



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:17 PM UTC

PDB ID : 7XNT / pdb_00007xnt
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

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

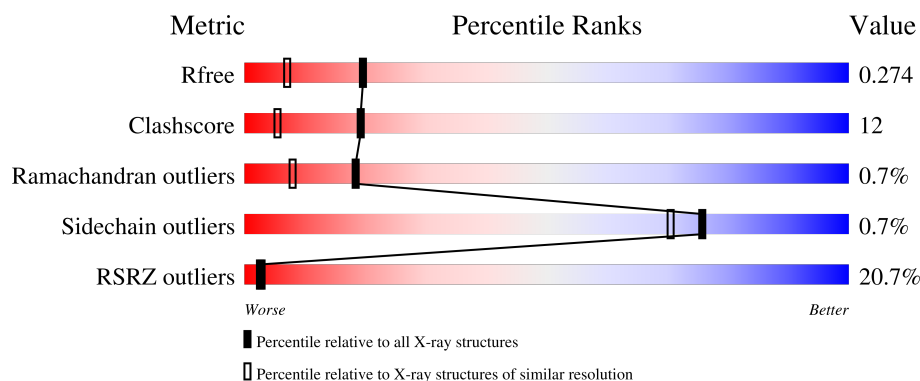
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	357	
1	B	357	
1	C	357	
1	G	357	

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 (CCD ID: CO) (formula: Co) (labeled as "Ligand of Interest" by depositor).

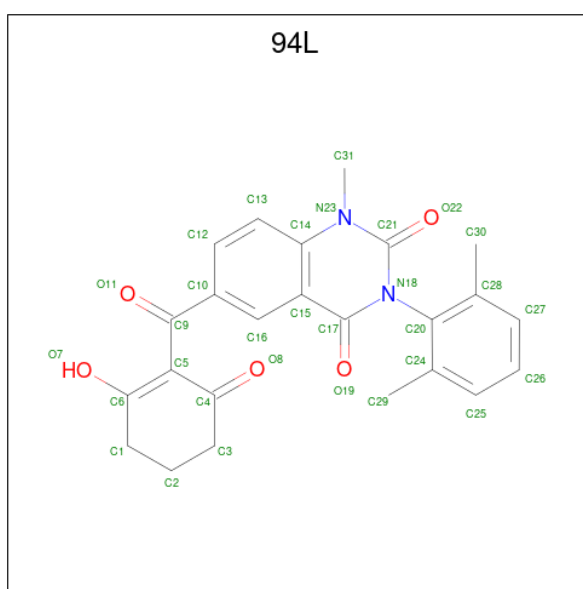
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Co	0	0
			1	1		

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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 (CCD ID: 94L) (formula: C₂₄H₂₂N₂O₅) (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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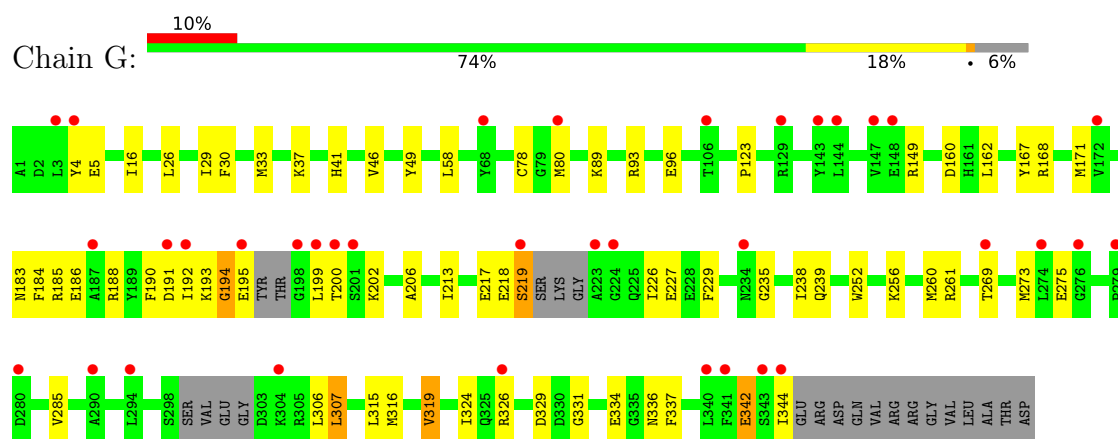
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	151	Total 151	O 151	0	0
4	B	49	Total 49	O 49	0	0
4	C	41	Total 41	O 41	0	0

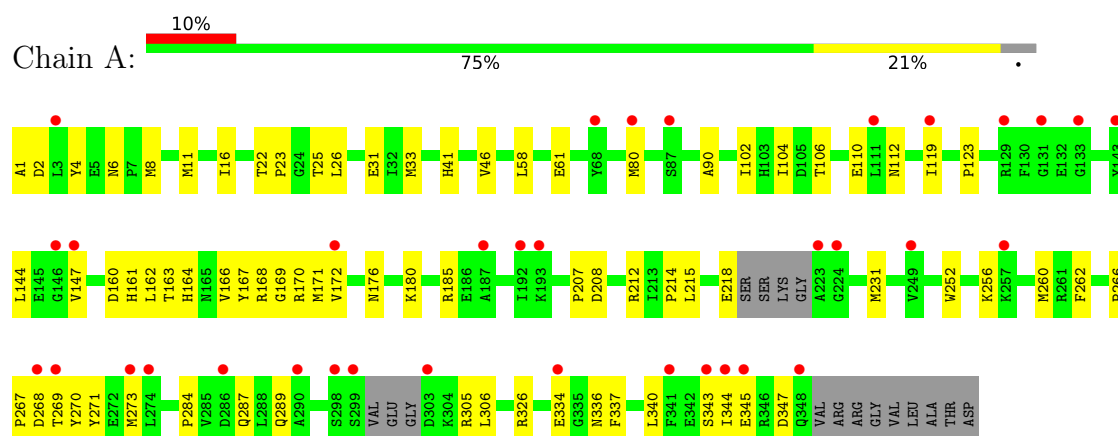
3 Residue-property plots [i](#)

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.

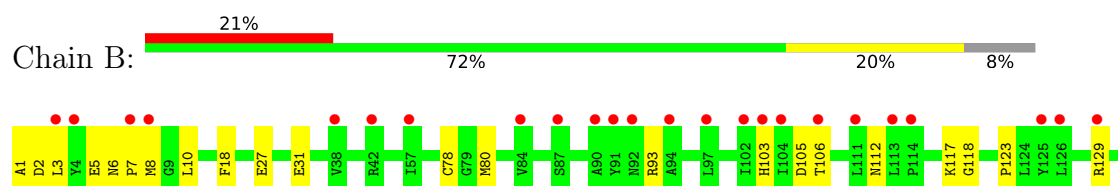
- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

