Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 08:10 pm BST

PDB ID	:	9I32 / pdb_00009i32
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with isobutanoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	1.94 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:

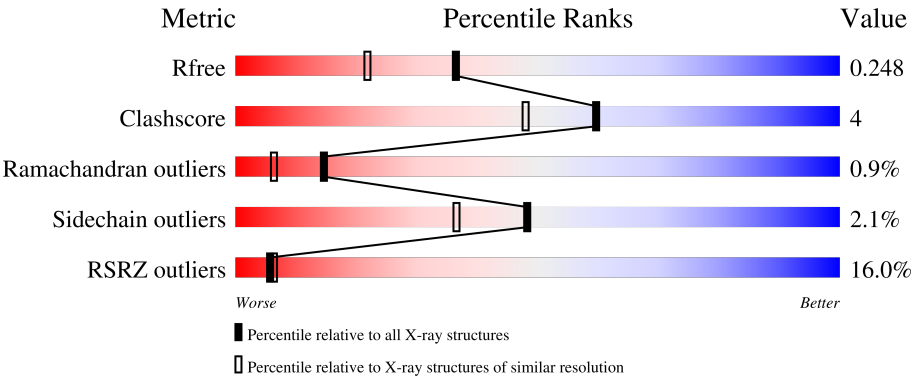
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	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 1.94 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.



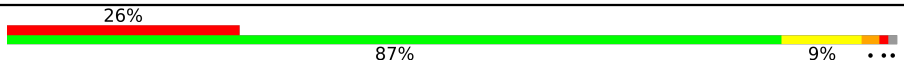
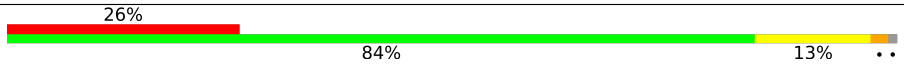
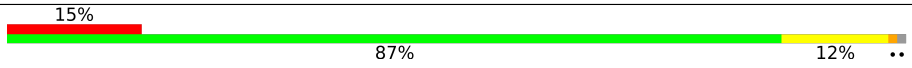
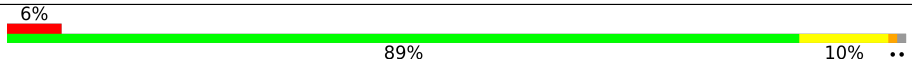
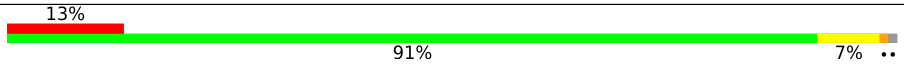
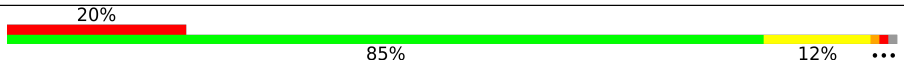
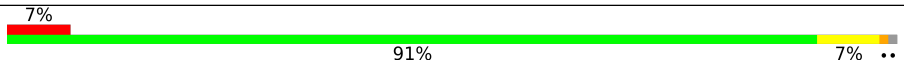
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	14% 88% 10%
1	B	364	12% 88% 9%
1	C	364	24% 87% 11%
1	D	364	12% 88% 10%
1	E	364	14% 85% 12%

Continued on next page...

Continued from previous page...

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 35372 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	360	Total	C	N	O	S	0	4	0
			2735	1713	490	516	16			
1	B	357	Total	C	N	O	S	0	2	0
			2707	1698	486	507	16			
1	C	360	Total	C	N	O	S	0	4	0
			2730	1710	488	516	16			
1	D	360	Total	C	N	O	S	0	1	0
			2719	1705	487	511	16			
1	E	359	Total	C	N	O	S	0	2	0
			2715	1703	487	509	16			
1	F	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	G	360	Total	C	N	O	S	0	3	0
			2726	1708	487	515	16			
1	H	360	Total	C	N	O	S	0	2	0
			2728	1710	489	513	16			
1	I	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	J	360	Total	C	N	O	S	0	1	0
			2719	1705	487	511	16			
1	K	360	Total	C	N	O	S	0	3	0
			2726	1708	488	514	16			
1	L	360	Total	C	N	O	S	0	3	0
			2732	1712	489	515	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

Continued on next page...

Continued from previous page...

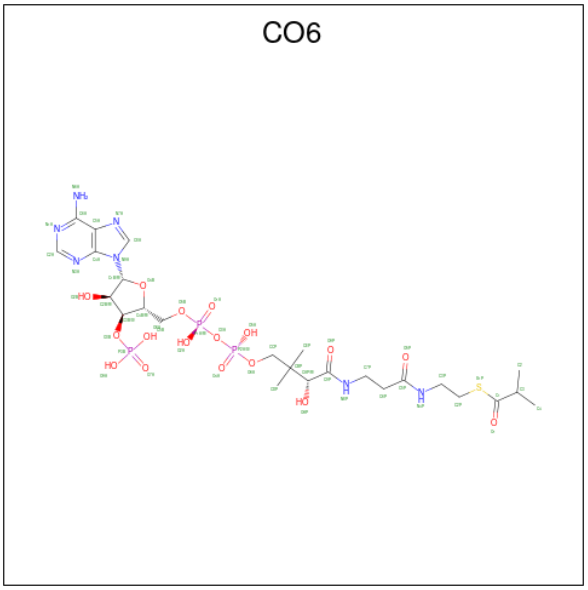
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is ISOBUTYRYL-COENZYME A (CCD ID: CO6) (formula: $C_{25}H_{42}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			53	25	7	17	3	1		

- Molecule 3 is water.

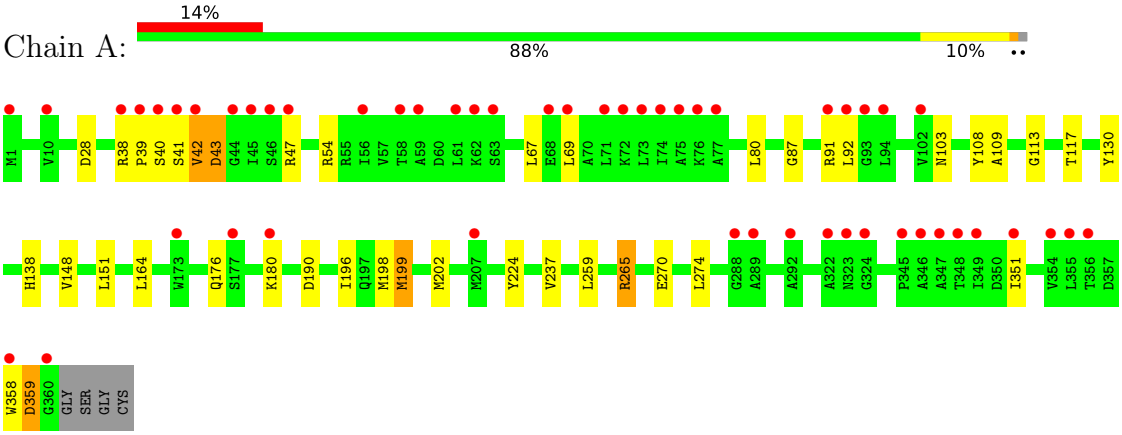
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	156	Total	O	0	0
			156	156		
3	C	152	Total	O	0	0
			152	152		
3	D	167	Total	O	0	0
			167	167		
3	E	166	Total	O	0	0
			166	166		
3	F	146	Total	O	0	0
			146	146		
3	G	151	Total	O	0	0
			151	151		
3	H	162	Total	O	0	0
			162	162		
3	I	215	Total	O	0	0
			215	215		
3	J	198	Total	O	0	0
			198	198		
3	K	184	Total	O	0	0
			184	184		
3	L	190	Total	O	0	0
			190	190		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

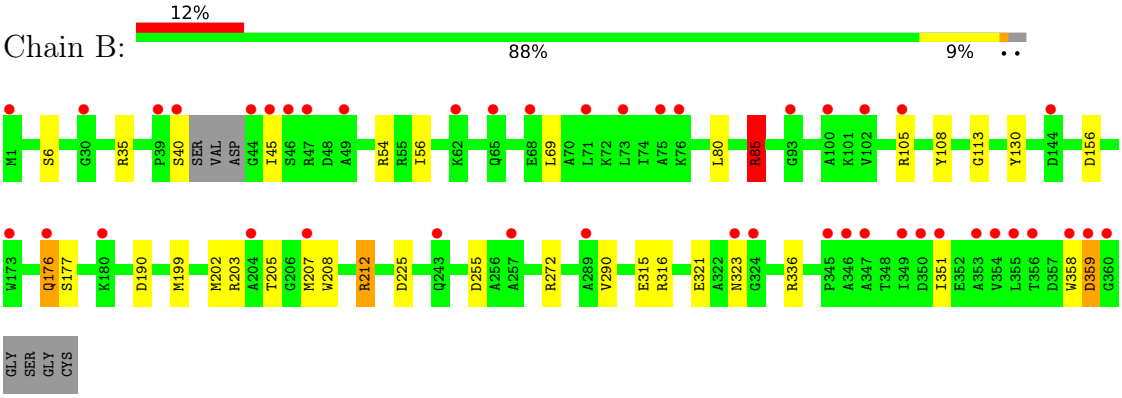
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



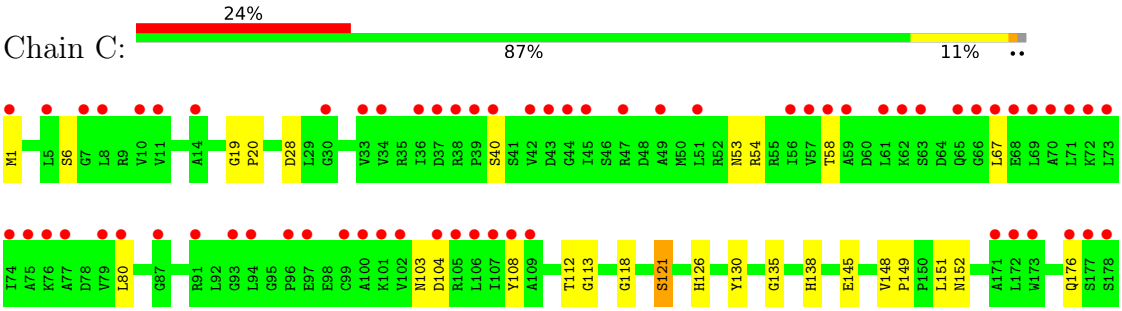
• Molecule 1: Alpha-methylacyl-CoA racemase

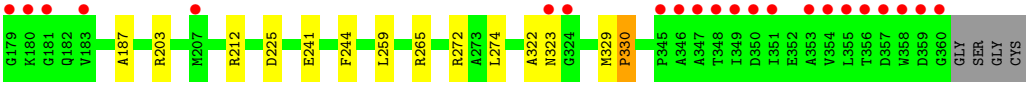
Chain B:



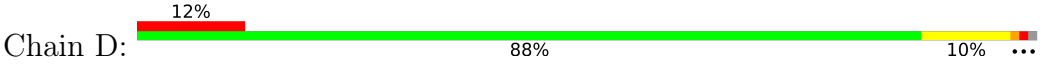
• Molecule 1: Alpha-methylacyl-CoA racemase

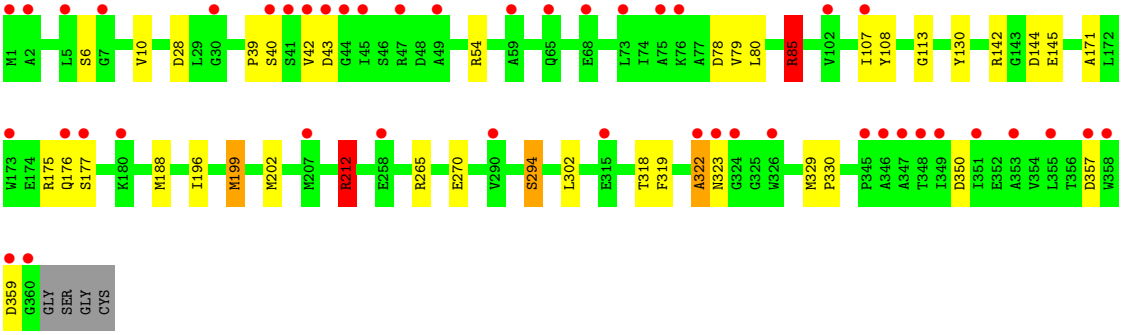
Chain C:



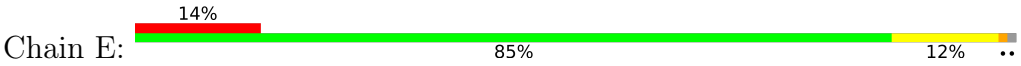


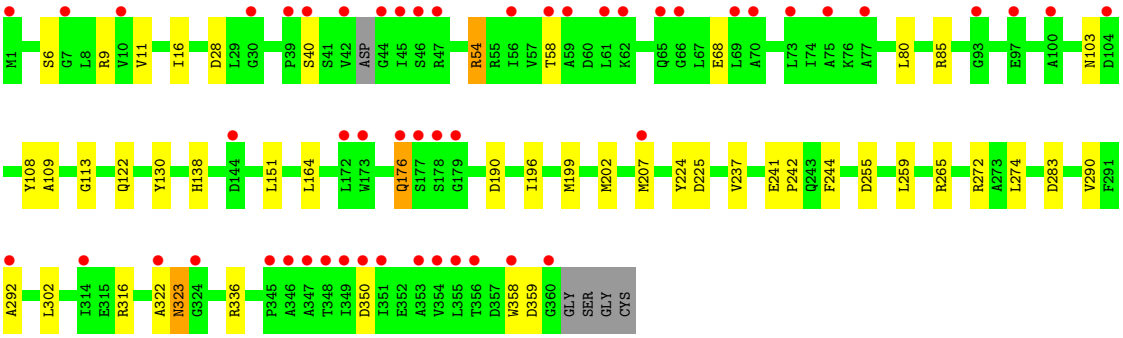
• Molecule 1: Alpha-methylacyl-CoA racemase



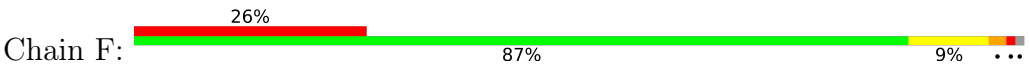


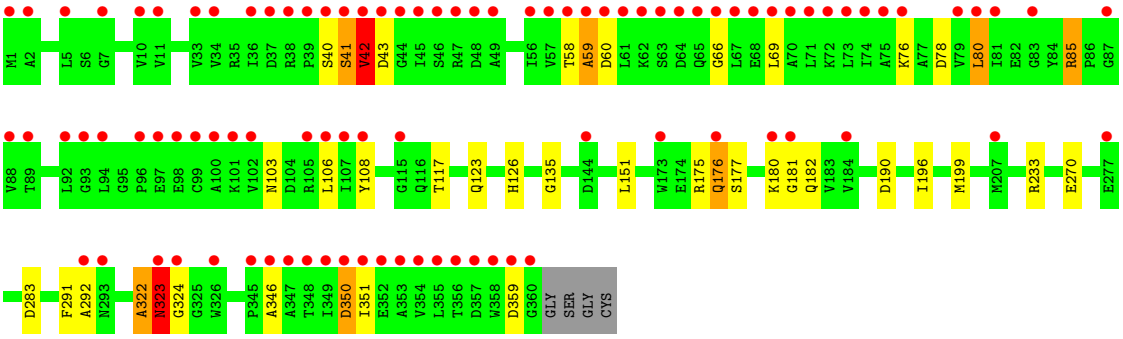
• Molecule 1: Alpha-methylacyl-CoA racemase



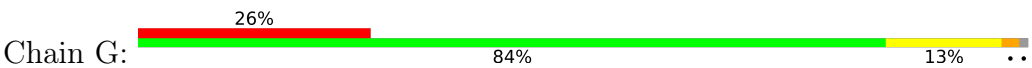


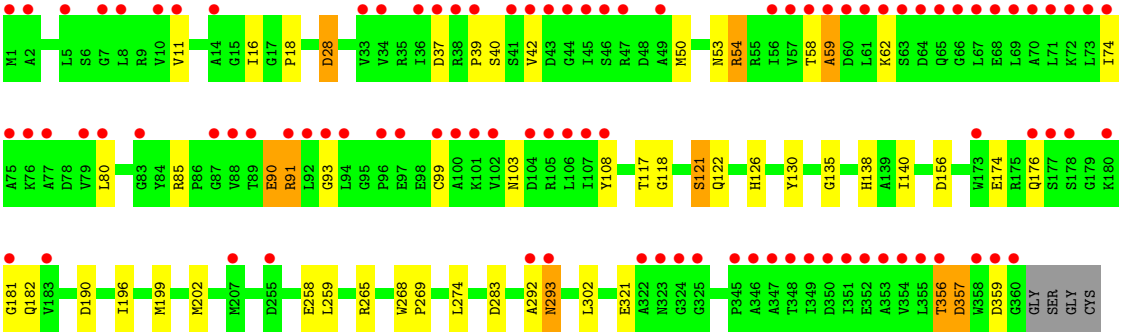
• Molecule 1: Alpha-methylacyl-CoA racemase





