Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 10:19 PM EDT

PDB ID	:	1TLS
Title	:	THYMIDYLATE SYNTHASE TERNARY COMPLEX WITH FDUMP AND METHYLENETETRAHYDROFOLATE
Authors	:	Hyatt, D.C.; Maley, F.; Montfort, W.R.
Deposited on	:	1996-12-03
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

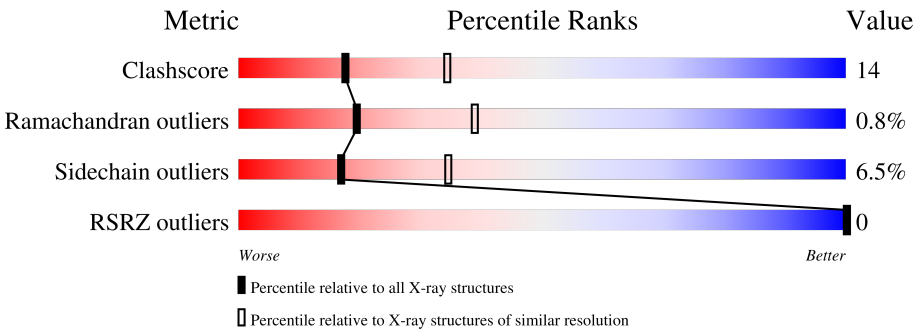
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	264	63% 31% 5% •
1	B	264	65% 29% 5% •

2 Entry composition (i)

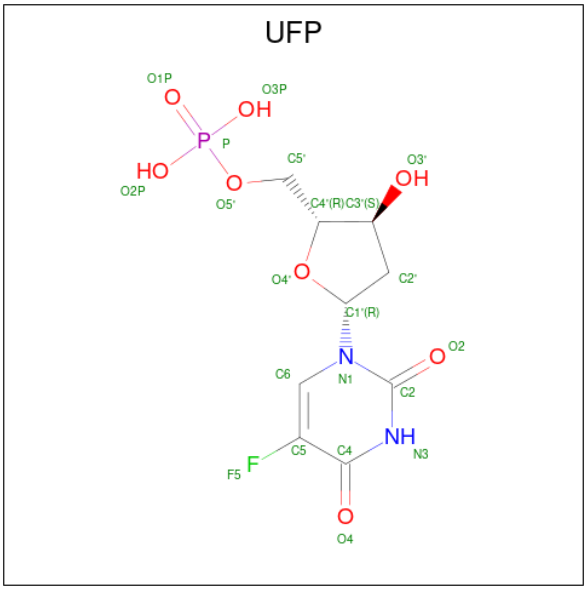
There are 4 unique types of molecules in this entry. The entry contains 4608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

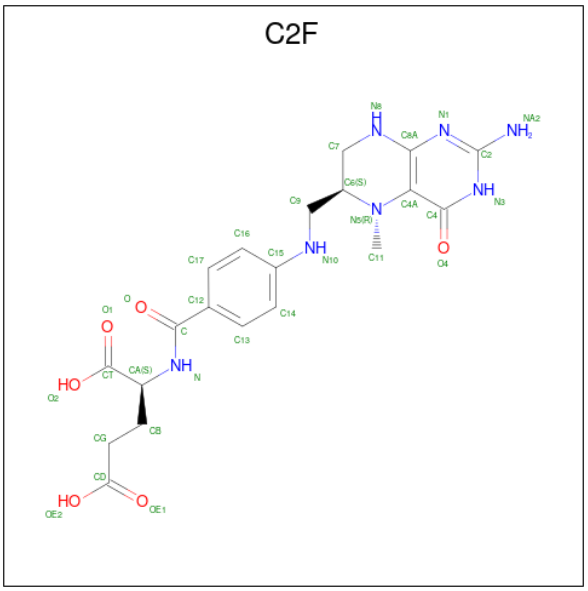
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2153	1375	371	395	12	0	0	0
1	B	264	2153	1375	371	395	12	0	0	0

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	21	9	1	2	8	1	0	0
2	B	1	21	9	1	2	8	1	0	0

- Molecule 3 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: $C_{20}H_{25}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	33	20	7	6	0	0
			Total	C	N	O		
3	B	1	33	20	7	6	0	0

- Molecule 4 is water.

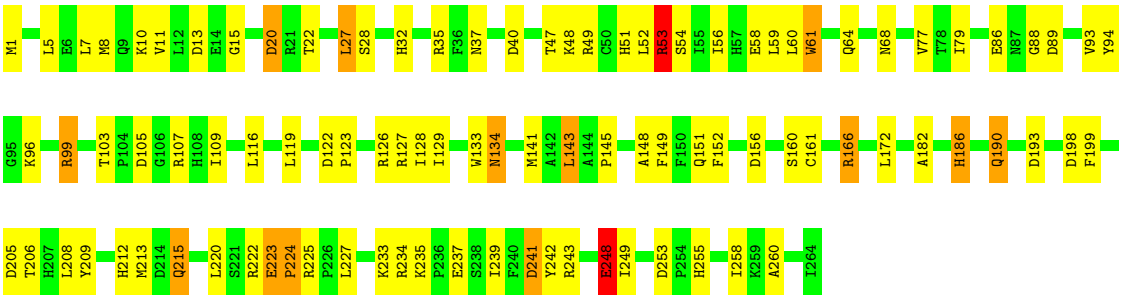
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	110	110	110	0	0
			Total	O		
4	B	84	84	84	0	0

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.

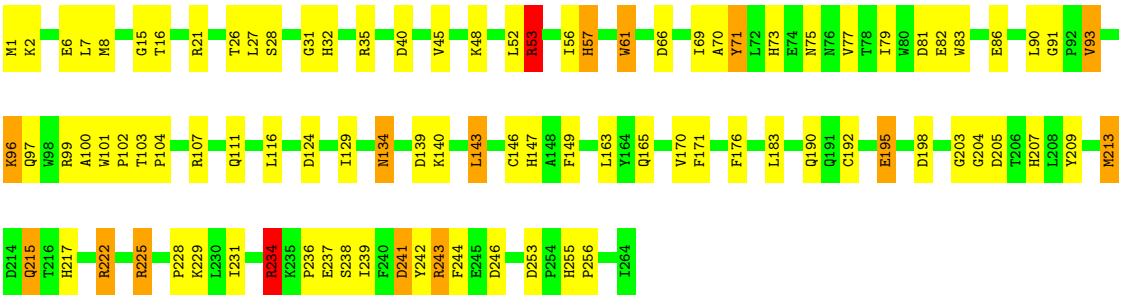
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A:



- Molecule 1: THYMIDYLATE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	126.78Å 126.78Å 67.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.80 – 2.60 14.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.80-2.60) 89.5 (14.85-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.61Å)	Xtriage
Refinement program	GPRLSA	Depositor
R, R_{free}	0.180 , (Not available) 0.161 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CXM, C2F, UFP

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	0.97	0/2202	1.87	47/2990 (1.6%)
1	B	0.96	0/2202	1.74	35/2990 (1.2%)
All	All	0.97	0/4404	1.80	82/5980 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ARG	NE-CZ-NH2	-18.01	111.29	120.30
1	A	198	ASP	CB-CG-OD1	14.30	131.17	118.30
1	A	35	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	243	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	A	53	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	B	99	ARG	NE-CZ-NH2	10.43	125.51	120.30
1	B	35	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	A	99	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	A	166	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	35	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	198	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	B	225	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	166	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	124	ASP	CB-CG-OD2	-8.32	110.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	B	21	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	B	53	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	59	LEU	CB-CG-CD2	-7.51	98.24	111.00
1	B	243	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	40	ASP	CB-CG-OD2	7.40	124.96	118.30
1	B	99	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	A	99	ARG	NH1-CZ-NH2	-7.31	111.36	119.40
1	B	139	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	107	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	241	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	198	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	61	TRP	CA-CB-CG	6.66	126.35	113.70
1	A	13	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	161	CYS	O-C-N	6.65	133.35	122.70
1	B	222	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	40	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	B	234	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	20	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	253	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	193	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	107	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	148	ALA	N-CA-CB	-6.37	101.18	110.10
1	A	205	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	195	GLU	N-CA-CB	-6.29	99.28	110.60
1	B	71	TYR	CB-CG-CD1	6.28	124.77	121.00
1	B	205	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	71	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	237	GLU	CG-CD-OE1	6.14	130.58	118.30
1	A	53	ARG	CD-NE-CZ	6.12	132.17	123.60
1	B	243	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	75	ASN	CB-CA-C	6.08	122.56	110.40
1	B	48	LYS	N-CA-CB	6.07	121.52	110.60
1	A	103	THR	CA-CB-CG2	6.05	120.86	112.40
1	A	53	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
1	A	105	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	126	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	99	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	160	SER	N-CA-CB	5.87	119.31	110.50
1	A	22	THR	CA-CB-CG2	5.69	120.37	112.40
1	B	6	GLU	CG-CD-OE2	-5.66	106.98	118.30
1	A	199	PHE	N-CA-CB	5.65	120.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	86	GLU	CA-CB-CG	5.62	125.76	113.40
1	B	35	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	227	LEU	N-CA-CB	-5.48	99.44	110.40
1	B	45	VAL	CA-CB-CG2	-5.45	102.72	110.90
1	A	94	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	16	THR	N-CA-CB	5.44	120.64	110.30
1	B	143	LEU	N-CA-CB	-5.35	99.70	110.40
1	A	156	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	A	61	TRP	CA-CB-CG	5.31	123.79	113.70
1	A	224	PRO	O-C-N	5.30	131.18	122.70
1	A	241	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	139	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	172	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	234	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	94	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	186	HIS	CA-CB-CG	5.15	122.36	113.60
1	B	246	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	48	LYS	CA-C-O	-5.14	109.31	120.10
1	B	195	GLU	CB-CA-C	-5.12	100.16	110.40
1	A	198	ASP	N-CA-CB	-5.10	101.43	110.60
1	A	86	GLU	CG-CD-OE2	5.09	128.49	118.30
1	B	190	GLN	CB-CG-CD	5.07	124.79	111.60
1	B	244	PHE	CB-CA-C	5.06	120.52	110.40
1	B	57	HIS	CA-CB-CG	-5.04	105.03	113.60
1	A	248	GLU	CG-CD-OE1	-5.02	108.26	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	ARG	Sidechain
1	A	99	ARG	Sidechain

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	2153	0	2079	66	0
1	B	2153	0	2079	52	0
2	A	21	0	9	1	0
2	B	21	0	9	1	0
3	A	33	0	21	5	0
3	B	33	0	21	1	0
4	A	110	0	0	3	0
4	B	84	0	0	2	0
All	All	4608	0	4218	118	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 14.