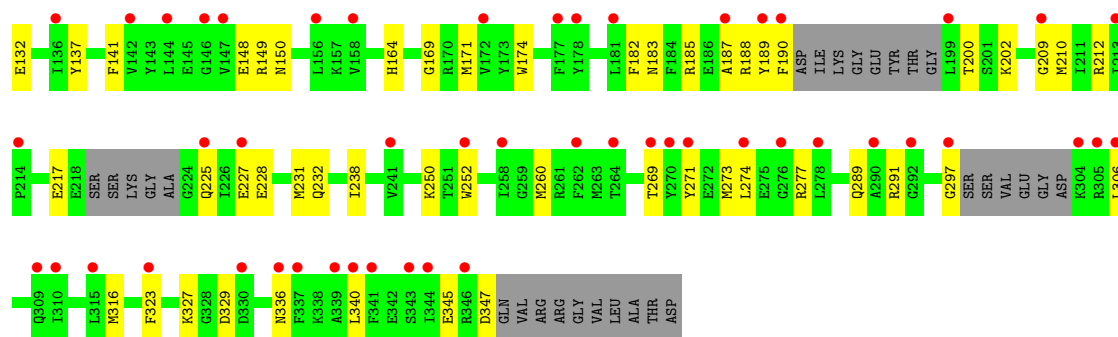


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase

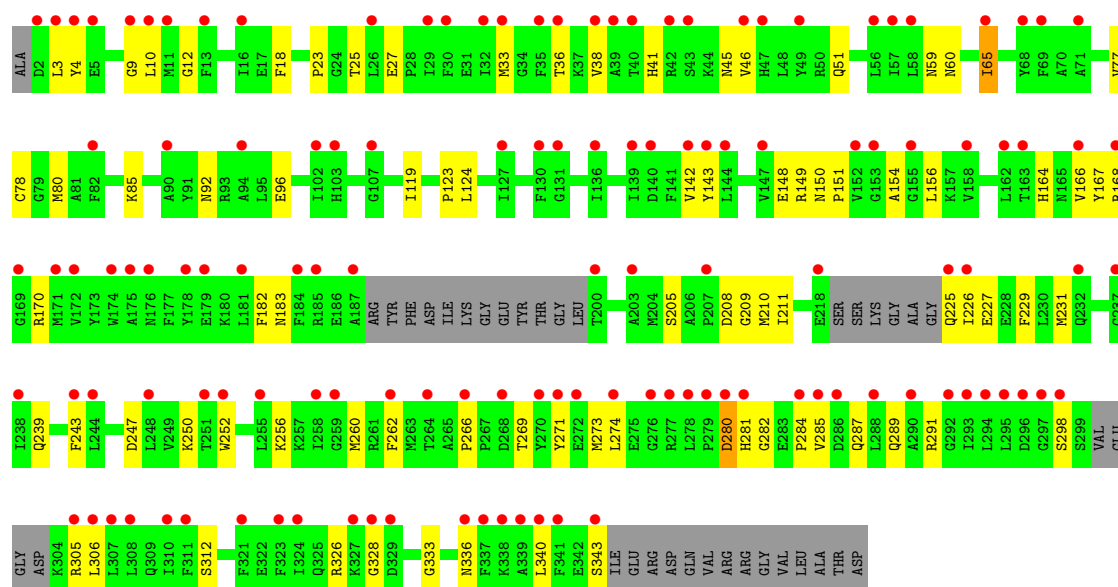


- Molecule 1: 4-hydroxyphenylpyruvate dioxygenase





• Molecule 1: 4-hydroxyphenylpyruvate dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.94Å 73.04Å 87.96Å 66.13° 79.56° 69.10°	Depositor
Resolution (Å)	34.90 – 1.82 34.90 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (34.90-1.82) 97.8 (34.90-1.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.238 , 0.271 0.241 , 0.274	Depositor DCC
R_{free} test set	6501 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: 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	0.53	2/2749 (0.1%)	0.73	1/3713 (0.0%)
1	B	0.30	0/2617	0.52	0/3538
1	C	0.30	0/2518	0.53	0/3409
1	G	0.54	2/2685 (0.1%)	0.69	2/3626 (0.1%)
All	All	0.43	4/10569 (0.0%)	0.63	3/14286 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	342	GLU	C-O	-5.73	1.17	1.24
1	A	336	ASN	C-O	-5.65	1.16	1.24
1	G	336	ASN	C-O	-5.53	1.16	1.24
1	A	11	MET	CG-SD	5.18	1.93	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	307	LEU	CA-CB-CG	5.39	135.16	116.30
1	G	319	VAL	CG1-CB-CG2	-5.37	98.99	110.80
1	A	11	MET	CB-CG-SD	-5.10	97.39	112.70

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	2684	0	2592	68	0
1	B	2555	0	2449	47	0
1	C	2458	0	2347	75	0
1	G	2622	0	2535	55	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	239	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 12.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:MET:HG2	1:A:260:MET:HE1	1.42	0.99
1:G:33:MET:HG2	1:G:260:MET:HE1	1.54	0.89
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: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
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:B:80:MET:HE2	1:B:238:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:186:GLU:CD	1:G:202:LYS:HD2	2.16	0.70
1:A:284:PRO:HB2	1:A:287:GLN:HG3	1.75	0.69
1:B:171:MET:HE3	1:B:217:GLU:HG2	1.74	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:C:208:ASP:HB2	1:C:210:MET:HE3	1.78	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: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:A:168:ARG:HB3	1:B:231:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:171:MET:HE3	1:G:202:LYS:HE2	1.86	0.58
1:C:80:MET:HE3	1:C:124:LEU:HD13	1.86	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: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:33:MET:HG2	1:G:260:MET:CE	2.33	0.55
1:G:261:ARG:HD2	1:A:23:PRO:HD2	1.87	0.55
1:G:219:SER:O	1:G:219:SER:OG	2.17	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:273:MET:HE1	1:G:342:GLU:HB3	1.89	0.55
1:G:167:TYR:OH	1:G:235:GLY:HA2	2.07	0.55
1:A:1:ALA:H3	1:A:6:ASN:HD22	1.55	0.54
1:B:345:GLU:C	4:B:512:HOH:O	2.50	0.54
1:A:334:GLU:C	4:A:505:HOH:O	2.51	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:8:MET:HE2	1:B:93:ARG:HG2	1.93	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:C:227:GLU:H	1:C:227:GLU:CD	2.19	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: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:C:260:MET:HA	1:C:260:MET:HE2	1.94	0.49
1:G:188:ARG:NH2	1:G:190:PHE:HB2	2.28	0.49
1:B:10:LEU:HD11	1:B:182:PHE:HB3	1.94	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:B:183:ASN:OD1	1:B:185:ARG:NH2	2.46	0.49
1:C:33:MET:HG2	1:C:260:MET:HE1	1.96	0.48
1:A:8:MET:HE1	1:A:90:ALA:O	2.13	0.48
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:HIS:HB2	1:G:46:VAL:CG2	2.40	0.47
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:B:80:MET:HE1	1:B:164:HIS:CE1	2.50	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:G:149:ARG:NH1	4:G:504:HOH:O	2.28	0.45
1:B:80:MET:HE1	1:B:164:HIS:HE1	1.80	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:B:117:LYS:HZ3	1:B:174:TRP:HH2	1.62	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: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:A:171:MET:HE2	1:A:215:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:260:MET:HE2	1:B:323:PHE:CZ	2.54	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:A:231:MET:HE3	1:B:169:GLY:HA3	2.01	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:A:41:HIS:HE1	1:A:110:GLU:CD	2.26	0.42
1:A:171:MET:HE3	1:A:171:MET:HB2	1.74	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:C:273:MET:HE1	1:C:343:SER:CB	2.49	0.42
1:A:268:ASP:OD1	4:A:501:HOH:O	2.22	0.42
1:G:171:MET:HE3	1:G:202:LYS:CE	2.50	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:A:305:ARG:C	1:A:306:LEU:HD12	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:163:THR:HB	1:A:214:PRO:HB2	2.03	0.40
1:B:18:PHE:CE2	1:B:316:MET:HE1	2.57	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:C:149:ARG:C	1:C:151:PRO:HD3	2.47	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

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	335/357 (94%)	328 (98%)	6 (2%)	1 (0%)	36	26
1	B	320/357 (90%)	312 (98%)	6 (2%)	2 (1%)	21	11
1	C	312/357 (87%)	302 (97%)	6 (2%)	4 (1%)	9	2
1	G	327/357 (92%)	316 (97%)	9 (3%)	2 (1%)	21	11
All	All	1294/1428 (91%)	1258 (97%)	27 (2%)	9 (1%)	18	8

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
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%)	276 (100%)	1 (0%)	84	81
1	B	259/296 (88%)	258 (100%)	1 (0%)	84	81
1	C	247/296 (83%)	246 (100%)	1 (0%)	84	81
1	G	270/296 (91%)	266 (98%)	4 (2%)	57	46
All	All	1053/1184 (89%)	1046 (99%)	7 (1%)	76	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	219	SER
1	G	306	LEU
1	G	307	LEU
1	G	344	ILE
1	A	347	ASP
1	B	200	THR
1	C	298	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	103	HIS

