12.90	126.75	120.30
1	C	171	ARG	NE-CZ-NH2	9.59	125.10	120.30
1	C	171	ARG	NE-CZ-NH1	-9.25	115.67	120.30
1	C	401	GLY	N-CA-C	6.23	128.68	113.10
1	C	126	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	97	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	97	LEU	CA-CB-CG	5.17	127.19	115.30

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	2695	0	2555	36	0
1	B	2673	0	2519	31	0
1	C	2758	0	2591	29	0
1	D	2697	0	2538	28	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	31	0	0	1	0
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
4	A	360	0	0	6	0
4	B	357	0	0	8	0
4	C	367	0	0	10	0
4	D	378	0	0	8	0
All	All	12413	0	10203	117	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 6.

All (117) 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:D:302:MET:SD	4:D:973:HOH:O	2.27	0.92
1:C:346:VAL:HG21	1:C:369:VAL:HG21	1.56	0.87
1:A:313:LEU:HD21	1:A:388:ILE:HG21	1.64	0.79
1:D:293:HIS:HD2	4:D:900:HOH:O	1.71	0.73
1:A:214:LEU:HD21	1:A:388:ILE:HD13	1.70	0.73
1:A:214:LEU:HD21	1:A:388:ILE:CD1	2.19	0.73
1:C:314:ARG:NH2	4:C:603:HOH:O	2.25	0.70
1:C:322:MET:HE1	1:D:209:ALA:HB1	1.74	0.69
1:D:126:ARG:NH1	4:D:601:HOH:O	2.26	0.68
1:A:65:ARG:HD2	1:B:64:GLY:HA3	1.76	0.67
1:A:248:THR:O	1:A:248:THR:HG22	1.94	0.67
1:B:279:HIS:ND1	4:B:604:HOH:O	2.28	0.67
1:B:217:PHE:CE2	1:B:302:MET:HE2	2.30	0.67
1:B:217:PHE:HE2	1:B:302:MET:HE2	1.60	0.66
1:D:220:ILE:HG12	1:D:302:MET:HG2	1.77	0.64
1:A:278:VAL:O	1:A:279:HIS:ND1	2.32	0.63
1:A:214:LEU:CD2	1:A:388:ILE:CD1	2.77	0.62
1:B:310:LEU:HD13	1:B:354:GLU:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:HG21	4:A:772:HOH:O	1.99	0.61
1:A:304:LEU:O	1:A:388:ILE:HD12	1.99	0.61
1:A:261:MET:HE2	1:A:263:LEU:HD21	1.81	0.61
1:C:165:ASP:HB2	1:C:171:ARG:NH1	2.16	0.61
1:C:281:THR:HG22	4:C:648:HOH:O	2.00	0.60
1:A:346:VAL:HG21	1:A:369:VAL:HG21	1.83	0.60
1:A:77:ARG:HD2	4:A:608:HOH:O	2.02	0.60
1:B:52:VAL:HG21	1:B:302:MET:HE3	1.84	0.59
1:A:104:PRO:HB3	1:A:119:PHE:HZ	1.66	0.59
1:A:57:ALA:HB2	1:B:57:ALA:HB3	1.86	0.58
1:C:340:ARG:NH2	4:C:612:HOH:O	2.37	0.56
1:B:340:ARG:NH2	4:B:609:HOH:O	2.37	0.56
1:C:281:THR:HG23	1:C:283:ARG:H	1.68	0.56
1:A:214:LEU:CD2	1:A:388:ILE:HD11	2.35	0.56
1:B:342:ARG:NH1	4:B:608:HOH:O	2.36	0.56
1:A:171:ARG:NH2	4:A:607:HOH:O	2.39	0.55
1:B:40:ARG:HD2	4:B:828:HOH:O	2.05	0.55
1:B:216:ARG:NH1	1:B:217:PHE:O	2.40	0.55
1:C:197:PHE:N	4:C:614:HOH:O	2.39	0.55
1:A:171:ARG:CZ	4:A:607:HOH:O	2.55	0.55
1:B:192:ALA:O	1:B:194:GLY:N	2.40	0.55
1:C:197:PHE:C	4:C:614:HOH:O	2.46	0.54
1:B:362:VAL:HG22	1:B:371:LEU:HD22	1.90	0.53
1:B:311:ARG:NH1	4:B:614:HOH:O	2.41	0.52
1:D:248:THR:HG22	1:D:258:LEU:H	1.75	0.52
1:B:149:PHE:O	1:B:153:VAL:HG13	2.09	0.52
1:D:192:ALA:HB3	4:D:916:HOH:O	2.10	0.52
1:C:217:PHE:HE2	1:C:302:MET:HE2	1.76	0.51
1:D:221:VAL:HG21	1:D:301:HIS:CE1	2.45	0.51
1:A:261:MET:HE3	1:A:263:LEU:HD11	1.93	0.51
1:A:322:MET:O	1:B:68:PHE:HB3	2.12	0.50
1:D:334:ASP:OD2	1:D:334:ASP:N	2.45	0.49
1:D:355:CYS:HA	1:D:360:VAL:HG13	1.93	0.49
1:B:316:MET:HE2	1:B:327:PHE:HZ	1.77	0.49
1:B:309:VAL:HB	1:B:390:GLN:HB2	1.94	0.49
1:C:242:GLU:OE2	4:C:601:HOH:O	2.20	0.49
1:A:373:ILE:HG22	1:A:388:ILE:HG23	1.94	0.49