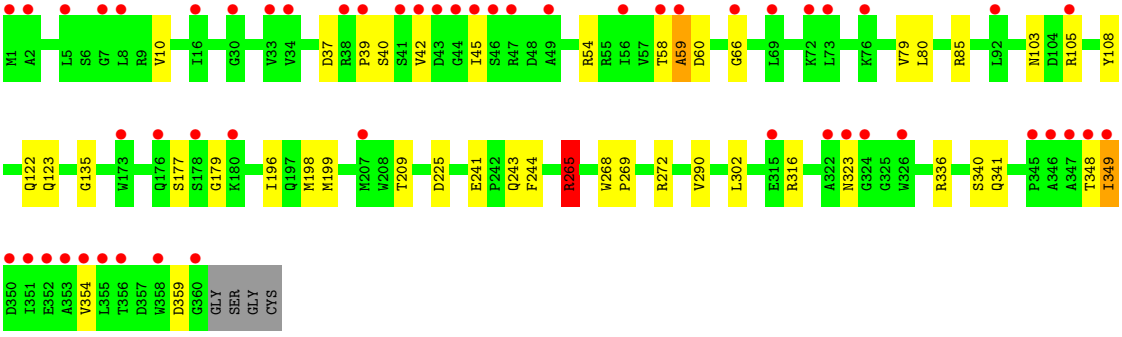
• Molecule 1: Alpha-methylacyl-CoA racemase





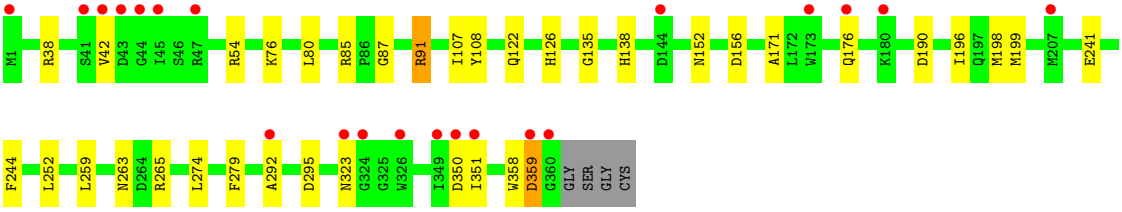
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain H:



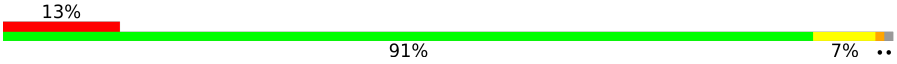
• Molecule 1: Alpha-methylacyl-CoA racemase

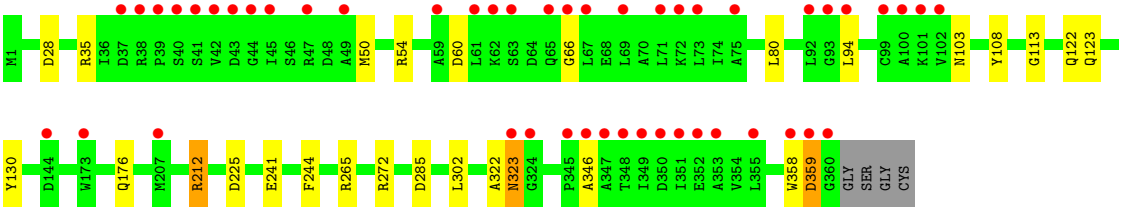
Chain I:



• Molecule 1: Alpha-methylacyl-CoA racemase

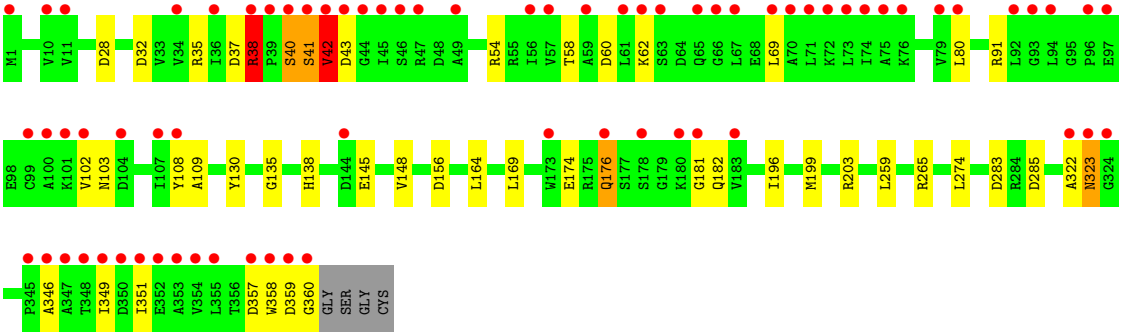
Chain J:





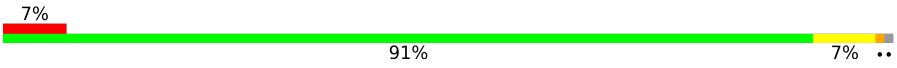
• Molecule 1: Alpha-methylacyl-CoA racemase

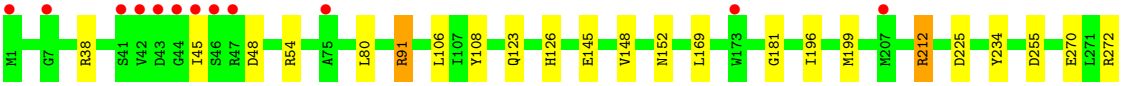
Chain K:

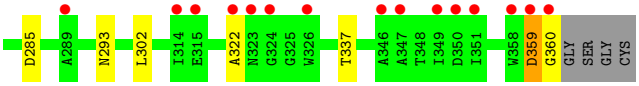


• Molecule 1: Alpha-methylacyl-CoA racemase

Chain L:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	276.49Å 276.49Å 390.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.58 – 1.94 225.58 – 1.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.58-1.94) 99.9 (225.58-1.94)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.207 , 0.238 0.218 , 0.248	Depositor DCC
R_{free} test set	27487 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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 0.007 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	35372	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 2.94% 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: CO6

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	0.66	0/2812	1.03	3/3825 (0.1%)
1	B	0.65	0/2773	1.04	5/3770 (0.1%)
1	C	0.65	0/2811	1.08	3/3824 (0.1%)
1	D	0.67	0/2786	1.06	5/3790 (0.1%)
1	E	0.65	0/2785	1.05	5/3787 (0.1%)
1	F	0.65	0/2795	1.04	4/3802 (0.1%)
1	G	0.64	0/2803	1.07	6/3813 (0.2%)
1	H	0.66	0/2795	1.05	4/3802 (0.1%)
1	I	0.67	0/2795	1.06	8/3802 (0.2%)
1	J	0.68	1/2786 (0.0%)	1.07	8/3790 (0.2%)
1	K	0.67	0/2803	1.08	4/3813 (0.1%)
1	L	0.65	0/2803	1.07	5/3813 (0.1%)
All	All	0.66	1/33547 (0.0%)	1.06	60/45631 (0.1%)

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	3
1	B	0	3
1	D	0	4
1	E	0	2
1	F	0	3
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	5
1	L	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	32

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	285	ASP	CG-OD1	5.87	1.36	1.25

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	123	GLN	CB-CA-C	11.12	127.96	109.84
1	J	123	GLN	CB-CA-C	8.34	123.43	109.84
1	B	203	ARG	CB-CA-C	-7.66	98.08	110.79
1	I	292	ALA	CA-C-N	-7.32	111.67	122.86
1	I	292	ALA	C-N-CA	-7.32	111.67	122.86
1	I	91	ARG	CB-CA-C	-7.07	97.10	110.67
1	B	255	ASP	CB-CA-C	6.99	121.89	110.22
1	C	203	ARG	CB-CA-C	-6.96	99.02	110.85
1	E	28	ASP	CA-CB-CG	6.87	119.47	112.60
1	H	265	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	D	265	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	28	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	156	ASP	CB-CA-C	-6.51	100.62	110.90
1	B	203	ARG	N-CA-CB	6.40	119.53	110.12
1	K	283	ASP	CA-CB-CG	6.38	118.98	112.60
1	D	28	ASP	CA-CB-CG	6.27	118.87	112.60
1	L	91	ARG	CB-CA-C	-6.19	100.15	110.68
1	L	123	GLN	N-CA-CB	-6.17	100.38	109.95
1	G	283[A]	ASP	CA-CB-CG	6.14	118.74	112.60
1	G	283[B]	ASP	CA-CB-CG	6.14	118.74	112.60
1	H	265	ARG	CB-CG-CD	6.09	125.31	111.30
1	L	123	GLN	CB-CG-CD	-5.92	102.54	112.60
1	H	123	GLN	CB-CA-C	5.84	119.36	109.84
1	D	265	ARG	CB-CG-CD	5.78	124.60	111.30
1	A	148	VAL	CA-C-O	5.68	123.03	119.51
1	F	283	ASP	CA-CB-CG	5.64	118.24	112.60
1	F	350	ASP	CB-CA-C	5.61	119.01	109.53
1	I	156	ASP	CB-CA-C	-5.61	102.08	110.88
1	A	190	ASP	CA-CB-CG	5.58	118.18	112.60
1	J	123	GLN	N-CA-CB	-5.58	101.30	109.95
1	I	38	ARG	CB-CA-C	-5.57	100.76	109.11
1	D	144	ASP	CA-CB-CG	5.55	118.15	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	293	ASN	CA-CB-CG	5.54	118.14	112.60
1	E	283	ASP	CA-CB-CG	5.52	118.12	112.60
1	G	28	ASP	CA-CB-CG	5.50	118.09	112.60
1	K	148	VAL	CA-C-O	5.47	122.90	119.51
1	I	190	ASP	CA-CB-CG	5.46	118.06	112.60
1	L	148	VAL	CA-C-O	5.44	122.88	119.51
1	K	28	ASP	CA-CB-CG	5.40	118.00	112.60
1	J	28	ASP	CA-CB-CG	5.39	117.99	112.60
1	G	190	ASP	CA-CB-CG	5.39	117.99	112.60
1	J	265	ARG	CB-CG-CD	5.36	123.63	111.30
1	C	330	PRO	CB-CA-C	-5.30	104.60	111.39
1	E	255	ASP	CB-CA-C	5.30	118.78	110.19
1	D	265	ARG	NE-CZ-NH1	-5.29	116.20	121.50
1	I	265	ARG	CB-CG-CD	5.25	123.37	111.30
1	J	265	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	E	190	ASP	CA-CB-CG	5.17	117.77	112.60
1	K	32	ASP	CA-CB-CG	5.14	117.74	112.60
1	J	54	ARG	CB-CA-C	-5.12	98.82	110.07
1	H	265	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	C	203	ARG	N-CA-CB	5.09	117.70	110.16
1	F	323	ASN	CB-CA-C	5.08	120.54	110.42
1	F	190	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	255	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	190	ASP	CA-CB-CG	5.06	117.66	112.60
1	I	156	ASP	CA-CB-CG	5.05	117.65	112.60
1	J	265	ARG	CB-CA-C	5.04	119.16	110.79
1	J	285	ASP	CB-CA-C	5.02	120.31	110.67
1	G	91	ARG	CB-CA-C	-5.01	100.45	110.42

