



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:08 PM UTC

PDB ID : 2YIM / pdb_00002yim
Title : The enolisation chemistry of a thioester-dependent racemase: the 1.4 Å crystal structure of a complex with a planar reaction intermediate analogue
Authors : Sharma, S.; Bhaumik, P.; Venkatesan, R.; Hiltunen, J.K.; Conzelmann, E.; Juffer, A.H.; Wierenga, R.K.
Deposited on : 2011-05-16
Resolution : 1.41 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

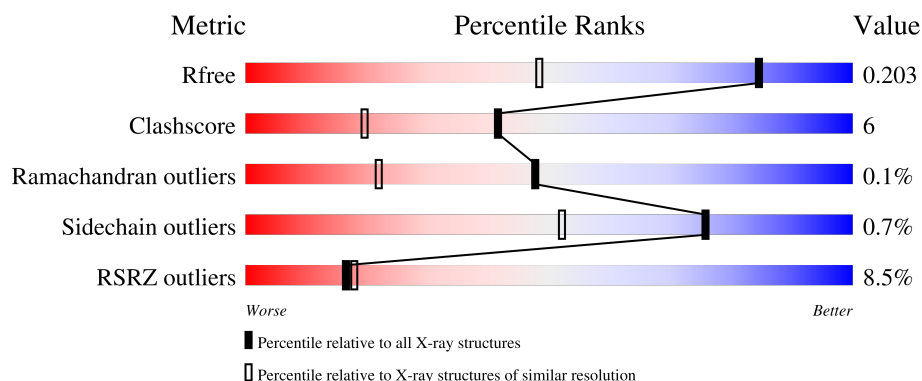
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	360	8% 92% 6%
1	B	360	9% 92% 6%
1	C	360	10% 92% 6%
1	D	360	7% 92% 6%

2 Entry composition [i](#)

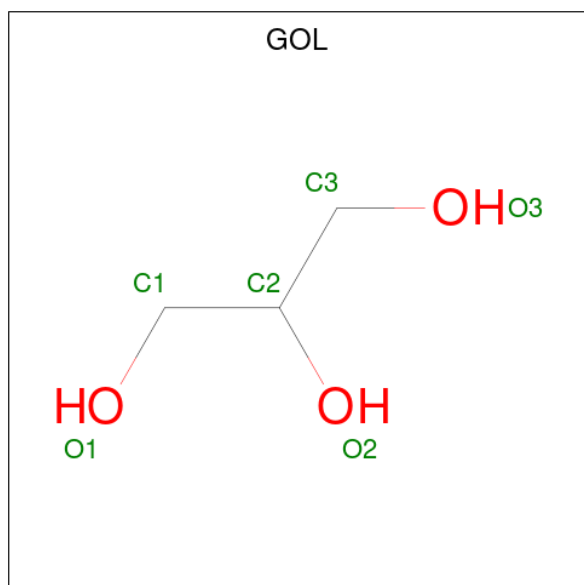
There are 5 unique types of molecules in this entry. The entry contains 13495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROBABLE ALPHA-METHYLACYL-COA RACEMASE MCR (2-METHYLACYL-COA RACEMASE) (2-ARYLPROPIONYL-COA EPIMERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	26	0
			2833	1797	502	513	21			
1	B	355	Total	C	N	O	S	0	29	0
			2857	1803	508	524	22			
1	C	355	Total	C	N	O	S	0	31	0
			2854	1805	503	524	22			
1	D	355	Total	C	N	O	S	0	31	0
			2866	1811	507	527	21			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



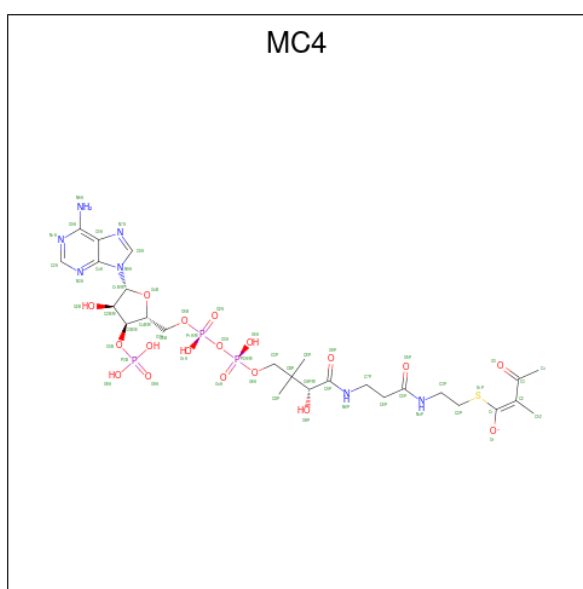
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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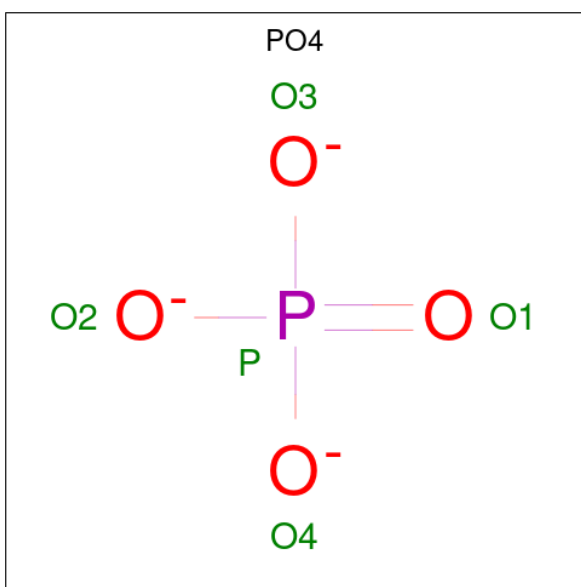
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-METHYLACETOACETYL COA (CCD ID: MC4) (formula: $C_{26}H_{41}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			55	26	7	18	3	1		

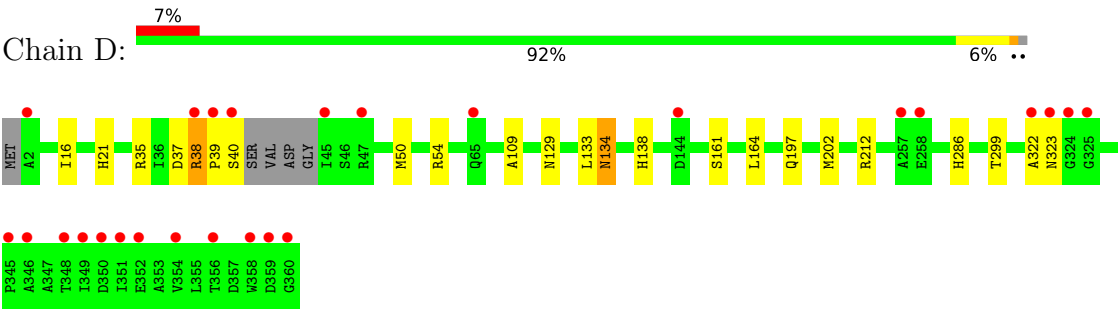
- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	515	Total	O	0	1
			516	516		
5	B	398	Total	O	0	0
			398	398		
5	C	483	Total	O	0	2
			485	485		
5	D	422	Total	O	0	4
			426	426		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 80.17Å 118.88Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	118.84 – 1.41 118.84 – 1.41	Depositor EDS
% Data completeness (in resolution range)	98.6 (118.84-1.41) 98.6 (118.84-1.41)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.205 0.185 , 0.203	Depositor DCC
R_{free} test set	16290 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.137 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13495	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1371e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MC4, PO4, GOL

