



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:54 PM UTC

PDB ID : 1TSN / pdb_00001tsn
Title : THYMIDYLATE SYNTHASE TERNARY COMPLEX WITH FDUMP AND METHYLENETETRAHYDROFOLATE
Authors : Hyatt, D.C.; Maley, F.; Montfort, W.R.
Deposited on : 1996-12-02
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

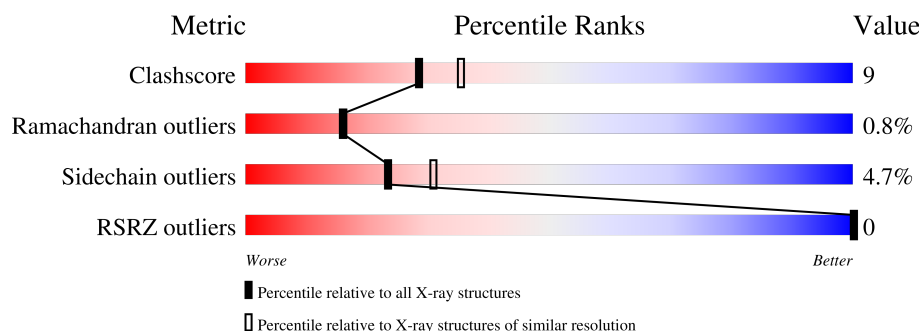
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	

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
2	PO4	A	267	-	X	-	-

2 Entry composition [i](#)

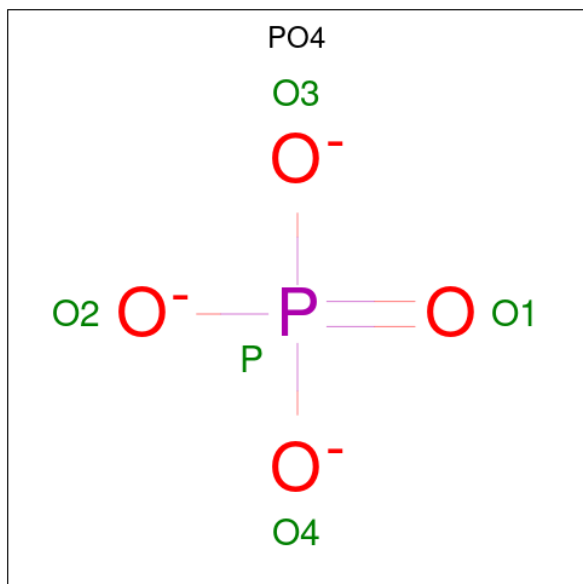
There are 5 unique types of molecules in this entry. The entry contains 2322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

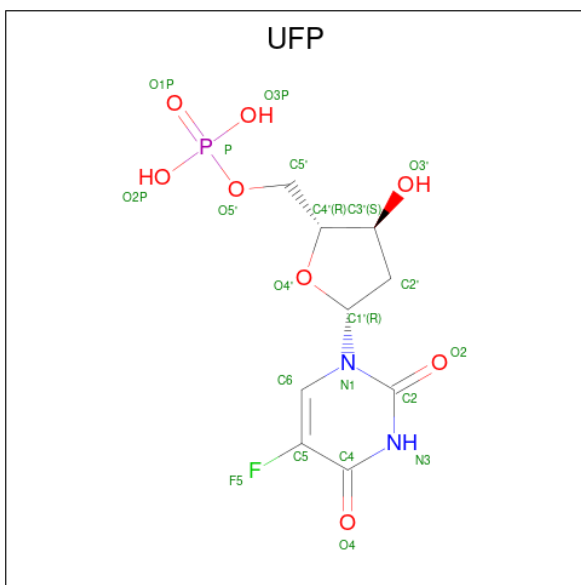
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2153	1375	371	395	12	0	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



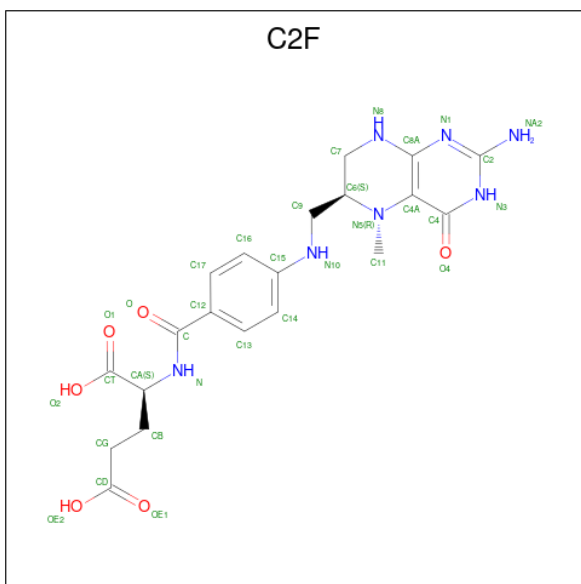
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: $C_9H_{12}FN_2O_8P$).