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	54	ARG	Peptide
1	B	212	ARG	Sidechain
1	B	54	ARG	Peptide
1	B	85	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	54	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	85	ARG	Sidechain
1	E	350	ASP	Peptide
1	E	54	ARG	Peptide
1	F	233	ARG	Sidechain
1	F	322	ALA	Peptide
1	F	85	ARG	Sidechain
1	G	54	ARG	Peptide
1	G	91	ARG	Sidechain
1	H	323	ASN	Peptide
1	H	54	ARG	Peptide
1	I	42	VAL	Peptide
1	I	54	ARG	Peptide
1	J	212	ARG	Sidechain
1	J	35	ARG	Sidechain
1	K	265	ARG	Sidechain
1	K	35	ARG	Sidechain
1	K	38	ARG	Sidechain
1	K	54	ARG	Peptide
1	K	91	ARG	Sidechain
1	L	212	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	2735	0	2670	29	0
1	B	2707	0	2651	25	0
1	C	2730	0	2663	26	0
1	D	2719	0	2663	26	0
1	E	2715	0	2660	26	0
1	F	2722	0	2661	28	0
1	G	2726	0	2661	37	0
1	H	2728	0	2670	25	0
1	I	2722	0	2661	22	0
1	J	2719	0	2663	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2726	0	2663	26	0
1	L	2732	0	2670	16	0
2	A	53	0	38	0	0
2	B	53	0	38	3	0
2	C	53	0	38	3	0
2	D	53	0	38	5	0
2	E	53	0	38	1	0
2	F	53	0	38	3	0
2	G	53	0	38	5	0
2	H	53	0	38	2	0
2	I	53	0	38	3	0
2	J	53	0	38	0	0
2	K	53	0	38	2	0
2	L	53	0	38	3	0
3	A	168	0	0	4	0
3	B	156	0	0	5	0
3	C	152	0	0	1	0
3	D	167	0	0	1	0
3	E	166	0	0	3	0
3	F	146	0	0	2	0
3	G	151	0	0	3	0
3	H	162	0	0	2	0
3	I	215	0	0	4	0
3	J	198	0	0	3	0
3	K	184	0	0	6	0
3	L	190	0	0	4	0
All	All	35372	0	32412	276	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 (276) 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)
2:L:401:CO6:S1P	2:L:401:CO6:C1	2.02	1.47
1:F:85:ARG:HD3	2:F:401:CO6:O1A	1.56	1.02
1:D:85:ARG:HD3	2:D:401:CO6:O1A	1.74	0.88
1:C:118:GLY:O	1:C:121:SER:OG	1.97	0.81
1:G:126:HIS:HA	2:G:401:CO6:H22	1.64	0.80
1:K:40:SER:OG	3:K:501:HOH:O	1.99	0.79
1:F:85:ARG:CD	2:F:401:CO6:O1A	2.31	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.04	0.75
1:E:199:MET:HE3	1:E:202:MET:HE1	1.69	0.75
1:F:80:LEU:HD22	1:F:108:TYR:CE2	2.22	0.74
1:A:199:MET:HE3	1:A:202:MET:HE1	1.71	0.73
1:C:1:MET:O	1:C:6:SER:OG	2.07	0.72
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.72	0.71
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.71	0.71
1:G:90:GLU:O	1:G:93:GLY:N	2.20	0.70
1:E:292:ALA:O	3:E:501:HOH:O	2.12	0.67
1:C:80:LEU:CD2	1:C:108:TYR:CE1	2.78	0.66
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.31	0.65
1:B:315:GLU:OE1	3:B:501:HOH:O	2.15	0.64
1:A:199:MET:HE3	1:A:202:MET:CE	2.27	0.64
1:D:199:MET:HE3	1:D:202:MET:HE1	1.80	0.63
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.13	0.62
1:G:85:ARG:NH1	1:G:122:GLN:O	2.31	0.62
1:K:176:GLN:HA	1:K:176:GLN:HE21	1.64	0.62
1:A:40:SER:OG	3:A:501:HOH:O	2.16	0.62
1:E:199:MET:HE3	1:E:202:MET:CE	2.29	0.61
1:G:199:MET:HE3	1:G:202:MET:CE	2.31	0.61
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.82	0.60
1:K:138:HIS:HD2	3:K:593:HOH:O	1.83	0.60
1:G:118:GLY:O	1:G:121:SER:OG	2.19	0.60
1:I:358:TRP:O	1:I:359:ASP:HB2	2.01	0.60
1:K:156:ASP:OD1	2:K:401:CO6:S1P	2.59	0.60
1:B:85:ARG:CD	2:B:401:CO6:O1A	2.51	0.59
1:J:322:ALA:O	1:J:323:ASN:C	2.45	0.59
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.85	0.58
1:G:80:LEU:CD2	1:G:108:TYR:CE2	2.86	0.58
1:K:346:ALA:HB3	3:K:548:HOH:O	2.03	0.58
1:G:80:LEU:HD23	1:G:108:TYR:CE2	2.39	0.57
1:B:85:ARG:HD2	2:B:401:CO6:O1A	2.04	0.57
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.39	0.57
1:G:39:PRO:HD2	3:G:518:HOH:O	2.03	0.57
1:A:47:ARG:HG2	1:B:205:THR:HG22	1.86	0.57
1:L:48:ASP:HB2	3:L:618:HOH:O	2.05	0.57
1:C:138:HIS:HD2	3:C:567:HOH:O	1.87	0.56
1:G:58:THR:O	1:G:59:ALA:HB2	2.04	0.56
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.40	0.56
1:F:58:THR:O	1:F:59:ALA:HB2	2.05	0.56
1:G:50:MET:HE1	1:H:198:MET:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLY:O	1:A:91:ARG:HG3	2.06	0.56
1:K:80:LEU:HD23	1:K:108:TYR:CE2	2.41	0.56
1:A:138:HIS:HD2	3:A:532:HOH:O	1.89	0.56
1:E:85:ARG:NH1	1:E:122:GLN:O	2.34	0.56
1:H:241:GLU:HB2	1:H:244:PHE:CD2	2.41	0.56
1:L:285:ASP:HB2	3:L:503:HOH:O	2.05	0.56
1:C:80:LEU:HD23	1:C:108:TYR:CE1	2.40	0.56
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.21	0.56
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.88	0.56
1:B:358:TRP:O	1:B:359:ASP:HB2	2.06	0.55
1:B:199:MET:HE3	1:B:202:MET:CE	2.36	0.55
1:D:39:PRO:O	1:D:42:VAL:HG12	2.06	0.55
1:K:38:ARG:HB2	3:K:501:HOH:O	2.06	0.55
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.42	0.55
1:L:152:ASN:HD22	2:L:401:CO6:H42	1.72	0.55
1:F:323:ASN:CG	1:F:324:GLY:H	2.15	0.54
1:I:152:ASN:HD22	2:I:401:CO6:H12	1.72	0.54
1:B:199:MET:HE3	1:B:202:MET:HE1	1.87	0.54
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.41	0.54
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.42	0.54
1:H:349:ILE:HD11	1:H:354:VAL:HG22	1.88	0.54
1:A:39:PRO:O	1:A:42:VAL:HG23	2.08	0.54
1:C:152:ASN:HD22	2:C:401:CO6:H42	1.72	0.54
1:E:138:HIS:HD2	3:E:583:HOH:O	1.92	0.53
1:F:323:ASN:CG	1:F:324:GLY:N	2.66	0.53
1:J:346:ALA:HB3	3:J:609:HOH:O	2.08	0.53
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.90	0.53
1:A:42:VAL:HG12	1:A:43:ASP:H	1.72	0.53
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.42	0.53
1:D:199:MET:HE3	1:D:202:MET:CE	2.39	0.53
1:F:346:ALA:HB3	3:F:529:HOH:O	2.08	0.53
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.40	0.53
1:A:69:LEU:HD13	1:A:351:ILE:CG2	2.39	0.52
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.90	0.52
1:J:122:GLN:HG2	3:J:503:HOH:O	2.09	0.52
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.92	0.52
1:D:85:ARG:CD	2:D:401:CO6:O1A	2.53	0.52
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.45	0.52
1:F:40:SER:O	1:F:41:SER:CB	2.58	0.52
1:F:106:LEU:O	1:F:181:GLY:HA3	2.10	0.52
1:K:358:TRP:O	1:K:360:GLY:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:HD13	1:A:351:ILE:HG21	1.92	0.51
1:D:294:SER:HB2	1:L:293:ASN:O	2.11	0.51
1:D:10:VAL:HG22	1:D:79:VAL:HB	1.92	0.51
1:G:265:ARG:NH2	3:G:508:HOH:O	2.41	0.51
1:I:198:MET:HB2	1:J:50:MET:HE1	1.93	0.51
1:A:80:LEU:CD2	1:A:108:TYR:CE2	2.94	0.51
1:B:105:ARG:NH1	3:B:507:HOH:O	2.44	0.51
1:F:196:ILE:HG12	1:F:199:MET:HB2	1.93	0.51
1:B:202:MET:HE3	1:B:208:TRP:CE3	2.45	0.51
1:G:199:MET:HE3	1:G:202:MET:HE1	1.91	0.51
1:C:126:HIS:CE1	2:C:401:CO6:H12	2.45	0.51
1:C:145:GLU:CD	1:D:145:GLU:OE1	2.54	0.51
1:E:109:ALA:HB1	1:E:164:LEU:HD11	1.92	0.50
1:E:322:ALA:O	1:E:323:ASN:C	2.53	0.50
1:G:39:PRO:HA	1:G:58:THR:HG23	1.94	0.50
2:H:401:CO6:H42	2:H:401:CO6:H21	1.94	0.50
1:K:41:SER:O	1:K:42:VAL:HG23	2.11	0.50
1:H:39:PRO:HD2	3:H:521:HOH:O	2.11	0.50
1:D:188:MET:HE1	2:D:401:CO6:H21	1.93	0.50
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.76	0.49
1:E:292:ALA:O	1:F:123:GLN:NE2	2.45	0.49
1:I:351:ILE:HG23	3:I:598:HOH:O	2.13	0.49
1:K:285:ASP:CB	3:K:502:HOH:O	2.60	0.49
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.47	0.49
1:F:291:PHE:O	1:F:292:ALA:C	2.55	0.49
2:H:401:CO6:H141	2:H:401:CO6:O9P	2.13	0.49
1:L:270:GLU:HG3	3:L:534:HOH:O	2.11	0.49
1:B:85:ARG:HD3	2:B:401:CO6:O1A	2.12	0.49
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.94	0.48
1:D:142:ARG:O	1:D:212:ARG:HD2	2.13	0.48
1:B:40:SER:C	3:B:525:HOH:O	2.55	0.48
1:C:322:ALA:O	1:C:323:ASN:C	2.56	0.48
1:G:199:MET:HE3	1:G:202:MET:HE2	1.94	0.48
1:K:259:LEU:CD2	1:K:274:LEU:HD13	2.43	0.48
1:D:318:THR:HG22	1:D:319:PHE:CE1	2.48	0.48
1:D:329:MET:HE3	1:D:330:PRO:HD2	1.95	0.48
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.29	0.48
1:E:176:GLN:HG3	1:F:176:GLN:NE2	2.28	0.48
1:K:69:LEU:HD13	1:K:351:ILE:HG21	1.94	0.48
1:G:39:PRO:CA	1:G:58:THR:HG23	2.44	0.48
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ASP:O	1:J:66:GLY:HA3	2.14	0.48
1:A:91:ARG:HD2	1:E:242:PRO:HB3	1.96	0.48
1:I:176:GLN:HE21	1:I:176:GLN:HA	1.79	0.47
1:I:241:GLU:HB2	1:I:244:PHE:CD2	2.49	0.47
1:K:285:ASP:HB2	3:K:502:HOH:O	2.13	0.47
1:G:156:ASP:OD2	2:G:401:CO6:C1	2.62	0.47
1:H:243[B]:GLN:HG2	3:H:630:HOH:O	2.12	0.47
1:I:138:HIS:HD2	3:I:528:HOH:O	1.98	0.47
1:I:351:ILE:CG2	3:I:598:HOH:O	2.62	0.47
1:F:40:SER:O	1:F:41:SER:HB3	2.15	0.47
1:I:85:ARG:NH1	1:I:122:GLN:O	2.45	0.47
1:A:198:MET:HG2	1:A:202:MET:HE2	1.95	0.47
1:A:270:GLU:HG3	3:A:559:HOH:O	2.13	0.47
1:L:126:HIS:ND1	2:L:401:CO6:H12	2.29	0.47
1:G:37:ASP:HB3	1:G:42:VAL:CG2	2.45	0.47
1:I:263:ASN:HB2	3:I:596:HOH:O	2.14	0.47
1:J:358:TRP:O	1:J:359:ASP:HB2	2.15	0.47
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.50	0.46
1:I:126:HIS:CE1	2:I:401:CO6:H42	2.51	0.46
1:B:212:ARG:HG2	3:B:523:HOH:O	2.15	0.46
1:H:45:ILE:HD12	1:H:45:ILE:H	1.80	0.46
1:K:109:ALA:HB1	1:K:164:LEU:HD11	1.98	0.46
1:K:196:ILE:HG12	1:K:199:MET:HB2	1.97	0.46
1:A:176:GLN:NE2	1:B:176:GLN:HG2	2.31	0.46
1:G:138:HIS:HD2	3:G:559:HOH:O	1.98	0.46
1:E:302:LEU:O	1:F:135:GLY:HA2	2.16	0.46
1:G:74:ILE:HG21	1:G:99:CYS:SG	2.56	0.46
1:A:39:PRO:HA	1:A:42:VAL:HG23	1.98	0.46
1:E:196:ILE:HG12	1:E:199:MET:HB2	1.97	0.46
1:G:356:THR:HG22	1:G:357:ASP:N	2.30	0.46
1:C:148:VAL:HG23	1:C:149:PRO:HD2	1.97	0.46
1:E:259:LEU:HD22	1:E:274:LEU:HD13	1.98	0.46
1:G:302:LEU:O	1:H:135:GLY:HA2	2.16	0.46
1:C:126:HIS:ND1	2:C:401:CO6:H12	2.31	0.45
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.51	0.45
1:C:176:GLN:CD	1:D:176:GLN:HG2	2.41	0.45
1:D:270:GLU:HG3	3:D:559:HOH:O	2.15	0.45
1:K:145:GLU:OE2	1:L:145:GLU:OE1	2.33	0.45
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.52	0.45
1:E:113:GLY:HA3	1:E:130:TYR:CZ	2.51	0.45
1:E:316:ARG:HD2	1:F:117:THR:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.99	0.45
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.98	0.45
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.81	0.45
1:B:80:LEU:CD2	1:B:108:TYR:CE2	2.99	0.45
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.32	0.45
1:H:37:ASP:O	1:H:58:THR:HA	2.17	0.45
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.49	0.45
1:D:318:THR:HG22	1:D:319:PHE:CD1	2.52	0.45
1:H:60:ASP:O	1:H:66:GLY:HA3	2.17	0.45
1:K:181:GLY:O	1:K:182:GLN:HB3	2.17	0.45
1:K:176:GLN:HE21	1:K:176:GLN:CA	2.30	0.44
1:K:169:LEU:HB3	1:L:169:LEU:HB3	1.98	0.44
1:D:107:ILE:HD12	1:D:171:ALA:HB1	1.98	0.44
1:A:117:THR:O	1:B:316:ARG:HD2	2.17	0.44
1:C:19:GLY:N	1:C:20:PRO:CD	2.81	0.44
1:G:176:GLN:HA	1:G:176:GLN:NE2	2.32	0.44
1:H:10:VAL:HG22	1:H:79:VAL:HB	1.99	0.44
1:K:174:GLU:HG3	1:L:337:THR:HG21	2.00	0.44
1:H:80:LEU:HD23	1:H:108:TYR:CD2	2.52	0.44
1:E:265:ARG:HD2	3:E:505:HOH:O	2.16	0.44
1:G:196:ILE:HG12	1:G:199:MET:HB2	2.00	0.44
1:F:322:ALA:O	1:F:323:ASN:C	2.60	0.43
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.99	0.43
1:F:76:LYS:HE3	1:F:359:ASP:HB2	2.01	0.43
1:L:234:TYR:OH	3:L:501:HOH:O	2.21	0.43
1:H:58:THR:O	1:H:59:ALA:HB2	2.19	0.43
1:H:340:SER:O	1:H:341:GLN:C	2.62	0.43
1:B:69:LEU:HD13	1:B:351:ILE:CG2	2.49	0.43
1:E:9:ARG:NH2	1:E:358:TRP:HA	2.32	0.43
1:E:80:LEU:CD2	1:E:108:TYR:CE2	3.01	0.43
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.52	0.43
1:G:181:GLY:O	1:G:182:GLN:HB3	2.19	0.43
1:G:176:GLN:HA	1:G:176:GLN:HE21	1.84	0.43
1:I:196:ILE:HG12	1:I:199:MET:HB2	2.01	0.43
1:L:225:ASP:OD2	1:L:272:ARG:NH1	2.52	0.43
1:D:85:ARG:HD3	2:D:401:CO6:P1A	2.59	0.43
1:G:11:VAL:HG12	1:G:80:LEU:HD12	2.00	0.43
1:G:18:PRO:HB3	1:G:156:ASP:O	2.19	0.43
1:H:196:ILE:HG12	1:H:199:MET:HB2	2.01	0.43
1:K:135:GLY:HA2	1:L:302:LEU:O	2.19	0.43
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ASP:OD1	1:F:175:ARG:NH2	2.43	0.42
1:K:37:ASP:O	1:K:58:THR:HA	2.19	0.42
1:B:45:ILE:HD12	1:B:45:ILE:H	1.84	0.42
1:B:359:ASP:HA	3:B:528:HOH:O	2.18	0.42
1:H:105:ARG:HG2	1:H:179:GLY:O	2.20	0.42
1:C:138:HIS:O	1:C:212:ARG:HD3	2.19	0.42
1:D:78:ASP:OD1	1:D:175:ARG:NH2	2.44	0.42
1:E:11:VAL:O	1:E:80:LEU:HA	2.19	0.42
1:H:265:ARG:HG2	1:H:268:TRP:CZ3	2.54	0.42
1:E:16:ILE:HD12	2:E:401:CO6:H43	2.01	0.42
1:G:62:LYS:NZ	2:G:401:CO6:O7A	2.52	0.42
1:H:85:ARG:NH2	1:H:122:GLN:O	2.51	0.42
1:I:126:HIS:ND1	2:I:401:CO6:H42	2.34	0.42
1:J:212:ARG:HG2	3:J:535:HOH:O	2.18	0.42
1:K:322:ALA:O	1:K:323:ASN:C	2.63	0.42
1:A:80:LEU:HD22	1:A:108:TYR:CE2	2.55	0.42
1:E:113:GLY:HA3	1:E:130:TYR:CE1	2.54	0.42
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.45	0.42
1:E:224:TYR:HA	1:E:237:VAL:O	2.19	0.42
1:F:80:LEU:HD22	1:F:108:TYR:CD2	2.55	0.42
1:C:67:LEU:HD12	1:C:67:LEU:O	2.19	0.41
1:F:60:ASP:O	1:F:66:GLY:HA3	2.20	0.41
1:G:16:ILE:HD12	2:G:401:CO6:C2	2.50	0.41
1:L:106:LEU:O	1:L:181:GLY:HA3	2.19	0.41
1:F:42:VAL:HG12	1:F:43:ASP:N	2.34	0.41
1:K:60:ASP:OD1	1:K:62:LYS:HB2	2.20	0.41
1:A:67:LEU:HD13	1:A:92:LEU:O	2.20	0.41
1:C:80:LEU:HD22	1:C:108:TYR:CE1	2.54	0.41
1:D:85:ARG:HD2	2:D:401:CO6:H10	2.02	0.41
1:I:135:GLY:HA2	1:J:302:LEU:O	2.20	0.41
1:C:112:THR:O	1:C:187:ALA:HA	2.20	0.41
1:G:174:GLU:OE1	1:G:174:GLU:C	2.63	0.41
1:I:252:LEU:HD21	1:I:279:PHE:CE1	2.56	0.41
1:J:94:LEU:HD23	1:J:94:LEU:HA	1.92	0.41
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.56	0.41
1:A:180:LYS:O	1:B:336:ARG:NH2	2.53	0.41
1:A:224:TYR:HA	1:A:237:VAL:O	2.21	0.41
1:F:270:GLU:HG3	3:F:544:HOH:O	2.19	0.41
1:I:87:GLY:O	1:I:91:ARG:HG3	2.20	0.41
1:F:126:HIS:HA	2:F:401:CO6:H32	2.03	0.41
1:I:107:ILE:HD12	1:I:171:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HB3	1:B:56:ILE:HD13	2.03	0.41
1:J:241:GLU:HB2	1:J:244:PHE:CD2	2.55	0.41
1:A:109:ALA:HB1	1:A:164:LEU:HD11	2.02	0.41
1:A:39:PRO:HA	1:A:42:VAL:CG2	2.51	0.41
1:A:265:ARG:NH2	3:A:517:HOH:O	2.53	0.41
1:D:322:ALA:O	1:D:323:ASN:C	2.63	0.41
1:L:359:ASP:O	1:L:360:GLY:C	2.63	0.41
1:C:135:GLY:HA2	1:D:302:LEU:O	2.21	0.40
1:G:58:THR:O	1:G:59:ALA:CB	2.69	0.40
1:G:135:GLY:HA2	1:H:302:LEU:O	2.21	0.40
1:H:268:TRP:N	1:H:269:PRO:CD	2.83	0.40
1:A:358:TRP:O	1:A:359:ASP:CB	2.69	0.40
1:B:69:LEU:HD13	1:B:351:ILE:HG21	2.03	0.40
1:K:130:TYR:HE2	2:K:401:CO6:H31	1.87	0.40
1:F:181:GLY:O	1:F:182:GLN:HB3	2.21	0.40
1:G:117:THR:O	1:H:316:ARG:HD2	2.22	0.40
1:G:130:TYR:HE2	2:G:401:CO6:H21	1.87	0.40
1:I:244:PHE:CD1	1:I:295:ASP:HB3	2.57	0.40
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.57	0.40
1:C:241:GLU:HB2	1:C:244:PHE:CD2	2.56	0.40
1:E:241:GLU:HB2	1:E:244:PHE:CD2	2.56	0.40
1:G:268:TRP:N	1:G:269:PRO:CD	2.84	0.40
1:H:42:VAL:HG11	1:H:348:THR:OG1	2.22	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	362/364 (100%)	342 (94%)	14 (4%)	6 (2%)	7 1
1	B	355/364 (98%)	341 (96%)	12 (3%)	2 (1%)	22 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	362/364 (100%)	348 (96%)	12 (3%)	2 (1%)	22 12
1	D	359/364 (99%)	343 (96%)	15 (4%)	1 (0%)	37 30
1	E	357/364 (98%)	338 (95%)	15 (4%)	4 (1%)	12 4
1	F	360/364 (99%)	338 (94%)	17 (5%)	5 (1%)	9 2
1	G	361/364 (99%)	335 (93%)	21 (6%)	5 (1%)	9 2
1	H	360/364 (99%)	342 (95%)	15 (4%)	3 (1%)	16 7
1	I	360/364 (99%)	346 (96%)	12 (3%)	2 (1%)	22 12
1	J	359/364 (99%)	347 (97%)	9 (2%)	3 (1%)	16 7
1	K	361/364 (99%)	346 (96%)	11 (3%)	4 (1%)	12 4
1	L	361/364 (99%)	346 (96%)	14 (4%)	1 (0%)	37 30
All	All	4317/4368 (99%)	4112 (95%)	167 (4%)	38 (1%)	14 6