1:C:87:HIS:HB3	1:C:119:PHE:CE2	2.48	0.49
1:C:192:ALA:HB2	4:C:740:HOH:O	2.12	0.48
1:A:261:MET:CE	1:A:263:LEU:HD11	2.44	0.48
1:B:354:GLU:HG2	4:B:612:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:VAL:HG21	1:C:302:MET:HE3	1.95	0.48
1:B:104:PRO:HB3	1:B:119:PHE:HZ	1.79	0.48
1:B:378:VAL:HG11	1:B:386:LEU:HD13	1.96	0.48
1:C:314:ARG:NH2	1:C:354:GLU:OE1	2.47	0.48
1:B:221:VAL:HG21	1:B:301:HIS:CE1	2.49	0.47
1:A:313:LEU:HD21	1:A:388:ILE:CG2	2.42	0.47
1:D:128:ALA:HA	4:D:669:HOH:O	2.14	0.47
1:C:217:PHE:CE2	1:C:302:MET:HE2	2.50	0.47
1:B:224:VAL:HG12	1:B:297:PRO:HB3	1.97	0.47
1:A:209:ALA:HB1	1:B:322:MET:SD	2.55	0.46
1:D:309:VAL:HB	1:D:390:GLN:HB2	1.97	0.46
1:B:338:GLY:O	1:B:342:ARG:HG3	2.15	0.46
1:D:378:VAL:HG11	1:D:386:LEU:HD13	1.98	0.46
1:C:106:ALA:HA	1:C:125:ARG:HH12	1.81	0.45
1:C:106:ALA:N	4:C:606:HOH:O	2.30	0.45
1:B:354:GLU:CG	4:B:612:HOH:O	2.65	0.45
1:D:342:ARG:HD2	4:D:606:HOH:O	2.17	0.45
1:C:171:ARG:CZ	4:C:633:HOH:O	2.66	0.44
1:A:416:ASN:HB3	1:A:419:GLN:NE2	2.33	0.44
1:D:342:ARG:NH1	4:D:606:HOH:O	2.33	0.44
1:D:93:ARG:HG3	4:D:614:HOH:O	2.18	0.44
1:A:104:PRO:HB3	1:A:119:PHE:CZ	2.49	0.44
1:A:214:LEU:HD21	1:A:388:ILE:HD11	1.92	0.44
1:C:80:LEU:HG	1:C:105:TYR:CZ	2.51	0.44
1:D:338:GLY:O	1:D:342:ARG:HG3	2.18	0.44
1:D:65:ARG:HA	1:D:68:PHE:CE2	2.53	0.44
1:D:242:GLU:OE1	1:D:245:GLU:OE2	2.36	0.43
1:D:311:ARG:O	1:D:315:GLU:HG3	2.17	0.43
1:A:68:PHE:CZ	1:A:319:ARG:HG3	2.53	0.43
1:C:336:TYR:CZ	1:C:356:GLN:HA	2.53	0.43
1:B:97:LEU:HD11	1:B:304:LEU:HD22	1.99	0.43
1:C:217:PHE:CE2	1:C:302:MET:CE	3.02	0.43
1:D:217:PHE:CE2	1:D:302:MET:HE3	2.54	0.43
1:D:242:GLU:OE1	1:D:245:GLU:HG3	2.19	0.43
1:A:309:VAL:HB	1:A:390:GLN:HB2	2.00	0.43
1:B:216:ARG:NH2	4:B:628:HOH:O	2.51	0.43
1:B:65:ARG:HA	1:B:68:PHE:CE2	2.53	0.42
1:C:97:LEU:HD11	1:C:304:LEU:HD22	2.01	0.42
1:A:416:ASN:HB3	1:A:419:GLN:HE21	1.84	0.42
1:B:163:PRO:HA	1:B:172:LEU:O	2.19	0.42
1:D:314:ARG:HH12	1:D:354:GLU:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:SER:O	1:C:206:SER:OG	2.38	0.42
1:C:220:ILE:HG12	1:C:302:MET:HG2	2.02	0.41
1:D:178:TYR:CZ	1:D:222:GLY:HA3	2.55	0.41
1:A:373:ILE:HG22	1:A:388:ILE:CG2	2.49	0.41
1:A:214:LEU:CD2	1:A:388:ILE:HD13	2.41	0.41
1:A:217:PHE:CE2	1:A:302:MET:CE	3.03	0.41
1:C:106:ALA:HB2	1:D:381:ARG:NH1	2.35	0.41
1:A:163:PRO:HA	1:A:172:LEU:O	2.21	0.41
1:C:171:ARG:NH1	4:C:633:HOH:O	2.53	0.41
1:C:322:MET:O	1:D:68:PHE:HB3	2.21	0.41
1:D:248:THR:HG22	1:D:258:LEU:HG	2.03	0.41
1:B:219:HIS:HB3	1:B:271:LEU:HB2	2.03	0.40
1:C:165:ASP:HB2	1:C:171:ARG:HH12	1.87	0.40
1:A:77:ARG:NH2	4:A:608:HOH:O	2.40	0.40
1:A:65:ARG:NH2	4:A:631:HOH:O	2.55	0.40
1:A:419:GLN:HE22	3:A:502:94L:C31	2.34	0.40
1:D:52:VAL:HG21	1:D:302:MET:HE3	2.04	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	356/444 (80%)	343 (96%)	13 (4%)	0	100	100
1	B	355/444 (80%)	341 (96%)	11 (3%)	3 (1%)	19	9
1	C	372/444 (84%)	357 (96%)	12 (3%)	3 (1%)	19	9
1	D	359/444 (81%)	345 (96%)	10 (3%)	4 (1%)	14	5
All	All	1442/1776 (81%)	1386 (96%)	46 (3%)	10 (1%)	22	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	ALA
1	C	207	PRO
1	C	398	ASP
1	D	193	ALA
1	D	207	PRO
1	B	207	PRO
1	D	197	PHE
1	D	192	ALA
1	B	197	PHE
1	C	197	PHE

