



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 1PD9 / pdb_00001pd9
Title : Analysis of Three Crystal Structure Determinations of a 5-Methyl-6-N-Methylthylanilino Pyridopyrimidine antifolate Complex with Human Dihydrofolate Reductase
Authors : Cody, V.; Luft, J.R.; Pangborn, W.; Gangjee, A.
Deposited on : 2003-05-19
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

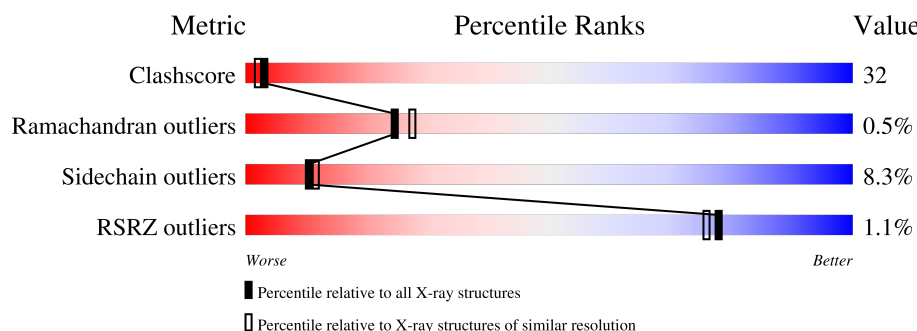
1 Overall quality at a glance

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	186	31% 45% 22% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CO4	A	187	X	-	-	-

2 Entry composition [i](#)

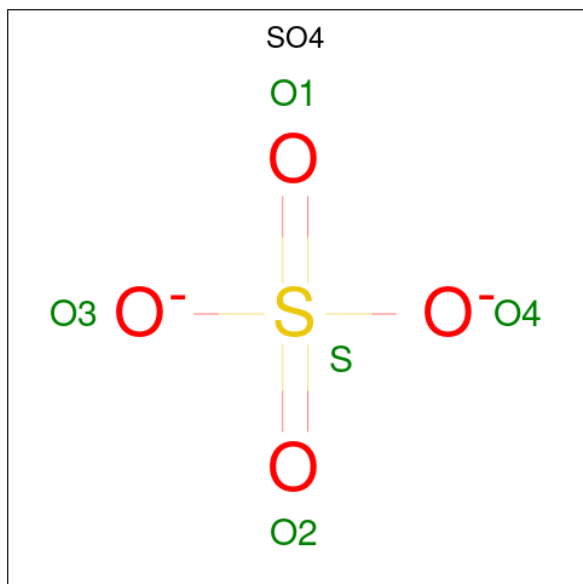
There are 4 unique types of molecules in this entry. The entry contains 1609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrofolate reductase.

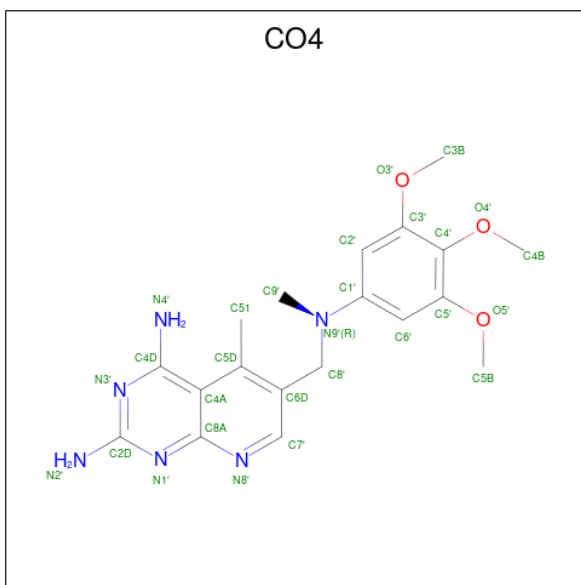
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 2,4-DIAMINO-5-METHYL-6-[(3,4,5-TRIMETHOXY-N-METHYLANILINO) METHYL]PYRIDO[2,3-D]PYRIMIDINE (CCD ID: CO4) (formula: C₁₉H₂₄N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	6	3		

