Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 07:55 pm BST

PDB ID	:	9I35 / pdb_00009i35
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with octanoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	2.08 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:

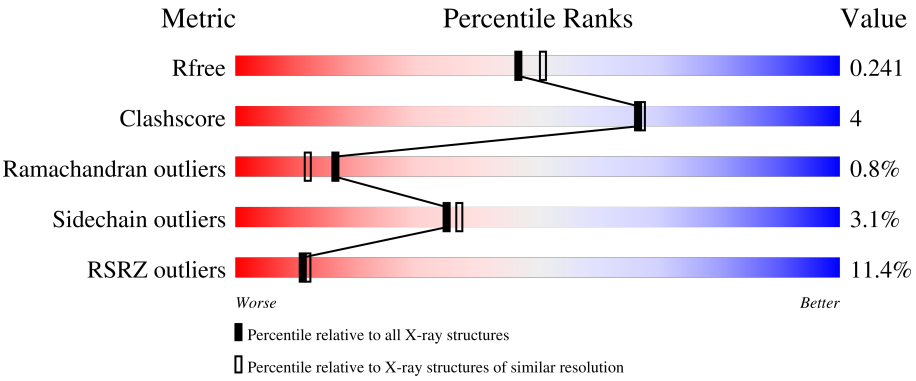
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.08 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}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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	364	8% 85% 12%
1	B	364	12% 87% 10%
1	C	364	19% 87% 10%
1	D	364	6% 88% 9%
1	E	364	10% 86% 11%

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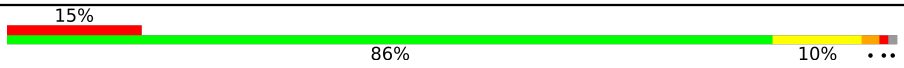
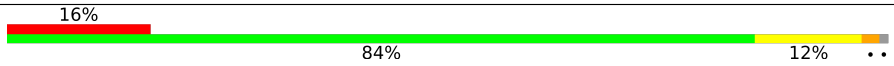
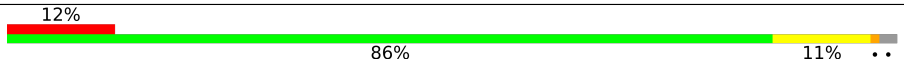
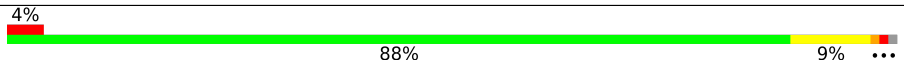
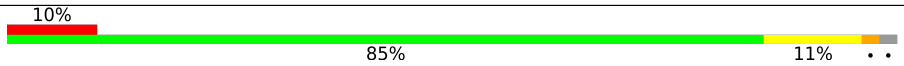
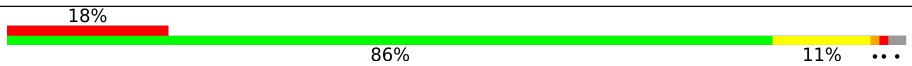
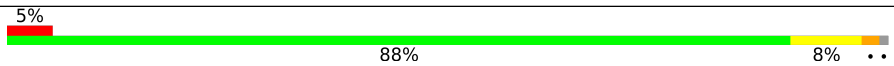
Mol	Chain	Length	Quality of chain
1	F	364	
1	G	364	
1	H	364	
1	I	364	
1	J	364	
1	K	364	
1	L	364	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35020 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 Alpha-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	B	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	C	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	356	Total	C	N	O	S	0	2	0
			2698	1692	483	507	16			
1	F	359	Total	C	N	O	S	0	2	0
			2724	1708	488	512	16			
1	G	359	Total	C	N	O	S	0	3	0
			2727	1709	488	514	16			
1	H	358	Total	C	N	O	S	0	2	0
			2713	1703	486	508	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	356	Total	C	N	O	S	0	1	0
			2695	1691	483	505	16			
1	K	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	L	359	Total	C	N	O	S	0	2	0
			2721	1707	487	511	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLY	-	expression tag	UNP O06543
A	362	SER	-	expression tag	UNP O06543
A	363	GLY	-	expression tag	UNP O06543
A	364	CYS	-	expression tag	UNP O06543
B	361	GLY	-	expression tag	UNP O06543

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	UNP O06543
D	361	GLY	-	expression tag	UNP O06543
D	362	SER	-	expression tag	UNP O06543
D	363	GLY	-	expression tag	UNP O06543
D	364	CYS	-	expression tag	UNP O06543
E	361	GLY	-	expression tag	UNP O06543
E	362	SER	-	expression tag	UNP O06543
E	363	GLY	-	expression tag	UNP O06543
E	364	CYS	-	expression tag	UNP O06543
F	361	GLY	-	expression tag	UNP O06543
F	362	SER	-	expression tag	UNP O06543
F	363	GLY	-	expression tag	UNP O06543
F	364	CYS	-	expression tag	UNP O06543
G	361	GLY	-	expression tag	UNP O06543
G	362	SER	-	expression tag	UNP O06543
G	363	GLY	-	expression tag	UNP O06543
G	364	CYS	-	expression tag	UNP O06543
H	361	GLY	-	expression tag	UNP O06543
H	362	SER	-	expression tag	UNP O06543
H	363	GLY	-	expression tag	UNP O06543
H	364	CYS	-	expression tag	UNP O06543
I	361	GLY	-	expression tag	UNP O06543
I	362	SER	-	expression tag	UNP O06543
I	363	GLY	-	expression tag	UNP O06543
I	364	CYS	-	expression tag	UNP O06543
J	361	GLY	-	expression tag	UNP O06543
J	362	SER	-	expression tag	UNP O06543
J	363	GLY	-	expression tag	UNP O06543
J	364	CYS	-	expression tag	UNP O06543
K	361	GLY	-	expression tag	UNP O06543
K	362	SER	-	expression tag	UNP O06543
K	363	GLY	-	expression tag	UNP O06543
K	364	CYS	-	expression tag	UNP O06543
L	361	GLY	-	expression tag	UNP O06543
L	362	SER	-	expression tag	UNP O06543
L	363	GLY	-	expression tag	UNP O06543

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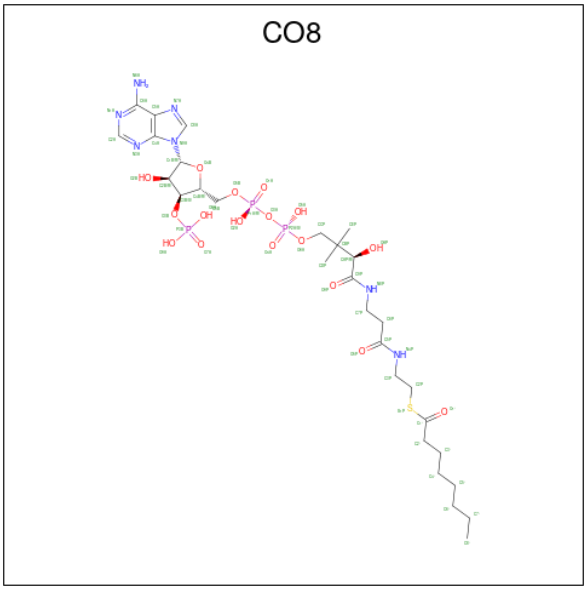
Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is OCTANOYL-COENZYME A (CCD ID: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			57	29	7	17	3	1		

- Molecule 3 is water.

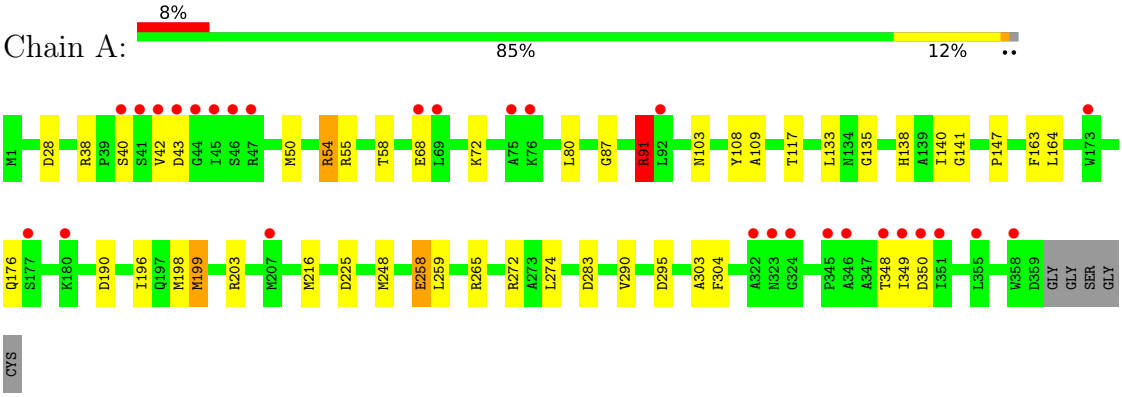
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	146	Total	O	0	0
			146	146		
3	C	147	Total	O	0	0
			147	147		
3	D	153	Total	O	0	0
			153	153		
3	E	133	Total	O	0	0
			133	133		
3	F	139	Total	O	0	0
			139	139		
3	G	128	Total	O	0	0
			128	128		
3	H	134	Total	O	0	0
			134	134		
3	I	166	Total	O	0	0
			166	166		
3	J	162	Total	O	0	0
			162	162		
3	K	151	Total	O	0	0
			151	151		
3	L	156	Total	O	0	0
			156	156		

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.

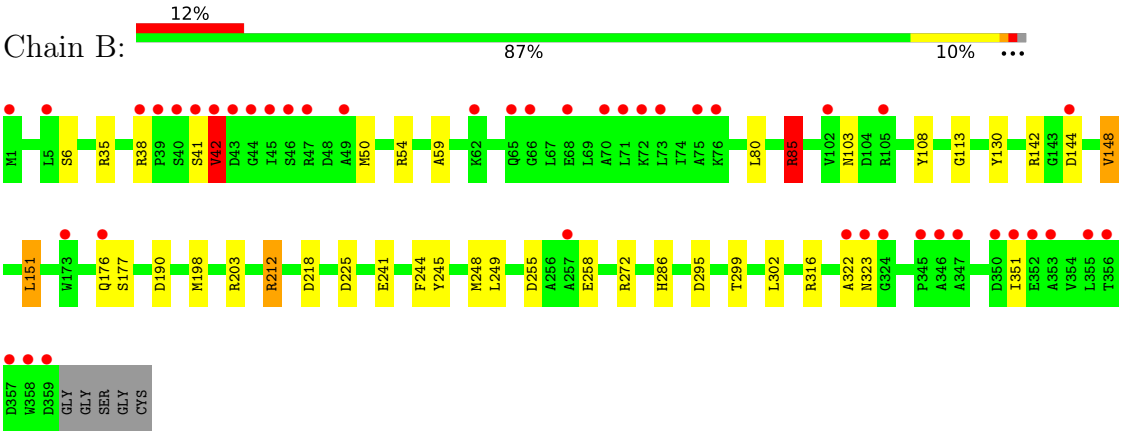
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



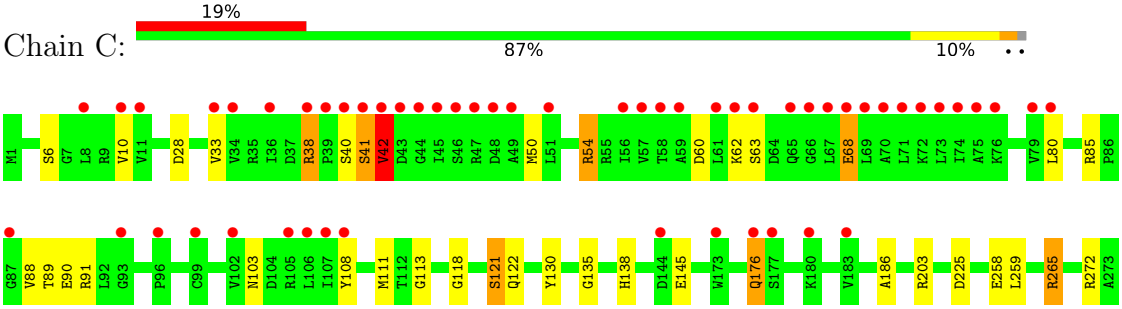
• Molecule 1: Alpha-methylacyl-CoA racemase

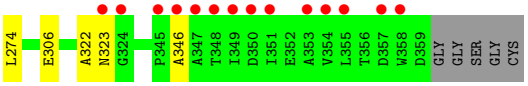
Chain B:



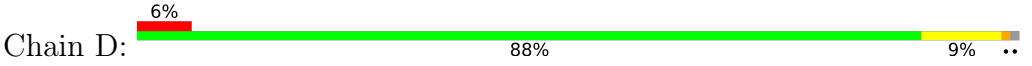
• Molecule 1: Alpha-methylacyl-CoA racemase

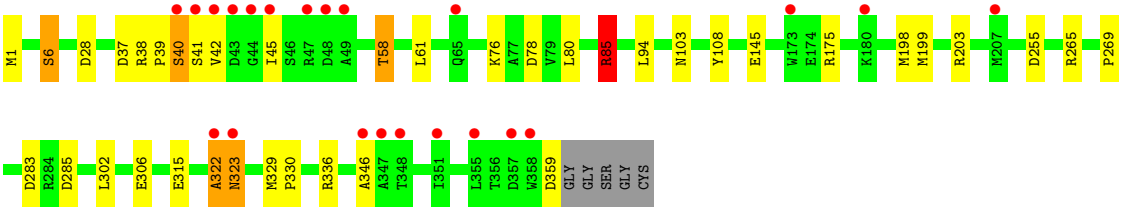
Chain C:



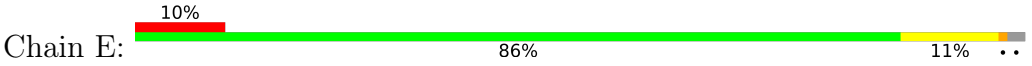


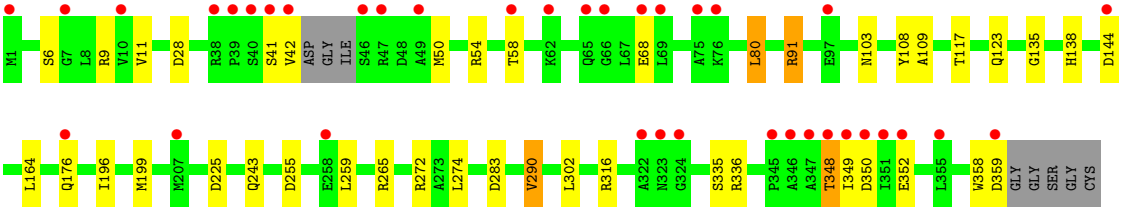
• Molecule 1: Alpha-methylacyl-CoA racemase



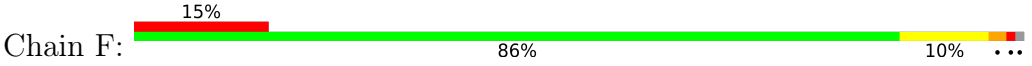


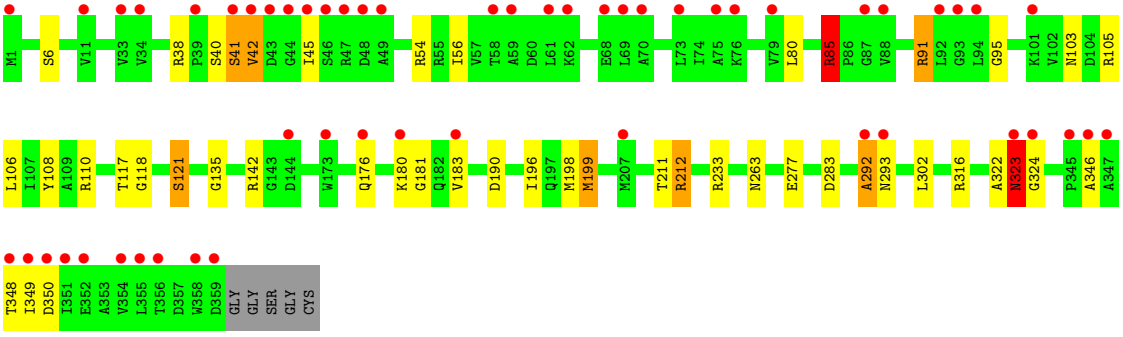
• Molecule 1: Alpha-methylacyl-CoA racemase



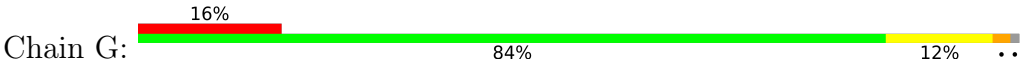


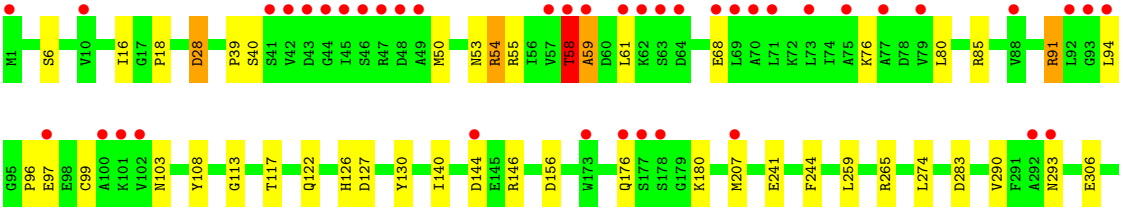
• Molecule 1: Alpha-methylacyl-CoA racemase

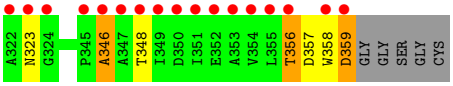




• Molecule 1: Alpha-methylacyl-CoA racemase

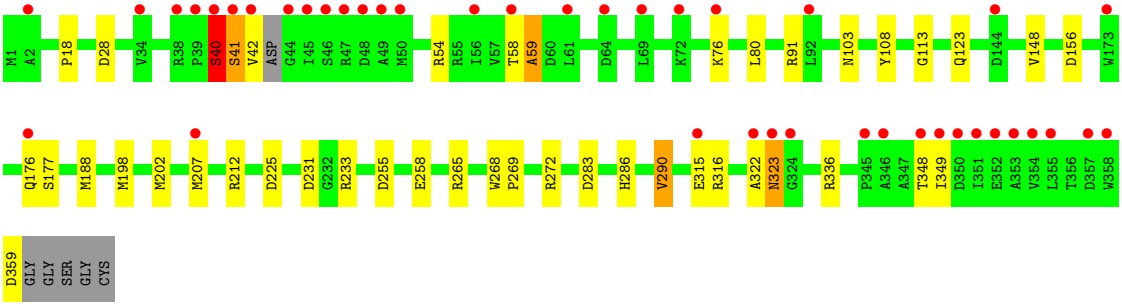






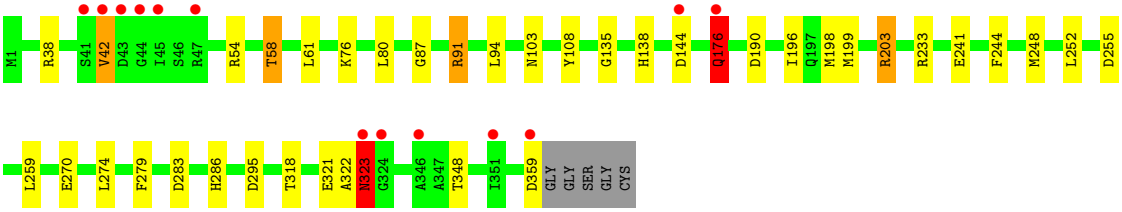
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain H:



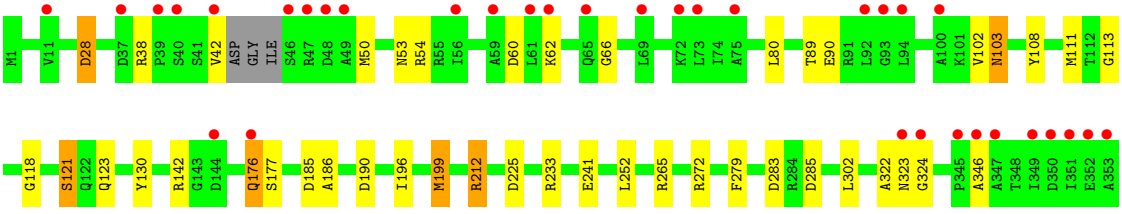
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain I:



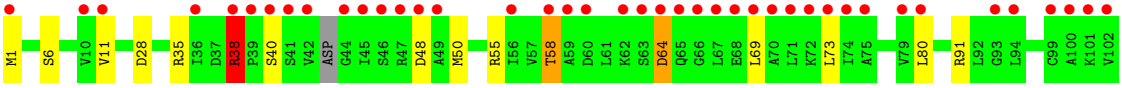
• Molecule 1: Alpha-methylacyl-CoA racemase

