



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 7X7L / pdb_00007x7l
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 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

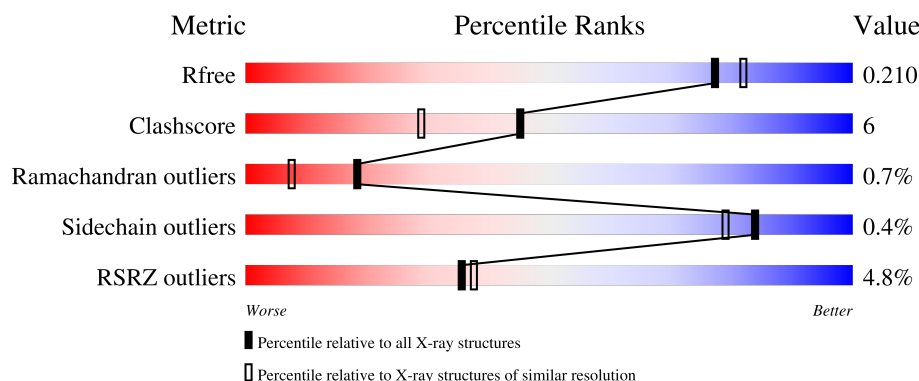
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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% 75% 7% 15%
1	B	444	 3% 72% 10% 15%
1	C	444	 5% 77% 7% 11%
1	D	444	 4% 74% 9% 13%

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			

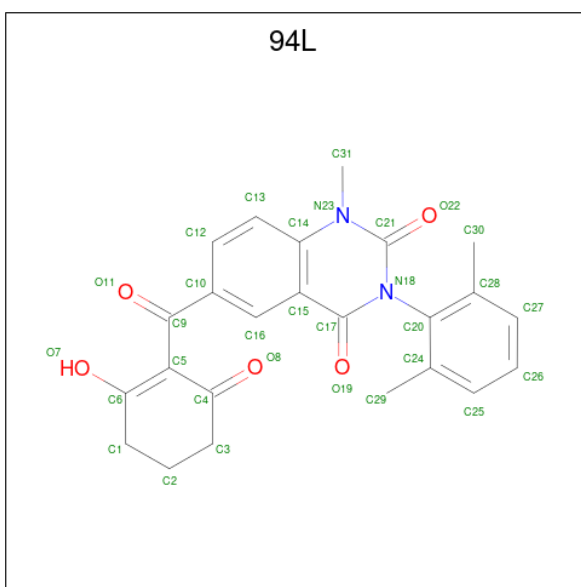
There are 4 discrepancies between the modelled and reference sequences:

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 (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		

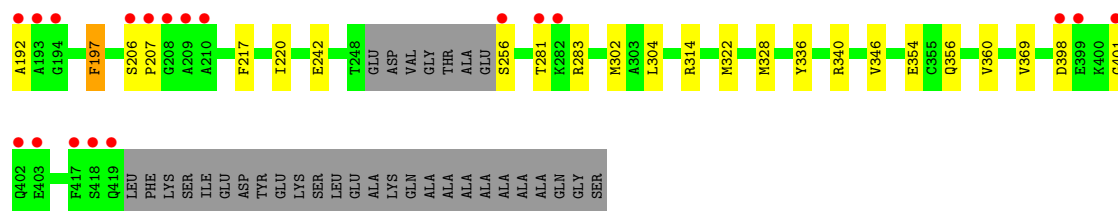
- Molecule 3 is 3-(2,6-dimethylphenyl)-1-methyl-6-(2-oxidanyl-6-oxidanylidene-cyclohexen-1-yl)carbonyl-quinazoline-2,4-dione (CCD ID: 94L) (formula: C₂₄H₂₂N₂O₅).



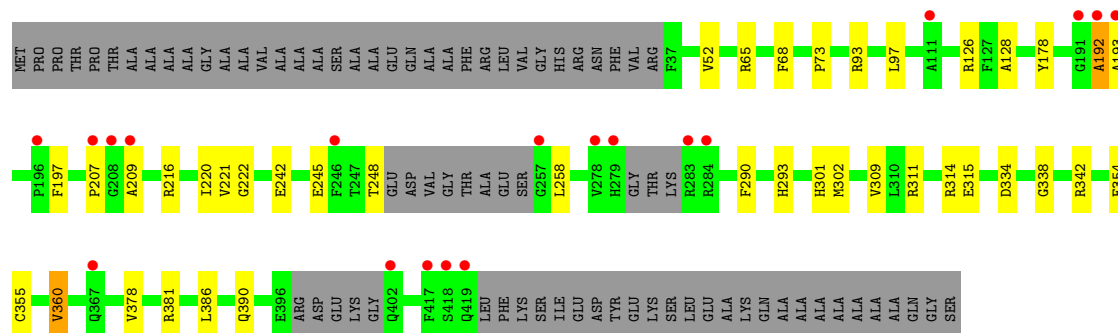
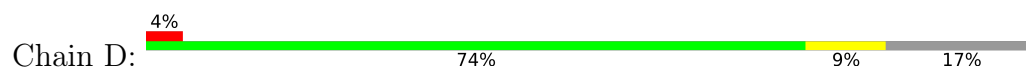
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	2	5		
3	B	1	Total	C	N	O	0	0
			31	24	2	5		
3	C	1	Total	C	N	O	0	0
			31	24	2	5		
3	D	1	Total	C	N	O	0	0
			31	24	2	5		

