



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2022 – 02:22 PM JST

PDB ID : 7XNT  
Title : Crystal structure of PfHPPD-Y13161 complex  
Authors : Lin, H.-Y.; Yang, G.-F.  
Deposited on : 2022-04-29  
Resolution : 1.82 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](mailto: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>.

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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 : 2.31.3  
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) : 2.31.3

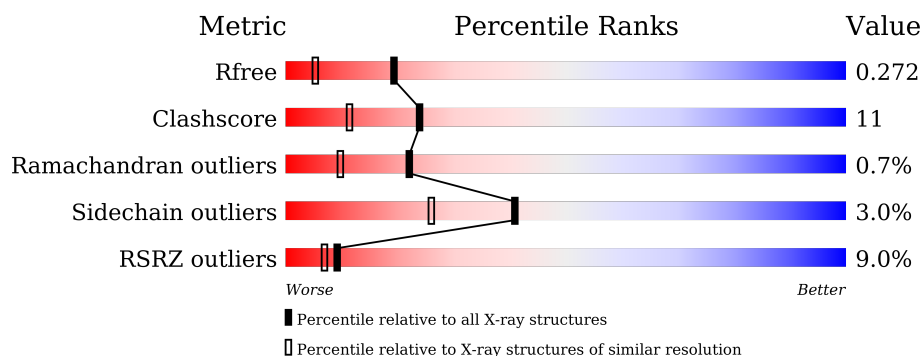
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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  $\geq 3$ , 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	357	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	357	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>• 8%</div> </div> </div>
1	C	357	<div> <div>15%</div> <div> <div></div> <div>67%</div> <div>22%</div> <div>• 10%</div> </div> </div>
1	G	357	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10832 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	G	335	Total	C	N	O	S	0	0	0
			2622	1689	435	484	14			
1	A	341	Total	C	N	O	S	0	0	0
			2684	1725	447	498	14			
1	B	328	Total	C	N	O	S	0	0	0
			2555	1645	428	468	14			
1	C	320	Total	C	N	O	S	0	0	0
			2458	1585	413	446	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	105	ASP	GLU	variant	UNP A0A0W0HIR1
G	280	ASP	ASN	variant	UNP A0A0W0HIR1
G	355	ALA	THR	variant	UNP A0A0W0HIR1
A	105	ASP	GLU	variant	UNP A0A0W0HIR1
A	280	ASP	ASN	variant	UNP A0A0W0HIR1
A	355	ALA	THR	variant	UNP A0A0W0HIR1
B	105	ASP	GLU	variant	UNP A0A0W0HIR1
B	280	ASP	ASN	variant	UNP A0A0W0HIR1
B	355	ALA	THR	variant	UNP A0A0W0HIR1
C	105	ASP	GLU	variant	UNP A0A0W0HIR1
C	280	ASP	ASN	variant	UNP A0A0W0HIR1
C	355	ALA	THR	variant	UNP A0A0W0HIR1

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

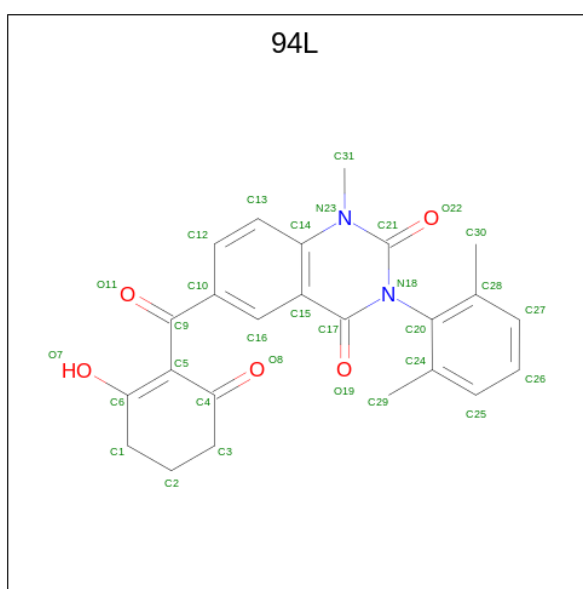
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Co	0	0
			1	1		

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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		

- 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: C<sub>24</sub>H<sub>22</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	144	Total	O	0	0
			144	144		

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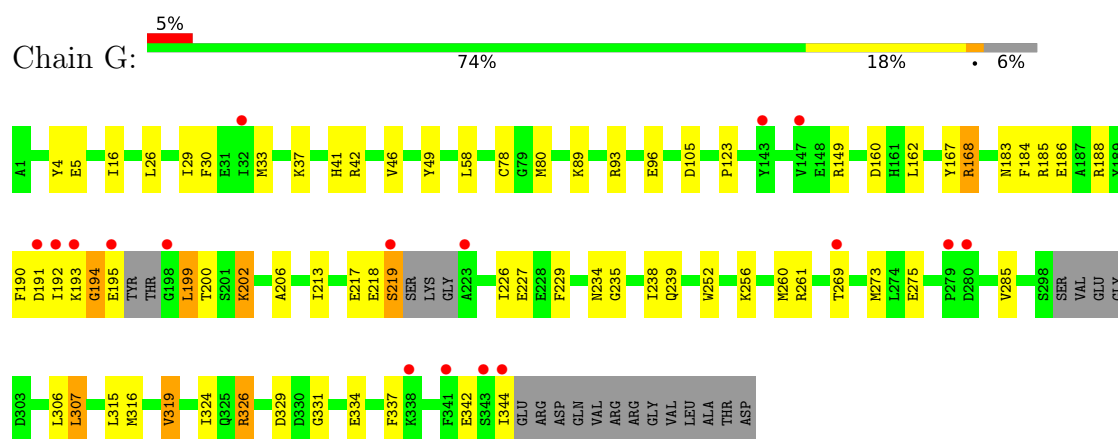
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total 151	O 151	0	0
4	B	49	Total 49	O 49	0	0
4	C	41	Total 41	O 41	0	0

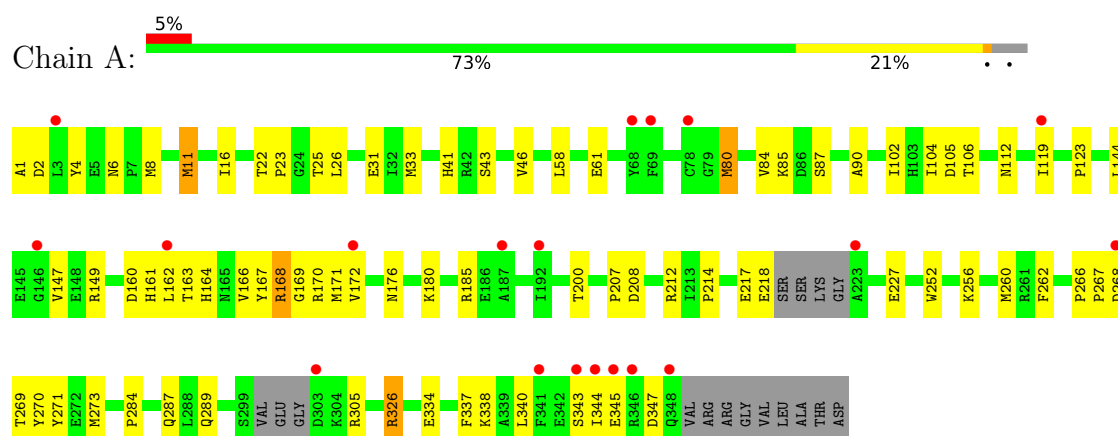
### 3 Residue-property plots [i](#)

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.

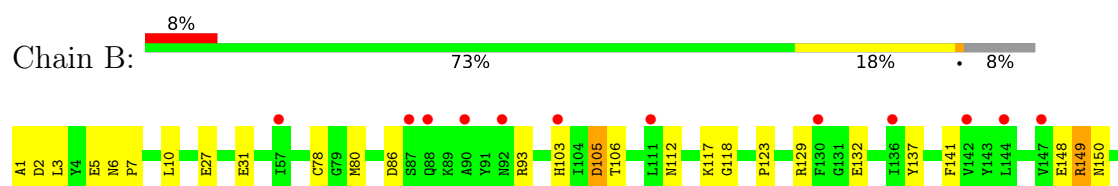
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