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	ASP
1	B	359	ASP
1	C	103	ASN
1	F	41	SER
1	F	103	ASN
1	G	103	ASN
1	I	359	ASP
1	A	41	SER
1	A	103	ASN
1	D	359	ASP
1	E	323	ASN
1	F	59	ALA
1	G	59	ALA
1	I	323	ASN
1	J	323	ASN
1	K	103	ASN
1	F	151	LEU
1	H	59	ALA
1	H	103	ASN
1	A	42	VAL
1	A	43	ASP
1	B	323	ASN
1	G	292	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	359	ASP
1	J	103	ASN
1	J	359	ASP
1	K	42	VAL
1	K	359	ASP
1	L	359	ASP
1	A	151	LEU
1	C	151	LEU
1	E	103	ASN
1	E	151	LEU
1	E	359	ASP
1	G	90	GLU
1	G	359	ASP
1	K	323	ASN
1	F	42	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	279/277 (101%)	278 (100%)	1 (0%)	89 89
1	B	274/277 (99%)	267 (97%)	7 (3%)	41 28
1	C	279/277 (101%)	273 (98%)	6 (2%)	47 35
1	D	276/277 (100%)	266 (96%)	10 (4%)	30 17
1	E	276/277 (100%)	268 (97%)	8 (3%)	37 24
1	F	277/277 (100%)	271 (98%)	6 (2%)	47 35
1	G	278/277 (100%)	269 (97%)	9 (3%)	34 22
1	H	277/277 (100%)	271 (98%)	6 (2%)	47 35
1	I	277/277 (100%)	275 (99%)	2 (1%)	81 79
1	J	276/277 (100%)	276 (100%)	0	100 100
1	K	278/277 (100%)	268 (96%)	10 (4%)	30 17
1	L	278/277 (100%)	274 (99%)	4 (1%)	62 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3325/3324 (100%)	3256 (98%)	69 (2%)	48 36

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	MET
1	B	6	SER
1	B	85	ARG
1	B	176	GLN
1	B	177	SER
1	B	207	MET
1	B	290	VAL
1	B	321	GLU
1	C	40	SER
1	C	54	ARG
1	C	58	THR
1	C	104	ASP
1	C	121	SER
1	C	265	ARG
1	D	6	SER
1	D	40	SER
1	D	43	ASP
1	D	85	ARG
1	D	177	SER
1	D	199	MET
1	D	212	ARG
1	D	294	SER
1	D	350	ASP
1	D	357	ASP
1	E	6	SER
1	E	40	SER
1	E	54	ARG
1	E	58	THR
1	E	68	GLU
1	E	176	GLN
1	E	207	MET
1	E	290	VAL
1	F	42	VAL
1	F	80	LEU
1	F	176	GLN
1	F	177	SER
1	F	323	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	350	ASP
1	G	40	SER
1	G	54	ARG
1	G	121	SER
1	G	140	ILE
1	G	258	GLU
1	G	293	ASN
1	G	321	GLU
1	G	356	THR
1	G	357	ASP
1	H	40	SER
1	H	177	SER
1	H	209	THR
1	H	265	ARG
1	H	290	VAL
1	H	349	ILE
1	I	76	LYS
1	I	350	ASP
1	K	38	ARG
1	K	40	SER
1	K	41	SER
1	K	42	VAL
1	K	43	ASP
1	K	102	VAL
1	K	176	GLN
1	K	203	ARG
1	K	349	ILE
1	K	357	ASP
1	L	38	ARG
1	L	45	ILE
1	L	212	ARG
1	L	255	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	176	GLN
1	A	286	HIS
1	A	309	ASN
1	A	327	GLN
1	B	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	286	HIS
1	B	293	ASN
1	B	308	HIS
1	C	116	GLN
1	C	138	HIS
1	C	176	GLN
1	C	282	HIS
1	C	327	GLN
1	D	65	GLN
1	D	323	ASN
1	E	116	GLN
1	E	138	HIS
1	E	176	GLN
1	E	293	ASN
1	E	327	GLN
1	F	282	HIS
1	F	293	ASN
1	G	138	HIS
1	G	176	GLN
1	G	263	ASN
1	G	282	HIS
1	G	286	HIS
1	G	308	HIS
1	G	323	ASN
1	G	327	GLN
1	H	176	GLN
1	H	282	HIS
1	H	286	HIS
1	H	323	ASN
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	323	ASN
1	I	327	GLN
1	J	123	GLN
1	J	134	ASN
1	J	176	GLN
1	J	286	HIS
1	K	138	HIS
1	K	176	GLN
1	K	327	GLN
1	L	123	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	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

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	CO6	E	401	-	46,55,55	0.90	1 (2%)	55,82,82	1.52	8 (14%)
2	CO6	J	401	-	46,55,55	1.38	3 (6%)	55,82,82	1.12	5 (9%)
2	CO6	K	401	-	46,55,55	0.91	2 (4%)	55,82,82	2.37	11 (20%)
2	CO6	H	401	-	46,55,55	1.18	1 (2%)	55,82,82	1.15	6 (10%)
2	CO6	C	401	-	46,55,55	1.29	2 (4%)	55,82,82	1.03	4 (7%)
2	CO6	G	401	-	46,55,55	1.19	1 (2%)	55,82,82	1.47	8 (14%)
2	CO6	L	401	-	46,55,55	1.42	2 (4%)	55,82,82	0.97	2 (3%)
2	CO6	I	401	-	46,55,55	1.34	1 (2%)	55,82,82	0.83	1 (1%)
2	CO6	B	401	-	46,55,55	1.05	2 (4%)	55,82,82	1.78	3 (5%)
2	CO6	D	401	-	46,55,55	1.00	3 (6%)	55,82,82	1.66	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CO6	F	401	-	46,55,55	1.05	2 (4%)	55,82,82	2.25	13 (23%)
2	CO6	A	401	-	46,55,55	0.94	1 (2%)	55,82,82	1.95	8 (14%)

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	CO6	E	401	-	-	9/51/71/71	0/3/3/3
2	CO6	J	401	-	-	11/51/71/71	0/3/3/3
2	CO6	K	401	-	-	10/51/71/71	0/3/3/3
2	CO6	H	401	-	-	6/51/71/71	0/3/3/3
2	CO6	C	401	-	-	6/51/71/71	0/3/3/3
2	CO6	G	401	-	-	9/51/71/71	0/3/3/3
2	CO6	L	401	-	-	5/51/71/71	0/3/3/3
2	CO6	I	401	-	-	7/51/71/71	0/3/3/3
2	CO6	B	401	-	-	5/51/71/71	0/3/3/3
2	CO6	D	401	-	-	4/51/71/71	0/3/3/3
2	CO6	F	401	-	-	13/51/71/71	0/3/3/3
2	CO6	A	401	-	-	8/51/71/71	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	CO6	C1-S1P	8.37	2.02	1.75
2	I	401	CO6	C1-S1P	7.69	2.00	1.75
2	J	401	CO6	C1-S1P	7.06	1.98	1.75
2	C	401	CO6	C1-S1P	7.04	1.98	1.75
2	H	401	CO6	C1-S1P	6.31	1.95	1.75
2	G	401	CO6	C1-S1P	6.15	1.95	1.75
2	F	401	CO6	C1-S1P	4.20	1.88	1.75
2	A	401	CO6	C1-S1P	4.01	1.88	1.75
2	D	401	CO6	C1-S1P	3.85	1.87	1.75
2	B	401	CO6	C1-S1P	3.63	1.86	1.75
2	E	401	CO6	C1-S1P	3.53	1.86	1.75
2	J	401	CO6	OAP-CAP	3.40	1.48	1.42
2	B	401	CO6	P3B-O3B	2.69	1.64	1.59
2	K	401	CO6	C1-S1P	2.47	1.83	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	CO6	P3B-O3B	2.39	1.63	1.59
2	L	401	CO6	P3B-O3B	2.36	1.63	1.59
2	D	401	CO6	P3B-O3B	2.36	1.63	1.59
2	F	401	CO6	P3B-O3B	2.16	1.63	1.59
2	D	401	CO6	C2P-S1P	-2.13	1.72	1.81
2	C	401	CO6	P3B-O3B	2.10	1.63	1.59
2	K	401	CO6	C7P-C6P	2.01	1.57	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	CO6	C2P-S1P-C1	12.49	139.33	101.75
2	B	401	CO6	C2P-S1P-C1	10.35	132.90	101.75
2	A	401	CO6	C2P-S1P-C1	10.10	132.14	101.75
2	D	401	CO6	C2P-S1P-C1	9.81	131.28	101.75
2	F	401	CO6	C7P-C6P-C5P	-9.35	96.78	112.36
2	E	401	CO6	C2P-S1P-C1	7.19	123.37	101.75
2	K	401	CO6	C6P-C5P-N4P	5.73	126.07	116.42
2	F	401	CO6	C6P-C5P-N4P	4.91	124.69	116.42
2	G	401	CO6	O5A-P2A-O4A	4.75	135.75	112.24
2	F	401	CO6	O5A-P2A-O4A	4.72	135.60	112.24
2	A	401	CO6	O5A-P2A-O4A	4.68	135.38	112.24
2	F	401	CO6	C7P-N8P-C9P	4.63	130.85	122.59
2	F	401	CO6	CAP-C9P-N8P	4.50	125.54	116.58
2	K	401	CO6	O5P-C5P-C6P	-4.33	114.09	122.02
2	B	401	CO6	O1-C1-S1P	4.28	129.56	123.80
2	F	401	CO6	C2P-S1P-C1	4.20	114.38	101.75
2	J	401	CO6	O5A-P2A-O4A	4.19	132.97	112.24
2	G	401	CO6	C2P-C3P-N4P	-4.14	103.72	112.42
2	K	401	CO6	O1-C1-S1P	-4.13	118.25	123.80
2	G	401	CO6	O1-C1-S1P	3.98	129.16	123.80
2	K	401	CO6	O5A-P2A-O4A	3.95	131.79	112.24
2	C	401	CO6	O5A-P2A-O4A	3.92	131.64	112.24
2	H	401	CO6	O5A-P2A-O4A	3.90	131.51	112.24
2	D	401	CO6	O1-C1-S1P	3.75	128.85	123.80
2	F	401	CO6	O9P-C9P-N8P	-3.65	115.17	122.99
2	A	401	CO6	O2B-C2B-C3B	3.62	121.45	111.17
2	E	401	CO6	O2B-C2B-C3B	3.52	121.15	111.17
2	L	401	CO6	O5A-P2A-O4A	3.33	128.70	112.24
2	G	401	CO6	C2P-S1P-C1	3.31	111.71	101.75
2	H	401	CO6	C2P-S1P-C1	3.27	111.59	101.75
2	B	401	CO6	O5A-P2A-O4A	3.16	127.88	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	401	CO6	O6A-P2A-O4A	-3.11	96.93	109.07
2	K	401	CO6	O3B-P3B-O7A	-3.01	97.76	109.39
2	F	401	CO6	O5P-C5P-C6P	-2.98	116.57	122.02
2	F	401	CO6	C5A-C6A-N6A	2.96	124.85	120.35
2	J	401	CO6	C5A-C6A-N6A	2.89	124.75	120.35
2	A	401	CO6	O6A-P2A-O4A	-2.86	97.88	109.07
2	G	401	CO6	C5A-C6A-N6A	2.84	124.67	120.35
2	E	401	CO6	C5A-C6A-N6A	2.83	124.65	120.35
2	H	401	CO6	C5A-C6A-N6A	2.80	124.61	120.35
2	A	401	CO6	O3B-P3B-O7A	-2.80	98.58	109.39
2	K	401	CO6	C5A-C6A-N6A	2.78	124.58	120.35
2	F	401	CO6	OAP-CAP-CBP	-2.72	103.85	110.25
2	C	401	CO6	C5A-C6A-N6A	2.67	124.41	120.35
2	I	401	CO6	O5A-P2A-O4A	2.65	125.33	112.24
2	G	401	CO6	O5A-P2A-O6A	-2.62	95.57	107.75
2	E	401	CO6	O2B-C2B-C1B	-2.56	101.41	110.85
2	E	401	CO6	O5A-P2A-O4A	2.50	124.59	112.24
2	J	401	CO6	OAP-CAP-CBP	-2.47	104.44	110.25
2	E	401	CO6	C7P-C6P-C5P	-2.42	108.33	112.36
2	D	401	CO6	O5A-P2A-O4A	2.41	124.17	112.24
2	F	401	CO6	O5P-C5P-N4P	-2.34	118.61	123.01
2	A	401	CO6	C5A-C6A-N6A	2.32	123.88	120.35
2	G	401	CO6	C6P-C5P-N4P	-2.31	112.53	116.42
2	A	401	CO6	O8A-P3B-O3B	2.31	116.34	105.99
2	G	401	CO6	O6A-CCP-CBP	-2.29	106.86	110.55
2	E	401	CO6	O6A-P2A-O4A	-2.28	100.18	109.07
2	F	401	CO6	O5A-P2A-O6A	-2.25	97.31	107.75
2	J	401	CO6	C2P-S1P-C1	2.21	108.39	101.75
2	C	401	CO6	O5A-P2A-O6A	-2.17	97.66	107.75
2	J	401	CO6	O5A-P2A-O6A	-2.17	97.68	107.75
2	E	401	CO6	O1-C1-S1P	2.15	126.69	123.80
2	C	401	CO6	O3B-P3B-O7A	-2.14	101.12	109.39
2	K	401	CO6	O9A-P3B-O3B	2.14	115.57	105.99
2	A	401	CO6	OAP-CAP-CBP	-2.12	105.25	110.25
2	H	401	CO6	O2B-C2B-C3B	2.12	117.19	111.17
2	L	401	CO6	O5A-P2A-O6A	-2.10	97.99	107.75
2	H	401	CO6	O5A-P2A-O6A	-2.09	98.04	107.75
2	K	401	CO6	O5P-C5P-N4P	-2.08	119.09	123.01
2	H	401	CO6	O1-C1-S1P	2.06	126.57	123.80
2	F	401	CO6	O6A-CCP-CBP	-2.04	107.27	110.55
2	K	401	CO6	OAP-CAP-CBP	-2.02	105.50	110.25

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CO6	C5P-C6P-C7P-N8P
2	A	401	CO6	S1P-C1-C3-C2
2	A	401	CO6	O1-C1-C3-C4
2	C	401	CO6	C5P-C6P-C7P-N8P
2	C	401	CO6	O1-C1-S1P-C2P
2	C	401	CO6	C3-C1-S1P-C2P
2	E	401	CO6	C3B-O3B-P3B-O7A
2	E	401	CO6	S1P-C1-C3-C2
2	E	401	CO6	S1P-C1-C3-C4
2	F	401	CO6	CAP-C9P-N8P-C7P
2	F	401	CO6	O9P-C9P-N8P-C7P
2	F	401	CO6	C5P-C6P-C7P-N8P
2	F	401	CO6	C6P-C5P-N4P-C3P
2	F	401	CO6	O5P-C5P-N4P-C3P
2	F	401	CO6	S1P-C1-C3-C2
2	F	401	CO6	S1P-C1-C3-C4
2	G	401	CO6	C5P-C6P-C7P-N8P
2	G	401	CO6	S1P-C2P-C3P-N4P
2	G	401	CO6	O1-C1-S1P-C2P
2	G	401	CO6	C3-C1-S1P-C2P
2	G	401	CO6	S1P-C1-C3-C2
2	H	401	CO6	O1-C1-S1P-C2P
2	H	401	CO6	C3-C1-S1P-C2P
2	I	401	CO6	O1-C1-S1P-C2P
2	I	401	CO6	C3-C1-S1P-C2P
2	J	401	CO6	C3B-O3B-P3B-O7A
2	J	401	CO6	O1-C1-S1P-C2P
2	J	401	CO6	C3-C1-S1P-C2P
2	J	401	CO6	S1P-C1-C3-C2
2	J	401	CO6	S1P-C1-C3-C4
2	J	401	CO6	O1-C1-C3-C2
2	K	401	CO6	C6P-C5P-N4P-C3P
2	K	401	CO6	O5P-C5P-N4P-C3P
2	K	401	CO6	S1P-C2P-C3P-N4P
2	K	401	CO6	O1-C1-S1P-C2P
2	K	401	CO6	C3-C1-S1P-C2P
2	L	401	CO6	O1-C1-S1P-C2P
2	L	401	CO6	C3-C1-S1P-C2P
2	B	401	CO6	C5P-C6P-C7P-N8P
2	D	401	CO6	C5P-C6P-C7P-N8P
2	J	401	CO6	C5P-C6P-C7P-N8P
2	K	401	CO6	C5P-C6P-C7P-N8P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	401	CO6	N8P-C9P-CAP-CBP
2	F	401	CO6	C6P-C7P-N8P-C9P
2	B	401	CO6	C3B-O3B-P3B-O7A
2	C	401	CO6	C3B-O3B-P3B-O7A
2	G	401	CO6	C3B-O3B-P3B-O7A
2	L	401	CO6	C5P-C6P-C7P-N8P
2	D	401	CO6	C5B-O5B-P1A-O3A
2	J	401	CO6	P2A-O3A-P1A-O1A
2	K	401	CO6	S1P-C1-C3-C4
2	I	401	CO6	CCP-O6A-P2A-O4A
2	A	401	CO6	O1-C1-C3-C2
2	C	401	CO6	O1-C1-C3-C2
2	E	401	CO6	O1-C1-C3-C4
2	H	401	CO6	O1-C1-C3-C4
2	I	401	CO6	O1-C1-C3-C4
2	J	401	CO6	O1-C1-C3-C4
2	K	401	CO6	O1-C1-C3-C4
2	L	401	CO6	O1-C1-C3-C2
2	E	401	CO6	C5P-C6P-C7P-N8P
2	H	401	CO6	S1P-C2P-C3P-N4P
2	E	401	CO6	O4B-C4B-C5B-O5B
2	A	401	CO6	C3P-C2P-S1P-C1
2	B	401	CO6	C3P-C2P-S1P-C1
2	D	401	CO6	C3P-C2P-S1P-C1
2	E	401	CO6	C3P-C2P-S1P-C1
2	F	401	CO6	C3P-C2P-S1P-C1
2	G	401	CO6	C3P-C2P-S1P-C1
2	K	401	CO6	C3P-C2P-S1P-C1
2	K	401	CO6	O4B-C4B-C5B-O5B
2	F	401	CO6	C3B-O3B-P3B-O7A
2	H	401	CO6	C3B-O3B-P3B-O7A
2	I	401	CO6	C5P-C6P-C7P-N8P
2	B	401	CO6	O4B-C4B-C5B-O5B
2	A	401	CO6	C3B-O3B-P3B-O9A
2	B	401	CO6	C5B-O5B-P1A-O3A
2	E	401	CO6	C3B-O3B-P3B-O8A
2	F	401	CO6	C3B-O3B-P3B-O8A
2	J	401	CO6	C3B-O3B-P3B-O9A
2	C	401	CO6	O4B-C4B-C5B-O5B
2	F	401	CO6	O4B-C4B-C5B-O5B
2	G	401	CO6	O4B-C4B-C5B-O5B
2	H	401	CO6	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	401	CO6	O4B-C4B-C5B-O5B
2	E	401	CO6	P2A-O3A-P1A-O2A
2	G	401	CO6	P2A-O3A-P1A-O2A
2	A	401	CO6	S1P-C1-C3-C4
2	A	401	CO6	O4B-C4B-C5B-O5B
2	D	401	CO6	O4B-C4B-C5B-O5B
2	I	401	CO6	O4B-C4B-C5B-O5B
2	L	401	CO6	O4B-C4B-C5B-O5B
2	I	401	CO6	C6P-C7P-N8P-C9P