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

- Molecule 4 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (CCD ID: C2F) (formula: $C_{20}H_{25}N_7O_6$).



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

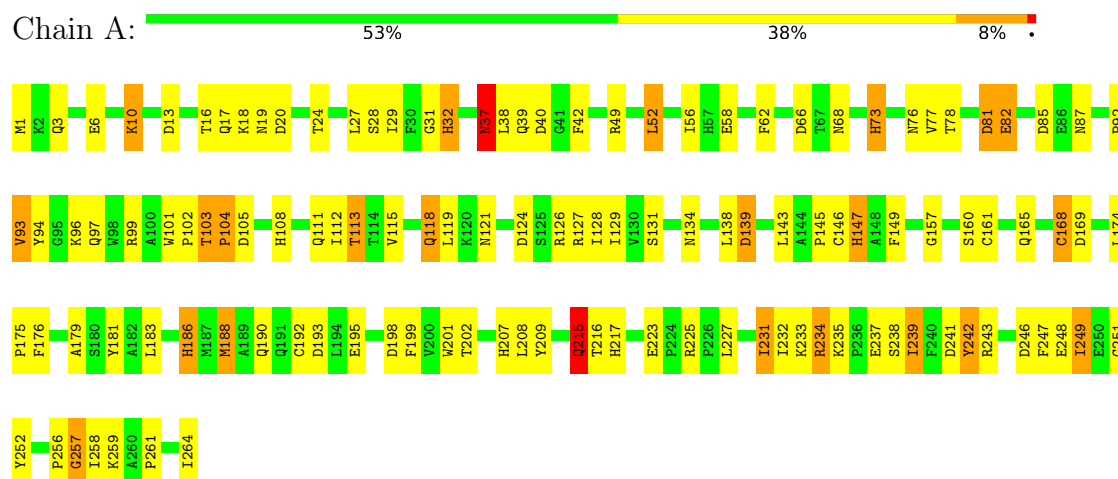
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total 110	O 110	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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 72.10Å 115.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.00 – 2.20 9.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (9.00-2.20) 88.3 (9.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.19Å)	Xtriage
Refinement program	GPRLSA	Depositor
R, R_{free}	0.178 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2322	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CXM, PO4, UFP, C2F

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	1.25	2/2202 (0.1%)	2.39	143/2990 (4.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	SER	CA-C	-5.26	1.46	1.52
1	A	231	ILE	C-N	-5.09	1.27	1.33