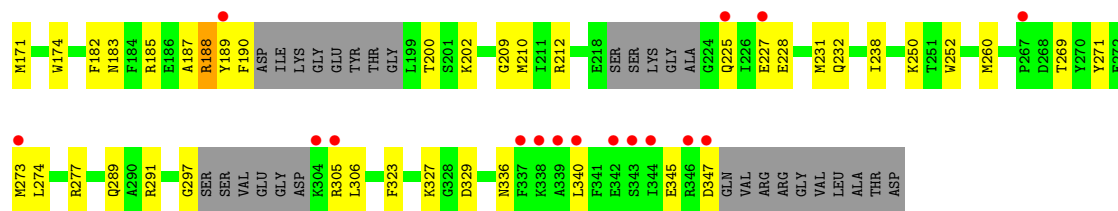


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

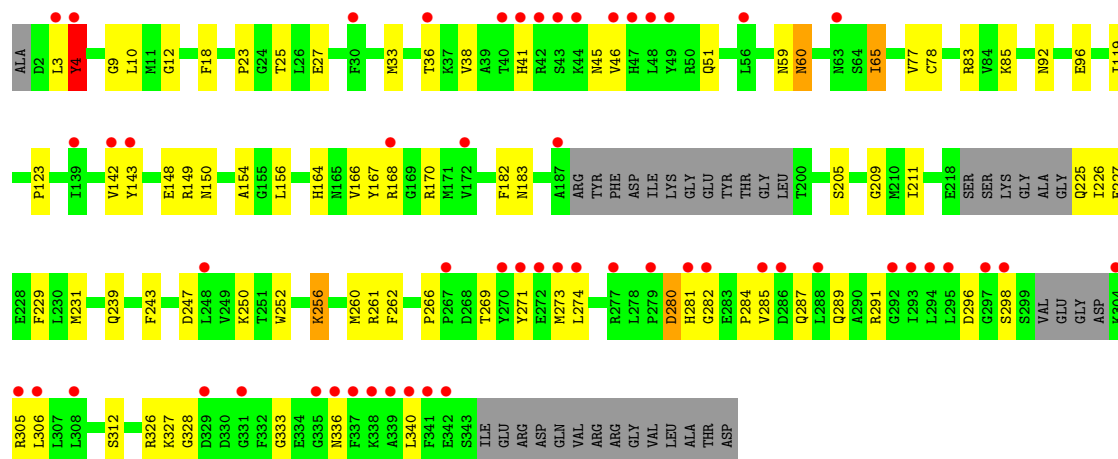


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





● Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.94Å 73.04Å 87.96Å 66.13° 79.56° 69.10°	Depositor
Resolution (Å)	34.90 – 1.82 49.63 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.90-1.82) 97.8 (49.63-1.82)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.238 , 0.271 0.240 , 0.272	Depositor DCC
$R_{free}$ test set	6501 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,-k+l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.56	1/2749 (0.0%)	0.72	3/3713 (0.1%)
1	B	0.38	0/2617	0.57	1/3538 (0.0%)
1	C	0.42	1/2518 (0.0%)	0.56	0/3409
1	G	0.55	1/2685 (0.0%)	0.70	3/3626 (0.1%)
All	All	0.49	3/10569 (0.0%)	0.64	7/14286 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	VAL	CB-CG2	5.63	1.64	1.52
1	C	4	TYR	CE2-CZ	-5.37	1.31	1.38
1	G	342	GLU	CD-OE1	-5.08	1.20	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	307	LEU	CA-CB-CG	8.63	135.16	115.30
1	G	319	VAL	CG1-CB-CG2	-7.44	98.99	110.90
1	A	326	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	326	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	86	ASP	CB-CG-OD1	5.70	123.42	118.30
1	G	326	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	A	11	MET	CB-CG-SD	-5.00	97.39	112.40

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	2684	0	2592	68	0
1	B	2555	0	2449	41	0
1	C	2458	0	2347	71	0
1	G	2622	0	2535	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
3	A	31	0	0	1	0
3	B	31	0	0	1	0
3	C	31	0	0	0	0
3	G	31	0	0	0	0
4	A	151	0	0	8	0
4	B	49	0	0	3	0
4	C	41	0	0	2	0
4	G	144	0	0	8	0
All	All	10832	0	9923	227	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 11.