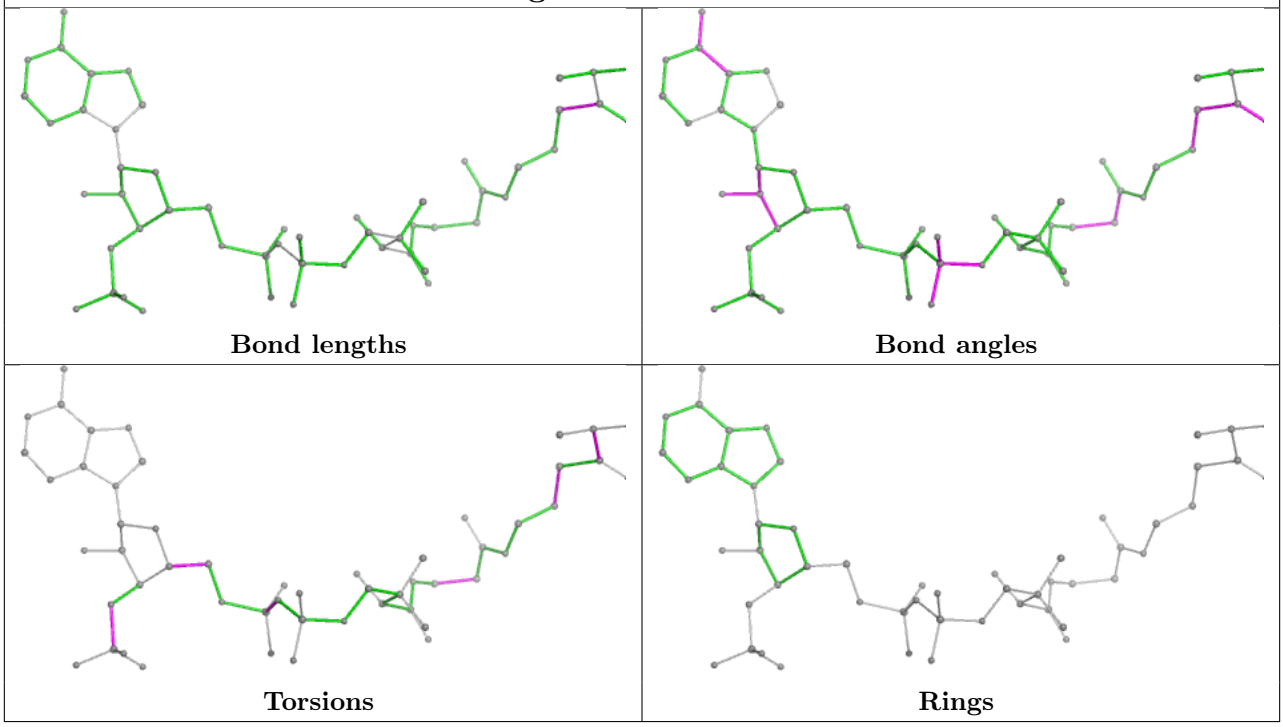
There are no ring outliers.

10 monomers are involved in 30 short contacts:

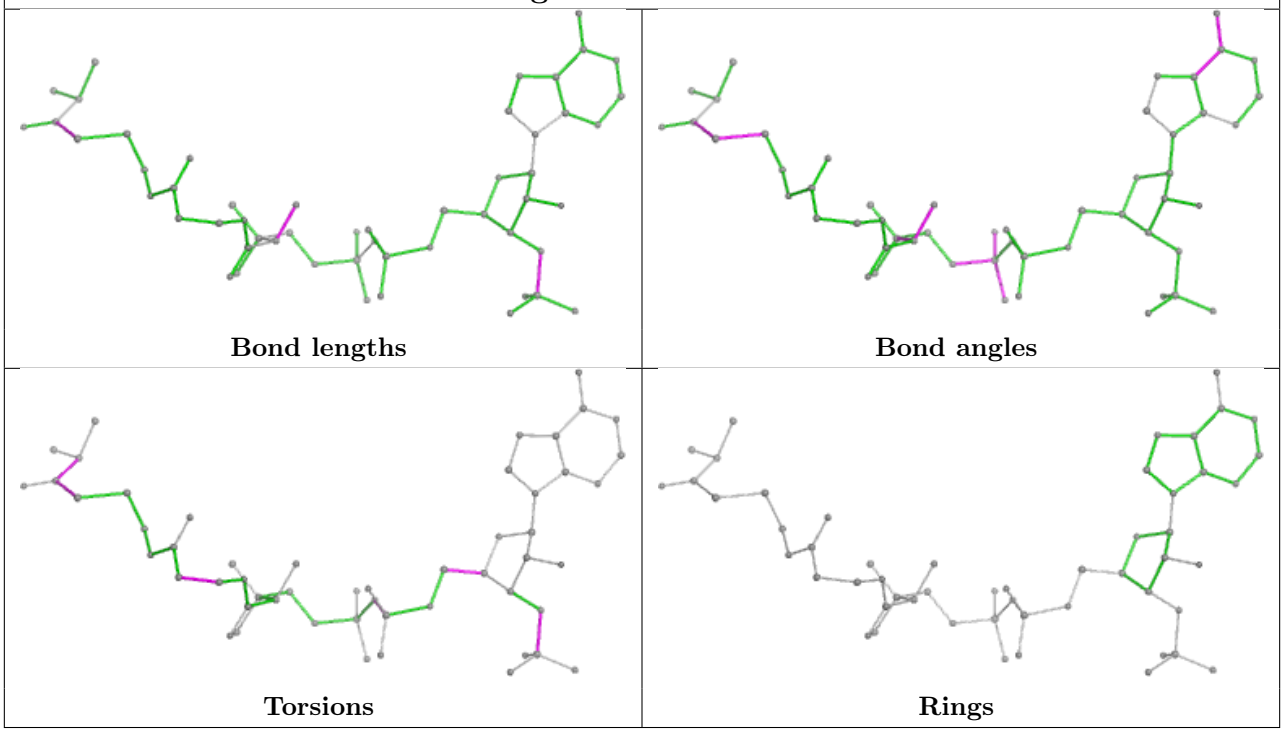
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	CO6	1	0
2	K	401	CO6	2	0
2	H	401	CO6	2	0
2	C	401	CO6	3	0
2	G	401	CO6	5	0
2	L	401	CO6	3	0
2	I	401	CO6	3	0
2	B	401	CO6	3	0
2	D	401	CO6	5	0
2	F	401	CO6	3	0

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.

