



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:51 am BST

PDB ID : 3UWL
Title : Crystal structure of Enterococcus faecalis thymidylate synthase (EfTS) in complex with 5-formyl tetrahydrofolate
Authors : Pozzi, C.; Catalano, A.; Cortesi, D.; Luciani, R.; Ferrari, S.; Fritz, T.; Costi, M.P.; Mangani, S.
Deposited on : 2011-12-02
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

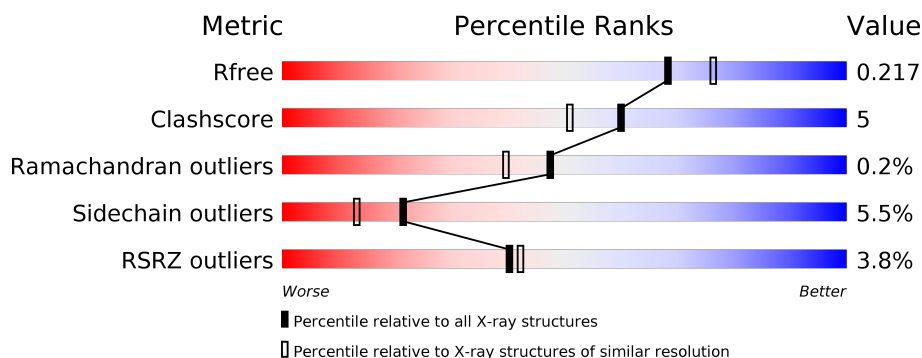
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 on 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	315	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>7%</div> </div> </div>
1	C	315	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>10%</div> </div> </div>
2	B	315	<div> <div></div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
2	D	315	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10751 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2380	1532	396	442	10			
1	C	282	Total	C	N	O	S	0	0	0
			2302	1486	382	424	10			

- Molecule 2 is a protein called Thymidylate synthase.

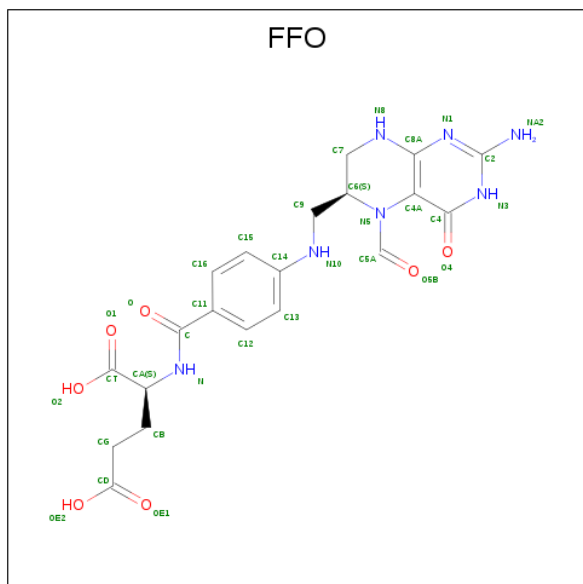
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	315	Total	C	N	O	S	0	0	0
			2573	1653	427	481	12			
2	D	315	Total	C	N	O	S	0	0	0
			2567	1651	427	477	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is N-[4-({[(6S)-2-amino-5-formyl-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (three-letter code: FFO) (formula: $C_{20}H_{23}N_7O_7$).





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

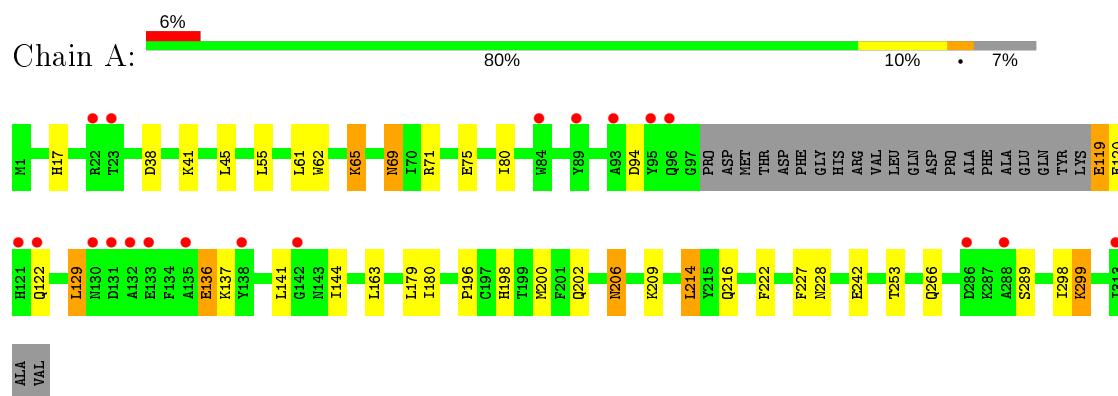
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total	O	0	0
			162	162		
6	B	244	Total	O	0	0
			244	244		
6	C	130	Total	O	0	0
			130	130		
6	D	263	Total	O	0	0
			263	263		