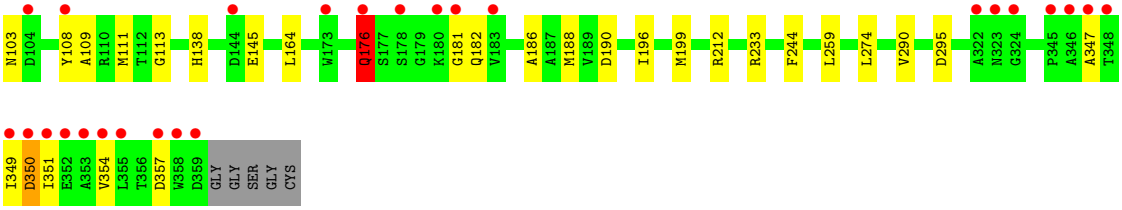
Chain J:



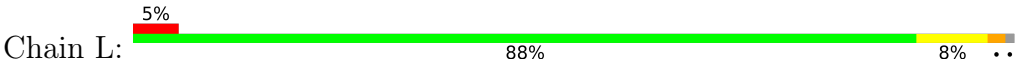
• Molecule 1: Alpha-methylacyl-CoA racemase

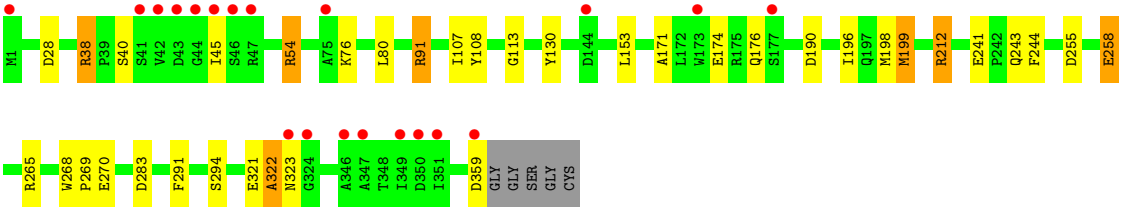
Chain K:





• Molecule 1: Alpha-methylacyl-CoA racemase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	276.31Å 276.31Å 390.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.59 – 2.08 225.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.59-2.08) 99.9 (225.59-2.08)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.201 , 0.233 0.212 , 0.241	Depositor DCC
R_{free} test set	22342 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.008 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35020	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO8

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	0.65	0/2791	1.18	16/3797 (0.4%)
1	B	0.66	0/2782	1.16	11/3785 (0.3%)
1	C	0.64	0/2791	1.19	11/3797 (0.3%)
1	D	0.65	0/2782	1.19	12/3785 (0.3%)
1	E	0.66	0/2770	1.15	9/3767 (0.2%)
1	F	0.65	0/2791	1.16	6/3797 (0.2%)
1	G	0.65	0/2800	1.21	14/3809 (0.4%)
1	H	0.66	0/2782	1.18	10/3783 (0.3%)
1	I	0.67	0/2791	1.16	12/3797 (0.3%)
1	J	0.66	0/2761	1.19	13/3755 (0.3%)
1	K	0.66	0/2782	1.19	9/3783 (0.2%)
1	L	0.66	0/2791	1.15	8/3797 (0.2%)
All	All	0.66	0/33414	1.18	131/45452 (0.3%)

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
1	B	0	4
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	6
1	G	0	3
1	H	0	4
1	I	0	2
1	J	0	2
1	K	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	5
All	All	0	37

There are no bond length outliers.

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	123	GLN	CB-CA-C	10.30	126.63	109.84
1	K	58	THR	CA-CB-OG1	-10.14	94.39	109.60
1	B	203	ARG	N-CA-CB	9.26	123.87	110.16
1	D	203	ARG	CB-CA-C	-8.92	95.98	110.79
1	B	203	ARG	CB-CA-C	-8.78	95.93	110.85
1	L	38	ARG	N-CA-CB	-8.64	97.95	110.14
1	J	123	GLN	N-CA-CB	-8.48	96.80	109.95
1	A	203	ARG	CB-CA-C	-8.47	96.73	110.79
1	A	258	GLU	CB-CA-C	-8.12	94.13	109.72
1	C	203	ARG	CB-CA-C	-8.09	97.11	110.85
1	H	265	ARG	NE-CZ-NH2	8.03	126.43	119.20
1	A	258	GLU	N-CA-CB	7.73	122.60	110.46
1	I	255	ASP	CB-CA-C	7.63	122.55	110.19
1	L	190	ASP	CA-CB-CG	7.57	120.17	112.60
1	C	203	ARG	N-CA-CB	7.57	121.37	110.16
1	A	203	ARG	N-CA-CB	7.54	121.20	110.12
1	D	58	THR	CA-CB-OG1	-7.47	98.40	109.60
1	A	91	ARG	CB-CA-C	-7.37	95.75	110.42
1	I	91	ARG	CB-CA-C	-7.34	96.58	110.67
1	J	265	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	G	91	ARG	N-CA-CB	7.27	122.45	110.39
1	C	38	ARG	CB-CA-C	-7.25	97.59	109.27
1	E	283	ASP	CB-CA-C	-7.21	94.89	109.68
1	L	38	ARG	CB-CA-C	7.20	119.85	109.26
1	J	185	ASP	CA-CB-CG	7.18	119.78	112.60
1	G	91	ARG	CB-CA-C	-7.15	95.37	110.31
1	B	255	ASP	CB-CA-C	7.04	121.98	110.22
1	H	123	GLN	CB-CA-C	7.00	121.25	109.84
1	K	64	ASP	CB-CA-C	6.95	121.03	109.56
1	D	283	ASP	CB-CA-C	6.86	123.48	110.51
1	K	350	ASP	CB-CA-C	6.86	121.92	109.37
1	B	190	ASP	CA-CB-CG	6.81	119.41	112.60
1	D	265	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	43	ASP	CB-CA-C	-6.64	103.20	111.43
1	I	38	ARG	CB-CA-C	-6.59	98.66	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	203	ARG	N-CA-CB	6.51	119.69	110.12
1	B	38	ARG	CB-CA-C	6.49	117.70	108.68
1	E	176	GLN	N-CA-CB	6.49	120.21	110.22
1	K	38	ARG	N-CA-CB	6.47	119.56	110.11
1	D	265	ARG	CD-NE-CZ	6.44	133.41	124.40
1	G	58	THR	CA-CB-OG1	-6.43	99.95	109.60
1	K	212	ARG	CB-CA-C	6.41	120.37	109.53
1	J	285	ASP	CB-CA-C	6.41	122.97	110.67
1	A	28	ASP	CA-CB-CG	6.38	118.98	112.60
1	I	190	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	190	ASP	CA-CB-CG	6.34	118.94	112.60
1	I	248	MET	CG-SD-CE	6.29	114.73	100.90
1	C	176	GLN	N-CA-CB	6.27	119.44	110.16
1	L	91	ARG	CB-CA-C	-6.27	100.02	110.68
1	H	28	ASP	CA-CB-CG	6.27	118.87	112.60
1	H	255	ASP	CB-CA-C	6.25	120.31	110.19
1	J	265	ARG	NE-CZ-NH1	-6.20	115.31	121.50
1	C	42	VAL	N-CA-CB	6.19	121.44	111.23
1	L	283	ASP	CB-CA-C	6.17	122.04	109.76
1	E	144	ASP	CA-CB-CG	6.14	118.74	112.60
1	L	258	GLU	CB-CA-C	-6.13	99.46	110.37
1	G	283	ASP	CA-CB-CG	6.12	118.72	112.60
1	J	190	ASP	CA-CB-CG	6.10	118.70	112.60
1	G	91	ARG	CG-CD-NE	6.09	125.40	112.00
1	I	203	ARG	CB-CA-C	-6.09	100.68	110.79
1	I	58	THR	CA-CB-OG1	-6.08	100.47	109.60
1	D	28	ASP	CA-CB-CG	6.07	118.67	112.60
1	E	255	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	283	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	60	ASP	CA-CB-CG	6.04	118.64	112.60
1	L	28	ASP	CA-CB-CG	6.01	118.61	112.60
1	I	91	ARG	N-CA-CB	5.99	119.56	110.28
1	D	38	ARG	CB-CA-C	5.98	117.47	108.86
1	G	28	ASP	CA-CB-CG	5.98	118.58	112.60
1	H	265	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	J	28	ASP	CA-CB-CG	5.93	118.53	112.60
1	I	176	GLN	N-CA-CB	5.87	118.85	110.16
1	H	258	GLU	CB-CA-C	-5.85	99.48	110.01
1	E	28	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	54	ARG	N-CA-CB	-5.84	100.67	111.13
1	G	207	MET	CG-SD-CE	5.83	113.73	100.90
1	H	123	GLN	N-CA-CB	-5.83	100.92	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	265	ARG	CD-NE-CZ	5.82	132.55	124.40
1	G	144	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	306	GLU	CB-CA-C	-5.80	99.56	109.65
1	G	54	ARG	N-CA-CB	-5.79	100.75	111.53
1	F	350	ASP	CB-CA-C	5.77	119.28	109.53
1	E	91	ARG	CB-CA-C	-5.74	101.09	110.85
1	G	293	ASN	CA-CB-CG	5.69	118.29	112.60
1	C	68	GLU	CB-CA-C	5.65	119.13	109.24
1	B	299	THR	OG1-CB-CG2	-5.65	98.00	109.30
1	I	144	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	163	PHE	CA-CB-CG	-5.62	108.18	113.80
1	F	91	ARG	CB-CA-C	-5.62	99.89	110.67
1	I	318	THR	CA-CB-OG1	-5.61	101.19	109.60
1	J	265	ARG	CA-CB-CG	-5.60	102.90	114.10
1	F	190	ASP	CA-CB-CG	5.59	118.19	112.60
1	J	283	ASP	CA-CB-CG	5.57	118.17	112.60
1	H	148	VAL	CA-C-O	5.57	123.16	119.38
1	C	258	GLU	CB-CA-C	-5.55	101.18	110.56
1	A	38	ARG	CB-CA-C	5.53	117.41	109.11
1	J	38	ARG	CB-CA-C	5.51	116.80	108.86
1	A	248	MET	CG-SD-CE	5.47	112.93	100.90
1	D	306	GLU	CB-CA-C	-5.46	100.16	109.65
1	F	38	ARG	CB-CA-C	-5.45	100.87	109.42
1	B	54	ARG	CB-CA-C	-5.43	97.51	109.56
1	A	147	PRO	CA-C-N	-5.42	118.61	123.33
1	A	147	PRO	C-N-CA	-5.42	118.61	123.33
1	B	218	ASP	CA-CB-CG	5.40	118.00	112.60
1	I	283	ASP	CB-CA-C	5.40	121.58	110.40
1	K	190	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	285	ASP	CB-CA-C	5.38	120.99	110.67
1	F	211	THR	CA-CB-OG1	-5.37	101.54	109.60
1	J	265	ARG	CD-NE-CZ	5.37	131.92	124.40
1	G	306	GLU	CB-CA-C	-5.37	100.31	109.65
1	B	248	MET	CG-SD-CE	5.35	112.68	100.90
1	D	85	ARG	CD-NE-CZ	5.35	131.89	124.40
1	H	91	ARG	CB-CA-C	-5.34	100.42	110.67
1	G	99	CYS	CB-CA-C	5.32	119.89	110.85
1	J	54	ARG	CB-CA-C	-5.30	98.40	110.07
1	A	55	ARG	CB-CA-C	5.30	118.49	109.75
1	L	54	ARG	CB-CA-C	-5.29	98.95	109.79
1	K	28	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	290	VAL	N-CA-CB	-5.24	103.92	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	146	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	258	GLU	CB-CA-C	-5.19	100.26	110.11
1	B	144	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	265	ARG	CD-NE-CZ	5.15	131.61	124.40
1	E	91	ARG	N-CA-CB	5.14	117.77	110.16
1	E	255	ASP	CB-CA-C	5.14	118.53	110.19
1	K	176	GLN	N-CA-CB	5.12	119.03	110.32
1	G	146	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	C	28	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	283	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	283	ASP	CA-CB-CG	5.03	117.63	112.60
1	K	145	GLU	CB-CG-CD	-5.03	104.05	112.60

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	322	ALA	Peptide
1	B	35	ARG	Sidechain
1	B	85	ARG	Sidechain
1	C	54	ARG	Peptide
1	C	91	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	85	ARG	Sidechain
1	E	54	ARG	Peptide
1	F	110	ARG	Sidechain
1	F	212	ARG	Sidechain
1	F	233	ARG	Sidechain
1	F	54	ARG	Peptide
1	F	85	ARG	Sidechain
1	F	91	ARG	Sidechain
1	G	346	ALA	Peptide
1	G	91	ARG	Sidechain
1	G	96	PRO	Peptide
1	H	212	ARG	Sidechain
1	H	233	ARG	Sidechain
1	H	323	ASN	Peptide
1	H	54	ARG	Peptide
1	I	233	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	54	ARG	Peptide
1	J	212	ARG	Sidechain
1	J	233	ARG	Sidechain
1	K	233	ARG	Sidechain
1	K	35	ARG	Sidechain
1	K	38	ARG	Sidechain
1	K	91	ARG	Sidechain
1	L	212	ARG	Sidechain
1	L	265	ARG	Sidechain
1	L	322	ALA	Peptide
1	L	54	ARG	Peptide
1	L	91	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	2718	0	2658	21	0
1	B	2715	0	2660	23	0
1	C	2718	0	2658	23	0
1	D	2715	0	2660	19	0
1	E	2698	0	2639	22	0
1	F	2724	0	2667	27	0
1	G	2727	0	2665	31	0
1	H	2713	0	2663	21	0
1	I	2718	0	2658	17	0
1	J	2695	0	2641	20	0
1	K	2710	0	2653	24	0
1	L	2721	0	2668	14	0
2	A	57	0	46	0	0
2	B	57	0	46	5	0
2	C	57	0	46	3	0
2	D	57	0	46	2	0
2	E	57	0	46	2	0
2	F	57	0	46	2	0
2	G	57	0	46	9	0
2	H	57	0	46	1	0
2	I	57	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	57	0	46	1	0
2	K	57	0	46	0	0
2	L	57	0	46	0	0
3	A	149	0	0	1	0
3	B	146	0	0	2	0
3	C	147	0	0	2	0
3	D	153	0	0	3	0
3	E	133	0	0	2	0
3	F	139	0	0	4	0
3	G	128	0	0	3	0
3	H	134	0	0	1	0
3	I	166	0	0	4	0
3	J	162	0	0	1	0
3	K	151	0	0	4	0
3	L	156	0	0	2	0
All	All	35020	0	32442	238	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 4.