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	0.44	0/2975	0.70	0/4040
1	B	0.45	0/2986	0.68	0/4051
1	C	0.44	0/2982	0.69	1/4053 (0.0%)
1	D	0.44	0/2999	0.68	0/4071
All	All	0.44	0/11942	0.69	1/16215 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	349	ILE	N-CA-C	5.11	115.31	109.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2833	0	2857	36	0
1	B	2857	0	2859	51	0
1	C	2854	0	2850	46	0
1	D	2866	0	2866	34	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	16	0	0
2	D	6	0	8	0	0
3	A	55	0	37	3	0
3	B	55	0	37	2	0
3	C	55	0	37	5	0
3	D	55	0	37	3	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	A	516	0	0	4	0
5	B	398	0	0	1	0
5	C	485	0	0	1	0
5	D	426	0	0	5	0
All	All	13495	0	11620	149	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 6.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347[B]:ALA:CB	1:C:348[B]:THR:OG1	1.83	1.26
1:C:347[A]:ALA:CB	1:C:348[A]:THR:HA	1.66	1.18
1:C:347[A]:ALA:HB1	1:C:348[A]:THR:CA	1.75	1.15
1:C:347[B]:ALA:HB1	1:C:348[B]:THR:OG1	0.96	1.11
1:A:91[B]:ARG:HG2	1:A:91[B]:ARG:HH11	1.18	1.09
1:A:91[B]:ARG:HH11	1:A:91[B]:ARG:CG	1.71	1.04
1:C:50[A]:MET:HA	1:D:197[A]:GLN:HE22	1.31	0.94
1:C:199[A]:MET:CE	1:C:202[A]:MET:HE1	1.98	0.93
1:C:347[B]:ALA:CB	1:C:348[B]:THR:HG1	1.74	0.91
1:B:199[A]:MET:HE2	1:B:202[A]:MET:HE1	1.53	0.90
1:C:199[A]:MET:HE2	1:C:202[A]:MET:HE1	1.54	0.90
1:B:50[A]:MET:O	1:B:51[A]:LEU:HB2	1.72	0.88
1:C:199[A]:MET:HE3	1:C:202[A]:MET:CE	2.04	0.88
1:B:199[A]:MET:CE	1:B:202[A]:MET:HE1	2.06	0.86
1:C:50[A]:MET:CA	1:D:197[A]:GLN:HE22	1.87	0.86
1:C:346[A]:ALA:O	1:C:347[A]:ALA:HB2	1.76	0.84
1:B:50[A]:MET:O	1:B:51[A]:LEU:HD13	1.75	0.84
1:B:54[A]:ARG:CG	1:B:54[A]:ARG:HH11	1.92	0.81
1:C:323[B]:ASN:HD22	1:C:323[B]:ASN:H	1.28	0.81
1:B:54[A]:ARG:HH11	1:B:54[A]:ARG:HG2	1.45	0.80
1:C:323[B]:ASN:HD22	1:C:323[B]:ASN:N	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50[A]:MET:HA	1:D:197[A]:GLN:NE2	1.96	0.80
1:B:199[A]:MET:HE3	1:B:202[A]:MET:CE	2.13	0.79
1:B:198[B]:MET:HE3	1:B:202[B]:MET:HE2	1.64	0.78
1:A:198[A]:MET:HE3	1:B:50[A]:MET:HE1	1.64	0.78
1:C:199[A]:MET:HE3	1:C:202[A]:MET:HE2	1.65	0.78
1:A:91[B]:ARG:CB	1:A:91[B]:ARG:NH1	2.48	0.77
1:A:315[A]:GLU:HG3	5:A:2457[A]:HOH:O	1.87	0.75
1:B:50[A]:MET:O	1:B:51[A]:LEU:CB	2.36	0.74
1:B:199[A]:MET:HE3	1:B:202[A]:MET:HE2	1.70	0.74
1:A:91[B]:ARG:HH11	1:A:91[B]:ARG:CB	2.00	0.73
1:C:347[A]:ALA:HB1	1:C:348[A]:THR:HA	0.79	0.73
1:D:38:ARG:HH11	1:D:38:ARG:HG3	1.53	0.73
1:A:91[B]:ARG:HG2	1:A:91[B]:ARG:NH1	1.98	0.73
1:C:199[A]:MET:CE	1:C:202[A]:MET:CE	2.64	0.73
1:B:50[A]:MET:O	1:B:51[A]:LEU:CD1	2.37	0.73
1:B:199[A]:MET:CE	1:B:202[A]:MET:CE	2.67	0.73
1:C:346[A]:ALA:O	1:C:347[A]:ALA:CB	2.38	0.72
1:B:322[A]:ALA:O	1:B:323[A]:ASN:C	2.34	0.71
1:C:129:ASN:HD22	1:D:299:THR:HG22	1.55	0.71
1:B:198[B]:MET:HE3	1:B:202[B]:MET:CE	2.22	0.70
1:D:133:LEU:HB2	5:D:2202:HOH:O	1.92	0.69
1:A:231:ASP:OD2	1:A:233[B]:ARG:HD3	1.93	0.69
1:B:51[A]:LEU:HA	1:B:54[A]:ARG:NH1	2.07	0.69
1:C:198[A]:MET:HE3	1:D:50[A]:MET:HE1	1.74	0.68
1:A:199[B]:MET:HE3	1:A:202[B]:MET:HE1	1.76	0.67
3:B:1363:MC4:H4A	3:B:1363:MC4:S1P	2.34	0.67
1:B:323[A]:ASN:C	1:B:323[A]:ASN:HD22	2.01	0.66
1:A:50[B]:MET:HE2	1:B:198[B]:MET:HA	1.79	0.64
1:A:283[A]:ASP:H	2:A:1361:GOL:H12	1.64	0.63
3:C:1363:MC4:C4	3:C:1363:MC4:S1P	2.87	0.62
1:A:50[B]:MET:HE2	1:B:198[B]:MET:CG	2.29	0.62
1:B:54[A]:ARG:CG	1:B:54[A]:ARG:NH1	2.56	0.62
1:B:198[B]:MET:CE	1:B:199[B]:MET:HE1	2.29	0.62
1:C:323[B]:ASN:N	1:C:323[B]:ASN:ND2	2.46	0.62
1:C:347[B]:ALA:HB1	1:C:348[B]:THR:HG1	0.79	0.61
1:A:283[B]:ASP:H	2:A:1361:GOL:H12	1.64	0.61
1:D:133:LEU:CB	5:D:2202:HOH:O	2.49	0.59
1:C:198[B]:MET:HG3	1:D:50[B]:MET:CE	2.32	0.59
3:A:1363:MC4:S1P	3:A:1363:MC4:C4	2.91	0.58
3:D:1363:MC4:S1P	3:D:1363:MC4:C4	2.93	0.57
1:C:50[B]:MET:HB2	1:D:197[B]:GLN:HE22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199[B]:MET:HA	1:A:202[B]:MET:HE3	1.87	0.56
1:D:50[B]:MET:O	1:D:54[B]:ARG:NH1	2.37	0.56
1:B:198[A]:MET:HG2	1:B:202[A]:MET:HE2	1.88	0.56
1:C:198[B]:MET:HA	1:D:50[B]:MET:HE2	1.87	0.56
1:C:129:ASN:HA	1:D:299:THR:HG21	1.87	0.55