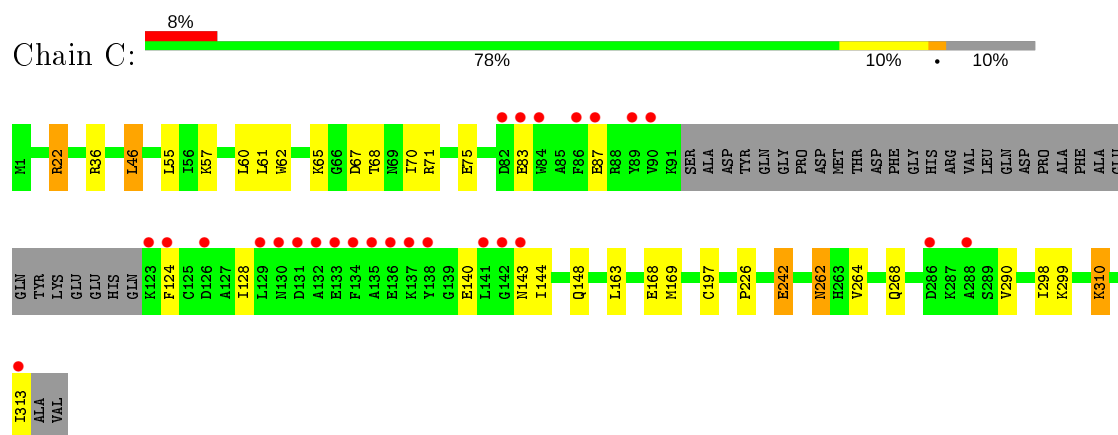
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

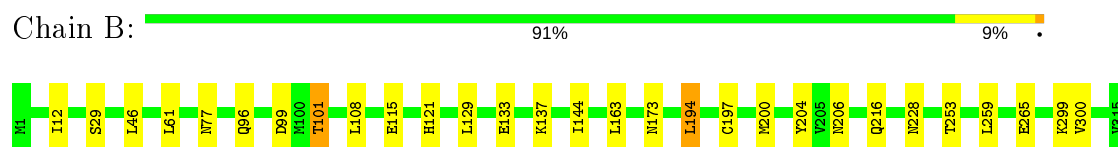
• Molecule 1: Thymidylate synthase



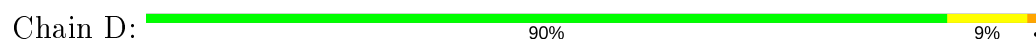
• Molecule 1: Thymidylate synthase



• Molecule 2: Thymidylate synthase



• Molecule 2: Thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.94Å 94.25Å 96.19Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	33.49 – 2.07 33.49 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.49-2.07) 96.2 (33.49-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.160 , 0.217 0.162 , 0.217	Depositor DCC
R_{free} test set	3757 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10751	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: FFO, CME, SO4, EDO

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	0.74	0/2445	0.73	0/3312
1	C	0.72	1/2365 (0.0%)	0.70	0/3204
2	B	0.78	0/2634	0.75	1/3568 (0.0%)
2	D	0.78	0/2628	0.76	2/3560 (0.1%)
All	All	0.75	1/10072 (0.0%)	0.74	3/13644 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	CYS	CB-SG	5.46	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	194	LEU	CA-CB-CG	5.81	128.67	115.30
2	D	30	LEU	CA-CB-CG	5.47	127.88	115.30
2	D	71	ARG	NE-CZ-NH1	5.22	122.91	120.30

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	2380	0	2289	28	0
1	C	2302	0	2230	27	0
2	B	2573	0	2467	15	0
2	D	2567	0	2463	23	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	B	34	0	21	2	0
4	D	34	0	21	0	0
5	B	16	0	24	0	0
5	C	8	0	12	2	0
5	D	8	0	12	0	0
6	A	162	0	0	4	0
6	B	244	0	0	5	0
6	C	130	0	0	7	0
6	D	263	0	0	5	0
All	All	10751	0	9539	90	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 5.