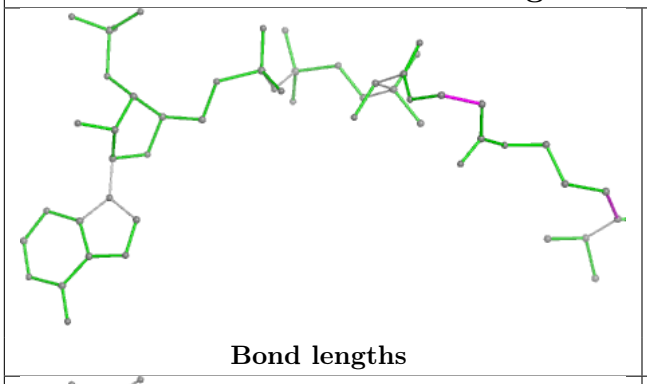
Ligand CO6 E 401



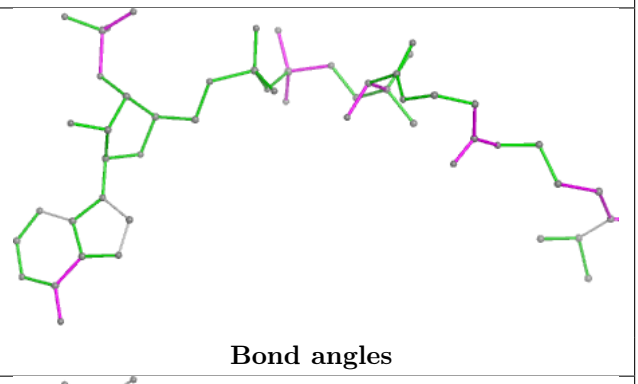
Ligand CO6 J 401



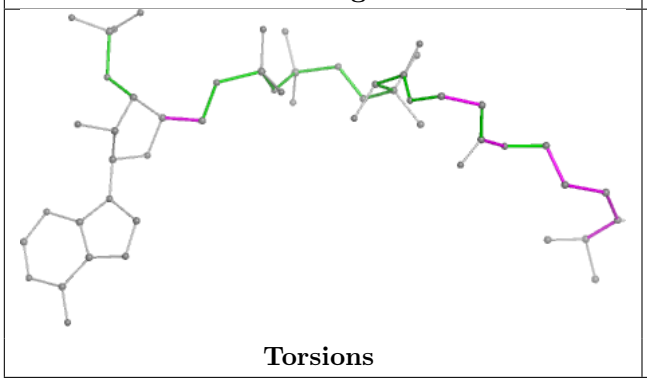
Ligand CO6 K 401



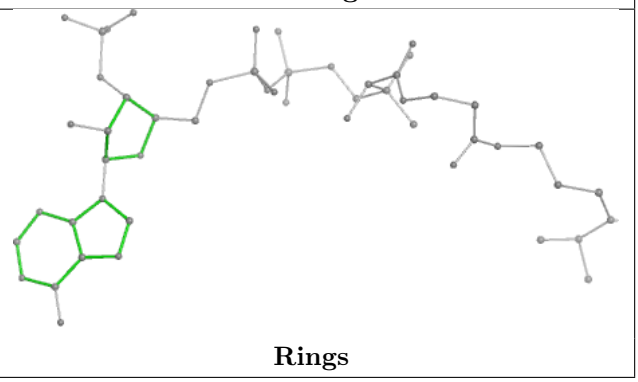
Bond lengths



Bond angles

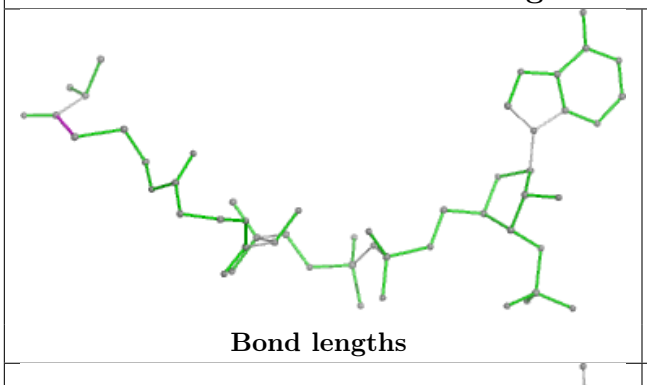


Torsions

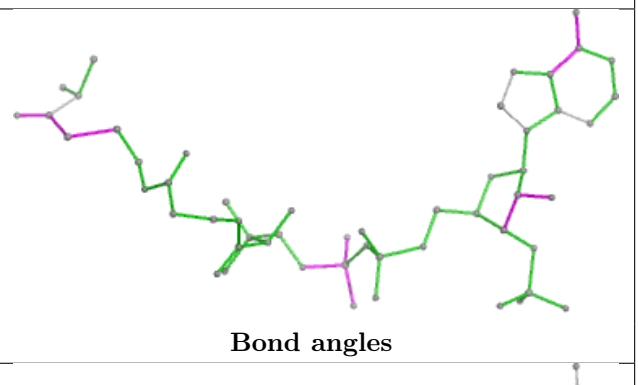


Rings

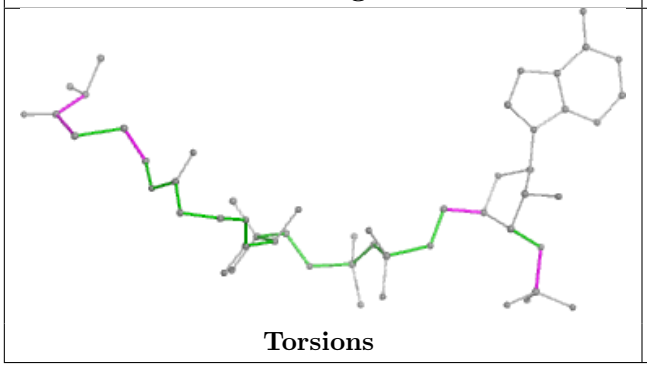
Ligand CO6 H 401



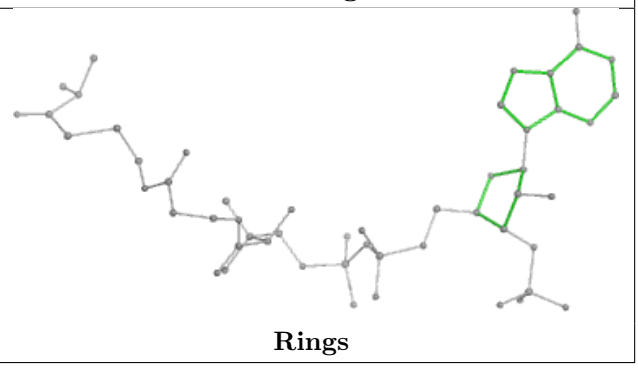
Bond lengths



Bond angles

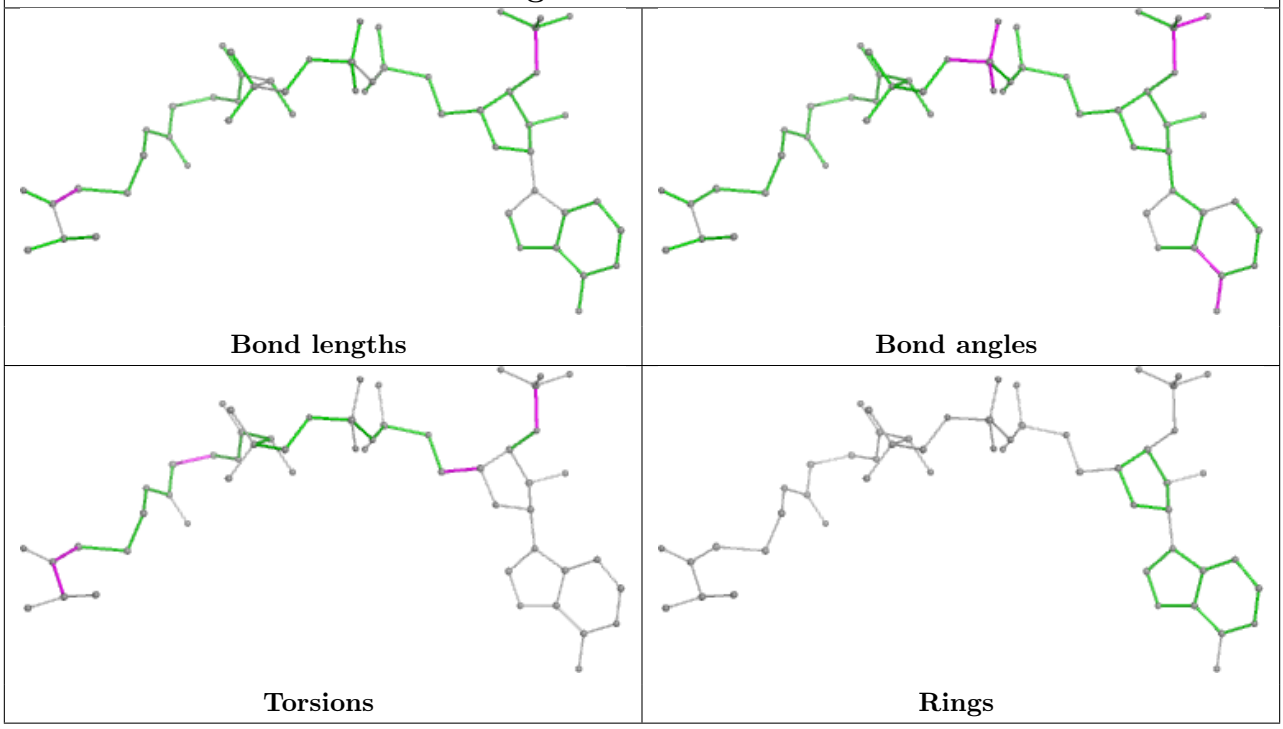


Torsions

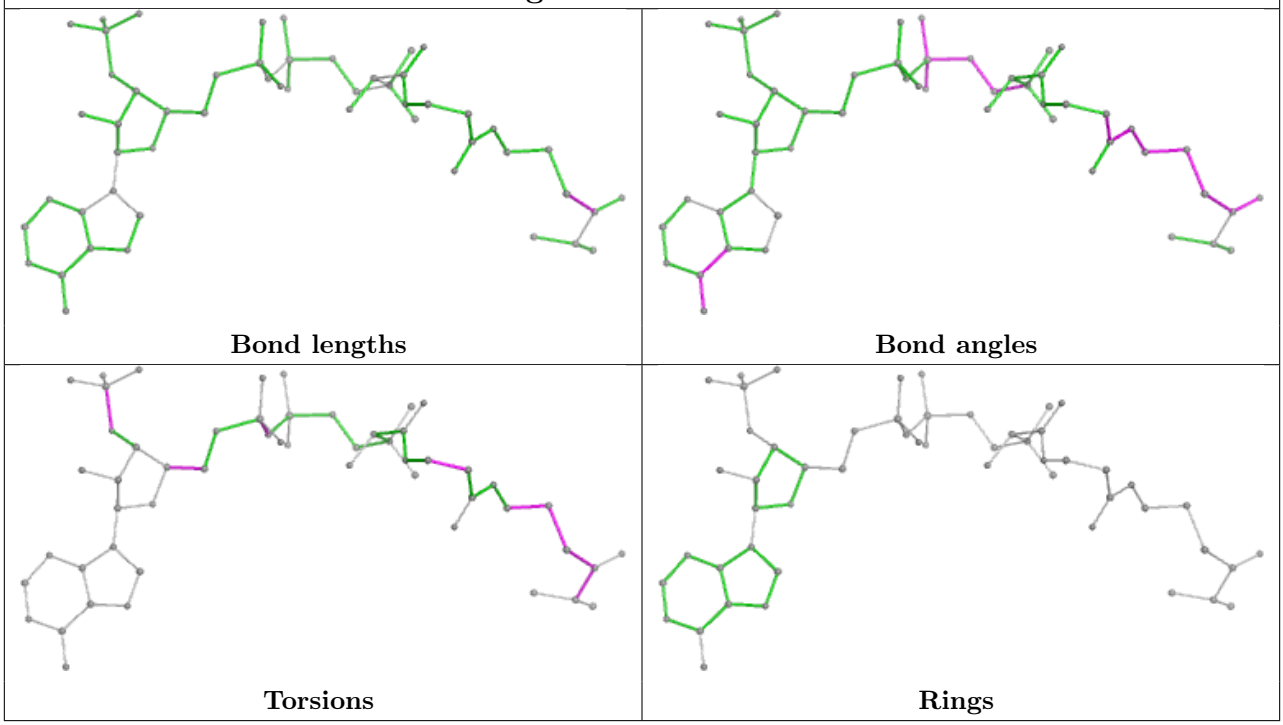


Rings

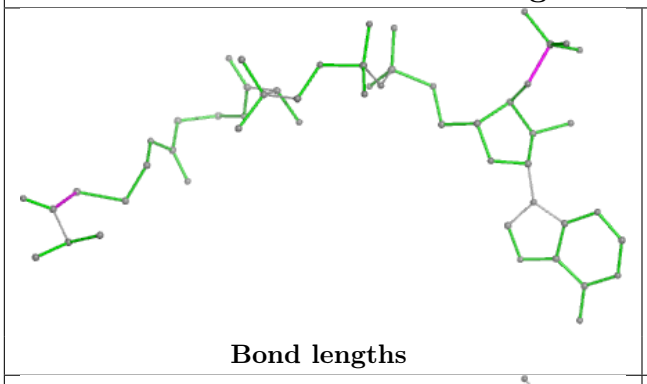
Ligand CO6 C 401



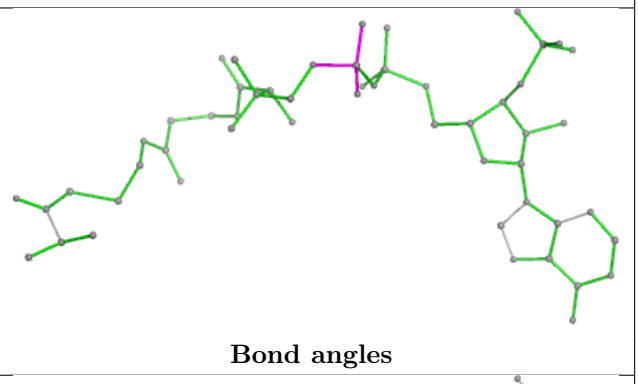
Ligand CO6 G 401



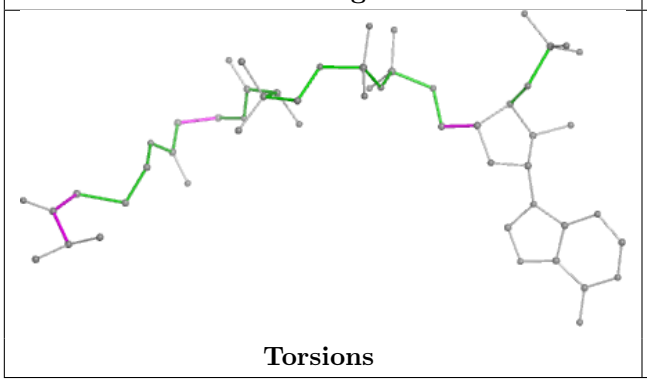
Ligand CO6 L 401



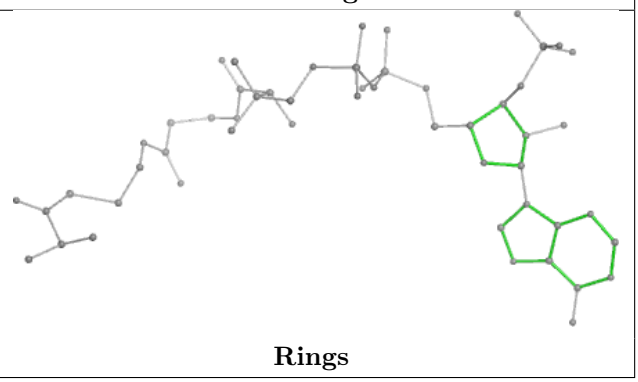
Bond lengths



Bond angles

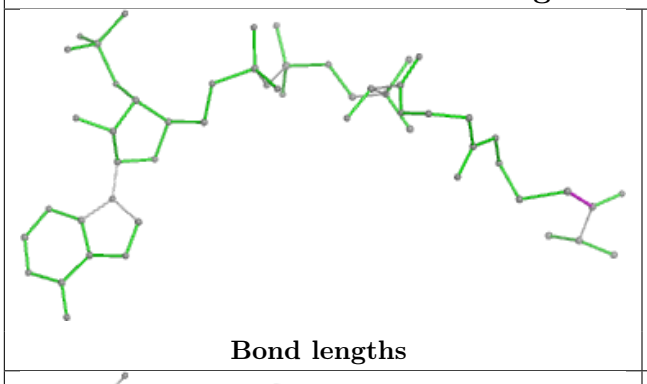


Torsions

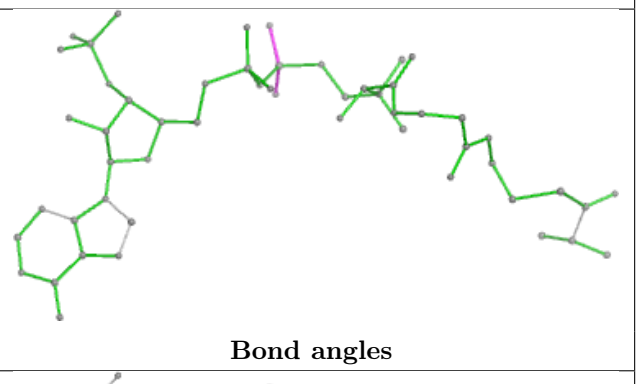


Rings

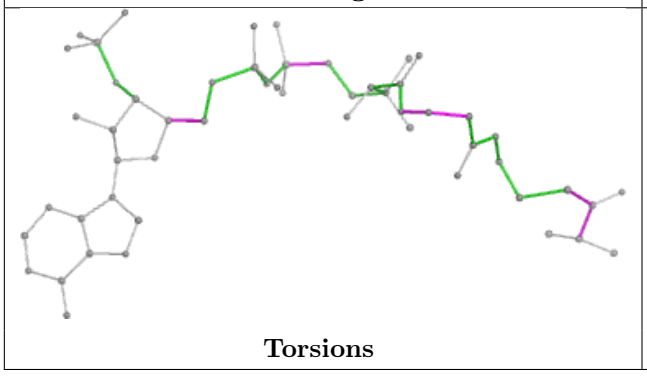
Ligand CO6 I 401



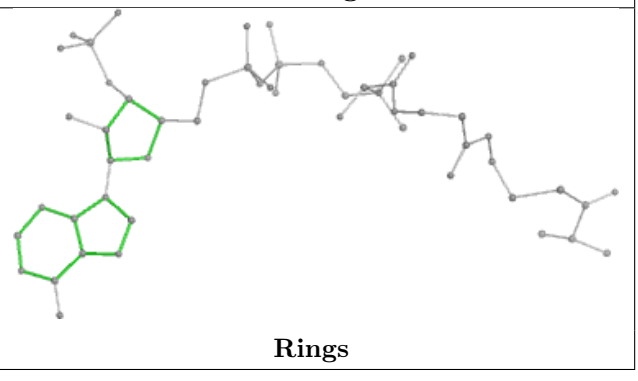
Bond lengths



Bond angles

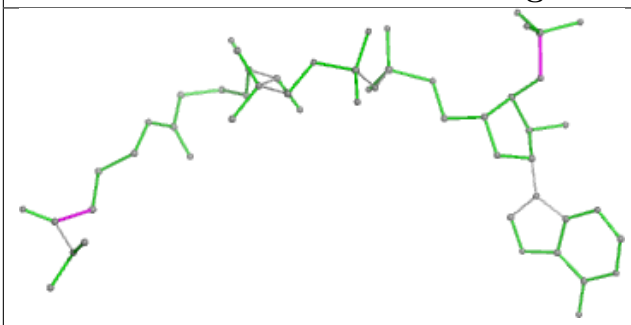


Torsions

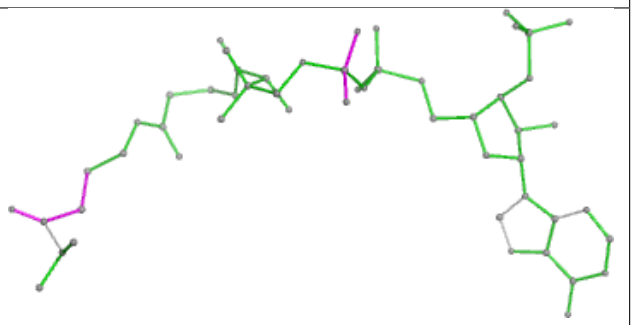


Rings

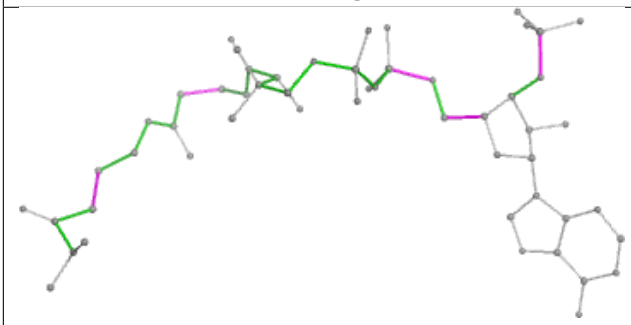
Ligand CO6 B 401