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Mol	Chain	Res	Type
1	G	232	GLN
1	G	336	ASN
1	A	6	ASN
1	A	103	HIS
1	A	164	HIS
1	B	6	ASN
1	B	216	ASN
1	B	336	ASN
1	C	51	GLN
1	C	183	ASN
1	C	216	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	94L	C	402	2	34,34,34	2.00	11 (32%)	47,51,51	1.75	12 (25%)
3	94L	G	402	2	34,34,34	2.05	10 (29%)	47,51,51	1.86	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	94L	A	402	2	34,34,34	2.02	9 (26%)	47,51,51	1.86	10 (21%)
3	94L	B	402	2	34,34,34	2.12	11 (32%)	47,51,51	1.90	11 (23%)

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

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	94L	C15-C17	-6.18	1.35	1.47
3	A	402	94L	C15-C17	-6.12	1.35	1.47
3	G	402	94L	C15-C17	-6.11	1.35	1.47
3	C	402	94L	C15-C17	-6.02	1.35	1.47
3	B	402	94L	C17-N18	-4.44	1.32	1.40
3	G	402	94L	C17-N18	-4.31	1.32	1.40
3	G	402	94L	C14-N23	-4.25	1.32	1.40
3	C	402	94L	C14-N23	-4.21	1.32	1.40
3	B	402	94L	C14-N23	-4.16	1.32	1.40
3	A	402	94L	C14-N23	-3.89	1.32	1.40
3	A	402	94L	C17-N18	-3.71	1.33	1.40
3	C	402	94L	C17-N18	-3.61	1.33	1.40
3	B	402	94L	C5-C4	3.24	1.53	1.45
3	C	402	94L	C5-C4	3.16	1.53	1.45
3	G	402	94L	C1-C6	2.99	1.54	1.49
3	A	402	94L	C5-C4	2.84	1.52	1.45
3	A	402	94L	C15-C14	-2.80	1.36	1.41
3	C	402	94L	O7-C6	2.75	1.40	1.32
3	G	402	94L	C5-C4	2.71	1.52	1.45
3	B	402	94L	C15-C14	-2.70	1.36	1.41
3	C	402	94L	C15-C14	-2.67	1.36	1.41
3	B	402	94L	O7-C6	2.67	1.40	1.32
3	A	402	94L	O7-C6	2.58	1.39	1.32
3	G	402	94L	C15-C14	-2.54	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	94L	C1-C6	2.52	1.53	1.49
3	B	402	94L	O22-C21	-2.48	1.17	1.22
3	A	402	94L	C21-N18	-2.45	1.35	1.40
3	G	402	94L	C21-N23	-2.45	1.35	1.38
3	C	402	94L	O11-C9	-2.40	1.18	1.23
3	G	402	94L	O7-C6	2.38	1.39	1.32
3	G	402	94L	O19-C17	-2.33	1.17	1.22
3	B	402	94L	O11-C9	-2.31	1.18	1.23
3	C	402	94L	C5-C6	-2.24	1.32	1.39
3	A	402	94L	C5-C6	-2.23	1.32	1.39
3	C	402	94L	C1-C6	2.15	1.53	1.49
3	C	402	94L	C10-C9	2.14	1.53	1.49
3	B	402	94L	O8-C4	-2.12	1.18	1.23
3	G	402	94L	C5-C6	-2.11	1.32	1.39
3	B	402	94L	C5-C6	-2.10	1.32	1.39
3	C	402	94L	O8-C4	-2.05	1.19	1.23
3	A	402	94L	C21-N23	-2.03	1.35	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	94L	C17-N18-C21	-6.20	119.12	125.45
3	C	402	94L	C17-N18-C21	-5.92	119.41	125.45
3	G	402	94L	C17-N18-C21	-5.32	120.03	125.45
3	A	402	94L	C1-C6-C5	-4.99	117.53	122.90
3	A	402	94L	O11-C9-C10	-4.72	110.03	120.58
3	G	402	94L	C2-C3-C4	-4.67	104.59	113.57
3	A	402	94L	C17-N18-C21	-4.60	120.75	125.45
3	A	402	94L	C10-C9-C5	4.27	129.83	120.06
3	G	402	94L	C15-C17-N18	4.16	120.38	114.69
3	B	402	94L	C15-C17-N18	4.08	120.27	114.69
3	C	402	94L	C15-C17-N18	3.89	120.02	114.69
3	G	402	94L	O11-C9-C10	-3.88	111.90	120.58
3	B	402	94L	O11-C9-C10	-3.81	112.05	120.58
3	C	402	94L	C10-C9-C5	3.63	128.37	120.06
3	B	402	94L	C10-C9-C5	3.57	128.24	120.06
3	B	402	94L	C31-N23-C21	3.32	120.77	117.34
3	A	402	94L	O7-C6-C5	-3.18	115.72	121.95
3	B	402	94L	O22-C21-N23	-3.14	119.43	122.10
3	C	402	94L	C31-N23-C21	3.10	120.54	117.34
3	G	402	94L	C10-C9-C5	3.02	126.96	120.06
3	A	402	94L	C15-C17-N18	2.99	118.78	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	94L	O11-C9-C10	-2.76	114.40	120.58
3	G	402	94L	C12-C10-C16	2.67	122.34	119.25
3	G	402	94L	O22-C21-N23	-2.62	119.88	122.10
3	B	402	94L	C28-C20-N18	2.60	122.05	118.73
3	G	402	94L	C31-N23-C21	2.44	119.87	117.34
3	C	402	94L	C28-C20-N18	2.42	121.81	118.73
3	B	402	94L	C14-N23-C21	-2.41	119.70	122.69
3	A	402	94L	C31-N23-C21	2.29	119.71	117.34
3	G	402	94L	C28-C20-N18	2.25	121.60	118.73
3	B	402	94L	C1-C6-C5	-2.23	120.50	122.90
3	A	402	94L	C28-C20-N18	2.21	121.54	118.73
3	C	402	94L	C3-C4-C5	2.20	120.99	116.94
3	C	402	94L	C25-C24-C20	2.19	121.07	117.99
3	C	402	94L	C14-N23-C21	-2.15	120.02	122.69
3	A	402	94L	C2-C1-C6	-2.15	110.28	112.49
3	C	402	94L	O8-C4-C3	-2.14	117.35	120.87
3	B	402	94L	C3-C4-C5	2.14	120.88	116.94
3	A	402	94L	C14-N23-C21	-2.12	120.05	122.69
3	C	402	94L	C2-C1-C6	2.03	114.58	112.49
3	G	402	94L	C30-C28-C20	-2.02	119.46	121.75
3	B	402	94L	O7-C6-C1	2.01	119.05	114.43
3	C	402	94L	C20-N18-C17	2.00	120.39	117.26

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

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

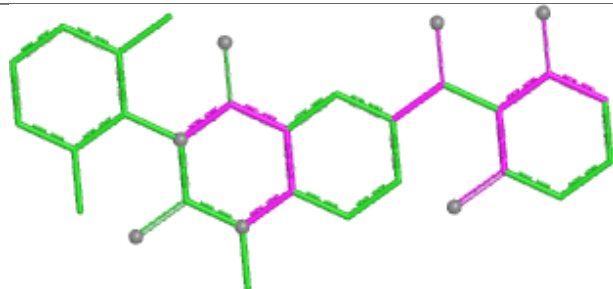
There are no ring outliers.

2 monomers are involved in 2 short contacts:

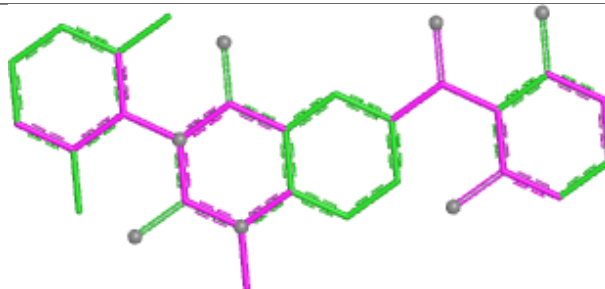
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	94L	1	0
3	B	402	94L	1	0

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.