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	GLN	OE1-CD-NE2	-13.07	109.53	122.60
1	A	127	ARG	NE-CZ-NH2	12.47	130.42	119.20
1	A	62	PHE	CA-CB-CG	11.80	125.60	113.80
1	A	258	ILE	CA-C-O	-11.45	108.71	120.27
1	A	176	PHE	CA-CB-CG	10.07	123.87	113.80
1	A	256	PRO	CA-C-N	8.75	128.41	120.10
1	A	256	PRO	C-N-CA	8.75	128.41	120.10
1	A	217	HIS	CA-CB-CG	-8.72	105.08	113.80
1	A	176	PHE	CA-C-N	7.99	130.82	120.44
1	A	176	PHE	C-N-CA	7.99	130.82	120.44
1	A	101	TRP	O-C-N	7.92	128.55	121.18
1	A	127	ARG	NE-CZ-NH1	-7.88	113.62	121.50
1	A	108	HIS	CA-CB-CG	-7.88	105.92	113.80
1	A	37	ASN	CB-CG-ND2	7.64	127.87	116.40
1	A	112	ILE	CA-C-N	7.55	131.02	120.29
1	A	112	ILE	C-N-CA	7.55	131.02	120.29
1	A	111	GLN	OE1-CD-NE2	7.53	130.13	122.60
1	A	28	SER	N-CA-C	7.37	121.55	109.24
1	A	32	HIS	CA-CB-CG	-7.36	106.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASP	O-C-N	7.36	132.43	123.16
1	A	3	GLN	CG-CD-NE2	-7.25	105.52	116.40
1	A	258	ILE	O-C-N	7.23	130.70	123.18
1	A	201	TRP	CA-C-O	-7.16	112.62	120.43
1	A	235	LYS	O-C-N	7.09	128.34	120.83
1	A	143	LEU	CA-C-O	-7.02	112.18	120.60
1	A	235	LYS	CA-C-O	-6.99	113.91	119.99
1	A	208	LEU	CA-C-O	-6.96	112.85	120.30
1	A	73	HIS	CA-CB-CG	-6.95	106.86	113.80
1	A	227	LEU	O-C-N	6.94	129.21	121.43
1	A	81	ASP	CA-C-O	-6.91	113.57	120.82
1	A	76	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	145	PRO	CA-C-O	-6.61	114.11	121.32
1	A	42	PHE	O-C-N	6.59	126.91	121.31
1	A	175	PRO	CA-C-N	6.55	128.96	120.44
1	A	175	PRO	C-N-CA	6.55	128.96	120.44
1	A	40	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	216	THR	CA-CB-OG1	-6.54	99.79	109.60
1	A	209	TYR	CA-C-O	-6.51	114.47	121.56
1	A	124	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	238	SER	O-C-N	6.47	131.11	122.96
1	A	215	GLN	CA-C-O	-6.45	113.71	120.55
1	A	161	CYS	O-C-N	6.43	130.93	123.41
1	A	19	ASN	N-CA-C	-6.42	101.89	110.55
1	A	207	HIS	N-CA-CB	-6.41	101.24	111.62
1	A	56	ILE	CA-C-N	6.36	128.80	120.28
1	A	56	ILE	C-N-CA	6.36	128.80	120.28
1	A	223	GLU	CB-CG-CD	6.35	123.40	112.60
1	A	195	GLU	CG-CD-OE1	-6.33	103.83	118.40
1	A	85	ASP	N-CA-CB	6.30	119.52	110.45
1	A	77	VAL	CB-CA-C	6.26	119.67	110.77
1	A	13	ASP	CA-C-O	-6.23	112.81	119.97
1	A	233	LYS	N-CA-C	6.22	119.04	111.82
1	A	225	ARG	N-CA-C	-6.20	102.87	110.31
1	A	126	ARG	N-CA-C	-6.17	105.68	112.72
1	A	231	ILE	CA-C-O	-6.17	113.92	120.39
1	A	138	LEU	CA-C-O	-6.16	113.97	120.63
1	A	3	GLN	CG-CD-OE1	6.16	133.12	120.80
1	A	225	ARG	CA-C-N	6.14	125.90	119.76
1	A	225	ARG	C-N-CA	6.14	125.90	119.76
1	A	160	SER	CA-C-O	-6.14	114.44	121.68
1	A	68	ASN	CB-CA-C	6.13	119.87	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	TYR	CA-C-O	-6.11	113.58	120.43
1	A	113	THR	CA-CB-CG2	6.10	120.87	110.50
1	A	131	SER	CA-C-O	-6.07	113.81	120.36
1	A	234	ARG	CA-CB-CG	6.04	126.17	114.10
1	A	169	ASP	CA-C-N	6.00	128.69	120.46
1	A	169	ASP	C-N-CA	6.00	128.69	120.46
1	A	147	HIS	CA-CB-CG	5.98	119.78	113.80
1	A	85	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	168	CYS	N-CA-C	5.93	118.10	108.26
1	A	202	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	31	GLY	CA-C-O	5.88	130.81	120.57
1	A	6	GLU	CA-C-O	-5.80	113.55	120.10