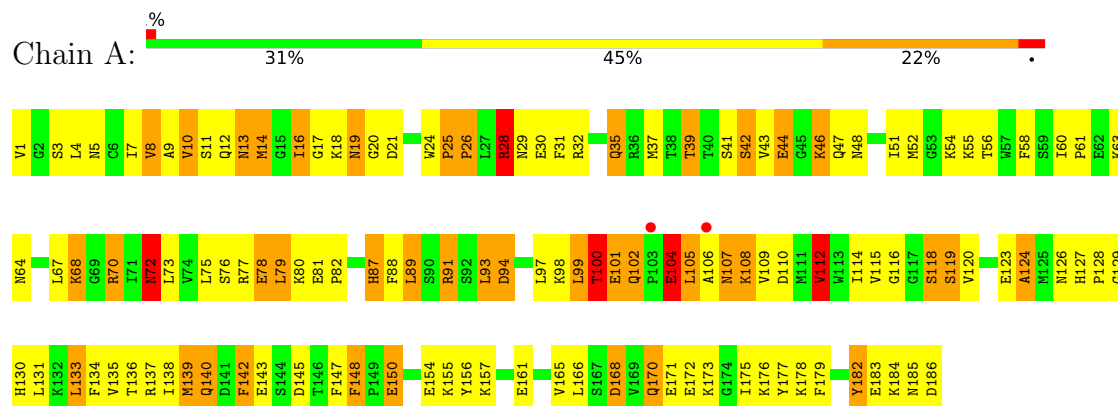
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0

3 Residue-property plots

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: Dihydrofolate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 85.43Å 78.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (8.00-2.20) 94.1 (8.00-2.20)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.20Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , 0.213 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 80.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1609	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: SO4, CO4

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	1.33	1/1537 (0.1%)	2.80	154/2073 (7.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLY	N-CA	6.53	1.51	1.45