All (90) 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:C:310:LYS:H	1:C:310:LYS:HD3	1.17	1.07
2:D:206:ASN:HB2	6:D:796:HOH:O	1.54	1.05
1:C:65:LYS:HB3	6:C:440:HOH:O	1.62	0.99
1:C:242:GLU:HG3	1:C:290:VAL:HG22	1.52	0.90
1:C:22:ARG:HH11	1:C:22:ARG:HG3	1.36	0.89
1:A:299:LYS:HE3	6:A:384:HOH:O	1.76	0.85
1:C:262:ASN:HD22	1:C:262:ASN:H	1.28	0.81
1:A:206:ASN:HB2	6:B:595:HOH:O	1.82	0.80
1:A:227:PHE:HB3	6:A:716:HOH:O	1.84	0.75
1:C:310:LYS:H	1:C:310:LYS:CD	1.93	0.75
2:D:99:ASP:OD1	2:D:101:THR:HG23	1.86	0.75
1:A:65:LYS:HD3	6:A:793:HOH:O	1.85	0.75
1:C:169:MET:HG2	6:C:672:HOH:O	1.87	0.75
2:B:99:ASP:OD1	2:B:101:THR:CG2	2.37	0.72
1:C:36:ARG:HG3	5:C:318:EDO:H12	1.73	0.69
2:B:99:ASP:OD1	2:B:101:THR:HG22	1.97	0.65
2:D:145:TYR:CZ	2:D:198:HIS:NE2	2.65	0.65
1:C:22:ARG:CG	1:C:22:ARG:HH11	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:TYR:CZ	2:D:198:HIS:CE1	2.86	0.63
2:B:265:GLU:HG3	2:D:265:GLU:HG3	1.80	0.63
1:A:298:ILE:O	1:A:299:LYS:HD2	1.98	0.63
2:D:216:GLN:HE22	2:D:228:ASN:ND2	1.96	0.62
1:C:46:LEU:HD22	1:C:226:PRO:HB3	1.80	0.61
1:A:69:ASN:HD22	1:A:71:ARG:H	1.48	0.61
2:B:77:ASN:HB3	6:B:772:HOH:O	2.00	0.61
2:B:99:ASP:OD1	2:B:101:THR:HG23	2.00	0.61
1:A:62:TRP:HH2	1:A:141:LEU:HD12	1.67	0.59
1:A:298:ILE:C	1:A:299:LYS:HD2	2.23	0.59
2:B:115:GLU:HG3	6:B:550:HOH:O	2.02	0.58
1:C:143:ASN:HB2	6:C:753:HOH:O	2.03	0.58
1:C:65:LYS:CG	1:C:67:ASP:HB2	2.34	0.57
1:A:242:GLU:OE2	1:A:289:SER:HA	2.04	0.57
2:D:145:TYR:HE1	2:D:198:HIS:O	1.88	0.57
1:A:65:LYS:HB3	1:A:65:LYS:NZ	2.19	0.56
1:A:75:GLU:HG3	1:A:129:LEU:HD11	1.87	0.56
1:A:198:HIS:HB3	1:A:214:LEU:HD21	1.86	0.56
2:D:145:TYR:CE1	2:D:198:HIS:CE1	2.93	0.56
4:B:316:FFO:C5A	6:B:365:HOH:O	2.53	0.55
1:A:38:ASP:HB3	1:A:41:LYS:HD2	1.89	0.55
2:D:198:HIS:CD2	2:D:198:HIS:H	2.23	0.54
2:D:77:ASN:ND2	6:D:441:HOH:O	2.40	0.53
2:D:56:ILE:HD13	2:D:230:ALA:HB3	1.90	0.53
2:D:197:CME:O	2:D:216:GLN:HG3	2.08	0.53
1:C:310:LYS:HE3	6:C:373:HOH:O	2.09	0.53
1:A:180:ILE:HD13	1:A:202:GLN:HB2	1.90	0.53
2:D:151:HIS:HE1	6:D:558:HOH:O	1.93	0.52
2:B:216:GLN:HE22	2:B:228:ASN:ND2	2.06	0.52
1:A:222:PHE:CZ	1:A:266:GLN:HB3	2.45	0.52
2:D:145:TYR:OH	2:D:198:HIS:CD2	2.63	0.52
1:C:310:LYS:HD3	1:C:310:LYS:N	2.03	0.52
2:D:173:ASN:HD22	2:D:176:SER:HB2	1.75	0.51
2:B:197:CME:SD	4:B:316:FFO:H5A	2.50	0.51
2:D:121:HIS:HD2	6:D:601:HOH:O	1.93	0.51
1:C:262:ASN:H	1:C:262:ASN:ND2	2.03	0.50
1:A:144:ILE:CD1	6:A:331:HOH:O	2.59	0.49
2:B:12:ILE:HG21	2:B:259:LEU:HB2	1.94	0.49
5:C:318:EDO:H11	6:C:795:HOH:O	2.12	0.49
1:C:62:TRP:CD1	1:C:67:ASP:HB3	2.48	0.49
1:C:124:PHE:O	1:C:128:ILE:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASN:HD22	1:C:262:ASN:N	2.06	0.47
1:A:216:GLN:HE22	1:A:228:ASN:ND2	2.11	0.47
1:A:65:LYS:HB3	1:A:65:LYS:HZ1	1.80	0.46
2:D:99:ASP:OD1	2:D:101:THR:CG2	2.60	0.46
1:A:209:LYS:HE3	1:A:209:LYS:HB2	1.64	0.46
1:A:75:GLU:CG	1:A:129:LEU:HD11	2.44	0.46
1:C:68:THR:HG23	1:C:140:GLU:OE1	2.16	0.46
1:C:242:GLU:HG3	1:C:290:VAL:CG2	2.36	0.46
2:D:71:ARG:NH2	2:D:129:LEU:O	2.50	0.45
2:B:137:LYS:HB2	2:B:137:LYS:HE3	1.56	0.45
1:C:264:VAL:O	1:C:268:GLN:HG3	2.17	0.45
1:C:310:LYS:HG3	6:C:769:HOH:O	2.17	0.45
1:A:200:MET:HE2	2:B:200:MET:HE1	1.99	0.44
2:B:121:HIS:HD2	6:B:625:HOH:O	2.00	0.44
1:A:119:GLU:HG3	1:A:120:GLU:N	2.33	0.43
1:C:22:ARG:HD2	6:C:495:HOH:O	2.17	0.43
1:C:65:LYS:HG3	1:C:67:ASP:HB2	2.00	0.42
1:A:200:MET:HE2	1:A:200:MET:HB3	1.97	0.42
2:D:155:LYS:HE2	6:D:560:HOH:O	2.20	0.42
2:D:214:LEU:HD22	2:D:232:TYR:CD2	2.54	0.42
1:C:57:LYS:NZ	1:C:298:ILE:O	2.51	0.41
1:A:136:GLU:HG2	1:A:136:GLU:H	1.60	0.41
1:A:200:MET:HE3	2:B:200:MET:HE3	2.02	0.41
1:A:17:HIS:HD2	2:B:204:TYR:OH	2.02	0.41
2:D:137:LYS:HG2	2:D:138:TYR:CE1	2.55	0.41
1:C:71:ARG:O	1:C:75:GLU:HG3	2.21	0.41
1:A:69:ASN:ND2	1:A:71:ARG:H	2.17	0.41
1:A:253:THR:HG21	2:B:253:THR:HG21	2.02	0.41
2:D:82:ASP:OD1	2:D:121:HIS:CE1	2.74	0.40
2:D:163:LEU:HD23	2:D:181:VAL:HG21	2.02	0.40
1:C:22:ARG:CG	1:C:22:ARG:NH1	2.79	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	288/315 (91%)	279 (97%)	9 (3%)	0	100	100
1	C	278/315 (88%)	268 (96%)	10 (4%)	0	100	100
2	B	312/315 (99%)	304 (97%)	7 (2%)	1 (0%)	41	32
2	D	312/315 (99%)	305 (98%)	6 (2%)	1 (0%)	41	32
All	All	1190/1260 (94%)	1156 (97%)	32 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	144	ILE
2	B	144	ILE