All (238) 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:F:85:ARG:HD3	2:F:401:CO8:O1A	1.66	0.96
1:C:118:GLY:O	1:C:121:SER:OG	1.94	0.83
1:I:286:HIS:ND1	3:I:502:HOH:O	2.18	0.77
1:C:41:SER:O	1:C:42:VAL:HG23	1.85	0.76
1:D:85:ARG:HD3	2:D:401:CO8:O1A	1.85	0.75
1:D:40:SER:OG	3:D:501:HOH:O	2.06	0.73
1:C:41:SER:O	1:C:42:VAL:CG2	2.40	0.70
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.73	0.70
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.27	0.70
1:J:346:ALA:HB3	3:J:546:HOH:O	1.93	0.69
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.08	0.69
1:G:50:MET:HE1	1:H:198:MET:HB2	1.74	0.68
1:F:80:LEU:HD23	1:F:108:TYR:CE2	2.29	0.68
1:D:346:ALA:HB3	3:D:509:HOH:O	1.93	0.68
1:G:80:LEU:HD23	1:G:108:TYR:CE2	2.29	0.67
1:K:176:GLN:OE1	1:L:176:GLN:HG2	1.95	0.67
1:I:323:ASN:OD1	1:I:323:ASN:N	2.28	0.66
2:I:401:CO8:O4A	3:I:501:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:322:ALA:O	1:J:324:GLY:N	2.29	0.66
1:A:42:VAL:HG21	1:A:58:THR:HG21	1.77	0.65
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.79	0.65
1:D:1:MET:O	1:D:6:SER:OG	2.14	0.65
1:G:58:THR:O	1:G:59:ALA:HB2	1.96	0.65
1:F:118:GLY:O	1:F:121:SER:OG	2.15	0.64
1:G:358:TRP:O	1:G:359:ASP:HB2	1.97	0.63
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.33	0.63
1:H:76:LYS:NZ	1:H:359:ASP:C	2.57	0.63
1:K:138:HIS:HD2	3:K:536:HOH:O	1.82	0.62
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.34	0.62
1:E:336:ARG:HG2	1:E:336:ARG:HH11	1.65	0.61
1:G:156:ASP:OD2	2:G:401:CO8:H3'1	2.01	0.61
1:C:138:HIS:HD2	3:C:549:HOH:O	1.84	0.61
1:D:85:ARG:CD	2:D:401:CO8:O1A	2.48	0.61
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.84	0.61
2:B:401:CO8:O7A	3:B:501:HOH:O	2.17	0.60
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.38	0.59
1:A:216:MET:HE1	2:B:401:CO8:H7'2	1.85	0.58
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.36	0.57
1:L:291:PHE:O	1:L:294:SER:HB3	2.05	0.57
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.30	0.57
1:I:198:MET:HB2	1:J:50:MET:HE1	1.87	0.57
1:E:259:LEU:HD22	1:E:274:LEU:HD13	1.87	0.56
1:G:346:ALA:HB3	3:G:504:HOH:O	2.06	0.56
1:I:322:ALA:O	1:I:323:ASN:C	2.49	0.55
1:F:322:ALA:O	1:F:324:GLY:N	2.39	0.55
1:G:85:ARG:NH1	1:G:122:GLN:O	2.38	0.55
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.90	0.55
1:I:270:GLU:HG3	3:I:583:HOH:O	2.07	0.55
1:C:50:MET:HE1	1:D:198:MET:HB2	1.88	0.55
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.87	0.55
1:G:176:GLN:HE21	1:G:176:GLN:HA	1.71	0.55
1:H:76:LYS:HZ3	1:H:359:ASP:C	2.15	0.55
2:G:401:CO8:O5P	2:G:401:CO8:C2P	2.56	0.54
1:F:346:ALA:HB3	3:F:581:HOH:O	2.08	0.54
1:E:91:ARG:NH2	2:E:401:CO8:O9A	2.41	0.54
1:C:322:ALA:O	1:C:323:ASN:C	2.50	0.53
1:F:85:ARG:CD	2:F:401:CO8:O1A	2.50	0.52
1:A:138:HIS:HD2	3:A:550:HOH:O	1.93	0.52
1:G:39:PRO:HB3	1:G:58:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HB2	1:B:50:MET:HE1	1.92	0.52
1:K:55:ARG:HG2	1:K:349:ILE:HD12	1.92	0.52
1:C:38:ARG:NH2	2:C:401:CO8:O4B	2.43	0.52
1:B:244:PHE:HB3	1:B:295:ASP:O	2.10	0.51
1:E:80:LEU:CD2	1:E:108:TYR:CE2	2.93	0.51
1:C:88:VAL:HG13	2:C:401:CO8:H3B	1.93	0.51
1:E:196:ILE:HG12	1:E:199:MET:HB2	1.92	0.51
1:J:118:GLY:O	1:J:121:SER:OG	2.21	0.51
1:J:111:MET:HE3	1:J:186:ALA:O	2.11	0.51
1:D:39:PRO:O	1:D:42:VAL:HG12	2.11	0.50
1:F:40:SER:O	1:F:41:SER:CB	2.58	0.50
1:J:102:VAL:O	1:J:103:ASN:HB2	2.11	0.50
1:A:50:MET:HE1	1:B:198:MET:HB2	1.91	0.50
1:K:113:GLY:CA	1:K:188:MET:HE3	2.42	0.50
2:J:401:CO8:O9P	2:J:401:CO8:H131	2.12	0.50
1:D:76:LYS:HE2	1:D:359:ASP:C	2.37	0.50
1:G:126:HIS:ND1	2:G:401:CO8:H4'2	2.27	0.50
1:I:196:ILE:HG12	1:I:199:MET:HB2	1.93	0.49
1:K:48:ASP:OD2	3:K:501:HOH:O	2.19	0.49
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.94	0.49
1:I:138:HIS:HD2	3:I:527:HOH:O	1.95	0.49
1:G:16:ILE:HG13	2:G:401:CO8:H21	1.93	0.49
1:E:138:HIS:HD2	3:E:576:HOH:O	1.96	0.49
1:F:40:SER:O	1:F:41:SER:HB3	2.11	0.49
1:G:265:ARG:HD2	3:G:587:HOH:O	2.11	0.49
2:G:401:CO8:O9P	2:G:401:CO8:H141	2.12	0.49
1:J:196:ILE:HG12	1:J:199:MET:HB2	1.94	0.49
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.48	0.49
1:F:42:VAL:N	3:F:505:HOH:O	2.44	0.49
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.95	0.48
1:A:176:GLN:HG3	1:B:176:GLN:HE21	1.78	0.48
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.28	0.48
1:C:80:LEU:HD23	1:C:108:TYR:CE2	2.48	0.48
1:G:356:THR:HG22	1:G:357:ASP:N	2.28	0.48
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.46	0.48
1:E:42:VAL:HG11	1:E:348:THR:OG1	2.14	0.48
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.46	0.48
1:F:323:ASN:CG	1:F:324:GLY:N	2.71	0.48
1:I:87:GLY:O	1:I:91:ARG:HG3	2.14	0.48
1:B:85:ARG:CD	2:B:401:CO8:O1A	2.62	0.48
1:G:61:LEU:HD13	1:G:94:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.49	0.47
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.29	0.47
1:I:61:LEU:HD22	1:I:94:LEU:HD11	1.96	0.47
1:F:106:LEU:O	1:F:181:GLY:HA3	2.14	0.47
2:I:401:CO8:H8'2	1:J:241:GLU:OE2	2.14	0.47
1:B:142:ARG:O	1:B:212:ARG:HD2	2.15	0.47
1:C:135:GLY:HA2	1:D:302:LEU:O	2.15	0.47
1:F:42:VAL:HG11	1:F:348:THR:OG1	2.14	0.47
1:C:111:MET:HE3	1:C:186:ALA:O	2.15	0.47
1:K:111:MET:HE3	1:K:186:ALA:O	2.15	0.47
1:E:117:THR:O	1:F:316:ARG:HD2	2.14	0.47
1:K:64:ASP:HA	3:K:503:HOH:O	2.15	0.46
1:D:45:ILE:HD12	1:D:45:ILE:H	1.80	0.46
1:A:117:THR:O	1:B:316:ARG:HD2	2.15	0.46
1:E:358:TRP:O	1:E:359:ASP:HB2	2.14	0.46
1:H:80:LEU:HD23	1:H:108:TYR:CD2	2.50	0.46
1:G:241:GLU:HB2	1:G:244:PHE:CD2	2.51	0.46
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.51	0.46
1:G:18:PRO:HB3	1:G:156:ASP:O	2.16	0.46
1:E:302:LEU:O	1:F:135:GLY:HA2	2.16	0.46
1:H:76:LYS:HZ1	1:H:359:ASP:C	2.24	0.46
1:K:113:GLY:HA2	1:K:188:MET:HE3	1.97	0.46
1:J:28:ASP:HA	1:J:53:ASN:ND2	2.31	0.45
1:L:241:GLU:HB2	1:L:244:PHE:CD2	2.51	0.45
1:B:85:ARG:HD3	2:B:401:CO8:O1A	2.16	0.45
1:D:315:GLU:HG3	3:D:537:HOH:O	2.15	0.45
1:L:322:ALA:O	1:L:323:ASN:C	2.59	0.45
1:G:176:GLN:CD	1:H:176:GLN:HG2	2.41	0.45
1:K:196:ILE:HG13	1:L:153:LEU:HD21	1.98	0.45
1:L:107:ILE:HD12	1:L:171:ALA:HB1	1.98	0.45
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.35	0.45
1:F:142:ARG:O	1:F:212:ARG:HD2	2.16	0.45
1:E:135:GLY:HA2	1:F:302:LEU:O	2.16	0.45
1:I:176:GLN:HG3	1:J:176:GLN:HE21	1.82	0.45
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.51	0.45
1:K:55:ARG:HD2	1:K:349:ILE:HD13	1.99	0.45
1:J:60:ASP:O	1:J:66:GLY:HA3	2.17	0.45
1:K:80:LEU:HD23	1:K:108:TYR:CE1	2.52	0.45
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.97	0.45
1:L:270:GLU:HG3	3:L:566:HOH:O	2.16	0.45
1:A:295:ASP:CG	1:B:85:ARG:HH22	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.50	0.45
1:G:156:ASP:OD1	2:G:401:CO8:H2'1	2.17	0.45
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.53	0.44
1:F:105:ARG:NH1	3:F:506:HOH:O	2.45	0.44
1:D:78:ASP:OD1	1:D:175:ARG:NH2	2.37	0.44
1:K:73:LEU:HD21	1:K:354:VAL:CG1	2.47	0.44
1:I:252:LEU:HD21	1:I:279:PHE:CE1	2.53	0.44
1:B:241:GLU:HB2	1:B:244:PHE:CD2	2.53	0.44
1:E:109:ALA:HB1	1:E:164:LEU:HD11	2.00	0.44
1:A:141:GLY:HA2	1:B:148:VAL:HG21	1.99	0.44
1:C:85:ARG:NH1	1:C:122:GLN:O	2.46	0.44
1:A:87:GLY:O	1:A:91:ARG:HG3	2.17	0.44
1:C:88:VAL:CG1	2:C:401:CO8:H3B	2.48	0.44
1:H:202:MET:HG2	1:H:207:MET:HE2	1.99	0.44
1:K:69:LEU:HB3	1:K:351:ILE:HD13	1.99	0.44
1:B:41:SER:O	1:B:42:VAL:HG23	2.18	0.44
1:I:135:GLY:HA2	1:J:302:LEU:O	2.17	0.44
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.52	0.43
1:C:80:LEU:HD22	1:C:108:TYR:CE2	2.51	0.43
1:H:58:THR:O	1:H:59:ALA:HB2	2.19	0.43
1:H:322:ALA:O	1:H:323:ASN:C	2.60	0.43
1:L:268:TRP:N	1:L:269:PRO:CD	2.81	0.43
1:B:80:LEU:CD2	1:B:108:TYR:CE2	3.01	0.43
1:E:11:VAL:O	1:E:80:LEU:HA	2.18	0.43
1:E:316:ARG:HD2	1:F:117:THR:O	2.19	0.43
1:F:263:ASN:ND2	3:F:515:HOH:O	2.52	0.43
1:I:241:GLU:HB2	1:I:244:PHE:CD2	2.53	0.43
1:K:109:ALA:HB1	1:K:164:LEU:HD11	2.00	0.43
1:E:336:ARG:HG2	1:E:336:ARG:NH1	2.33	0.43
1:I:259:LEU:HD22	1:I:274:LEU:HD13	2.00	0.43
1:K:181:GLY:O	1:K:182:GLN:HB3	2.18	0.43
1:A:196:ILE:HG12	1:A:199:MET:HB2	2.01	0.43
1:D:61:LEU:HD22	1:D:94:LEU:HD11	1.99	0.43
1:H:231:ASP:CG	1:H:283:ASP:HB2	2.44	0.43
2:I:401:CO8:H2'1	2:I:401:CO8:H21	1.89	0.43
1:B:245:TYR:CE2	1:B:249:LEU:HD11	2.54	0.43
1:K:1:MET:O	1:K:6:SER:OG	2.27	0.43
1:K:11:VAL:HG12	1:K:80:LEU:HD12	1.99	0.43
1:A:135:GLY:HA2	1:B:302:LEU:O	2.19	0.43
1:D:329:MET:HE3	1:D:330:PRO:HD2	2.00	0.43
1:G:113:GLY:HA3	1:G:130:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:196:ILE:HG12	1:K:199:MET:HB2	2.01	0.43
1:L:243[B]:GLN:HG2	3:L:602:HOH:O	2.18	0.43
1:E:335:SER:OG	1:F:183:VAL:HB	2.19	0.43
1:J:142:ARG:O	1:J:212:ARG:HD2	2.19	0.43
1:L:113:GLY:HA3	1:L:130:TYR:CE1	2.54	0.43
1:B:85:ARG:NH1	2:B:401:CO8:O5A	2.52	0.42
1:F:196:ILE:HG12	1:F:199:MET:HB2	2.01	0.42
1:G:127:ASP:H	2:G:401:CO8:C2'	2.31	0.42
1:C:10:VAL:HB	1:C:33:VAL:HG22	2.00	0.42
1:G:76:LYS:NZ	1:G:359:ASP:HB3	2.34	0.42
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.54	0.42
1:C:259:LEU:CD2	1:C:274:LEU:HD13	2.49	0.42
1:J:111:MET:HE3	1:J:111:MET:HA	2.02	0.42
1:K:50:MET:HE1	1:L:198:MET:HB2	2.01	0.42
1:A:68:GLU:OE2	1:A:72:LYS:HE3	2.20	0.42
1:A:140:ILE:CD1	1:B:151:LEU:HG	2.49	0.42
1:L:174:GLU:OE1	1:L:174:GLU:C	2.62	0.42
1:E:50:MET:CE	1:F:198:MET:HB2	2.50	0.42
1:G:117:THR:O	1:H:316:ARG:HD2	2.20	0.42
1:K:73:LEU:HD21	1:K:354:VAL:HG12	2.00	0.42
1:E:123:GLN:NE2	1:F:292:ALA:O	2.53	0.42
2:E:401:CO8:O9P	2:E:401:CO8:H131	2.19	0.42
1:F:293:ASN:HB2	1:G:290:VAL:O	2.19	0.42
1:E:272:ARG:NH1	3:E:509:HOH:O	2.51	0.42
1:I:244:PHE:HB3	1:I:295:ASP:O	2.19	0.41
1:C:259:LEU:HD22	1:C:274:LEU:HD13	2.02	0.41
1:C:346:ALA:HB3	3:C:514:HOH:O	2.19	0.41
1:F:80:LEU:HD23	1:F:108:TYR:CD2	2.54	0.41
1:K:69:LEU:HD13	1:K:351:ILE:HG21	2.02	0.41
1:G:55:ARG:HA	3:G:504:HOH:O	2.20	0.41
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.86	0.41
1:A:225:ASP:OD2	1:A:272:ARG:NH1	2.53	0.41
1:G:28:ASP:HA	1:G:53:ASN:HD22	1.86	0.41
1:G:126:HIS:HB3	2:G:401:CO8:H2'2	2.01	0.41
1:G:127:ASP:H	2:G:401:CO8:H2'1	1.85	0.41
1:J:80:LEU:CD2	1:J:108:TYR:CE2	3.04	0.41
1:A:109:ALA:HB1	1:A:164:LEU:HD11	2.03	0.41
1:A:303:ALA:O	1:A:304:PHE:C	2.63	0.41
1:C:89:THR:O	1:C:90:GLU:C	2.63	0.41
1:E:9:ARG:NH2	1:E:358:TRP:HA	2.35	0.41
1:H:18:PRO:HB3	1:H:156:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:GLY:HA2	1:H:188:MET:HB2	2.03	0.41
1:H:286:HIS:CE1	1:H:290:VAL:HG21	2.56	0.41
1:D:336:ARG:HG2	1:D:336:ARG:HH11	1.85	0.41
1:G:180:LYS:HB2	1:H:336:ARG:NH2	2.36	0.41
1:K:244:PHE:HB3	1:K:295:ASP:O	2.21	0.41
1:D:37:ASP:O	1:D:58:THR:HA	2.20	0.40
1:D:322:ALA:O	1:D:323:ASN:C	2.64	0.40
1:J:89:THR:O	1:J:90:GLU:C	2.63	0.40
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.54	0.40
1:K:50:MET:HB3	3:K:501:HOH:O	2.20	0.40
1:B:286:HIS:HE1	3:B:637:HOH:O	2.05	0.40
1:H:268:TRP:N	1:H:269:PRO:CD	2.84	0.40
1:H:40:SER:O	1:H:41:SER:CB	2.70	0.40
2:H:401:CO8:OAP	3:H:501:HOH:O	2.22	0.40
1:J:252:LEU:HD21	1:J:279:PHE:CE1	2.57	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	359/364 (99%)	341 (95%)	16 (4%)	2 (1%)	22	18
1	B	358/364 (98%)	343 (96%)	10 (3%)	5 (1%)	9	5
1	C	359/364 (99%)	339 (94%)	18 (5%)	2 (1%)	22	18
1	D	358/364 (98%)	337 (94%)	20 (6%)	1 (0%)	37	36
1	E	354/364 (97%)	336 (95%)	15 (4%)	3 (1%)	16	12
1	F	359/364 (99%)	338 (94%)	15 (4%)	6 (2%)	7	3
1	G	360/364 (99%)	342 (95%)	15 (4%)	3 (1%)	16	12
1	H	356/364 (98%)	338 (95%)	13 (4%)	5 (1%)	9	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	359/364 (99%)	345 (96%)	11 (3%)	3 (1%)	16 12
1	J	353/364 (97%)	339 (96%)	12 (3%)	2 (1%)	22 18
1	K	356/364 (98%)	333 (94%)	21 (6%)	2 (1%)	22 18
1	L	359/364 (99%)	343 (96%)	16 (4%)	0	100 100
All	All	4290/4368 (98%)	4074 (95%)	182 (4%)	34 (1%)	16 12

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	VAL
1	F	41	SER
1	G	97	GLU
1	H	40	SER
1	H	41	SER
1	J	103	ASN
1	J	323	ASN
1	B	42	VAL
1	E	348	THR
1	F	323	ASN
1	G	59	ALA
1	K	103	ASN
1	K	347	ALA
1	A	103	ASN
1	B	103	ASN
1	B	323	ASN
1	C	103	ASN
1	E	41	SER
1	E	103	ASN
1	F	103	ASN
1	H	59	ALA
1	I	323	ASN
1	B	151	LEU
1	G	103	ASN
1	H	103	ASN
1	H	348	THR
1	D	103	ASN
1	I	103	ASN
1	B	59	ALA
1	F	292	ALA
1	A	290	VAL
1	I	42	VAL

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Mol	Chain	Res	Type
1	F	42	VAL
1	F	95	GLY

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	277/277 (100%)	269 (97%)	8 (3%)	37	40
1	B	276/277 (100%)	270 (98%)	6 (2%)	47	51
1	C	277/277 (100%)	267 (96%)	10 (4%)	30	31
1	D	276/277 (100%)	268 (97%)	8 (3%)	37	40
1	E	275/277 (99%)	265 (96%)	10 (4%)	30	31
1	F	277/277 (100%)	267 (96%)	10 (4%)	30	31
1	G	278/277 (100%)	268 (96%)	10 (4%)	30	31
1	H	276/277 (100%)	270 (98%)	6 (2%)	47	51
1	I	277/277 (100%)	268 (97%)	9 (3%)	34	36
1	J	274/277 (99%)	267 (97%)	7 (3%)	41	44
1	K	276/277 (100%)	269 (98%)	7 (2%)	42	46
1	L	277/277 (100%)	267 (96%)	10 (4%)	30	31
All	All	3316/3324 (100%)	3215 (97%)	101 (3%)	35	38

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	54	ARG
1	A	133	LEU
1	A	199	MET
1	A	258	GLU
1	A	348	THR
1	A	349	ILE
1	A	350	ASP

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Mol	Chain	Res	Type
1	B	6	SER
1	B	42	VAL
1	B	85	ARG
1	B	148	VAL
1	B	177	SER
1	B	351	ILE
1	C	6	SER
1	C	40	SER
1	C	41	SER
1	C	54	ARG
1	C	62	LYS
1	C	63	SER
1	C	68	GLU
1	C	121	SER
1	C	176	GLN
1	C	265	ARG
1	D	6	SER
1	D	40	SER
1	D	41	SER
1	D	85	ARG
1	D	199	MET
1	D	255	ASP
1	D	269	PRO
1	D	323	ASN
1	E	6	SER
1	E	58	THR
1	E	68	GLU
1	E	80	LEU
1	E	243	GLN
1	E	265	ARG
1	E	290	VAL
1	E	349	ILE
1	E	350	ASP
1	E	352	GLU
1	F	6	SER
1	F	45	ILE
1	F	56	ILE
1	F	85	ARG
1	F	121	SER
1	F	176	GLN
1	F	199	MET
1	F	277	GLU

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Mol	Chain	Res	Type
1	F	323	ASN
1	F	349	ILE
1	G	6	SER
1	G	40	SER
1	G	54	ARG
1	G	58	THR
1	G	68	GLU
1	G	140	ILE
1	G	323	ASN
1	G	348	THR
1	G	356	THR
1	G	359	ASP
1	H	40	SER
1	H	42	VAL
1	H	177	SER
1	H	290	VAL
1	H	315	GLU
1	H	349	ILE
1	I	42	VAL
1	I	58	THR
1	I	76	LYS
1	I	176	GLN
1	I	203	ARG
1	I	321	GLU
1	I	323	ASN
1	I	348	THR
1	I	359	ASP
1	J	42	VAL
1	J	62	LYS
1	J	121	SER
1	J	176	GLN
1	J	177	SER
1	J	199	MET
1	J	357	ASP
1	K	38	ARG
1	K	40	SER
1	K	58	THR
1	K	176	GLN
1	K	290	VAL
1	K	350	ASP
1	K	357	ASP
1	L	38	ARG

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Mol	Chain	Res	Type
1	L	40	SER
1	L	45	ILE
1	L	76	LYS
1	L	199	MET
1	L	212	ARG
1	L	255	ASP
1	L	258	GLU
1	L	321	GLU
1	L	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	138	HIS
1	A	176	GLN
1	A	263	ASN
1	A	323	ASN
1	A	327	GLN
1	B	176	GLN
1	B	282	HIS
1	B	286	HIS
1	C	138	HIS
1	C	176	GLN
1	C	263	ASN
1	C	327	GLN
1	D	282	HIS
1	D	308	HIS
1	D	323	ASN
1	E	116	GLN
1	E	138	HIS
1	E	243	GLN
1	E	263	ASN
1	E	293	ASN
1	E	323	ASN
1	E	327	GLN
1	F	122	GLN
1	F	293	ASN
1	G	138	HIS
1	G	176	GLN
1	G	263	ASN
1	G	282	HIS

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Mol	Chain	Res	Type
1	G	286	HIS
1	G	323	ASN
1	G	327	GLN
1	H	176	GLN
1	H	282	HIS
1	H	286	HIS
1	I	122	GLN
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	282	HIS
1	I	327	GLN
1	J	176	GLN
1	J	282	HIS
1	J	286	HIS
1	K	116	GLN
1	K	138	HIS
1	K	327	GLN
1	L	122	GLN
1	L	282	HIS
1	L	323	ASN
1	L	341	GLN

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

12 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	$\#\|Z\| > 2$
2	CO8	I	401	-	51,59,59	1.61	3 (5%)	62,85,85	1.55	5 (8%)
2	CO8	K	401	-	51,59,59	1.58	3 (5%)	62,85,85	1.77	11 (17%)
2	CO8	A	401	-	51,59,59	1.52	3 (5%)	62,85,85	1.69	7 (11%)
2	CO8	G	401	-	51,59,59	1.20	2 (3%)	62,85,85	2.42	14 (22%)
2	CO8	C	401	-	51,59,59	1.48	3 (5%)	62,85,85	1.65	10 (16%)
2	CO8	L	401	-	51,59,59	1.65	3 (5%)	62,85,85	1.58	5 (8%)
2	CO8	E	401	-	51,59,59	1.54	3 (5%)	62,85,85	1.46	6 (9%)
2	CO8	F	401	-	51,59,59	1.03	3 (5%)	62,85,85	1.65	8 (12%)
2	CO8	J	401	-	51,59,59	1.03	3 (5%)	62,85,85	2.06	12 (19%)
2	CO8	D	401	-	51,59,59	1.01	4 (7%)	62,85,85	1.70	7 (11%)
2	CO8	B	401	-	51,59,59	1.70	3 (5%)	62,85,85	1.66	7 (11%)
2	CO8	H	401	-	51,59,59	1.62	3 (5%)	62,85,85	2.05	10 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CO8	I	401	-	-	7/54/74/74	0/3/3/3
2	CO8	K	401	-	-	8/54/74/74	0/3/3/3
2	CO8	A	401	-	-	9/54/74/74	0/3/3/3
2	CO8	G	401	-	-	16/54/74/74	0/3/3/3
2	CO8	C	401	-	-	13/54/74/74	0/3/3/3
2	CO8	L	401	-	-	10/54/74/74	0/3/3/3
2	CO8	E	401	-	-	12/54/74/74	0/3/3/3
2	CO8	F	401	-	-	9/54/74/74	0/3/3/3
2	CO8	J	401	-	-	18/54/74/74	0/3/3/3
2	CO8	D	401	-	-	9/54/74/74	0/3/3/3
2	CO8	B	401	-	-	12/54/74/74	0/3/3/3
2	CO8	H	401	-	-	13/54/74/74	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	CO8	C1'-S1P	9.30	1.98	1.76
2	B	401	CO8	C1'-S1P	9.08	1.98	1.76
2	I	401	CO8	C1'-S1P	9.06	1.98	1.76
2	H	401	CO8	C1'-S1P	8.86	1.97	1.76
2	E	401	CO8	C1'-S1P	8.64	1.97	1.76
2	K	401	CO8	C1'-S1P	8.57	1.97	1.76
2	A	401	CO8	C1'-S1P	8.43	1.96	1.76
2	C	401	CO8	C1'-S1P	7.70	1.94	1.76
2	B	401	CO8	O1'-C1'	5.21	1.29	1.21
2	G	401	CO8	C2'-C1'	4.99	1.55	1.50
2	I	401	CO8	O1'-C1'	4.95	1.29	1.21
2	L	401	CO8	O1'-C1'	4.92	1.29	1.21
2	H	401	CO8	O1'-C1'	4.83	1.28	1.21
2	A	401	CO8	O1'-C1'	4.71	1.28	1.21
2	K	401	CO8	O1'-C1'	4.65	1.28	1.21
2	E	401	CO8	O1'-C1'	4.49	1.28	1.21
2	G	401	CO8	O1'-C1'	4.29	1.28	1.21
2	C	401	CO8	O1'-C1'	4.25	1.27	1.21
2	J	401	CO8	C1'-S1P	3.79	1.85	1.76
2	F	401	CO8	C1'-S1P	3.75	1.85	1.76
2	D	401	CO8	C1'-S1P	3.31	1.84	1.76
2	B	401	CO8	C2'-C1'	2.94	1.53	1.50
2	J	401	CO8	C2'-C1'	2.93	1.53	1.50
2	H	401	CO8	C2'-C1'	2.69	1.53	1.50
2	F	401	CO8	O1'-C1'	2.58	1.25	1.21
2	E	401	CO8	C2'-C1'	2.54	1.53	1.50
2	K	401	CO8	C2'-C1'	2.43	1.53	1.50
2	D	401	CO8	C2P-C3P	2.41	1.61	1.51
2	I	401	CO8	C2'-C1'	2.34	1.53	1.50
2	C	401	CO8	C2'-C1'	2.30	1.53	1.50
2	F	401	CO8	C2'-C1'	2.28	1.53	1.50
2	L	401	CO8	C2'-C1'	2.18	1.53	1.50
2	D	401	CO8	P3B-O3B	2.18	1.63	1.59
2	A	401	CO8	C2'-C1'	2.11	1.53	1.50
2	J	401	CO8	O1'-C1'	2.04	1.24	1.21
2	D	401	CO8	O1'-C1'	2.03	1.24	1.21