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	CD-NE-CZ	22.33	155.66	124.40
1	A	123	GLU	CB-CG-CD	14.94	138.00	112.60
1	A	124	ALA	CA-C-N	12.08	137.68	120.28
1	A	124	ALA	C-N-CA	12.08	137.68	120.28
1	A	28	ARG	NE-CZ-NH2	11.94	129.95	119.20
1	A	21	ASP	CA-CB-CG	11.93	124.53	112.60
1	A	89	LEU	CA-C-O	-11.31	107.66	120.66
1	A	142	PHE	CA-CB-CG	9.84	123.64	113.80
1	A	104	GLU	CB-CG-CD	9.36	128.51	112.60
1	A	44	GLU	CB-CG-CD	9.24	128.31	112.60
1	A	107	ASN	CA-CB-CG	9.19	121.79	112.60
1	A	88	PHE	O-C-N	9.18	133.92	123.27
1	A	29	ASN	CA-CB-CG	8.84	121.44	112.60
1	A	136	THR	N-CA-CB	8.75	124.29	110.55
1	A	120	VAL	O-C-N	8.67	130.91	121.90
1	A	140	GLN	OE1-CD-NE2	8.63	131.23	122.60
1	A	93	LEU	CA-C-N	8.62	131.64	120.44
1	A	93	LEU	C-N-CA	8.62	131.64	120.44
1	A	116	GLY	CA-C-O	-8.58	113.13	122.14
1	A	140	GLN	N-CA-CB	8.54	124.55	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	CA-CB-OG1	-8.45	96.93	109.60
1	A	145	ASP	CA-C-O	8.39	128.27	118.79
1	A	48	ASN	CA-CB-CG	8.34	120.94	112.60
1	A	47	GLN	CA-C-O	-8.29	111.74	121.44
1	A	3	SER	O-C-N	8.22	132.22	122.85
1	A	118	SER	O-C-N	8.20	130.81	122.12
1	A	88	PHE	CA-C-O	-8.19	111.56	121.06
1	A	109	VAL	N-CA-C	8.05	119.44	108.17
1	A	58	PHE	CA-CB-CG	-8.05	105.75	113.80
1	A	148	PHE	CB-CA-C	7.93	120.05	108.87
1	A	77	ARG	CA-CB-CG	7.90	129.91	114.10
1	A	48	ASN	CA-C-N	7.83	134.01	123.05
1	A	48	ASN	C-N-CA	7.83	134.01	123.05
1	A	12	GLN	OE1-CD-NE2	7.76	130.37	122.60
1	A	161	GLU	CA-C-O	7.53	129.38	121.10
1	A	127	HIS	CA-C-O	7.51	126.87	119.51
1	A	102	GLN	N-CA-C	-7.47	99.33	110.24
1	A	25	PRO	CB-CA-C	7.46	120.02	110.92
1	A	127	HIS	CA-CB-CG	7.45	121.25	113.80
1	A	145	ASP	CB-CA-C	7.38	121.67	109.80
1	A	179	PHE	CA-C-O	-7.32	112.68	120.80
1	A	35	GLN	CG-CD-NE2	7.27	127.31	116.40
1	A	68	LYS	O-C-N	7.26	131.43	122.86
1	A	3	SER	CA-C-O	-7.12	113.41	121.81
1	A	32	ARG	CA-C-O	7.11	128.28	120.82
1	A	99	LEU	CA-C-O	7.04	128.04	119.31
1	A	115	VAL	N-CA-C	7.03	118.85	112.17
1	A	120	VAL	CA-C-O	-7.02	113.26	121.05
1	A	87	HIS	ND1-CE1-NE2	-6.96	101.44	108.40
1	A	101	GLU	CB-CA-C	-6.80	96.42	109.95
1	A	5	ASN	CA-C-O	-6.79	113.73	121.40
1	A	30	GLU	CA-C-O	6.49	127.30	120.42
1	A	42	SER	CA-C-N	6.49	132.63	122.70
1	A	42	SER	C-N-CA	6.49	132.63	122.70
1	A	168	ASP	CA-C-N	6.44	129.20	120.63
1	A	168	ASP	C-N-CA	6.44	129.20	120.63
1	A	87	HIS	CA-C-O	-6.43	112.27	119.67
1	A	12	GLN	CG-CD-NE2	-6.38	106.83	116.40
1	A	73	LEU	CA-C-O	-6.34	113.51	120.30
1	A	126	ASN	N-CA-C	-6.34	105.67	113.41
1	A	133	LEU	CA-C-O	-6.34	113.34	120.32
1	A	118	SER	CA-CB-OG	-6.32	98.46	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	GLN	CA-C-N	-6.32	110.90	121.64
1	A	170	GLN	C-N-CA	-6.32	110.90	121.64
1	A	80	LYS	CA-CB-CG	6.29	126.67	114.10
1	A	172	GLU	CA-CB-CG	6.24	126.58	114.10
1	A	182	TYR	O-C-N	6.24	131.30	123.19
1	A	70	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	168	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	147	PHE	N-CA-C	6.16	119.58	109.85
1	A	134	PHE	CA-C-O	-6.16	114.19	120.84
1	A	13	ASN	CA-C-O	6.15	126.87	119.43
1	A	101	GLU	N-CA-CB	6.13	120.71	110.41
1	A	41	SER	CA-C-O	6.10	127.58	120.80
1	A	137	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	118	SER	N-CA-C	6.09	117.92	111.28
1	A	11	SER	N-CA-C	-6.06	101.99	110.35
1	A	70	ARG	NH1-CZ-NH2	6.04	127.15	119.30