All (118) 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:52:LEU:CD1	1:A:249:ILE:HD13	1.54	1.33
1:A:52:LEU:HD11	1:A:249:ILE:CD1	1.84	1.08
1:B:129:ILE:HG21	1:B:149:PHE:CZ	2.02	0.95
1:A:52:LEU:CD1	1:A:249:ILE:CD1	2.42	0.94
1:A:215:GLN:HE21	1:A:215:GLN:H	1.19	0.90
1:B:215:GLN:HE21	1:B:215:GLN:N	1.69	0.90
1:B:215:GLN:H	1:B:215:GLN:NE2	1.68	0.90
1:A:52:LEU:HD11	1:A:249:ILE:HD13	0.87	0.84
1:B:215:GLN:HE21	1:B:215:GLN:H	0.85	0.82
1:B:96:LYS:NZ	1:B:102:PRO:HG3	1.96	0.80
1:B:27:LEU:HD12	1:B:213:MET:HE1	1.68	0.76
1:A:215:GLN:H	1:A:215:GLN:NE2	1.85	0.75
3:B:266:C2F:O2	4:B:346:HOH:O	2.08	0.71
1:A:222:ARG:NH1	1:A:258:ILE:HD11	2.06	0.71
1:A:53:ARG:HH11	1:A:53:ARG:HB2	1.56	0.71
1:B:56:ILE:HG12	1:B:183:LEU:HD21	1.73	0.71
1:A:129:ILE:HG21	1:A:149:PHE:CE2	2.26	0.70
1:A:5:LEU:HD23	1:A:8:MET:HE2	1.76	0.67
1:B:129:ILE:CG2	1:B:149:PHE:CZ	2.75	0.67
1:B:134:ASN:HD22	1:B:134:ASN:C	1.98	0.67
1:B:96:LYS:HZ3	1:B:102:PRO:HG3	1.61	0.66
1:A:52:LEU:HD13	1:A:249:ILE:HD13	1.71	0.66
1:A:233:LYS:NZ	1:A:248:GLU:HG3	2.12	0.64
1:A:10:LYS:HE2	1:A:32:HIS:CD2	2.34	0.63
1:A:52:LEU:HD21	1:A:249:ILE:HD11	1.81	0.63
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:HE2	1:A:32:HIS:HD2	1.65	0.60
1:A:129:ILE:CG2	1:A:149:PHE:CE2	2.84	0.59
1:A:52:LEU:CD2	1:A:249:ILE:CD1	2.80	0.59
1:B:238:SER:O	1:B:241:ASP:HB2	2.02	0.59
1:A:233:LYS:HZ2	1:A:248:GLU:HG3	1.69	0.58
1:A:151:GLN:HE22	1:B:204:GLY:HA3	1.69	0.57
1:B:57:HIS:HD2	1:B:71:TYR:OH	1.86	0.57
1:A:52:LEU:HD21	1:A:249:ILE:CD1	2.34	0.57
1:A:52:LEU:HD13	1:A:249:ILE:CD1	2.30	0.57
1:B:96:LYS:HZ1	1:B:102:PRO:HG3	1.69	0.56
1:A:7:LEU:HD11	1:A:206:THR:HG21	1.87	0.56
1:B:26:THR:HG22	1:B:209:TYR:CD1	2.41	0.55
1:A:53:ARG:HB2	1:A:53:ARG:NH1	2.19	0.55
1:A:129:ILE:HG13	1:A:151:GLN:HG3	1.88	0.55
1:A:215:GLN:HE21	1:A:215:GLN:N	1.98	0.55
1:B:27:LEU:HD12	1:B:213:MET:CE	2.36	0.54
1:B:69:ILE:HD12	1:B:73:HIS:CE1	2.42	0.54
1:B:27:LEU:CD1	1:B:213:MET:HE1	2.38	0.54
1:B:171:PHE:CZ	1:B:215:GLN:HB3	2.43	0.54
1:B:82:GLU:HG2	1:B:83:TRP:CZ3	2.43	0.54
1:A:47:THR:HA	1:A:255:HIS:CD2	2.44	0.53
1:B:147:HIS:HB2	1:B:163:LEU:HD11	1.91	0.53
1:B:53:ARG:HG3	1:B:53:ARG:NH1	2.23	0.52
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.45	0.52
1:A:5:LEU:HD23	1:A:8:MET:CE	2.38	0.52
1:A:134:ASN:C	1:A:134:ASN:HD22	2.14	0.51
1:A:47:THR:HA	1:A:255:HIS:HD2	1.75	0.51
1:B:242:TYR:O	1:B:243:ARG:HG2	2.11	0.51
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.46	0.51
1:A:143:LEU:CD2	3:A:266:C2F:H72	2.41	0.50
1:A:11:VAL:HG12	1:A:27:LEU:HD13	1.93	0.50
1:A:68:ASN:ND2	1:A:89:ASP:OD1	2.34	0.49
1:A:5:LEU:HD11	1:A:47:THR:HG21	1.94	0.48
1:A:8:MET:HE3	1:A:220:LEU:HG	1.94	0.48
1:A:53:ARG:HH11	1:A:53:ARG:CB	2.23	0.48
1:B:116:LEU:HD23	1:B:192:CYS:SG	2.53	0.48
1:A:56:ILE:O	1:A:60:LEU:HG	2.13	0.48
1:A:235:LYS:NZ	4:A:455:HOH:O	2.34	0.48
1:A:129:ILE:HG21	1:A:149:PHE:CZ	2.48	0.48
1:B:73:HIS:NE2	1:B:81:ASP:OD1	2.35	0.48
1:B:236:PRO:HG2	1:B:242:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:CD2	3:A:266:C2F:C7	2.92	0.47
1:B:129:ILE:HD13	1:B:149:PHE:CZ	2.49	0.47
1:B:165:GLN:O	1:B:203:GLY:HA2	2.15	0.47
1:A:11:VAL:HG12	1:A:27:LEU:CD1	2.46	0.46
1:A:127:ARG:HH22	1:B:143:LEU:HD12	1.81	0.46
1:B:234:ARG:O	1:B:236:PRO:HD3	2.14	0.46
1:A:133:TRP:CZ3	1:A:166:ARG:HD3	2.50	0.46
1:A:11:VAL:O	1:A:15:GLY:N	2.48	0.46
1:A:119:LEU:HD23	1:A:128:ILE:HD13	1.98	0.45
1:A:143:LEU:HD21	3:A:266:C2F:N8	2.31	0.45
1:B:239:ILE:HA	1:B:242:TYR:HE1	1.81	0.45
1:B:70:ALA:O	1:B:73:HIS:HB2	2.16	0.45
1:B:100:ALA:O	1:B:102:PRO:HD3	2.16	0.45
1:A:64:GLN:HG2	4:A:404:HOH:O	2.15	0.45
1:A:77:VAL:HG13	1:A:79:ILE:HG12	1.98	0.45
1:B:7:LEU:HD13	1:B:32:HIS:ND1	2.32	0.45
1:B:103:THR:HB	1:B:104:PRO:HD2	1.98	0.45
1:B:27:LEU:CD1	1:B:213:MET:CE	2.95	0.44
1:A:51:HIS:CE1	1:A:54:SER:HG	2.36	0.44
1:A:128:ILE:CG2	1:A:152:PHE:HB2	2.48	0.44
1:B:91:GLY:O	1:B:93:VAL:N	2.46	0.43
1:B:101:TRP:CH2	1:B:134:ASN:HA	2.53	0.43
1:B:134:ASN:C	1:B:134:ASN:ND2	2.69	0.43
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.31	0.43
1:B:15:GLY:HA2	1:B:28:SER:O	2.19	0.43
1:A:223:GLU:HA	1:A:224:PRO:HD3	1.86	0.42
1:A:58:GLU:O	1:A:61:TRP:HB3	2.19	0.42
1:A:64:GLN:CG	4:A:404:HOH:O	2.67	0.42
1:B:231:ILE:HA	4:B:463:HOH:O	2.20	0.42
1:A:166:ARG:NH2	2:A:265:UFP:O3P	2.41	0.42
1:A:11:VAL:CG1	1:A:208:LEU:HD12	2.50	0.42
1:A:20:ASP:OD2	1:A:209:TYR:HE1	2.02	0.42
1:A:129:ILE:HD13	1:A:149:PHE:HZ	1.85	0.42
1:A:239:ILE:O	1:A:242:TYR:HD1	2.03	0.42
1:A:141:MET:SD	1:A:145:PRO:HD3	2.60	0.42
1:A:68:ASN:HA	1:A:88:GLY:O	2.19	0.41
1:B:213:MET:O	1:B:217:HIS:CD2	2.73	0.41
1:B:146:CYS:HB2	2:B:265:UFP:C4	2.50	0.41
1:A:143:LEU:HD23	3:A:266:C2F:H72	2.02	0.41
1:A:182:ALA:O	1:A:186:HIS:HD2	2.04	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:CD2	1:A:260:ALA:HB1	2.55	0.41
1:B:77:VAL:CG1	1:B:79:ILE:HG12	2.51	0.41
3:A:266:C2F:H92	3:A:266:C2F:H16	1.82	0.41
1:B:69:ILE:HG23	1:B:90:LEU:HD11	2.02	0.41
1:B:255:HIS:HB3	1:B:256:PRO:CD	2.51	0.40
1:B:97:GLN:O	1:B:111:GLN:NE2	2.46	0.40
1:B:165:GLN:O	1:B:204:GLY:N	2.49	0.40
1:B:170:VAL:HG23	1:B:207:HIS:O	2.21	0.40
1:B:70:ALA:O	1:B:73:HIS:N	2.54	0.40
1:A:122:ASP:N	1:A:123:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	34	57
1	B	262/264 (99%)	248 (95%)	11 (4%)	3 (1%)	14	30
All	All	524/528 (99%)	497 (95%)	23 (4%)	4 (1%)	19	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	B	228	PRO
1	B	31	GLY
1	B	93	VAL