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	260/322 (81%)	256 (98%)	4 (2%)	65	59
1	B	257/322 (80%)	254 (99%)	3 (1%)	71	67
1	C	263/322 (82%)	260 (99%)	3 (1%)	73	70
1	D	258/322 (80%)	254 (98%)	4 (2%)	62	56
All	All	1038/1288 (81%)	1024 (99%)	14 (1%)	69	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	TYR
1	A	246	PHE
1	A	319	ARG
1	A	364	ARG
1	B	120	SER
1	B	178	TYR
1	B	319	ARG
1	C	120	SER
1	C	126	ARG
1	C	178	TYR
1	D	77	ARG
1	D	178	TYR

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Mol	Chain	Res	Type
1	D	319	ARG
1	D	360	VAL

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	419	GLN
1	D	293	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	94L	B	502	2	32,34,34	3.12	12 (37%)	38,51,51	3.31	19 (50%)
3	94L	D	502	2	32,34,34	3.12	12 (37%)	38,51,51	3.18	18 (47%)
3	94L	C	502	2	32,34,34	3.11	11 (34%)	38,51,51	3.76	20 (52%)
3	94L	A	502	2	32,34,34	3.05	11 (34%)	38,51,51	3.49	20 (52%)

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	94L	B	502	2	-	7/12/26/26	0/4/4/4
3	94L	D	502	2	-	7/12/26/26	0/4/4/4
3	94L	C	502	2	-	7/12/26/26	0/4/4/4
3	94L	A	502	2	-	7/12/26/26	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	94L	O8-C4	9.35	1.42	1.23
3	B	502	94L	O8-C4	8.99	1.41	1.23
3	C	502	94L	O11-C9	8.63	1.41	1.23
3	A	502	94L	O8-C4	8.58	1.40	1.23
3	B	502	94L	O11-C9	8.57	1.41	1.23
3	A	502	94L	O11-C9	8.45	1.41	1.23
3	C	502	94L	O8-C4	7.64	1.38	1.23
3	D	502	94L	O11-C9	7.61	1.39	1.23
3	C	502	94L	C15-C14	-6.37	1.36	1.41
3	C	502	94L	O19-C17	6.27	1.40	1.24
3	A	502	94L	O19-C17	6.08	1.39	1.24
3	D	502	94L	O19-C17	6.06	1.39	1.24
3	D	502	94L	C15-C14	-6.02	1.36	1.41
3	B	502	94L	O19-C17	5.90	1.39	1.24
3	B	502	94L	C15-C14	-5.85	1.36	1.41
3	A	502	94L	C15-C14	-4.84	1.37	1.41
3	C	502	94L	C5-C6	4.69	1.53	1.39
3	A	502	94L	C5-C6	4.48	1.53	1.39
3	D	502	94L	C5-C6	4.45	1.52	1.39
3	B	502	94L	C5-C6	4.35	1.52	1.39
3	C	502	94L	C5-C4	3.97	1.55	1.46
3	D	502	94L	C5-C4	3.94	1.55	1.46
3	B	502	94L	C5-C4	3.66	1.54	1.46
3	A	502	94L	C5-C4	3.34	1.53	1.46
3	C	502	94L	C3-C4	3.29	1.55	1.50
3	D	502	94L	C14-N23	-3.25	1.36	1.40
3	A	502	94L	C14-N23	-3.20	1.36	1.40
3	D	502	94L	O7-C6	3.13	1.40	1.32
3	C	502	94L	C14-N23	-3.11	1.36	1.40
3	A	502	94L	C1-C6	2.99	1.54	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	94L	O7-C6	2.83	1.40	1.32
3	D	502	94L	C1-C6	2.76	1.54	1.49
3	B	502	94L	C3-C4	2.67	1.54	1.50
3	A	502	94L	O7-C6	2.66	1.39	1.32
3	C	502	94L	O7-C6	2.65	1.39	1.32
3	B	502	94L	C14-N23	-2.64	1.37	1.40
3	A	502	94L	C3-C4	2.54	1.54	1.50
3	A	502	94L	C16-C15	2.46	1.45	1.41
3	B	502	94L	C1-C6	2.42	1.53	1.49
3	C	502	94L	C5-C9	2.35	1.55	1.48
3	C	502	94L	C1-C6	2.20	1.53	1.49
3	B	502	94L	C17-N18	-2.15	1.33	1.37
3	D	502	94L	C5-C9	2.11	1.54	1.48
3	D	502	94L	C17-N18	-2.09	1.34	1.37
3	B	502	94L	C5-C9	2.07	1.54	1.48
3	D	502	94L	C10-C9	2.07	1.53	1.49