- 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 45.62 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.62-1.89) 96.8 (45.62-1.89)	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 0.175 , 0.210	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 , 41.9	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 94L, 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	0.32	0/2760	0.52	0/3746
1	B	0.30	0/2737	0.55	2/3717 (0.1%)
1	C	0.36	0/2825	0.61	3/3839 (0.1%)
1	D	0.30	0/2760	0.52	0/3749
All	All	0.32	0/11082	0.55	5/15051 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	401	GLY	N-CA-C	10.36	128.68	115.21
1	B	216	ARG	NE-CZ-NH2	-10.16	110.06	119.20
1	C	171	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	C	171	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	B	216	ARG	NE-CZ-NH1	5.25	126.75	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	37	0
1	B	2673	0	2519	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2758	0	2591	34	0
1	D	2697	0	2538	31	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	7	0
4	C	367	0	0	12	0
4	D	378	0	0	8	0
All	All	12413	0	10203	124	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 (124) 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:A:261:MET:HE2	1:A:263:LEU:HD21	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:217:PHE:CE2	1:B:302:MET:HE2	2.30	0.66
1:B:217:PHE:HE2	1:B:302:MET:HE2	1.61	0.65
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
1:C:52:VAL:HG21	1:C:302:MET:HE3	1.81	0.62
1:A:248:THR:HG21	4:A:772:HOH:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:O	1:A:388:ILE:HD12	1.99	0.61
1:B:52:VAL:HG21	1:B:302:MET:HE3	1.83	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:A:104:PRO:HB3	1:A:119:PHE:HZ	1.66	0.59
1:C:322:MET:HE2	1:C:322:MET:HA	1.84	0.59
1:C:197:PHE:C	4:C:614:HOH:O	2.46	0.58
1:A:57:ALA:HB2	1:B:57:ALA:HB3	1.86	0.58
1:C:217:PHE:HE2	1:C:302:MET:HE2	1.69	0.57
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:217:PHE:CE2	1:C:302:MET:HE2	2.41	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: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:A:52:VAL:HG21	1:A:302:MET:HE3	1.92	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:D:221:VAL:HG21	1:D:301:HIS:CE1	2.45	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: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
1:B:104:PRO:HB3	1:B:119:PHE:HZ	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:MET:HE1	1:D:73:PRO:HB3	1.95	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:52:VAL:HG21	1:D:302:MET:HE3	1.96	0.47
1:D:128:ALA:HA	4:D:669:HOH:O	2.14	0.47
1:B:224:VAL:HG12	1:B:297:PRO:HB3	1.97	0.47
1:B:70:LEU:HD23	1:B:316:MET:HE3	1.97	0.47
1:A:209:ALA:HB1	1:B:322:MET:SD	2.55	0.46
1:C:322:MET:HE1	1:D:73:PRO:CB	2.45	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:322:MET:HE3	1:D:209:ALA:HB1	1.98	0.45
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:C:256:SER:C	4:C:616:HOH:O	2.60	0.44
1:D:342:ARG:NH1	4:D:606:HOH:O	2.33	0.44
1:D:97:LEU:HD13	1:D:216:ARG:C	2.42	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:A:261:MET:HE2	1:A:263:LEU:CD2	2.44	0.43
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:B:290:PHE:CD1	1:B:290:PHE:C	2.96	0.43
1:C:217:PHE:CE2	1:C:302:MET:CE	3.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:MET:HE1	4:C:965:HOH:O	2.18	0.42
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
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:D:290:PHE:CD1	1:D:290:PHE:C	2.98	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

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	356/444 (80%)	343 (96%)	13 (4%)	0	100	100
1	B	355/444 (80%)	341 (96%)	11 (3%)	3 (1%)	16	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	372/444 (84%)	357 (96%)	12 (3%)	3 (1%)	16	5
1	D	359/444 (81%)	345 (96%)	10 (3%)	4 (1%)	11	3
All	All	1442/1776 (81%)	1386 (96%)	46 (3%)	10 (1%)	18	7

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%)	260 (100%)	0	100	100
1	B	257/322 (80%)	255 (99%)	2 (1%)	73	68
1	C	263/322 (82%)	262 (100%)	1 (0%)	84	79
1	D	258/322 (80%)	257 (100%)	1 (0%)	84	79
All	All	1038/1288 (81%)	1034 (100%)	4 (0%)	84	79

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	VAL
1	B	360	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	360	VAL
1	D	360	VAL

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	405	GLN
1	A	419	GLN
1	B	288	GLN
1	B	293	HIS
1	C	405	GLN
1	D	45	HIS
1	D	293	HIS

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	94L	C	502	2	34,34,34	3.21	16 (47%)	47,51,51	4.10	20 (42%)
3	94L	D	502	2	34,34,34	3.25	17 (50%)	47,51,51	3.57	19 (40%)
3	94L	B	502	2	34,34,34	3.26	17 (50%)	47,51,51	3.71	19 (40%)
3	94L	A	502	2	34,34,34	3.21	16 (47%)	47,51,51	3.77	21 (44%)