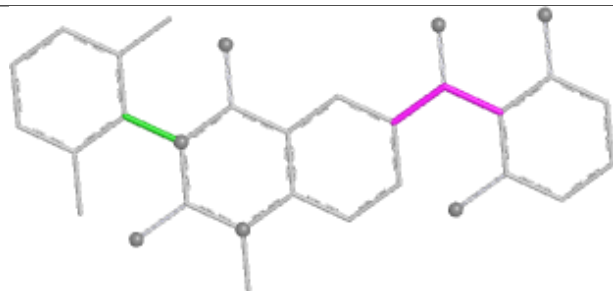
Ligand 94L C 402



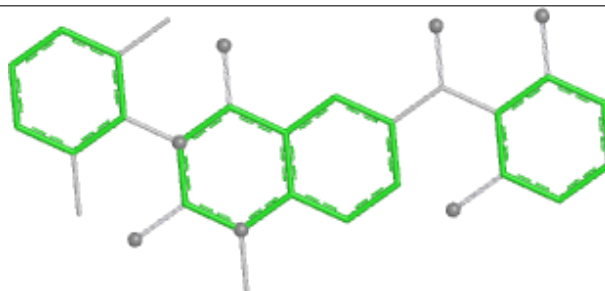
Bond lengths



Bond angles

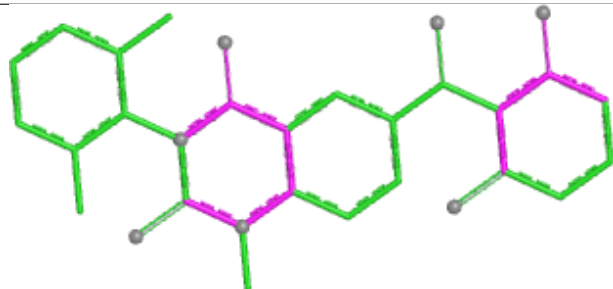


Torsions

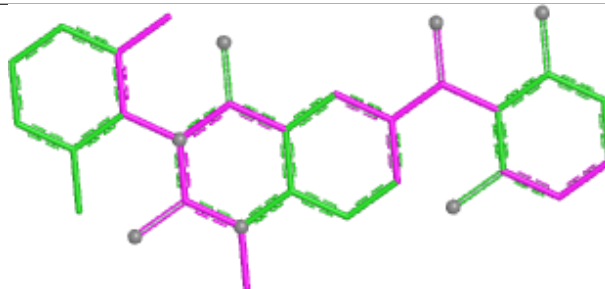


Rings

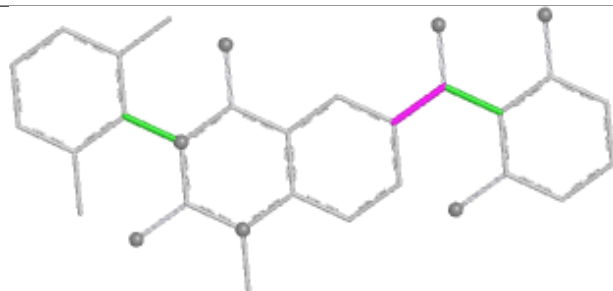
Ligand 94L G 402



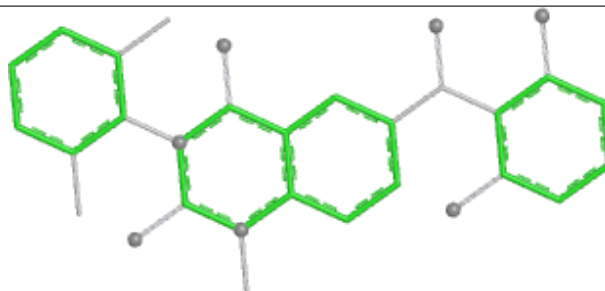
Bond lengths



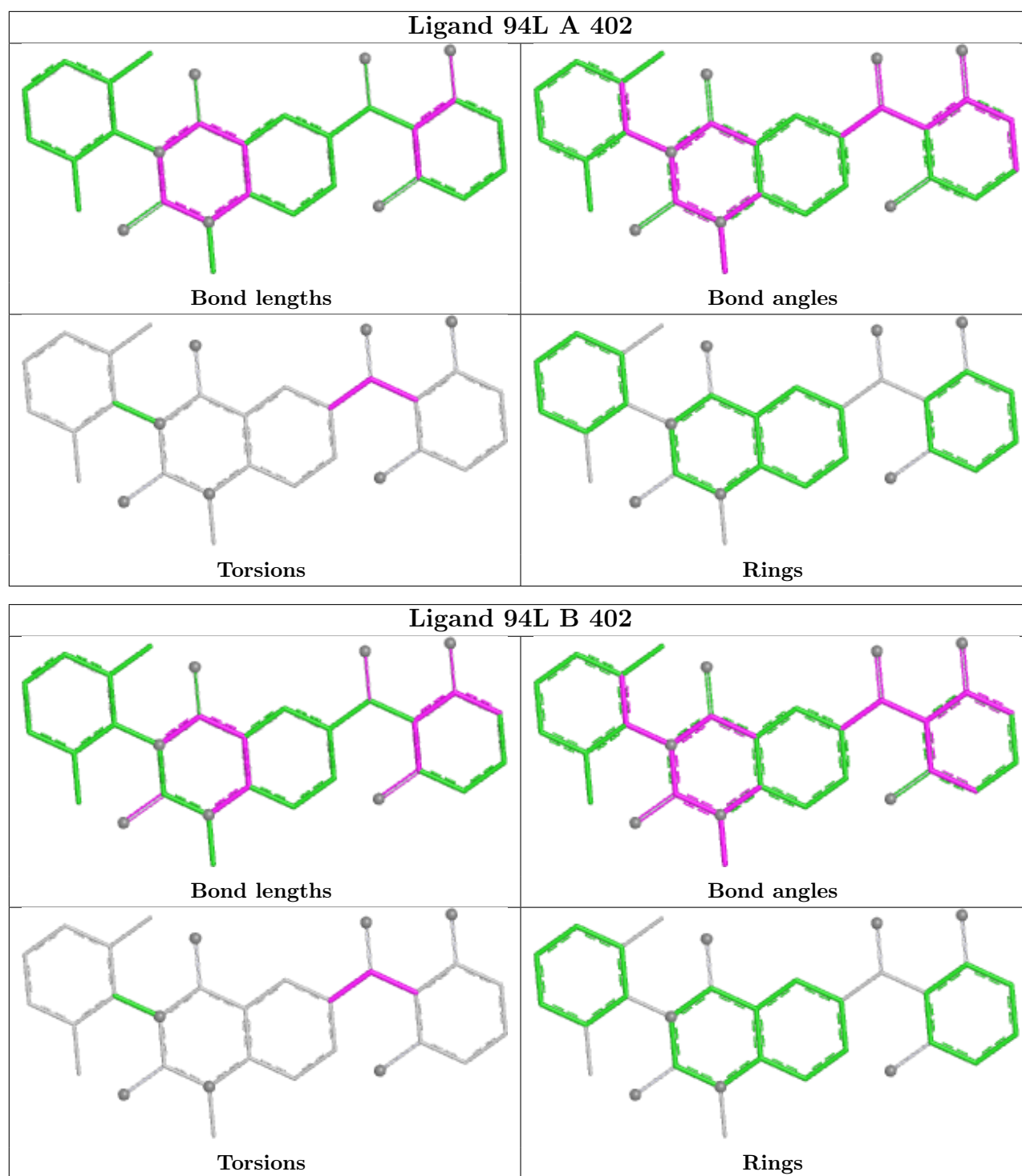
Bond angles



Torsions



Rings



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, 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	341/357 (95%)	0.86	35 (10%) 12 13	25, 36, 58, 84	0
1	B	328/357 (91%)	1.50	74 (22%) 2 2	39, 52, 72, 88	0
1	C	320/357 (89%)	1.92	129 (40%) 0 0	39, 58, 84, 92	0
1	G	335/357 (93%)	0.85	36 (10%) 11 12	23, 36, 60, 78	0
All	All	1324/1428 (92%)	1.27	274 (20%) 2 3	23, 47, 73, 92	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	ALA	7.2
1	C	172	VAL	6.3
1	G	192	ILE	6.0
1	A	192	ILE	5.6
1	C	175	ALA	5.3
1	C	308	LEU	5.1
1	C	56	LEU	5.0
1	G	143	TYR	4.9
1	A	146	GLY	4.9
1	C	341	PHE	4.8
1	C	3	LEU	4.8
1	A	223	ALA	4.6
1	B	214	PRO	4.6
1	G	195	GLU	4.5
1	C	288	LEU	4.5
1	C	292	GLY	4.5
1	B	142	VAL	4.4
1	C	297	GLY	4.4
1	C	4	TYR	4.3
1	G	234	ASN	4.3
1	C	293	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	90	ALA	4.1
1	A	3	LEU	4.1
1	A	299	SER	4.1
1	B	190	PHE	4.0
1	C	46	VAL	4.0
1	C	290	ALA	4.0
1	A	348	GLN	4.0
1	C	248	LEU	4.0
1	C	329	ASP	3.9
1	B	297	GLY	3.9
1	C	42	ARG	3.9
1	B	136	ILE	3.9
1	C	306	LEU	3.8
1	B	341	PHE	3.8
1	A	268	ASP	3.8
1	C	142	VAL	3.7
1	C	147	VAL	3.7
1	C	298	SER	3.7
1	C	285	VAL	3.7
1	C	30	PHE	3.7
1	C	279	PRO	3.6
1	G	223	ALA	3.6
1	B	337	PHE	3.5
1	B	111	LEU	3.5
1	G	172	VAL	3.5
1	B	126	LEU	3.5
1	B	343	SER	3.5
1	G	147	VAL	3.5
1	C	310	ILE	3.4
1	C	184	PHE	3.4
1	A	68	TYR	3.4
1	C	271	TYR	3.3
1	A	298	SER	3.3
1	C	286	ASP	3.3
1	C	2	ASP	3.3
1	C	143	TYR	3.3
1	C	169	GLY	3.3
1	C	272	GLU	3.2
1	C	178	TYR	3.2
1	C	281	HIS	3.2
1	B	158	VAL	3.2
1	B	181	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	323	PHE	3.2
1	C	337	PHE	3.2
1	A	143	TYR	3.2
1	B	340	LEU	3.2
1	B	269	THR	3.1
1	C	65	ILE	3.1
1	C	252	TRP	3.1
1	B	227	GLU	3.1
1	A	341	PHE	3.1
1	G	200	THR	3.1
1	B	3	LEU	3.1
1	B	274	LEU	3.1
1	C	49	TYR	3.1
1	C	340	LEU	3.1
1	A	343	SER	3.1
1	C	274	LEU	3.0
1	B	178	TYR	3.0
1	B	189	TYR	3.0
1	C	43	SER	3.0
1	C	140	ASP	3.0
1	A	80	MET	3.0
1	A	129	ARG	3.0
1	C	176	ASN	3.0
1	C	158	VAL	2.9
1	G	198	GLY	2.9
1	A	269	THR	2.9
1	A	345	GLU	2.9
1	B	344	ILE	2.9
1	C	162	LEU	2.9
1	C	9	GLY	2.9
1	C	58	LEU	2.9
1	G	224	GLY	2.9
1	B	4	TYR	2.9
1	C	321	PHE	2.9
1	A	303	ASP	2.9
1	C	268	ASP	2.9
1	B	125	TYR	2.8
1	G	280	ASP	2.8
1	B	57	ILE	2.8
1	C	32	ILE	2.8
1	C	295	LEU	2.8
1	G	219	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	225	GLN	2.8
1	A	119	ILE	2.8
1	C	26	LEU	2.8
1	C	294	LEU	2.8
1	B	144	LEU	2.8
1	C	307	LEU	2.8
1	A	344	ILE	2.8
1	B	187	ALA	2.7