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	CO8	C2P-S1P-C1'	10.36	134.11	101.87
2	J	401	CO8	C2P-S1P-C1'	10.31	133.96	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	CO8	O1'-C1'-S1P	-10.16	109.42	122.61
2	F	401	CO8	C2P-S1P-C1'	9.11	130.23	101.87
2	G	401	CO8	C7P-C6P-C5P	-8.43	98.32	112.36
2	H	401	CO8	CDP-CBP-CCP	7.90	121.12	108.23
2	L	401	CO8	O1'-C1'-C2'	-7.38	115.27	123.99
2	G	401	CO8	C2'-C1'-S1P	6.70	121.26	113.46
2	L	401	CO8	O1'-C1'-S1P	6.67	131.28	122.61
2	I	401	CO8	O1'-C1'-C2'	-6.45	116.38	123.99
2	A	401	CO8	O1'-C1'-S1P	6.36	130.88	122.61
2	I	401	CO8	O1'-C1'-S1P	6.32	130.82	122.61
2	H	401	CO8	O1'-C1'-S1P	6.23	130.70	122.61
2	K	401	CO8	O1'-C1'-S1P	6.19	130.66	122.61
2	H	401	CO8	CEP-CBP-CCP	-6.17	98.17	108.23
2	A	401	CO8	O1'-C1'-C2'	-6.12	116.77	123.99
2	C	401	CO8	O1'-C1'-S1P	6.05	130.47	122.61
2	K	401	CO8	O1'-C1'-C2'	-5.94	116.98	123.99
2	E	401	CO8	O1'-C1'-C2'	-5.80	117.14	123.99
2	B	401	CO8	O1'-C1'-S1P	5.73	130.06	122.61
2	B	401	CO8	O1'-C1'-C2'	-5.60	117.37	123.99
2	E	401	CO8	O1'-C1'-S1P	5.60	129.89	122.61
2	J	401	CO8	C2'-C1'-S1P	5.56	119.93	113.46
2	B	401	CO8	C3P-N4P-C5P	-5.51	112.62	122.84
2	H	401	CO8	O1'-C1'-C2'	-5.46	117.54	123.99
2	C	401	CO8	O5A-P2A-O4A	5.00	136.94	112.24
2	J	401	CO8	O5A-P2A-O4A	4.76	135.77	112.24
2	H	401	CO8	O5A-P2A-O4A	4.73	135.64	112.24
2	A	401	CO8	O5A-P2A-O4A	4.57	134.82	112.24
2	K	401	CO8	O5A-P2A-O4A	4.51	134.56	112.24
2	G	401	CO8	O1'-C1'-C2'	4.25	129.00	123.99
2	H	401	CO8	O6A-P2A-O4A	-4.21	92.60	109.07
2	C	401	CO8	O1'-C1'-C2'	-4.13	119.11	123.99
2	G	401	CO8	O5A-P2A-O4A	3.99	131.95	112.24
2	F	401	CO8	O5A-P2A-O4A	3.91	131.59	112.24
2	A	401	CO8	O6A-CCP-CBP	-3.80	104.43	110.55
2	B	401	CO8	O5A-P2A-O4A	3.75	130.78	112.24
2	K	401	CO8	O6A-CCP-CBP	-3.73	104.56	110.55
2	L	401	CO8	O5A-P2A-O4A	3.67	130.38	112.24
2	G	401	CO8	O6A-P2A-O4A	-3.43	95.66	109.07
2	J	401	CO8	O6A-CCP-CBP	-3.33	105.19	110.55
2	I	401	CO8	O5A-P2A-O4A	3.33	128.68	112.24
2	E	401	CO8	O5A-P2A-O4A	3.32	128.66	112.24
2	C	401	CO8	O6A-CCP-CBP	-3.28	105.28	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	CO8	O9P-C9P-N8P	-3.26	116.00	122.99
2	F	401	CO8	OAP-CAP-CBP	-3.17	102.79	110.25
2	D	401	CO8	O5A-P2A-O4A	3.17	127.89	112.24
2	J	401	CO8	O1'-C1'-C2'	-3.16	120.25	123.99
2	K	401	CO8	O9A-P3B-O7A	2.97	122.32	110.68
2	K	401	CO8	O6A-P2A-O4A	-2.97	97.46	109.07
2	A	401	CO8	OAP-CAP-CBP	-2.96	103.29	110.25
2	E	401	CO8	O6A-CCP-CBP	-2.95	105.81	110.55
2	J	401	CO8	C5A-C6A-N6A	2.95	124.83	120.35
2	G	401	CO8	C3'-C2'-C1'	2.94	118.86	112.33
2	G	401	CO8	C6P-C7P-N8P	-2.94	105.95	111.90
2	D	401	CO8	O1'-C1'-S1P	2.91	126.39	122.61
2	K	401	CO8	C5A-C6A-N6A	2.89	124.74	120.35
2	F	401	CO8	O6A-CCP-CBP	-2.87	105.93	110.55
2	C	401	CO8	O8A-P3B-O3B	-2.86	93.17	105.99
2	J	401	CO8	OAP-CAP-CBP	-2.80	103.66	110.25
2	F	401	CO8	C5A-C6A-N6A	2.76	124.54	120.35
2	K	401	CO8	O2B-C2B-C3B	2.75	118.97	111.17
2	K	401	CO8	O8A-P3B-O7A	-2.74	99.97	110.68
2	C	401	CO8	C5A-C6A-N6A	2.70	124.46	120.35
2	E	401	CO8	C5A-C6A-N6A	2.70	124.45	120.35
2	D	401	CO8	O9A-P3B-O8A	2.68	117.87	107.64
2	E	401	CO8	C1B-N9A-C4A	-2.66	121.96	126.64
2	L	401	CO8	O9A-P3B-O8A	2.66	117.82	107.64
2	C	401	CO8	C2'-C1'-S1P	-2.61	110.42	113.46
2	C	401	CO8	O6A-P2A-O4A	-2.59	98.94	109.07
2	K	401	CO8	CEP-CBP-CCP	2.53	112.35	108.23
2	H	401	CO8	O5A-P2A-O6A	2.47	119.21	107.75
2	F	401	CO8	O6A-P2A-O4A	-2.41	99.65	109.07
2	G	401	CO8	C5A-C6A-N6A	2.40	124.00	120.35
2	H	401	CO8	C2P-S1P-C1'	2.39	109.32	101.87
2	D	401	CO8	CDP-CBP-CAP	2.38	112.95	108.82
2	G	401	CO8	O8A-P3B-O7A	2.38	120.00	110.68
2	H	401	CO8	C5A-C6A-N6A	2.38	123.97	120.35
2	J	401	CO8	O9A-P3B-O7A	2.36	119.91	110.68
2	F	401	CO8	O1'-C1'-S1P	2.35	125.67	122.61
2	C	401	CO8	CEP-CBP-CAP	2.34	112.88	108.82
2	J	401	CO8	CDP-CBP-CCP	2.31	112.00	108.23
2	K	401	CO8	O9A-P3B-O8A	2.30	116.42	107.64
2	F	401	CO8	O1'-C1'-C2'	-2.29	121.29	123.99
2	D	401	CO8	O1'-C1'-C2'	-2.25	121.33	123.99
2	J	401	CO8	C3'-C2'-C1'	2.23	117.28	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	CO8	C5A-C6A-N6A	2.22	123.72	120.35
2	J	401	CO8	O1'-C1'-S1P	-2.19	119.77	122.61
2	B	401	CO8	O2B-C2B-C1B	-2.17	102.84	110.85
2	G	401	CO8	O8A-P3B-O3B	-2.16	96.29	105.99
2	B	401	CO8	O2B-C2B-C3B	2.16	117.31	111.17
2	G	401	CO8	O6A-CCP-CBP	-2.15	107.08	110.55
2	I	401	CO8	O3B-P3B-O7A	-2.15	101.09	109.39
2	A	401	CO8	C3P-N4P-C5P	-2.15	118.85	122.84
2	G	401	CO8	C2P-S1P-C1'	-2.09	95.38	101.87
2	C	401	CO8	C3B-C2B-C1B	2.08	104.51	99.89
2	L	401	CO8	O3B-P3B-O7A	-2.06	101.45	109.39
2	J	401	CO8	O3B-C3B-C2B	2.04	119.09	111.68
2	B	401	CO8	O9A-P3B-O3B	2.04	115.14	105.99
2	A	401	CO8	CEP-CBP-CCP	-2.03	104.92	108.23
2	H	401	CO8	CEP-CBP-CAP	2.01	112.31	108.82
2	D	401	CO8	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CO8	C5B-O5B-P1A-O1A
2	A	401	CO8	C5P-C6P-C7P-N8P
2	A	401	CO8	O1'-C1'-S1P-C2P
2	A	401	CO8	C2'-C1'-S1P-C2P
2	B	401	CO8	C5B-O5B-P1A-O3A
2	B	401	CO8	C5P-C6P-C7P-N8P
2	B	401	CO8	C3P-C2P-S1P-C1'
2	B	401	CO8	O1'-C1'-S1P-C2P
2	B	401	CO8	C2'-C1'-S1P-C2P
2	C	401	CO8	C3B-O3B-P3B-O7A
2	C	401	CO8	C5B-O5B-P1A-O1A
2	C	401	CO8	O1'-C1'-S1P-C2P
2	C	401	CO8	C2'-C1'-S1P-C2P
2	D	401	CO8	C3P-C2P-S1P-C1'
2	E	401	CO8	C3B-O3B-P3B-O7A
2	E	401	CO8	O1'-C1'-S1P-C2P
2	E	401	CO8	C2'-C1'-S1P-C2P
2	E	401	CO8	C1'-C2'-C3'-C4'
2	F	401	CO8	C3P-C2P-S1P-C1'
2	G	401	CO8	CAP-C9P-N8P-C7P
2	G	401	CO8	O9P-C9P-N8P-C7P

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Mol	Chain	Res	Type	Atoms
2	G	401	CO8	C5P-C6P-C7P-N8P
2	G	401	CO8	C2P-C3P-N4P-C5P
2	G	401	CO8	S1P-C1'-C2'-C3'
2	G	401	CO8	O1'-C1'-C2'-C3'
2	H	401	CO8	C3B-O3B-P3B-O7A
2	H	401	CO8	CCP-O6A-P2A-O5A
2	H	401	CO8	C9P-CAP-CBP-CCP
2	H	401	CO8	O1'-C1'-S1P-C2P
2	H	401	CO8	C2'-C1'-S1P-C2P
2	I	401	CO8	CCP-O6A-P2A-O4A
2	I	401	CO8	O1'-C1'-S1P-C2P
2	I	401	CO8	C2'-C1'-S1P-C2P
2	J	401	CO8	C2B-C3B-O3B-P3B
2	J	401	CO8	C3B-O3B-P3B-O7A
2	J	401	CO8	O4B-C4B-C5B-O5B
2	J	401	CO8	C5B-O5B-P1A-O1A
2	J	401	CO8	C5B-O5B-P1A-O3A
2	J	401	CO8	C1'-C2'-C3'-C4'
2	K	401	CO8	O1'-C1'-S1P-C2P
2	K	401	CO8	C2'-C1'-S1P-C2P
2	L	401	CO8	CCP-O6A-P2A-O4A
2	L	401	CO8	O1'-C1'-S1P-C2P
2	L	401	CO8	C2'-C1'-S1P-C2P
2	C	401	CO8	C4B-C3B-O3B-P3B
2	E	401	CO8	C4'-C5'-C6'-C7'
2	C	401	CO8	C2B-C3B-O3B-P3B
2	J	401	CO8	C4B-C3B-O3B-P3B
2	A	401	CO8	C2'-C3'-C4'-C5'
2	E	401	CO8	C2'-C3'-C4'-C5'
2	K	401	CO8	C3'-C4'-C5'-C6'
2	K	401	CO8	C4'-C5'-C6'-C7'
2	L	401	CO8	C4'-C5'-C6'-C7'
2	D	401	CO8	C2'-C3'-C4'-C5'
2	G	401	CO8	C4'-C5'-C6'-C7'
2	C	401	CO8	C2'-C3'-C4'-C5'
2	J	401	CO8	C2'-C3'-C4'-C5'
2	H	401	CO8	C2'-C3'-C4'-C5'
2	C	401	CO8	C4'-C5'-C6'-C7'
2	K	401	CO8	C2'-C3'-C4'-C5'
2	L	401	CO8	C2'-C3'-C4'-C5'
2	I	401	CO8	C2'-C3'-C4'-C5'
2	G	401	CO8	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	B	401	CO8	C2'-C3'-C4'-C5'
2	C	401	CO8	C5P-C6P-C7P-N8P
2	K	401	CO8	C5P-C6P-C7P-N8P
2	D	401	CO8	C4'-C5'-C6'-C7'
2	J	401	CO8	C5'-C6'-C7'-C8'
2	A	401	CO8	C5'-C6'-C7'-C8'
2	B	401	CO8	C5'-C6'-C7'-C8'
2	F	401	CO8	O4B-C4B-C5B-O5B
2	A	401	CO8	C4'-C5'-C6'-C7'
2	G	401	CO8	N8P-C9P-CAP-CBP
2	I	401	CO8	C5'-C6'-C7'-C8'
2	G	401	CO8	O1'-C1'-S1P-C2P
2	J	401	CO8	O1'-C1'-S1P-C2P
2	J	401	CO8	S1P-C1'-C2'-C3'
2	J	401	CO8	O1'-C1'-C2'-C3'
2	F	401	CO8	C1'-C2'-C3'-C4'
2	B	401	CO8	O4B-C4B-C5B-O5B
2	G	401	CO8	C2'-C1'-S1P-C2P
2	A	401	CO8	C5B-O5B-P1A-O3A
2	C	401	CO8	C5B-O5B-P1A-O3A
2	F	401	CO8	C5B-O5B-P1A-O3A
2	H	401	CO8	C3B-O3B-P3B-O9A
2	L	401	CO8	CCP-O6A-P2A-O3A
2	H	401	CO8	CCP-O6A-P2A-O4A
2	G	401	CO8	S1P-C2P-C3P-N4P
2	H	401	CO8	OAP-CAP-CBP-CCP
2	J	401	CO8	C3'-C4'-C5'-C6'
2	H	401	CO8	C4'-C5'-C6'-C7'
2	I	401	CO8	C3'-C4'-C5'-C6'
2	C	401	CO8	P2A-O3A-P1A-O2A
2	J	401	CO8	P2A-O3A-P1A-O2A
2	F	401	CO8	C4'-C5'-C6'-C7'
2	E	401	CO8	C5P-C6P-C7P-N8P
2	A	401	CO8	O4B-C4B-C5B-O5B
2	C	401	CO8	O4B-C4B-C5B-O5B
2	D	401	CO8	C5'-C6'-C7'-C8'
2	J	401	CO8	C3P-C2P-S1P-C1'
2	F	401	CO8	C3'-C4'-C5'-C6'
2	D	401	CO8	S1P-C1'-C2'-C3'
2	D	401	CO8	O1'-C1'-C2'-C3'
2	F	401	CO8	S1P-C1'-C2'-C3'
2	F	401	CO8	O1'-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
2	B	401	CO8	C1'-C2'-C3'-C4'
2	D	401	CO8	C1'-C2'-C3'-C4'
2	K	401	CO8	C1'-C2'-C3'-C4'
2	D	401	CO8	O5P-C5P-N4P-C3P
2	G	401	CO8	O4B-C4B-C5B-O5B
2	F	401	CO8	C2'-C3'-C4'-C5'
2	J	401	CO8	C2'-C1'-S1P-C2P
2	C	401	CO8	C3'-C4'-C5'-C6'
2	H	401	CO8	C6P-C7P-N8P-C9P
2	E	401	CO8	C3B-O3B-P3B-O8A
2	H	401	CO8	CCP-O6A-P2A-O3A
2	J	401	CO8	C3B-O3B-P3B-O9A
2	D	401	CO8	O4B-C4B-C5B-O5B
2	E	401	CO8	O4B-C4B-C5B-O5B
2	K	401	CO8	O4B-C4B-C5B-O5B
2	L	401	CO8	O4B-C4B-C5B-O5B
2	B	401	CO8	P2A-O3A-P1A-O2A
2	E	401	CO8	P2A-O3A-P1A-O1A
2	E	401	CO8	P2A-O3A-P1A-O2A
2	G	401	CO8	P2A-O3A-P1A-O2A
2	L	401	CO8	P2A-O3A-P1A-O1A
2	J	401	CO8	C4'-C5'-C6'-C7'
2	B	401	CO8	C5B-O5B-P1A-O1A
2	B	401	CO8	C5B-O5B-P1A-O2A
2	E	401	CO8	C5B-O5B-P1A-O1A
2	G	401	CO8	C5B-O5B-P1A-O1A
2	L	401	CO8	C5B-O5B-P1A-O1A
2	L	401	CO8	CCP-O6A-P2A-O5A
2	H	401	CO8	O4B-C4B-C5B-O5B
2	I	401	CO8	O4B-C4B-C5B-O5B
2	G	401	CO8	O9P-C9P-CAP-CBP

There are no ring outliers.