1:D:21:HIS:HD2	1:D:161:SER:OG	1.90	0.55
1:B:198[B]:MET:HE2	1:B:199[B]:MET:SD	2.46	0.55
3:B:1363:MC4:S1P	3:B:1363:MC4:C4	2.93	0.55
1:A:91[B]:ARG:NH1	1:A:91[B]:ARG:HB2	2.20	0.55
1:A:91[B]:ARG:HB2	1:A:91[B]:ARG:CZ	2.37	0.55
1:B:198[B]:MET:CE	1:B:199[B]:MET:CE	2.84	0.55
1:C:198[B]:MET:HG3	1:D:50[B]:MET:HE2	1.87	0.55
1:C:299[B]:THR:CG2	1:D:129:ASN:HD22	2.19	0.54
1:C:198[B]:MET:CG	1:D:50[B]:MET:HE2	2.38	0.54
1:C:299[B]:THR:HG23	1:D:129:ASN:HD22	1.73	0.54
1:A:16:ILE:HD12	3:A:1363:MC4:H4A	1.89	0.54
1:A:199[B]:MET:CE	1:A:202[B]:MET:HE1	2.38	0.54
1:C:347[B]:ALA:CA	1:C:348[B]:THR:OG1	2.53	0.54
1:A:199[B]:MET:HA	1:A:202[B]:MET:CE	2.39	0.53
1:C:21:HIS:HD2	1:C:161:SER:OG	1.91	0.53
1:A:21:HIS:HD2	1:A:161:SER:OG	1.92	0.53
1:B:323[A]:ASN:HD22	1:B:324[A]:GLY:N	2.06	0.53
1:B:21:HIS:HD2	1:B:161:SER:OG	1.92	0.52
3:A:1363:MC4:S1P	3:A:1363:MC4:H4B	2.50	0.51
1:D:286:HIS:HE1	5:D:2342:HOH:O	1.92	0.51
3:C:1363:MC4:S1P	3:C:1363:MC4:H4A	2.51	0.51
1:A:140[A]:ILE:HD13	1:A:150:PRO:HG3	1.93	0.50
1:B:198[B]:MET:HE1	1:B:199[B]:MET:HE1	1.93	0.50
1:D:202[A]:MET:CE	5:D:2239:HOH:O	2.60	0.50
1:B:323[A]:ASN:C	1:B:323[A]:ASN:ND2	2.70	0.50
1:A:56:ILE:HG23	5:A:2043:HOH:O	2.12	0.49
1:C:123[B]:GLN:OE1	5:C:2207:HOH:O	2.18	0.49
1:A:37:ASP:HB2	5:A:2043:HOH:O	2.13	0.49
1:A:199[B]:MET:SD	1:A:202[B]:MET:CE	3.01	0.49
1:B:50[B]:MET:O	1:B:54[B]:ARG:NH1	2.45	0.49
3:D:1363:MC4:S1P	3:D:1363:MC4:H4A	2.53	0.49
1:D:138:HIS:O	1:D:212:ARG:HD3	2.13	0.48
1:A:51:LEU:HB2	5:A:2072:HOH:O	2.12	0.48
1:A:50[B]:MET:CE	1:B:198[B]:MET:CG	2.92	0.47
1:B:199[A]:MET:HA	1:B:202[A]:MET:HE3	1.96	0.47
1:B:323[B]:ASN:HD22	1:B:323[B]:ASN:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199[B]:MET:SD	1:A:202[B]:MET:HE1	2.55	0.47
1:A:134:ASN:C	1:A:134:ASN:HD22	2.22	0.47
1:D:134:ASN:C	1:D:134:ASN:HD22	2.23	0.47
1:A:50[B]:MET:CE	1:B:198[B]:MET:HG3	2.44	0.46
1:D:16:ILE:HD12	3:D:1363:MC4:H4A	1.98	0.46
1:C:199[A]:MET:HA	1:C:202[A]:MET:CE	2.46	0.46
1:C:196:ILE:HG12	1:C:199[A]:MET:HB2	1.97	0.46
1:D:39:PRO:O	1:D:40:SER:C	2.59	0.46
1:A:50[B]:MET:HE2	1:B:198[B]:MET:HG2	1.98	0.46
1:C:12:GLU:OE1	1:C:54[B]:ARG:HD3	2.16	0.45
1:A:50[B]:MET:HE2	1:B:198[B]:MET:HG3	1.98	0.45
1:C:134:ASN:HD22	1:C:134:ASN:C	2.24	0.45
1:C:50[B]:MET:CB	1:D:197[B]:GLN:HE22	2.30	0.44
1:B:134:ASN:HD22	1:B:134:ASN:C	2.25	0.44
1:C:129:ASN:HD22	1:D:299:THR:CG2	2.28	0.44
1:B:51[A]:LEU:CA	1:B:54[A]:ARG:NH1	2.79	0.44
1:C:199[A]:MET:HA	1:C:202[A]:MET:HE3	2.00	0.43
1:C:16:ILE:HD12	3:C:1363:MC4:H4A	2.00	0.43
1:B:50[A]:MET:C	1:B:51[A]:LEU:CD1	2.92	0.43
1:B:196:ILE:HG12	1:B:199[A]:MET:HB2	1.99	0.43
1:C:126:HIS:HB3	3:C:1363:MC4:H52B	2.01	0.42
1:A:196:ILE:HG12	1:A:199[A]:MET:HB2	1.99	0.42
1:D:35:ARG:HG2	1:D:37[B]:ASP:OD1	2.20	0.42
1:B:109:ALA:HB1	1:B:164:LEU:HD11	2.02	0.42
1:B:54[A]:ARG:NH1	1:B:54[A]:ARG:HG3	2.32	0.42
1:B:248[B]:MET:HE2	1:B:248[B]:MET:HB3	1.94	0.41
1:C:194:VAL:O	1:D:21:HIS:HE1	2.02	0.41
1:A:259[A]:LEU:HD22	1:A:274:LEU:HD13	2.02	0.41
1:B:323[B]:ASN:HD22	1:B:323[B]:ASN:H	1.67	0.41
1:B:214:ALA:O	1:B:265[B]:ARG:NH2	2.47	0.41
1:C:299[B]:THR:HG21	1:D:129:ASN:HB3	2.01	0.41
3:C:1363:MC4:S1P	3:C:1363:MC4:H4B	2.60	0.41
1:D:109:ALA:HB1	1:D:164:LEU:HD11	2.03	0.41
1:D:322[A]:ALA:O	1:D:323[A]:ASN:C	2.62	0.41
1:A:50[B]:MET:HE3	1:B:201:ALA:HB3	2.03	0.41
1:A:194:VAL:O	1:B:21:HIS:HE1	2.03	0.41
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.56	0.41
1:A:302:LEU:O	1:B:135:GLY:HA2	2.21	0.40
1:B:199[A]:MET:HA	1:B:202[A]:MET:CE	2.52	0.40
1:B:198[B]:MET:CE	1:B:199[B]:MET:SD	3.09	0.40
1:B:293[B]:ASN:ND2	5:B:2341:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ILE:HG12	1:C:199[B]:MET:HB2	2.03	0.40
1:D:202[A]:MET:HE1	5:D:2239:HOH:O	2.19	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	377/360 (105%)	366 (97%)	11 (3%)	0	100	100
1	B	380/360 (106%)	369 (97%)	11 (3%)	0	100	100
1	C	382/360 (106%)	367 (96%)	13 (3%)	2 (0%)	24	7
1	D	382/360 (106%)	367 (96%)	15 (4%)	0	100	100
All	All	1521/1440 (106%)	1469 (97%)	50 (3%)	2 (0%)	48	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	323[A]	ASN
1	C	323[B]	ASN