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

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	94L	O8-C4	9.32	1.42	1.23
3	B	502	94L	O8-C4	8.96	1.41	1.23
3	C	502	94L	O11-C9	8.75	1.41	1.23
3	C	502	94L	O19-C17	8.74	1.40	1.22
3	B	502	94L	O11-C9	8.69	1.41	1.23
3	A	502	94L	O11-C9	8.57	1.41	1.23
3	A	502	94L	O8-C4	8.55	1.40	1.23
3	A	502	94L	O19-C17	8.50	1.39	1.22
3	D	502	94L	O19-C17	8.48	1.39	1.22
3	B	502	94L	O19-C17	8.29	1.39	1.22
3	D	502	94L	O11-C9	7.72	1.39	1.23
3	C	502	94L	O8-C4	7.62	1.38	1.23
3	C	502	94L	C5-C6	4.79	1.53	1.39
3	A	502	94L	C5-C6	4.57	1.53	1.39
3	D	502	94L	C5-C6	4.54	1.52	1.39
3	B	502	94L	C5-C6	4.43	1.52	1.39
3	C	502	94L	C5-C4	3.93	1.55	1.45
3	D	502	94L	C5-C4	3.90	1.55	1.45
3	D	502	94L	C21-N23	-3.79	1.33	1.38
3	A	502	94L	C16-C15	3.65	1.45	1.39
3	B	502	94L	C5-C4	3.62	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	94L	C21-N23	-3.53	1.34	1.38
3	B	502	94L	C17-N18	-3.49	1.33	1.40
3	D	502	94L	C17-N18	-3.44	1.34	1.40
3	B	502	94L	C21-N23	-3.43	1.34	1.38
3	C	502	94L	C21-N23	-3.34	1.34	1.38
3	A	502	94L	C5-C4	3.32	1.53	1.45
3	C	502	94L	C17-N18	-3.23	1.34	1.40
3	C	502	94L	C3-C4	3.21	1.55	1.50
3	A	502	94L	C17-N18	-3.16	1.34	1.40
3	C	502	94L	C16-C15	3.09	1.44	1.39
3	C	502	94L	C15-C14	-3.02	1.36	1.41
3	A	502	94L	C1-C6	2.97	1.54	1.49
3	D	502	94L	O7-C6	2.96	1.40	1.32
3	B	502	94L	C21-N18	-2.92	1.34	1.40
3	D	502	94L	C21-N18	-2.89	1.34	1.40
3	D	502	94L	C15-C14	-2.84	1.36	1.41
3	D	502	94L	C15-C17	-2.80	1.42	1.47
3	B	502	94L	C16-C15	2.79	1.44	1.39
3	A	502	94L	C13-C14	2.77	1.43	1.39
3	B	502	94L	C15-C14	-2.75	1.36	1.41
3	D	502	94L	C1-C6	2.75	1.54	1.49
3	B	502	94L	C15-C17	-2.69	1.42	1.47
3	B	502	94L	O7-C6	2.68	1.40	1.32
3	C	502	94L	C21-N18	-2.66	1.34	1.40
3	D	502	94L	C16-C15	2.65	1.44	1.39
3	B	502	94L	C3-C4	2.60	1.54	1.50
3	A	502	94L	O7-C6	2.52	1.39	1.32
3	C	502	94L	O7-C6	2.51	1.39	1.32
3	A	502	94L	C3-C4	2.48	1.54	1.50
3	B	502	94L	C13-C14	2.47	1.43	1.39
3	C	502	94L	C15-C17	-2.45	1.42	1.47
3	B	502	94L	C1-C6	2.42	1.53	1.49
3	C	502	94L	C5-C9	2.38	1.55	1.48
3	A	502	94L	C21-N18	-2.36	1.35	1.40
3	D	502	94L	C13-C14	2.26	1.43	1.39
3	A	502	94L	C15-C14	-2.23	1.37	1.41
3	D	502	94L	C10-C9	2.22	1.53	1.49
3	C	502	94L	C13-C14	2.20	1.43	1.39
3	C	502	94L	C1-C6	2.19	1.53	1.49
3	A	502	94L	C15-C17	-2.18	1.43	1.47
3	D	502	94L	C5-C9	2.14	1.54	1.48
3	B	502	94L	C5-C9	2.10	1.54	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	94L	C5-C9	2.02	1.54	1.48
3	B	502	94L	C10-C9	2.01	1.53	1.49
3	D	502	94L	C14-N23	-2.01	1.36	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	94L	C1-C6-C5	-15.35	106.41	122.90
3	B	502	94L	C1-C6-C5	-14.48	107.35	122.90
3	D	502	94L	C1-C6-C5	-14.27	107.58	122.90
3	C	502	94L	C4-C5-C6	-13.84	103.76	119.13
3	A	502	94L	C1-C6-C5	-13.60	108.29	122.90
3	D	502	94L	C4-C5-C6	-8.77	109.39	119.13
3	C	502	94L	O8-C4-C3	-8.50	106.94	120.87
3	B	502	94L	O7-C6-C5	-8.36	105.58	121.95
3	A	502	94L	O7-C6-C5	-8.28	105.73	121.95
3	A	502	94L	O8-C4-C3	-8.05	107.67	120.87
3	C	502	94L	O11-C9-C10	-7.98	102.75	120.58
