



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 03:24 PM EST

PDB ID : 3C3D  
Title : Crystal structure of 2-phospho-(S)-lactate transferase from *Methanosarcina mazei* in complex with Fo and phosphate. Northeast Structural Genomics Consortium target MaR46  
Authors : Forouhar, F.; Abashidze, M.; Xu, H.; Grochowski, L.L.; Seetharaman, J.; Hussain, M.; Kuzin, A.P.; Chen, Y.; Zhou, W.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Galinier, A.; White, R.H.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-01-28  
Resolution : 2.50 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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11

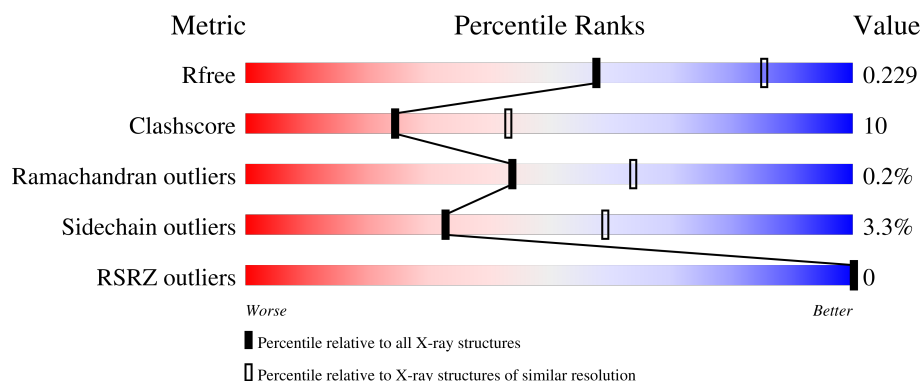
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)


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	311	 80% 17% ..
1	B	311	 74% 23% ..
1	C	311	 77% 20% ..

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.39

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Mol	Chain	Length	Quality of chain
1	D	311	 <div>79% 18% ..</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FO1	A	401	-	X	-	-
3	FO1	B	401	-	X	-	-
3	FO1	C	401	-	X	-	-
3	FO1	D	401	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10077 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 2-phospho-L-lactate transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	B	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	C	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			
1	D	306	Total	C	N	O	S	Se	0	0	0
			2371	1506	392	463	2	8			

There are 32 discrepancies between the modelled and reference sequences:

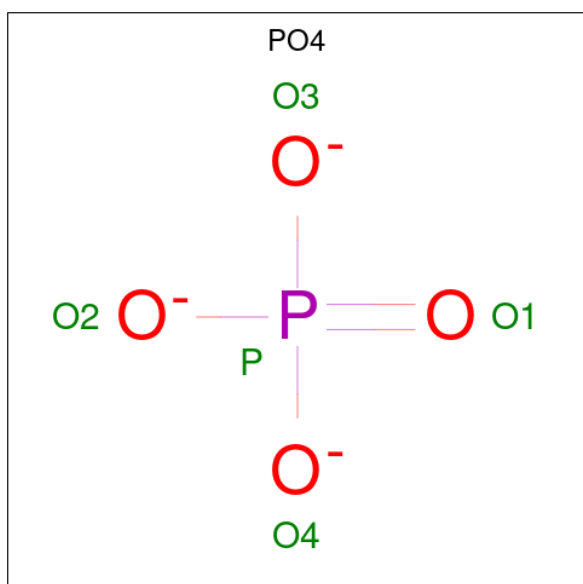
Chain	Residue	Modelled	Actual	Comment	Reference
A	304	LEU	-	expression tag	UNP Q8PVT6
A	305	GLU	-	expression tag	UNP Q8PVT6
A	306	HIS	-	expression tag	UNP Q8PVT6
A	307	HIS	-	expression tag	UNP Q8PVT6
A	308	HIS	-	expression tag	UNP Q8PVT6
A	309	HIS	-	expression tag	UNP Q8PVT6
A	310	HIS	-	expression tag	UNP Q8PVT6
A	311	HIS	-	expression tag	UNP Q8PVT6
B	304	LEU	-	expression tag	UNP Q8PVT6
B	305	GLU	-	expression tag	UNP Q8PVT6
B	306	HIS	-	expression tag	UNP Q8PVT6
B	307	HIS	-	expression tag	UNP Q8PVT6
B	308	HIS	-	expression tag	UNP Q8PVT6
B	309	HIS	-	expression tag	UNP Q8PVT6
B	310	HIS	-	expression tag	UNP Q8PVT6
B	311	HIS	-	expression tag	UNP Q8PVT6
C	304	LEU	-	expression tag	UNP Q8PVT6
C	305	GLU	-	expression tag	UNP Q8PVT6
C	306	HIS	-	expression tag	UNP Q8PVT6
C	307	HIS	-	expression tag	UNP Q8PVT6
C	308	HIS	-	expression tag	UNP Q8PVT6

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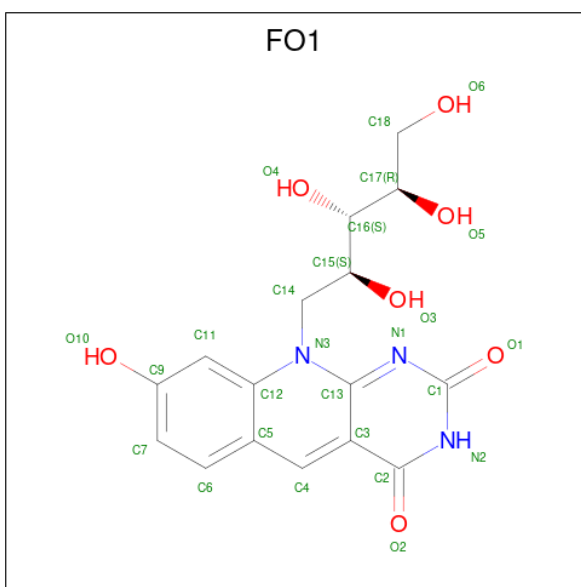
Chain	Residue	Modelled	Actual	Comment	Reference
C	309	HIS	-	expression tag	UNP Q8PVT6
C	310	HIS	-	expression tag	UNP Q8PVT6
C	311	HIS	-	expression tag	UNP Q8PVT6
D	304	LEU	-	expression tag	UNP Q8PVT6
D	305	GLU	-	expression tag	UNP Q8PVT6
D	306	HIS	-	expression tag	UNP Q8PVT6
D	307	HIS	-	expression tag	UNP Q8PVT6
D	308	HIS	-	expression tag	UNP Q8PVT6
D	309	HIS	-	expression tag	UNP Q8PVT6
D	310	HIS	-	expression tag	UNP Q8PVT6
D	311	HIS	-	expression tag	UNP Q8PVT6

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1-deoxy-1-(8-hydroxy-2,4-dioxo-3,4-dihydropyrimido[4,5-b]quinolin-10(2H)-yl)-D-ribose (three-letter code: FO1) (formula: C<sub>16</sub>H<sub>17</sub>N<sub>3</sub>O<sub>7</sub>).