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	296/275 (108%)	294 (99%)	2 (1%)	76	52
1	B	297/275 (108%)	294 (99%)	3 (1%)	68	39
1	C	296/275 (108%)	294 (99%)	2 (1%)	76	52
1	D	298/275 (108%)	296 (99%)	2 (1%)	76	52
All	All	1187/1100 (108%)	1178 (99%)	9 (1%)	76	47

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	134	ASN
1	B	54[A]	ARG
1	B	54[B]	ARG
1	B	134	ASN
1	C	58	THR
1	C	134	ASN
1	D	38	ARG
1	D	134	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	103	ASN
1	A	116	GLN
1	A	176	GLN
1	A	262	GLN
1	A	263	ASN
1	A	308	HIS
1	A	327	GLN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	309	ASN
1	B	327	GLN
1	C	21	HIS
1	C	103	ASN
1	C	134	ASN
1	C	176	GLN
1	C	308	HIS

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Mol	Chain	Res	Type
1	C	327	GLN
1	D	21	HIS
1	D	65	GLN
1	D	103	ASN
1	D	134	ASN
1	D	286	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	MC4	A	1363	-	53,57,57	2.29	13 (24%)	73,85,85	1.43	8 (10%)
4	PO4	B	1361	-	4,4,4	0.95	0	6,6,6	0.45	0
3	MC4	B	1363	-	53,57,57	2.29	14 (26%)	73,85,85	1.43	7 (9%)
3	MC4	C	1363	-	53,57,57	2.31	13 (24%)	73,85,85	1.41	8 (10%)
3	MC4	D	1363	-	53,57,57	2.29	12 (22%)	73,85,85	1.44	8 (10%)
4	PO4	D	1361	-	4,4,4	0.98	0	6,6,6	0.50	0
2	GOL	C	1361	-	5,5,5	0.36	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	1362	-	5,5,5	0.36	0	5,5,5	0.25	0
2	GOL	A	1361	-	5,5,5	0.39	0	5,5,5	0.24	0
2	GOL	B	1362	-	5,5,5	0.35	0	5,5,5	0.37	0
2	GOL	C	1362	-	5,5,5	0.34	0	5,5,5	0.42	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	MC4	A	1363	-	-	2/53/75/75	0/3/3/3
3	MC4	B	1363	-	-	6/53/75/75	0/3/3/3
3	MC4	C	1363	-	-	2/53/75/75	0/3/3/3
3	MC4	D	1363	-	-	1/53/75/75	0/3/3/3
2	GOL	C	1361	-	-	0/4/4/4	-
2	GOL	D	1362	-	-	0/4/4/4	-
2	GOL	A	1361	-	-	2/4/4/4	-
2	GOL	B	1362	-	-	1/4/4/4	-
2	GOL	C	1362	-	-	0/4/4/4	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1363	MC4	P3B-O9A	6.34	1.70	1.50
3	A	1363	MC4	P3B-O9A	6.33	1.70	1.50
3	B	1363	MC4	P3B-O9A	6.31	1.70	1.50
3	D	1363	MC4	P3B-O9A	6.28	1.70	1.50
3	A	1363	MC4	O3-C3	6.04	1.37	1.23
3	D	1363	MC4	O3-C3	6.02	1.36	1.23
3	B	1363	MC4	O3-C3	5.97	1.36	1.23
3	C	1363	MC4	O3-C3	5.95	1.36	1.23
3	A	1363	MC4	O1-C1	-5.78	1.23	1.30
3	D	1363	MC4	O1-C1	-5.64	1.23	1.30
3	C	1363	MC4	O1-C1	-5.62	1.23	1.30
3	C	1363	MC4	C4-C3	-5.61	1.39	1.50
3	A	1363	MC4	C4-C3	-5.51	1.39	1.50
3	B	1363	MC4	O1-C1	-5.49	1.24	1.30
3	B	1363	MC4	C4-C3	-5.46	1.39	1.50
3	D	1363	MC4	C4-C3	-5.42	1.39	1.50
3	C	1363	MC4	P2A-O4A	5.26	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1363	MC4	P2A-O4A	5.24	1.69	1.50
3	D	1363	MC4	P2A-O4A	5.20	1.68	1.50
3	C	1363	MC4	P1A-O2A	5.19	1.68	1.50
3	A	1363	MC4	P2A-O4A	5.18	1.68	1.50
3	A	1363	MC4	P1A-O2A	5.16	1.68	1.50
3	B	1363	MC4	P1A-O2A	5.16	1.68	1.50
3	D	1363	MC4	P1A-O2A	5.09	1.68	1.50
3	C	1363	MC4	C5A-C4A	4.12	1.46	1.39
3	B	1363	MC4	P3B-O8A	4.09	1.70	1.54
3	D	1363	MC4	P3B-O8A	4.05	1.69	1.54
3	C	1363	MC4	P3B-O8A	4.04	1.69	1.54
3	A	1363	MC4	C5A-C4A	4.04	1.46	1.39
3	B	1363	MC4	C5A-C4A	4.03	1.46	1.39
3	D	1363	MC4	C5A-C4A	4.03	1.46	1.39
3	A	1363	MC4	P3B-O8A	4.00	1.69	1.54
3	D	1363	MC4	C1-S1P	3.18	1.78	1.74
3	A	1363	MC4	C5A-N7A	-2.96	1.33	1.39
3	B	1363	MC4	C5A-N7A	-2.95	1.33	1.39
3	D	1363	MC4	C5A-N7A	-2.94	1.33	1.39
3	C	1363	MC4	C5A-N7A	-2.91	1.33	1.39
3	B	1363	MC4	C1-S1P	2.71	1.77	1.74
3	C	1363	MC4	C5A-C6A	2.69	1.48	1.41
3	B	1363	MC4	C5A-C6A	2.64	1.48	1.41
3	D	1363	MC4	C5A-C6A	2.59	1.48	1.41
3	A	1363	MC4	C5A-C6A	2.56	1.48	1.41
3	C	1363	MC4	C1-S1P	2.46	1.77	1.74
3	C	1363	MC4	P2A-O3A	2.42	1.62	1.59
3	B	1363	MC4	P1A-O3A	2.31	1.62	1.59
3	C	1363	MC4	P1A-O3A	2.23	1.61	1.59
3	B	1363	MC4	P2A-O3A	2.21	1.61	1.59
3	A	1363	MC4	P1A-O3A	2.14	1.61	1.59
3	D	1363	MC4	C4A-N9A	-2.14	1.33	1.37
3	A	1363	MC4	P2A-O3A	2.13	1.61	1.59
3	A	1363	MC4	C4A-N9A	-2.07	1.33	1.37
3	B	1363	MC4	C4A-N9A	-2.02	1.33	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1363	MC4	C5A-C4A-N3A	-5.89	118.61	126.72
3	B	1363	MC4	C5A-C4A-N3A	-5.88	118.62	126.72
3	C	1363	MC4	C5A-C4A-N3A	-5.70	118.86	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1363	MC4	C5A-C4A-N3A	-5.68	118.90	126.72
3	B	1363	MC4	N3A-C4A-N9A	5.60	136.70	127.17
3	A	1363	MC4	N3A-C4A-N9A	5.56	136.62	127.17
3	C	1363	MC4	N3A-C4A-N9A	5.45	136.43	127.17
3	D	1363	MC4	N3A-C4A-N9A	5.43	136.40	127.17
3	A	1363	MC4	C2A-N3A-C4A	3.36	120.05	111.83
3	C	1363	MC4	C2A-N3A-C4A	3.32	119.93	111.83
3	B	1363	MC4	C2A-N3A-C4A	3.31	119.91	111.83
3	D	1363	MC4	C2A-N3A-C4A	3.27	119.82	111.83
3	D	1363	MC4	O3-C3-C2	-3.16	115.90	121.88
3	B	1363	MC4	O3-C3-C2	-3.09	116.04	121.88
3	A	1363	MC4	N3A-C2A-N1A	-3.05	123.96	128.58
3	C	1363	MC4	N3A-C2A-N1A	-3.03	124.00	128.58
3	D	1363	MC4	C4A-N9A-C8A	3.01	108.90	105.74
3	D	1363	MC4	N3A-C2A-N1A	-2.98	124.06	128.58
3	B	1363	MC4	N3A-C2A-N1A	-2.90	124.19	128.58
3	C	1363	MC4	O3-C3-C2	-2.90	116.40	121.88
3	B	1363	MC4	C4A-N9A-C8A	2.87	108.75	105.74
3	A	1363	MC4	O3-C3-C2	-2.86	116.47	121.88
3	C	1363	MC4	C4A-N9A-C8A	2.85	108.73	105.74
3	A	1363	MC4	C4A-N9A-C8A	2.80	108.68	105.74
3	D	1363	MC4	C3-C2-C1	2.71	124.01	119.02
3	A	1363	MC4	C3-C2-C1	2.60	123.81	119.02
3	C	1363	MC4	C3-C2-C1	2.44	123.51	119.02
3	B	1363	MC4	C3-C2-C1	2.35	123.34	119.02
3	D	1363	MC4	C2A-N1A-C6A	2.21	122.36	118.73
3	A	1363	MC4	C2A-N1A-C6A	2.16	122.28	118.73
3	C	1363	MC4	C2A-N1A-C6A	2.14	122.25	118.73