3	A	502	94L	O11-C9-C10	-7.55	103.70	120.58
3	B	502	94L	O8-C4-C3	-7.32	108.87	120.87
3	B	502	94L	O11-C9-C10	-7.17	104.55	120.58
3	A	502	94L	C4-C5-C6	-7.05	111.30	119.13
3	D	502	94L	O8-C4-C3	-6.69	109.90	120.87
3	A	502	94L	O8-C4-C5	-6.54	112.12	122.77
3	D	502	94L	O11-C9-C10	-6.43	106.22	120.58
3	D	502	94L	O7-C6-C5	-6.37	109.47	121.95
3	B	502	94L	C4-C5-C6	-6.08	112.38	119.13
3	B	502	94L	O8-C4-C5	-5.81	113.30	122.77
3	C	502	94L	O7-C6-C5	-5.33	111.50	121.95
3	D	502	94L	O8-C4-C5	-5.25	114.23	122.77
3	A	502	94L	C3-C4-C5	-5.00	107.70	116.94
3	C	502	94L	C3-C4-C5	-4.59	108.46	116.94
3	A	502	94L	C17-N18-C21	-4.58	120.78	125.45
3	B	502	94L	C3-C4-C5	-4.40	108.82	116.94
3	D	502	94L	C3-C4-C5	-4.36	108.89	116.94
3	C	502	94L	C17-N18-C21	-4.33	121.03	125.45
3	A	502	94L	C15-C17-N18	4.28	120.54	114.69
3	B	502	94L	C15-C17-N18	4.27	120.53	114.69
3	B	502	94L	C10-C9-C5	4.25	129.79	120.06
3	C	502	94L	C15-C17-N18	4.25	120.50	114.69
3	A	502	94L	C12-C10-C9	-4.24	110.93	120.42
3	D	502	94L	C17-N18-C21	-4.18	121.19	125.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	94L	O8-C4-C5	-3.99	116.27	122.77
3	B	502	94L	C17-N18-C21	-3.99	121.38	125.45
3	B	502	94L	C12-C10-C9	-3.97	111.54	120.42
3	D	502	94L	C15-C17-N18	3.92	120.05	114.69
3	A	502	94L	C14-C15-C17	-3.72	116.12	121.60
3	C	502	94L	C14-C15-C17	-3.69	116.16	121.60
3	B	502	94L	C14-C15-C17	-3.59	116.30	121.60
3	C	502	94L	C10-C9-C5	3.57	128.23	120.06
3	C	502	94L	C12-C10-C9	-3.43	112.75	120.42
3	B	502	94L	C16-C10-C9	3.40	127.26	119.97
3	D	502	94L	C14-C15-C17	-3.31	116.72	121.60
3	B	502	94L	C31-N23-C21	3.28	120.73	117.34
3	D	502	94L	O11-C9-C5	-3.25	114.02	119.89
3	A	502	94L	C10-C9-C5	3.21	127.40	120.06
3	A	502	94L	C16-C10-C9	3.19	126.81	119.97
3	B	502	94L	O11-C9-C5	-3.07	114.36	119.89
3	A	502	94L	O22-C21-N23	-3.04	119.52	122.10
3	C	502	94L	C16-C10-C9	2.97	126.34	119.97
3	C	502	94L	O11-C9-C5	-2.96	114.56	119.89
3	D	502	94L	C12-C10-C9	-2.93	113.87	120.42
3	D	502	94L	C10-C9-C5	2.84	126.55	120.06
3	C	502	94L	C13-C14-N23	-2.76	117.37	121.04
3	C	502	94L	C16-C15-C17	2.75	123.84	118.37
3	A	502	94L	C16-C15-C17	2.75	123.82	118.37
3	C	502	94L	C31-N23-C21	2.71	120.14	117.34
3	D	502	94L	C20-N18-C17	2.69	121.47	117.26
3	C	502	94L	O7-C6-C1	-2.66	108.34	114.43
3	B	502	94L	C20-N18-C17	2.49	121.15	117.26
3	A	502	94L	C13-C14-N23	-2.47	117.76	121.04
3	D	502	94L	C16-C10-C9	2.46	125.24	119.97
3	C	502	94L	O22-C21-N23	-2.40	120.06	122.10
3	B	502	94L	C16-C15-C17	2.39	123.12	118.37
3	C	502	94L	C15-C14-N23	2.35	121.76	119.80
3	A	502	94L	C20-N18-C17	2.34	120.92	117.26
3	A	502	94L	C31-N23-C21	2.26	119.68	117.34
3	A	502	94L	C12-C10-C16	2.22	121.82	119.25
3	D	502	94L	O22-C21-N23	-2.18	120.25	122.10
3	B	502	94L	C24-C20-N18	2.18	121.50	118.73
3	A	502	94L	O7-C6-C1	-2.17	109.45	114.43
3	D	502	94L	C16-C15-C17	2.16	122.66	118.37
3	A	502	94L	C25-C24-C20	2.14	120.99	117.99
3	D	502	94L	C14-N23-C21	-2.05	120.14	122.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	94L	C13-C14-N23	-2.04	118.32	121.04
3	B	502	94L	C13-C14-N23	-2.01	118.37	121.04