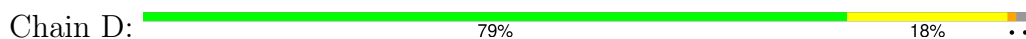
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	13	3	4		
3	B	1	Total	C	N	O	0	0
			20	13	3	4		
3	C	1	Total	C	N	O	0	0
			20	13	3	4		
3	D	1	Total	C	N	O	0	0
			20	13	3	4		

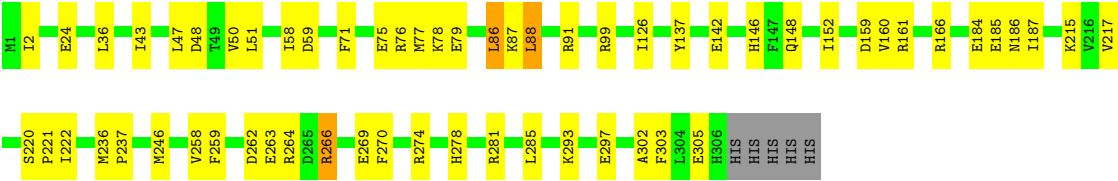
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	85	Total	O	0	0
			85	85		
4	C	90	Total	O	0	0
			90	90		
4	D	156	Total	O	0	0
			156	156		



- Molecule 1: 2-phospho-L-lactate transferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.28Å 185.28Å 67.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.50 29.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.59-2.50) 97.2 (29.59-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.195 , 0.231 0.195 , 0.229	Depositor DCC
$R_{free}$ test set	8536 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l 0.021 for h,-h-k,-l 0.021 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: PO4, FO1

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	0.39	0/2408	0.58	0/3247
1	B	0.36	0/2408	0.55	0/3247
1	C	0.36	0/2408	0.55	0/3247
1	D	0.39	0/2408	0.59	0/3247
All	All	0.37	0/9632	0.57	0/12988

There are no bond length outliers.

There are no bond angle outliers.

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	2371	0	2376	44	0
1	B	2371	0	2376	54	0
1	C	2371	0	2376	46	0
1	D	2371	0	2376	47	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	8	0	0
3	C	20	0	8	0	0
3	D	20	0	8	0	0
4	A	162	0	0	5	0
4	B	85	0	0	3	0
4	C	90	0	0	3	0
4	D	156	0	0	6	0
All	All	10077	0	9536	185	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 10.