1	C	155	GLY	2.7
1	G	269	THR	2.7
1	B	278	LEU	2.7
1	C	255	LEU	2.7
1	A	286	ASP	2.7
1	C	136	ILE	2.7
1	C	171	MET	2.7
1	B	172	VAL	2.7
1	B	264	THR	2.7
1	C	258	ILE	2.7
1	B	304	LYS	2.7
1	A	133	GLY	2.7
1	C	39	ALA	2.6
1	C	270	TYR	2.6
1	A	87	SER	2.6
1	B	104	ILE	2.6
1	C	29	ILE	2.6
1	B	146	GLY	2.6
1	C	71	ALA	2.6
1	B	252	TRP	2.6
1	C	278	LEU	2.6
1	G	80	MET	2.6
1	C	131	GLY	2.6
1	A	257	LYS	2.6
1	B	114	PRO	2.6
1	B	315	LEU	2.6
1	C	107	GLY	2.6
1	B	147	VAL	2.6
1	C	33	MET	2.5
1	G	144	LEU	2.5
1	G	344	ILE	2.5
1	B	213	ILE	2.5
1	C	336	ASN	2.5
1	B	241	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	68	TYR	2.5
1	B	91	TYR	2.5
1	C	296	ASP	2.5
1	C	13	PHE	2.5
1	C	276	GLY	2.5
1	B	258	ILE	2.5
1	C	174	TRP	2.5
1	G	343	SER	2.5
1	C	203	ALA	2.5
1	A	172	VAL	2.5
1	C	200	THR	2.5
1	C	225	GLN	2.5
1	A	224	GLY	2.5
1	B	306	LEU	2.5
1	B	305	ARG	2.5
1	B	346	ARG	2.5
1	C	5	GLU	2.5
1	G	290	ALA	2.5
1	G	304	LYS	2.5
1	C	237	GLY	2.4
1	C	181	LEU	2.4
1	C	40	THR	2.4
1	C	327	LYS	2.4
1	G	279	PRO	2.4
1	C	152	VAL	2.4
1	C	10	LEU	2.4
1	C	163	THR	2.4
1	G	187	ALA	2.4
1	G	340	LEU	2.4
1	C	244	LEU	2.4
1	B	106	THR	2.4
1	C	57	ILE	2.4
1	A	334	GLU	2.4
1	B	87	SER	2.4
1	C	218	GLU	2.3
1	C	251	THR	2.3
1	C	264	THR	2.3
1	B	310	ILE	2.3
1	C	90	ALA	2.3
1	C	47	HIS	2.3
1	C	338	LYS	2.3
1	B	38	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	168	ARG	2.3
1	G	274	LEU	2.3
1	C	144	LEU	2.3
1	B	271	TYR	2.3
1	B	323	PHE	2.3
1	C	243	PHE	2.3
1	A	290	ALA	2.3
1	B	209	GLY	2.3
1	G	148	GLU	2.3
1	B	199	LEU	2.3
1	C	36	THR	2.3
1	B	262	PHE	2.3
1	B	270	TYR	2.3
1	C	35	PHE	2.3
1	C	69	PHE	2.3
1	C	262	PHE	2.3
1	B	7	PRO	2.3
1	C	266	PRO	2.3
1	G	129	ARG	2.3
1	B	42	ARG	2.3
1	C	343	SER	2.3
1	G	3	LEU	2.3
1	G	4	TYR	2.2
1	C	38	VAL	2.2
1	G	199	LEU	2.2
1	B	276	GLY	2.2
1	C	284	PRO	2.2
1	C	82	PHE	2.2
1	B	102	ILE	2.2
1	B	8	MET	2.2
1	B	336	ASN	2.2
1	C	11	MET	2.2
1	C	305	ARG	2.2
1	B	84	VAL	2.2
1	C	153	GLY	2.2
1	B	290	ALA	2.2
1	C	94	ALA	2.2
1	B	177	PHE	2.2
1	C	16	ILE	2.2
1	C	127	ILE	2.2
1	B	92	ASN	2.2
1	C	103	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	179	GLU	2.2
1	C	166	VAL	2.2
1	B	97	LEU	2.2
1	A	187	ALA	2.2
1	G	326	ARG	2.2
1	C	185	ARG	2.2
1	A	273	MET	2.1
1	G	341	PHE	2.1
1	C	130	PHE	2.1
1	G	106	THR	2.1
1	B	292	GLY	2.1
1	C	339	ALA	2.1
1	C	139	ILE	2.1
1	C	324	ILE	2.1
1	G	201	SER	2.1
1	A	131	GLY	2.1
1	B	156	LEU	2.1
1	B	309	GLN	2.1
1	B	339	ALA	2.1
1	G	191	ASP	2.1
1	C	102	ILE	2.1
1	B	129	ARG	2.1
1	C	259	GLY	2.1
1	B	103	HIS	2.1
1	C	232	GLN	2.1
1	G	294	LEU	2.1
1	B	113	LEU	2.1
1	B	330	ASP	2.1
1	C	280	ASP	2.1
1	C	277	ARG	2.1
1	C	238	ILE	2.0
1	C	311	PHE	2.0
1	C	68	TYR	2.0
1	G	276	GLY	2.0
1	A	111	LEU	2.0
1	A	274	LEU	2.0
1	B	94	ALA	2.0
1	A	193	LYS	2.0
1	C	226	ILE	2.0
1	C	328	GLY	2.0
1	C	207	PRO	2.0
1	A	147	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	249	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