There are no chirality outliers.

All (28) torsion outliers are listed below:

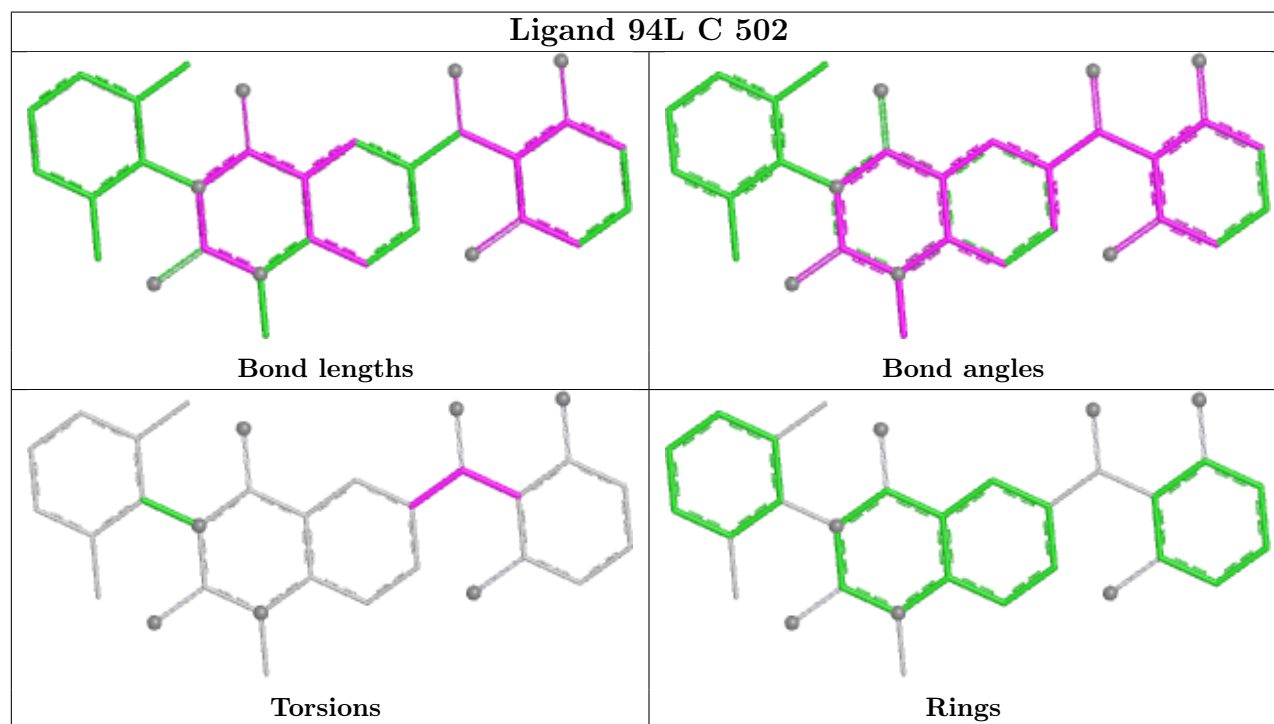
Mol	Chain	Res	Type	Atoms
3	A	502	94L	C4-C5-C9-C10
3	A	502	94L	C4-C5-C9-O11
3	A	502	94L	C6-C5-C9-C10
3	B	502	94L	C4-C5-C9-O11
3	B	502	94L	C6-C5-C9-C10
3	C	502	94L	C4-C5-C9-O11
3	C	502	94L	C6-C5-C9-C10
3	D	502	94L	C4-C5-C9-C10
3	D	502	94L	C4-C5-C9-O11
3	D	502	94L	C6-C5-C9-C10
3	B	502	94L	C12-C10-C9-O11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

There are no ring outliers.

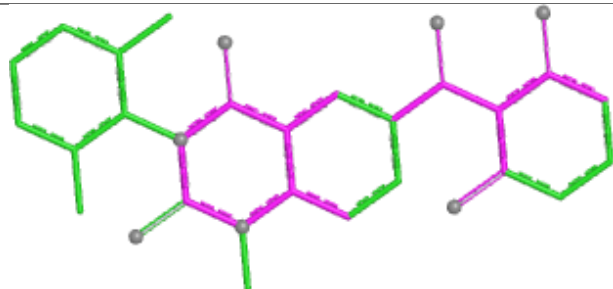
1 monomer is involved in 1 short contact:

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

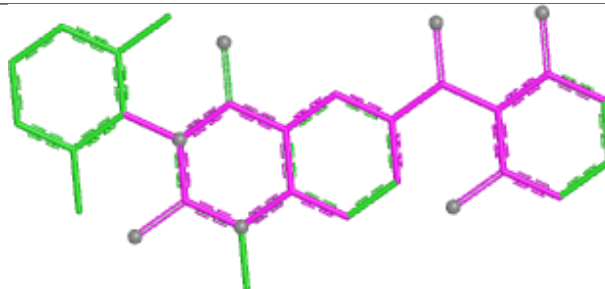
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