All (185) 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:2:ILE:HG13	1:A:184:GLU:HG3	1.38	1.05
1:C:221:PRO:HG2	1:C:222:ILE:HD12	1.45	0.94
1:D:2:ILE:HG13	1:D:184:GLU:HG3	1.53	0.91
1:B:227:PRO:HG3	1:B:232:ALA:HB3	1.52	0.91
1:B:221:PRO:HG2	1:B:222:ILE:HD12	1.50	0.91
1:C:227:PRO:HG3	1:C:232:ALA:HB3	1.55	0.89
1:A:159:ASP:HB3	1:A:161:ARG:NH1	1.96	0.80
1:B:266:ARG:HD3	1:B:281:ARG:NH2	1.97	0.79
1:C:266:ARG:HD3	1:C:281:ARG:NH2	1.98	0.78
1:A:221:PRO:HG2	1:A:222:ILE:HD12	1.64	0.77
1:D:266:ARG:HB2	1:D:266:ARG:HH11	1.51	0.76
1:D:221:PRO:HG2	1:D:222:ILE:HD12	1.67	0.75
1:D:146:HIS:HB2	4:D:527:HOH:O	1.87	0.74
1:A:146:HIS:HB2	4:A:511:HOH:O	1.86	0.74
1:A:266:ARG:HH11	1:A:266:ARG:HB2	1.52	0.74
1:B:278:HIS:HB3	4:B:486:HOH:O	1.87	0.73
1:B:266:ARG:HH11	1:B:281:ARG:HH22	1.39	0.69
1:C:48:ASP:OD2	1:C:99:ARG:NH2	2.26	0.68
1:D:146:HIS:CD2	1:D:148:GLN:H	2.12	0.68
1:D:48:ASP:OD2	1:D:99:ARG:NH2	2.26	0.67
1:B:48:ASP:OD2	1:B:99:ARG:NH2	2.29	0.66
1:A:146:HIS:CD2	1:A:148:GLN:H	2.14	0.66
1:B:86:LEU:HD23	1:B:86:LEU:N	2.12	0.65
1:A:48:ASP:OD2	1:A:99:ARG:NH2	2.29	0.64
1:D:278:HIS:HB3	4:D:556:HOH:O	1.97	0.64
1:C:221:PRO:HG2	1:C:222:ILE:CD1	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ASP:HB3	1:D:161:ARG:NH1	2.13	0.63
1:B:146:HIS:CD2	1:B:148:GLN:H	2.17	0.63
1:A:262:ASP:OD1	1:A:264:ARG:HD3	2.01	0.61
1:D:266:ARG:NH1	1:D:281:ARG:HH22	1.99	0.61
1:A:184:GLU:HG2	4:A:461:HOH:O	2.00	0.60
1:A:217:VAL:HG22	1:A:258:VAL:HB	1.82	0.60
1:B:186:ASN:C	1:B:187:ILE:HD12	2.21	0.60
1:D:220:SER:HB2	1:D:259:PHE:CZ	2.36	0.60
1:C:86:LEU:HG	1:C:88:LEU:HD13	1.83	0.60
1:D:266:ARG:HH11	1:D:281:ARG:HH22	1.49	0.60
1:D:146:HIS:HD2	1:D:148:GLN:H	1.50	0.60
1:C:86:LEU:N	1:C:86:LEU:HD23	2.16	0.59
1:D:217:VAL:HG22	1:D:258:VAL:HB	1.84	0.59
1:C:24:GLU:H	1:C:24:GLU:CD	2.05	0.59
1:C:149:ASP:O	1:C:154:LYS:HG2	2.02	0.59
1:B:262:ASP:OD1	1:B:264:ARG:HD3	2.04	0.58
1:B:42:LEU:O	1:B:99:ARG:NH1	2.36	0.58
1:A:242:GLU:HG2	4:A:528:HOH:O	2.02	0.58
1:C:266:ARG:HD3	1:C:281:ARG:HH22	1.68	0.57
1:C:186:ASN:C	1:C:187:ILE:HD12	2.24	0.57
1:B:221:PRO:HG2	1:B:222:ILE:CD1	2.30	0.57
1:D:186:ASN:C	1:D:187:ILE:HD12	2.26	0.57
1:C:278:HIS:HB3	4:C:486:HOH:O	2.05	0.56
1:A:86:LEU:HG	1:A:88:LEU:HD13	1.89	0.55
1:B:71:PHE:CE2	1:B:87:LYS:HG2	2.41	0.55
1:A:266:ARG:HH11	1:A:281:ARG:HH22	1.54	0.55
1:A:146:HIS:HD2	1:A:148:GLN:H	1.52	0.55
1:B:86:LEU:HG	1:B:88:LEU:HD13	1.89	0.55
1:B:266:ARG:HD3	1:B:281:ARG:HH22	1.71	0.54
1:C:146:HIS:CD2	1:C:148:GLN:H	2.24	0.54
1:D:274:ARG:HH11	1:D:274:ARG:HG3	1.72	0.54
1:A:186:ASN:C	1:A:187:ILE:HD12	2.28	0.54
1:C:165:ILE:HD13	1:C:200:PRO:HG3	1.90	0.54
1:A:266:ARG:NH1	1:A:281:ARG:HH22	2.05	0.53
1:C:261:PHE:HE1	1:C:279:ALA:HB1	1.74	0.53
1:D:86:LEU:HG	1:D:88:LEU:HD13	1.91	0.53
1:C:169:SER:HB2	1:C:170:GLU:OE2	2.09	0.53
1:B:164:ASP:OD1	1:B:166:ARG:HD3	2.10	0.52
1:B:220:SER:HB2	1:B:259:PHE:CZ	2.44	0.52
1:A:221:PRO:HG2	1:A:222:ILE:CD1	2.37	0.52
1:B:266:ARG:NH1	1:B:281:ARG:HH22	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.75	0.52
1:B:217:VAL:HG22	1:B:258:VAL:HB	1.92	0.52
1:D:51:LEU:HD23	1:D:126:ILE:HD12	1.93	0.51
1:D:146:HIS:HE1	4:D:485:HOH:O	1.93	0.51
1:D:24:GLU:H	1:D:24:GLU:CD	2.14	0.51
1:A:148:GLN:HG3	1:A:152:ILE:HD12	1.91	0.51
1:B:146:HIS:HD2	1:B:148:GLN:H	1.56	0.50
1:B:290:GLU:O	1:B:294:GLU:HG3	2.11	0.50
1:A:76:ARG:HD3	1:B:91:ARG:CZ	2.41	0.50
1:A:186:ASN:HB3	1:A:303:PHE:CE1	2.46	0.50
1:A:220:SER:HB2	1:A:259:PHE:CZ	2.46	0.50
1:B:44:SER:HB3	1:B:47:LEU:HB2	1.93	0.50
1:C:220:SER:HB2	1:C:259:PHE:CZ	2.47	0.50
1:D:50:VAL:HG12	1:D:126:ILE:HD13	1.95	0.49
1:C:187:ILE:HD11	1:C:214:LYS:HD2	1.94	0.49
1:D:78:LYS:HB3	1:D:78:LYS:NZ	2.27	0.49
1:D:184:GLU:HG2	4:D:464:HOH:O	2.12	0.49
1:B:59:ASP:OD2	1:B:62:ARG:HD3	2.13	0.48
1:B:146:HIS:HE1	4:B:469:HOH:O	1.96	0.48
1:B:24:GLU:CD	1:B:24:GLU:H	2.16	0.48
1:C:213:LYS:O	1:C:214:LYS:HG2	2.13	0.48
1:C:266:ARG:HH11	1:C:281:ARG:HH22	1.61	0.48
1:A:2:ILE:CG1	1:A:184:GLU:HG3	2.27	0.48
1:B:256:LEU:HD21	1:B:259:PHE:CD1	2.49	0.47
1:A:146:HIS:HE1	4:A:486:HOH:O	1.98	0.47
1:D:75:GLU:O	1:D:79:GLU:HG3	2.15	0.47
1:D:142:GLU:HG3	4:D:472:HOH:O	2.15	0.47
1:A:293:LYS:O	1:A:297:GLU:HG3	2.15	0.47
1:B:271:ALA:O	1:B:274:ARG:HB2	2.14	0.47
1:C:58:ILE:HG13	1:C:59:ASP:N	2.29	0.47
1:C:146:HIS:HE1	4:C:464:HOH:O	1.97	0.46
1:B:75:GLU:O	1:B:79:GLU:HG3	2.16	0.46
1:D:186:ASN:HB3	1:D:303:PHE:CE1	2.51	0.46
1:B:157:GLU:N	1:B:158:PRO:CD	2.79	0.46
1:C:217:VAL:HG22	1:C:258:VAL:HB	1.98	0.46
1:C:262:ASP:OD1	1:C:264:ARG:HD3	2.16	0.46
1:D:293:LYS:O	1:D:297:GLU:HG3	2.16	0.46
1:A:48:ASP:CG	1:A:99:ARG:HH22	2.19	0.46
1:B:102:ILE:HG22	1:B:107:ALA:HB3	1.98	0.46
1:B:165:ILE:HD13	1:B:200:PRO:HG3	1.98	0.46
1:B:213:LYS:O	1:B:214:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:SER:HB2	1:B:170:GLU:OE2	2.16	0.46
1:B:187:ILE:HD11	1:B:214:LYS:HD2	1.98	0.46
1:A:86:LEU:HD23	1:A:86:LEU:N	2.31	0.45
1:D:187:ILE:HD12	1:D:187:ILE:N	2.31	0.45
1:D:221:PRO:HG2	1:D:222:ILE:CD1	2.42	0.45
1:D:258:VAL:HG11	1:D:302:ALA:HB1	1.99	0.45
1:B:185:GLU:HA	1:B:214:LYS:HD3	1.98	0.45
1:D:236:MSE:N	1:D:237:PRO:HD2	2.31	0.45
1:A:215:LYS:NZ	1:A:306:HIS:HA	2.32	0.45
1:C:185:GLU:HA	1:C:214:LYS:HD3	1.99	0.45
1:A:137:TYR:CD2	1:A:166:ARG:HD2	2.51	0.45
1:A:185:GLU:N	1:A:185:GLU:CD	2.70	0.45
1:C:44:SER:HB3	1:C:47:LEU:HB2	1.97	0.45
1:C:76:ARG:HD3	1:D:91:ARG:CZ	2.46	0.45
1:C:157:GLU:N	1:C:158:PRO:CD	2.80	0.45
1:C:266:ARG:HD3	1:C:281:ARG:CZ	2.46	0.45
1:A:43:ILE:HD11	1:A:88:LEU:HD21	1.99	0.44
1:C:146:HIS:CE1	4:C:464:HOH:O	2.70	0.44
1:C:42:LEU:O	1:C:99:ARG:NH1	2.48	0.44
1:C:86:LEU:HG	1:C:88:LEU:CD1	2.48	0.44
1:D:148:GLN:HG3	1:D:152:ILE:HD12	1.99	0.44
1:B:43:ILE:HG12	1:B:96:HIS:CE1	2.53	0.44
1:B:149:ASP:O	1:B:154:LYS:HG2	2.18	0.44
1:D:36:LEU:HD11	1:D:146:HIS:CD2	2.53	0.44
1:B:58:ILE:HG13	1:B:59:ASP:N	2.32	0.44
1:C:62:ARG:HB3	1:C:64:TRP:NE1	2.32	0.44
1:C:236:MSE:N	1:C:237:PRO:HD2	2.33	0.44
1:A:58:ILE:HG13	1:A:59:ASP:N	2.32	0.44
1:C:91:ARG:CZ	1:D:76:ARG:HD3	2.48	0.44
1:D:262:ASP:OD1	1:D:264:ARG:HD3	2.17	0.44
1:A:263:GLU:H	1:A:263:GLU:HG3	1.65	0.43
1:B:10:THR:OG1	1:B:190:GLY:HA3	2.18	0.43
1:B:46:ASP:HA	4:B:455:HOH:O	2.18	0.43
1:A:236:MSE:N	1:A:237:PRO:HD2	2.33	0.43
1:B:266:ARG:HD3	1:B:281:ARG:CZ	2.48	0.43
1:D:71:PHE:CE2	1:D:87:LYS:HG2	2.54	0.43
1:A:91:ARG:CZ	1:B:76:ARG:HD3	2.49	0.43
1:D:160:VAL:O	1:D:161:ARG:HD2	2.19	0.43
1:B:187:ILE:HD12	1:B:187:ILE:N	2.33	0.43
1:C:86:LEU:N	1:C:86:LEU:CD2	2.81	0.42
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:HB2	1:C:61:LYS:HE3	1.87	0.42
1:A:50:VAL:HG12	1:A:126:ILE:HD13	2.01	0.42
1:C:48:ASP:CG	1:C:99:ARG:HH22	2.23	0.42
1:D:58:ILE:HG13	1:D:59:ASP:N	2.33	0.42
1:A:262:ASP:HA	1:A:282:ALA:O	2.19	0.42
1:B:10:THR:N	1:B:11:PRO:HD2	2.35	0.42
1:D:263:GLU:H	1:D:263:GLU:HG3	1.70	0.42
1:C:91:ARG:NH1	1:D:76:ARG:HD3	2.35	0.42
1:C:33:ALA:HB1	1:C:136:THR:OG1	2.19	0.42
1:D:186:ASN:HD22	1:D:215:LYS:HB3	1.85	0.42
1:A:258:VAL:HG11	1:A:302:ALA:HB1	2.02	0.42
1:B:126:ILE:O	1:B:127:LEU:HD23	2.20	0.42
1:A:215:LYS:CE	1:A:306:HIS:HA	2.49	0.42
1:A:154:LYS:HB3	1:A:158:PRO:HD3	2.02	0.41
1:D:43:ILE:HD11	1:D:88:LEU:HD21	2.02	0.41
1:D:266:ARG:HA	1:D:281:ARG:NH2	2.36	0.41
1:B:261:PHE:CD1	1:B:261:PHE:N	2.89	0.41
1:B:264:ARG:HD3	1:B:264:ARG:H	1.85	0.41
1:B:285:LEU:HD22	1:B:287:THR:HG23	2.01	0.41
1:C:285:LEU:HD22	1:C:287:THR:HG23	2.03	0.41
1:D:246:MSE:HB2	4:D:523:HOH:O	2.20	0.41
1:A:266:ARG:HD3	1:A:281:ARG:NH2	2.35	0.41
1:B:7:GLY:HA3	2:B:402:PO4:O3	2.21	0.41
1:C:71:PHE:CE2	1:C:87:LYS:HG2	2.55	0.41
1:C:94:ALA:HB1	1:D:77:MSE:HG3	2.03	0.41
1:A:62:ARG:HB3	1:A:64:TRP:NE1	2.35	0.41
1:A:142:GLU:HG3	4:A:445:HOH:O	2.21	0.41
1:B:33:ALA:HB1	1:B:136:THR:OG1	2.21	0.41
1:D:137:TYR:CD2	1:D:166:ARG:HD2	2.57	0.40
1:D:266:ARG:HD3	1:D:281:ARG:NH2	2.36	0.40
1:B:174:SER:HB3	1:B:177:VAL:HG23	2.02	0.40
1:A:51:LEU:HD23	1:A:126:ILE:HD12	2.04	0.40
1:C:141:ALA:HB2	1:C:161:ARG:HE	1.87	0.40
1:C:150:PHE:CE2	1:C:156:GLY:HA2	2.56	0.40
1:C:10:THR:N	1:C:11:PRO:HD2	2.36	0.40
1:B:236:MSE:N	1:B:237:PRO:HD2	2.36	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	304/311 (98%)	296 (97%)	8 (3%)	0	100	100
1	B	304/311 (98%)	293 (96%)	11 (4%)	0	100	100
1	C	304/311 (98%)	291 (96%)	12 (4%)	1 (0%)	37	56
1	D	304/311 (98%)	292 (96%)	11 (4%)	1 (0%)	37	56
All	All	1216/1244 (98%)	1172 (96%)	42 (4%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	268	ASP
1	D	305	GLU