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	253/273 (93%)	235 (93%)	18 (7%)	14	7
1	C	246/273 (90%)	229 (93%)	17 (7%)	15	8
2	B	272/272 (100%)	258 (95%)	14 (5%)	24	15
2	D	270/272 (99%)	262 (97%)	8 (3%)	41	35
All	All	1041/1090 (96%)	984 (94%)	57 (6%)	21	13

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	55	LEU
1	A	61	LEU
1	A	65	LYS
1	A	69	ASN
1	A	80	ILE

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Mol	Chain	Res	Type
1	A	94	ASP
1	A	119	GLU
1	A	122	GLN
1	A	129	LEU
1	A	136	GLU
1	A	137	LYS
1	A	163	LEU
1	A	179	LEU
1	A	196	PRO
1	A	206	ASN
1	A	214	LEU
1	A	299	LYS
2	B	29	SER
2	B	46	LEU
2	B	61	LEU
2	B	96	GLN
2	B	101	THR
2	B	108	LEU
2	B	129	LEU
2	B	133	GLU
2	B	163	LEU
2	B	173	ASN
2	B	194	LEU
2	B	206	ASN
2	B	299	LYS
2	B	300	VAL
1	C	22	ARG
1	C	46	LEU
1	C	55	LEU
1	C	60	LEU
1	C	61	LEU
1	C	70	ILE
1	C	83	GLU
1	C	87	GLU
1	C	144	ILE
1	C	148	GLN
1	C	163	LEU
1	C	168	GLU
1	C	242	GLU
1	C	262	ASN
1	C	299	LYS
1	C	310	LYS

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Mol	Chain	Res	Type
1	C	313	ILE
2	D	30	LEU
2	D	61	LEU
2	D	65	LYS
2	D	101	THR
2	D	119	GLU
2	D	129	LEU
2	D	163	LEU
2	D	179	LEU

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

Mol	Chain	Res	Type
1	A	17	HIS
1	A	69	ASN
1	A	121	HIS
1	A	130	ASN
1	A	148	GLN
1	A	151	HIS
1	A	228	ASN
1	A	261	GLN
2	B	121	HIS
2	B	228	ASN
2	B	270	GLN
1	C	17	HIS
1	C	148	GLN
1	C	261	GLN
1	C	262	ASN
1	C	270	GLN
2	D	77	ASN
2	D	121	HIS
2	D	151	HIS
2	D	173	ASN
2	D	228	ASN
2	D	268	GLN
2	D	270	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CME	B	197	2	8,9,10	0.71	0	5,9,11	1.45	1 (20%)
2	CME	D	197	2	8,9,10	0.74	0	5,9,11	1.78	2 (40%)