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	94L	C4-C5-C6	-14.06	103.76	119.27
3	D	502	94L	C4-C5-C6	-8.96	109.39	119.27
3	C	502	94L	O8-C4-C3	-8.49	106.94	120.86
3	A	502	94L	O8-C4-C3	-8.05	107.67	120.86
3	B	502	94L	O7-C6-C5	-7.91	105.58	121.91
3	A	502	94L	O7-C6-C5	-7.83	105.73	121.91
3	C	502	94L	O11-C9-C10	-7.80	102.75	120.58
3	A	502	94L	O11-C9-C10	-7.39	103.70	120.58
3	B	502	94L	O8-C4-C3	-7.32	108.87	120.86
3	A	502	94L	C4-C5-C6	-7.23	111.30	119.27
3	B	502	94L	O11-C9-C10	-7.01	104.55	120.58
3	D	502	94L	O8-C4-C3	-6.69	109.90	120.86
3	D	502	94L	O11-C9-C10	-6.28	106.22	120.58
3	B	502	94L	C4-C5-C6	-6.25	112.38	119.27
3	A	502	94L	O8-C4-C5	-6.22	112.12	122.75
3	D	502	94L	O7-C6-C5	-6.02	109.47	121.91
3	B	502	94L	O8-C4-C5	-5.53	113.30	122.75
3	C	502	94L	C13-C14-N23	-5.42	117.37	121.71
3	C	502	94L	O7-C6-C5	-5.04	111.50	121.91
3	D	502	94L	O8-C4-C5	-4.99	114.23	122.75
3	A	502	94L	C13-C14-N23	-4.93	117.76	121.71
3	A	502	94L	C3-C4-C5	-4.92	107.70	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	94L	C3-C4-C5	-4.52	108.46	116.95
3	B	502	94L	C10-C9-C5	4.41	129.79	119.93
3	B	502	94L	C3-C4-C5	-4.33	108.82	116.95
3	D	502	94L	C3-C4-C5	-4.29	108.89	116.95
3	D	502	94L	C13-C14-N23	-4.22	118.32	121.71
3	A	502	94L	C12-C10-C9	-4.19	110.93	120.42
3	B	502	94L	C13-C14-N23	-4.17	118.37	121.71
3	A	502	94L	C25-C24-C20	4.10	120.99	117.12
3	B	502	94L	C24-C20-N18	3.96	121.50	118.25
3	A	502	94L	C28-C20-C24	-3.95	119.20	123.10
3	B	502	94L	C12-C10-C9	-3.92	111.54	120.42
3	C	502	94L	O8-C4-C5	-3.79	116.27	122.75
3	C	502	94L	C10-C9-C5	3.72	128.23	119.93
3	D	502	94L	C28-C20-C24	-3.66	119.48	123.10
3	D	502	94L	C24-C20-N18	3.64	121.23	118.25
3	A	502	94L	C10-C16-C15	-3.52	117.76	121.82
3	B	502	94L	C9-C5-C6	-3.48	114.93	118.34
3	B	502	94L	C27-C28-C20	3.44	120.37	117.12
3	D	502	94L	C25-C24-C20	3.40	120.33	117.12
3	C	502	94L	C12-C10-C9	-3.39	112.75	120.42
3	A	502	94L	C24-C20-N18	3.37	121.02	118.25
3	A	502	94L	C10-C9-C5	3.34	127.40	119.93
3	C	502	94L	C28-C20-C24	-3.34	119.80	123.10
3	B	502	94L	C10-C16-C15	-3.31	118.00	121.82
3	B	502	94L	C28-C20-C24	-3.23	119.91	123.10
3	D	502	94L	C10-C16-C15	-3.19	118.14	121.82
3	D	502	94L	C27-C28-C20	3.15	120.09	117.12
3	A	502	94L	C27-C28-C20	3.12	120.07	117.12
3	C	502	94L	C27-C28-C20	3.12	120.06	117.12
3	D	502	94L	O11-C9-C5	-3.11	114.02	119.96
3	D	502	94L	C10-C9-C5	2.96	126.55	119.93
3	B	502	94L	O11-C9-C5	-2.94	114.36	119.96
3	C	502	94L	C10-C16-C15	-2.92	118.46	121.82
3	D	502	94L	C12-C10-C9	-2.89	113.87	120.42
3	C	502	94L	O11-C9-C5	-2.83	114.56	119.96
3	C	502	94L	C25-C24-C20	2.70	119.67	117.12
3	C	502	94L	C15-C14-N23	2.70	121.76	119.57
3	C	502	94L	O7-C6-C1	-2.68	108.34	114.49
3	B	502	94L	C25-C24-C20	2.64	119.61	117.12
3	A	502	94L	C14-C15-C17	-2.49	116.12	119.39
3	A	502	94L	C9-C5-C6	-2.46	115.93	118.34
3	C	502	94L	C14-C15-C17	-2.45	116.16	119.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	94L	C14-C15-C17	-2.35	116.30	119.39
3	C	502	94L	C28-C20-N18	2.34	120.17	118.25
3	A	502	94L	C15-C14-N23	2.30	121.44	119.57
3	B	502	94L	C16-C10-C9	2.30	127.26	121.41
3	A	502	94L	O7-C6-C1	-2.19	109.45	114.49
3	A	502	94L	C12-C10-C16	2.18	121.82	119.23
3	D	502	94L	C31-N23-C14	2.17	120.89	118.06
3	C	502	94L	C24-C20-N18	2.17	120.03	118.25
3	D	502	94L	C15-C14-N23	2.16	121.33	119.57
3	A	502	94L	C16-C10-C9	2.12	126.81	121.41
3	B	502	94L	C15-C14-N23	2.09	121.27	119.57
3	C	502	94L	C2-C3-C4	-2.09	109.86	113.58
3	D	502	94L	C14-C15-C17	-2.03	116.72	119.39

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	94L	C4-C5-C9-C10
3	A	502	94L	C4-C5-C9-O11
3	A	502	94L	C6-C5-C9-C10
3	B	502	94L	C4-C5-C9-O11
3	B	502	94L	C6-C5-C9-C10
3	C	502	94L	C4-C5-C9-C10
3	C	502	94L	C4-C5-C9-O11
3	C	502	94L	C6-C5-C9-C10
3	D	502	94L	C4-C5-C9-C10
3	D	502	94L	C4-C5-C9-O11
3	D	502	94L	C6-C5-C9-C10
3	B	502	94L	C12-C10-C9-O11
3	C	502	94L	C12-C10-C9-O11
3	A	502	94L	C12-C10-C9-O11
3	D	502	94L	C16-C10-C9-C5
3	A	502	94L	C16-C10-C9-C5
3	B	502	94L	C16-C10-C9-C5
3	B	502	94L	C4-C5-C9-C10
3	B	502	94L	C16-C10-C9-O11
3	D	502	94L	C12-C10-C9-C5
3	C	502	94L	C16-C10-C9-O11
3	A	502	94L	C16-C10-C9-O11
3	C	502	94L	C16-C10-C9-C5
3	D	502	94L	C12-C10-C9-O11