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1363	MC4	C1-C2-C3-O3
3	B	1363	MC4	C1-C2-C3-C4
2	A	1361	GOL	O1-C1-C2-C3
2	A	1361	GOL	O1-C1-C2-O2
3	B	1363	MC4	C52-C2-C3-C4
3	B	1363	MC4	C3B-O3B-P3B-O8A
2	B	1362	GOL	O1-C1-C2-C3
3	B	1363	MC4	P2A-O3A-P1A-O1A
3	C	1363	MC4	P2A-O3A-P1A-O2A

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Mol	Chain	Res	Type	Atoms
3	D	1363	MC4	P2A-O3A-P1A-O1A
3	A	1363	MC4	C5P-C6P-C7P-N8P
3	B	1363	MC4	C5P-C6P-C7P-N8P
3	C	1363	MC4	C5P-C6P-C7P-N8P
3	A	1363	MC4	P2A-O3A-P1A-O1A

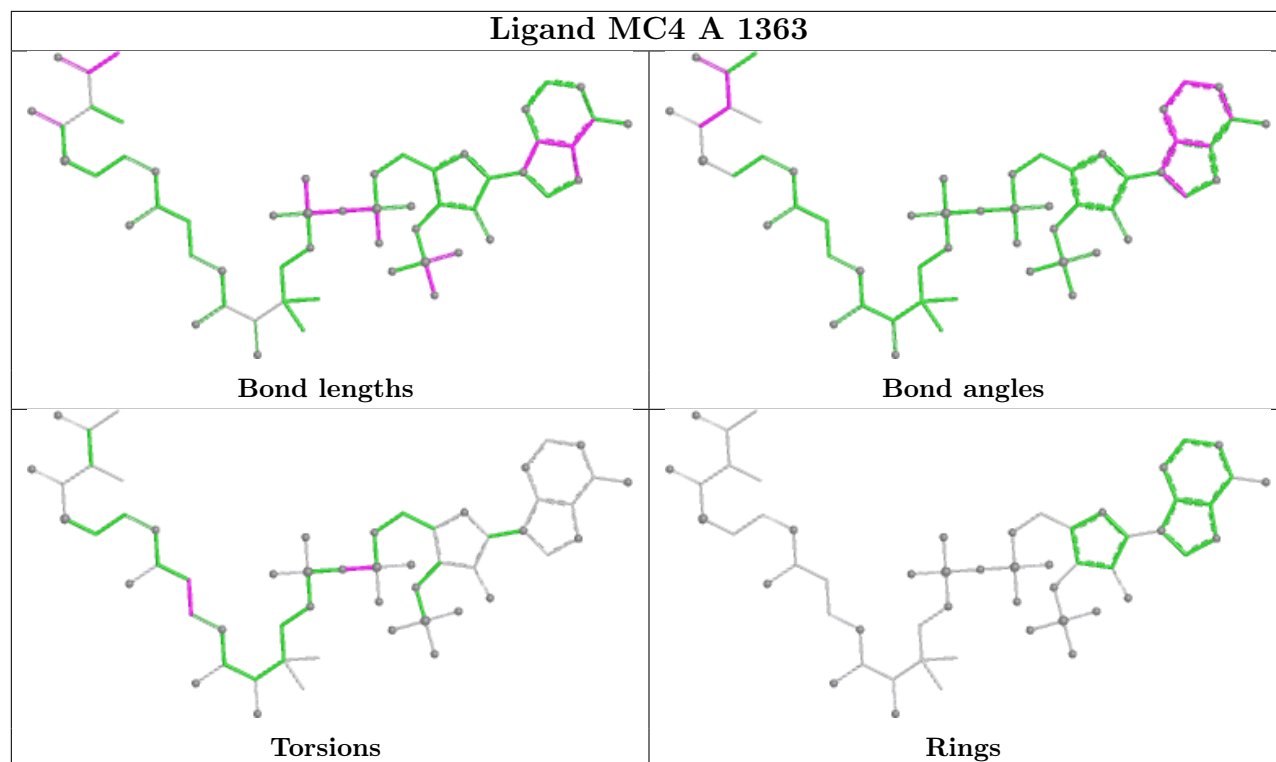
There are no ring outliers.

5 monomers are involved in 15 short contacts:

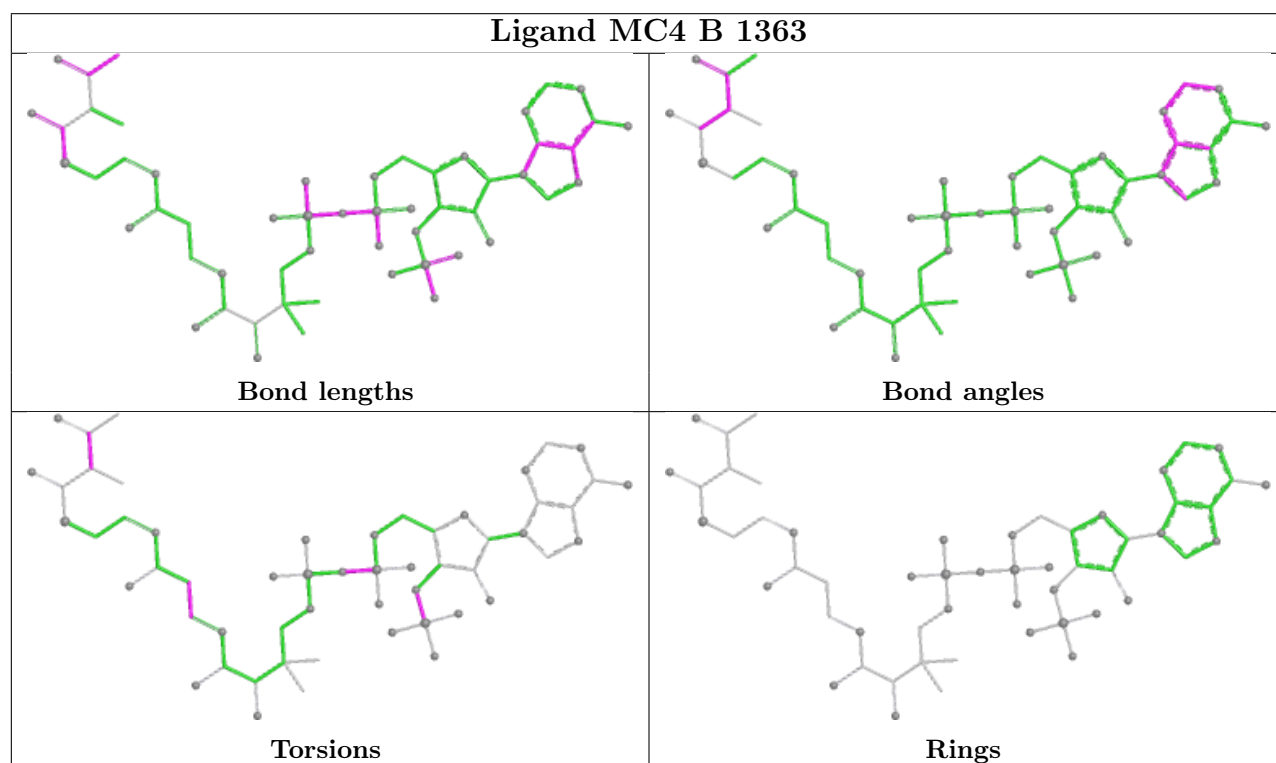
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1363	MC4	3	0
3	B	1363	MC4	2	0
3	C	1363	MC4	5	0
3	D	1363	MC4	3	0
2	A	1361	GOL	2	0