5.3.2 Protein sidechains (i)

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	232/232 (100%)	218 (94%)	14 (6%)	19	39
1	B	232/232 (100%)	216 (93%)	16 (7%)	15	31
All	All	464/464 (100%)	434 (94%)	30 (6%)	17	34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	53	ARG
1	A	96	LYS
1	A	109	ILE
1	A	134	ASN
1	A	190	GLN
1	A	213	MET
1	A	215	GLN
1	A	223	GLU
1	A	225	ARG
1	A	241	ASP
1	A	248	GLU
1	B	2	LYS
1	B	8	MET
1	B	52	LEU
1	B	53	ARG
1	B	96	LYS
1	B	134	ASN
1	B	140	LYS
1	B	176	PHE
1	B	195	GLU
1	B	213	MET
1	B	215	GLN
1	B	225	ARG
1	B	229	LYS

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Mol	Chain	Res	Type
1	B	234	ARG
1	B	237	GLU
1	B	253	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	97	GLN
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	190	GLN
1	A	215	GLN
1	A	217	HIS
1	B	32	HIS
1	B	57	HIS
1	B	117	ASN
1	B	118	GLN
1	B	121	ASN
1	B	134	ASN
1	B	151	GLN
1	B	215	GLN
1	B	217	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
1	CXM	A	1	1	9,10,11	1.22	1 (11%)	9,11,13	1.87	2 (22%)
1	CXM	B	1	1	9,10,11	1.03	1 (11%)	9,11,13	2.90	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	A	1	1	-	1/9/10/12	-
1	CXM	B	1	1	-	1/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CXM	CN-N	-2.54	1.30	1.35
1	B	1	CXM	ON1-CN	2.16	1.25	1.21

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1	CXM	O-C-CA	-6.04	109.24	124.77
1	B	1	CXM	ON1-CN-N	-4.12	118.11	124.86
1	B	1	CXM	C-CA-N	-3.91	101.95	109.50
1	A	1	CXM	O-C-CA	-3.79	115.02	124.77
1	A	1	CXM	C-CA-N	-3.41	102.91	109.50
1	B	1	CXM	CB-CA-N	2.60	115.26	110.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	O-C-CA-CB
1	B	1	CXM	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
3	C2F	A	266	2	33,35,35	2.34	14 (42%)	35,49,49	2.38	15 (42%)
2	UFP	B	265	1,3	22,22,22	5.90	5 (22%)	32,33,33	4.45	12 (37%)
2	UFP	A	265	1,3	22,22,22	5.64	5 (22%)	32,33,33	4.28	12 (37%)
3	C2F	B	266	2	33,35,35	2.32	11 (33%)	35,49,49	3.21	9 (25%)