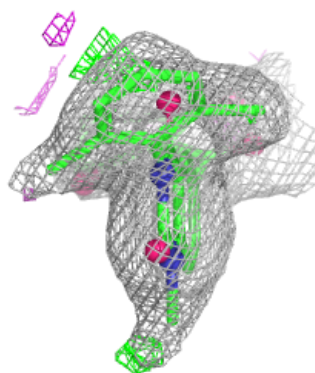
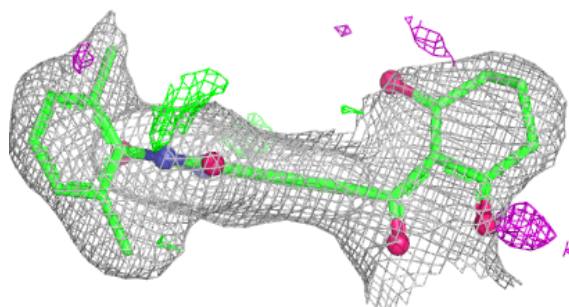
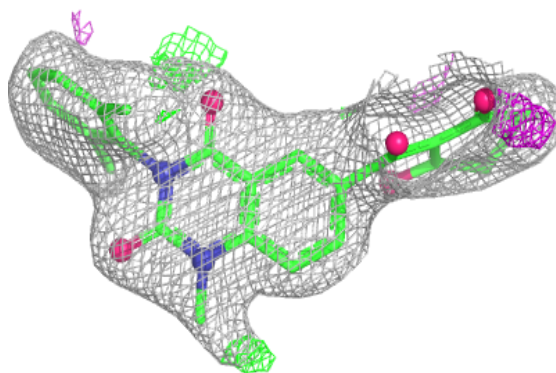
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	94L	B	402	31/31	0.84	0.13	49,54,57,58	0
3	94L	C	402	31/31	0.88	0.12	53,60,66,70	0
3	94L	G	402	31/31	0.90	0.11	33,40,44,50	0
3	94L	A	402	31/31	0.92	0.10	34,41,45,46	0
2	CO	C	401	1/1	0.98	0.07	64,64,64,64	0
2	CO	B	401	1/1	0.99	0.04	58,58,58,58	0
2	CO	G	401	1/1	0.99	0.03	27,27,27,27	0
2	CO	A	401	1/1	0.99	0.02	30,30,30,30	0

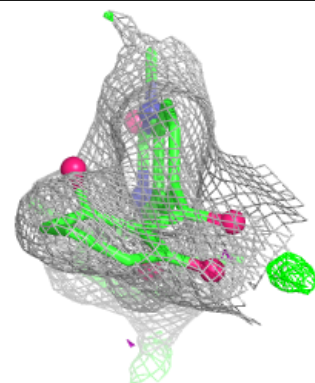
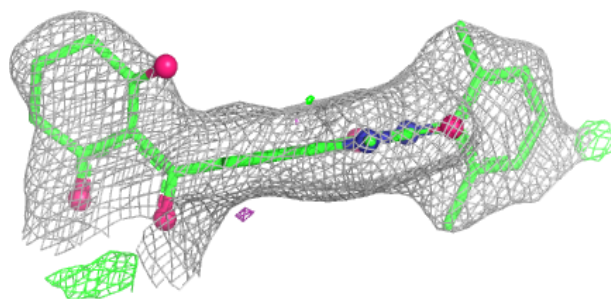
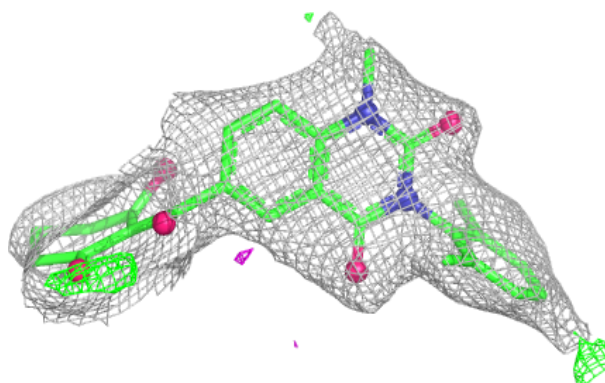
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 94L B 402:

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

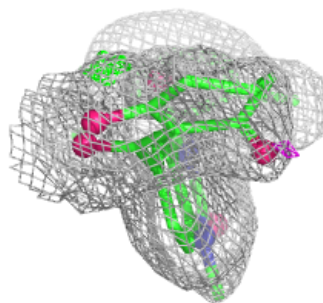
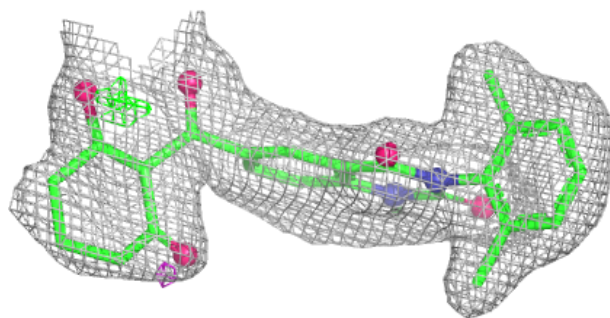
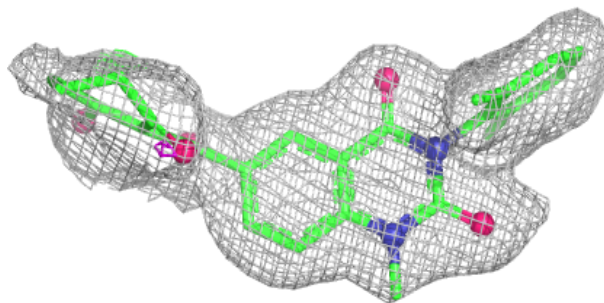
**Electron density around 94L C 402:**