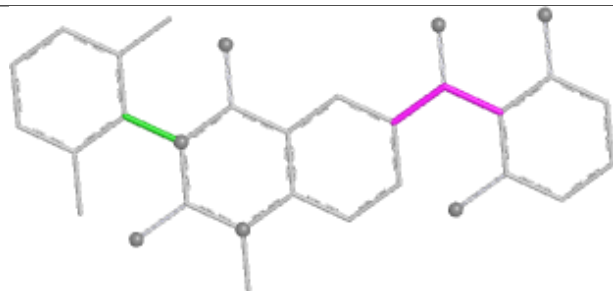
Ligand 94L D 502



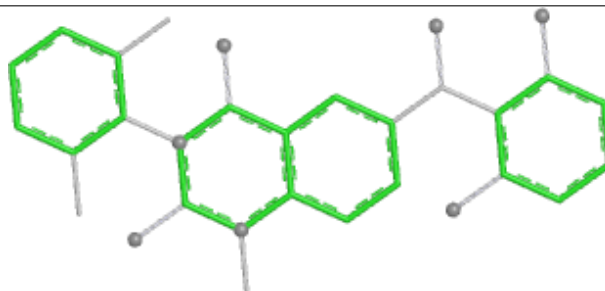
Bond lengths



Bond angles

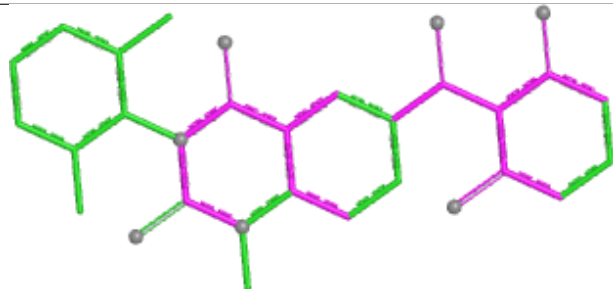


Torsions

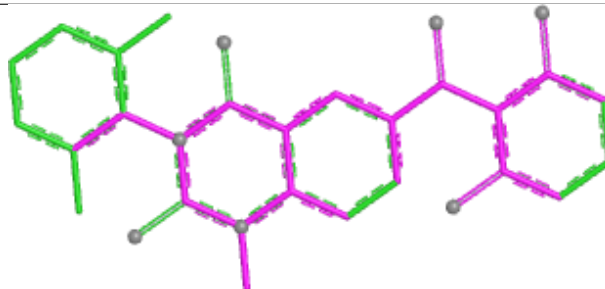


Rings

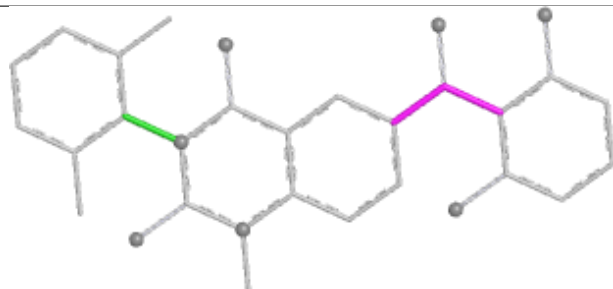
Ligand 94L B 502



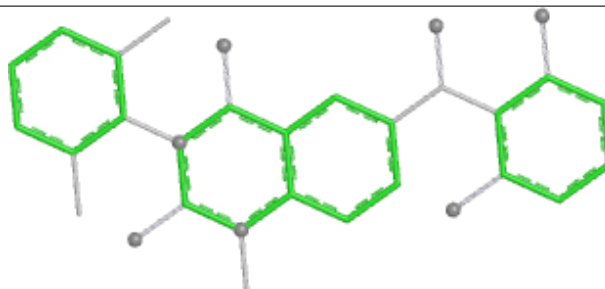
Bond lengths



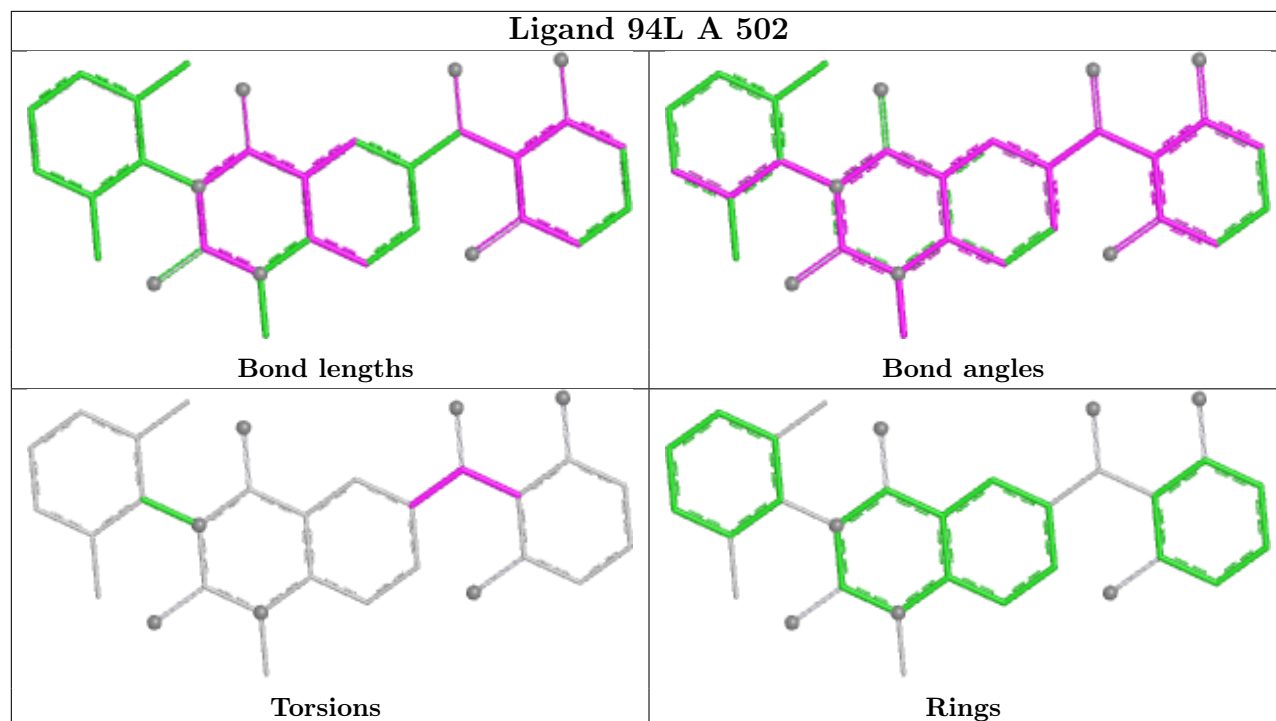
Bond angles



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%)	0.05	13 (3%) 46 50	14, 22, 38, 58	0
1	B	363/444 (81%)	0.05	15 (4%) 41 45	14, 23, 43, 57	0
1	C	376/444 (84%)	0.06	24 (6%) 25 28	14, 22, 48, 57	0
1	D	367/444 (82%)	0.11	19 (5%) 33 34	16, 24, 46, 63	0
All	All	1470/1776 (82%)	0.07	71 (4%) 35 37	14, 23, 45, 63	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ALA	9.5
1	C	208	GLY	8.0
1	B	417	PHE	6.0
1	B	193	ALA	5.8
1	B	192	ALA	5.5
1	D	193	ALA	5.0
1	A	248	THR	5.0
1	A	209	ALA	4.9
1	D	417	PHE	4.8
1	C	193	ALA	4.7
1	C	108	GLY	4.4
1	C	192	ALA	4.3
1	D	419	GLN	4.3
1	A	208	GLY	4.3
1	C	109	ALA	4.2
1	C	207	PRO	4.2
1	D	192	ALA	4.0
1	B	279	HIS	3.9
1	C	107	HIS	3.8
1	B	404	TYR	3.8
1	B	207	PRO	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	418	SER	3.7
1	C	110	ASP	3.7
1	A	247	THR	3.6
1	C	398	ASP	3.5
1	D	279	HIS	3.4
1	D	207	PRO	3.4
1	B	191	GLY	3.3
1	B	246	PHE	3.3