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	C2F	A	266	2	-	1/22/35/35	0/3/3/3
2	UFP	B	265	1,3	-	0/10/22/22	0/2/2/2
2	UFP	A	265	1,3	-	2/10/22/22	0/2/2/2
3	C2F	B	266	2	-	2/22/35/35	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	265	UFP	C6-C5	20.76	1.62	1.33
2	A	265	UFP	C6-C5	18.89	1.59	1.33
2	A	265	UFP	C4-C5	15.35	1.63	1.44
2	B	265	UFP	C4-C5	14.88	1.63	1.44
2	B	265	UFP	C6-N1	8.70	1.52	1.38
2	A	265	UFP	C6-N1	8.18	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	266	C2F	C9-N10	5.88	1.56	1.45
3	B	266	C2F	C4-N3	5.46	1.42	1.33
3	A	266	C2F	C4-N3	5.30	1.42	1.33
3	B	266	C2F	C8A-N1	4.58	1.42	1.34
2	A	265	UFP	F5-C5	-4.29	1.27	1.35
3	A	266	C2F	C8A-N1	4.16	1.42	1.34
3	B	266	C2F	C6-N5	-4.05	1.42	1.47
3	A	266	C2F	C2-NA2	3.94	1.41	1.33
3	A	266	C2F	C9-N10	3.90	1.52	1.45
3	A	266	C2F	C6-N5	-3.89	1.43	1.47
2	B	265	UFP	O4'-C4'	3.39	1.52	1.45
3	A	266	C2F	C2-N3	3.37	1.41	1.35
3	B	266	C2F	CG-CD	3.35	1.58	1.50
3	A	266	C2F	C-N	3.25	1.41	1.34
3	A	266	C2F	C2-N1	3.11	1.40	1.35
3	B	266	C2F	C7-C6	-2.96	1.48	1.52
3	B	266	C2F	C2-N3	2.90	1.40	1.35
3	B	266	C2F	C-N	2.77	1.40	1.34
2	B	265	UFP	O3'-C3'	-2.75	1.37	1.43
3	A	266	C2F	C14-C15	2.66	1.43	1.39
3	B	266	C2F	C2-N1	2.58	1.39	1.35
2	A	265	UFP	P-O2P	-2.57	1.45	1.54
3	B	266	C2F	C15-N10	2.45	1.45	1.38
3	A	266	C2F	CA-CT	2.36	1.58	1.52
3	A	266	C2F	C14-C13	-2.31	1.35	1.38
3	A	266	C2F	C12-C	2.21	1.55	1.50
3	A	266	C2F	CG-CD	2.20	1.55	1.50
3	A	266	C2F	O2-CT	-2.14	1.23	1.30
3	B	266	C2F	C16-C15	2.03	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	265	UFP	C6-C5-C4	-19.86	104.45	122.57
2	A	265	UFP	C6-C5-C4	-18.29	105.89	122.57
3	B	266	C2F	C8A-C4A-C4	11.38	123.25	114.44
3	B	266	C2F	CG-CB-CA	10.30	132.15	113.16
2	A	265	UFP	C5-C4-N3	7.53	119.52	112.64
2	A	265	UFP	O4-C4-C5	-7.27	119.50	125.69
2	B	265	UFP	O4-C4-C5	-7.19	119.57	125.69
3	A	266	C2F	C8A-C4A-C4	6.76	119.68	114.44
3	B	266	C2F	C11-N5-C4A	6.71	122.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	265	UFP	C5-C4-N3	6.51	118.59	112.64
2	A	265	UFP	F5-C5-C6	-5.52	116.34	120.99
2	B	265	UFP	C5-C6-N1	-5.38	113.86	120.32
2	B	265	UFP	F5-C5-C6	-5.23	116.58	120.99
3	A	266	C2F	C11-N5-C4A	5.13	120.28	113.30
2	A	265	UFP	C5-C6-N1	-4.79	114.57	120.32
3	A	266	C2F	C2-N3-C4	4.30	121.94	115.96
2	A	265	UFP	O4'-C1'-N1	4.10	115.14	107.86
3	A	266	C2F	CA-N-C	-3.94	112.12	121.56
2	B	265	UFP	C1'-N1-C6	-3.89	114.20	120.74
2	B	265	UFP	N3-C2-N1	3.87	119.93	114.89
2	A	265	UFP	N3-C2-N1	3.84	119.89	114.89
3	B	266	C2F	C2-N3-C4	3.70	121.10	115.96
3	A	266	C2F	O2-CT-O1	3.54	132.12	124.08
2	B	265	UFP	C1'-N1-C2	3.41	124.33	117.66
3	A	266	C2F	OE1-CD-CG	-3.40	112.30	123.09
3	B	266	C2F	O2-CT-O1	3.11	131.14	124.08
2	B	265	UFP	O2-C2-N3	-3.00	115.95	121.49
2	A	265	UFP	C1'-N1-C6	-2.94	115.81	120.74
3	A	266	C2F	CB-CA-N	-2.91	105.16	110.91
2	A	265	UFP	C2'-C3'-C4'	-2.79	97.13	102.80
2	B	265	UFP	O3P-P-O2P	2.78	118.24	107.80
2	A	265	UFP	C4-N3-C2	-2.76	123.73	127.34
3	A	266	C2F	N1-C2-N3	-2.74	121.29	125.48
3	B	266	C2F	NA2-C2-N1	2.73	121.32	117.22
3	B	266	C2F	C2-N1-C8A	2.72	121.05	114.59
3	A	266	C2F	CB-CG-CD	-2.70	105.30	112.49
2	B	265	UFP	O4'-C1'-C2'	2.65	111.20	106.25
3	A	266	C2F	CT-CA-N	-2.62	104.50	110.57
2	A	265	UFP	O3P-P-O1P	-2.52	101.00	110.83
3	B	266	C2F	CT-CA-N	-2.49	104.80	110.57
3	A	266	C2F	NA2-C2-N3	2.44	120.88	117.22
3	A	266	C2F	C2-N1-C8A	2.41	120.31	114.59
3	A	266	C2F	O1-CT-CA	-2.31	114.80	122.26
2	A	265	UFP	C1'-N1-C2	2.29	122.13	117.66
3	A	266	C2F	CG-CB-CA	2.15	117.12	113.16
3	A	266	C2F	C9-N10-C15	-2.13	116.58	122.00
2	B	265	UFP	C4'-O4'-C1'	-2.07	104.60	109.51
3	B	266	C2F	C11-N5-C6	-2.04	112.23	117.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	266	C2F	C6-C9-N10-C15
3	A	266	C2F	C6-C9-N10-C15
3	B	266	C2F	N-CA-CB-CG
2	A	265	UFP	O4'-C4'-C5'-O5'
2	A	265	UFP	C4'-C5'-O5'-P

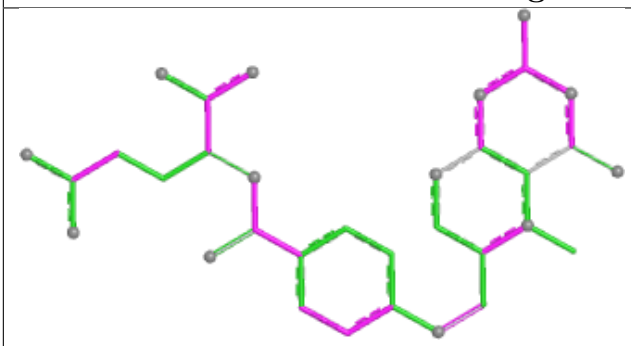
There are no ring outliers.

4 monomers are involved in 8 short contacts:

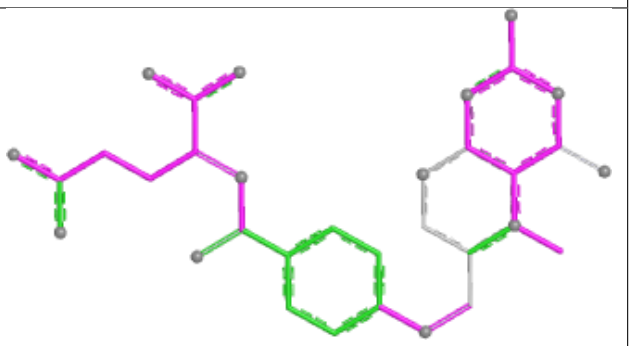
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	266	C2F	5	0
2	B	265	UFP	1	0
2	A	265	UFP	1	0
3	B	266	C2F	1	0

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 then 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.