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

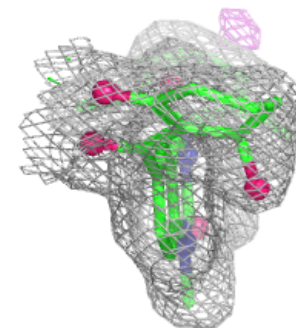
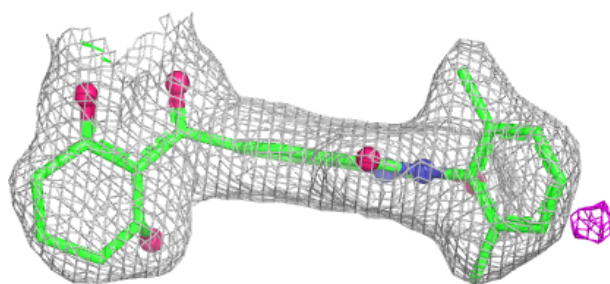
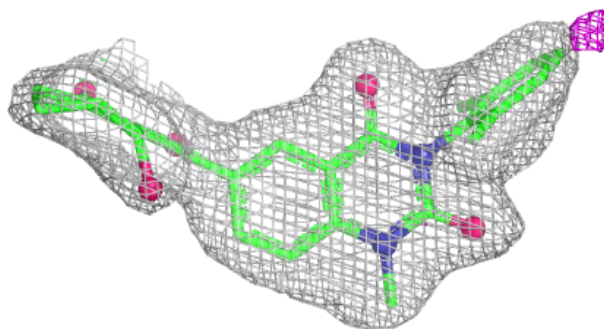


Electron density around 94L G 402:

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

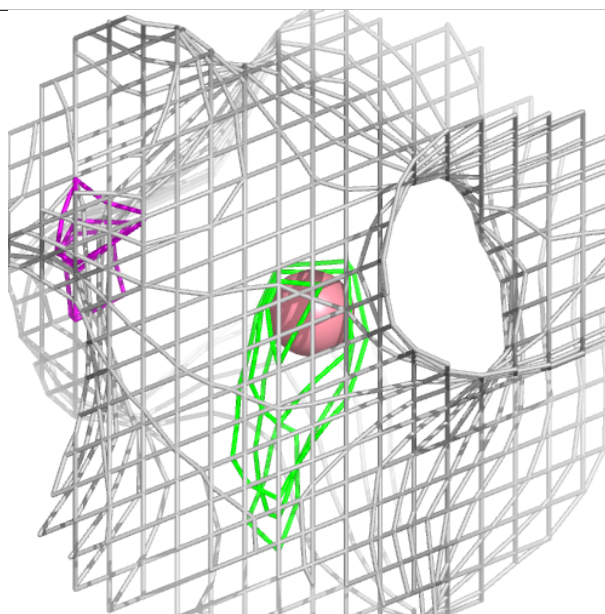
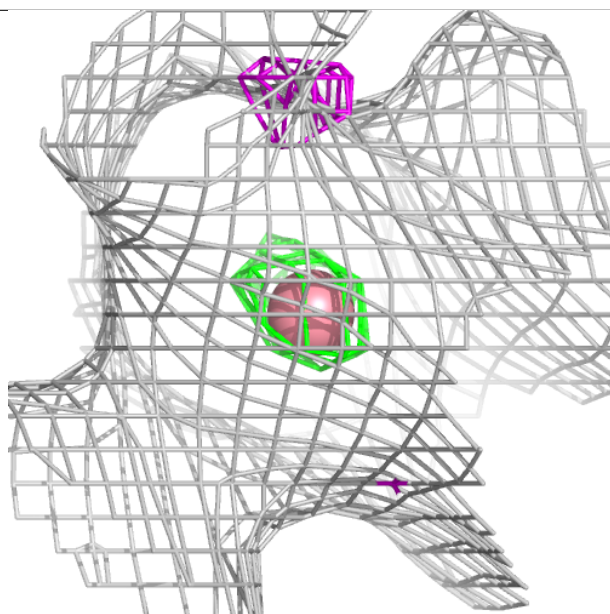
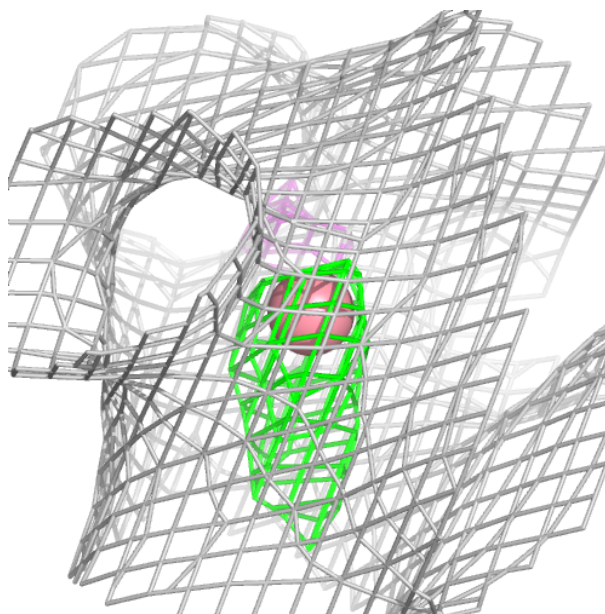
**Electron density around 94L A 402:**

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



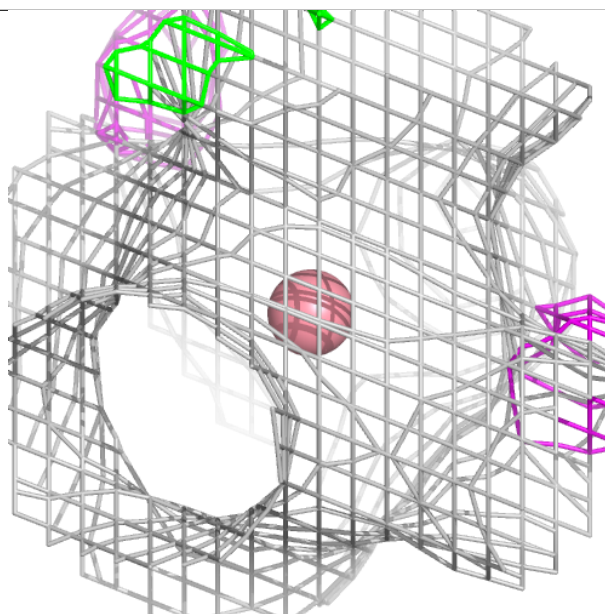
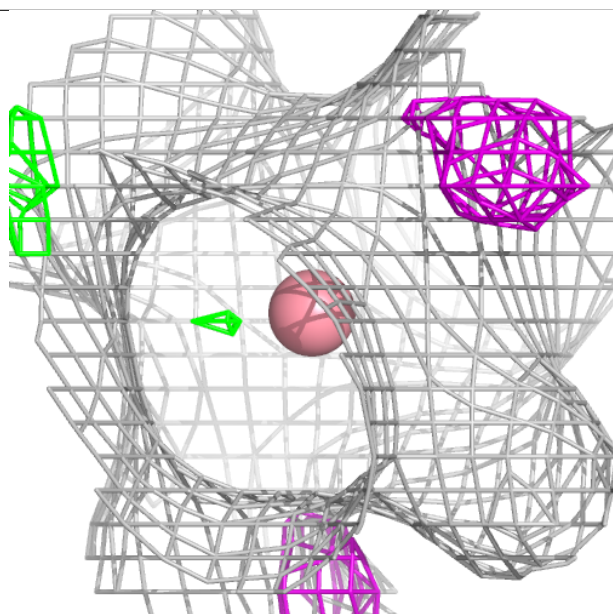
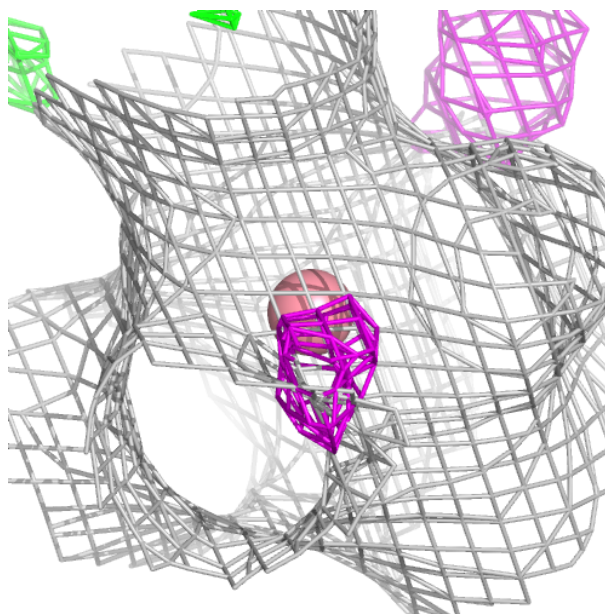
Electron density around CO C 401:

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



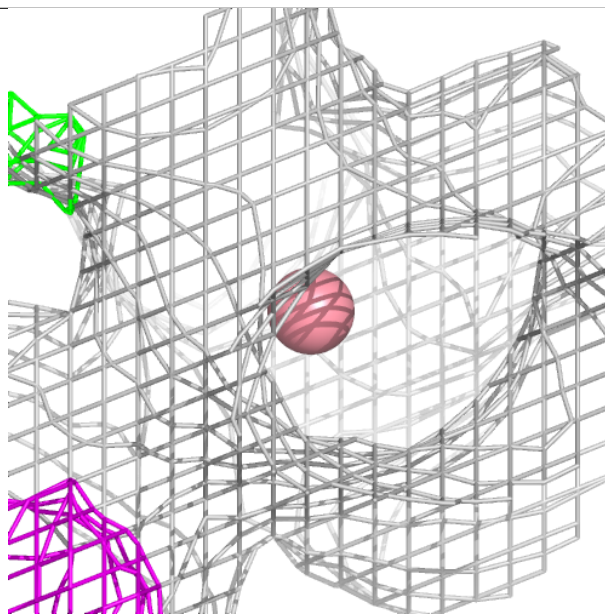
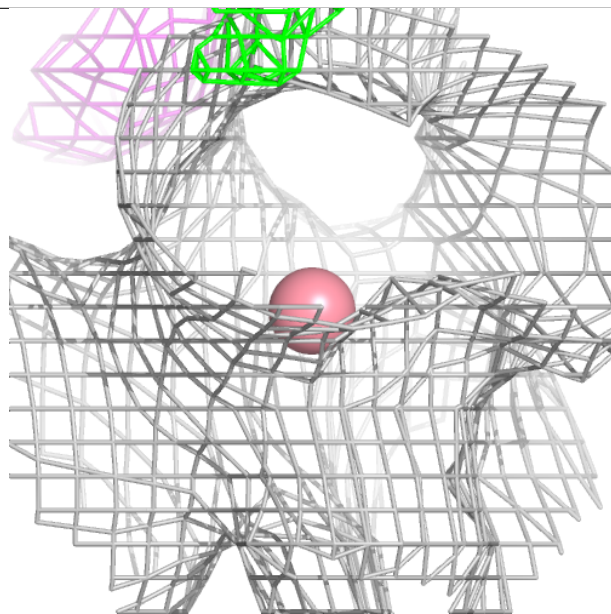
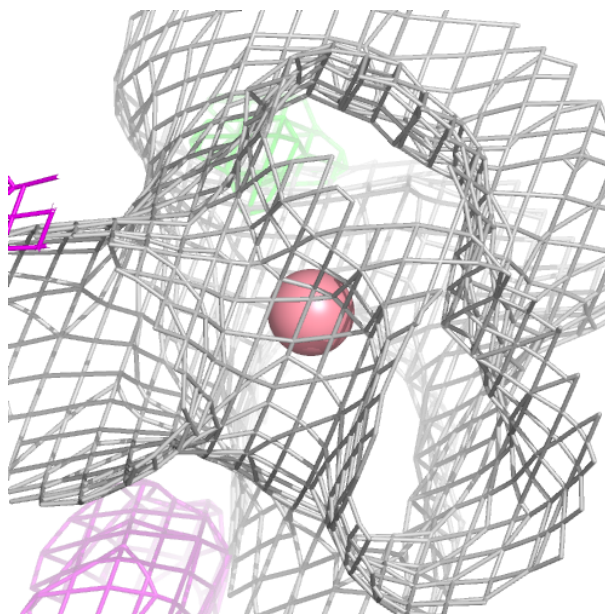
Electron density around CO B 401:

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



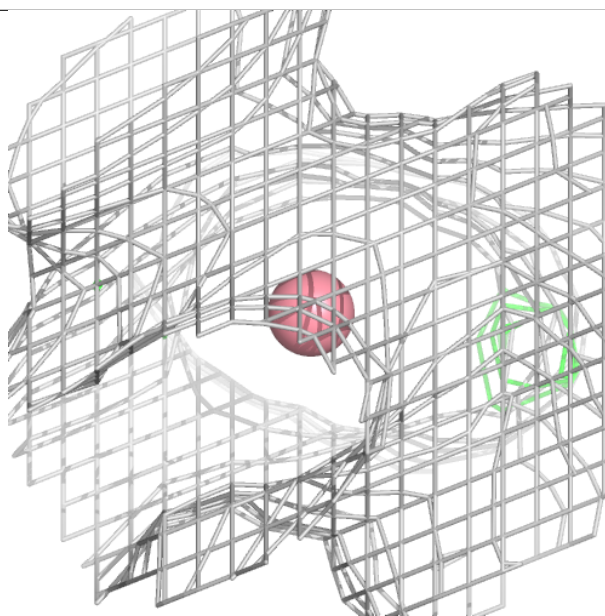
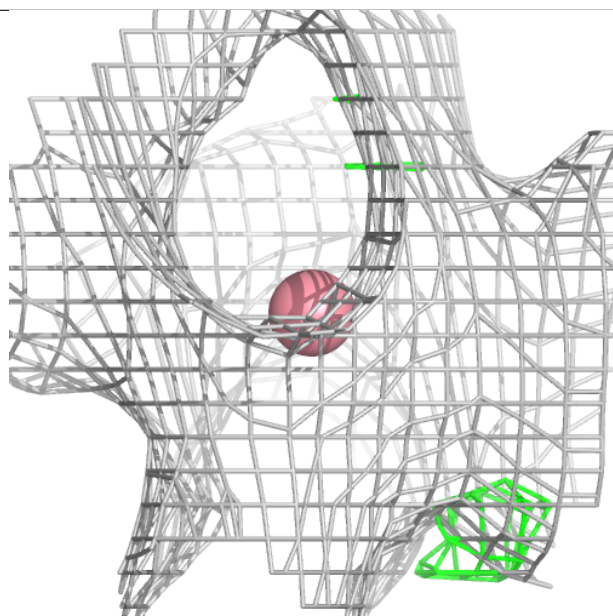
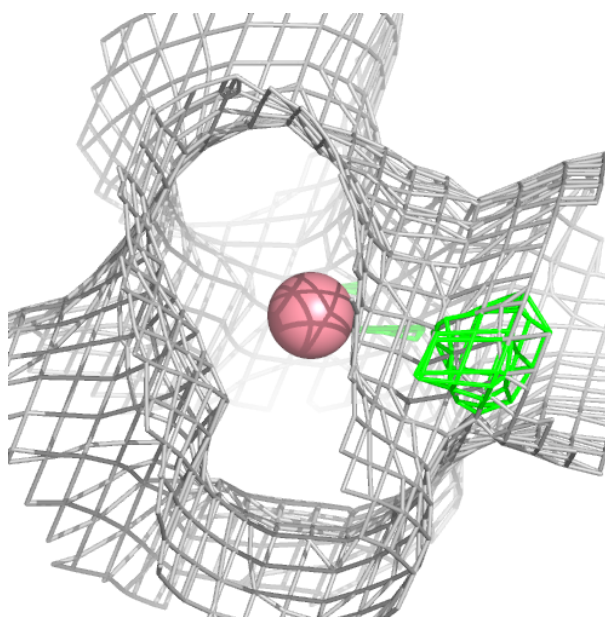
Electron density around CO G 401:

$2mF_o-DF_c$ (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.