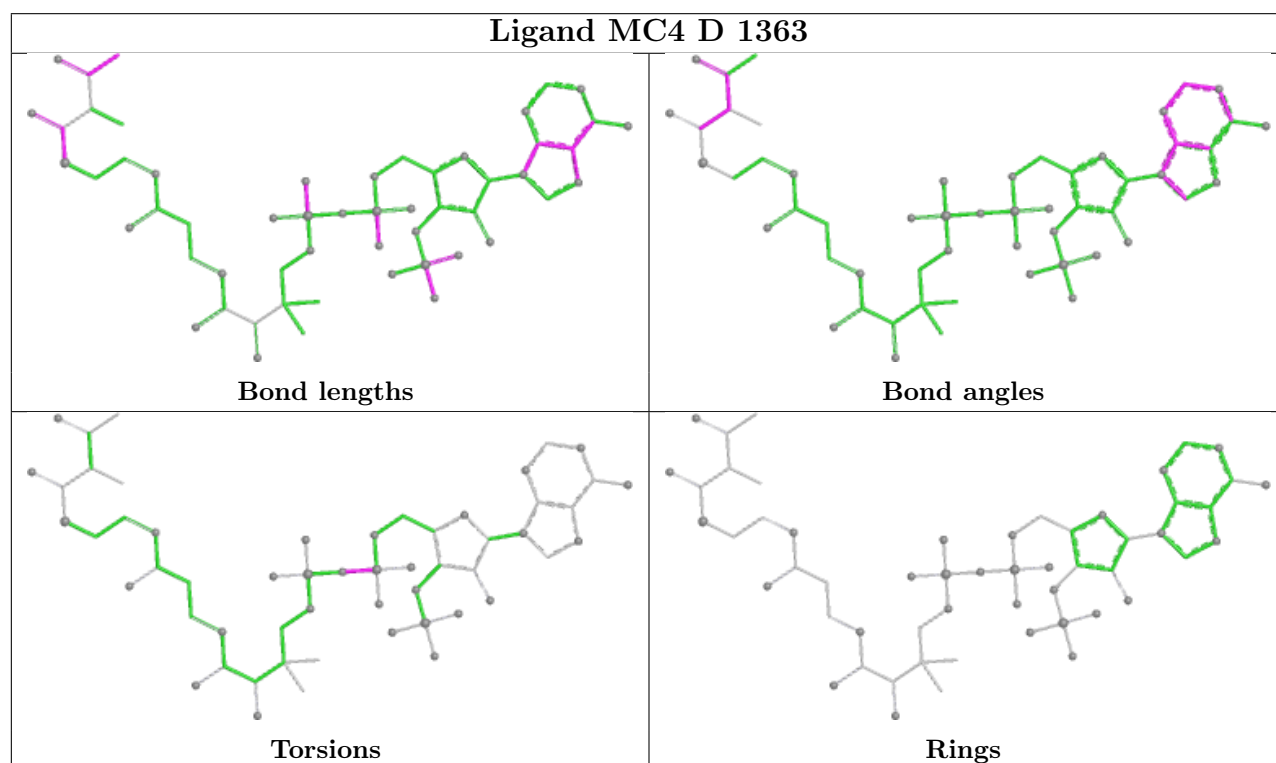
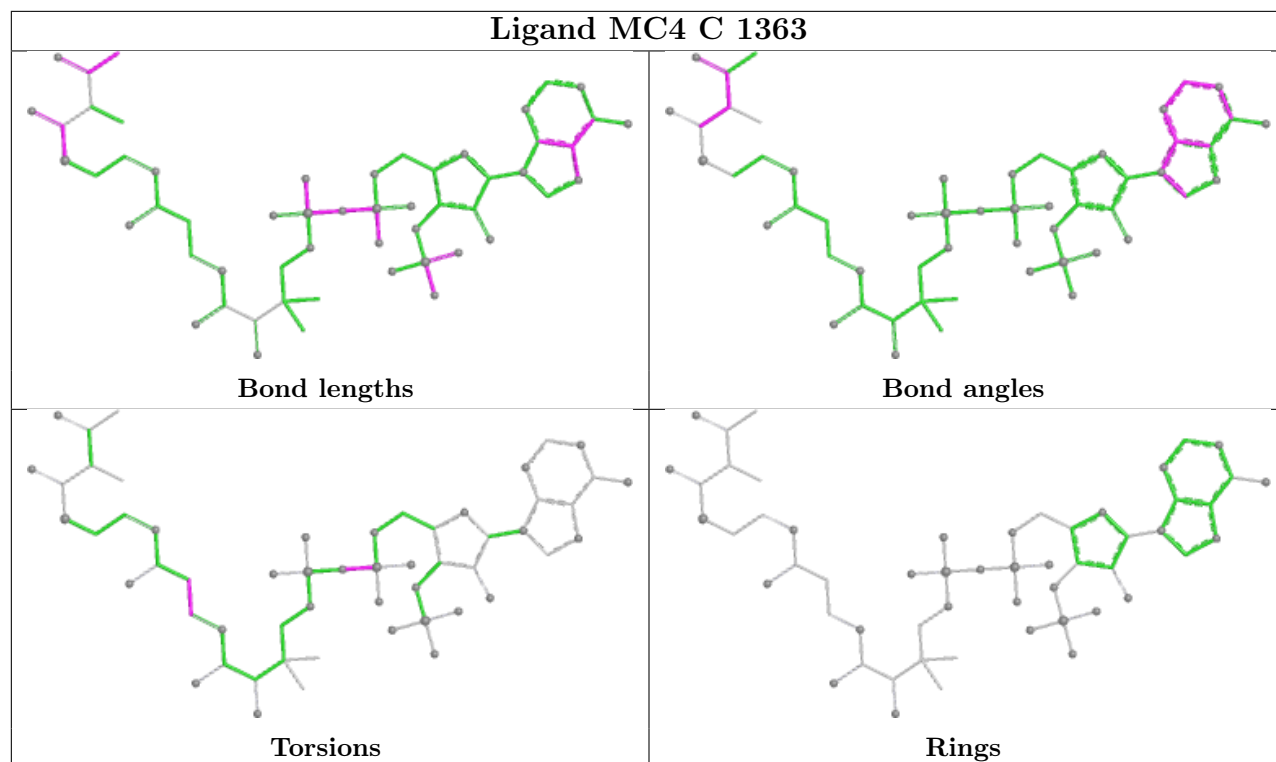
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand MC4 A 1363