All (227) 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:G:33:MET:HG2	1:G:260:MET:HE1	1.47	0.96
1:B:5:GLU:HG3	1:B:7:PRO:HD3	1.57	0.87
1:A:337:PHE:HD1	4:A:505:HOH:O	1.62	0.82
1:G:192:ILE:HD11	1:G:334:GLU:HB3	1.62	0.82
1:G:316:MET:O	1:G:319:VAL:HG12	1.79	0.80
1:A:337:PHE:CD1	4:A:505:HOH:O	2.35	0.80
1:G:337:PHE:CD2	4:G:515:HOH:O	2.38	0.77
1:A:33:MET:HG2	1:A:260:MET:HE1	1.65	0.76
1:G:218:GLU:HG2	1:G:226:ILE:HB	1.69	0.75
1:B:106:THR:HG21	1:B:112:ASN:HA	1.69	0.75
1:A:1:ALA:HB3	1:A:208:ASP:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:HIS:NE2	1:B:105:ASP:OD1	2.20	0.74
1:G:41:HIS:HB2	1:G:46:VAL:HG22	1.67	0.74
1:C:269:THR:OG1	1:C:273:MET:SD	2.47	0.73
1:A:41:HIS:HB2	1:A:46:VAL:HG22	1.70	0.72
1:G:89:LYS:NZ	4:G:501:HOH:O	2.23	0.72
1:C:3:LEU:HD12	1:C:4:TYR:CD1	2.25	0.71
4:G:535:HOH:O	1:A:25:THR:HG22	1.92	0.70
1:A:284:PRO:HB2	1:A:287:GLN:HG3	1.75	0.69
1:C:274:LEU:HD23	1:C:285:VAL:HG13	1.76	0.68
1:C:3:LEU:HD23	1:C:209:GLY:CA	2.23	0.67
1:A:119:ILE:HG21	1:A:164:HIS:CD2	2.29	0.67
1:C:119:ILE:HD13	1:C:164:HIS:HB3	1.77	0.67
1:C:65:ILE:HD12	1:C:65:ILE:H	1.60	0.67
1:A:104:ILE:HB	4:A:520:HOH:O	1.93	0.66
1:C:269:THR:O	1:C:273:MET:SD	2.53	0.66
1:A:345:GLU:O	1:A:345:GLU:HG2	1.95	0.65
1:G:186:GLU:CD	1:G:202:LYS:HD2	2.16	0.65
1:C:3:LEU:HD12	1:C:4:TYR:HD1	1.61	0.65
1:A:22:THR:OG1	1:A:25:THR:HG21	1.97	0.65
1:A:169:GLY:O	1:A:172:VAL:HG12	1.96	0.65
1:G:30:PHE:CE2	1:G:58:LEU:HD22	2.32	0.64
1:G:30:PHE:HE2	1:G:58:LEU:HD22	1.63	0.63
1:G:5:GLU:HG2	1:G:183:ASN:ND2	2.14	0.63
1:A:168:ARG:NH1	1:A:218:GLU:O	2.30	0.63
1:G:160:ASP:OD2	1:G:326:ARG:NH2	2.25	0.63
1:A:163:THR:HG21	3:A:402:94L:O8	1.98	0.62
1:A:4:TYR:HB2	1:A:207:PRO:HB3	1.81	0.62
1:A:1:ALA:N	1:A:6:ASN:HD22	1.97	0.62
1:G:80:MET:SD	1:G:162:LEU:HD21	2.40	0.62
1:A:31:GLU:HG3	4:A:522:HOH:O	1.99	0.62
1:C:3:LEU:HD11	1:C:4:TYR:HE1	1.65	0.62
1:C:280:ASP:O	1:C:282:GLY:N	2.32	0.61
1:C:252:TRP:CH2	1:C:256:LYS:HG3	2.36	0.61
1:B:80:MET:HE2	1:B:238:ILE:HD11	1.81	0.60
1:A:161:HIS:HD2	1:A:163:THR:HG23	1.66	0.60
1:B:306:LEU:HB3	1:B:327:LYS:HB3	1.83	0.60
1:B:1:ALA:HB3	1:B:6:ASN:HD22	1.66	0.60
1:B:227:GLU:O	1:B:231:MET:HG3	2.01	0.60
1:B:252:TRP:CE2	1:B:291:ARG:HB3	2.36	0.60
1:B:269:THR:HG21	1:B:347:ASP:HB2	1.84	0.60
1:B:171:MET:SD	1:B:202:LYS:HB2	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:LEU:HD13	1:G:238:ILE:HG12	1.83	0.59
1:C:3:LEU:HD11	1:C:4:TYR:CE1	2.37	0.59
1:C:305:ARG:O	1:C:306:LEU:HG	2.02	0.59
1:G:93:ARG:HA	1:G:96:GLU:HG2	1.84	0.59
1:A:33:MET:HG2	1:A:260:MET:CE	2.32	0.59
1:G:219:SER:OG	1:G:219:SER:O	2.17	0.59
1:C:119:ILE:HD13	1:C:164:HIS:CG	2.38	0.58
1:A:119:ILE:HG12	1:A:164:HIS:HD2	1.68	0.58
1:C:3:LEU:CD1	1:C:4:TYR:CE1	2.86	0.58
1:A:144:LEU:O	1:A:147:VAL:HG12	2.03	0.58
1:C:41:HIS:HB2	1:C:46:VAL:HG22	1.86	0.58
1:G:186:GLU:OE1	1:G:202:LYS:HD2	2.03	0.58
1:B:1:ALA:CB	1:B:6:ASN:HD22	2.17	0.57
1:A:271:TYR:CD2	1:A:289:GLN:HG3	2.40	0.57
1:G:26:LEU:HD12	1:G:58:LEU:HD11	1.86	0.57
1:A:144:LEU:HB2	1:A:147:VAL:CG1	2.34	0.57
1:C:33:MET:HG2	1:C:260:MET:HE1	1.87	0.57
1:A:163:THR:HG22	1:A:214:PRO:HG2	1.87	0.57
1:G:252:TRP:CH2	1:G:256:LYS:HG3	2.40	0.56
1:B:7:PRO:HB2	1:B:93:ARG:NH1	2.19	0.56
1:B:228:GLU:OE1	1:B:232:GLN:NE2	2.38	0.56
1:A:167:TYR:HB2	1:A:170:ARG:HG3	1.87	0.56
1:G:200:THR:HG23	1:G:217:GLU:HG3	1.87	0.56
1:B:80:MET:CE	1:B:238:ILE:HD11	2.36	0.56
1:G:261:ARG:HD2	1:A:23:PRO:HD2	1.87	0.55
1:B:336:ASN:O	1:B:340:LEU:HB2	2.05	0.55
1:C:46:VAL:HG12	1:C:59:ASN:HA	1.88	0.55
1:G:26:LEU:HD12	1:G:58:LEU:CD1	2.37	0.55
1:B:210:MET:O	1:B:212:ARG:NH1	2.40	0.55
1:G:167:TYR:OH	1:G:235:GLY:HA2	2.07	0.55
1:G:275:GLU:HG2	4:G:524:HOH:O	2.08	0.53
1:A:119:ILE:HG21	1:A:164:HIS:NE2	2.24	0.53
1:G:227:GLU:OE2	1:C:168:ARG:HD2	2.08	0.53
1:A:119:ILE:HD11	1:A:166:VAL:HG12	1.91	0.53
1:C:271:TYR:HA	1:C:274:LEU:HB2	1.90	0.53
1:A:270:TYR:HA	1:A:343:SER:OG	2.08	0.53
1:A:161:HIS:HB3	1:A:212:ARG:HB2	1.91	0.52
1:A:26:LEU:HD12	1:A:58:LEU:HD13	1.91	0.52
1:C:119:ILE:HD13	1:C:164:HIS:CB	2.39	0.52
1:B:187:ALA:O	1:C:183:ASN:ND2	2.44	0.51
1:A:252:TRP:CH2	1:A:256:LYS:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HZ3	1:B:174:TRP:HH2	1.57	0.51
1:C:3:LEU:CD2	1:C:209:GLY:HA2	2.40	0.51
1:C:33:MET:HG2	1:C:260:MET:CE	2.40	0.51
1:A:26:LEU:HD12	1:A:58:LEU:CD1	2.41	0.51
1:C:143:TYR:CG	1:C:149:ARG:HD3	2.45	0.51
1:B:277:ARG:NH1	4:B:509:HOH:O	2.37	0.51
1:B:189:TYR:O	1:B:190:PHE:HB2	2.11	0.50
1:C:148:GLU:OE1	1:C:150:ASN:N	2.36	0.50
1:A:161:HIS:HD2	1:A:163:THR:CG2	2.24	0.50
1:B:27:GLU:O	1:B:31:GLU:HG3	2.11	0.50
1:C:3:LEU:HD23	1:C:209:GLY:HA2	1.93	0.50
1:G:193:LYS:O	1:G:195:GLU:N	2.40	0.50
1:G:218:GLU:HG3	1:G:227:GLU:HB2	1.92	0.50
1:A:8:MET:HE1	1:A:90:ALA:O	2.11	0.50
1:C:271:TYR:CD2	1:C:289:GLN:HG3	2.47	0.50
1:C:247:ASP:OD2	1:C:250:LYS:N	2.28	0.50
1:C:3:LEU:CD1	1:C:4:TYR:CD1	2.92	0.50
1:G:188:ARG:NH2	1:G:190:PHE:HB2	2.28	0.49
1:A:1:ALA:H1	1:A:6:ASN:HD22	1.58	0.49
1:B:10:LEU:HD11	1:B:182:PHE:HB3	1.94	0.49
1:B:345:GLU:C	4:B:512:HOH:O	2.50	0.49
1:A:144:LEU:HB2	1:A:147:VAL:HG11	1.94	0.49
1:A:106:THR:HG21	1:A:112:ASN:HA	1.95	0.49
1:C:10:LEU:HD11	1:C:182:PHE:HB3	1.94	0.49
1:A:334:GLU:C	4:A:505:HOH:O	2.51	0.49
1:B:183:ASN:OD1	1:B:185:ARG:NH2	2.46	0.49
1:B:117:LYS:HE2	1:B:118:GLY:O	2.14	0.48
1:C:271:TYR:CE2	1:C:289:GLN:HG3	2.49	0.48
1:C:9:GLY:HA3	1:C:85:LYS:HG2	1.96	0.48
1:C:92:ASN:O	1:C:96:GLU:HG3	2.14	0.48
1:A:16:ILE:HG22	1:A:80:MET:HB2	1.95	0.48
1:A:334:GLU:HA	4:A:505:HOH:O	2.14	0.48
1:G:188:ARG:HH22	1:G:190:PHE:HB2	1.79	0.48
1:G:194:GLY:O	1:G:195:GLU:HG3	2.13	0.47
1:A:171:MET:HE3	1:A:217:GLU:HG2	1.96	0.47
1:C:260:MET:HA	1:C:260:MET:HE2	1.96	0.47
1:A:163:THR:HG22	1:A:214:PRO:CG	2.43	0.47
1:C:262:PHE:HA	1:C:312:SER:HA	1.96	0.47
1:C:41:HIS:HB2	1:C:46:VAL:CG2	2.45	0.47
1:C:142:VAL:HA	4:C:501:HOH:O	2.15	0.47
1:G:41:HIS:HB2	1:G:46:VAL:CG2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:LEU:O	1:G:213:ILE:HA	2.14	0.47
1:A:267:PRO:HG3	1:A:344:ILE:HD13	1.96	0.47
1:B:129:ARG:HD3	4:B:510:HOH:O	2.15	0.46
1:B:148:GLU:OE1	1:B:149:ARG:N	2.49	0.46
1:A:102:ILE:HG21	1:A:123:PRO:HB3	1.97	0.46
1:C:167:TYR:HB2	1:C:170:ARG:HG3	1.96	0.46
1:A:267:PRO:HG2	1:A:343:SER:HB3	1.98	0.46
1:A:160:ASP:OD2	1:A:326:ARG:NH2	2.37	0.46
1:A:269:THR:O	1:A:273:MET:HG3	2.16	0.46
1:C:227:GLU:O	1:C:231:MET:HG3	2.16	0.46
1:G:337:PHE:HD2	4:G:515:HOH:O	1.89	0.46
1:C:225:GLN:N	1:C:227:GLU:OE2	2.49	0.46
1:G:26:LEU:CD1	1:G:58:LEU:CD1	2.93	0.46
1:A:61:GLU:OE2	1:A:61:GLU:HA	2.16	0.46
1:C:227:GLU:H	1:C:227:GLU:CD	2.19	0.46
1:G:149:ARG:NH1	4:G:504:HOH:O	2.28	0.45
1:G:316:MET:HB2	1:G:319:VAL:CG1	2.46	0.45
1:C:119:ILE:CD1	1:C:164:HIS:HB3	2.46	0.45
1:C:27:GLU:OE1	1:C:27:GLU:N	2.43	0.45
1:C:271:TYR:HD1	1:C:274:LEU:HD22	1.80	0.45
1:G:78:CYS:O	1:G:123:PRO:HD2	2.17	0.45
1:A:260:MET:HG2	1:A:262:PHE:CE1	2.52	0.45
1:C:45:ASN:ND2	1:C:60:ASN:OD1	2.49	0.45
1:A:23:PRO:O	1:A:25:THR:HG23	2.17	0.45
1:G:324:ILE:HD13	1:G:326:ARG:NH2	2.32	0.44
1:B:225:GLN:NE2	3:B:402:94L:C27	2.80	0.44
1:C:4:TYR:OH	1:C:205:SER:O	2.34	0.44
1:A:176:ASN:O	1:A:180:LYS:HG3	2.18	0.44
1:C:51:GLN:NE2	1:C:154:ALA:H	2.16	0.44
1:A:144:LEU:HB2	1:A:147:VAL:HG12	1.98	0.44
1:G:269:THR:O	1:G:273:MET:HG3	2.18	0.44
1:C:225:GLN:HG3	1:C:226:ILE:HD13	1.99	0.44
1:C:340:LEU:HD12	1:C:340:LEU:HA	1.83	0.44
1:B:269:THR:O	1:B:273:MET:HG3	2.18	0.44
1:A:119:ILE:HG21	1:A:164:HIS:HE2	1.82	0.44
1:A:171:MET:HE1	1:A:200:THR:O	2.18	0.44
1:A:305:ARG:NH1	4:A:528:HOH:O	2.51	0.44
1:B:274:LEU:HD23	1:B:274:LEU:HA	1.90	0.44
1:C:36:THR:O	1:C:38:VAL:HG13	2.17	0.44
1:C:78:CYS:O	1:C:123:PRO:HD2	2.17	0.44
1:C:266:PRO:HB3	1:C:340:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LEU:HD23	1:C:209:GLY:HA3	1.99	0.44
1:C:23:PRO:O	1:C:25:THR:HG23	2.18	0.44
1:B:7:PRO:HB2	1:B:93:ARG:HH12	1.83	0.43
1:B:78:CYS:O	1:B:123:PRO:HD2	2.18	0.43
1:C:305:ARG:HD3	1:C:328:GLY:O	2.17	0.43
1:G:329:ASP:OD1	1:G:331:GLY:N	2.44	0.43
1:C:45:ASN:O	1:C:60:ASN:HB3	2.18	0.43
1:B:137:TYR:O	1:B:141:PHE:HB2	2.17	0.43
1:G:285:VAL:HG21	4:G:524:HOH:O	2.18	0.43
1:B:80:MET:HB2	1:B:80:MET:HE3	1.80	0.43
1:G:4:TYR:CE1	1:G:185:ARG:HD2	2.54	0.42
1:G:190:PHE:CD1	1:G:334:GLU:HB2	2.54	0.42
1:B:260:MET:HE2	1:B:323:PHE:CZ	2.54	0.42
1:C:287:GLN:HB3	1:C:291:ARG:NH1	2.34	0.42
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.88	0.42
1:C:143:TYR:N	4:C:501:HOH:O	2.34	0.42
1:B:271:TYR:CE2	1:B:289:GLN:HG3	2.54	0.42
1:C:119:ILE:HD11	1:C:166:VAL:HG12	2.02	0.42
1:G:37:LYS:HB2	1:G:49:TYR:CE2	2.55	0.42
1:B:250:LYS:HB2	1:B:250:LYS:HE2	1.94	0.42
1:G:184:PHE:CZ	1:G:206:ALA:HB2	2.55	0.42
1:A:41:HIS:HB2	1:A:46:VAL:CG2	2.43	0.42
1:A:268:ASP:OD1	4:A:501:HOH:O	2.22	0.42
1:G:191:ASP:N	4:G:508:HOH:O	2.35	0.42
1:B:132:GLU:OE2	1:B:150:ASN:ND2	2.40	0.42
1:B:269:THR:CG2	1:B:347:ASP:HB2	2.48	0.42
1:C:252:TRP:CE2	1:C:291:ARG:HB3	2.55	0.42
1:A:80:MET:SD	1:A:162:LEU:HD12	2.60	0.41
1:C:119:ILE:HD13	1:C:164:HIS:CD2	2.55	0.41
1:C:333:GLY:O	1:C:336:ASN:HB2	2.20	0.41
1:G:168:ARG:HG2	1:C:231:MET:CE	2.49	0.41
1:A:268:ASP:OD1	1:A:268:ASP:N	2.53	0.41
1:C:143:TYR:CD1	1:C:149:ARG:HD3	2.55	0.41
1:G:229:PHE:CE2	1:G:239:GLN:HA	2.55	0.41
1:C:12:GLY:HA2	1:C:211:ILE:HG13	2.01	0.41
1:C:143:TYR:CD2	1:C:149:ARG:HD3	2.55	0.41
1:A:266:PRO:HB3	1:A:340:LEU:CD2	2.51	0.41
1:C:229:PHE:CE2	1:C:239:GLN:HA	2.55	0.41
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.86	0.41
1:G:29:ILE:HG23	1:G:315:LEU:HD13	2.02	0.41
1:A:41:HIS:CB	1:A:46:VAL:HG22	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG23	1:A:119:ILE:O	2.21	0.41
1:G:200:THR:CG2	1:G:217:GLU:HG3	2.48	0.41
1:A:185:ARG:HH11	1:A:185:ARG:HD3	1.76	0.40
1:B:3:LEU:HG	1:B:209:GLY:CA	2.51	0.40
1:A:11:MET:HE2	1:A:85:LYS:HB2	2.03	0.40
1:A:163:THR:HB	1:A:214:PRO:HB2	2.03	0.40
1:G:16:ILE:HG22	1:G:80:MET:HG3	2.03	0.40
1:B:297:GLY:HA2	1:B:329:ASP:OD2	2.21	0.40
1:C:18:PHE:CE2	1:C:77:VAL:HG22	2.56	0.40
1:A:1:ALA:H3	1:A:6:ASN:HD22	1.68	0.40
1:C:156:LEU:HD13	1:C:243:PHE:CB	2.52	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	335/357 (94%)	328 (98%)	6 (2%)	1 (0%)	41	27
1	B	320/357 (90%)	312 (98%)	6 (2%)	2 (1%)	25	12
1	C	312/357 (87%)	302 (97%)	6 (2%)	4 (1%)	12	3
1	G	327/357 (92%)	316 (97%)	9 (3%)	2 (1%)	25	12
All	All	1294/1428 (91%)	1258 (97%)	27 (2%)	9 (1%)	22	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	B	2	ASP
1	C	281	HIS
1	G	199	LEU