1	D	209	ALA	3.2
1	A	419	GLN	3.2
1	B	367	GLN	3.1
1	D	402	GLN	3.1
1	C	194	GLY	3.1
1	A	279	HIS	3.1
1	A	278	VAL	3.1
1	D	257	GLY	3.0
1	B	248	THR	3.0
1	D	367	GLN	2.9
1	B	415	GLY	2.9
1	C	401	GLY	2.9
1	D	208	GLY	2.9
1	A	207	PRO	2.8
1	C	256	SER	2.8
1	C	210	ALA	2.7
1	D	246	PHE	2.7
1	B	208	GLY	2.7
1	D	191	GLY	2.6
1	C	417	PHE	2.6
1	A	109	ALA	2.6
1	C	206	SER	2.6
1	C	399	GLU	2.5
1	C	281	THR	2.5
1	D	283	ARG	2.4
1	A	246	PHE	2.4
1	B	257	GLY	2.4
1	C	106	ALA	2.3
1	C	419	GLN	2.3
1	C	403	GLU	2.3
1	D	284	ARG	2.2
1	D	196	PRO	2.2
1	D	111	ALA	2.2
1	D	278	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	282	LYS	2.2
1	A	257	GLY	2.1
1	B	416	ASN	2.1
1	C	402	GLN	2.1
1	A	417	PHE	2.1
1	D	418	SER	2.1
1	B	205	ALA	2.0
1	C	418	SER	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](#)

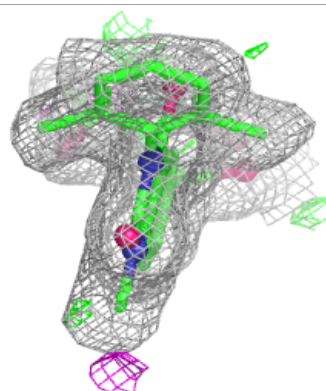
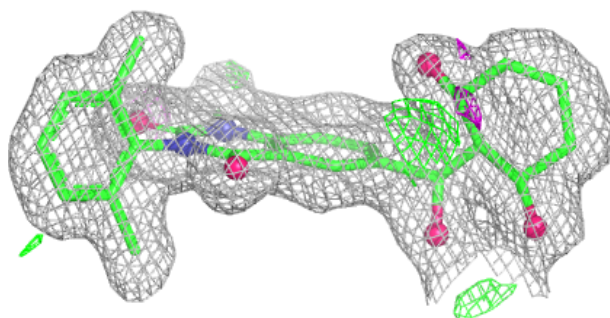
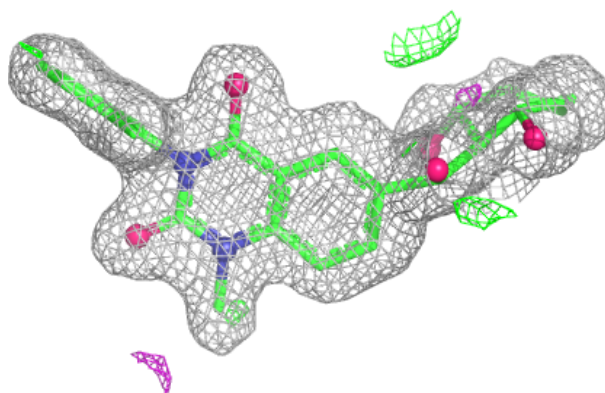
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	94L	A	502	31/31	0.93	0.08	16,20,25,26	0
3	94L	C	502	31/31	0.93	0.07	17,21,26,28	0
3	94L	D	502	31/31	0.93	0.08	19,24,29,31	0
3	94L	B	502	31/31	0.94	0.08	17,20,23,28	0
2	CO	A	501	1/1	1.00	0.01	15,15,15,15	0
2	CO	B	501	1/1	1.00	0.02	14,14,14,14	0
2	CO	C	501	1/1	1.00	0.01	18,18,18,18	0
2	CO	D	501	1/1	1.00	0.01	19,19,19,19	0