1	A	16	ILE	CA-C-N	-6.00	111.22	121.17
1	A	16	ILE	C-N-CA	-6.00	111.22	121.17
1	A	28	ARG	NH1-CZ-NH2	-5.95	111.56	119.30
1	A	47	GLN	O-C-N	5.95	130.89	123.15
1	A	78	GLU	CA-CB-CG	5.95	126.00	114.10
1	A	105	LEU	N-CA-CB	-5.94	101.13	110.46
1	A	150	GLU	N-CA-CB	-5.94	101.23	109.97
1	A	139	MET	CA-CB-CG	5.92	125.94	114.10
1	A	182	TYR	CA-C-O	-5.92	114.43	121.11
1	A	99	LEU	CA-CB-CG	5.91	136.99	116.30
1	A	72	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	9	ALA	CA-C-N	5.89	131.19	122.71
1	A	9	ALA	C-N-CA	5.89	131.19	122.71
1	A	30	GLU	N-CA-C	-5.86	104.97	111.36
1	A	51	ILE	O-C-N	-5.84	117.05	123.18
1	A	148	PHE	CA-C-O	-5.83	115.29	120.19
1	A	154	GLU	N-CA-C	-5.81	106.02	113.23
1	A	70	ARG	NE-CZ-NH2	-5.78	114.00	119.20
1	A	35	GLN	OE1-CD-NE2	-5.76	116.84	122.60
1	A	112	VAL	CG1-CB-CG2	5.73	123.42	110.80
1	A	115	VAL	CA-CB-CG2	5.73	120.14	110.40
1	A	13	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	72	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	A	39	THR	N-CA-C	5.66	118.65	111.69
1	A	170	GLN	N-CA-CB	5.66	119.13	110.70
1	A	10	VAL	N-CA-CB	5.65	120.72	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLY	CA-C-O	-5.63	115.23	121.37
1	A	94	ASP	N-CA-C	-5.61	105.07	111.07
1	A	80	LYS	N-CA-CB	5.58	118.73	110.53
1	A	118	SER	CB-CA-C	-5.55	101.57	110.79
1	A	46	LYS	CA-CB-CG	-5.55	103.00	114.10
1	A	135	VAL	CA-CB-CG1	5.53	119.80	110.40
1	A	147	PHE	N-CA-CB	-5.52	102.25	111.20
1	A	7	ILE	CB-CA-C	5.52	119.00	110.50
1	A	104	GLU	CA-CB-CG	5.48	125.06	114.10
1	A	91	ARG	N-CA-C	-5.48	105.72	112.90
1	A	179	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	8	VAL	CA-CB-CG2	5.46	119.68	110.40
1	A	120	VAL	CB-CA-C	5.46	119.17	112.02
1	A	21	ASP	N-CA-CB	-5.45	102.64	110.87
1	A	67	LEU	N-CA-C	-5.43	101.61	109.59
1	A	82	PRO	N-CA-CB	5.42	106.22	103.19
1	A	81	GLU	CG-CD-OE1	5.41	130.84	118.40
1	A	100	THR	N-CA-C	-5.41	105.55	111.82
1	A	13	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	107	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	137	ARG	CD-NE-CZ	-5.32	116.95	124.40
1	A	79	LEU	CA-C-O	-5.28	115.03	121.05
1	A	5	ASN	O-C-N	5.28	129.56	123.17
1	A	44	GLU	CA-C-O	5.27	127.13	121.55
1	A	51	ILE	N-CA-CB	-5.25	104.11	111.25
1	A	123	GLU	O-C-N	-5.25	115.21	122.46
1	A	3	SER	N-CA-C	5.24	117.62	110.55
1	A	134	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	9	ALA	N-CA-C	-5.22	100.39	108.90
1	A	177	TYR	CA-C-O	-5.18	115.73	121.33
1	A	172	GLU	CA-C-N	5.18	131.43	121.54
1	A	172	GLU	C-N-CA	5.18	131.43	121.54
1	A	172	GLU	CG-CD-OE1	5.15	130.25	118.40
1	A	12	GLN	CB-CG-CD	-5.14	103.86	112.60
1	A	46	LYS	N-CA-CB	5.13	118.74	110.85
1	A	161	GLU	CB-CG-CD	5.12	121.31	112.60
1	A	136	THR	N-CA-C	-5.11	100.19	108.52
1	A	157	LYS	O-C-N	5.11	129.70	123.21
1	A	19	ASN	CA-CB-CG	-5.11	107.50	112.60
1	A	14	MET	CA-C-O	-5.10	114.45	120.57
1	A	10	VAL	CA-CB-CG1	5.09	119.06	110.40
1	A	129	GLY	N-CA-C	-5.09	104.86	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	MET	CA-C-N	5.07	128.22	121.01
1	A	52	MET	C-N-CA	5.07	128.22	121.01
1	A	3	SER	CB-CA-C	-5.05	99.71	109.76
1	A	131	LEU	CB-CA-C	5.05	118.95	109.86
1	A	129	GLY	O-C-N	5.04	127.99	123.00
1	A	133	LEU	N-CA-CB	-5.04	102.64	110.55
1	A	108	LYS	CA-C-O	-5.03	113.42	119.15
1	A	102	GLN	CA-CB-CG	5.00	124.10	114.10