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Mol	Chain	Res	Type
1	B	188	ARG
1	C	280	ASP
1	C	65	ILE
1	G	194	GLY
1	C	284	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/296 (94%)	268 (97%)	9 (3%)	39	24
1	B	259/296 (88%)	254 (98%)	5 (2%)	57	45
1	C	247/296 (83%)	239 (97%)	8 (3%)	39	24
1	G	270/296 (91%)	260 (96%)	10 (4%)	34	19
All	All	1053/1184 (89%)	1021 (97%)	32 (3%)	41	26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	42	ARG
1	G	105	ASP
1	G	168	ARG
1	G	199	LEU
1	G	202	LYS
1	G	219	SER
1	G	234	ASN
1	G	306	LEU
1	G	307	LEU
1	G	344	ILE
1	A	43	SER
1	A	80	MET
1	A	87	SER
1	A	105	ASP
1	A	149	ARG
1	A	168	ARG

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Mol	Chain	Res	Type
1	A	227	GLU
1	A	338	LYS
1	A	347	ASP
1	B	105	ASP
1	B	149	ARG
1	B	188	ARG
1	B	200	THR
1	B	305	ARG
1	C	4	TYR
1	C	60	ASN
1	C	83	ARG
1	C	256	LYS
1	C	261	ARG
1	C	296	ASP
1	C	298	SER
1	C	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	232	GLN
1	A	6	ASN
1	A	164	HIS
1	B	6	ASN
1	C	51	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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	G	402	2	34,34,34	2.02	10 (29%)	47,51,51	1.99	12 (25%)
3	94L	B	402	2	34,34,34	2.10	10 (29%)	47,51,51	2.09	10 (21%)
3	94L	A	402	2	34,34,34	1.99	9 (26%)	47,51,51	1.88	11 (23%)
3	94L	C	402	2	34,34,34	1.97	10 (29%)	47,51,51	1.94	13 (27%)

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	G	402	2	-	4/12/26/26	0/4/4/4
3	94L	B	402	2	-	8/12/26/26	0/4/4/4
3	94L	A	402	2	-	8/12/26/26	0/4/4/4
3	94L	C	402	2	-	8/12/26/26	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	94L	C15-C17	-6.10	1.35	1.47
3	A	402	94L	C15-C17	-6.04	1.35	1.47
3	G	402	94L	C15-C17	-6.03	1.35	1.47
3	C	402	94L	C15-C17	-5.94	1.35	1.47
3	B	402	94L	C17-N18	-4.57	1.32	1.40
3	G	402	94L	C17-N18	-4.43	1.32	1.40
3	G	402	94L	C14-N23	-3.92	1.32	1.40
3	C	402	94L	C14-N23	-3.89	1.32	1.40
3	B	402	94L	C14-N23	-3.84	1.32	1.40
3	A	402	94L	C17-N18	-3.81	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	94L	C17-N18	-3.70	1.33	1.40
3	A	402	94L	C14-N23	-3.60	1.32	1.40
3	B	402	94L	C5-C4	3.27	1.53	1.46
3	C	402	94L	C5-C4	3.19	1.53	1.46
3	G	402	94L	C1-C6	3.00	1.54	1.49
3	C	402	94L	O7-C6	2.91	1.40	1.32
3	A	402	94L	C5-C4	2.86	1.52	1.46
3	B	402	94L	O7-C6	2.82	1.40	1.32
3	A	402	94L	C15-C14	-2.77	1.36	1.41
3	G	402	94L	C5-C4	2.74	1.52	1.46
3	A	402	94L	O7-C6	2.73	1.39	1.32
3	B	402	94L	C15-C14	-2.68	1.36	1.41
3	C	402	94L	C15-C14	-2.65	1.36	1.41
3	B	402	94L	C1-C6	2.53	1.53	1.49
3	B	402	94L	O22-C21	-2.51	1.17	1.22
3	G	402	94L	O7-C6	2.51	1.39	1.32
3	G	402	94L	C15-C14	-2.51	1.37	1.41
3	A	402	94L	C21-N18	-2.45	1.35	1.40
3	G	402	94L	O19-C17	-2.44	1.17	1.22
3	G	402	94L	C21-N23	-2.42	1.35	1.38
3	C	402	94L	O11-C9	-2.36	1.18	1.23
3	B	402	94L	O11-C9	-2.27	1.18	1.23
3	C	402	94L	C1-C6	2.16	1.53	1.49
3	B	402	94L	O8-C4	-2.11	1.18	1.23
3	C	402	94L	C5-C6	-2.11	1.32	1.39
3	A	402	94L	C5-C6	-2.10	1.32	1.39
3	C	402	94L	O8-C4	-2.04	1.19	1.23
3	A	402	94L	C21-N23	-2.01	1.35	1.38
3	G	402	94L	C21-N18	-2.00	1.36	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	94L	C17-N18-C21	-6.02	119.12	125.38
3	C	402	94L	C17-N18-C21	-5.75	119.41	125.38
3	B	402	94L	C14-N23-C21	-5.65	119.70	123.39
3	C	402	94L	C14-N23-C21	-5.17	120.02	123.39
3	G	402	94L	C17-N18-C21	-5.15	120.03	125.38
3	A	402	94L	C14-N23-C21	-5.11	120.05	123.39
3	G	402	94L	C2-C3-C4	-5.06	104.59	113.58
3	A	402	94L	O11-C9-C10	-4.61	110.03	120.58
3	G	402	94L	C14-N23-C21	-4.47	120.47	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	94L	C17-N18-C21	-4.45	120.75	125.38
3	A	402	94L	C10-C9-C5	4.43	129.83	119.93
3	G	402	94L	C15-C17-N18	4.38	120.38	114.60
3	B	402	94L	C15-C17-N18	4.30	120.27	114.60
3	B	402	94L	C9-C5-C6	4.17	122.42	118.34
3	C	402	94L	C15-C17-N18	4.11	120.02	114.60
3	G	402	94L	O11-C9-C10	-3.80	111.90	120.58
3	C	402	94L	C10-C9-C5	3.78	128.37	119.93
3	C	402	94L	C9-C5-C6	3.76	122.02	118.34
3	B	402	94L	O11-C9-C10	-3.73	112.05	120.58
3	B	402	94L	C10-C9-C5	3.72	128.24	119.93
3	B	402	94L	C31-N23-C21	3.25	120.77	117.35
3	A	402	94L	C15-C17-N18	3.17	118.78	114.60
3	G	402	94L	C10-C9-C5	3.15	126.96	119.93
3	B	402	94L	O22-C21-N23	-3.04	119.43	122.08
3	C	402	94L	C31-N23-C21	3.03	120.54	117.35
3	A	402	94L	O7-C6-C5	-3.00	115.72	121.91
3	A	402	94L	C9-C5-C6	2.77	121.05	118.34
3	C	402	94L	O11-C9-C10	-2.70	114.40	120.58
3	G	402	94L	C12-C10-C16	2.62	122.34	119.24
3	G	402	94L	O22-C21-N23	-2.53	119.88	122.08
3	B	402	94L	C28-C20-N18	2.50	122.05	118.73
3	G	402	94L	C9-C5-C6	2.40	120.69	118.34
3	G	402	94L	C31-N23-C21	2.39	119.87	117.35
3	C	402	94L	C28-C20-N18	2.32	121.81	118.73
3	C	402	94L	C20-N18-C17	2.25	120.39	117.29
3	A	402	94L	C31-N23-C21	2.24	119.71	117.35
3	G	402	94L	C28-C20-N18	2.16	121.60	118.73
3	C	402	94L	C25-C24-C20	2.16	121.07	118.00
3	C	402	94L	C3-C4-C5	2.15	120.99	116.95
3	C	402	94L	O8-C4-C3	-2.14	117.35	120.86
3	A	402	94L	C2-C1-C6	-2.12	110.28	112.48
3	A	402	94L	C28-C20-N18	2.12	121.54	118.73
3	B	402	94L	C3-C4-C5	2.09	120.88	116.95
3	A	402	94L	C20-N18-C17	2.04	120.10	117.29
3	G	402	94L	C30-C28-C20	-2.04	119.46	121.75
3	C	402	94L	C2-C1-C6	2.02	114.58	112.48