Ligand MC4 B 1363





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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	355/360 (98%)	0.14	28 (7%)	18	20	4, 11, 26, 34	26 (7%)
1	B	355/360 (98%)	0.27	31 (8%)	16	17	4, 11, 26, 36	29 (8%)
1	C	355/360 (98%)	0.26	35 (9%)	13	14	4, 11, 26, 36	31 (8%)
1	D	355/360 (98%)	0.13	26 (7%)	21	23	4, 11, 24, 33	31 (8%)
All	All	1420/1440 (98%)	0.20	120 (8%)	16	18	4, 11, 26, 36	117 (8%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346[A]	ALA	7.9
1	C	347[A]	ALA	7.0
1	C	348[A]	THR	6.1
1	D	40	SER	5.6
1	A	45	ILE	5.6
1	C	40	SER	5.6
1	B	40	SER	5.5
1	C	351	ILE	5.2
1	A	351	ILE	5.2
1	B	45	ILE	5.1
1	D	322[A]	ALA	5.1
1	B	323[A]	ASN	5.0
1	A	350	ASP	4.9
1	C	49	ALA	4.8
1	C	359	ASP	4.8
1	A	40	SER	4.7
1	C	45	ILE	4.7
1	B	351	ILE	4.6
1	A	346	ALA	4.6
1	D	45	ILE	4.6
1	C	350	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	354	VAL	4.5
1	B	350	ASP	4.4
1	B	322[A]	ALA	4.4
1	B	49	ALA	4.3
1	D	323[A]	ASN	4.3
1	C	345[A]	PRO	4.2
1	B	359	ASP	4.1
1	C	324[A]	GLY	4.1
1	B	51[A]	LEU	4.1
1	C	349	ILE	4.1
1	C	2	ALA	4.1
1	C	322[A]	ALA	4.0
1	D	350	ASP	4.0
1	D	2	ALA	3.9
1	B	346	ALA	3.8
1	D	351	ILE	3.8
1	B	355	LEU	3.6
1	A	2	ALA	3.6
1	B	2	ALA	3.6
1	D	346	ALA	3.6
1	C	50[A]	MET	3.5
1	A	47	ARG	3.5
1	B	39	PRO	3.5
1	B	358	TRP	3.4
1	A	322	ALA	3.4
1	B	47	ARG	3.4
1	B	50[A]	MET	3.3
1	D	360	GLY	3.3
1	D	38	ARG	3.3
1	C	354	VAL	3.3
1	A	323	ASN	3.3
1	C	356	THR	3.3
1	D	258	GLU	3.2
1	A	359	ASP	3.1
1	A	348	THR	3.1
1	D	359	ASP	3.1
1	C	355	LEU	3.1
1	A	352	GLU	3.0
1	A	258	GLU	3.0
1	D	47[A]	ARG	2.9
1	B	65	GLN	2.9
1	A	358	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	65	GLN	2.8
1	C	358	TRP	2.8
1	D	358	TRP	2.8
1	B	352	GLU	2.8
1	C	323[A]	ASN	2.8
1	A	39	PRO	2.8
1	A	354	VAL	2.7
1	C	48	ASP	2.7
1	C	325[A]	GLY	2.7
1	A	353	ALA	2.7
1	A	345	PRO	2.7
1	D	354	VAL	2.7
1	A	324	GLY	2.6
1	B	321[A]	GLU	2.6
1	A	349	ILE	2.6
1	D	324[A]	GLY	2.6
1	C	58	THR	2.6
1	D	65	GLN	2.5
1	D	257	ALA	2.5
1	B	68	GLU	2.5
1	B	360	GLY	2.5
1	C	258	GLU	2.5
1	D	356	THR	2.5
1	C	357	ASP	2.5
1	D	325[A]	GLY	2.4
1	A	355	LEU	2.4
1	A	360	GLY	2.4
1	C	39	PRO	2.4
1	D	345	PRO	2.4
1	B	345	PRO	2.3
1	C	67	LEU	2.3
1	C	68	GLU	2.3
1	C	47	ARG	2.3
1	B	356	THR	2.3
1	C	360	GLY	2.3
1	B	56	ILE	2.3
1	C	176	GLN	2.3
1	D	144	ASP	2.3
1	D	348	THR	2.3
1	C	353	ALA	2.2
1	C	144	ASP	2.2
1	B	258	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	324[A]	GLY	2.2
1	B	38	ARG	2.2
1	B	325[A]	GLY	2.1
1	A	46	SER	2.1
1	D	39	PRO	2.1
1	D	349	ILE	2.1
1	C	326	TRP	2.1
1	A	325	GLY	2.1
1	B	73	LEU	2.1
1	A	180	LYS	2.1
1	A	48	ASP	2.1
1	A	347	ALA	2.0
1	B	48[A]	ASP	2.0
1	A	326	TRP	2.0
1	D	352	GLU	2.0

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.

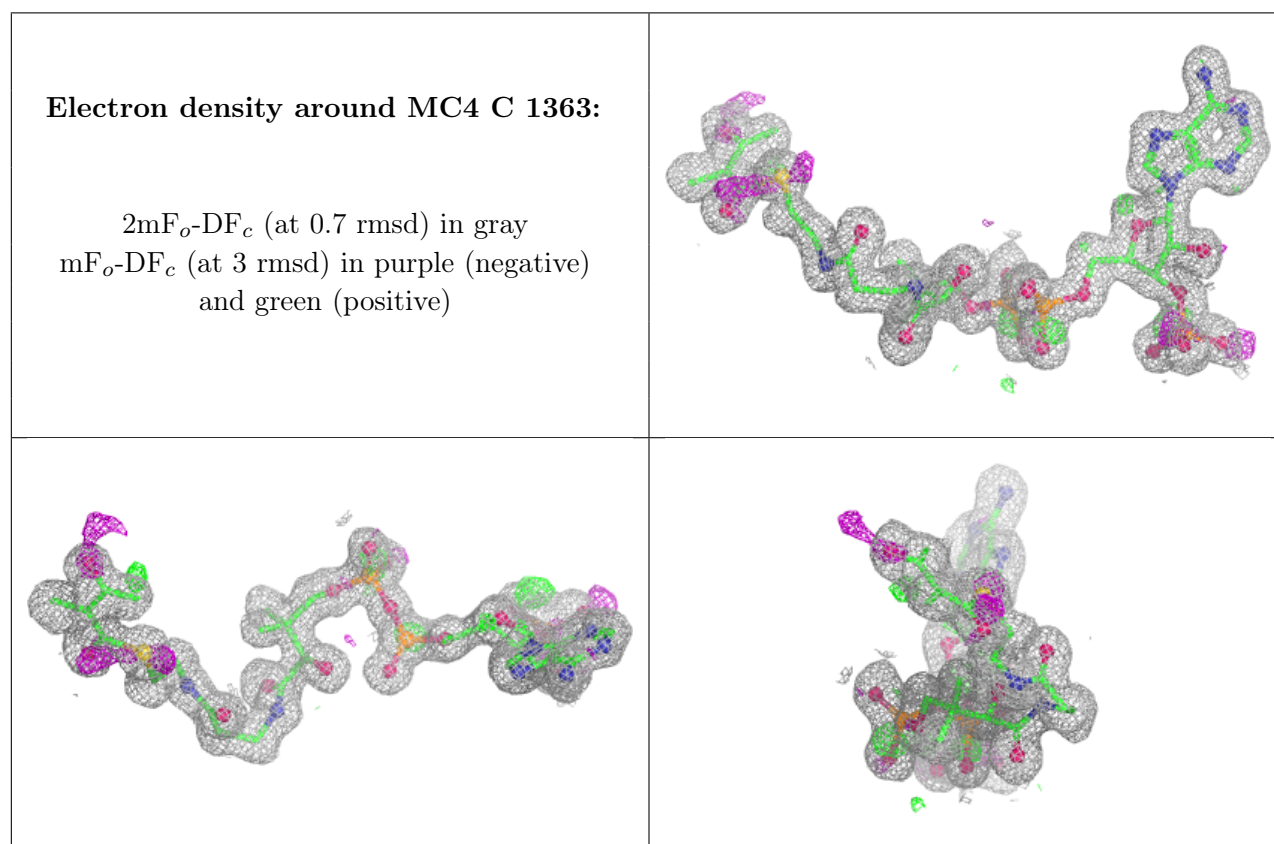
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1361	6/6	0.62	0.26	39,40,40,41	0
4	PO4	B	1361	5/5	0.65	0.26	85,85,85,85	0
2	GOL	B	1362	6/6	0.84	0.13	17,19,20,20	0
2	GOL	D	1362	6/6	0.87	0.11	26,26,27,28	0
2	GOL	C	1361	6/6	0.89	0.12	26,27,27,28	0
4	PO4	D	1361	5/5	0.89	0.14	35,36,36,36	0
2	GOL	C	1362	6/6	0.90	0.12	15,17,18,18	0
3	MC4	C	1363	55/55	0.96	0.07	9,14,21,21	0