9 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	CO8	3	0
2	G	401	CO8	9	0
2	C	401	CO8	3	0
2	E	401	CO8	2	0
2	F	401	CO8	2	0
2	J	401	CO8	1	0

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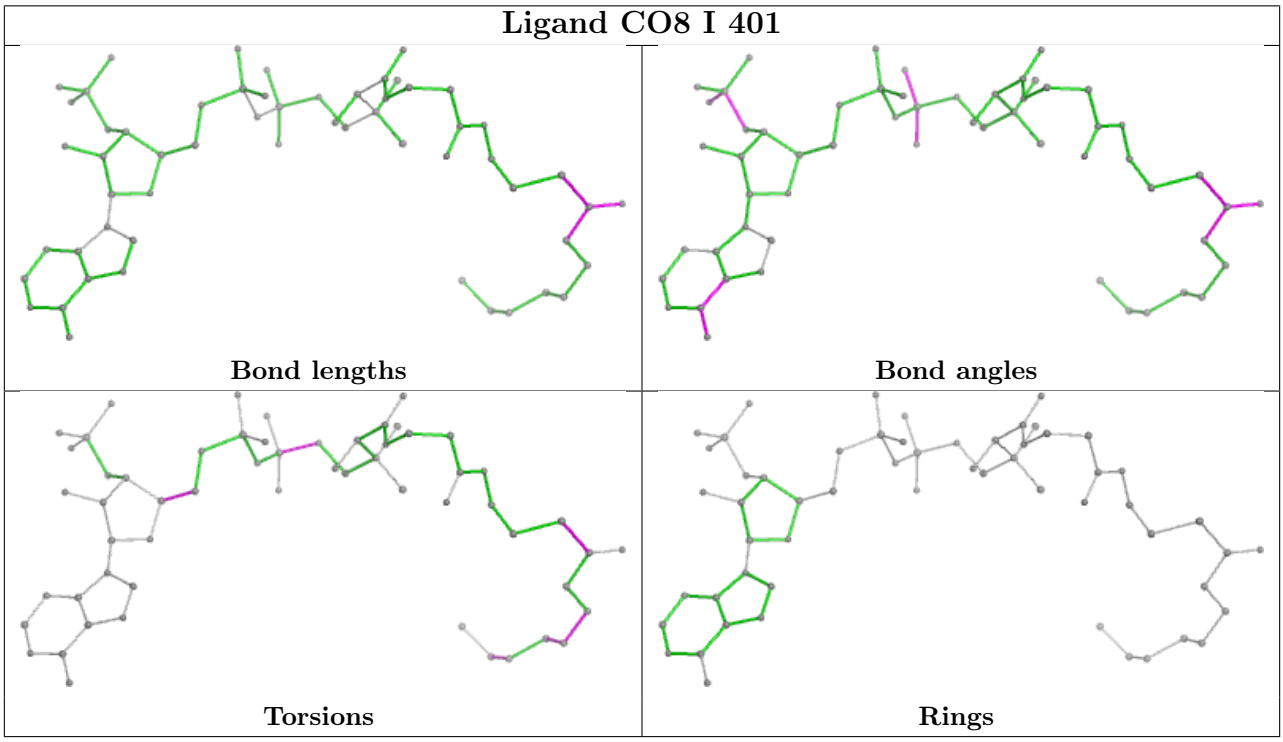
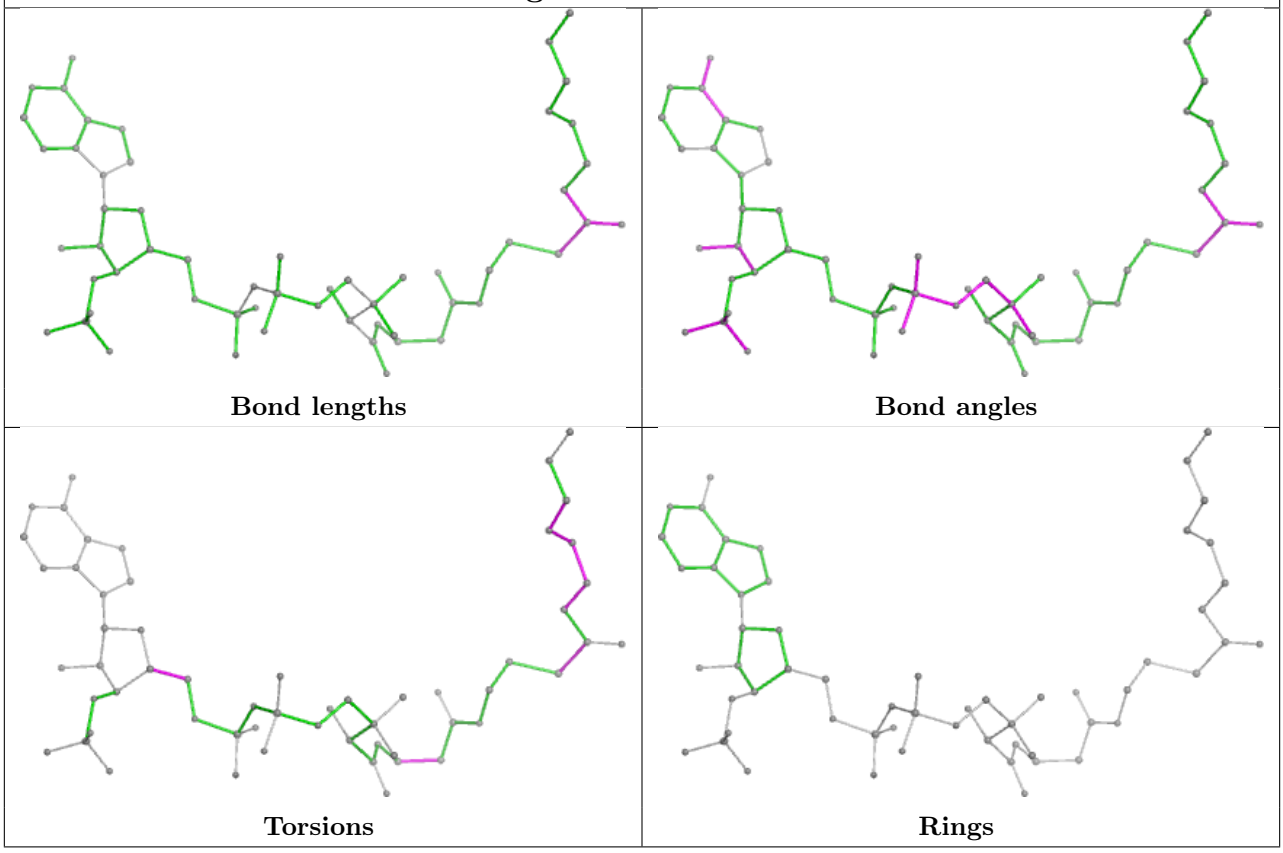
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	CO8	2	0
2	B	401	CO8	5	0
2	H	401	CO8	1	0

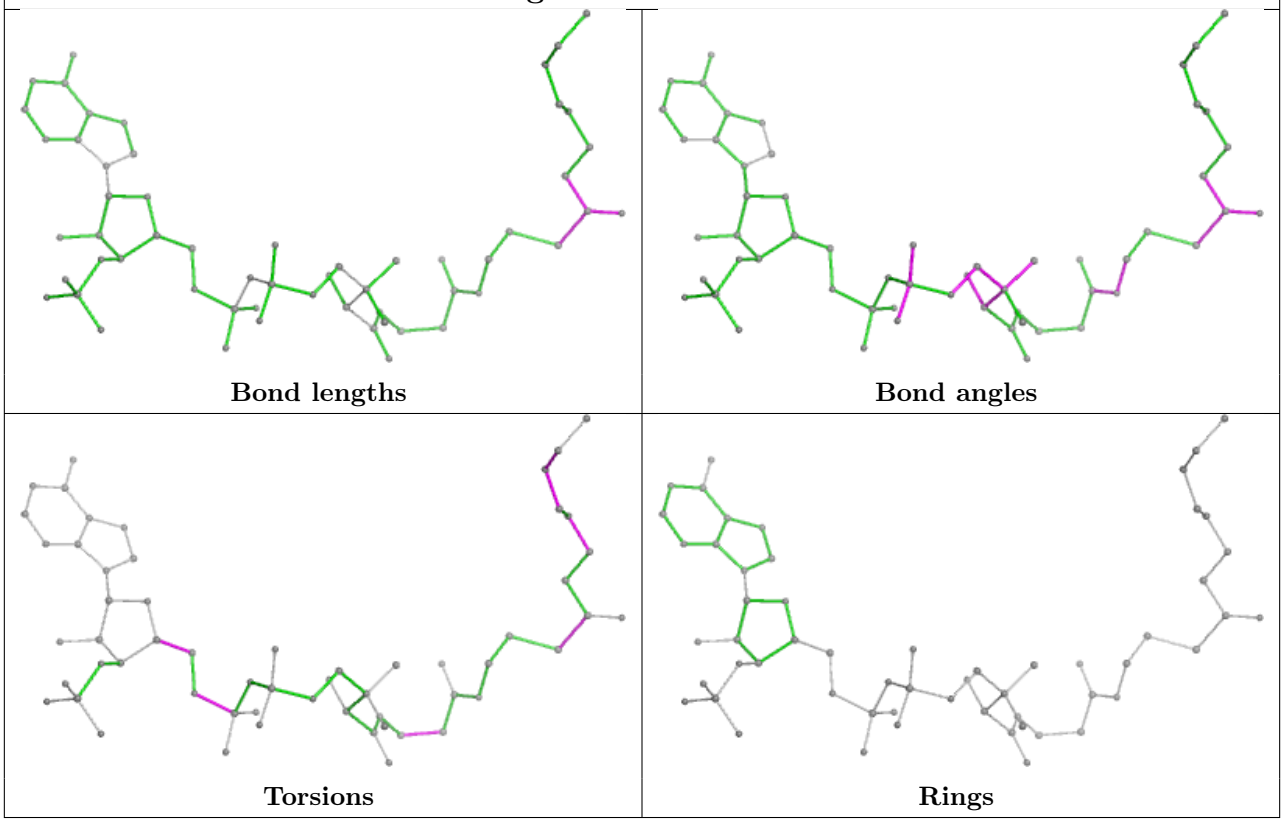
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