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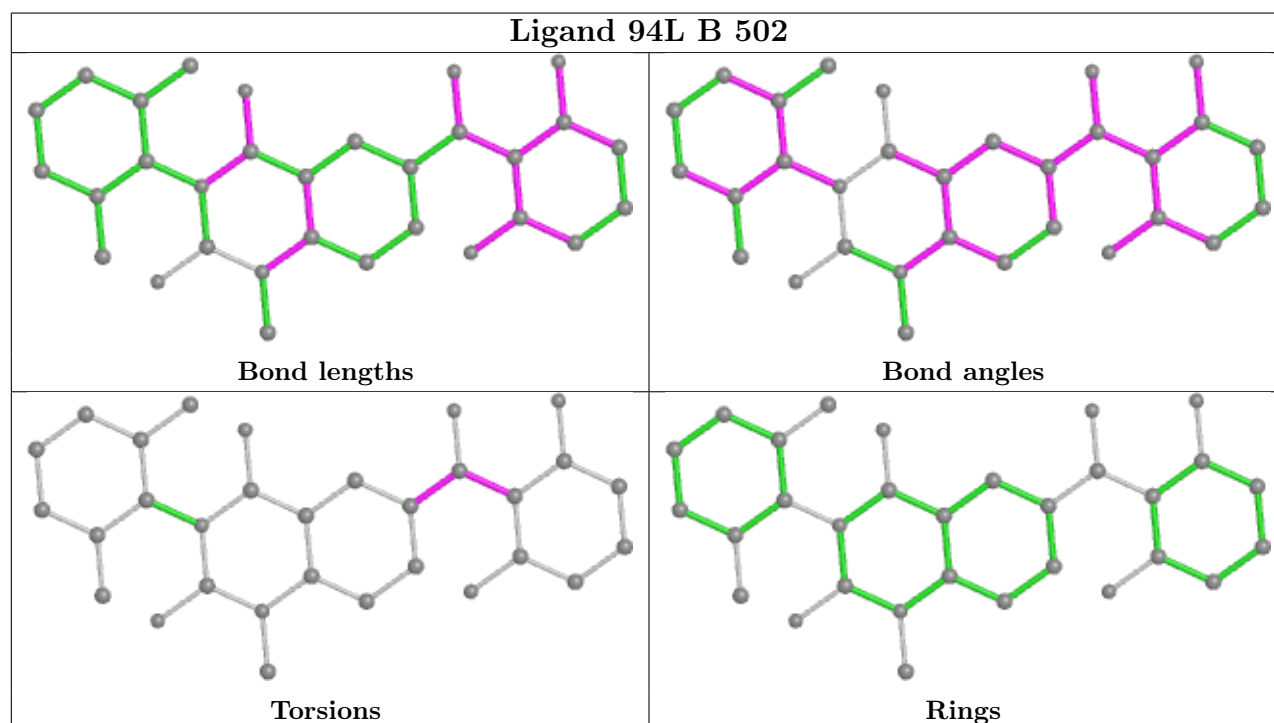
Mol	Chain	Res	Type	Atoms
3	A	502	94L	C12-C10-C9-C5
3	B	502	94L	C12-C10-C9-C5
3	D	502	94L	C16-C10-C9-O11
3	C	502	94L	C12-C10-C9-C5

There are no ring outliers.

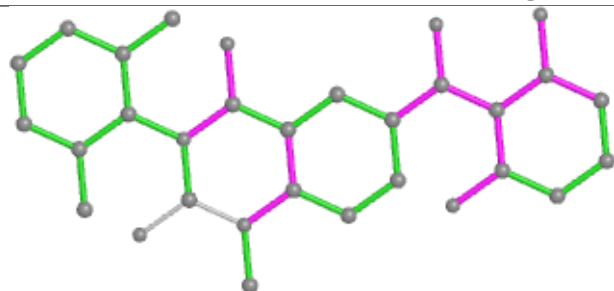
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	94L	1	0

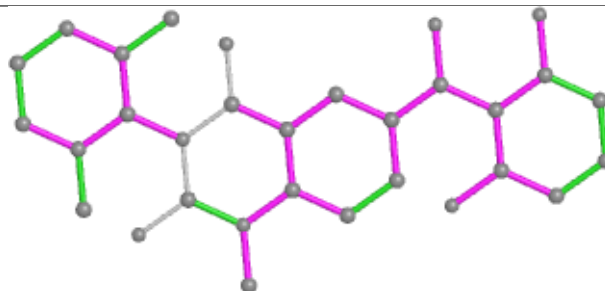
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