### 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	262/259 (101%)	252 (96%)	10 (4%)	28	53
1	B	262/259 (101%)	254 (97%)	8 (3%)	35	62
1	C	262/259 (101%)	253 (97%)	9 (3%)	32	58
1	D	262/259 (101%)	254 (97%)	8 (3%)	35	62
All	All	1048/1036 (101%)	1013 (97%)	35 (3%)	33	59

All (35) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	47	LEU
1	A	80	LEU
1	A	86	LEU
1	A	88	LEU
1	A	185	GLU
1	A	266	ARG
1	A	269	GLU
1	A	270	PHE
1	A	278	HIS
1	A	285	LEU
1	B	83	GLU
1	B	86	LEU
1	B	166	ARG
1	B	185	GLU
1	B	254	ASP
1	B	269	GLU
1	B	270	PHE
1	B	285	LEU
1	C	53	LEU
1	C	86	LEU
1	C	88	LEU
1	C	161	ARG
1	C	169	SER
1	C	208	ARG
1	C	254	ASP
1	C	269	GLU
1	C	270	PHE
1	D	47	LEU
1	D	86	LEU
1	D	88	LEU
1	D	185	GLU
1	D	266	ARG
1	D	269	GLU
1	D	270	PHE
1	D	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	125	ASN
1	A	146	HIS
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	253	GLN
1	B	57	GLN
1	B	125	ASN
1	B	146	HIS
1	B	186	ASN
1	B	253	GLN
1	B	301	GLN
1	C	57	GLN
1	C	125	ASN
1	C	146	HIS
1	C	186	ASN
1	C	253	GLN
1	C	301	GLN
1	D	57	GLN
1	D	125	ASN
1	D	146	HIS
1	D	186	ASN
1	D	253	GLN
1	D	301	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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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	$\# Z  > 2$
2	PO4	B	402	-	4,4,4	1.72	1 (25%)	6,6,6	0.46	0
2	PO4	D	402	-	4,4,4	1.79	1 (25%)	6,6,6	0.47	0
3	FO1	A	401	-	22,22,28	3.97	13 (59%)	30,32,41	2.95	14 (46%)
2	PO4	A	402	-	4,4,4	1.79	1 (25%)	6,6,6	0.48	0
2	PO4	C	402	-	4,4,4	1.67	1 (25%)	6,6,6	0.48	0
3	FO1	C	401	-	22,22,28	4.08	13 (59%)	30,32,41	2.92	14 (46%)
3	FO1	B	401	-	22,22,28	4.04	13 (59%)	30,32,41	2.88	14 (46%)
3	FO1	D	401	-	22,22,28	3.93	13 (59%)	30,32,41	2.93	15 (50%)