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	1502	0	1511	95	0
2	A	10	0	0	0	0
3	A	28	0	24	4	0
4	A	69	0	0	10	1
All	All	1609	0	1535	97	1

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 32.

All (97) 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:1:VAL:HG21	1:A:100:THR:CG2	1.79	1.11
1:A:184:LYS:HA	4:A:254:HOH:O	1.52	1.07
1:A:35:GLN:HE21	1:A:70:ARG:HH12	1.03	1.03
1:A:26:PRO:O	1:A:173:LYS:HE3	1.63	0.99
1:A:1:VAL:HG21	1:A:100:THR:HG23	1.00	0.98
1:A:1:VAL:CG2	1:A:100:THR:HG23	1.94	0.97
1:A:19:ASN:O	4:A:257:HOH:O	1.80	0.96
1:A:99:LEU:HD23	1:A:105:LEU:HD12	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLN:NE2	1:A:70:ARG:HH12	1.70	0.88
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.59	0.85
1:A:79:LEU:O	1:A:91:ARG:NH1	2.12	0.83
1:A:130:HIS:HE1	1:A:183:GLU:HG3	1.42	0.83
1:A:130:HIS:HB2	4:A:215:HOH:O	1.78	0.83
1:A:61:PRO:HG2	1:A:64:ASN:HD22	1.42	0.82
1:A:130:HIS:ND1	1:A:184:LYS:O	2.11	0.81
1:A:102:GLN:O	1:A:106:ALA:HB2	1.85	0.76
1:A:184:LYS:HG2	1:A:185:ASN:N	2.00	0.76
1:A:35:GLN:HE21	1:A:70:ARG:NH1	1.84	0.74
1:A:119:SER:OG	4:A:251:HOH:O	2.04	0.74
1:A:28:ARG:HH12	1:A:173:LYS:NZ	1.86	0.73
1:A:72:ASN:H	1:A:87:HIS:HD2	1.36	0.73
1:A:104:GLU:O	1:A:108:LYS:HE2	1.89	0.73
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.25	0.72
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.02	0.72
1:A:31:PHE:HE1	3:A:187:CO4:H7'	1.54	0.71
1:A:78:GLU:OE1	4:A:256:HOH:O	2.09	0.70
1:A:171:GLU:CD	1:A:176:LYS:HZ3	2.00	0.69
1:A:100:THR:O	1:A:106:ALA:HA	1.93	0.69
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.75	0.67
1:A:105:LEU:HA	1:A:108:LYS:HD2	1.77	0.67
1:A:104:GLU:O	1:A:108:LYS:CE	2.44	0.65
1:A:97:LEU:O	1:A:100:THR:HB	1.98	0.64
1:A:75:LEU:O	4:A:244:HOH:O	2.14	0.64
1:A:72:ASN:H	1:A:87:HIS:CD2	2.15	0.64
1:A:78:GLU:CD	4:A:256:HOH:O	2.42	0.63
1:A:99:LEU:HD23	1:A:105:LEU:CD1	2.27	0.62
1:A:94:ASP:O	1:A:98:LYS:HE3	2.00	0.62
1:A:61:PRO:HG2	1:A:64:ASN:ND2	2.14	0.61
1:A:139:MET:HE3	1:A:178:LYS:HD3	1.83	0.60
1:A:43:VAL:HG11	1:A:46:LYS:CE	2.32	0.59
1:A:184:LYS:HE3	1:A:186:ASP:OD1	2.01	0.59
1:A:94:ASP:C	1:A:98:LYS:HE3	2.28	0.59
1:A:26:PRO:HB2	1:A:28:ARG:NH1	2.17	0.59
1:A:42:SER:OG	1:A:110:ASP:OD1	2.18	0.58
1:A:55:LYS:HG2	4:A:246:HOH:O	2.04	0.57
1:A:114:ILE:CD1	1:A:124:ALA:HB2	2.34	0.57