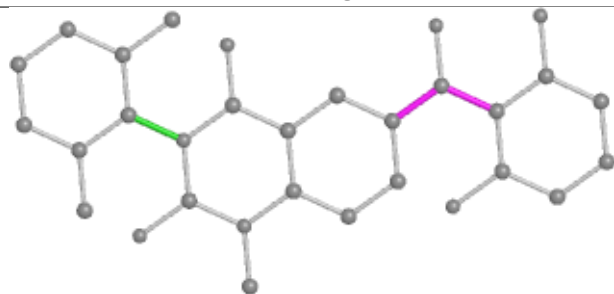
Ligand 94L D 502



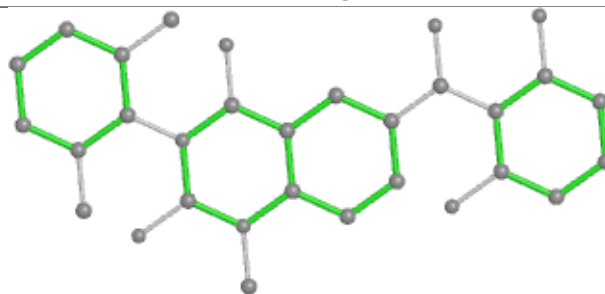
Bond lengths



Bond angles

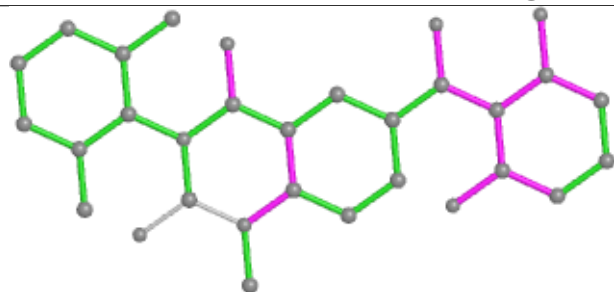


Torsions

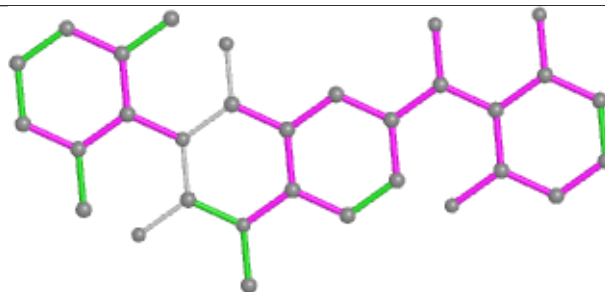


Rings

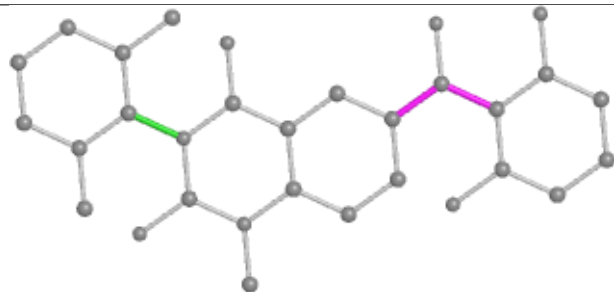
Ligand 94L C 502



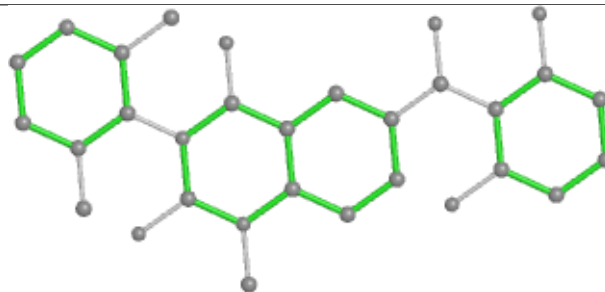
Bond lengths



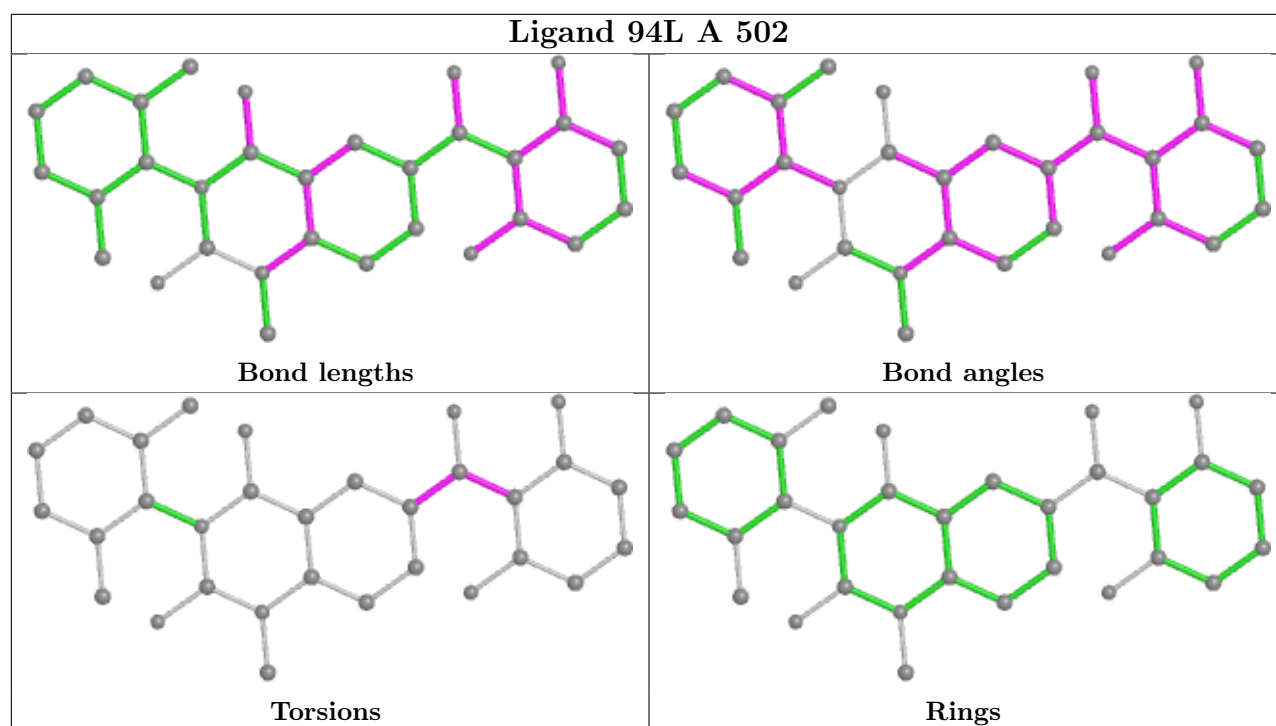
Bond angles



Torsions



Rings



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	364/444 (81%)	-0.25	9 (2%) 57 59	14, 22, 38, 58	0
1	B	363/444 (81%)	-0.17	11 (3%) 50 51	14, 23, 43, 57	0
1	C	376/444 (84%)	-0.16	15 (3%) 38 39	14, 22, 48, 57	0
1	D	367/444 (82%)	-0.14	19 (5%) 27 28	16, 24, 46, 63	0
All	All	1470/1776 (82%)	-0.18	54 (3%) 41 43	14, 23, 45, 63	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	GLY	12.1
1	C	209	ALA	11.9
1	B	417	PHE	9.3
1	D	419	GLN	8.4
1	D	193	ALA	8.4
1	B	193	ALA	7.7
1	D	417	PHE	7.0
1	A	208	GLY	6.8