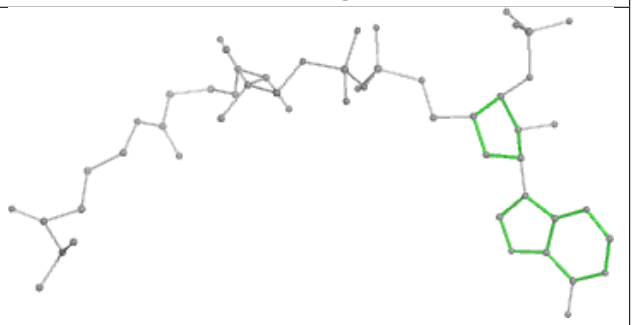
Bond lengths



Bond angles

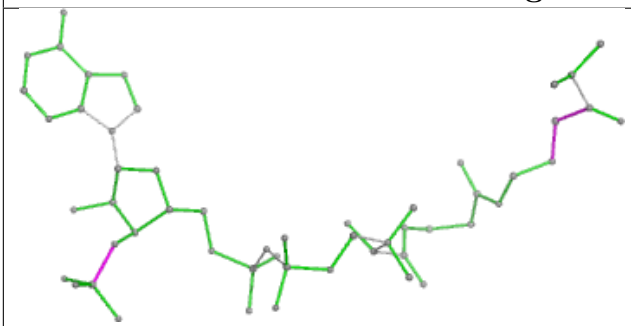


Torsions

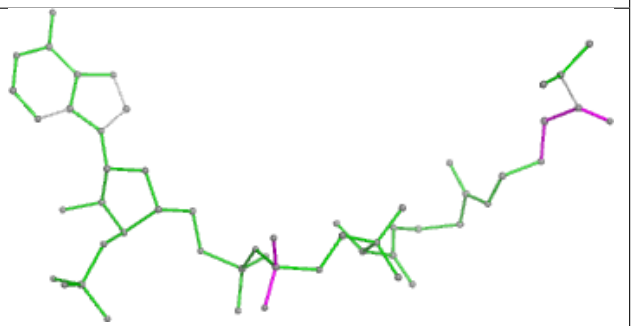


Rings

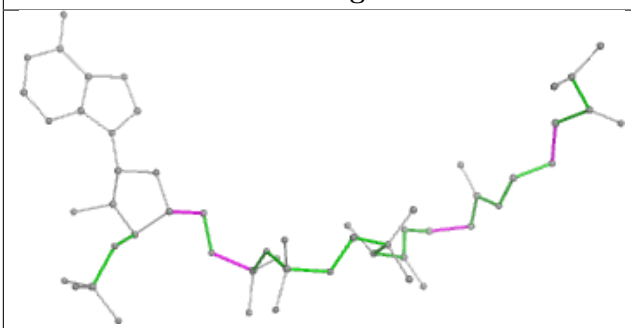
Ligand CO6 D 401



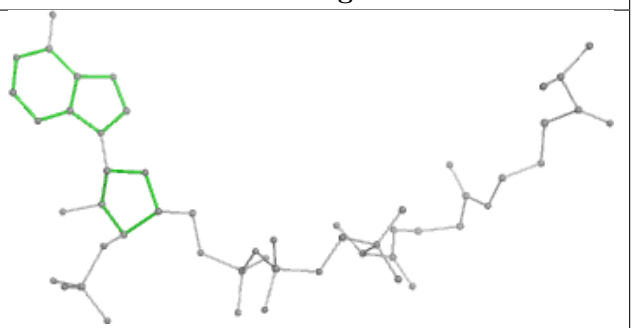
Bond lengths



Bond angles

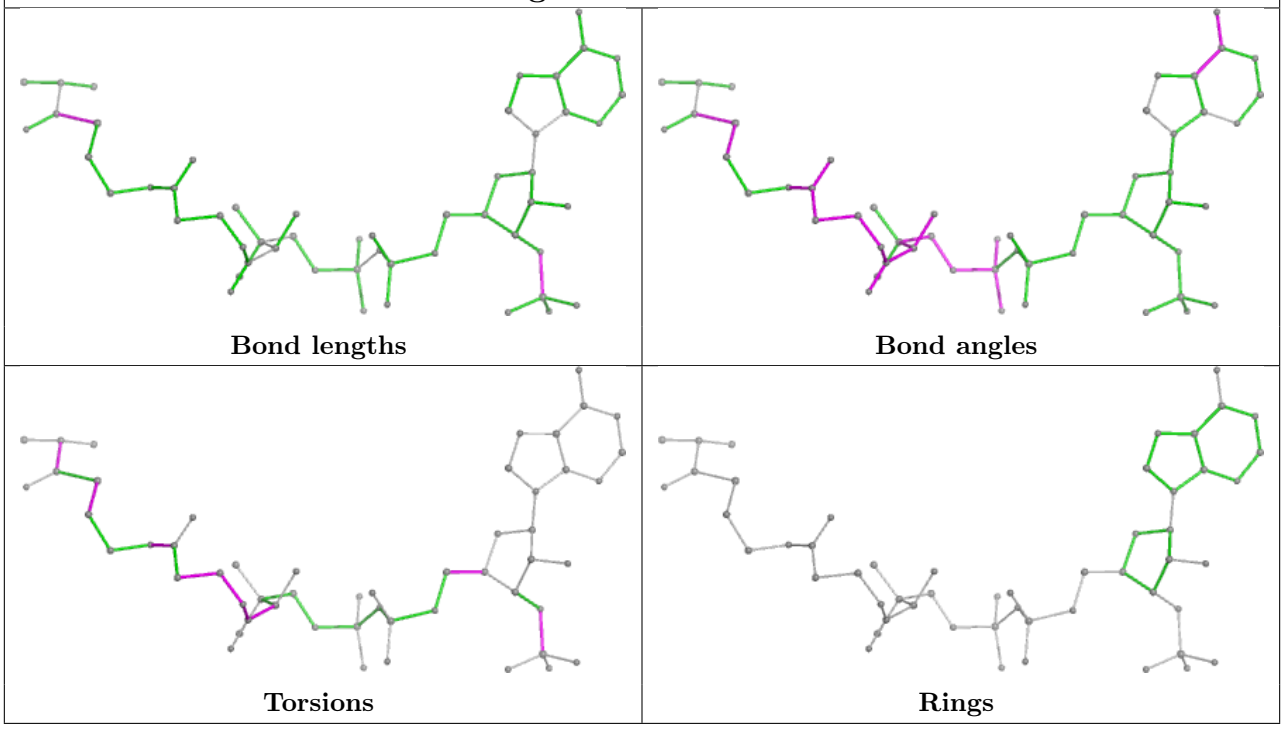


Torsions

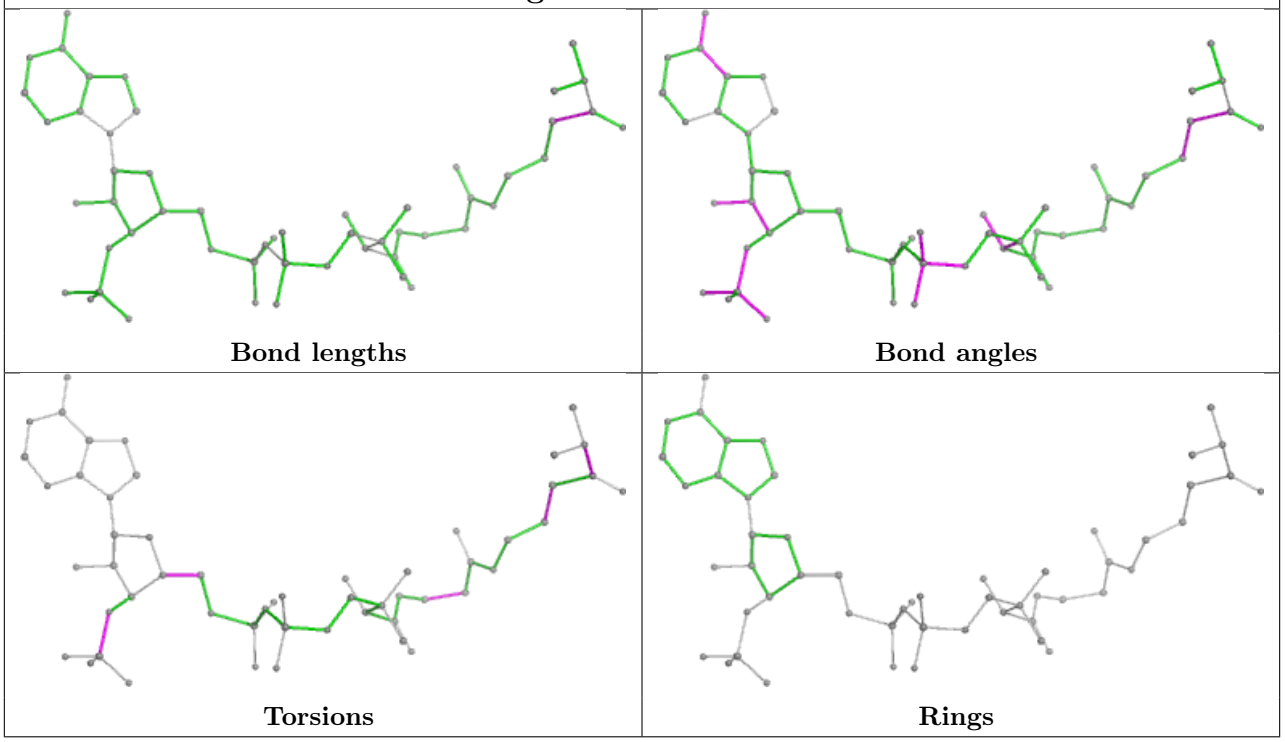


Rings

Ligand CO6 F 401



Ligand CO6 A 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	360/364 (98%)	0.72	52 (14%) 7 8	13, 34, 70, 123	4 (1%)
1	B	357/364 (98%)	0.64	44 (12%) 9 11	13, 34, 70, 109	2 (0%)
1	C	360/364 (98%)	0.95	88 (24%) 2 2	18, 35, 73, 115	4 (1%)
1	D	360/364 (98%)	0.66	45 (12%) 9 11	20, 34, 67, 118	1 (0%)
1	E	359/364 (98%)	0.78	52 (14%) 7 8	19, 36, 75, 119	2 (0%)
1	F	360/364 (98%)	1.06	94 (26%) 2 2	20, 36, 77, 123	2 (0%)
1	G	360/364 (98%)	1.12	95 (26%) 2 2	21, 37, 80, 134	3 (0%)
1	H	360/364 (98%)	0.75	53 (14%) 7 8	14, 35, 80, 113	2 (0%)
1	I	360/364 (98%)	0.34	21 (5%) 30 33	19, 31, 59, 104	2 (0%)
1	J	360/364 (98%)	0.56	48 (13%) 8 10	20, 32, 71, 114	1 (0%)
1	K	360/364 (98%)	0.83	72 (20%) 3 3	19, 33, 75, 105	3 (0%)
1	L	360/364 (98%)	0.45	27 (7%) 22 24	13, 33, 61, 112	3 (0%)
All	All	4316/4368 (98%)	0.74	691 (16%) 6 6	13, 34, 73, 134	29 (0%)