1	A	139	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	207	HIS	N-CA-C	5.78	117.75	109.14
1	A	42	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	24	THR	CA-C-O	-5.70	113.92	120.24
1	A	27	LEU	N-CA-C	-5.67	99.28	108.52
1	A	113	THR	N-CA-C	-5.66	105.19	111.36
1	A	92	PRO	CB-CA-C	5.66	120.30	112.89
1	A	247	PHE	CA-C-O	-5.63	114.80	121.16
1	A	261	PRO	N-CA-CB	-5.62	97.85	103.19
1	A	149	PHE	N-CA-CB	-5.61	101.00	110.49
1	A	126	ARG	N-CA-CB	-5.59	102.37	110.70
1	A	186	HIS	CA-C-N	5.56	127.67	120.44
1	A	186	HIS	C-N-CA	5.56	127.67	120.44
1	A	259	LYS	CA-C-O	-5.56	115.08	121.47
1	A	121	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	246	ASP	CA-C-O	-5.53	112.03	119.11
1	A	176	PHE	O-C-N	-5.50	116.40	122.07
1	A	232	ILE	N-CA-C	-5.50	99.82	107.80
1	A	58	GLU	N-CA-C	-5.49	105.30	111.28
1	A	128	ILE	N-CA-CB	-5.48	106.74	112.06
1	A	252	TYR	CA-C-N	-5.48	116.42	123.16
1	A	252	TYR	C-N-CA	-5.48	116.42	123.16
1	A	238	SER	CA-C-O	-5.46	115.39	121.51
1	A	76	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	A	243	ARG	CA-C-O	-5.45	115.07	121.44
1	A	87	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	A	104	PRO	N-CA-C	-5.43	104.98	113.78
1	A	169	ASP	CA-C-O	-5.42	115.13	120.98
1	A	111	GLN	CB-CG-CD	-5.38	103.46	112.60
1	A	199	PHE	N-CA-CB	5.35	118.95	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	TYR	CA-C-O	-5.33	114.77	120.42
1	A	82	GLU	CA-C-O	-5.32	113.05	119.49
1	A	93	VAL	CB-CA-C	5.32	120.01	111.29
1	A	10	LYS	CA-C-O	-5.31	114.92	120.55
1	A	129	ILE	N-CA-CB	-5.29	102.14	111.93
1	A	28	SER	N-CA-CB	-5.28	101.45	111.00
1	A	207	HIS	CA-CB-CG	5.26	119.06	113.80
1	A	96	LYS	CB-CG-CD	5.25	123.39	111.30
1	A	66	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	99	ARG	N-CA-C	5.23	119.93	113.50
1	A	96	LYS	CB-CA-C	5.23	119.74	110.85
1	A	251	GLY	O-C-N	5.20	128.42	122.34
1	A	102	PRO	CA-C-O	-5.19	115.25	121.48
1	A	97	GLN	CG-CD-NE2	5.19	124.19	116.40
1	A	237	GLU	CG-CD-OE2	-5.17	106.51	118.40
1	A	181	TYR	N-CA-CB	5.16	117.80	110.16
1	A	16	THR	N-CA-C	-5.16	101.75	109.95
1	A	78	THR	CA-CB-OG1	-5.16	101.87	109.60
1	A	237	GLU	CB-CA-C	-5.15	100.78	110.67
1	A	49	ARG	CA-C-O	-5.14	114.62	120.58
1	A	113	THR	CA-C-O	-5.13	114.98	120.42
1	A	242	TYR	O-C-N	5.12	128.90	122.86
1	A	105	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	257	GLY	CA-C-O	-5.08	115.92	121.71
1	A	118	GLN	CA-C-O	-5.08	115.04	120.42
1	A	239	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	A	215	GLN	N-CA-C	-5.06	105.76	111.28
1	A	179	ALA	CA-C-N	5.06	127.37	120.54
1	A	179	ALA	C-N-CA	5.06	127.37	120.54
1	A	96	LYS	CA-CB-CG	5.05	124.20	114.10
1	A	241	ASP	CA-C-O	-5.05	113.99	119.95
1	A	246	ASP	O-C-N	5.03	129.77	122.43
1	A	103	THR	CA-CB-CG2	5.03	119.04	110.50
1	A	157	GLY	CA-C-O	-5.02	113.05	119.58
1	A	143	LEU	O-C-N	5.01	129.40	123.33
1	A	225	ARG	CB-CG-CD	-5.01	99.78	111.30
1	A	223	GLU	N-CA-CB	5.01	117.61	109.90
1	A	165	GLN	CA-C-N	5.00	127.48	120.28
1	A	165	GLN	C-N-CA	5.00	127.48	120.28
1	A	246	ASP	N-CA-CB	5.00	118.82	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2080	36	0
2	A	5	0	0	1	0
3	A	21	0	10	4	0
4	A	33	0	21	2	0
5	A	110	0	0	4	2
All	All	2322	0	2111	38	2