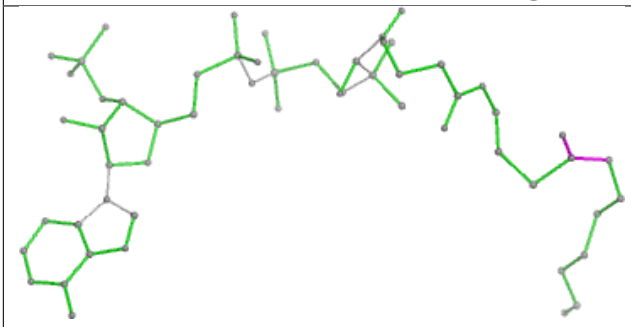
Ligand CO8 K 401



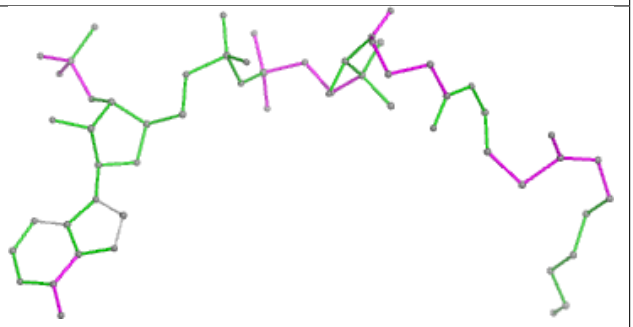
Ligand CO8 A 401



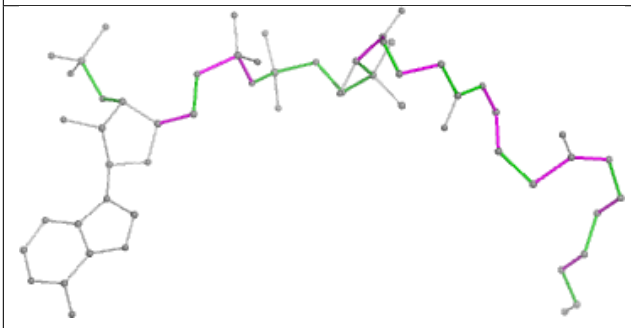
Ligand CO8 G 401



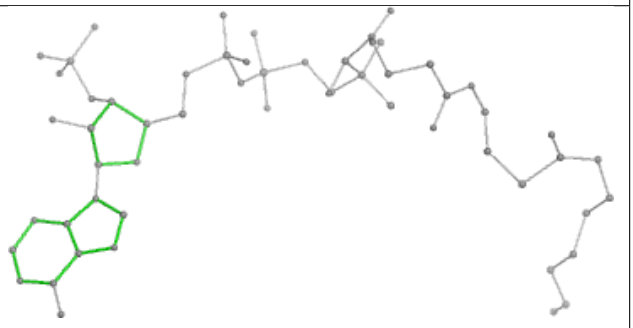
Bond lengths



Bond angles

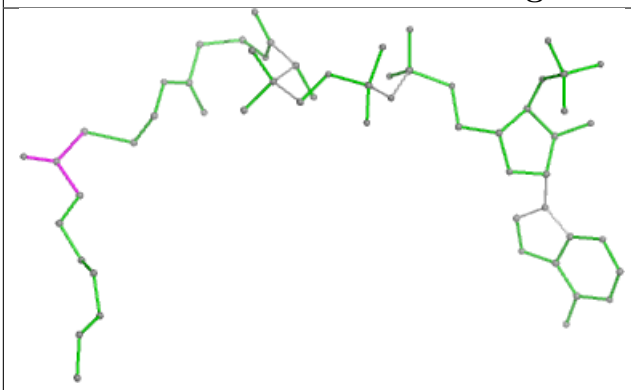


Torsions

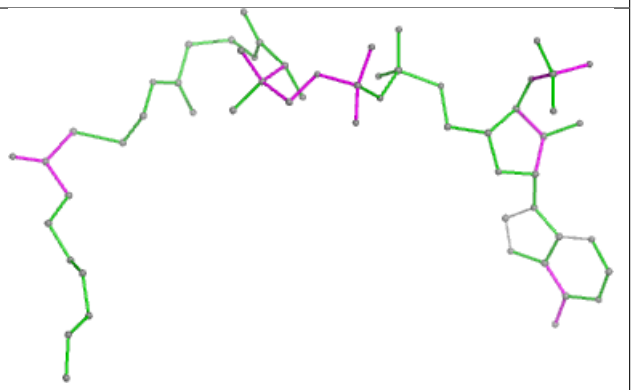


Rings

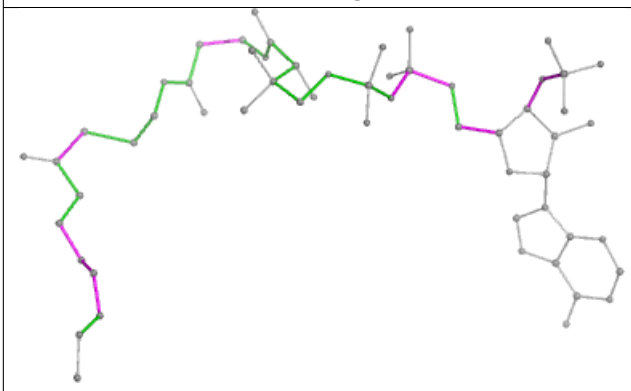
Ligand CO8 C 401



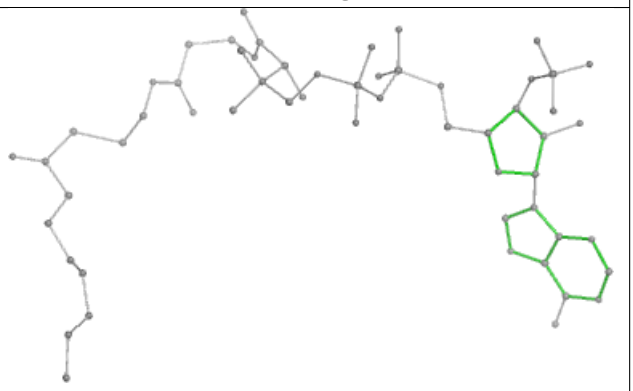
Bond lengths



Bond angles

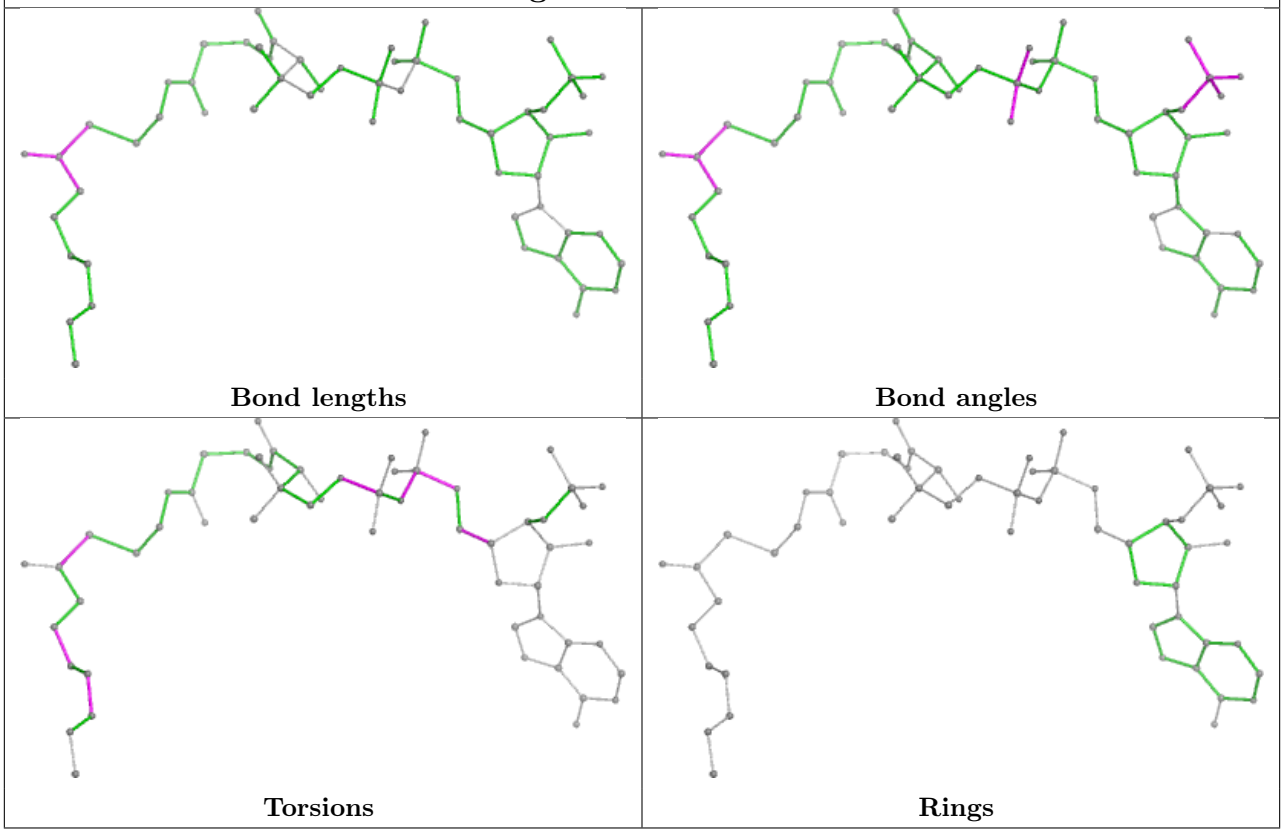


Torsions

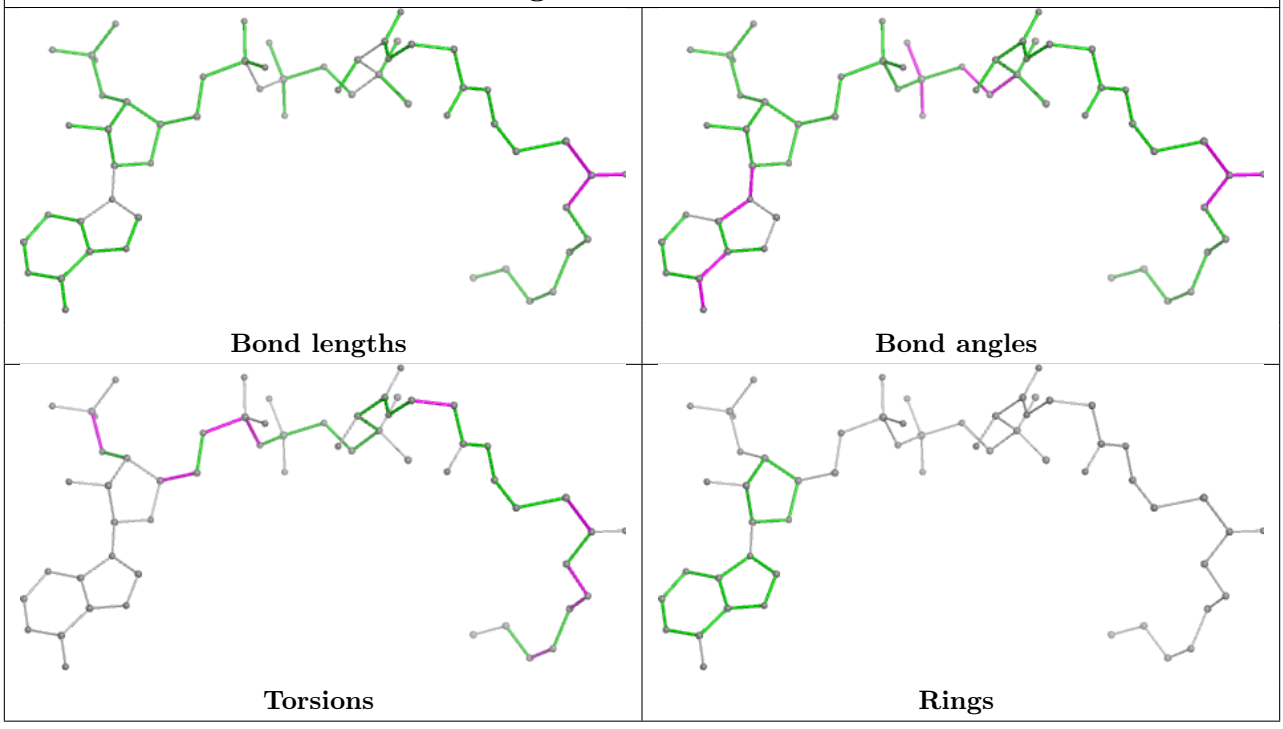


Rings

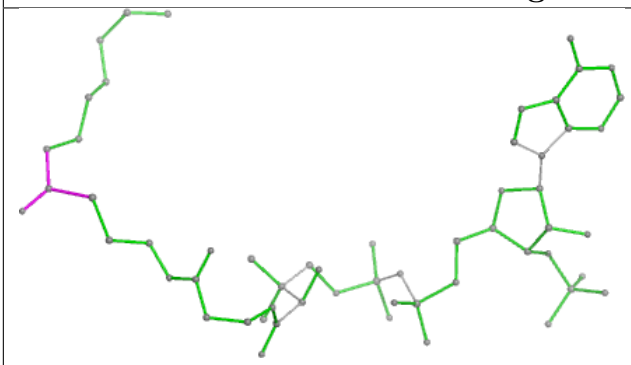
Ligand CO8 L 401



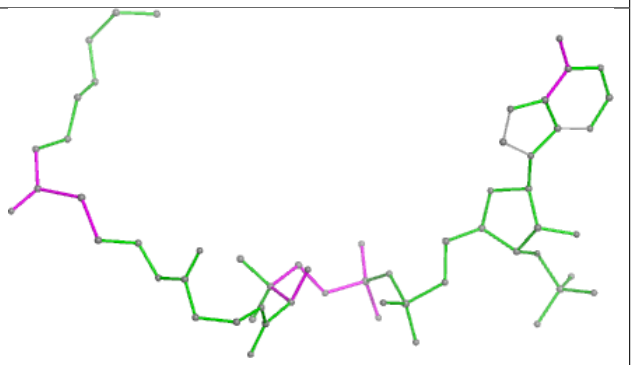
Ligand CO8 E 401



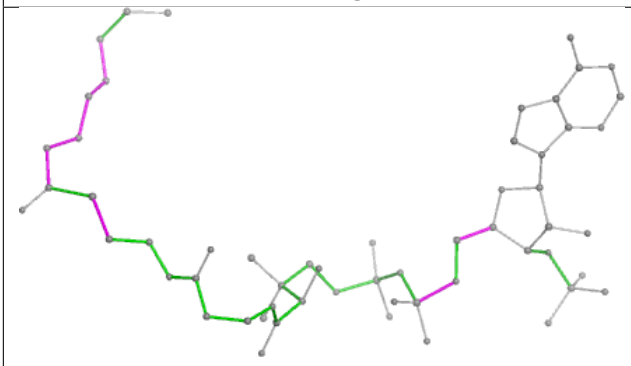
Ligand CO8 F 401



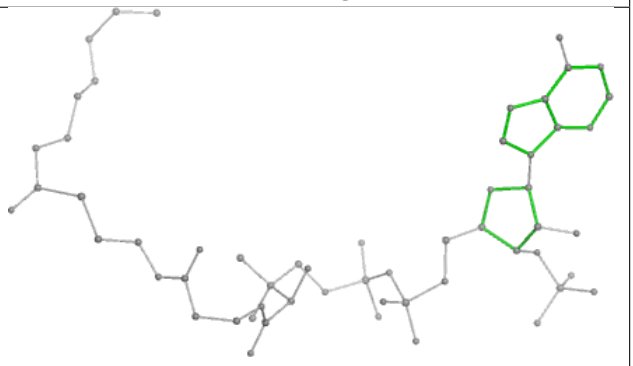
Bond lengths



Bond angles

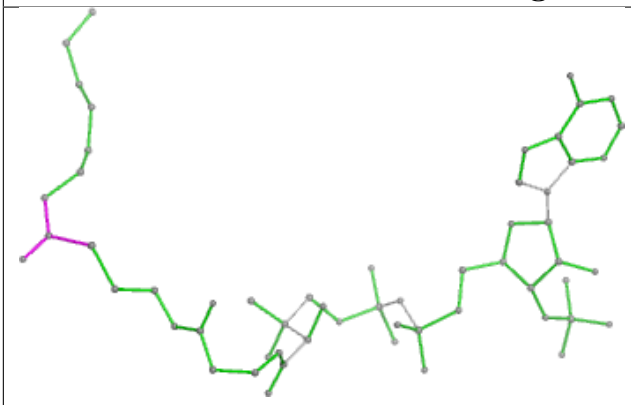


Torsions

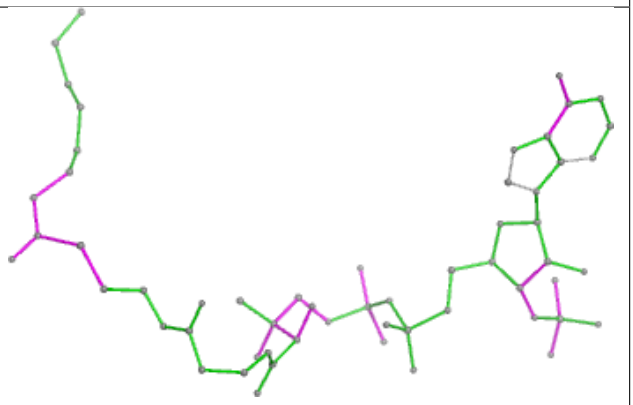


Rings

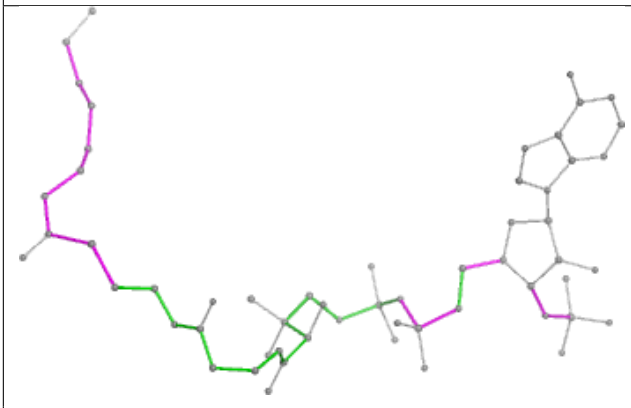
Ligand CO8 J 401



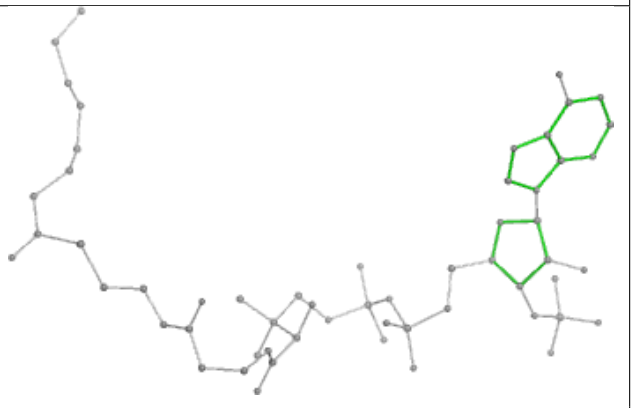
Bond lengths



Bond angles

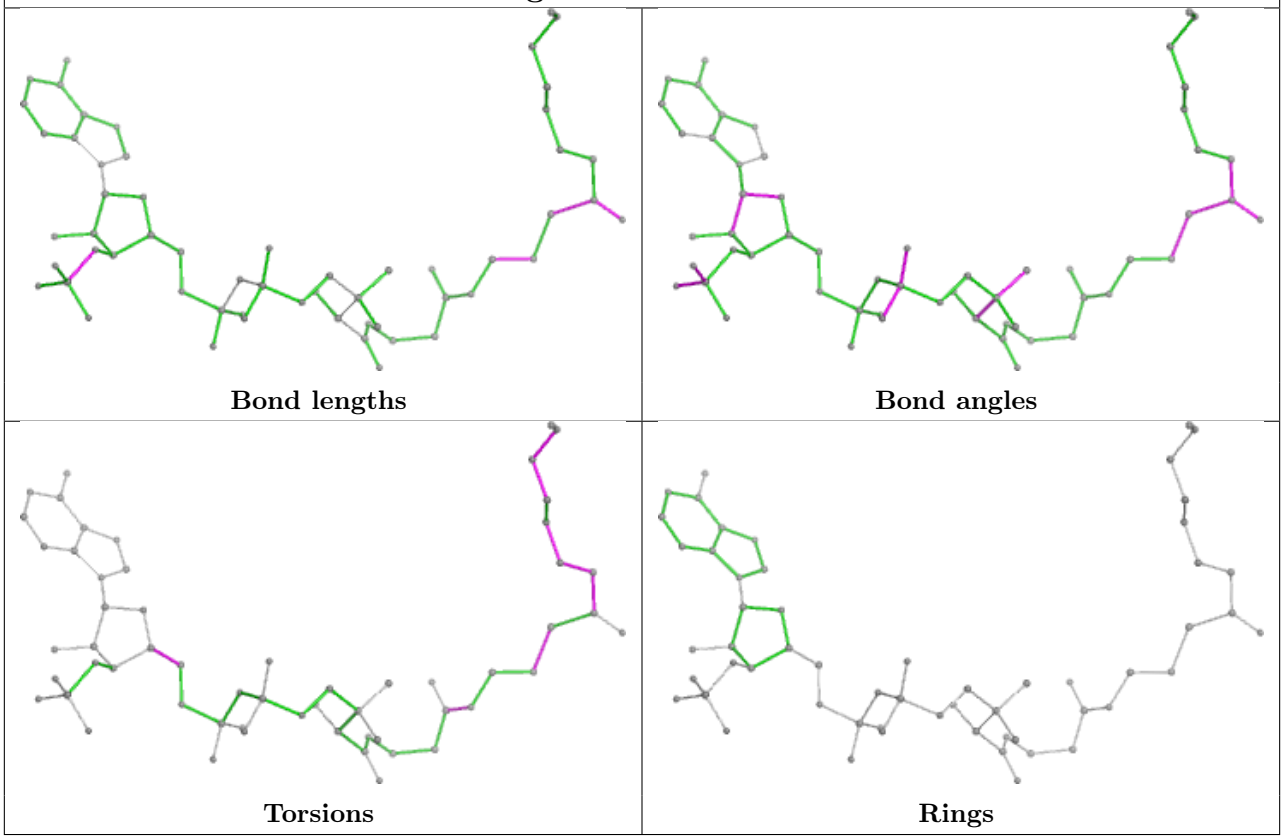


Torsions

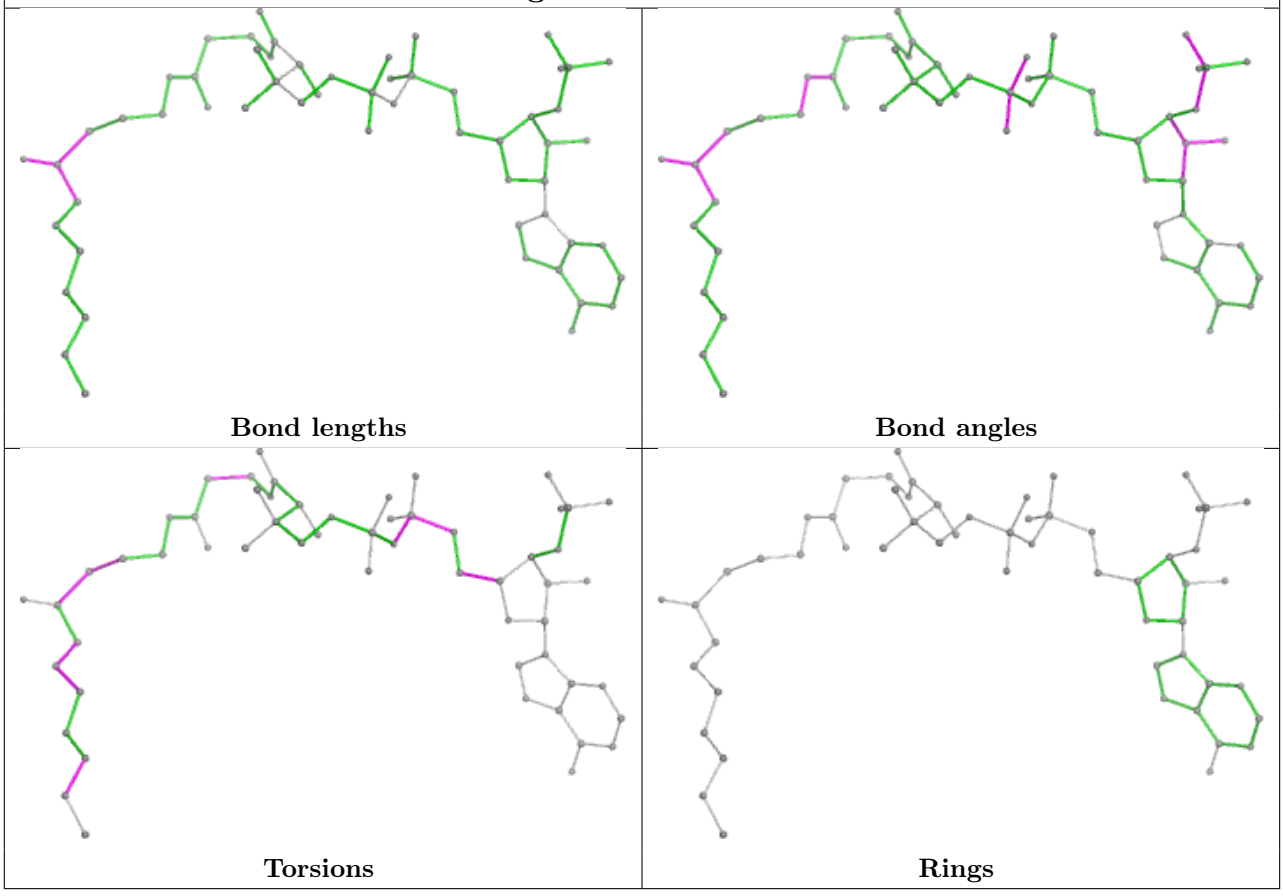


Rings

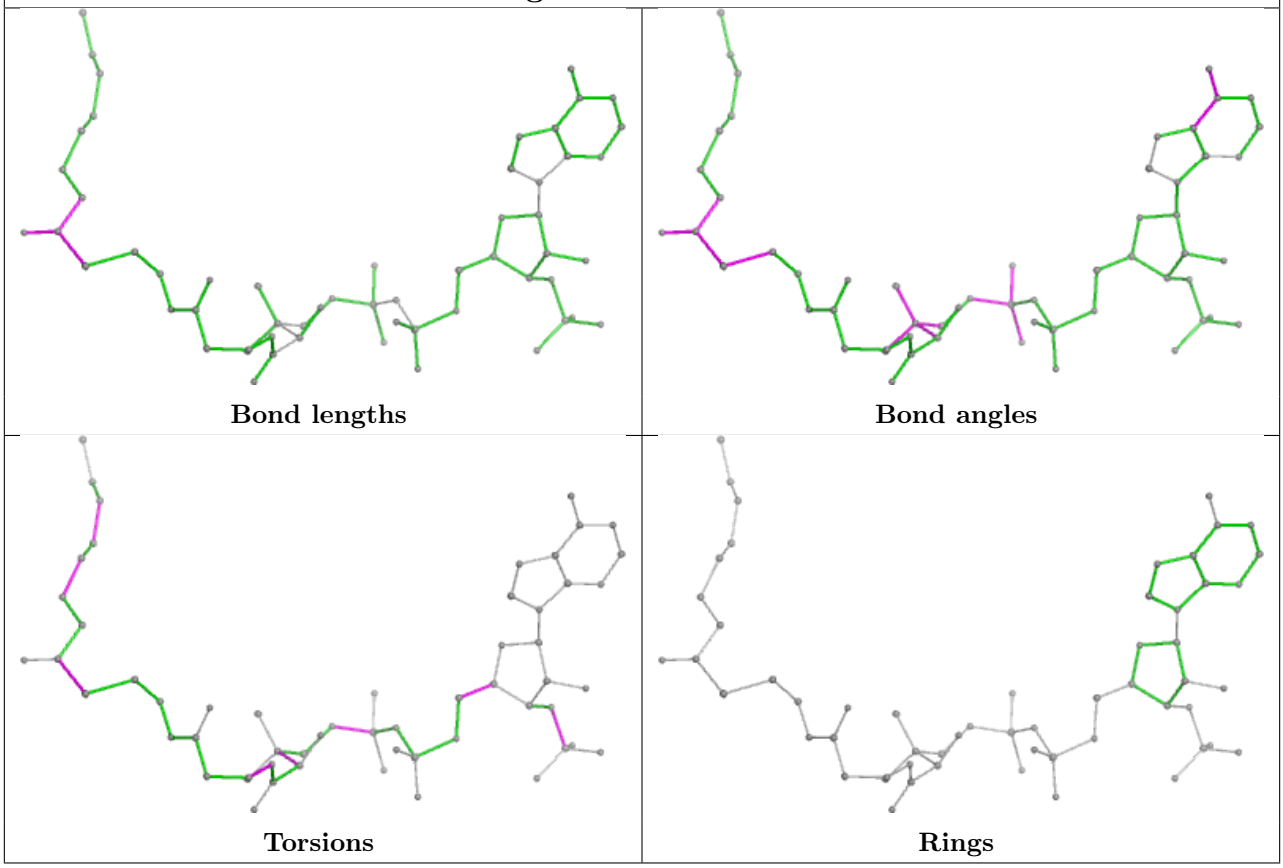
Ligand CO8 D 401



Ligand CO8 B 401



Ligand CO8 H 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	359/364 (98%)	0.46	28 (7%) 20 22	21, 35, 71, 106	2 (0%)
1	B	359/364 (98%)	0.56	44 (12%) 9 10	21, 36, 76, 116	1 (0%)
1	C	359/364 (98%)	0.70	69 (19%) 4 4	21, 35, 75, 114	2 (0%)
1	D	359/364 (98%)	0.35	22 (6%) 28 30	21, 34, 69, 115	1 (0%)
1	E	356/364 (97%)	0.47	37 (10%) 13 14	21, 35, 73, 101	2 (0%)
1	F	359/364 (98%)	0.64	54 (15%) 6 7	14, 36, 75, 111	2 (0%)
1	G	359/364 (98%)	0.70	59 (16%) 5 6	15, 37, 75, 113	3 (0%)
1	H	358/364 (98%)	0.51	42 (11%) 10 11	18, 36, 82, 113	2 (0%)
1	I	359/364 (98%)	0.19	13 (3%) 46 48	20, 32, 62, 98	2 (0%)
1	J	356/364 (97%)	0.40	37 (10%) 13 14	21, 33, 69, 103	1 (0%)
1	K	358/364 (98%)	0.70	67 (18%) 4 4	20, 34, 77, 113	2 (0%)
1	L	359/364 (98%)	0.29	20 (5%) 31 33	16, 34, 64, 106	2 (0%)
All	All	4300/4368 (98%)	0.50	492 (11%) 11 12	14, 35, 73, 116	22 (0%)