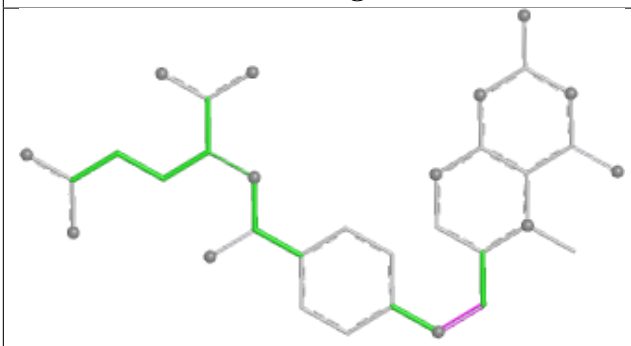
Ligand C2F A 266



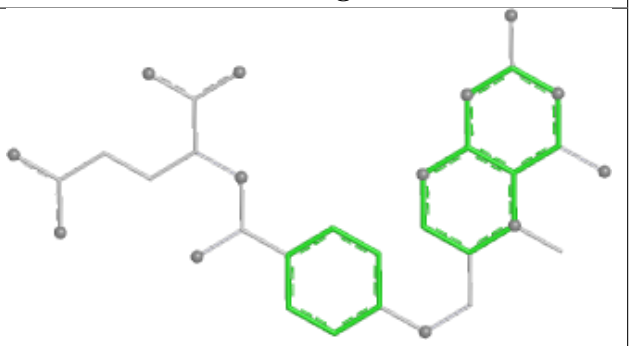
Bond lengths



Bond angles

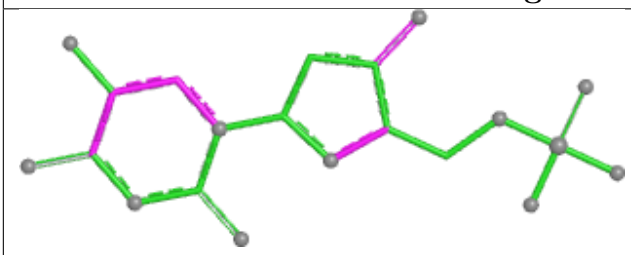


Torsions

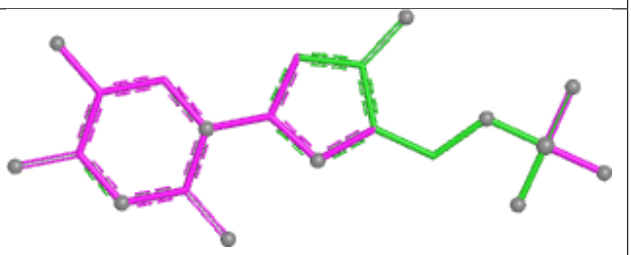


Rings

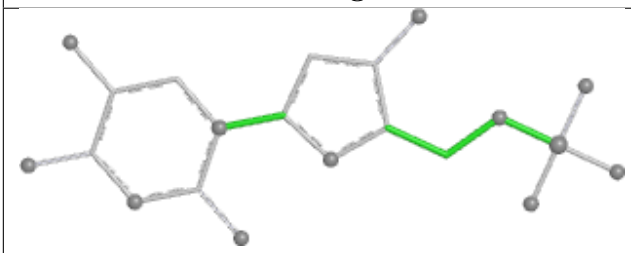
Ligand UFP B 265



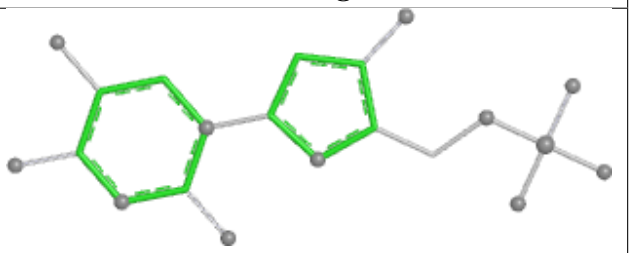
Bond lengths



Bond angles

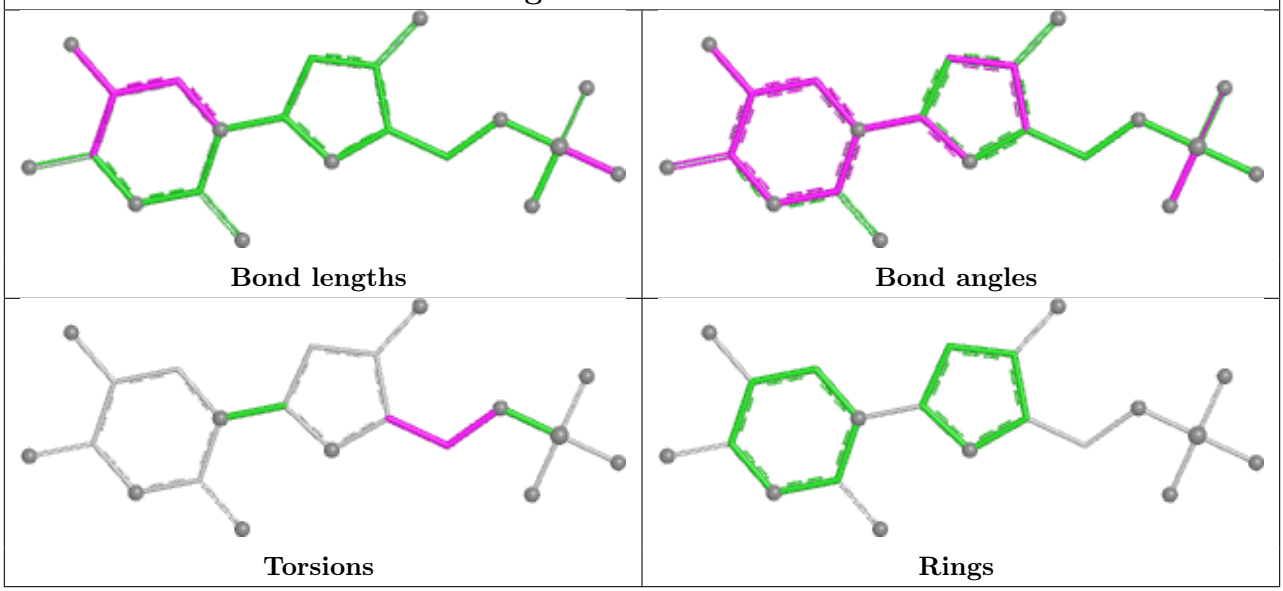


Torsions

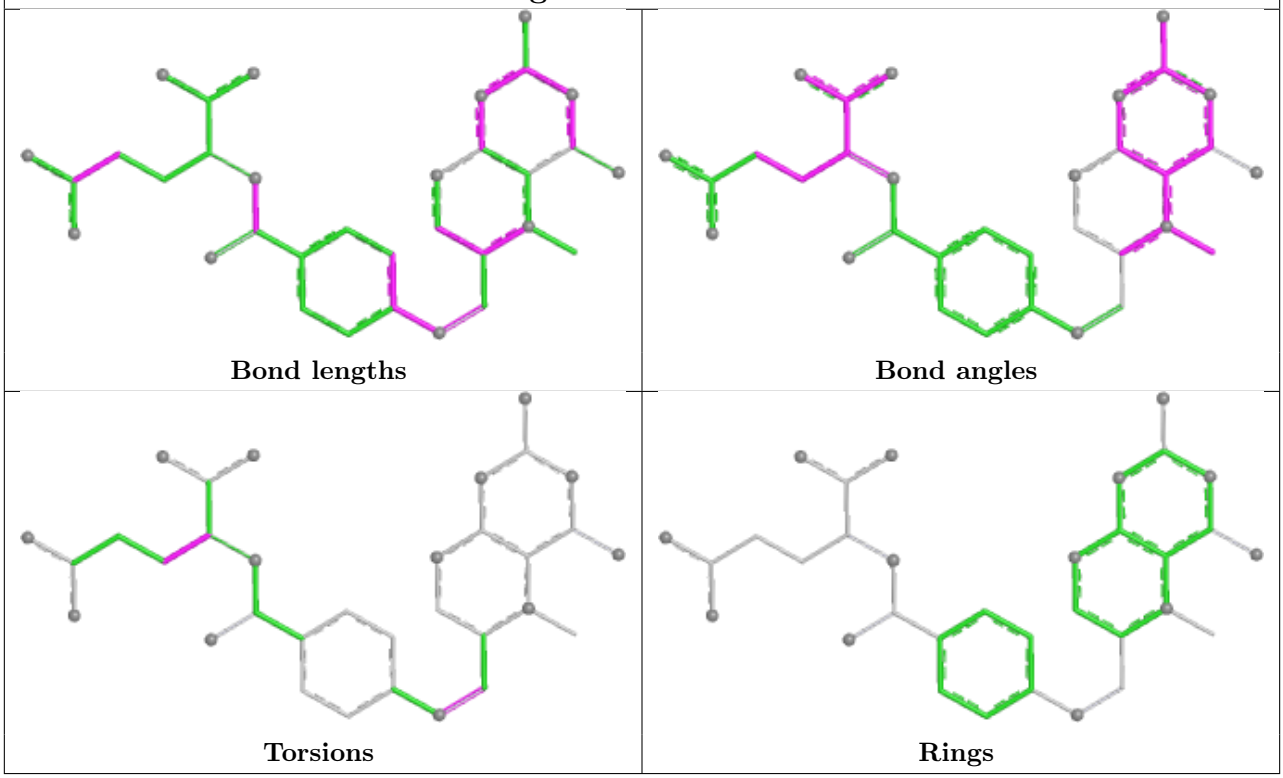


Rings

Ligand UFP A 265



Ligand C2F B 266



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, 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	263/264 (99%)	-1.06	0	100	100	2, 13, 28, 45	0