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 9.

All (38) 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:146:CYS:SG	3:A:265:UFP:C6	2.17	1.33
1:A:146:CYS:SG	3:A:265:UFP:H6	1.71	1.25
1:A:215:GLN:HE21	1:A:215:GLN:H	1.03	0.97
1:A:215:GLN:H	1:A:215:GLN:NE2	1.83	0.77
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.20	0.75
1:A:215:GLN:HE21	1:A:215:GLN:N	1.85	0.68
4:A:266:C2F:OE2	5:A:270:HOH:O	2.13	0.65
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.83	0.62
1:A:52:LEU:HD22	1:A:249:ILE:HD13	1.82	0.61
1:A:73:HIS:CE1	1:A:81:ASP:OD1	2.55	0.59
1:A:231:ILE:HB	1:A:248:GLU:HB3	1.86	0.56
1:A:186:HIS:CE1	5:A:282:HOH:O	2.59	0.56
1:A:10:LYS:NZ	1:A:32:HIS:HD2	2.05	0.55
1:A:37:ASN:HD21	1:A:39:GLN:HG3	1.72	0.54
1:A:37:ASN:ND2	1:A:39:GLN:H	2.07	0.52
1:A:186:HIS:HE1	5:A:282:HOH:O	1.91	0.52
1:A:37:ASN:HD22	1:A:39:GLN:H	1.59	0.50
1:A:10:LYS:HE2	1:A:29:ILE:HD13	1.93	0.50
1:A:103:THR:HB	1:A:104:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:CYS:O	1:A:193:ASP:HB2	2.12	0.49
1:A:82:GLU:HG2	1:A:264:ILE:CD1	2.45	0.46
1:A:82:GLU:HG2	1:A:264:ILE:HD13	1.96	0.46
1:A:248:GLU:HG3	5:A:374:HOH:O	2.16	0.45
1:A:146:CYS:SG	3:A:265:UFP:C5	3.04	0.44
1:A:37:ASN:HD22	1:A:38:LEU:N	2.16	0.43
1:A:188:MET:HE2	1:A:188:MET:HB3	1.88	0.43
1:A:10:LYS:HZ2	1:A:32:HIS:HD2	1.65	0.43
1:A:134:ASN:C	1:A:134:ASN:HD22	2.26	0.43
1:A:168:CYS:SG	1:A:174:LEU:HB2	2.59	0.43
1:A:37:ASN:HD22	1:A:37:ASN:C	2.27	0.42
1:A:257:GLY:N	2:A:267:PO4:O4	2.33	0.42
1:A:103:THR:HB	1:A:104:PRO:CD	2.50	0.41
1:A:119:LEU:CD1	1:A:188:MET:HE2	2.50	0.41
1:A:139:ASP:N	1:A:139:ASP:OD1	2.52	0.41
4:A:266:C2F:H92	4:A:266:C2F:H14	1.85	0.41
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.97	0.41
1:A:147:HIS:HD2	3:A:265:UFP:O4	2.04	0.40
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:296:HOH:O	5:A:296:HOH:O[5_555]	0.51	1.69
5:A:296:HOH:O	5:A:341:HOH:O[5_555]	2.11	0.09

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	262/264 (99%)	253 (97%)	7 (3%)	2 (1%)	16 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	A	93	VAL

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	232/232 (100%)	221 (95%)	11 (5%)	23 31

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	18	LYS
1	A	20	ASP
1	A	37	ASN
1	A	52	LEU
1	A	113	THR
1	A	188	MET
1	A	215	GLN
1	A	234	ARG
1	A	239	ILE
1	A	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	ASN
1	A	64	GLN
1	A	73	HIS
1	A	97	GLN
1	A	108	HIS
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	118	GLN
1	A	134	ASN
1	A	162	GLN
1	A	186	HIS
1	A	190	GLN
1	A	215	GLN
1	A	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	1.18	0	9,11,13	2.00	3 (33%)

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	-	0/9/10/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	ON1-CN-N	-4.26	117.88	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	O-C-CA	-2.72	117.77	124.77
1	A	1	CXM	C-CA-N	-2.27	105.12	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	C2F	A	266	3	32,35,35	2.29	12 (37%)	36,49,49	2.57	12 (33%)
3	UFP	A	265	4	22,22,22	5.94	5 (22%)	32,33,33	4.39	10 (31%)
2	PO4	A	267	-	4,4,4	2.63	2 (50%)	6,6,6	3.28	4 (66%)