All (492) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	ALA	8.7
1	E	346	ALA	7.2
1	E	42	VAL	6.6
1	K	42	VAL	6.6
1	D	42	VAL	6.4
1	B	42	VAL	6.3
1	K	45	ILE	6.1
1	D	346	ALA	6.1
1	B	45	ILE	6.0
1	C	42	VAL	5.9
1	H	45	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	F	42	VAL	5.8
1	G	42	VAL	5.8
1	G	97	GLU	5.7
1	H	39	PRO	5.6
1	H	42	VAL	5.6
1	A	44	GLY	5.6
1	B	43	ASP	5.5
1	A	42	VAL	5.5
1	G	44	GLY	5.5
1	C	45	ILE	5.5
1	L	45	ILE	5.3
1	E	349	ILE	5.2
1	F	45	ILE	5.2
1	I	47	ARG	5.2
1	F	176	GLN	5.0
1	B	345	PRO	4.9
1	E	39	PRO	4.9
1	B	46	SER	4.8
1	H	49	ALA	4.8
1	K	347	ALA	4.6
1	D	45	ILE	4.6
1	L	323	ASN	4.6
1	A	324	GLY	4.6
1	K	324	GLY	4.6
1	C	346	ALA	4.6
1	B	346	ALA	4.5
1	F	44	GLY	4.5
1	C	43	ASP	4.4
1	G	45	ILE	4.4
1	E	40	SER	4.3
1	K	176	GLN	4.3
1	K	47	ARG	4.3
1	K	349	ILE	4.3
1	J	346	ALA	4.2
1	A	45	ILE	4.2
1	G	177	SER	4.2
1	D	43	ASP	4.2
1	A	40	SER	4.2
1	K	93	GLY	4.2
1	D	323	ASN	4.2
1	L	359	ASP	4.1
1	C	93	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	323	ASN	4.1
1	J	42	VAL	4.1
1	C	44	GLY	4.1
1	F	346	ALA	4.1
1	J	49	ALA	4.1
1	L	44	GLY	4.0
1	K	75	ALA	4.0
1	B	41	SER	4.0
1	A	349	ILE	4.0
1	K	49	ALA	4.0
1	C	176	GLN	4.0
1	G	355	LEU	4.0
1	H	47	ARG	3.9
1	L	41	SER	3.9
1	D	44	GLY	3.9
1	K	345	PRO	3.9
1	H	44	GLY	3.9
1	C	59	ALA	3.9
1	C	66	GLY	3.9
1	C	47	ARG	3.9
1	A	346	ALA	3.9
1	G	176	GLN	3.8
1	E	351	ILE	3.8
1	C	69	LEU	3.8
1	I	41	SER	3.8
1	K	73	LEU	3.8
1	G	346	ALA	3.8
1	I	43	ASP	3.8
1	G	61	LEU	3.8
1	C	323	ASN	3.7
1	G	293	ASN	3.7
1	H	346	ALA	3.7
1	G	351	ILE	3.7
1	I	45	ILE	3.7
1	I	42	VAL	3.7
1	J	176	GLN	3.7
1	F	62	LYS	3.7
1	H	349	ILE	3.6
1	F	47	ARG	3.6
1	C	75	ALA	3.6
1	C	347	ALA	3.6
1	G	59	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	75	ALA	3.6
1	K	72	LYS	3.6
1	C	349	ILE	3.6
1	H	351	ILE	3.6
1	G	43	ASP	3.6
1	C	49	ALA	3.6
1	H	207	MET	3.6
1	B	44	GLY	3.5
1	A	351	ILE	3.5
1	F	359	ASP	3.5
1	K	69	LEU	3.5
1	C	70	ALA	3.5
1	G	347	ALA	3.5
1	L	346	ALA	3.5
1	K	44	GLY	3.5
1	K	180	LYS	3.5
1	J	351	ILE	3.5
1	F	92	LEU	3.5
1	H	355	LEU	3.5
1	B	351	ILE	3.4
1	B	347	ALA	3.4
1	G	324	GLY	3.4
1	I	44	GLY	3.4
1	B	47	ARG	3.4
1	F	351	ILE	3.4
1	A	177	SER	3.4
1	F	41	SER	3.4
1	F	207	MET	3.4
1	H	48	ASP	3.4
1	H	348	THR	3.3
1	K	348	THR	3.3
1	F	349	ILE	3.3
1	K	354	VAL	3.3
1	C	68	GLU	3.3
1	C	353	ALA	3.3
1	J	48	ASP	3.3
1	J	144	ASP	3.3
1	E	324	GLY	3.3
1	K	66	GLY	3.3
1	F	61	LEU	3.3
1	B	350	ASP	3.2
1	F	43	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	144	ASP	3.2
1	E	345	PRO	3.2
1	C	351	ILE	3.2
1	F	292	ALA	3.2
1	J	75	ALA	3.2
1	E	355	LEU	3.2
1	K	39	PRO	3.2
1	K	322	ALA	3.2
1	C	41	SER	3.2
1	B	65	GLN	3.2
1	G	94	LEU	3.2
1	D	351	ILE	3.2
1	G	349	ILE	3.2
1	L	42	VAL	3.1
1	K	46	SER	3.1
1	G	62	LYS	3.1
1	G	359	ASP	3.1
1	K	102	VAL	3.1
1	F	49	ALA	3.1
1	L	324	GLY	3.1
1	B	75	ALA	3.1
1	A	348	THR	3.1
1	J	47	ARG	3.1
1	C	71	LEU	3.0
1	F	324	GLY	3.0
1	K	71	LEU	3.0
1	D	49	ALA	3.0
1	H	46	SER	3.0
1	G	58	THR	3.0
1	E	323	ASN	3.0
1	B	49	ALA	3.0
1	A	41	SER	3.0
1	F	345	PRO	3.0
1	H	176	GLN	3.0
1	G	101	LYS	3.0
1	H	350	ASP	3.0
1	G	207	MET	3.0
1	D	41	SER	3.0
1	G	354	VAL	3.0
1	E	68	GLU	3.0
1	H	144	ASP	2.9
1	F	354	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	292	ALA	2.9
1	G	348	THR	2.9
1	F	39	PRO	2.9
1	A	68	GLU	2.9
1	B	73	LEU	2.9
1	C	61	LEU	2.9
1	B	359	ASP	2.9
1	G	178	SER	2.9
1	K	74	ILE	2.9
1	K	101	LYS	2.9
1	F	355	LEU	2.9
1	E	144	ASP	2.9
1	F	48	ASP	2.9
1	K	65	GLN	2.9
1	L	46	SER	2.9
1	F	323	ASN	2.9
1	J	323	ASN	2.9
1	C	76	LYS	2.9
1	F	76	LYS	2.9
1	K	62	LYS	2.9
1	H	41	SER	2.8
1	K	63	SER	2.8
1	A	47	ARG	2.8
1	L	47	ARG	2.8
1	K	351	ILE	2.8
1	L	349	ILE	2.8
1	I	324	GLY	2.8
1	C	108	TYR	2.8
1	J	355	LEU	2.8
1	D	322	ALA	2.8
1	D	347	ALA	2.8
1	G	47	ARG	2.8
1	F	180	LYS	2.8
1	I	351	ILE	2.8
1	H	58	THR	2.8
1	A	43	ASP	2.8
1	G	92	LEU	2.8
1	J	69	LEU	2.8
1	F	93	GLY	2.8
1	G	93	GLY	2.8
1	C	58	THR	2.8
1	D	348	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	345	PRO	2.8
1	J	92	LEU	2.8
1	F	358	TRP	2.8
1	H	352	GLU	2.8
1	G	353	ALA	2.7
1	I	323	ASN	2.7
1	K	41	SER	2.8
1	A	180	LYS	2.7
1	E	348	THR	2.7
1	A	345	PRO	2.7
1	K	359	ASP	2.7
1	D	180	LYS	2.7
1	C	177	SER	2.7
1	F	59	ALA	2.7
1	G	70	ALA	2.7
1	J	324	GLY	2.7
1	K	48	ASP	2.7
1	L	144	ASP	2.7
1	A	69	LEU	2.7
1	J	94	LEU	2.7
1	A	173	TRP	2.7
1	E	47	ARG	2.7
1	C	107	ILE	2.7
1	J	349	ILE	2.7
1	I	144	ASP	2.7
1	F	101	LYS	2.7
1	F	46	SER	2.7
1	F	69	LEU	2.7
1	G	1	MET	2.7
1	J	61	LEU	2.7
1	K	178	SER	2.7
1	L	173	TRP	2.7
1	L	351	ILE	2.7
1	B	40	SER	2.6
1	E	41	SER	2.6
1	A	322	ALA	2.6
1	C	79	VAL	2.6
1	K	100	ALA	2.6
1	K	350	ASP	2.6
1	C	74	ILE	2.6
1	C	63	SER	2.6
1	D	40	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	80	LEU	2.6
1	C	33	VAL	2.6
1	C	34	VAL	2.6
1	F	70	ALA	2.6
1	H	324	GLY	2.6
1	G	345	PRO	2.6
1	D	358	TRP	2.6
1	H	358	TRP	2.6
1	K	56	ILE	2.6
1	A	46	SER	2.6
1	E	69	LEU	2.6
1	J	93	GLY	2.6
1	E	347	ALA	2.6
1	J	353	ALA	2.6
1	C	10	VAL	2.6
1	C	48	ASP	2.6
1	E	359	ASP	2.6
1	K	60	ASP	2.6
1	F	1	MET	2.6
1	K	1	MET	2.6
1	C	39	PRO	2.6
1	K	36	ILE	2.6
1	K	323	ASN	2.6
1	J	46	SER	2.6
1	E	352	GLU	2.6
1	B	66	GLY	2.5
1	H	72	LYS	2.5
1	B	144	ASP	2.5
1	C	183	VAL	2.5
1	E	350	ASP	2.5
1	J	350	ASP	2.5
1	K	144	ASP	2.5
1	C	96	PRO	2.5
1	G	323	ASN	2.5
1	C	173	TRP	2.5
1	G	68	GLU	2.5
1	C	106	LEU	2.5
1	J	73	LEU	2.5
1	B	322	ALA	2.5
1	C	144	ASP	2.5
1	E	58	THR	2.5
1	I	176	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	68	GLU	2.5
1	H	40	SER	2.5
1	H	315	GLU	2.5
1	K	40	SER	2.5
1	B	355	LEU	2.5
1	D	173	TRP	2.5
1	B	357	ASP	2.5
1	E	207	MET	2.5
1	H	2	ALA	2.5
1	E	176	GLN	2.5
1	F	293	ASN	2.5
1	H	345	PRO	2.5
1	K	181	GLY	2.5
1	K	80	LEU	2.5
1	K	355	LEU	2.5
1	D	48	ASP	2.5
1	G	48	ASP	2.5
1	G	358	TRP	2.5
1	F	75	ALA	2.5
1	L	75	ALA	2.5
1	C	354	VAL	2.5
1	G	79	VAL	2.5
1	K	79	VAL	2.5
1	C	40	SER	2.4
1	C	324	GLY	2.4
1	A	350	ASP	2.4
1	B	5	LEU	2.4
1	H	38	ARG	2.4
1	B	358	TRP	2.4
1	H	353	ALA	2.4
1	J	100	ALA	2.4
1	K	353	ALA	2.4
1	B	356	THR	2.4
1	B	352	GLU	2.4
1	F	68	GLU	2.4
1	F	352	GLU	2.4
1	G	352	GLU	2.4
1	B	71	LEU	2.4
1	G	69	LEU	2.4
1	C	358	TRP	2.4
1	C	72	LYS	2.4
1	C	102	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	10	VAL	2.4
1	K	11	VAL	2.4
1	K	183	VAL	2.4
1	J	39	PRO	2.4
1	L	350	ASP	2.4
1	B	323	ASN	2.4
1	C	348	THR	2.4
1	E	38	ARG	2.4
1	K	38	ARG	2.4
1	B	176	GLN	2.4
1	D	357	ASP	2.4
1	E	97	GLU	2.3
1	H	61	LEU	2.3
1	B	72	LYS	2.3
1	G	49	ALA	2.3
1	G	100	ALA	2.3
1	F	356	THR	2.3
1	F	88	VAL	2.3
1	G	46	SER	2.3
1	C	350	ASP	2.3
1	E	66	GLY	2.3
1	K	357	ASP	2.3
1	L	43	ASP	2.3
1	K	352	GLU	2.3
1	C	67	LEU	2.3
1	B	70	ALA	2.3
1	B	257	ALA	2.3
1	F	58	THR	2.3
1	F	347	ALA	2.3
1	B	39	PRO	2.3
1	C	46	SER	2.3
1	G	88	VAL	2.3
1	G	173	TRP	2.3
1	F	73	LEU	2.3
1	G	73	LEU	2.3
1	G	322	ALA	2.3
1	I	346	ALA	2.3
1	J	59	ALA	2.3
1	G	41	SER	2.3
1	J	40	SER	2.3
1	G	102	VAL	2.3
1	G	144	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	350	ASP	2.3
1	I	359	ASP	2.3
1	J	352	GLU	2.3
1	K	358	TRP	2.3
1	C	56	ILE	2.3
1	K	108	TYR	2.3
1	A	75	ALA	2.3
1	C	65	GLN	2.3
1	L	177	SER	2.3
1	K	99	CYS	2.2
1	G	64	ASP	2.2
1	B	102	VAL	2.2
1	F	33	VAL	2.2
1	F	79	VAL	2.2
1	C	62	LYS	2.2
1	E	76	LYS	2.2
1	A	323	ASN	2.2
1	K	173	TRP	2.2
1	F	348	THR	2.2
1	G	77	ALA	2.2
1	J	345	PRO	2.2
1	C	11	VAL	2.2
1	E	10	VAL	2.2
1	F	11	VAL	2.2
1	G	10	VAL	2.2
1	G	57	VAL	2.2
1	D	207	MET	2.2
1	F	173	TRP	2.2
1	J	65	GLN	2.2
1	C	51	LEU	2.2
1	C	73	LEU	2.2
1	K	68	GLU	2.2
1	E	46	SER	2.2
1	L	347	ALA	2.2
1	H	76	LYS	2.2
1	C	105	ARG	2.2
1	F	34	VAL	2.2
1	J	56	ILE	2.2
1	E	49	ALA	2.2
1	E	322	ALA	2.2
1	H	322	ALA	2.2
1	J	347	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	87	GLY	2.2
1	C	99	CYS	2.2
1	A	207	MET	2.2
1	B	1	MET	2.2
1	E	1	MET	2.2
1	L	1	MET	2.2
1	E	65	GLN	2.2
1	A	92	LEU	2.1
1	D	355	LEU	2.1
1	G	71	LEU	2.1
1	K	67	LEU	2.1
1	A	76	LYS	2.1
1	A	358	TRP	2.1
1	B	173	TRP	2.1
1	J	72	LYS	2.1
1	F	350	ASP	2.1
1	J	359	ASP	2.1
1	K	59	ALA	2.1
1	K	64	ASP	2.1
1	K	70	ALA	2.1
1	K	104	ASP	2.1
1	C	57	VAL	2.1
1	H	354	VAL	2.1
1	C	355	LEU	2.1
1	B	38	ARG	2.1
1	C	357	ASP	2.1
1	D	47	ARG	2.1
1	J	37	ASP	2.1
1	K	58	THR	2.1
1	B	353	ALA	2.1
1	B	105	ARG	2.1
1	G	63	SER	2.1
1	G	356	THR	2.1
1	H	357	ASP	2.1
1	K	94	LEU	2.1
1	E	75	ALA	2.1
1	E	258	GLU	2.1
1	H	34	VAL	2.1
1	C	180	LYS	2.1
1	E	62	LYS	2.1
1	J	62	LYS	2.1
1	H	64	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	LEU	2.1
1	F	94	LEU	2.1
1	H	92	LEU	2.1
1	C	36	ILE	2.1
1	B	324	GLY	2.0
1	C	87	GLY	2.0
1	H	173	TRP	2.0
1	B	62	LYS	2.0
1	F	183	VAL	2.0
1	J	11	VAL	2.0
1	C	8	LEU	2.0
1	D	65	GLN	2.0
1	H	69	LEU	2.0
1	H	56	ILE	2.0
1	E	7	GLY	2.0
1	B	76	LYS	2.0
1	C	38	ARG	2.0
1	J	354	VAL	2.0
1	H	50	MET	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 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, 95^{th} 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
2	CO8	E	401	57/57	0.92	0.14	28,45,101,103	0
2	CO8	F	401	57/57	0.92	0.14	25,44,89,96	0
2	CO8	H	401	57/57	0.92	0.15	31,45,96,106	0
2	CO8	J	401	57/57	0.92	0.14	26,43,77,95	0

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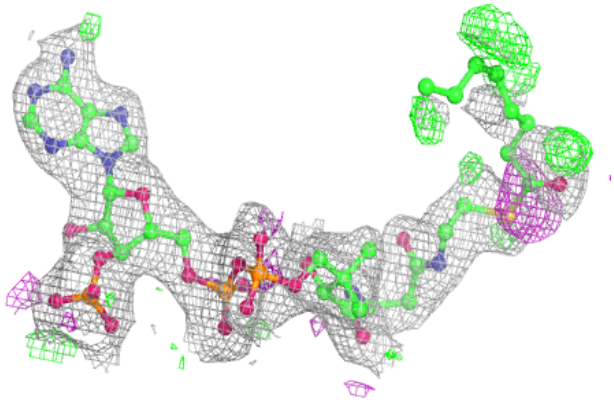
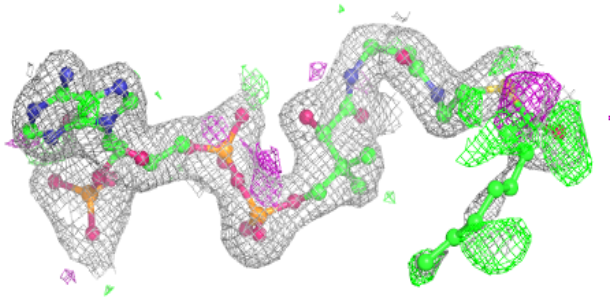
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO8	B	401	57/57	0.93	0.14	24,44,81,91	0
2	CO8	G	401	57/57	0.93	0.14	24,42,73,79	0
2	CO8	C	401	57/57	0.93	0.14	26,44,88,97	0
2	CO8	A	401	57/57	0.93	0.13	24,41,81,85	0
2	CO8	K	401	57/57	0.94	0.13	25,44,83,93	0
2	CO8	L	401	57/57	0.95	0.12	21,31,82,93	0
2	CO8	I	401	57/57	0.96	0.10	21,32,76,81	0
2	CO8	D	401	57/57	0.96	0.11	20,31,90,97	0

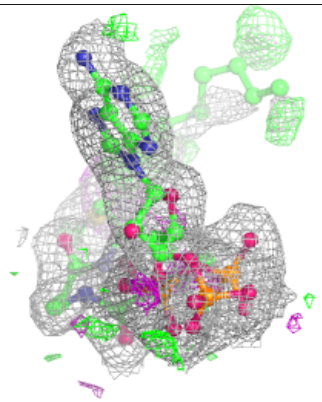
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CO8 E 401:

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

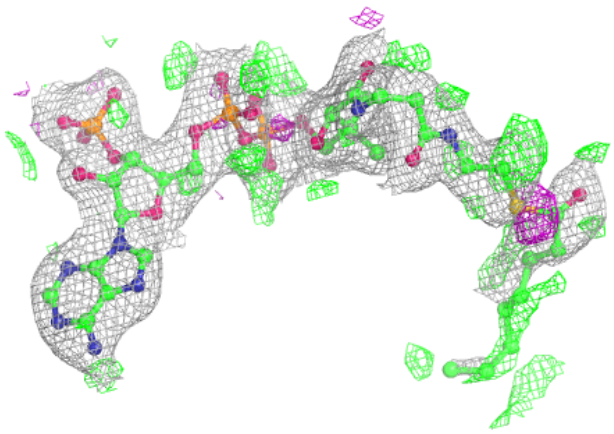


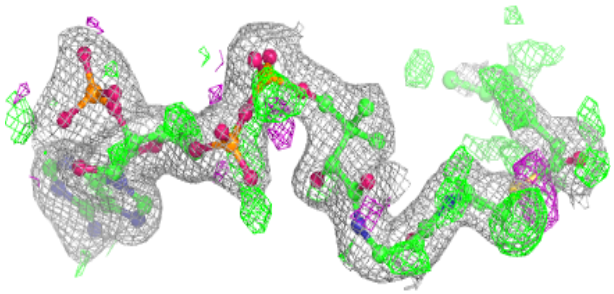




Electron density around CO8 F 401:

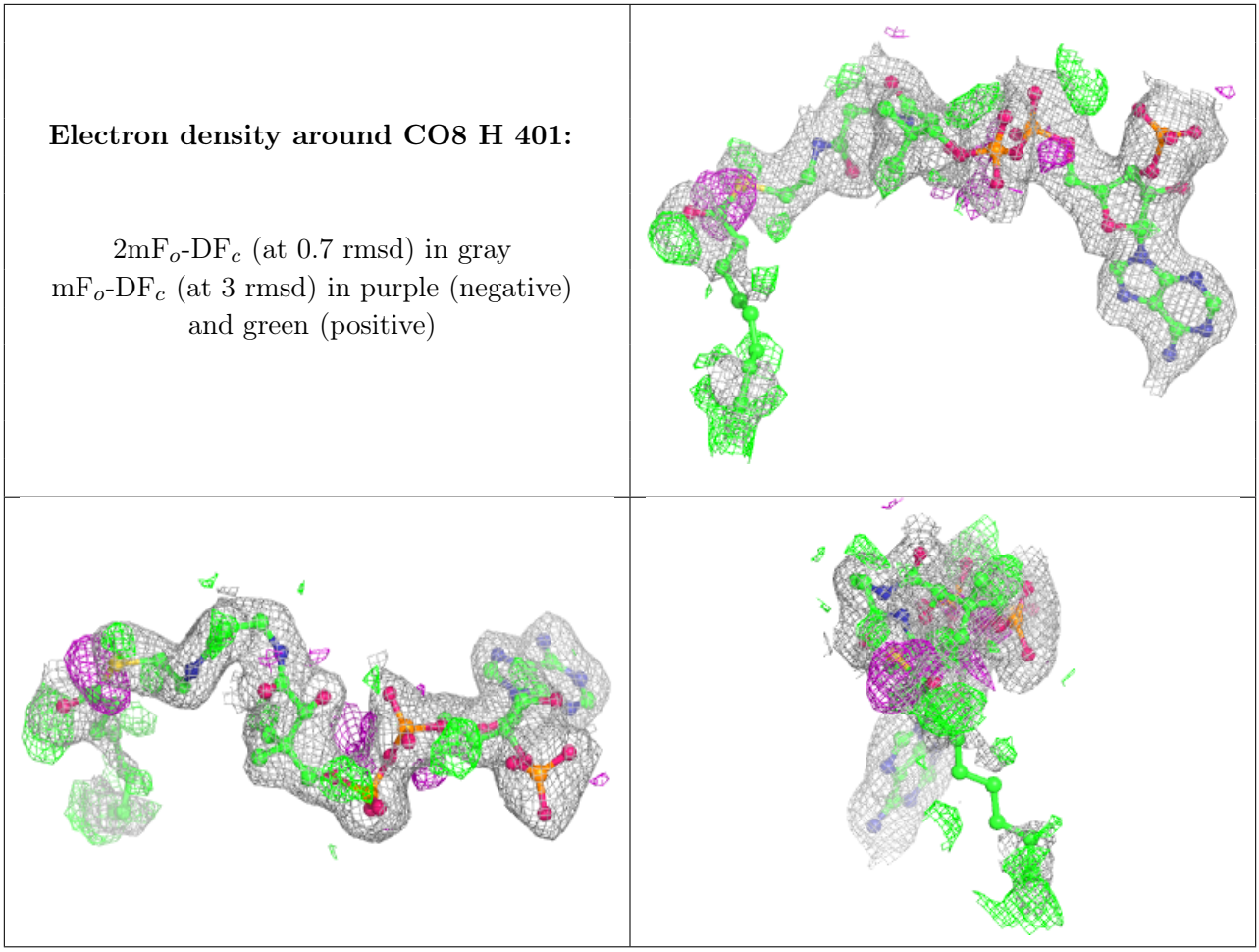
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