1:A:28:ARG:HH12	1:A:173:LYS:HZ2	1.54	0.56
1:A:155:LYS:HE3	4:A:214:HOH:O	2.05	0.56
1:A:43:VAL:HG11	1:A:46:LYS:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLU:CD	1:A:176:LYS:NZ	2.65	0.55
1:A:35:GLN:NE2	1:A:70:ARG:NH1	2.47	0.55
1:A:8:VAL:HG21	1:A:148:PHE:CD1	2.42	0.54
1:A:98:LYS:HA	1:A:101:GLU:HG2	1.87	0.54
3:A:187:CO4:H4'2	3:A:187:CO4:H513	1.72	0.54
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.91	0.53
1:A:44:GLU:HB2	4:A:243:HOH:O	2.09	0.52
1:A:31:PHE:HE1	3:A:187:CO4:C7'	2.22	0.50
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.33	0.50
1:A:99:LEU:CD2	1:A:105:LEU:CD1	2.89	0.50
1:A:60:ILE:O	1:A:61:PRO:C	2.55	0.50
1:A:54:LYS:NZ	1:A:78:GLU:OE1	2.44	0.50
1:A:138:ILE:HG21	1:A:142:PHE:HE2	1.77	0.49
1:A:155:LYS:HD3	1:A:186:ASP:OD2	2.13	0.49
1:A:76:SER:HB3	1:A:89:LEU:HD11	1.96	0.47
1:A:140:GLN:HG3	1:A:142:PHE:CE2	2.49	0.47
1:A:156:TYR:CE2	1:A:184:LYS:HB2	2.51	0.46
1:A:138:ILE:CG2	1:A:142:PHE:HE2	2.28	0.46
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.98	0.45
1:A:43:VAL:HG11	1:A:46:LYS:HE2	1.98	0.45
1:A:114:ILE:CD1	1:A:124:ALA:CB	2.94	0.45
1:A:105:LEU:O	1:A:106:ALA:C	2.60	0.44
1:A:139:MET:CE	1:A:178:LYS:HD3	2.46	0.44
1:A:10:VAL:HG11	1:A:148:PHE:HB3	1.99	0.44
1:A:37:MET:CE	1:A:165:VAL:HG22	2.47	0.44
1:A:26:PRO:C	1:A:28:ARG:HH11	2.25	0.44
1:A:184:LYS:CG	1:A:185:ASN:N	2.78	0.44
1:A:13:ASN:O	1:A:14:MET:HB2	2.19	0.43
1:A:168:ASP:OD2	1:A:168:ASP:N	2.48	0.43
1:A:139:MET:HE3	1:A:178:LYS:CD	2.48	0.43
1:A:35:GLN:HE22	1:A:70:ARG:HH22	1.66	0.43
3:A:187:CO4:H9'1	3:A:187:CO4:H2'	1.53	0.42
1:A:28:ARG:NH1	1:A:173:LYS:NZ	2.62	0.42
1:A:93:LEU:O	1:A:97:LEU:HG	2.19	0.42
1:A:138:ILE:HG21	1:A:142:PHE:CE2	2.55	0.42
1:A:170:GLN:O	1:A:176:LYS:HA	2.20	0.42
1:A:102:GLN:C	1:A:104:GLU:N	2.75	0.42
1:A:133:LEU:HB2	1:A:182:TYR:HB2	2.02	0.42
1:A:20:GLY:HA2	1:A:55:LYS:HE2	2.02	0.42
1:A:18:LYS:HD3	1:A:143:GLU:O	2.20	0.42
1:A:171:GLU:HA	1:A:175:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:O	1:A:26:PRO:C	2.63	0.41
1:A:104:GLU:O	1:A:108:LYS:HD2	2.20	0.41
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.81	0.41
1:A:16:ILE:HD13	1:A:16:ILE:HG21	1.83	0.40
1:A:28:ARG:NH1	1:A:173:LYS:CE	2.85	0.40
1:A:168:ASP:O	1:A:170:GLN:NE2	2.54	0.40
1:A:184:LYS:HG2	1:A:185:ASN:H	1.84	0.40