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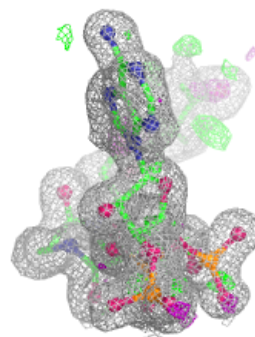
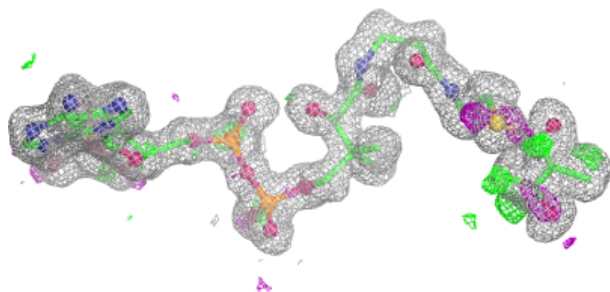
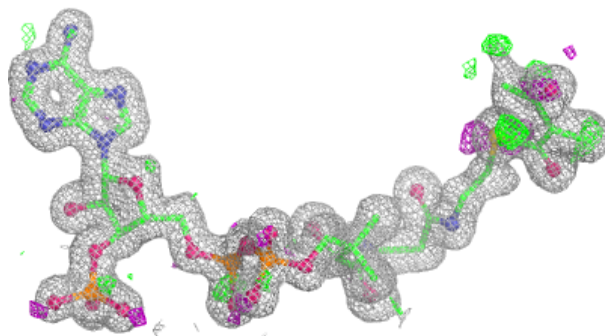
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MC4	D	1363	55/55	0.96	0.07	8,14,18,20	0
3	MC4	A	1363	55/55	0.96	0.07	9,14,20,20	0
3	MC4	B	1363	55/55	0.96	0.08	9,15,22,22	0

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.

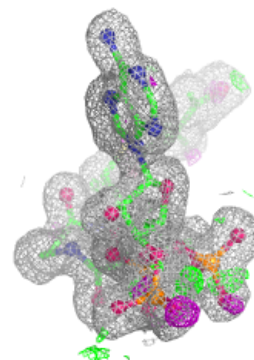
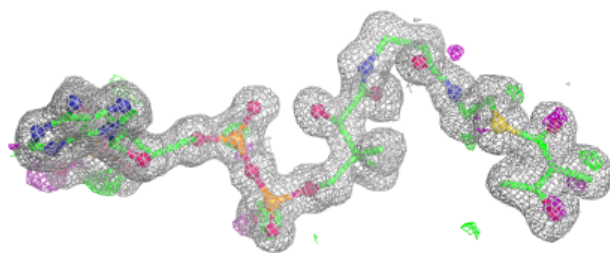
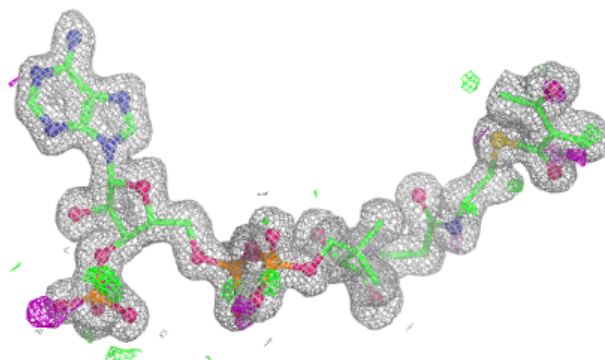


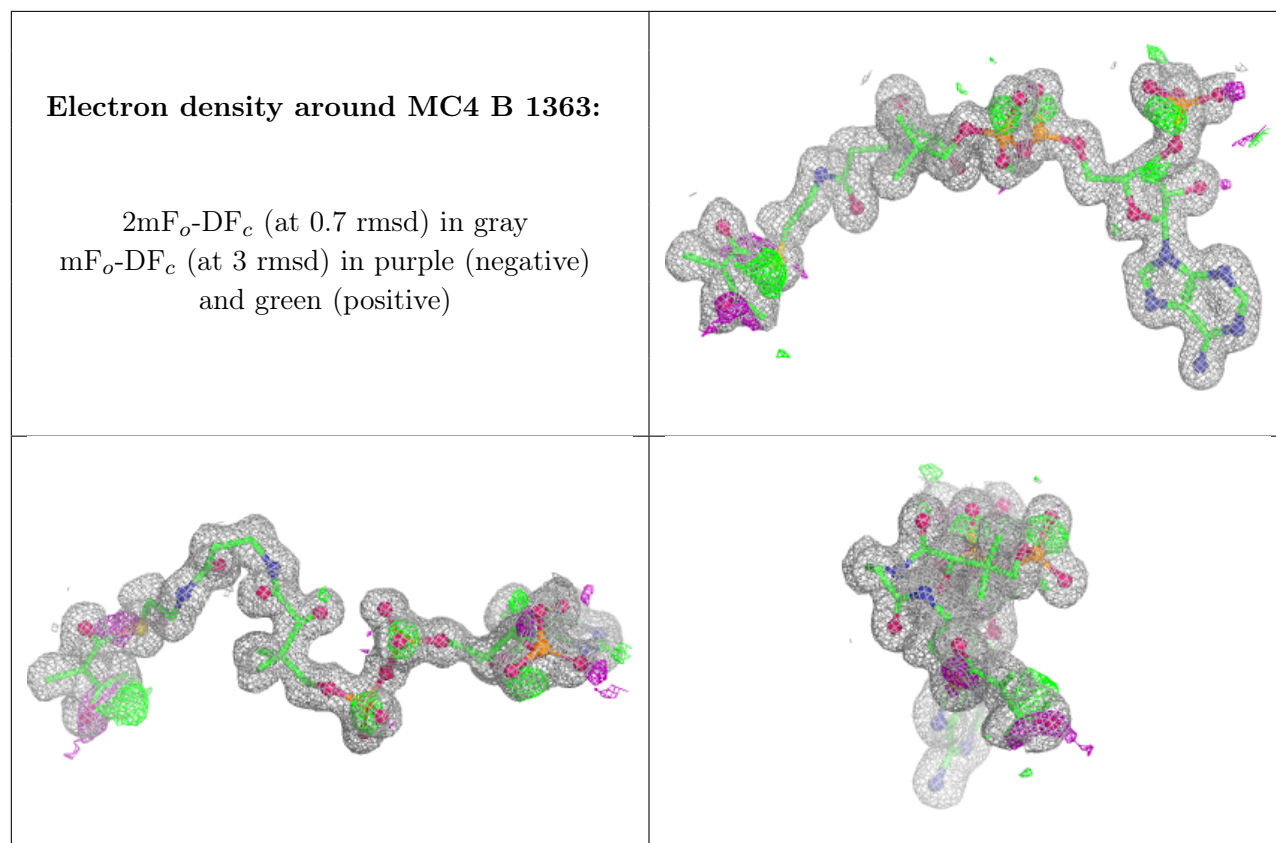
Electron density around MC4 D 1363:

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

**Electron density around MC4 A 1363:**

$2mF_o-DF_c$ (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.