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	FO1	D	401	-	-	0/3/3/14	0/3/3/3
3	FO1	A	401	-	-	0/3/3/14	0/3/3/3
3	FO1	B	401	-	-	0/3/3/14	0/3/3/3
3	FO1	C	401	-	-	0/3/3/14	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	FO1	C5-C12	10.77	1.58	1.41
3	B	401	FO1	C5-C12	10.64	1.58	1.41
3	A	401	FO1	C5-C12	10.58	1.58	1.41
3	D	401	FO1	C5-C12	10.53	1.58	1.41
3	C	401	FO1	C7-C9	6.58	1.51	1.39
3	D	401	FO1	C7-C9	6.56	1.51	1.39
3	A	401	FO1	C7-C9	6.45	1.51	1.39
3	B	401	FO1	C7-C9	6.42	1.51	1.39
3	C	401	FO1	C11-C12	5.42	1.48	1.39
3	B	401	FO1	C11-C12	5.40	1.48	1.39
3	A	401	FO1	C12-N3	5.37	1.50	1.41
3	C	401	FO1	C12-N3	5.32	1.50	1.41
3	C	401	FO1	C4-C3	5.11	1.46	1.35
3	D	401	FO1	C12-N3	5.11	1.50	1.41
3	B	401	FO1	C12-N3	5.09	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	FO1	C7-C6	5.07	1.47	1.38
3	D	401	FO1	C4-C3	5.04	1.46	1.35
3	A	401	FO1	C11-C12	5.03	1.47	1.39
3	A	401	FO1	C4-C3	4.99	1.46	1.35
3	B	401	FO1	C4-C3	4.96	1.45	1.35
3	B	401	FO1	C7-C6	4.88	1.46	1.38
3	D	401	FO1	C7-C6	4.81	1.46	1.38
3	A	401	FO1	C7-C6	4.76	1.46	1.38
3	D	401	FO1	C11-C12	4.59	1.47	1.39
3	B	401	FO1	C3-C2	4.54	1.53	1.45
3	C	401	FO1	C3-C2	4.53	1.53	1.45
3	C	401	FO1	C13-N3	4.12	1.46	1.37
3	B	401	FO1	C13-N3	4.11	1.46	1.37
3	D	401	FO1	C13-N1	4.00	1.41	1.33
3	A	401	FO1	C3-C2	3.96	1.52	1.45
3	D	401	FO1	C3-C13	3.95	1.52	1.44
3	B	401	FO1	C13-N1	3.94	1.41	1.33
3	B	401	FO1	C3-C13	3.90	1.52	1.44
3	A	401	FO1	C3-C13	3.88	1.52	1.44
3	D	401	FO1	C3-C2	3.82	1.52	1.45
3	A	401	FO1	C13-N3	3.79	1.45	1.37
3	C	401	FO1	C13-N1	3.78	1.40	1.33
3	A	401	FO1	C13-N1	3.75	1.40	1.33
3	C	401	FO1	C3-C13	3.75	1.52	1.44
3	D	401	FO1	C13-N3	3.63	1.45	1.37
3	D	401	FO1	C1-N2	2.95	1.45	1.39
3	A	401	FO1	C6-C5	2.92	1.46	1.41
3	C	401	FO1	C6-C5	2.81	1.45	1.41
3	D	401	FO1	C6-C5	2.75	1.45	1.41
3	B	401	FO1	C14-N3	2.71	1.53	1.47
3	B	401	FO1	C1-N2	2.70	1.44	1.39
3	A	401	FO1	C1-N2	2.64	1.44	1.39
3	C	401	FO1	C1-N2	2.64	1.44	1.39
3	C	401	FO1	C14-N3	2.55	1.53	1.47
3	B	401	FO1	C6-C5	2.50	1.45	1.41
3	A	401	FO1	C14-N3	2.32	1.53	1.47
3	D	401	FO1	C14-N3	2.19	1.52	1.47
2	A	402	PO4	P-O3	-2.17	1.48	1.54
2	D	402	PO4	P-O2	-2.07	1.48	1.54
2	B	402	PO4	P-O2	-2.00	1.48	1.54
2	C	402	PO4	P-O2	-2.00	1.48	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	FO1	C2-C3-C13	-8.11	113.23	117.48
3	C	401	FO1	C2-C3-C13	-7.74	113.43	117.48
3	D	401	FO1	C2-C3-C13	-7.71	113.44	117.48
3	D	401	FO1	O2-C2-C3	-7.45	109.56	125.98
3	B	401	FO1	C2-C3-C13	-7.38	113.61	117.48
3	A	401	FO1	O2-C2-C3	-7.27	109.96	125.98
3	C	401	FO1	O2-C2-C3	-7.16	110.20	125.98
3	B	401	FO1	O2-C2-C3	-7.09	110.36	125.98
3	D	401	FO1	C3-C2-N2	4.60	122.49	114.45
3	A	401	FO1	C3-C2-N2	4.55	122.42	114.45
3	C	401	FO1	C3-C2-N2	4.50	122.32	114.45
3	B	401	FO1	C3-C2-N2	4.47	122.27	114.45
3	B	401	FO1	C15-C14-N3	4.27	122.96	111.93
3	B	401	FO1	C13-N1-C1	4.20	125.95	116.85
3	D	401	FO1	O2-C2-N2	4.17	127.95	120.11
3	C	401	FO1	C13-N1-C1	4.16	125.86	116.85
3	A	401	FO1	C13-N1-C1	4.15	125.84	116.85
3	C	401	FO1	C15-C14-N3	4.05	122.38	111.93
3	A	401	FO1	O2-C2-N2	3.99	127.62	120.11
3	D	401	FO1	C13-N1-C1	3.97	125.44	116.85
3	C	401	FO1	O2-C2-N2	3.92	127.48	120.11
3	B	401	FO1	O2-C2-N2	3.86	127.37	120.11
3	A	401	FO1	C15-C14-N3	3.58	121.17	111.93
3	D	401	FO1	C15-C14-N3	3.52	121.01	111.93
3	B	401	FO1	C2-N2-C1	-3.39	119.61	125.64
3	C	401	FO1	C2-N2-C1	-3.38	119.64	125.64
3	D	401	FO1	C2-N2-C1	-3.32	119.74	125.64
3	C	401	FO1	C4-C3-C2	3.27	126.38	119.30
3	A	401	FO1	C2-N2-C1	-3.25	119.87	125.64
3	A	401	FO1	C4-C3-C2	3.24	126.31	119.30
3	B	401	FO1	C4-C3-C2	3.20	126.22	119.30
3	D	401	FO1	C4-C3-C2	3.03	125.84	119.30
3	A	401	FO1	O1-C1-N1	-2.97	116.87	121.80
3	B	401	FO1	O1-C1-N1	-2.96	116.88	121.80
3	C	401	FO1	O1-C1-N1	-2.94	116.92	121.80
3	D	401	FO1	O10-C9-C11	-2.93	112.19	119.85
3	D	401	FO1	O1-C1-N1	-2.92	116.95	121.80
3	A	401	FO1	O10-C9-C11	-2.82	112.48	119.85
3	A	401	FO1	O1-C1-N2	2.73	123.83	118.58
3	C	401	FO1	O10-C9-C11	-2.72	112.74	119.85
3	D	401	FO1	O1-C1-N2	2.64	123.66	118.58
3	B	401	FO1	O10-C9-C11	-2.61	113.01	119.85
3	A	401	FO1	C7-C9-C11	2.60	123.04	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	FO1	O1-C1-N2	2.58	123.53	118.58
3	B	401	FO1	O1-C1-N2	2.57	123.51	118.58
3	B	401	FO1	C11-C12-N3	2.56	125.30	121.85
3	C	401	FO1	C11-C12-N3	2.56	125.30	121.85
3	D	401	FO1	C7-C9-C11	2.54	122.98	120.19
3	A	401	FO1	C11-C12-N3	2.42	125.10	121.85
3	C	401	FO1	C7-C9-C11	2.39	122.81	120.19
3	B	401	FO1	C7-C9-C11	2.31	122.72	120.19
3	B	401	FO1	C11-C12-C5	-2.28	117.32	119.81
3	C	401	FO1	C11-C12-C5	-2.22	117.38	119.81
3	D	401	FO1	C11-C12-N3	2.20	124.81	121.85
3	D	401	FO1	C11-C12-C5	-2.17	117.44	119.81
3	A	401	FO1	C11-C12-C5	-2.17	117.44	119.81
3	D	401	FO1	C12-C11-C9	2.03	120.97	117.95

There are no chirality outliers.

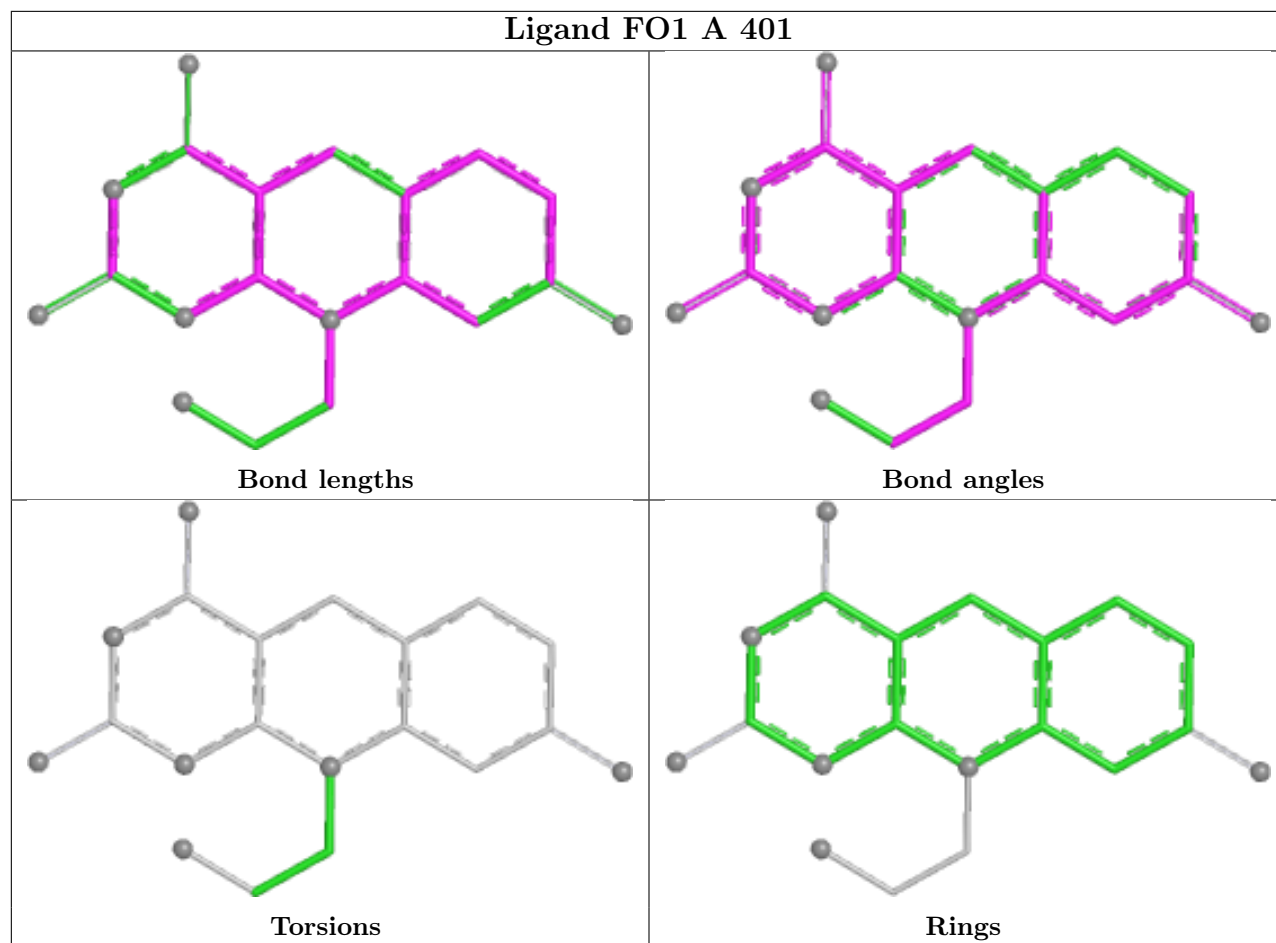
There are no torsion outliers.