All (1) 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)
4:A:238:HOH:O	4:A:255:HOH:O[6_555]	1.56	0.64

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	184/186 (99%)	178 (97%)	5 (3%)	1 (0%)	24 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU

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	168/168 (100%)	154 (92%)	14 (8%)	10	11

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	A	28	ARG
1	A	39	THR
1	A	63	LYS
1	A	68	LYS
1	A	72	ASN
1	A	100	THR
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	128	PRO
1	A	150	GLU
1	A	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	35	GLN
1	A	87	HIS
1	A	127	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
3	CO4	A	187	-	29,30,30	1.59	6 (20%)	40,43,43	3.75	23 (57%)
2	SO4	A	188	-	4,4,4	0.48	0	6,6,6	0.64	0
2	SO4	A	189	-	4,4,4	0.77	0	6,6,6	0.87	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
3	CO4	A	187	-	1/1/1/1	2/14/14/14	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	CO4	C7'-N8'	3.57	1.37	1.31
3	A	187	CO4	C8A-N8'	3.31	1.42	1.37
3	A	187	CO4	C8'-C6D	2.93	1.56	1.51
3	A	187	CO4	C7'-C6D	2.74	1.43	1.37
3	A	187	CO4	C2D-N2'	-2.50	1.29	1.33
3	A	187	CO4	C3'-C4'	-2.02	1.36	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	CO4	C5B-O5'-C5'	-8.94	104.40	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	CO4	O5'-C5'-C6'	-8.06	110.21	124.08
3	A	187	CO4	N2'-C2D-N3'	7.61	128.63	117.22
3	A	187	CO4	O4'-C4'-C3'	7.05	130.24	120.12
3	A	187	CO4	O5'-C5'-C4'	5.94	125.33	115.14
3	A	187	CO4	O4'-C4'-C5'	-5.74	111.89	120.12
3	A	187	CO4	C6D-C8'-N9'	5.58	122.86	114.49
3	A	187	CO4	N2'-C2D-N1'	-5.55	109.13	117.79
3	A	187	CO4	C5D-C4A-C8A	-4.72	113.99	118.22
3	A	187	CO4	N1'-C2D-N3'	-4.06	122.04	127.21
3	A	187	CO4	O3'-C3'-C4'	4.06	122.10	115.14
3	A	187	CO4	C6'-C5'-C4'	3.79	124.44	120.22
3	A	187	CO4	C9'-N9'-C1'	-3.41	113.96	119.59
3	A	187	CO4	C2D-N1'-C8A	3.30	119.04	115.48
3	A	187	CO4	O3'-C3'-C2'	-3.13	118.68	124.08
3	A	187	CO4	C9'-N9'-C8'	2.99	122.89	115.11
3	A	187	CO4	C51-C5D-C4A	-2.98	117.69	122.17
3	A	187	CO4	C8'-C6D-C7'	-2.91	117.13	121.30
3	A	187	CO4	N4'-C4D-N3'	-2.68	109.91	117.11
3	A	187	CO4	C5D-C4A-C4D	2.27	131.57	126.44
3	A	187	CO4	C4A-C4D-N4'	2.25	126.70	122.70
3	A	187	CO4	C51-C5D-C6D	-2.10	118.42	120.81
3	A	187	CO4	C8'-C6D-C5D	2.08	124.26	120.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	187	CO4	N9'

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	187	CO4	C5'-C4'-O4'-C4B
3	A	187	CO4	C3'-C4'-O4'-C4B

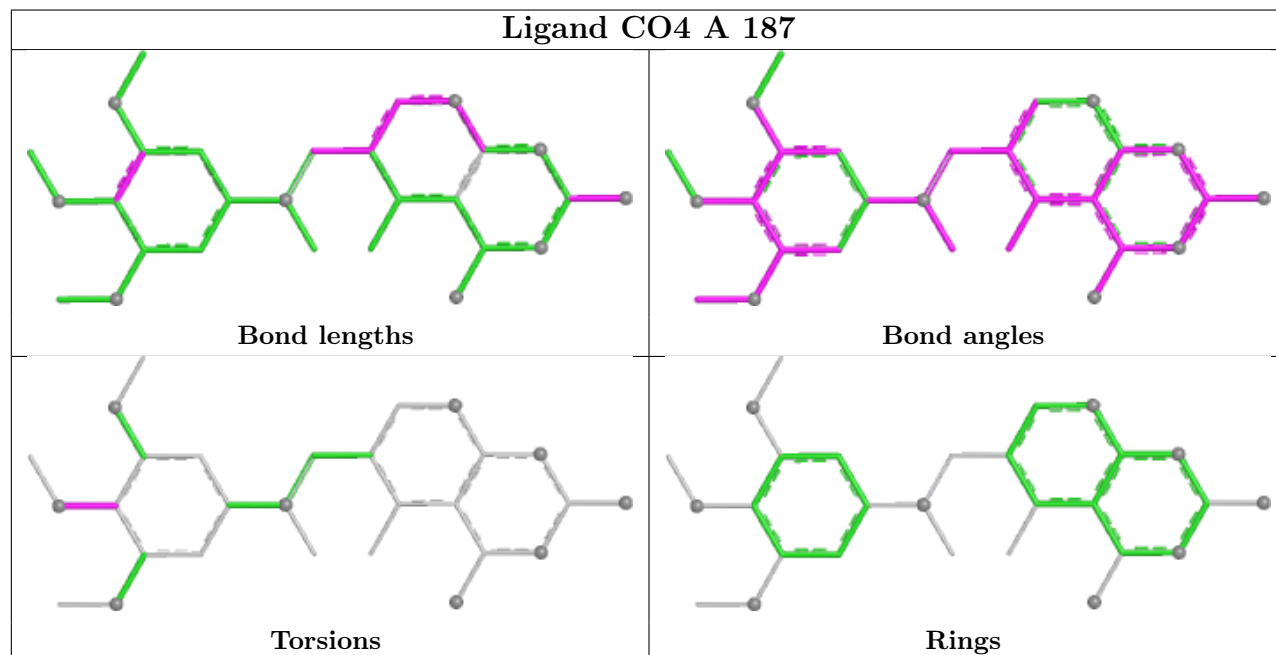
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	187	CO4	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	186/186 (100%)	-0.49	2 (1%) 78 76	9, 21, 43, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	2.4
1	A	103	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