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	94L	C4-C5-C9-C10
3	A	402	94L	C4-C5-C9-O11
3	A	402	94L	C6-C5-C9-C10
3	A	402	94L	C6-C5-C9-O11
3	B	402	94L	C4-C5-C9-C10
3	B	402	94L	C4-C5-C9-O11
3	B	402	94L	C6-C5-C9-C10
3	B	402	94L	C6-C5-C9-O11
3	C	402	94L	C4-C5-C9-C10
3	C	402	94L	C4-C5-C9-O11
3	C	402	94L	C6-C5-C9-C10
3	C	402	94L	C6-C5-C9-O11
3	A	402	94L	C12-C10-C9-O11
3	C	402	94L	C12-C10-C9-O11
3	C	402	94L	C16-C10-C9-O11
3	A	402	94L	C16-C10-C9-O11
3	G	402	94L	C12-C10-C9-O11
3	B	402	94L	C12-C10-C9-O11
3	B	402	94L	C16-C10-C9-O11
3	G	402	94L	C16-C10-C9-O11
3	C	402	94L	C12-C10-C9-C5
3	A	402	94L	C12-C10-C9-C5
3	C	402	94L	C16-C10-C9-C5
3	A	402	94L	C16-C10-C9-C5
3	B	402	94L	C12-C10-C9-C5
3	G	402	94L	C12-C10-C9-C5
3	B	402	94L	C16-C10-C9-C5
3	G	402	94L	C16-C10-C9-C5

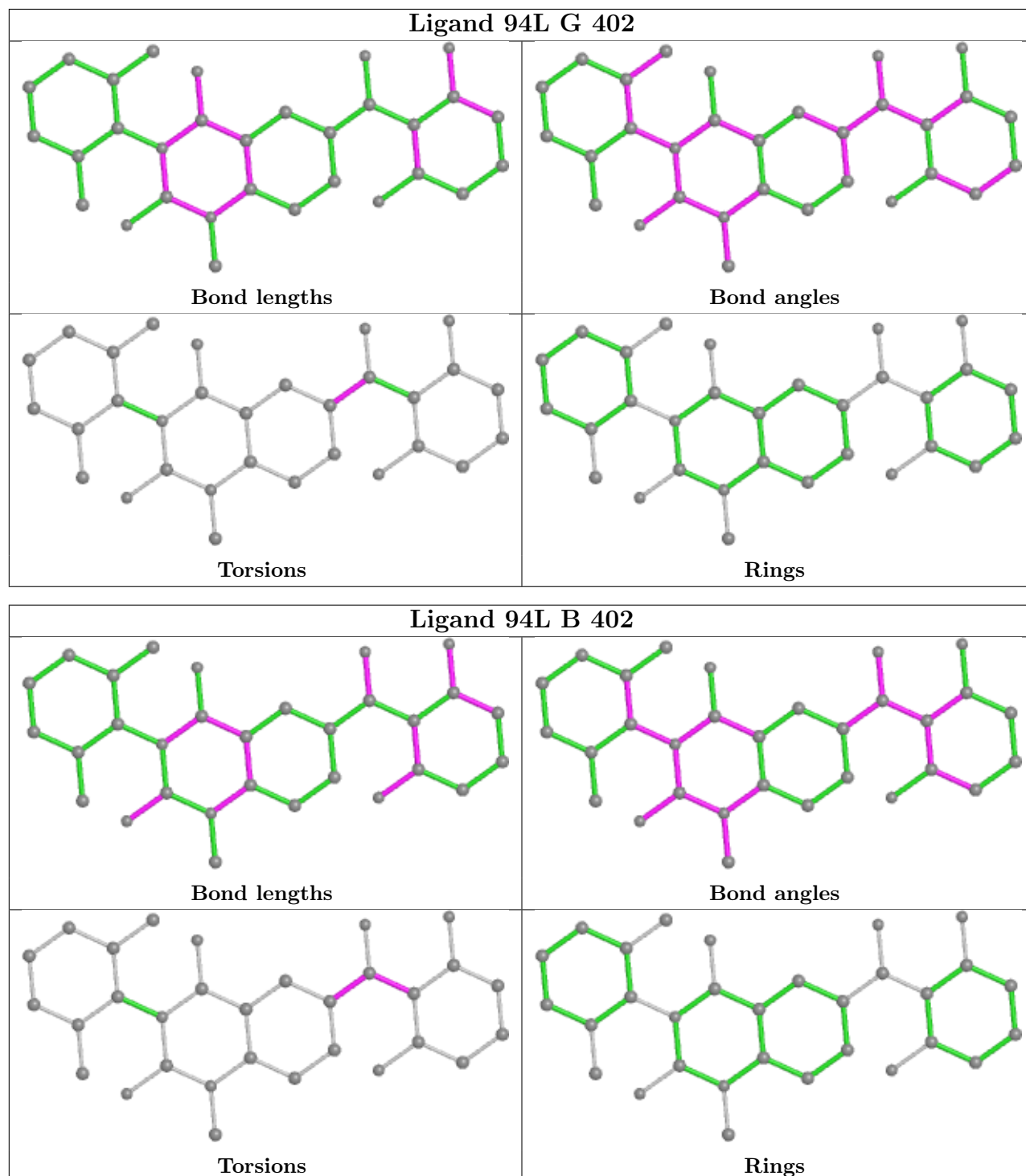
There are no ring outliers.