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
2	CME	B	197	2	-	2/5/8/10	-
2	CME	D	197	2	-	2/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	197	CME	CE-SD-SG	2.71	115.94	103.45
2	B	197	CME	CB-SG-SD	2.54	110.41	103.82
2	D	197	CME	CB-SG-SD	2.21	109.55	103.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	197	CME	SD-CE-CZ-OH
2	B	197	CME	SD-CE-CZ-OH
2	B	197	CME	CZ-CE-SD-SG
2	D	197	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	197	CME	1	0
2	D	197	CME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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
5	EDO	B	323	-	3,3,3	0.47	0	2,2,2	0.62	0
3	SO4	B	319	-	4,4,4	0.18	0	6,6,6	0.18	0
5	EDO	B	322	-	3,3,3	0.60	0	2,2,2	0.12	0
5	EDO	C	319	-	3,3,3	0.39	0	2,2,2	0.52	0
3	SO4	B	317	-	4,4,4	0.25	0	6,6,6	0.19	0
3	SO4	D	317	-	4,4,4	0.21	0	6,6,6	0.33	0
4	FFO	D	316	-	28,36,36	1.65	5 (17%)	28,50,50	1.90	9 (32%)
4	FFO	B	316	-	28,36,36	1.74	3 (10%)	28,50,50	2.05	8 (28%)
5	EDO	B	321	-	3,3,3	0.68	0	2,2,2	0.22	0
5	EDO	C	318	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	D	321	-	3,3,3	0.30	0	2,2,2	1.31	0
3	SO4	B	318	-	4,4,4	0.21	0	6,6,6	0.96	0
5	EDO	D	320	-	3,3,3	0.60	0	2,2,2	0.24	0
5	EDO	B	320	-	3,3,3	0.49	0	2,2,2	0.38	0
3	SO4	C	317	-	4,4,4	0.23	0	6,6,6	0.48	0
3	SO4	D	318	-	4,4,4	0.07	0	6,6,6	0.24	0

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
5	EDO	B	323	-	-	0/1/1/1	-
5	EDO	C	318	-	-	1/1/1/1	-
5	EDO	B	322	-	-	1/1/1/1	-
4	FFO	B	316	-	-	4/18/37/37	0/2/3/3
4	FFO	D	316	-	-	5/18/37/37	0/2/3/3
5	EDO	B	321	-	-	1/1/1/1	-
5	EDO	D	321	-	-	0/1/1/1	-
5	EDO	C	319	-	-	0/1/1/1	-
5	EDO	D	320	-	-	1/1/1/1	-
5	EDO	B	320	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	316	FFO	C4-C4A	5.41	1.48	1.41
4	D	316	FFO	C4-C4A	4.82	1.48	1.41
4	B	316	FFO	C5A-N5	4.68	1.41	1.35
4	D	316	FFO	C5A-N5	4.00	1.41	1.35
4	D	316	FFO	C4A-C8A	3.81	1.48	1.41
4	B	316	FFO	C4A-C8A	3.68	1.48	1.41
4	D	316	FFO	C4-N3	2.27	1.37	1.33
4	D	316	FFO	C7-C6	2.04	1.54	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	316	FFO	O5B-C5A-N5	-5.77	117.00	125.36
4	D	316	FFO	O5B-C5A-N5	-5.35	117.62	125.36
4	B	316	FFO	C4-N3-C2	3.71	121.83	115.93
4	B	316	FFO	C4-C4A-C8A	3.65	117.30	114.44
4	D	316	FFO	C2-N1-C8A	3.47	122.32	114.54
4	D	316	FFO	C4A-N5-C6	-3.37	113.34	119.31
4	B	316	FFO	C4A-N5-C6	-3.08	113.84	119.31
4	B	316	FFO	C2-N1-C8A	3.08	121.44	114.54
4	D	316	FFO	C4-N3-C2	3.06	120.79	115.93
4	B	316	FFO	CB-CA-N	3.00	114.56	110.19
4	D	316	FFO	C4-C4A-C8A	2.85	116.67	114.44
4	B	316	FFO	C4A-C4-N3	-2.79	117.40	123.14
4	B	316	FFO	C11-C-N	2.29	121.45	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	316	FFO	CB-CA-N	2.10	113.25	110.19
4	D	316	FFO	C4A-C4-N3	-2.09	118.84	123.14
4	D	316	FFO	CB-CG-CD	-2.04	109.21	113.59
4	D	316	FFO	C11-C-N	2.02	120.94	117.06

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	316	FFO	O5B-C5A-N5-C6
4	D	316	FFO	N5-C6-C9-N10
4	B	316	FFO	O5B-C5A-N5-C6
5	B	322	EDO	O1-C1-C2-O2
5	B	321	EDO	O1-C1-C2-O2
5	C	318	EDO	O1-C1-C2-O2
4	D	316	FFO	O5B-C5A-N5-C4A
4	B	316	FFO	O5B-C5A-N5-C4A
5	D	320	EDO	O1-C1-C2-O2
4	D	316	FFO	C6-C9-N10-C14
4	B	316	FFO	C6-C9-N10-C14
4	D	316	FFO	CT-CA-N-C
4	B	316	FFO	CT-CA-N-C