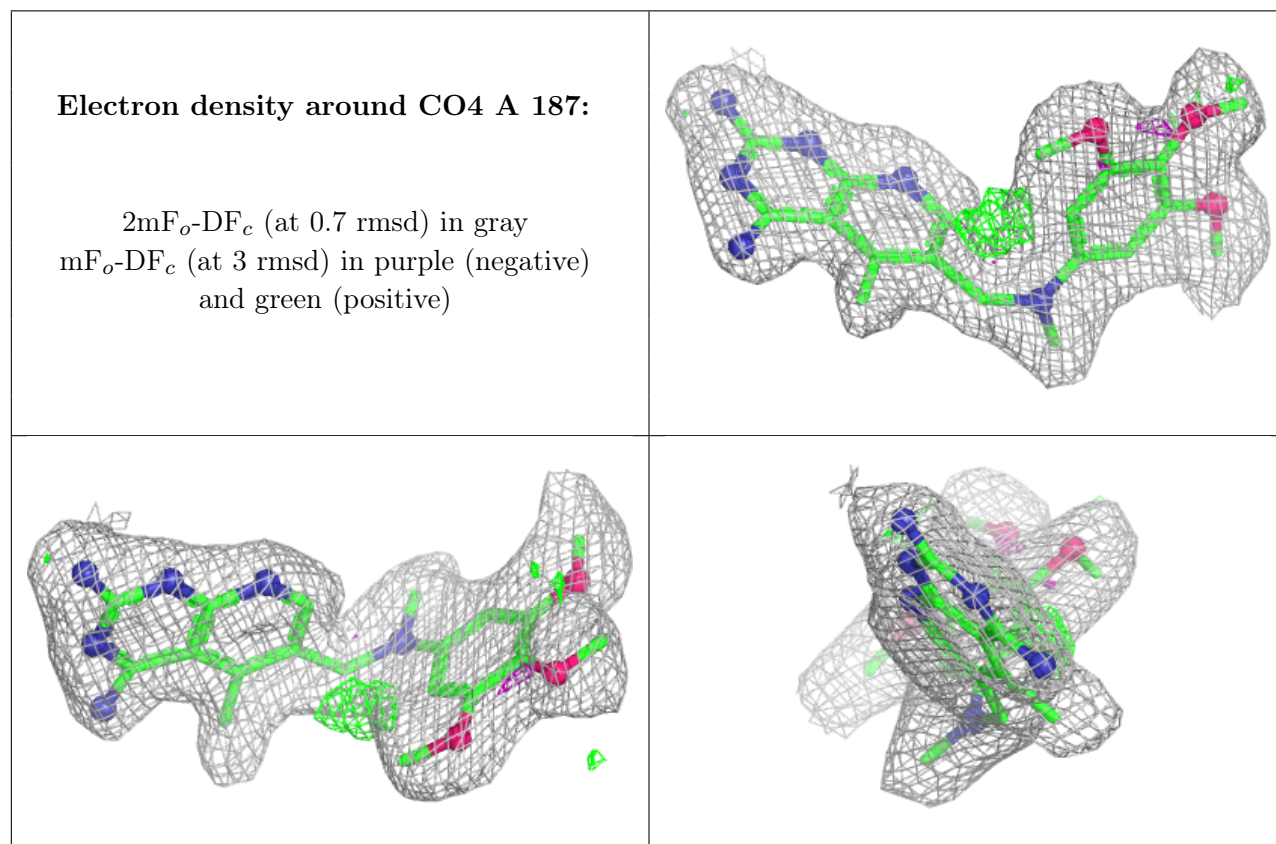
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CO4	A	187	28/28	0.89	0.07	15,21,26,27	0
2	SO4	A	189	5/5	0.96	0.07	46,46,47,47	0
2	SO4	A	188	5/5	0.99	0.04	22,22,23,23	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.