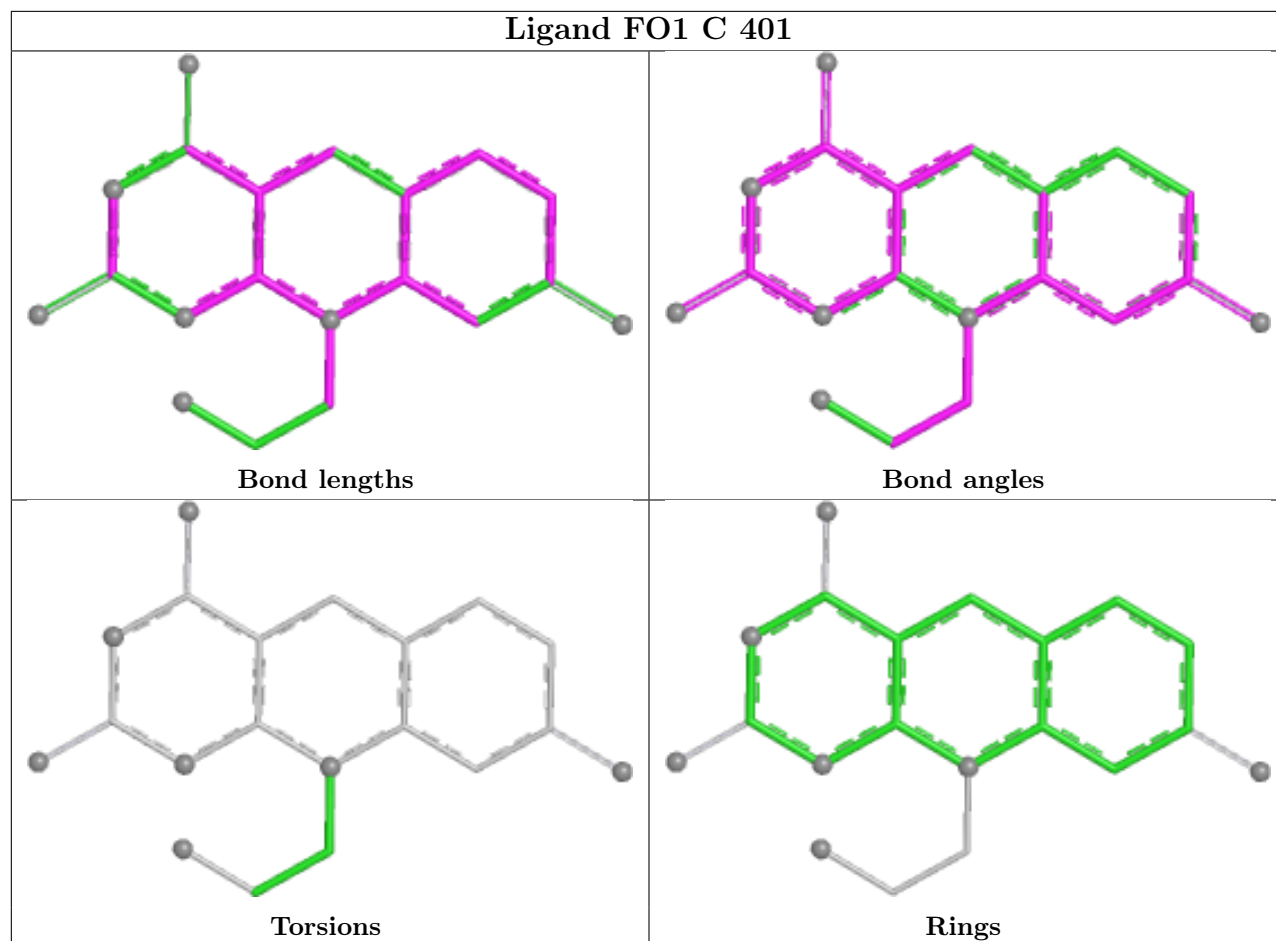
There are no ring outliers.

1 monomer is involved in 1 short contact:

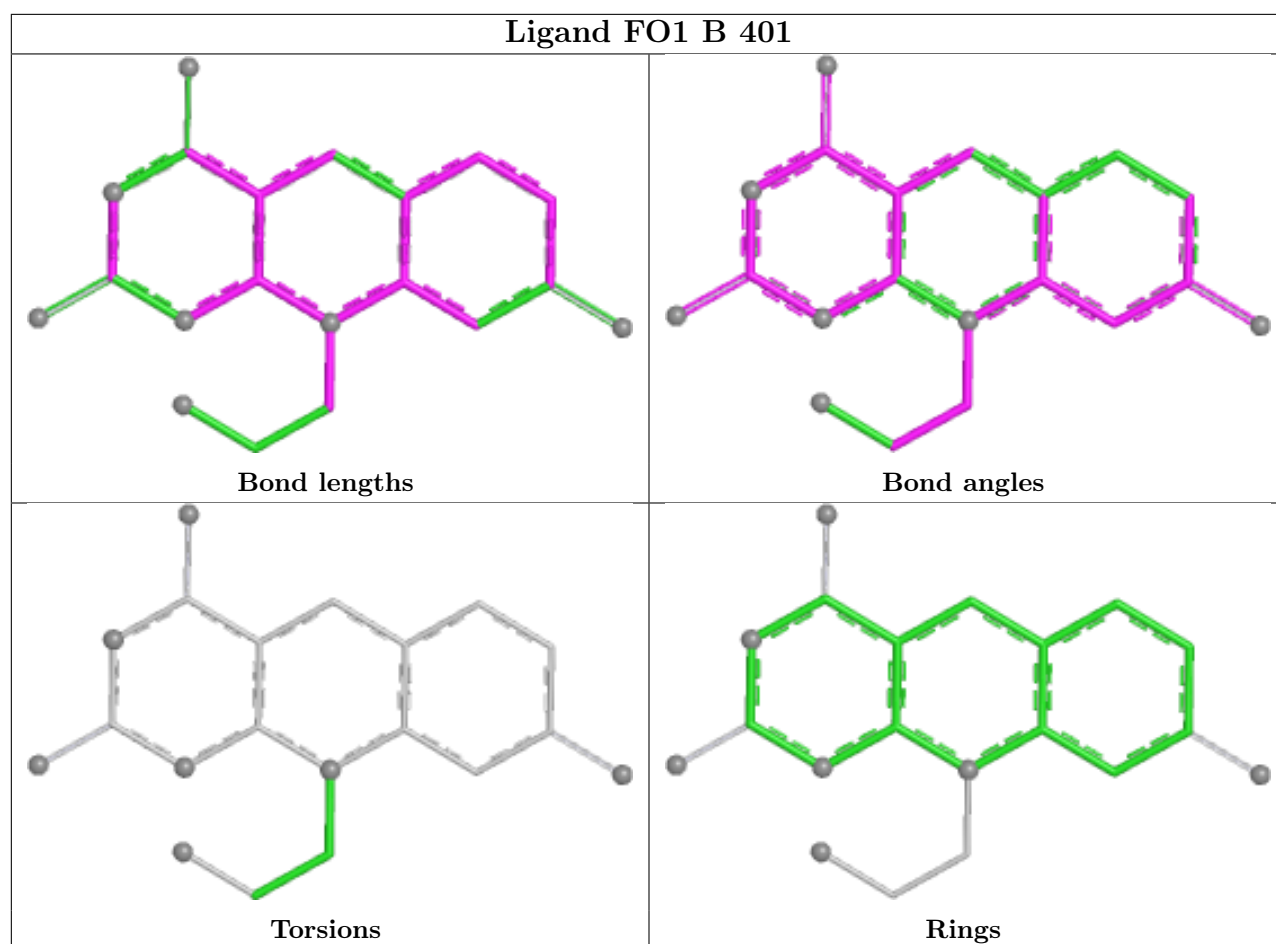
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	PO4	1	0