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
4	C2F	A	266	3	-	5/22/35/35	0/3/3/3
3	UFP	A	265	4	-	0/10/22/22	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	265	UFP	C6-C5	20.00	1.61	1.33
3	A	265	UFP	C4-C5	16.31	1.64	1.44
3	A	265	UFP	C6-N1	9.41	1.54	1.38
4	A	266	C2F	C6-N5	-7.40	1.38	1.48
2	A	267	PO4	P-O1	4.56	1.61	1.50
4	A	266	C2F	C9-N10	3.81	1.52	1.45
4	A	266	C2F	C4A-C4	3.22	1.51	1.43
4	A	266	C2F	CG-CD	3.21	1.58	1.50
4	A	266	C2F	C4-N3	3.11	1.44	1.38
4	A	266	C2F	C-N	2.92	1.41	1.34
4	A	266	C2F	C8A-N1	2.79	1.40	1.36
3	A	265	UFP	O4'-C1'	2.64	1.48	1.42
4	A	266	C2F	C15-N10	2.60	1.46	1.38
2	A	267	PO4	P-O2	-2.53	1.47	1.54
4	A	266	C2F	C17-C12	2.48	1.43	1.39
4	A	266	C2F	C2-N1	2.29	1.38	1.33
3	A	265	UFP	P-O2P	-2.25	1.46	1.54
4	A	266	C2F	C16-C15	2.19	1.42	1.39
4	A	266	C2F	C2-NA2	2.06	1.39	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	265	UFP	C6-C5-C4	-19.00	105.25	122.57
4	A	266	C2F	CG-CB-CA	10.37	132.28	113.16
3	A	265	UFP	O4-C4-C5	-8.25	118.67	125.69
3	A	265	UFP	F5-C5-C6	-5.78	116.12	120.99
2	A	267	PO4	O3-P-O2	5.66	125.51	107.91
3	A	265	UFP	C5-C4-N3	5.61	117.77	112.64
3	A	265	UFP	C5-C6-N1	-4.82	114.53	120.32
3	A	265	UFP	O3P-P-O5'	-4.62	94.63	106.67
4	A	266	C2F	CA-N-C	-4.57	110.61	121.56
4	A	266	C2F	C2-N1-C8A	4.40	121.13	113.36
3	A	265	UFP	N3-C2-N1	4.33	120.53	114.89
2	A	267	PO4	O4-P-O3	-3.83	96.01	107.91
3	A	265	UFP	C1'-N1-C6	-3.58	114.73	120.74
3	A	265	UFP	C1'-N1-C2	3.39	124.29	117.66
3	A	265	UFP	O2-C2-N3	-3.30	115.40	121.49
4	A	266	C2F	O4-C4-C4A	-3.25	119.64	127.62
4	A	266	C2F	O1-CT-CA	-3.03	112.49	122.26
2	A	267	PO4	O4-P-O2	2.82	116.69	107.91
4	A	266	C2F	O2-CT-O1	2.80	130.44	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	266	C2F	OE1-CD-CG	-2.72	114.46	123.09
2	A	267	PO4	O3-P-O1	-2.60	101.74	110.95
4	A	266	C2F	C4A-C4-N3	2.58	115.49	110.94
4	A	266	C2F	O4-C4-N3	2.53	124.88	120.11
4	A	266	C2F	CB-CA-N	-2.51	105.95	110.91
4	A	266	C2F	C2-N3-C4	-2.49	120.59	125.11
4	A	266	C2F	CB-CA-CT	2.05	115.21	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