1	B	263/264 (99%)	-0.90	0	100	100	3, 18, 39, 54	0
All	All	526/528 (99%)	-0.98	0	100	100	2, 15, 35, 54	0

There are no RSRZ outliers to report.

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(Å^2)	Q<0.9
1	CXM	B	1	11/12	0.96	0.10	17,20,26,26	0
1	CXM	A	1	11/12	0.98	0.08	13,17,20,20	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

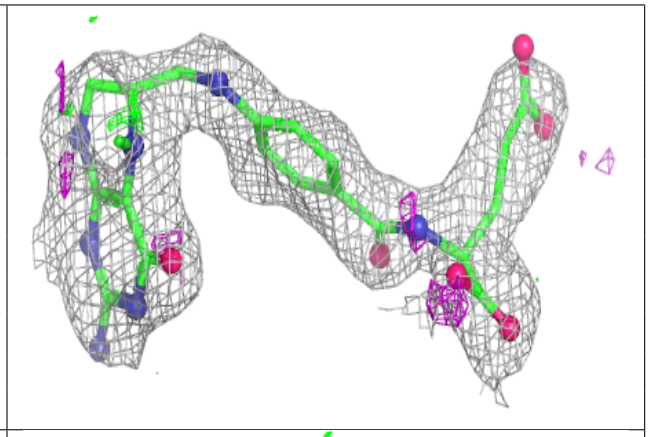
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

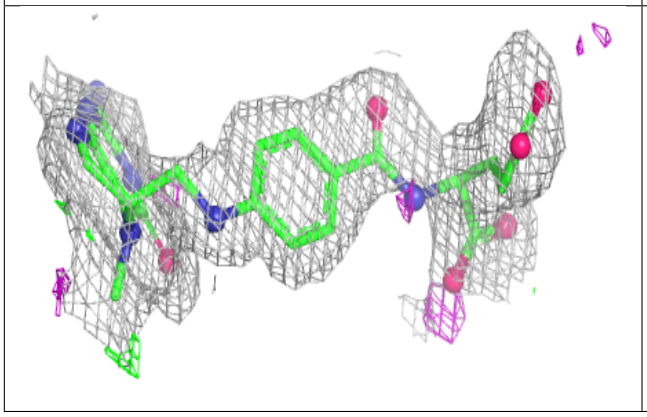
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C2F	B	266	33/33	0.86	0.18	20,33,50,53	0
3	C2F	A	266	33/33	0.87	0.15	15,26,46,47	0
2	UFP	A	265	21/21	0.96	0.12	8,13,16,18	0
2	UFP	B	265	21/21	0.96	0.12	13,17,19,20	0