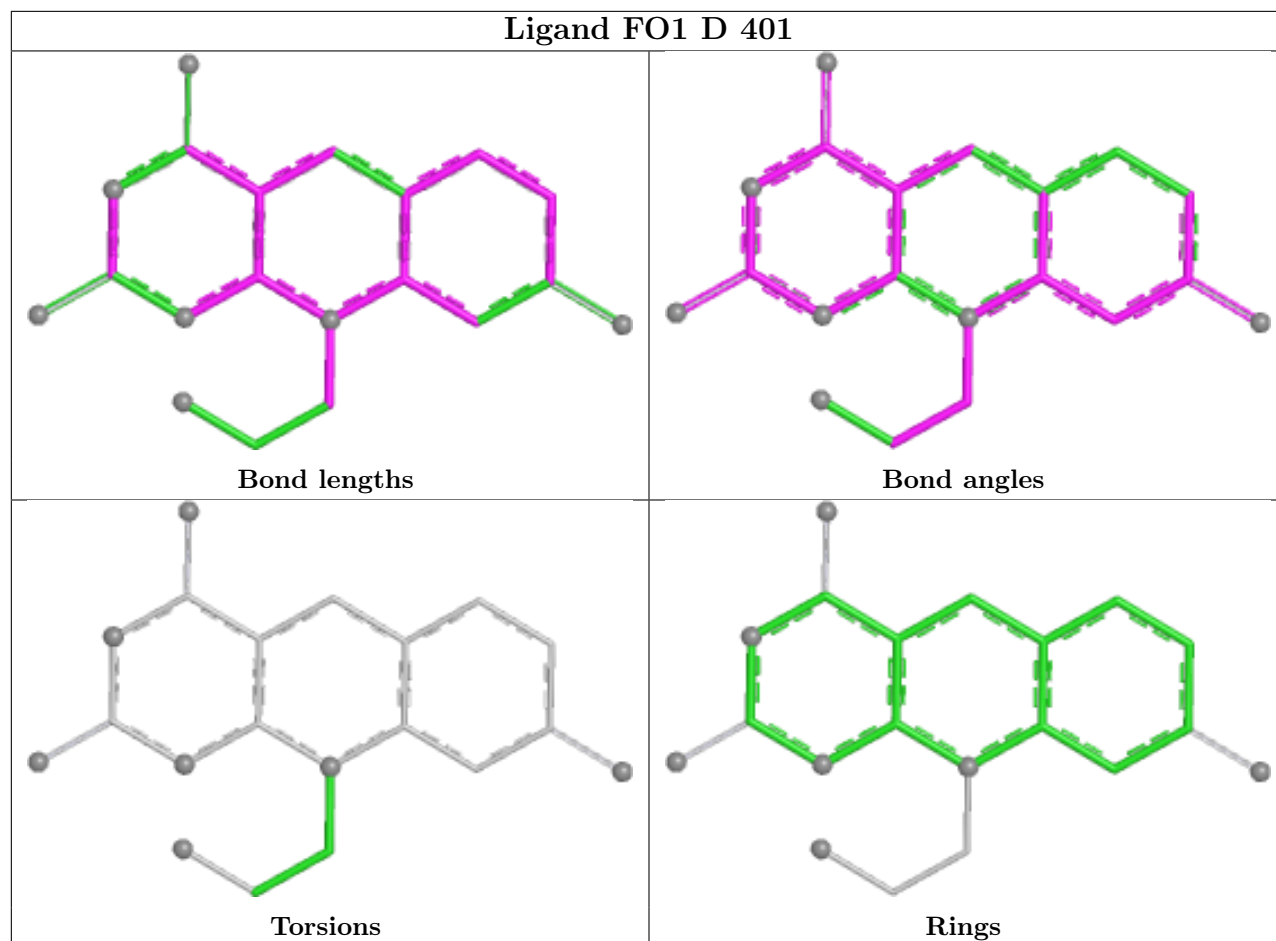
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	298/311 (95%)	-1.69	0 100 100	18, 31, 53, 89	0
1	B	298/311 (95%)	-1.54	0 100 100	22, 41, 76, 98	0
1	C	298/311 (95%)	-1.56	0 100 100	21, 41, 77, 99	0
1	D	298/311 (95%)	-1.69	0 100 100	18, 31, 53, 87	0
All	All	1192/1244 (95%)	-1.62	0 100 100	18, 34, 72, 99	0

There are no RSRZ outliers to report.

### 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
2	PO4	A	402	5/5	0.99	0.04	64,64,64,66	0
2	PO4	B	402	5/5	0.99	0.05	72,73,74,75	0
2	PO4	C	402	5/5	0.99	0.04	70,71,72,73	0
2	PO4	D	402	5/5	0.99	0.05	70,70,71,72	0

*Continued on next page...*

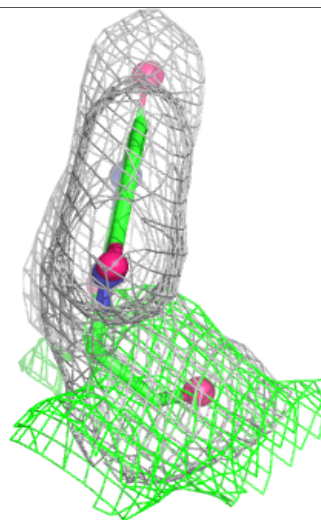
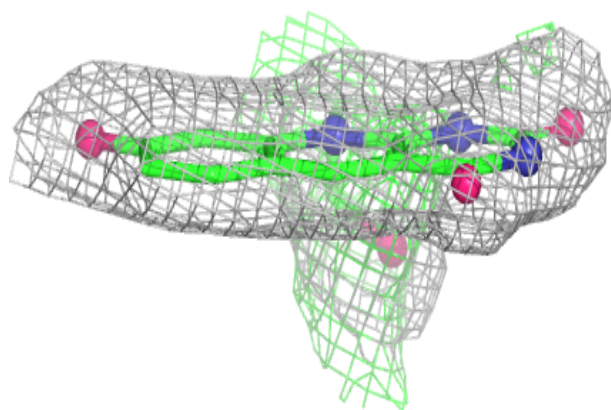
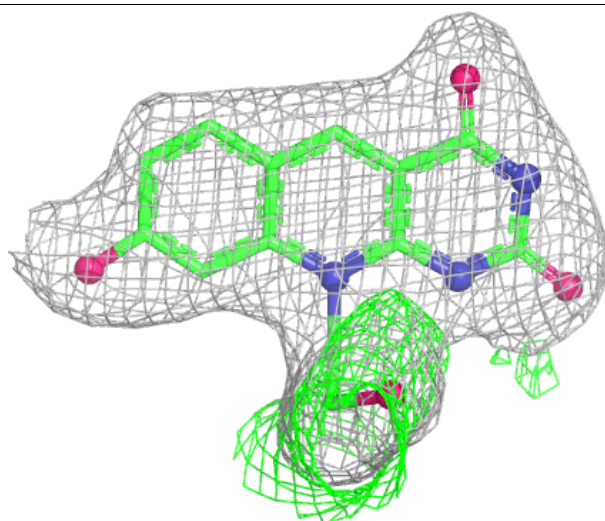
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FO1	A	401	20/26	0.99	0.04	16,20,30,32	20
3	FO1	B	401	20/26	0.99	0.04	25,33,39,40	20
3	FO1	C	401	20/26	0.99	0.04	28,34,39,42	20
3	FO1	D	401	20/26	0.99	0.04	17,21,31,33	20

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.