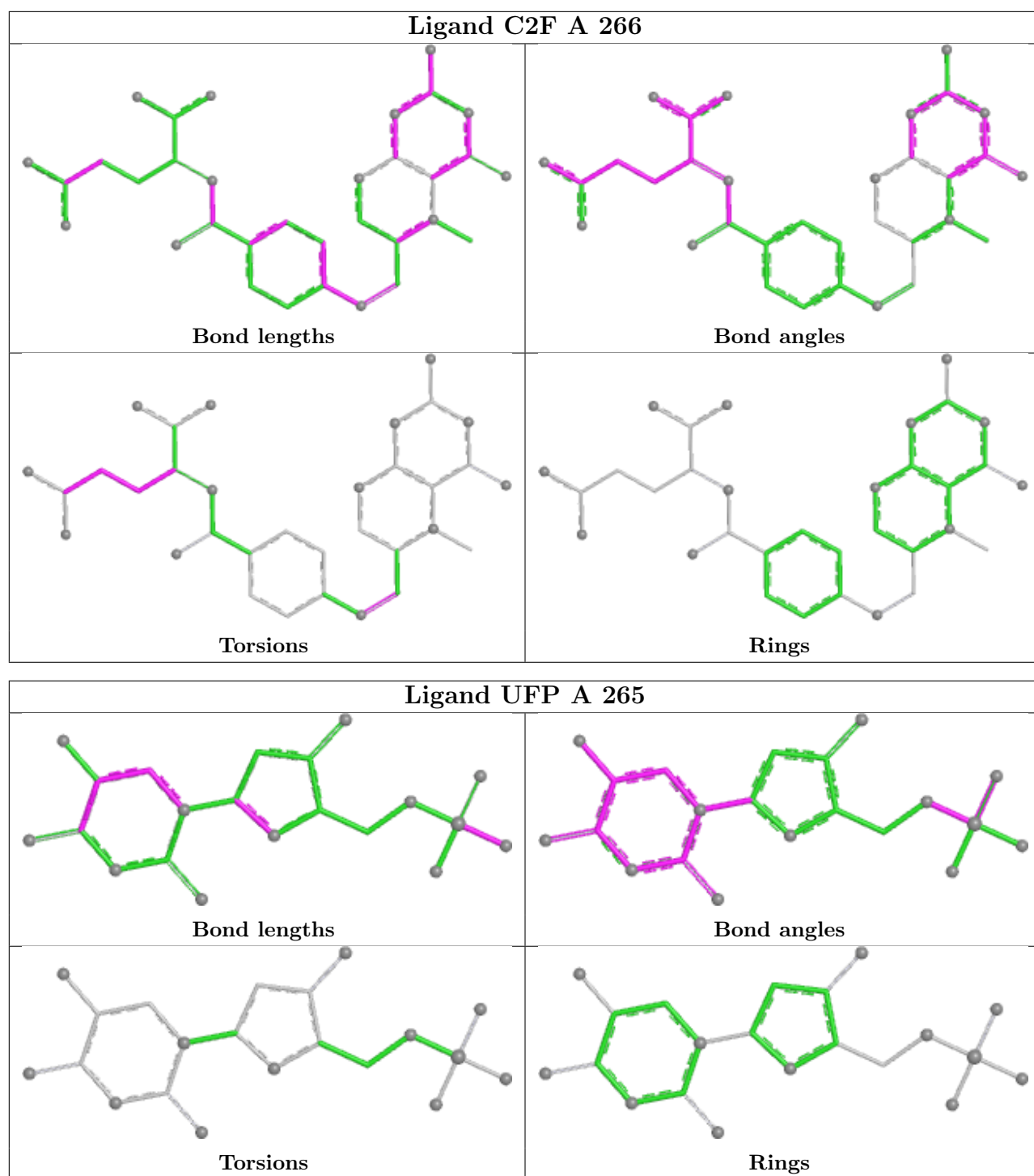
Mol	Chain	Res	Type	Atoms
4	A	266	C2F	N-CA-CB-CG
4	A	266	C2F	CT-CA-CB-CG
4	A	266	C2F	C6-C9-N10-C15
4	A	266	C2F	CA-CB-CG-CD
4	A	266	C2F	OE2-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	266	C2F	2	0
3	A	265	UFP	4	0
2	A	267	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 ⓘ

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%)	-0.78	0 100 100	9, 18, 33, 48	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	A	1	11/12	0.97	0.05	18,19,21,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

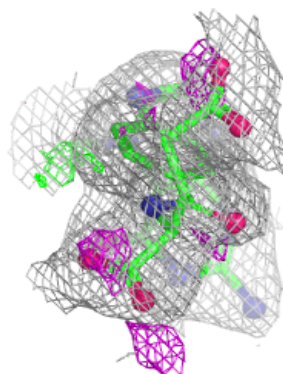
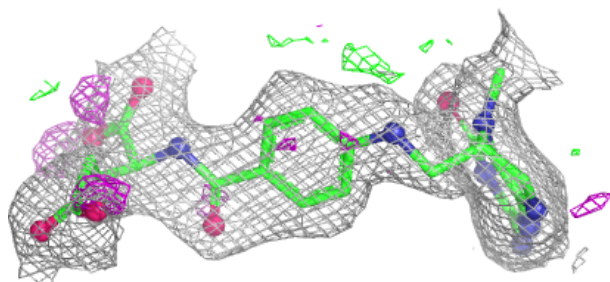
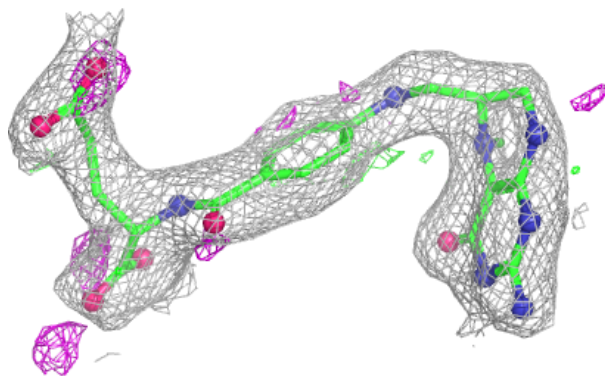
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