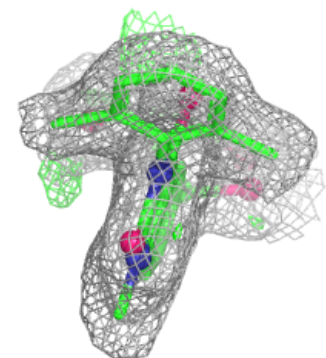
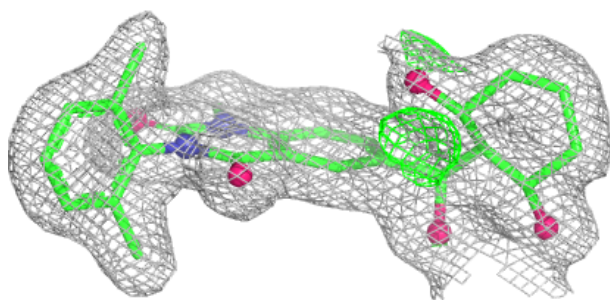
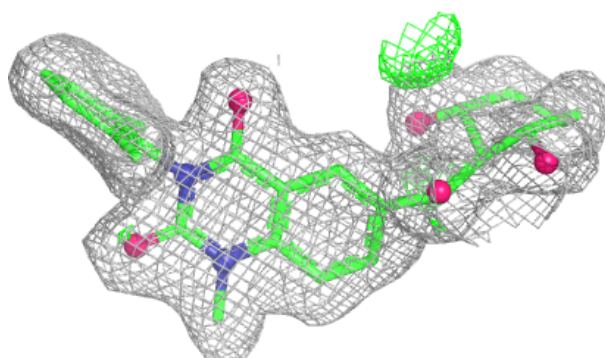
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

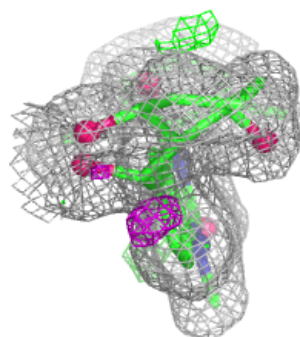
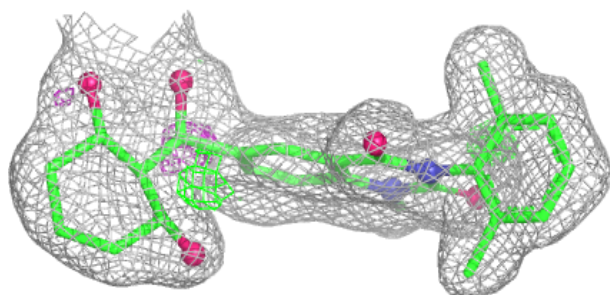
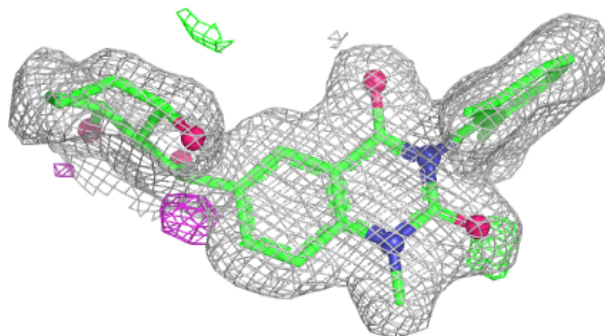
**Electron density around 94L C 502:**

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

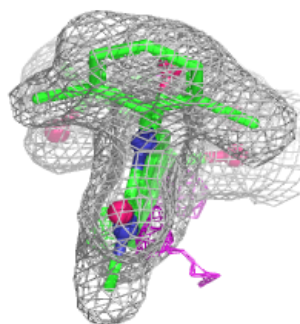
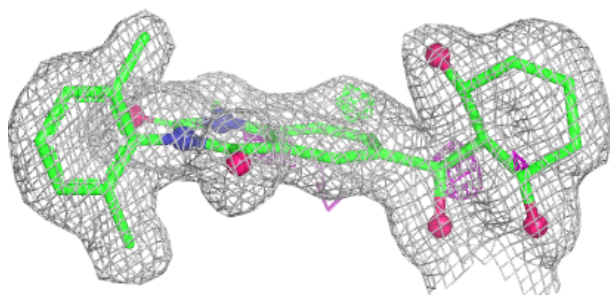
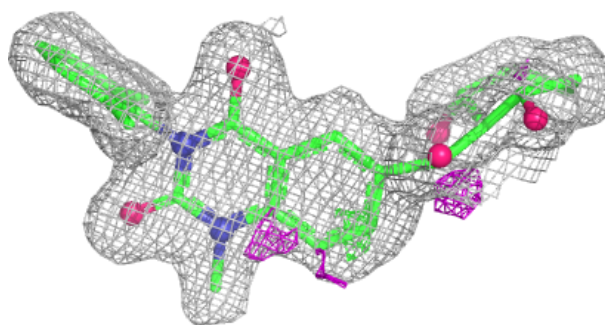


Electron density around 94L D 502:

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

**Electron density around 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 ⓘ

There are no such residues in this entry.