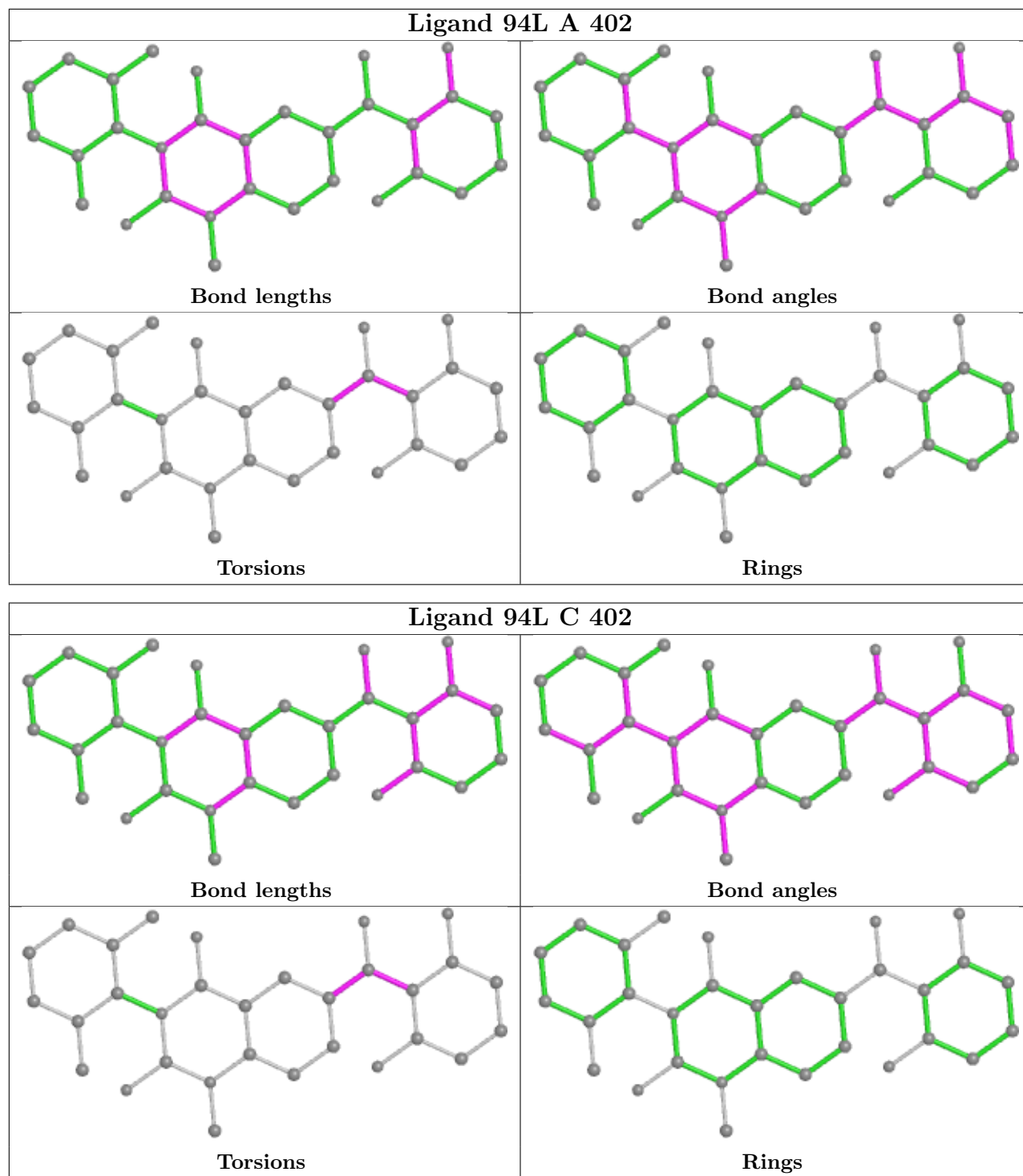
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	94L	1	0
3	A	402	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	341/357 (95%)	0.44	19 (5%)	24 19	25, 36, 58, 84	0
1	B	328/357 (91%)	0.63	28 (8%)	10 8	39, 52, 72, 88	0
1	C	320/357 (89%)	0.97	55 (17%)	1 1	39, 58, 84, 92	0
1	G	335/357 (93%)	0.41	17 (5%)	28 22	23, 36, 60, 78	0
All	All	1324/1428 (92%)	0.61	119 (8%)	9 7	23, 47, 73, 92	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	PHE	10.3
1	A	223	ALA	9.4
1	G	192	ILE	7.8
1	C	297	GLY	7.2
1	G	223	ALA	6.8
1	A	192	ILE	6.5
1	C	292	GLY	5.8
1	C	337	PHE	5.6
1	B	344	ILE	5.3
1	B	343	SER	5.3
1	C	308	LEU	5.2
1	G	195	GLU	5.1
1	C	288	LEU	5.0
1	C	142	VAL	4.8
1	B	346	ARG	4.7
1	A	348	GLN	4.7
1	C	271	TYR	4.7
1	A	345	GLU	4.6
1	B	142	VAL	4.6
1	G	198	GLY	4.2
1	A	341	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	172	VAL	4.1
1	C	285	VAL	4.1
1	C	339	ALA	4.1
1	G	344	ILE	4.0
1	C	286	ASP	4.0
1	A	343	SER	4.0
1	G	147	VAL	4.0
1	B	347	ASP	3.9
1	C	143	TYR	3.9
1	B	340	LEU	3.8
1	G	343	SER	3.7
1	A	146	GLY	3.7
1	B	339	ALA	3.7
1	B	90	ALA	3.7
1	C	279	PRO	3.6
1	C	273	MET	3.6
1	C	298	SER	3.6
1	B	273	MET	3.5
1	A	344	ILE	3.4
1	C	274	LEU	3.4
1	B	88	GLN	3.4
1	A	68	TYR	3.4
1	C	56	LEU	3.4
1	C	43	SER	3.3
1	B	267	PRO	3.3
1	C	277	ARG	3.2
1	G	143	TYR	3.2
1	C	295	LEU	3.2
1	C	267	PRO	3.1
1	C	42	ARG	3.1
1	C	46	VAL	3.1
1	C	272	GLU	3.1
1	A	268	ASP	3.0
1	C	306	LEU	3.0
1	B	136	ILE	3.0
1	C	41	HIS	3.0
1	B	189	TYR	3.0
1	B	144	LEU	2.9
1	B	87	SER	2.9
1	B	111	LEU	2.9
1	C	342	GLU	2.9
1	B	130	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	341	PHE	2.9
1	C	40	THR	2.8
1	C	248	LEU	2.8
1	C	30	PHE	2.7
1	B	147	VAL	2.7
1	C	187	ALA	2.6
1	C	304	LYS	2.6
1	C	336	ASN	2.6
1	G	193	LYS	2.6
1	G	219	SER	2.6
1	C	168	ARG	2.6
1	A	303	ASP	2.6
1	C	335	GLY	2.5
1	C	294	LEU	2.5
1	B	305	ARG	2.5
1	C	282	GLY	2.5
1	A	346	ARG	2.5
1	G	191	ASP	2.5
1	A	162	LEU	2.5
1	C	3	LEU	2.5
1	C	4	TYR	2.5
1	C	48	LEU	2.5
1	G	338	LYS	2.4
1	B	92	ASN	2.4
1	A	172	VAL	2.4
1	C	49	TYR	2.4
1	B	342	GLU	2.3
1	A	3	LEU	2.3
1	G	279	PRO	2.3
1	B	227	GLU	2.3
1	B	225	GLN	2.3
1	C	36	THR	2.3
1	A	69	PHE	2.3
1	G	269	THR	2.3
1	B	337	PHE	2.3
1	C	305	ARG	2.3
1	A	187	ALA	2.3
1	B	57	ILE	2.2
1	C	281	HIS	2.2
1	C	293	ILE	2.2
1	C	44	LYS	2.2
1	C	47	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	329	ASP	2.1
1	C	270	TYR	2.1
1	G	32	ILE	2.1
1	A	119	ILE	2.1
1	B	338	LYS	2.1
1	C	63	ASN	2.1
1	C	340	LEU	2.1
1	C	139	ILE	2.1
1	B	103	HIS	2.1
1	C	338	LYS	2.0
1	C	331	GLY	2.0
1	G	280	ASP	2.0
1	B	304	LYS	2.0
1	A	78	CYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

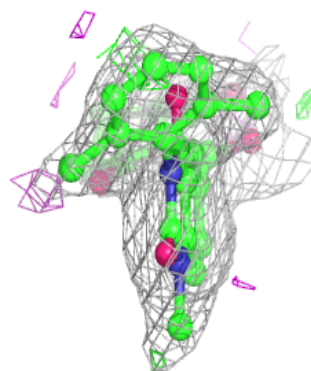
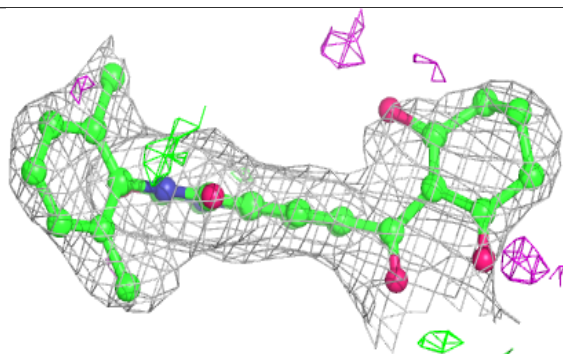
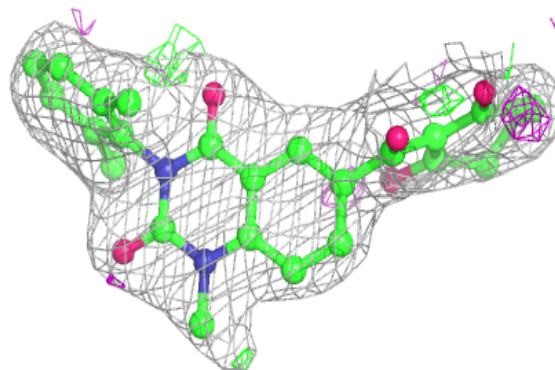
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	94L	B	402	31/31	0.89	0.14	49,54,57,58	0
3	94L	G	402	31/31	0.90	0.12	33,40,44,50	0
3	94L	C	402	31/31	0.91	0.14	53,60,66,70	0
3	94L	A	402	31/31	0.94	0.11	34,41,45,46	0
2	CO	C	401	1/1	0.96	0.15	64,64,64,64	0
2	CO	B	401	1/1	0.99	0.10	58,58,58,58	0
2	CO	G	401	1/1	1.00	0.07	27,27,27,27	0
2	CO	A	401	1/1	1.00	0.10	30,30,30,30	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.