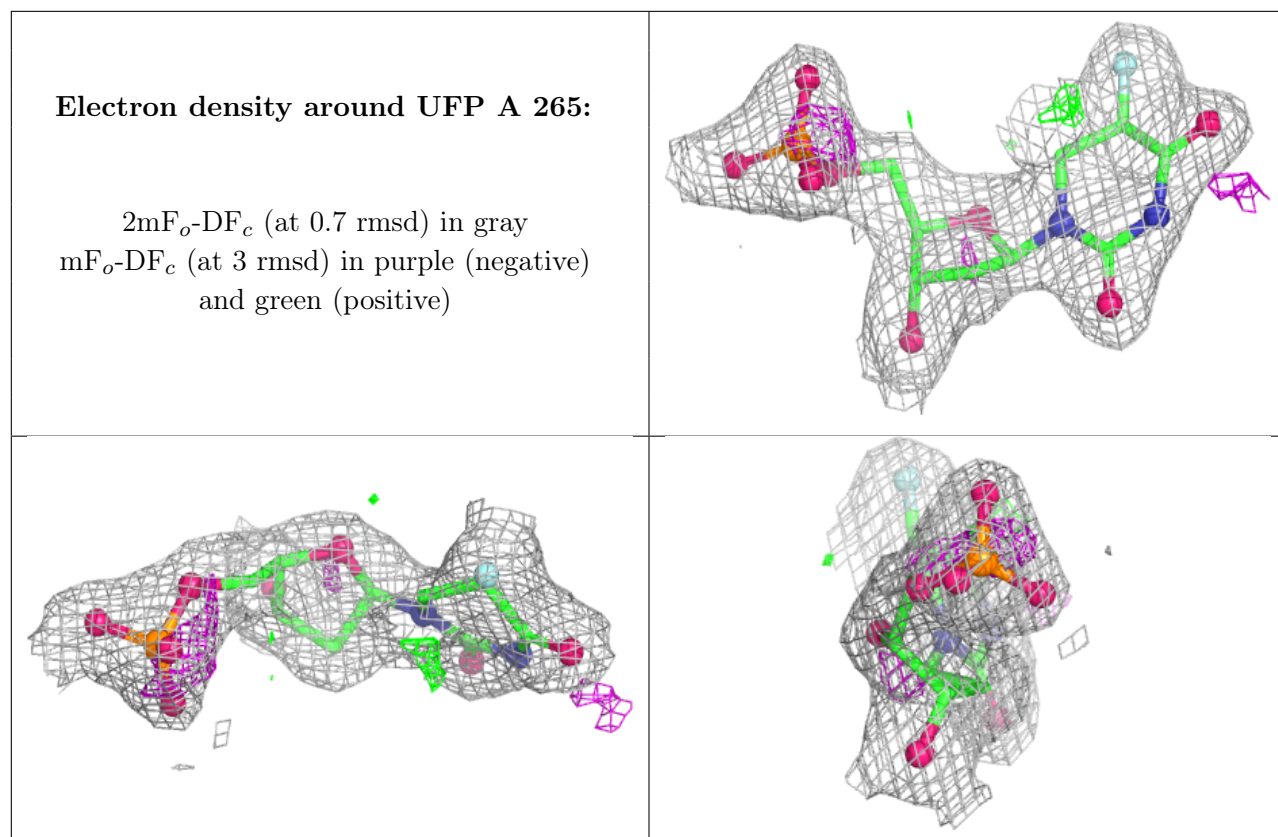
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	C2F	A	266	33/33	0.91	0.07	17,24,37,41	0
2	PO4	A	267	5/5	0.93	0.08	43,44,47,48	0
3	UFP	A	265	21/21	0.96	0.07	13,15,19,19	0

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 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.