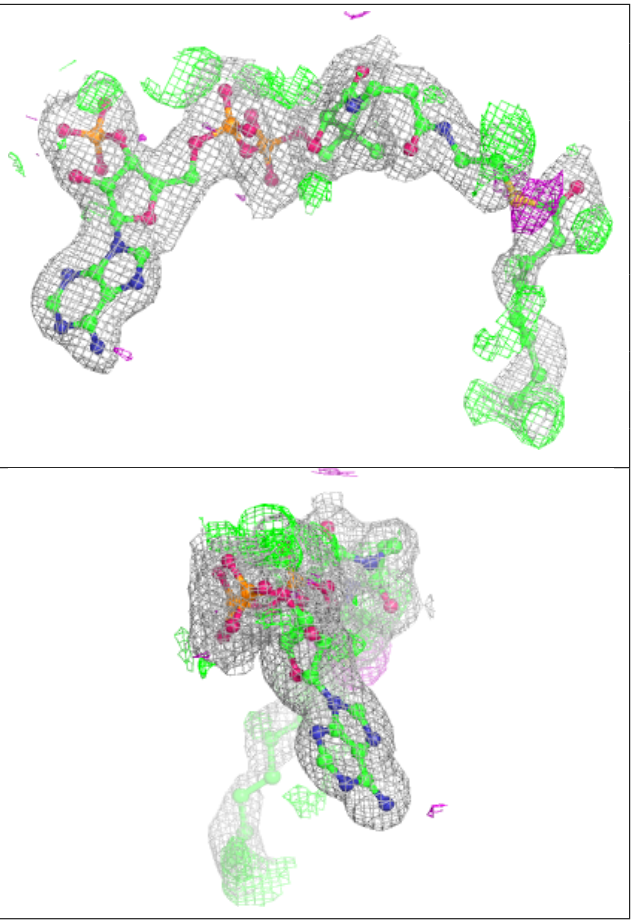
Electron density around CO8 H 401:

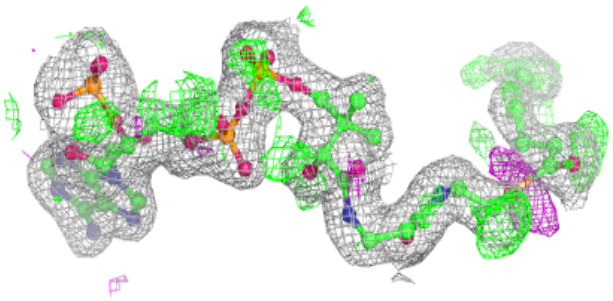
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CO8 J 401:

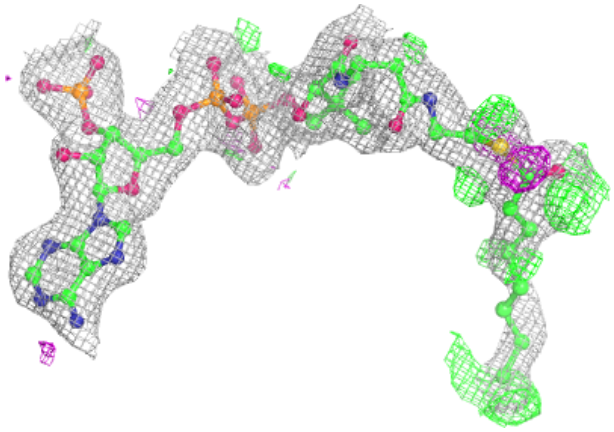
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

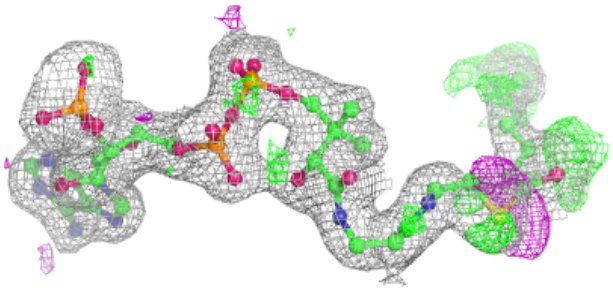


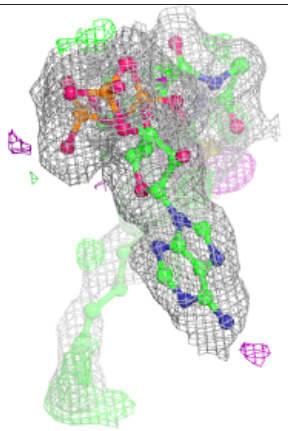


Electron density around CO8 B 401:

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

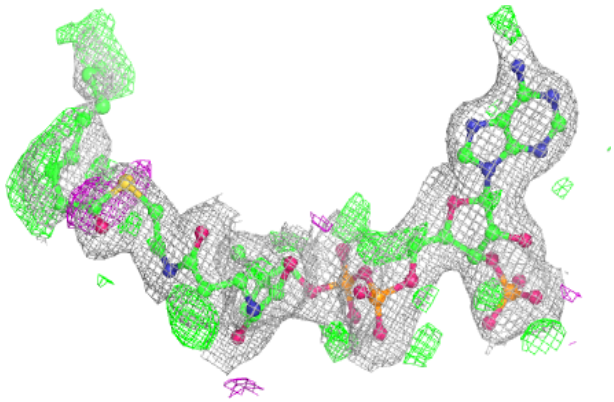


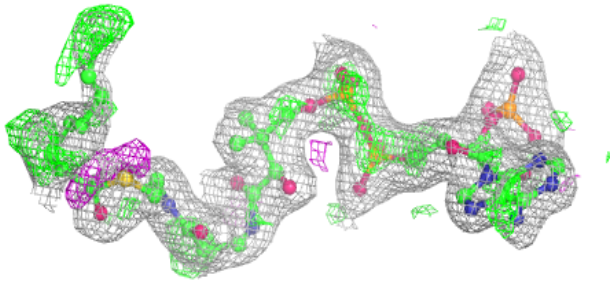


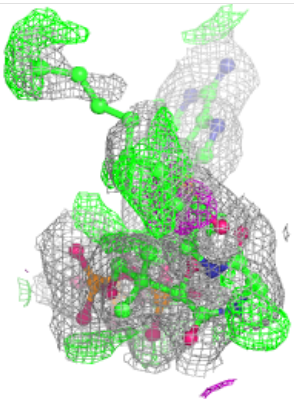


Electron density around CO8 G 401:

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

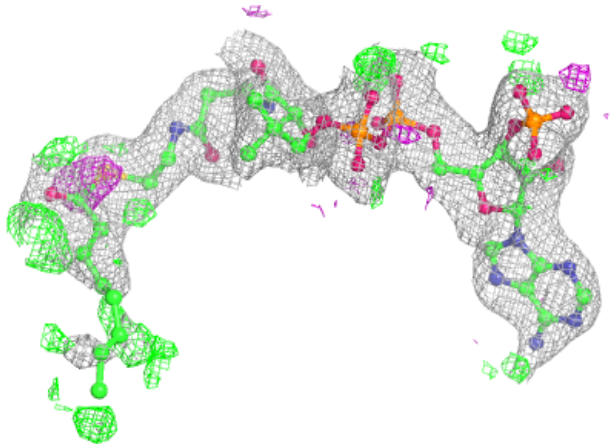


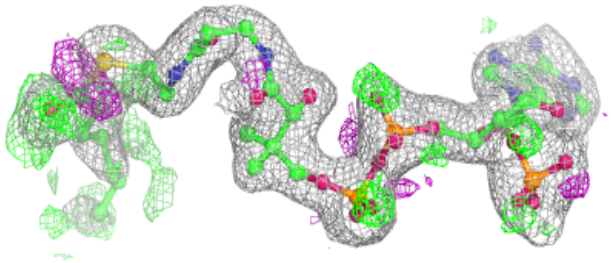


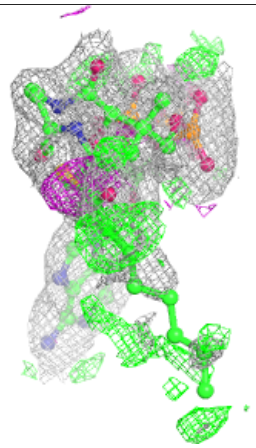


Electron density around CO8 C 401:

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

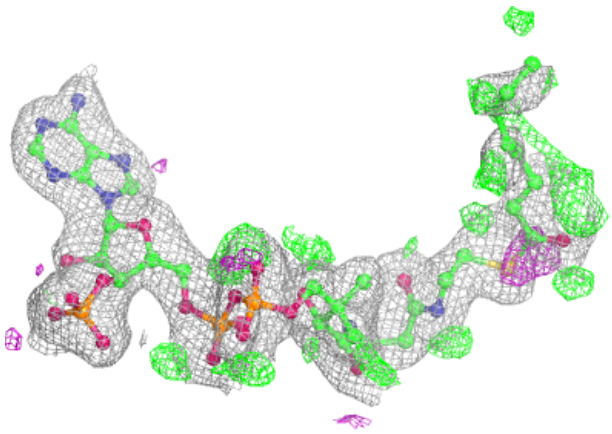


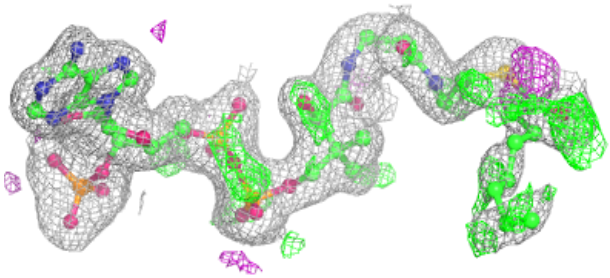


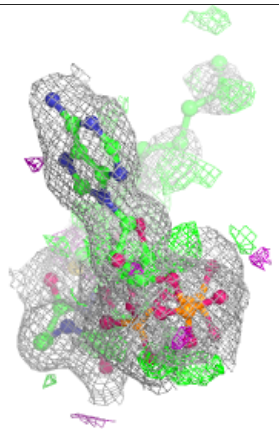


Electron density around CO8 A 401:

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

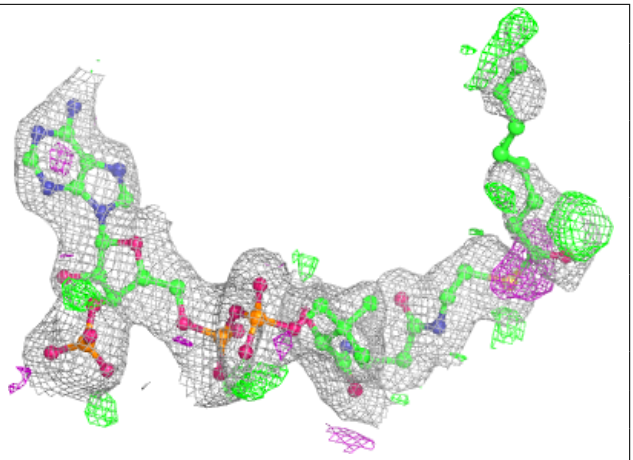


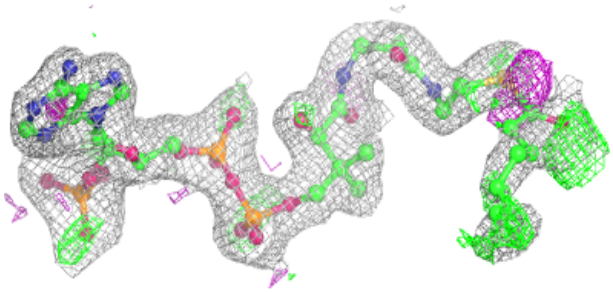


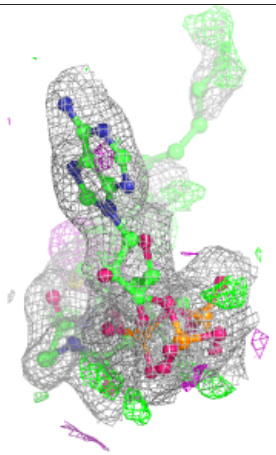


Electron density around CO8 K 401:

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

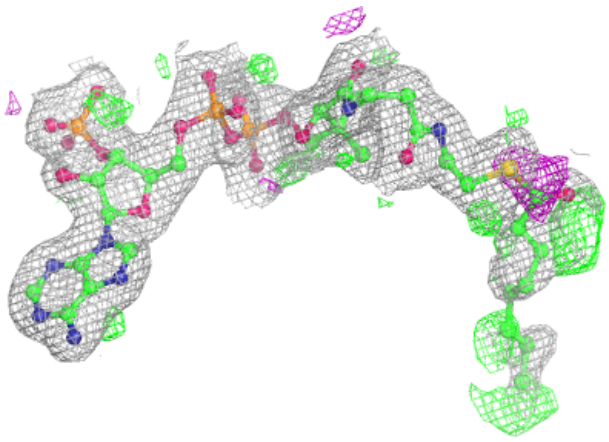


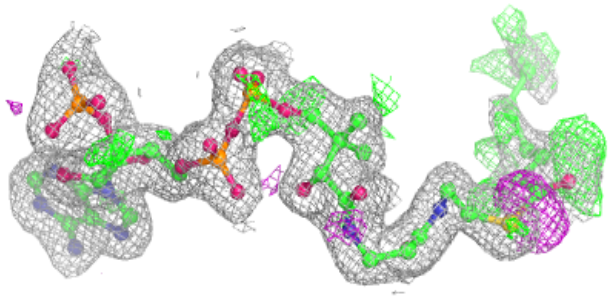


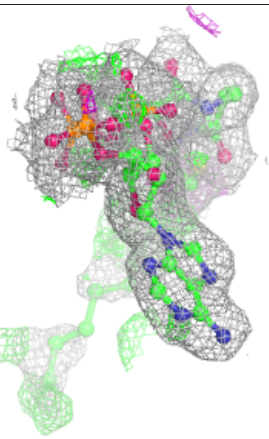


Electron density around CO8 L 401:

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

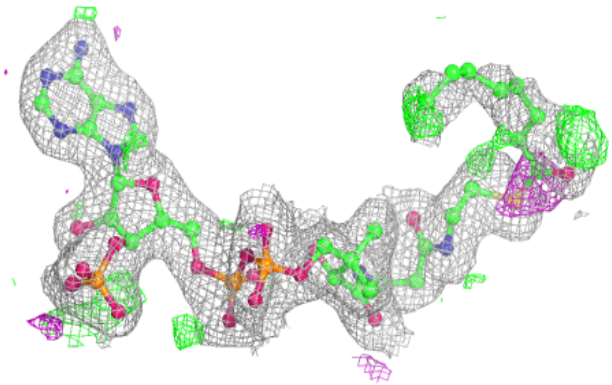


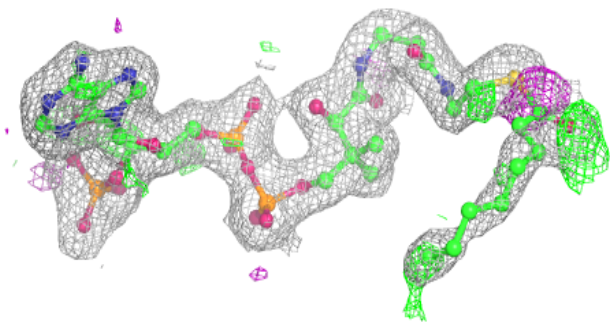


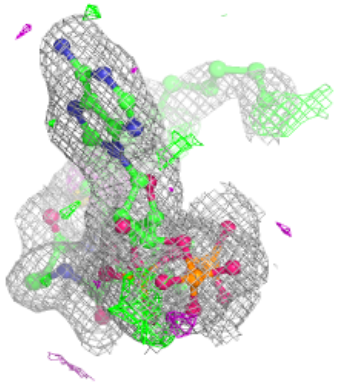


Electron density around CO8 I 401:

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

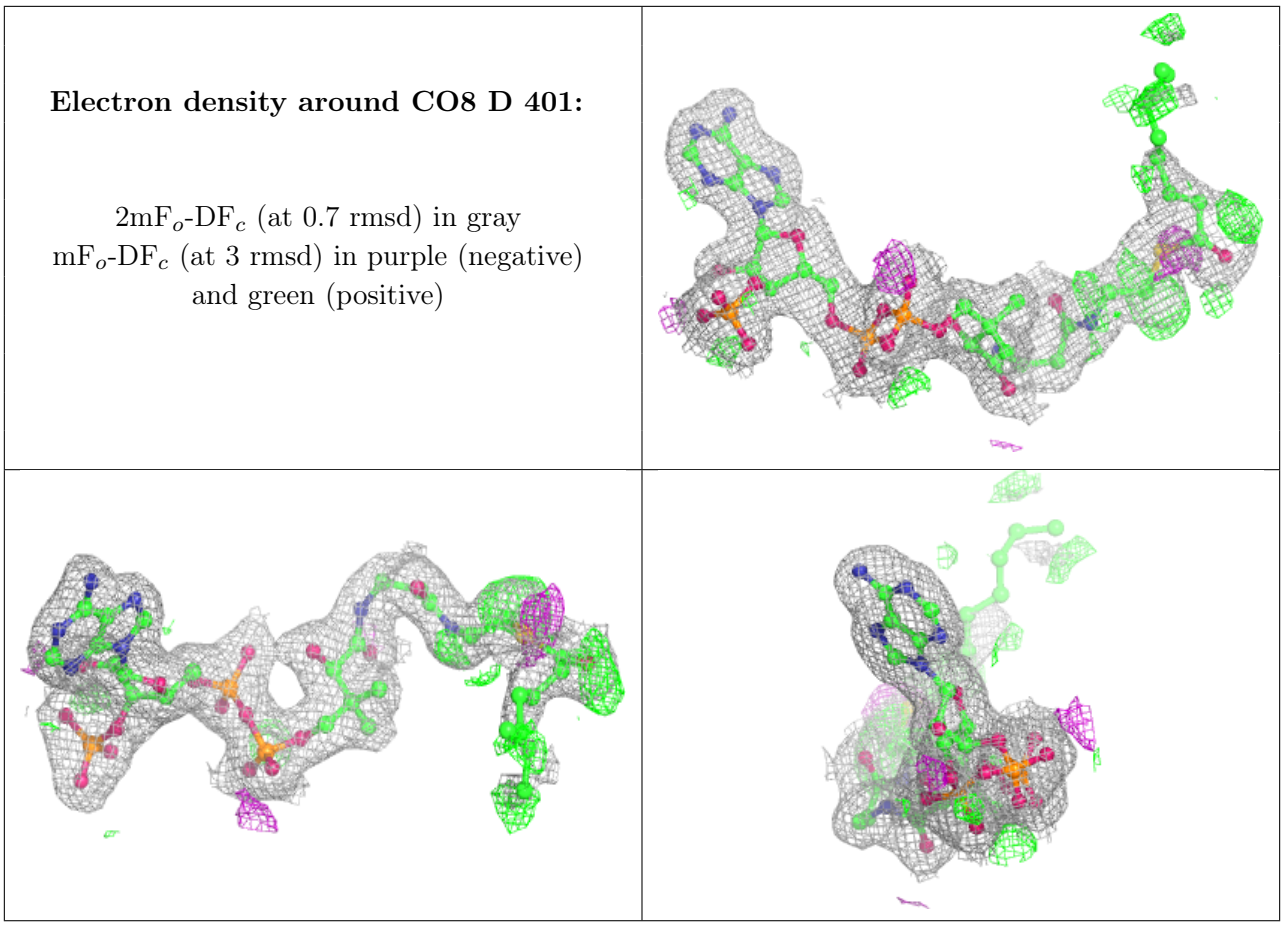






Electron density around CO8 D 401:

$2mF_o$-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.