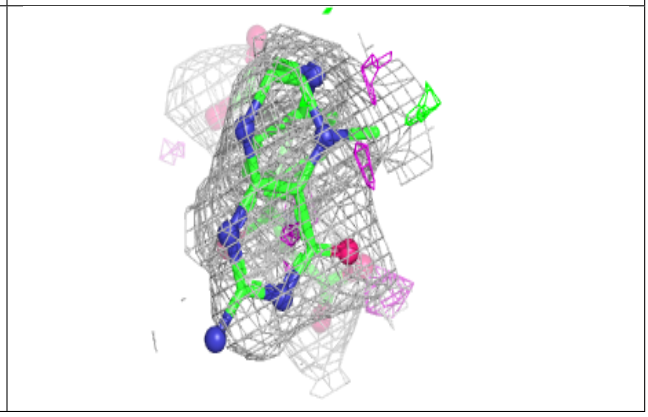
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C2F B 266:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

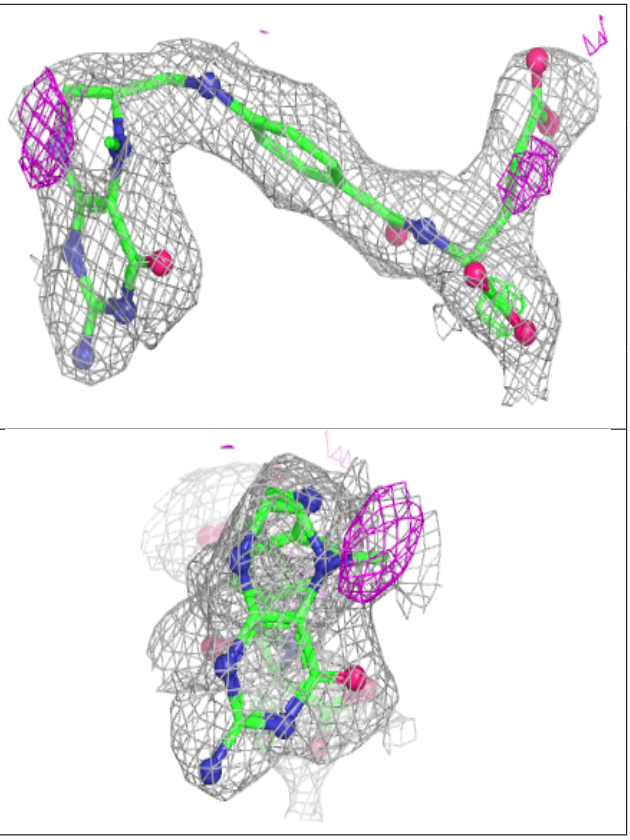






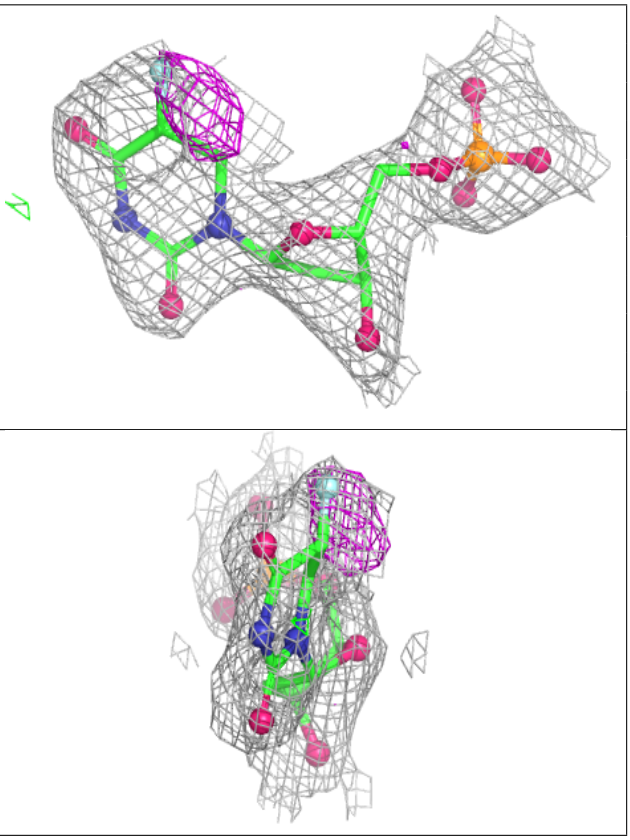
Electron density around C2F A 266:

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



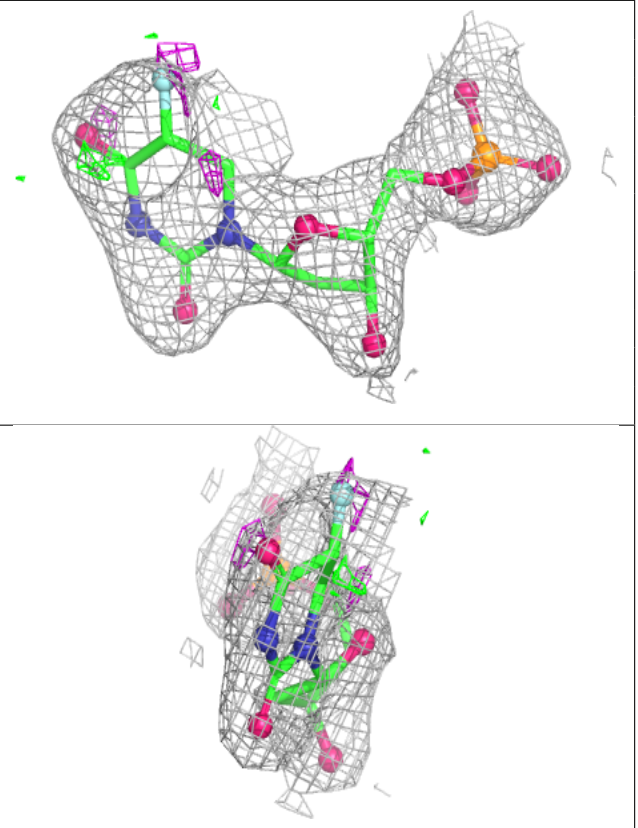
Electron density around UFP A 265:

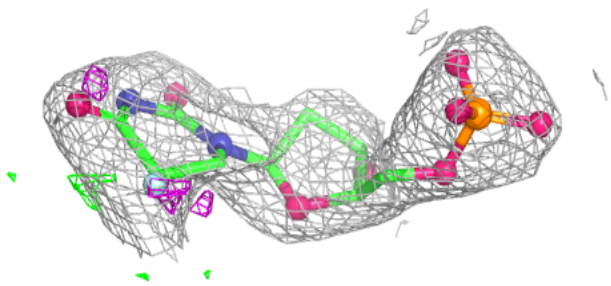
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UFP B 265:

$2mF_o$-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.