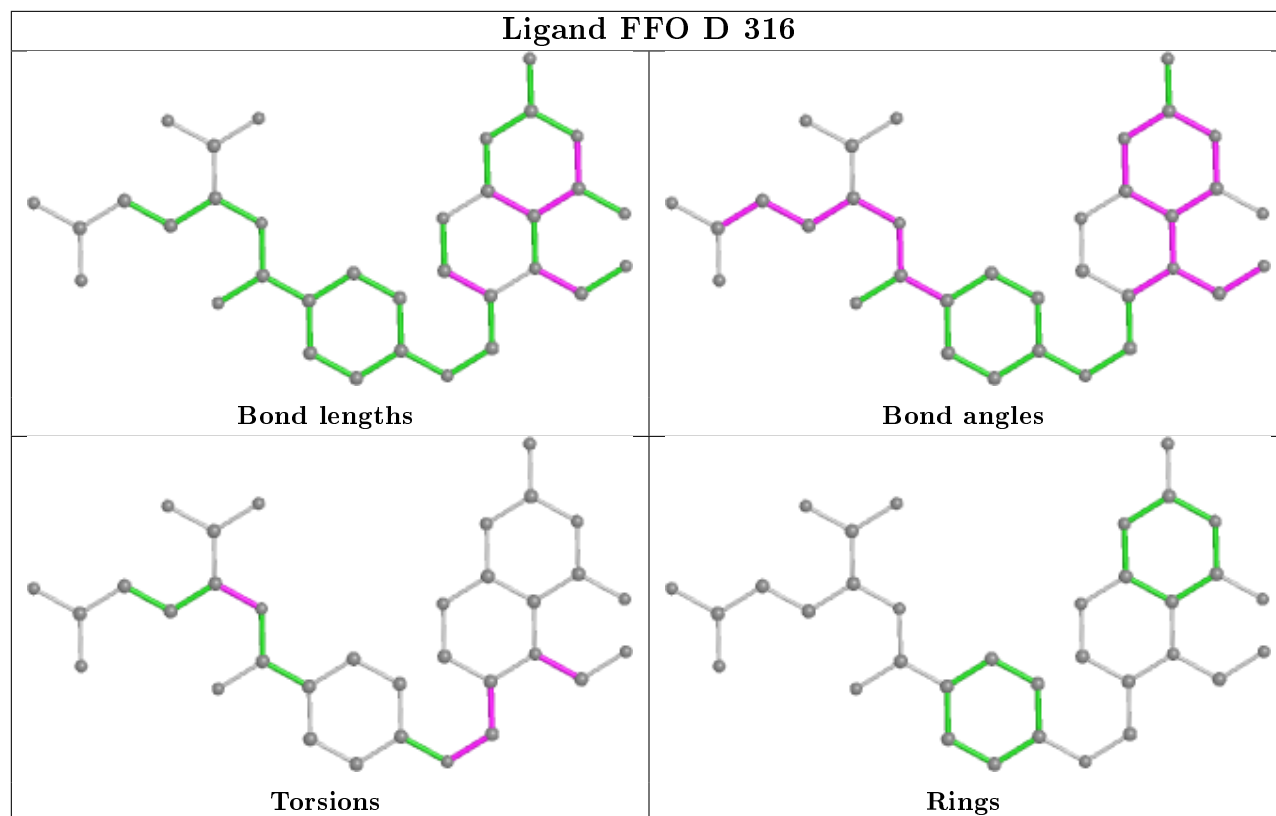
There are no ring outliers.

2 monomers are involved in 4 short contacts:

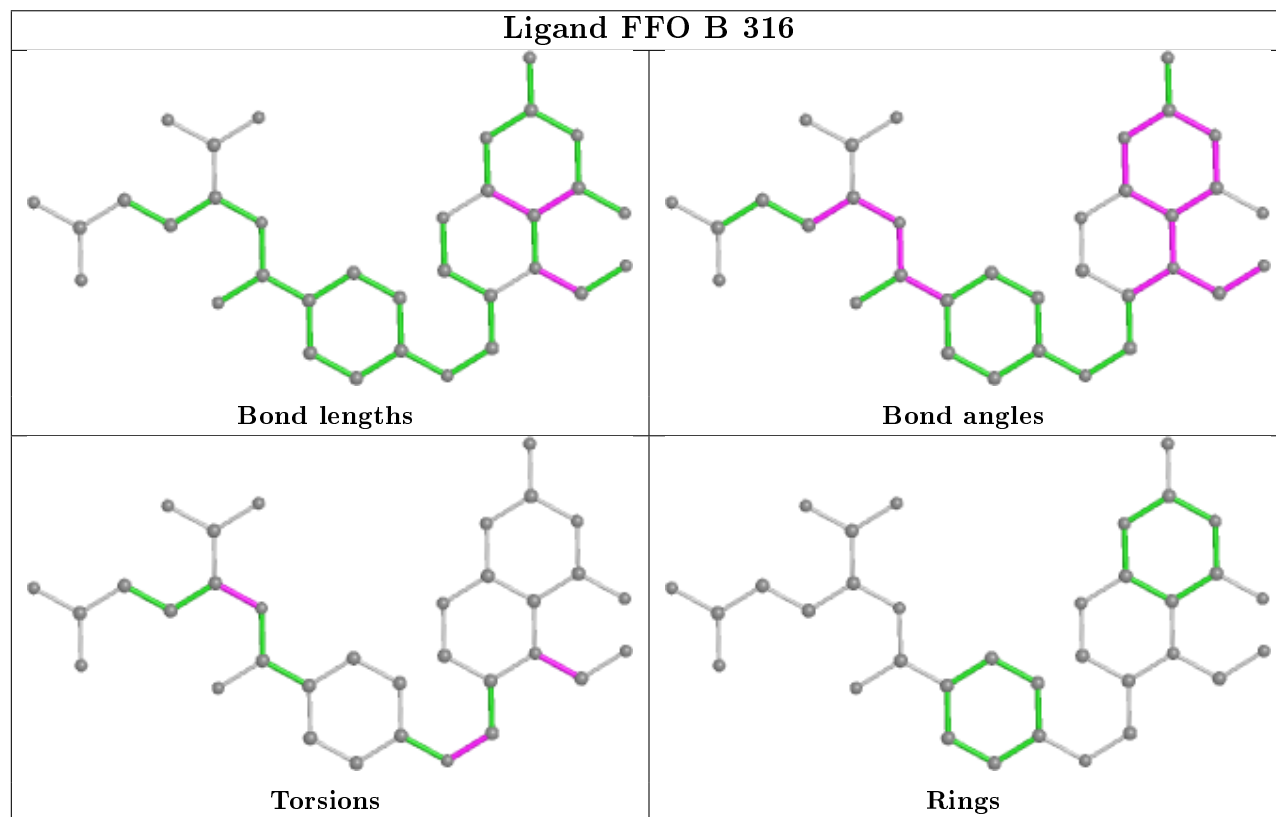
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	316	FFO	2	0
5	C	318	EDO	2	0

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 FFO D 316



Ligand FFO B 316



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	292/315 (92%)	-0.05	19 (6%) 18 19	5, 16, 56, 78	0
1	C	282/315 (89%)	0.07	26 (9%) 9 9	6, 17, 67, 83	0
2	B	314/315 (99%)	-0.51	0 100 100	5, 10, 23, 39	0
2	D	314/315 (99%)	-0.51	1 (0%) 94 94	5, 10, 23, 37	0
All	All	1202/1260 (95%)	-0.26	46 (3%) 40 42	5, 13, 45, 83	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	GLY	6.6
1	C	138	TYR	5.3
1	C	89	TYR	5.1
1	C	133	GLU	4.8
1	A	84	TRP	4.8
1	C	132	ALA	4.7
1	C	136	GLU	4.6
1	C	86	PHE	4.5
1	C	288	ALA	4.3
1	A	132	ALA	3.5
1	C	286	ASP	3.2
1	C	134	PHE	3.2
1	C	141	LEU	3.2
1	C	90	VAL	3.2
1	A	22	ARG	3.2
1	A	121	HIS	2.9
1	A	133	GLU	2.9
1	C	124	PHE	2.8
1	A	93	ALA	2.8
1	A	23	THR	2.7
1	A	313	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	89	TYR	2.6
1	C	123	LYS	2.6
2	D	198	HIS	2.5
1	A	288	ALA	2.5
1	A	96	GLN	2.4
1	A	130	ASN	2.4
1	C	126	ASP	2.4
1	A	286	ASP	2.4
1	C	82	ASP	2.4
1	C	87	GLU	2.4
1	C	313	ILE	2.4
1	C	131	ASP	2.3
1	C	137	LYS	2.3
1	A	135	ALA	2.2
1	C	83	GLU	2.2
1	C	84	TRP	2.2
1	A	95	TYR	2.2
1	C	130	ASN	2.2
1	C	129	LEU	2.1
1	A	138	TYR	2.1
1	A	142	GLY	2.1
1	A	122	GLN	2.1
1	C	143	ASN	2.0
1	C	135	ALA	2.0
1	A	131	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	CME	B	197	10/11	0.94	0.12	11,14,23,31	0
2	CME	D	197	10/11	0.95	0.14	11,14,22,31	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