1	D	192	ALA	6.6
1	B	192	ALA	6.5
1	C	193	ALA	6.0
1	C	192	ALA	5.8
1	A	209	ALA	5.6
1	B	367	GLN	4.9
1	D	418	SER	4.7
1	C	207	PRO	4.6
1	C	194	GLY	4.6
1	A	248	THR	4.5
1	A	247	THR	4.4
1	A	279	HIS	4.3
1	D	367	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	207	PRO	4.2
1	C	108	GLY	4.0
1	D	402	GLN	4.0
1	D	207	PRO	4.0
1	C	109	ALA	4.0
1	B	279	HIS	3.6
1	C	110	ASP	3.5
1	B	191	GLY	3.0
1	B	246	PHE	2.9
1	D	284	ARG	2.9
1	D	209	ALA	2.9
1	D	191	GLY	2.9
1	D	404	TYR	2.8
1	C	107	HIS	2.8
1	D	283	ARG	2.8
1	B	418	SER	2.8
1	A	367	GLN	2.8
1	B	419	GLN	2.7
1	A	207	PRO	2.7
1	D	257	GLY	2.6
1	B	415	GLY	2.6
1	D	194	GLY	2.5
1	D	190	ASP	2.4
1	C	398	ASP	2.3
1	C	417	PHE	2.3
1	D	403	GLU	2.3
1	D	196	PRO	2.3
1	A	404	TYR	2.2
1	C	256	SER	2.2
1	C	402	GLN	2.1
1	D	258	LEU	2.1
1	C	281	THR	2.1
1	A	419	GLN	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 ⓘ

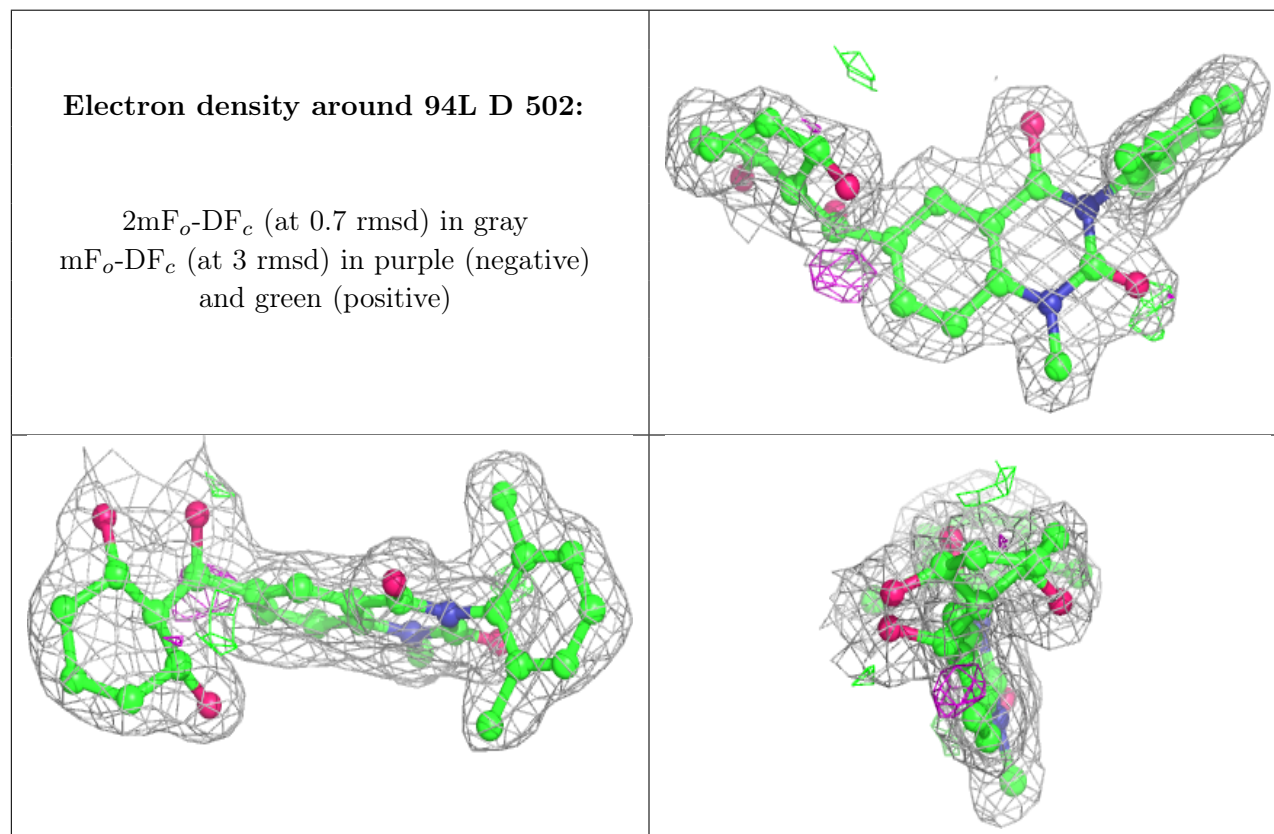
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