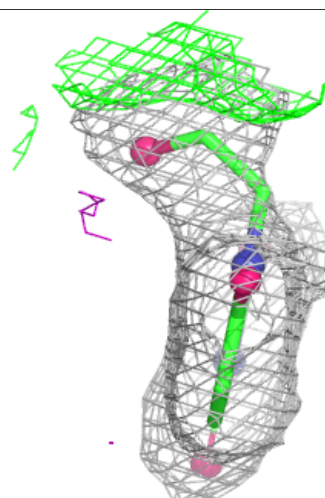
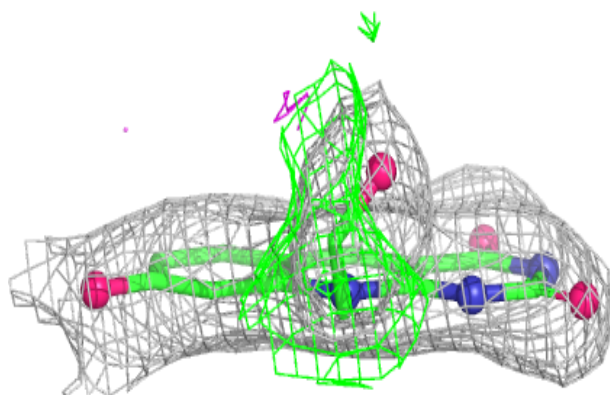
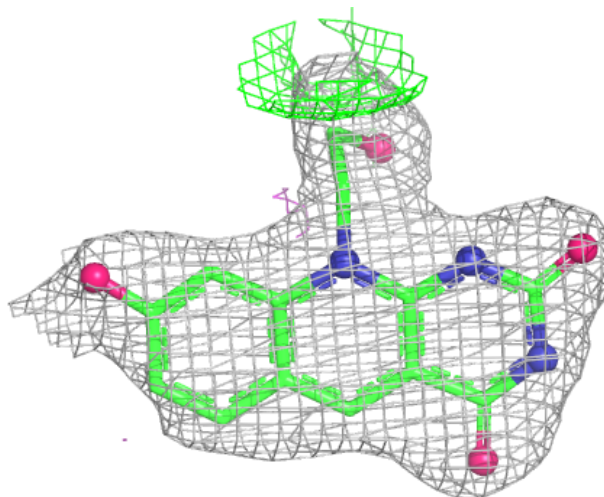
**Electron density around FO1 A 401:**

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)



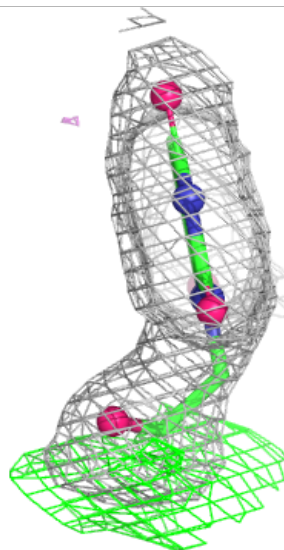
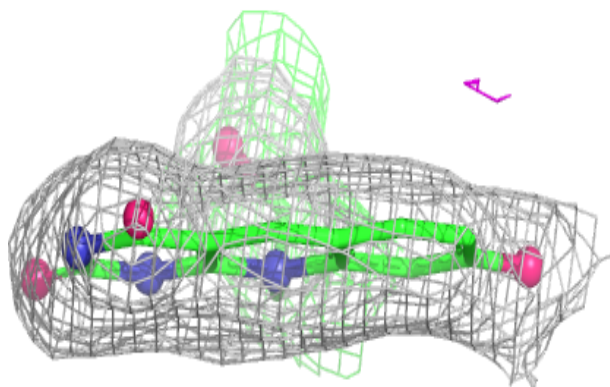
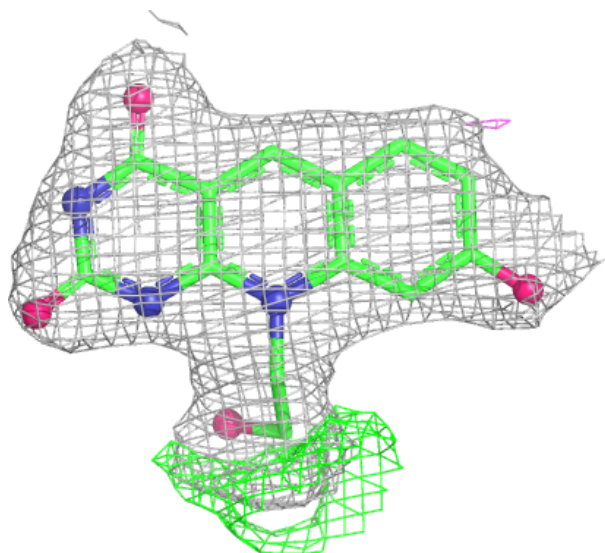
**Electron density around FO1 B 401:**

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



**Electron density around FO1 C 401:**

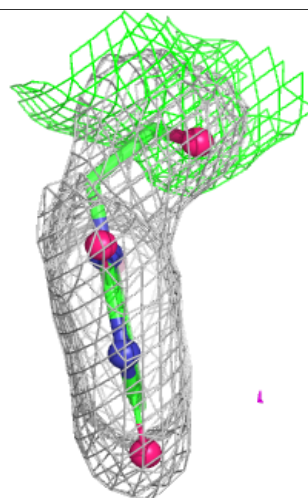
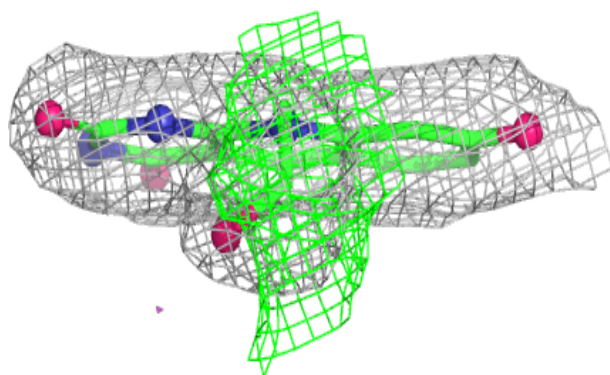
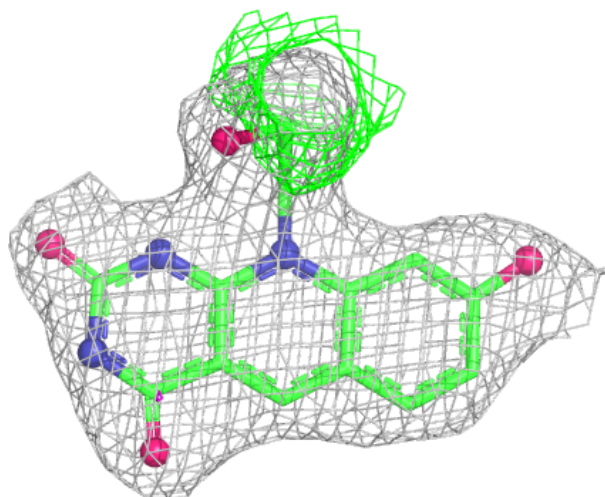
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FO1 D 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 [i](#)

There are no such residues in this entry.