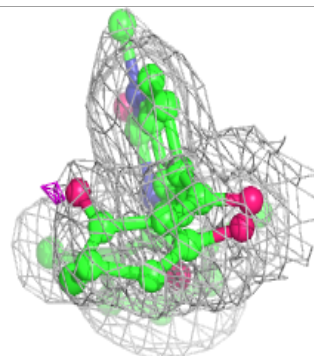
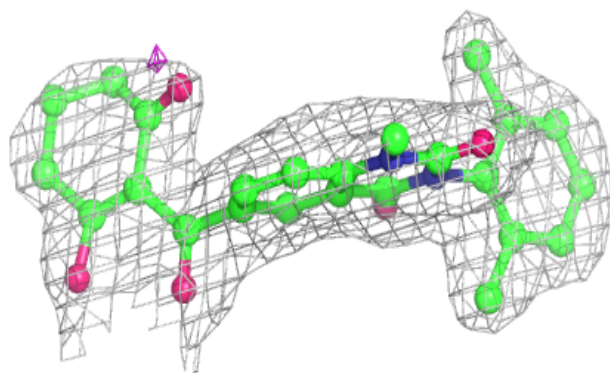
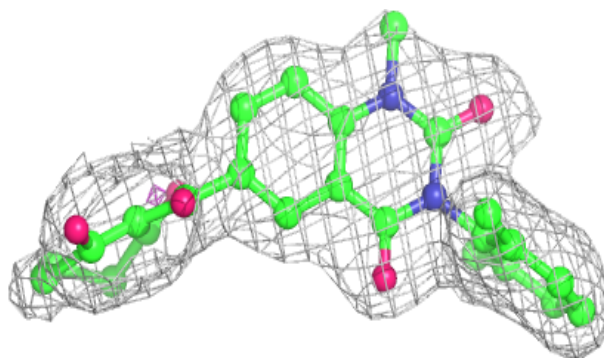
**Electron density around 94L B 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

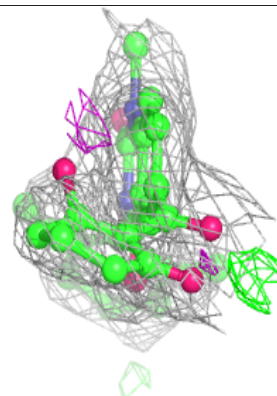
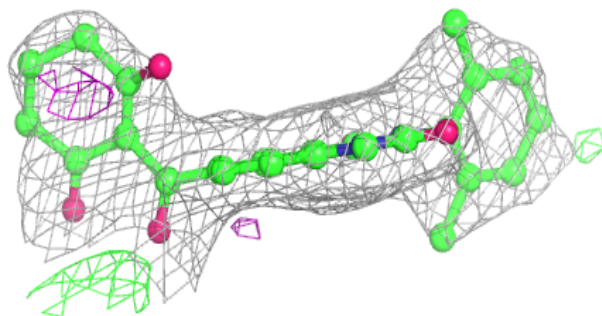
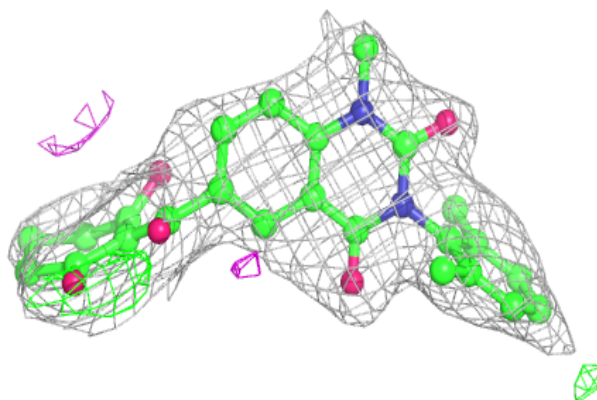


**Electron density around 94L G 402:**

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

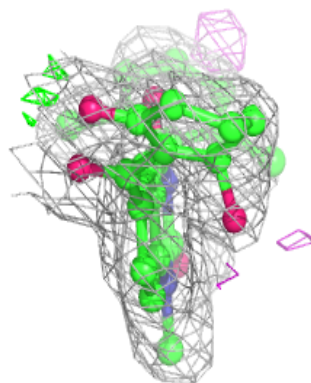
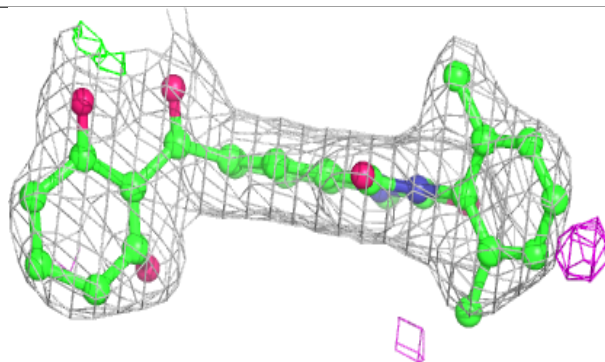
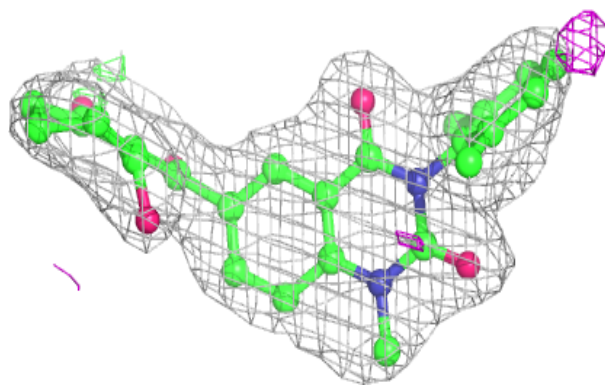
**Electron density around 94L C 402:**

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



**Electron density around 94L A 402:**

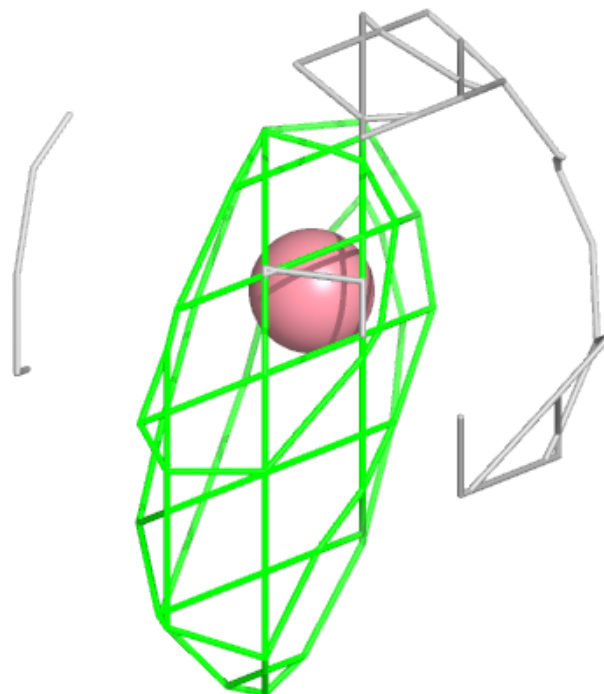
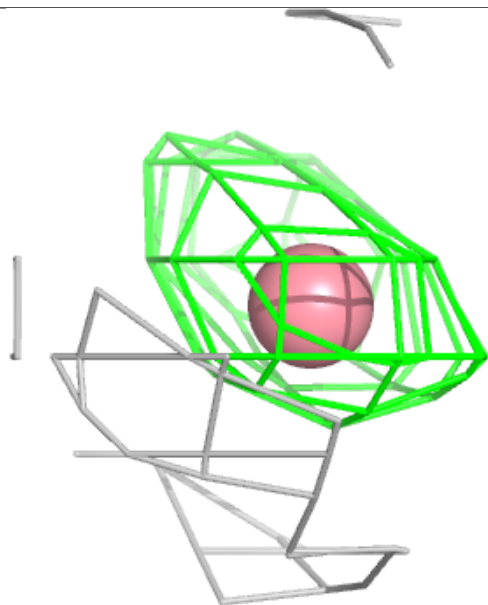
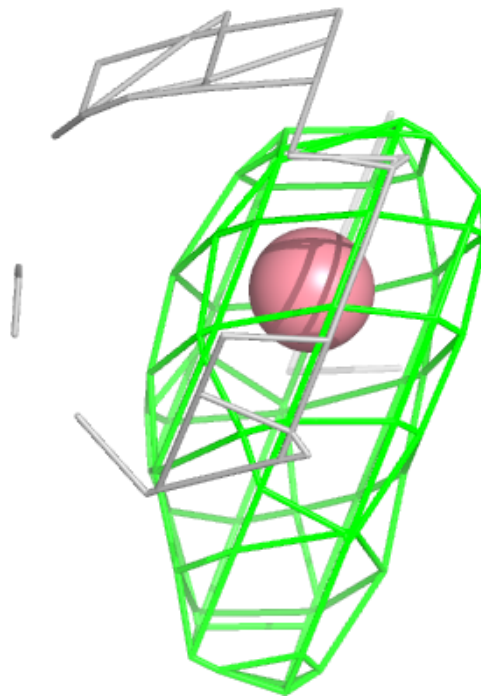
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