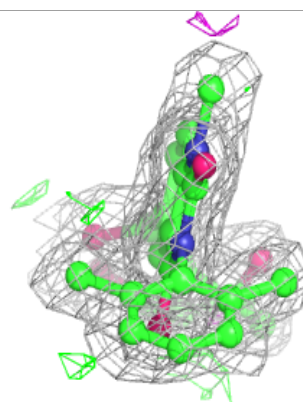
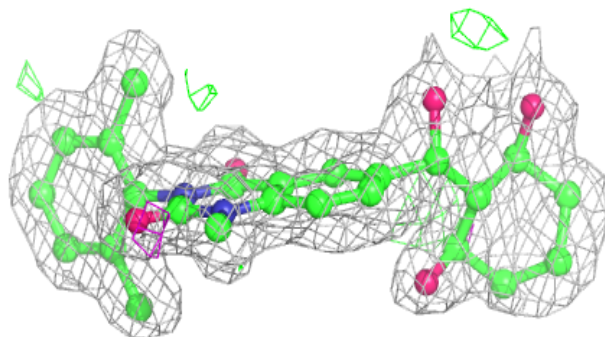
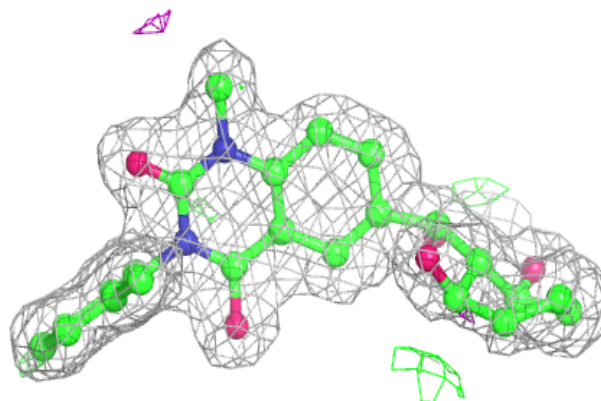
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	94L	D	502	31/31	0.91	0.10	19,24,29,31	0
3	94L	A	502	31/31	0.92	0.10	16,20,25,26	0
3	94L	C	502	31/31	0.93	0.10	17,21,26,28	0
3	94L	B	502	31/31	0.94	0.11	17,20,23,28	0
2	CO	A	501	1/1	1.00	0.06	15,15,15,15	0
2	CO	B	501	1/1	1.00	0.06	14,14,14,14	0
2	CO	C	501	1/1	1.00	0.07	18,18,18,18	0
2	CO	D	501	1/1	1.00	0.07	19,19,19,19	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.

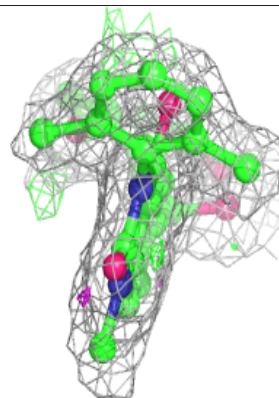
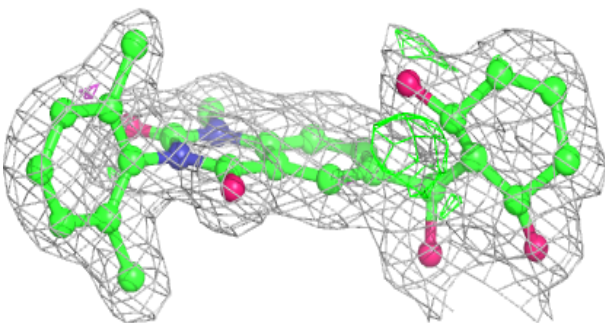
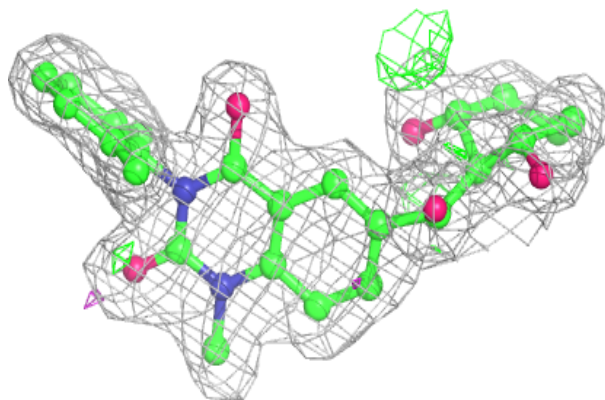


Electron density around 94L A 502:

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

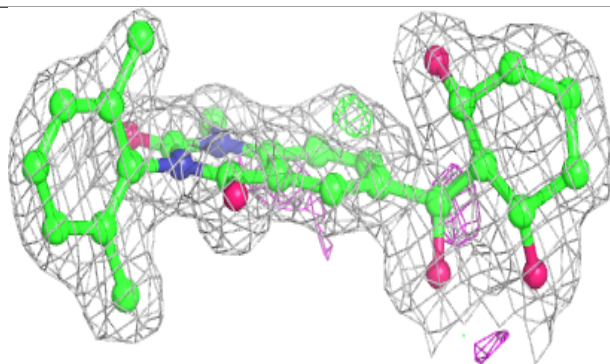
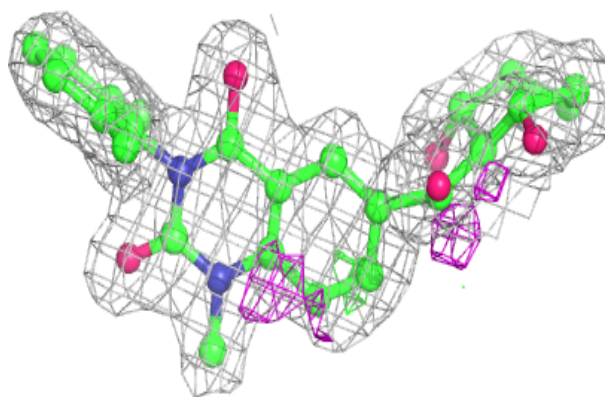
**Electron density around 94L C 502:**

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



Electron density around 94L 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 [i](#)

There are no such residues in this entry.