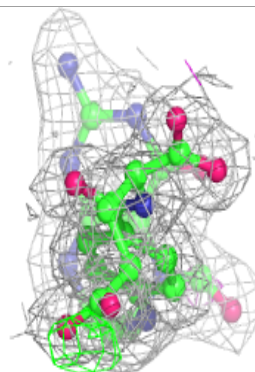
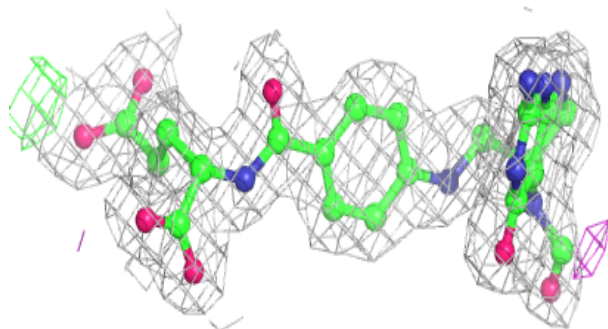
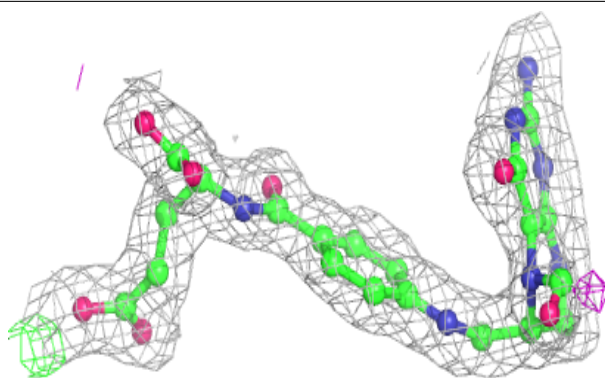
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	321	4/4	0.65	0.21	31,32,34,36	0
5	EDO	B	322	4/4	0.79	0.18	27,27,28,28	0
5	EDO	C	318	4/4	0.89	0.19	21,29,29,31	0
5	EDO	D	321	4/4	0.90	0.13	20,22,22,23	0
4	FFO	D	316	34/34	0.94	0.11	11,15,19,24	0
5	EDO	D	320	4/4	0.94	0.11	20,21,22,24	0
4	FFO	B	316	34/34	0.95	0.10	6,13,17,20	0
5	EDO	B	323	4/4	0.96	0.10	16,19,19,19	0
3	SO4	B	319	5/5	0.97	0.20	46,47,48,48	0
5	EDO	B	320	4/4	0.97	0.11	18,20,21,26	0
3	SO4	D	318	5/5	0.97	0.20	46,47,48,48	0
3	SO4	C	317	5/5	0.97	0.10	33,34,37,37	0
5	EDO	C	319	4/4	0.98	0.10	23,24,25,26	0
3	SO4	B	318	5/5	0.98	0.10	26,28,30,32	0
3	SO4	B	317	5/5	0.99	0.08	17,18,21,21	0
3	SO4	D	317	5/5	1.00	0.08	15,15,16,18	0

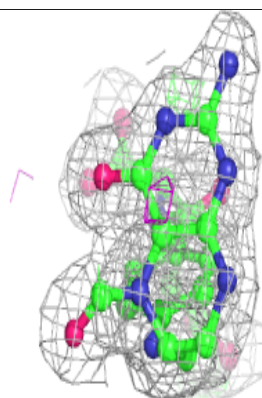
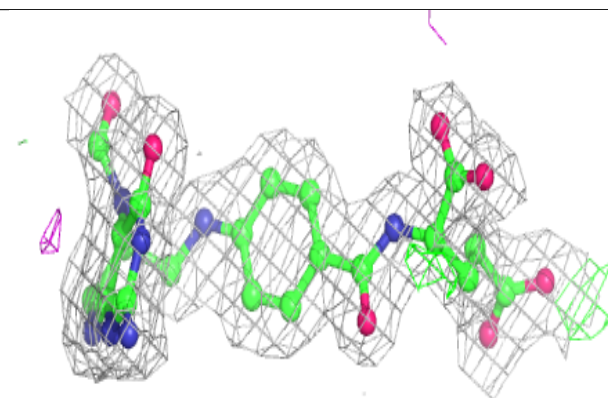
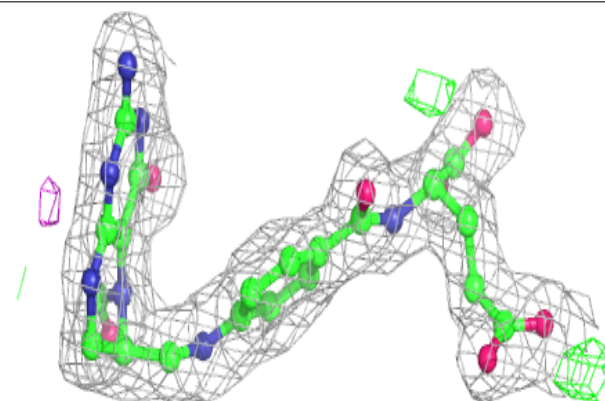
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FFO D 316:

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

**Electron density around FFO B 316:**

$2mF_o-DF_c$ (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.