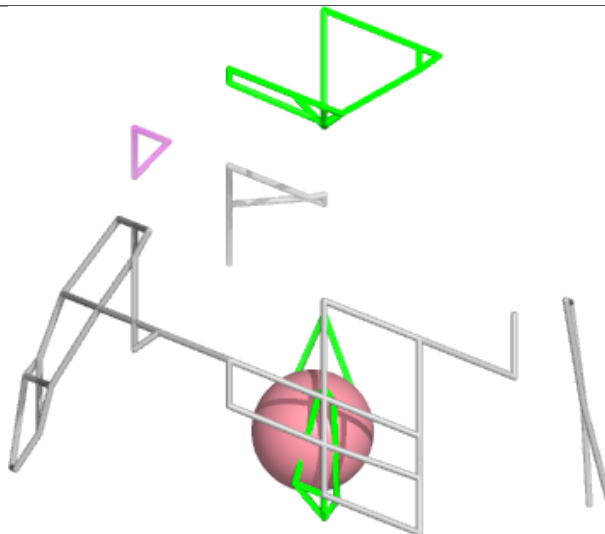
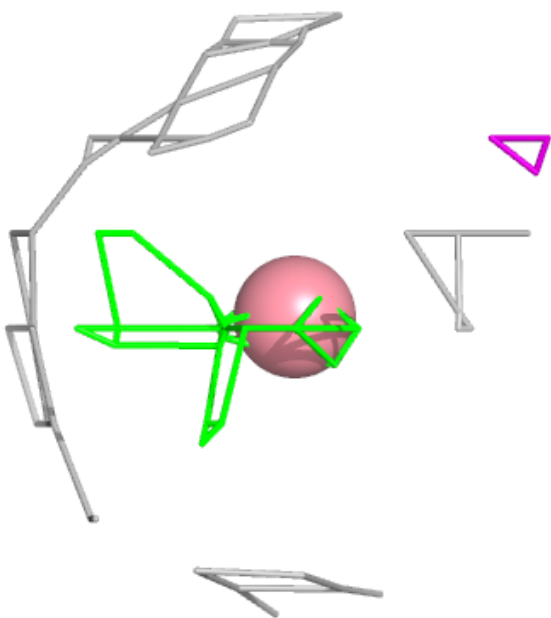
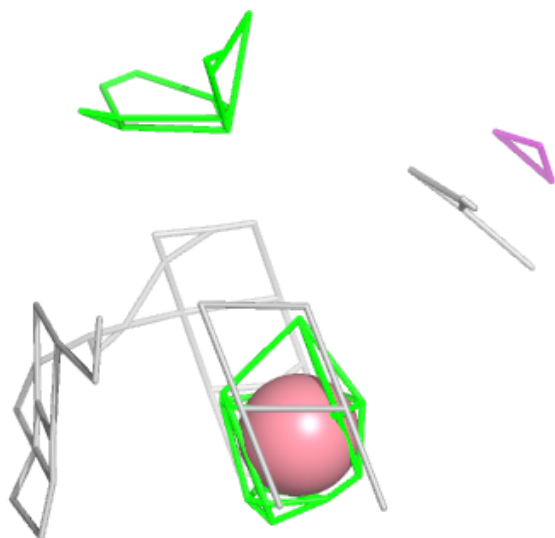
**Electron density around CO C 401:**

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



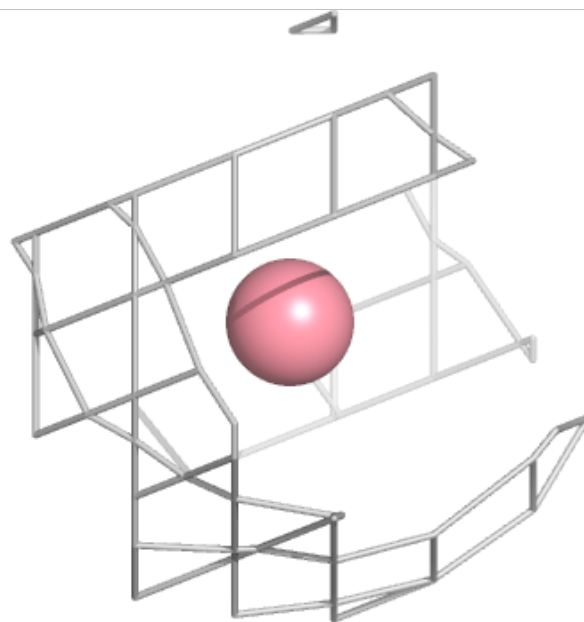
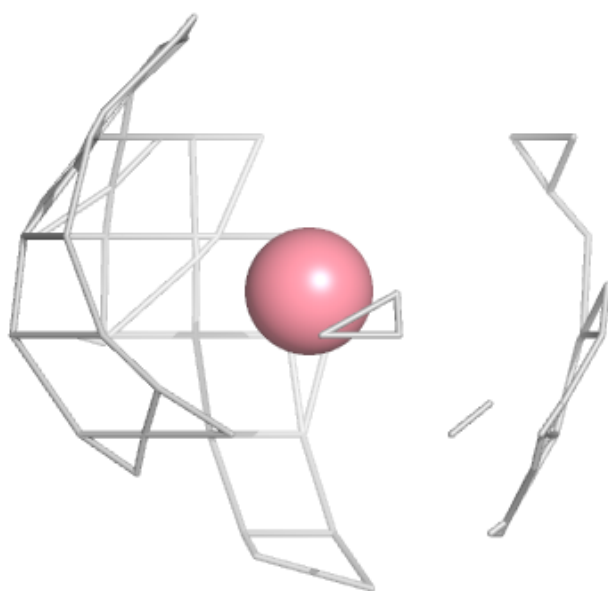
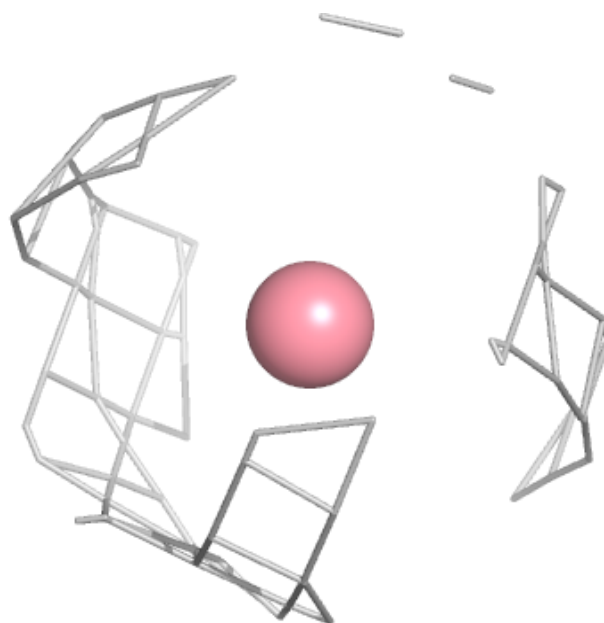
**Electron density around CO B 401:**

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



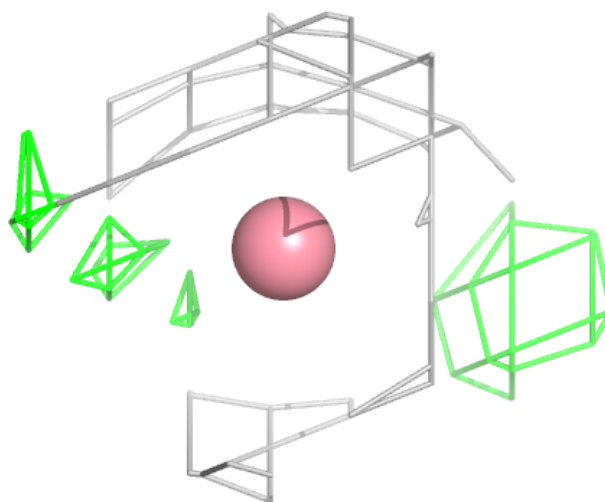
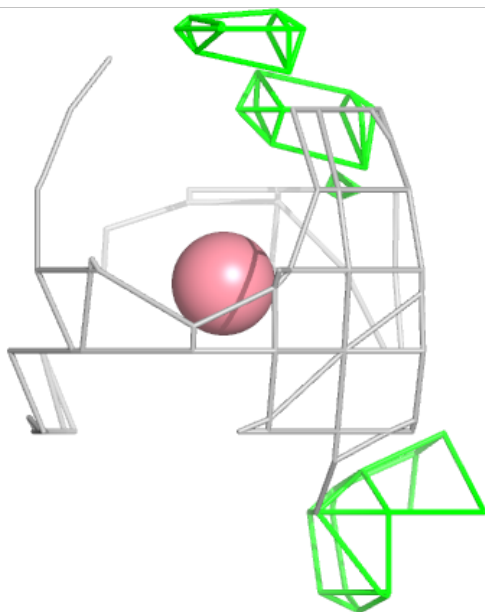
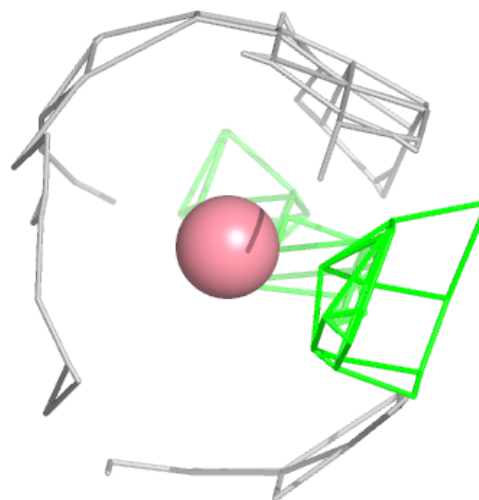
**Electron density around CO G 401:**

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



**Electron density around CO A 401:**

$2mF_o-DF_c$  (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.