All (691) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	360	GLY	9.7
1	J	360	GLY	8.7
1	A	42	VAL	8.4
1	H	360	GLY	8.0
1	D	42	VAL	7.7
1	B	360	GLY	7.5
1	F	346	ALA	7.2
1	K	346	ALA	6.7
1	E	42	VAL	6.7
1	C	360	GLY	6.5
1	F	42	VAL	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	360	GLY	6.3
1	K	42	VAL	6.3
1	E	360	GLY	6.2
1	L	360	GLY	6.2
1	G	351	ILE	6.1
1	K	45	ILE	6.1
1	B	45	ILE	5.9
1	H	45	ILE	5.9
1	F	351	ILE	5.8
1	F	93	GLY	5.7
1	J	346	ALA	5.7
1	I	360	GLY	5.6
1	L	45	ILE	5.6
1	J	207	MET	5.6
1	A	360	GLY	5.6
1	F	360	GLY	5.5
1	D	346	ALA	5.4
1	E	351	ILE	5.4
1	H	351	ILE	5.4
1	G	42	VAL	5.4
1	A	324	GLY	5.3
1	J	45	ILE	5.2
1	A	351	ILE	5.2
1	E	349	ILE	5.2
1	D	45	ILE	5.1
1	F	292	ALA	5.1
1	K	75	ALA	5.1
1	G	93	GLY	5.1
1	G	349	ILE	5.1
1	J	351	ILE	5.1
1	H	42	VAL	5.0
1	C	42	VAL	5.0
1	G	102	VAL	4.9
1	G	75	ALA	4.8
1	G	346	ALA	4.8
1	E	44	GLY	4.7
1	C	75	ALA	4.7
1	C	351	ILE	4.6
1	G	61	LEU	4.6
1	G	293	ASN	4.6
1	G	355	LEU	4.6
1	B	351	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	62	LYS	4.5
1	F	45	ILE	4.4
1	K	349	ILE	4.4
1	G	347	ALA	4.3
1	G	92	LEU	4.3
1	G	58	THR	4.3
1	C	207	MET	4.3
1	C	45	ILE	4.3
1	C	347	ALA	4.3
1	F	293	ASN	4.3
1	F	69	LEU	4.3
1	K	102	VAL	4.3
1	C	66	GLY	4.3
1	E	324	GLY	4.3
1	G	324	GLY	4.3
1	F	101	LYS	4.2
1	K	72	LYS	4.2
1	K	180	LYS	4.2
1	B	346	ALA	4.2
1	B	207	MET	4.1
1	A	349	ILE	4.1
1	J	42	VAL	4.1
1	F	207	MET	4.1
1	G	59	ALA	4.1
1	G	72	LYS	4.1
1	F	349	ILE	4.0
1	J	349	ILE	4.0
1	G	69	LEU	4.0
1	C	93	GLY	4.0
1	K	47	ARG	4.0
1	L	207	MET	4.0
1	G	94	LEU	4.0
1	K	324	GLY	4.0
1	H	358	TRP	4.0
1	F	70	ALA	4.0
1	A	62	LYS	4.0
1	H	349	ILE	4.0
1	F	61	LEU	4.0
1	E	345	PRO	4.0
1	F	358	TRP	4.0
1	K	345	PRO	3.9
1	I	41	SER	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	45	ILE	3.9
1	I	207	MET	3.9
1	B	46	SER	3.9
1	G	57	VAL	3.9
1	G	354	VAL	3.9
1	K	360	GLY	3.9
1	F	92	LEU	3.9
1	A	346	ALA	3.9
1	C	102	VAL	3.9
1	C	69	LEU	3.9
1	G	45	ILE	3.9
1	J	75	ALA	3.8
1	F	354	VAL	3.8
1	L	359	ASP	3.8
1	C	358	TRP	3.8
1	F	62	LYS	3.8
1	G	101	LYS	3.8
1	K	41	SER	3.8
1	C	349	ILE	3.8
1	K	71	LEU	3.8
1	F	347	ALA	3.8
1	H	353	ALA	3.8
1	H	39	PRO	3.8
1	L	323	ASN	3.8
1	F	73	LEU	3.8
1	L	173	TRP	3.8
1	C	346	ALA	3.8
1	J	347	ALA	3.8
1	A	180	LYS	3.8
1	G	88	VAL	3.8
1	D	323	ASN	3.7
1	C	61	LEU	3.7
1	G	207	MET	3.7
1	F	180	LYS	3.7
1	J	350	ASP	3.7
1	D	347	ALA	3.7
1	H	346	ALA	3.7
1	G	73	LEU	3.7
1	F	59	ALA	3.7
1	J	49	ALA	3.7
1	D	358	TRP	3.7
1	D	44	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	359	ASP	3.6
1	K	44	GLY	3.6
1	K	93	GLY	3.6
1	E	45	ILE	3.6
1	E	207	MET	3.6
1	K	73	LEU	3.6
1	D	349	ILE	3.6
1	K	351	ILE	3.6
1	G	1	MET	3.6
1	G	177	SER	3.6
1	G	353	ALA	3.6
1	J	44	GLY	3.6
1	G	358	TRP	3.6
1	E	346	ALA	3.5
1	G	292	ALA	3.5
1	F	44	GLY	3.5
1	L	42	VAL	3.5
1	D	40	SER	3.5
1	A	92	LEU	3.5
1	K	49	ALA	3.5
1	F	324	GLY	3.5
1	F	33	VAL	3.5
1	J	323	ASN	3.5
1	K	348	THR	3.5
1	K	347	ALA	3.5
1	G	176	GLN	3.5
1	F	39	PRO	3.5
1	H	47	ARG	3.5
1	I	45	ILE	3.5
1	L	324	GLY	3.5
1	C	323	ASN	3.5
1	K	66	GLY	3.5
1	B	44	GLY	3.4
1	H	324	GLY	3.4
1	A	39	PRO	3.4
1	L	351	ILE	3.4
1	C	176	GLN	3.4
1	E	176	GLN	3.4
1	F	356	THR	3.4
1	F	79	VAL	3.4
1	B	347	ALA	3.4
1	C	49	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	67	LEU	3.4
1	G	76	LYS	3.4
1	K	59	ALA	3.4
1	E	40	SER	3.4
1	A	69	LEU	3.4
1	C	59	ALA	3.4
1	G	77	ALA	3.4
1	H	69	LEU	3.4
1	K	46	SER	3.4
1	F	176	GLN	3.4
1	G	10	VAL	3.3
1	G	34	VAL	3.3
1	J	93	GLY	3.3
1	I	292	ALA	3.3
1	K	100	ALA	3.3
1	I	47	ARG	3.3
1	K	94	LEU	3.3
1	H	207	MET	3.3
1	G	44	GLY	3.3
1	F	173	TRP	3.3
1	F	57	VAL	3.3
1	C	70	ALA	3.3
1	D	322	ALA	3.3
1	A	355	LEU	3.3
1	C	350	ASP	3.3
1	A	68	GLU	3.3
1	C	108	TYR	3.3
1	D	351	ILE	3.3
1	K	56	ILE	3.3
1	D	348	THR	3.3
1	H	323	ASN	3.3
1	G	79	VAL	3.3
1	F	75	ALA	3.3
1	G	100	ALA	3.3
1	B	73	LEU	3.3
1	F	1	MET	3.3
1	F	355	LEU	3.3
1	C	99	CYS	3.3
1	F	99	CYS	3.3
1	A	47	ARG	3.3
1	C	47	ARG	3.3
1	F	66	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	66	GLY	3.3
1	K	1	MET	3.2
1	C	94	LEU	3.2
1	F	76	LYS	3.2
1	C	173	TRP	3.2
1	G	99	CYS	3.2
1	A	44	GLY	3.2
1	G	97	GLU	3.2
1	G	359	ASP	3.2
1	K	76	LYS	3.2
1	J	100	ALA	3.2
1	A	61	LEU	3.2
1	J	73	LEU	3.2
1	A	93	GLY	3.2
1	J	324	GLY	3.2
1	K	181	GLY	3.2
1	G	64	ASP	3.2
1	G	178	SER	3.2
1	C	76	LYS	3.2
1	B	345	PRO	3.2
1	E	353	ALA	3.2
1	G	70	ALA	3.2
1	K	354	VAL	3.2
1	K	69	LEU	3.2
1	E	178	SER	3.2
1	C	74	ILE	3.2
1	H	5	LEU	3.1
1	L	44	GLY	3.1
1	F	41	SER	3.1
1	G	350	ASP	3.1
1	L	346	ALA	3.1
1	G	11	VAL	3.1
1	C	101	LYS	3.1
1	A	177	SER	3.1
1	F	65	GLN	3.1
1	D	173	TRP	3.1
1	G	36	ILE	3.1
1	K	74	ILE	3.1
1	E	39	PRO	3.1
1	B	257	ALA	3.1
1	E	1	MET	3.1
1	B	47	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	87	GLY	3.1
1	F	46	SER	3.1
1	K	63	SER	3.1
1	C	56	ILE	3.1
1	A	173	TRP	3.1
1	A	40	SER	3.1
1	F	67	LEU	3.1
1	G	71	LEU	3.1
1	C	10	VAL	3.1
1	G	107	ILE	3.0
1	I	349	ILE	3.0
1	I	351	ILE	3.0
1	J	62	LYS	3.0
1	G	49	ALA	3.0
1	B	350	ASP	3.0
1	C	43	ASP	3.0
1	G	108	TYR	3.0
1	H	173	TRP	3.0
1	D	41	SER	3.0
1	C	355	LEU	3.0
1	F	106	LEU	3.0
1	K	61	LEU	3.0
1	K	67	LEU	3.0
1	C	79	VAL	3.0
1	C	354	VAL	3.0
1	G	91	ARG	3.0
1	G	39	PRO	3.0
1	H	49	ALA	3.0
1	G	352	GLU	3.0
1	K	10	VAL	3.0
1	A	72	LYS	3.0
1	B	176	GLN	3.0
1	I	359	ASP	3.0
1	D	324	GLY	3.0
1	G	56	ILE	3.0
1	A	292	ALA	3.0
1	B	355	LEU	3.0
1	C	71	LEU	3.0
1	F	47	ARG	3.0
1	F	94	LEU	3.0
1	C	72	LYS	3.0
1	K	11	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	324	GLY	2.9
1	C	353	ALA	2.9
1	G	38	ARG	2.9
1	K	101	LYS	2.9
1	H	355	LEU	2.9
1	K	355	LEU	2.9
1	E	358	TRP	2.9
1	F	34	VAL	2.9
1	C	44	GLY	2.9
1	A	75	ALA	2.9
1	C	107	ILE	2.9
1	E	347	ALA	2.9
1	F	353	ALA	2.9
1	I	323	ASN	2.9
1	D	180	LYS	2.9
1	F	58	THR	2.9
1	F	348	THR	2.9
1	F	71	LEU	2.9
1	G	67	LEU	2.9
1	D	357	ASP	2.9
1	F	350	ASP	2.9
1	A	358	TRP	2.9
1	G	173	TRP	2.9
1	K	173	TRP	2.9
1	C	7	GLY	2.9
1	G	87	GLY	2.9
1	G	345	PRO	2.9
1	H	44	GLY	2.9
1	C	178	SER	2.9
1	H	1	MET	2.9
1	D	49	ALA	2.9
1	H	350	ASP	2.9
1	K	359	ASP	2.9
1	G	80	LEU	2.9
1	J	355	LEU	2.9
1	F	11	VAL	2.9
1	F	102	VAL	2.9
1	G	96	PRO	2.9
1	B	75	ALA	2.9
1	C	171	ALA	2.9
1	E	292	ALA	2.9
1	F	49	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	56	ILE	2.8
1	E	355	LEU	2.8
1	E	66	GLY	2.8
1	D	43	ASP	2.8
1	F	89	THR	2.8
1	C	105	ARG	2.8
1	C	34	VAL	2.8
1	H	34	VAL	2.8
1	F	100	ALA	2.8
1	H	59	ALA	2.8
1	J	353	ALA	2.8
1	E	348	THR	2.8
1	F	36	ILE	2.8
1	F	56	ILE	2.8
1	F	81	ILE	2.8
1	G	7	GLY	2.8
1	G	180	LYS	2.8
1	J	72	LYS	2.8
1	C	73	LEU	2.8
1	L	47	ARG	2.8
1	A	356	THR	2.8
1	C	58	THR	2.8
1	D	107	ILE	2.8
1	E	56	ILE	2.8
1	G	74	ILE	2.8
1	C	177	SER	2.8
1	J	92	LEU	2.7
1	K	79	VAL	2.7
1	A	322	ALA	2.7
1	A	348	THR	2.7
1	E	58	THR	2.7
1	B	349	ILE	2.7
1	F	107	ILE	2.7
1	B	358	TRP	2.7
1	C	39	PRO	2.7
1	F	345	PRO	2.7
1	K	96	PRO	2.7
1	F	43	ASP	2.7
1	K	176	GLN	2.7
1	A	289	ALA	2.7
1	H	2	ALA	2.7
1	H	322	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	180	LYS	2.7
1	B	40	SER	2.7
1	C	96	PRO	2.7
1	D	345	PRO	2.7
1	G	106	LEU	2.7
1	B	1	MET	2.7
1	B	68	GLU	2.7
1	E	97	GLU	2.7
1	C	100	ALA	2.7
1	E	59	ALA	2.7
1	A	323	ASN	2.7
1	E	177	SER	2.7
1	J	40	SER	2.7
1	E	179	GLY	2.7
1	A	56	ILE	2.7
1	C	36	ILE	2.7
1	C	104	ASP	2.7
1	G	60	ASP	2.7
1	H	176	GLN	2.7
1	I	43	ASP	2.7
1	C	106	LEU	2.7
1	A	207	MET	2.7
1	F	38	ARG	2.6
1	F	323	ASN	2.6
1	H	58	THR	2.6
1	F	63	SER	2.6
1	H	41	SER	2.6
1	H	46	SER	2.6
1	L	349	ILE	2.6
1	C	80	LEU	2.6
1	H	105	ARG	2.6
1	J	38	ARG	2.6
1	K	358	TRP	2.6
1	G	322	ALA	2.6
1	I	44	GLY	2.6
1	H	43	ASP	2.6
1	B	180	LYS	2.6
1	C	180	LYS	2.6
1	F	96	PRO	2.6
1	H	345	PRO	2.6
1	A	46	SER	2.6
1	A	58	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	65	GLN	2.6
1	B	353	ALA	2.6
1	L	322	ALA	2.6
1	K	43	ASP	2.6
1	A	76	LYS	2.6
1	D	47	ARG	2.6
1	K	39	PRO	2.6
1	C	65	GLN	2.6
1	J	63	SER	2.6
1	C	356	THR	2.6
1	G	348	THR	2.6
1	G	68	GLU	2.6
1	J	352	GLU	2.6
1	D	75	ALA	2.6
1	F	72	LYS	2.5
1	J	102	VAL	2.5
1	E	173	TRP	2.5
1	K	99	CYS	2.5
1	D	65	GLN	2.5
1	J	61	LEU	2.5
1	C	68	GLU	2.5
1	F	98	GLU	2.5
1	H	352	GLU	2.5
1	C	30	GLY	2.5
1	E	356	THR	2.5
1	D	207	MET	2.5
1	K	322	ALA	2.5
1	C	11	VAL	2.5
1	I	42	VAL	2.5
1	K	183	VAL	2.5
1	K	108	TYR	2.5
1	C	97	GLU	2.5
1	F	40	SER	2.5
1	F	74	ILE	2.5
1	K	92	LEU	2.5
1	C	324	GLY	2.5
1	D	7	GLY	2.5
1	E	93	GLY	2.5
1	C	348	THR	2.5
1	E	350	ASP	2.5
1	F	48	ASP	2.5
1	J	43	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	2.5
1	B	49	ALA	2.5
1	G	33	VAL	2.5
1	I	176	GLN	2.5
1	J	345	PRO	2.5
1	F	326	TRP	2.5
1	G	63	SER	2.5
1	A	91	ARG	2.5
1	E	47	ARG	2.5
1	C	51	LEU	2.5
1	K	36	ILE	2.5
1	B	356	THR	2.5
1	D	59	ALA	2.5
1	J	59	ALA	2.5
1	E	65	GLN	2.5
1	G	65	GLN	2.5
1	B	323	ASN	2.5
1	D	102	VAL	2.5
1	F	184	VAL	2.5
1	K	34	VAL	2.5
1	J	39	PRO	2.4
1	A	41	SER	2.4
1	L	41	SER	2.4
1	J	47	ARG	2.4
1	K	350	ASP	2.4
1	B	204	ALA	2.4
1	D	2	ALA	2.4
1	H	76	LYS	2.4
1	K	178	SER	2.4
1	C	359	ASP	2.4
1	D	359	ASP	2.4
1	J	37	ASP	2.4
1	E	69	LEU	2.4
1	J	69	LEU	2.4
1	J	94	LEU	2.4
1	E	100	ALA	2.4
1	K	70	ALA	2.4
1	B	76	LYS	2.4
1	E	354	VAL	2.4
1	D	5	LEU	2.4
1	C	77	ALA	2.4
1	B	62	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	101	LYS	2.4
1	K	62	LYS	2.4
1	A	345	PRO	2.4
1	C	345	PRO	2.4
1	A	102	VAL	2.4
1	C	87	GLY	2.4
1	G	83	GLY	2.4
1	G	181	GLY	2.4
1	J	65	GLN	2.4
1	K	65	GLN	2.4
1	C	183	VAL	2.4
1	G	323	ASN	2.3
1	G	105	ARG	2.3
1	H	38	ARG	2.3
1	C	8	LEU	2.3
1	G	8	LEU	2.3
1	D	76	LYS	2.3
1	L	1	MET	2.3
1	A	77	ALA	2.3
1	D	353	ALA	2.3
1	C	37	ASP	2.3
1	C	63	SER	2.3
1	E	144	ASP	2.3
1	F	60	ASP	2.3
1	F	144	ASP	2.3
1	J	173	TRP	2.3
1	L	350	ASP	2.3
1	B	39	PRO	2.3
1	B	324	GLY	2.3
1	F	277	GLU	2.3
1	H	7	GLY	2.3
1	G	183	VAL	2.3
1	G	356	THR	2.3
1	H	348	THR	2.3
1	C	62	LYS	2.3
1	E	62	LYS	2.3
1	H	72	LYS	2.3
1	F	80	LEU	2.3
1	H	73	LEU	2.3
1	J	67	LEU	2.3
1	E	75	ALA	2.3
1	L	46	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	258	GLU	2.3
1	D	315	GLU	2.3
1	H	315	GLU	2.3
1	K	97	GLU	2.3
1	I	173	TRP	2.3
1	G	47	ARG	2.3
1	B	354	VAL	2.3
1	C	57	VAL	2.3
1	I	1	MET	2.3
1	D	355	LEU	2.3
1	K	357	ASP	2.3
1	L	43	ASP	2.3
1	A	74	ILE	2.3
1	A	347	ALA	2.3
1	H	16	ILE	2.3
1	K	107	ILE	2.3
1	B	93	GLY	2.3
1	E	7	GLY	2.3
1	K	323	ASN	2.3
1	J	359	ASP	2.3
1	G	41	SER	2.3
1	H	178	SER	2.3
1	G	2	ALA	2.2
1	B	30	GLY	2.2
1	C	181	GLY	2.2
1	A	1	MET	2.2
1	G	89	THR	2.2
1	B	173	TRP	2.2
1	D	326	TRP	2.2
1	F	68	GLU	2.2
1	G	43	ASP	2.2
1	C	5	LEU	2.2
1	K	80	LEU	2.2
1	L	75	ALA	2.2
1	F	7	GLY	2.2
1	H	30	GLY	2.2
1	H	356	THR	2.2
1	K	104	ASP	2.2
1	C	33	VAL	2.2
1	C	91	ARG	2.2
1	D	177	SER	2.2
1	K	57	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	2.2
1	E	61	LEU	2.2
1	E	172	LEU	2.2
1	E	322	ALA	2.2
1	H	347	ALA	2.2
1	E	314	ILE	2.2
1	D	176	GLN	2.2
1	F	97	GLU	2.2
1	C	357	ASP	2.2
1	J	144	ASP	2.2
1	K	38	ARG	2.2
1	F	88	VAL	2.2
1	C	179	GLY	2.2
1	H	66	GLY	2.2
1	A	71	LEU	2.2
1	A	94	LEU	2.2
1	C	172	LEU	2.2
1	G	14	ALA	2.2
1	H	8	LEU	2.2
1	B	105	ARG	2.2
1	C	38	ARG	2.2
1	E	104	ASP	2.1
1	A	63	SER	2.1
1	C	40	SER	2.1
1	K	40	SER	2.1
1	A	288	GLY	2.1
1	E	30	GLY	2.1
1	F	83	GLY	2.1
1	K	352	GLU	2.1
1	L	315	GLU	2.1
1	B	289	ALA	2.1
1	C	14	ALA	2.1
1	D	73	LEU	2.1
1	E	77	ALA	2.1
1	B	359	ASP	2.1
1	F	64	ASP	2.1
1	G	46	SER	2.1
1	C	1	MET	2.1
1	D	68	GLU	2.1
1	H	354	VAL	2.1
1	E	73	LEU	2.1
1	K	353	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	255	ASP	2.1
1	H	326	TRP	2.1
1	E	46	SER	2.1
1	H	180	LYS	2.1
1	F	181	GLY	2.1
1	J	66	GLY	2.1
1	A	10	VAL	2.1
1	B	102	VAL	2.1
1	H	33	VAL	2.1
1	B	100	ALA	2.1
1	B	144	ASP	2.1
1	F	2	ALA	2.1
1	K	144	ASP	2.1
1	L	347	ALA	2.1
1	H	92	LEU	2.1
1	J	41	SER	2.1
1	D	1	MET	2.1
1	F	352	GLU	2.1
1	I	326	TRP	2.1
1	J	348	THR	2.1
1	L	358	TRP	2.1
1	A	38	ARG	2.1
1	F	105	ARG	2.1
1	F	115	GLY	2.1
1	G	325	GLY	2.1
1	F	37	ASP	2.0
1	I	350	ASP	2.0
1	A	354	VAL	2.0
1	D	290	VAL	2.0
1	E	10	VAL	2.0
1	F	10	VAL	2.0
1	J	99	CYS	2.0
1	E	70	ALA	2.0
1	L	289	ALA	2.0
1	F	5	LEU	2.0
1	G	5	LEU	2.0
1	B	243[A]	GLN	2.0
1	L	314	ILE	2.0
1	F	108	TYR	2.0
1	J	358	TRP	2.0
1	L	326	TRP	2.0
1	D	30	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	7	GLY	2.0
1	F	357	ASP	2.0
1	G	37	ASP	2.0
1	G	104	ASP	2.0
1	I	144	ASP	2.0
1	C	109	ALA	2.0
1	B	71	LEU	2.0
1	J	71	LEU	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.

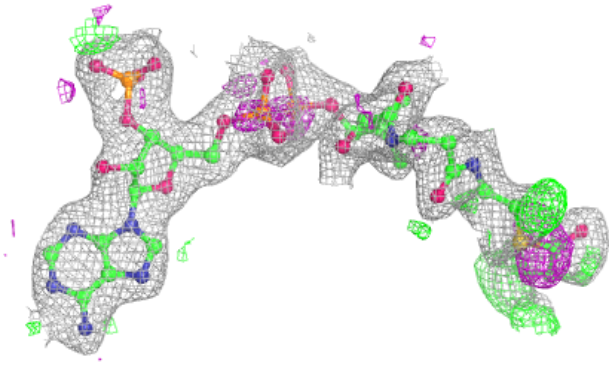
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CO6	E	401	53/53	0.88	0.15	33,44,85,91	0
2	CO6	F	401	53/53	0.89	0.15	27,45,74,78	0
2	CO6	H	401	53/53	0.90	0.14	32,45,79,91	0
2	CO6	C	401	53/53	0.91	0.13	27,41,61,65	0
2	CO6	G	401	53/53	0.91	0.15	25,42,74,83	0
2	CO6	A	401	53/53	0.91	0.14	28,42,73,76	0
2	CO6	K	401	53/53	0.92	0.14	27,40,74,97	0
2	CO6	J	401	53/53	0.93	0.12	23,37,66,84	0
2	CO6	B	401	53/53	0.93	0.12	24,34,75,82	0
2	CO6	D	401	53/53	0.94	0.10	20,31,67,76	0
2	CO6	L	401	53/53	0.94	0.10	21,29,63,74	0
2	CO6	I	401	53/53	0.95	0.10	21,30,55,71	0

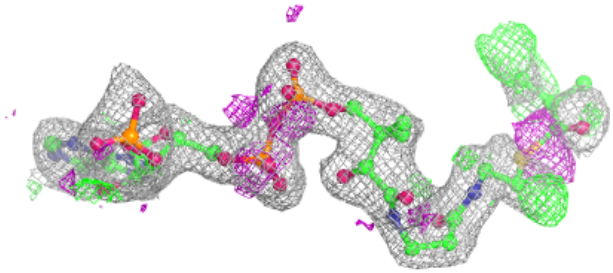
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

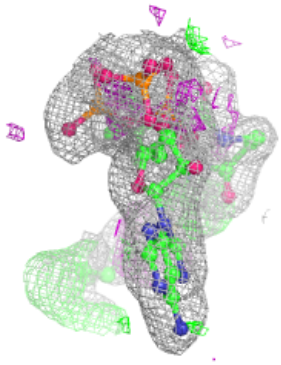
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CO6 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)

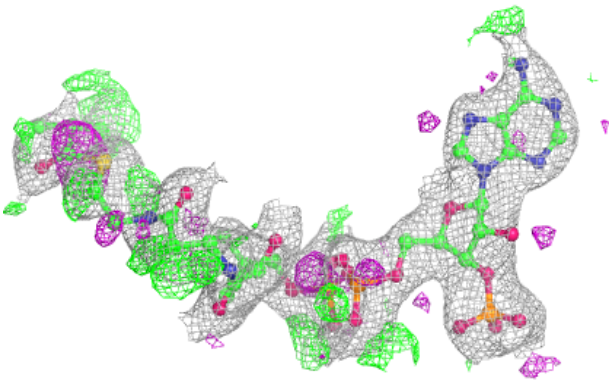


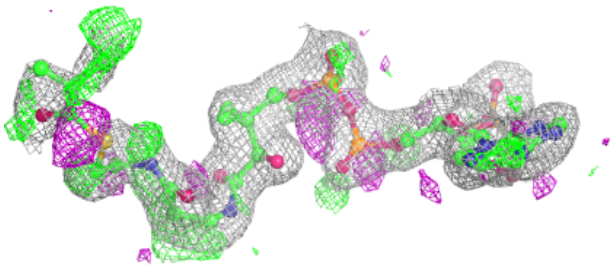


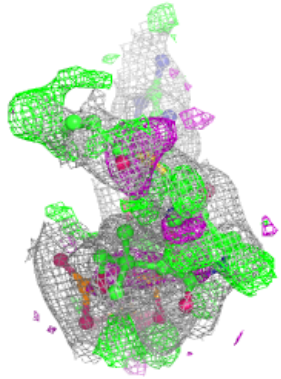


Electron density around CO6 F 401:

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

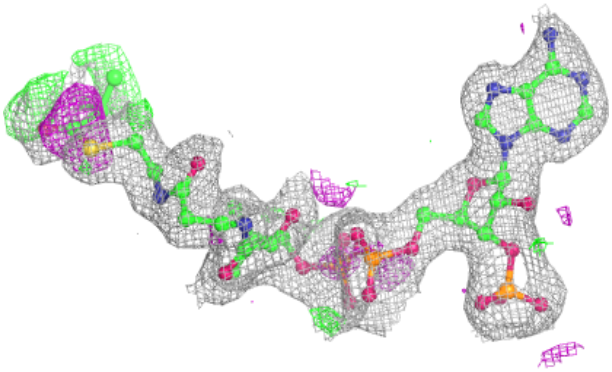


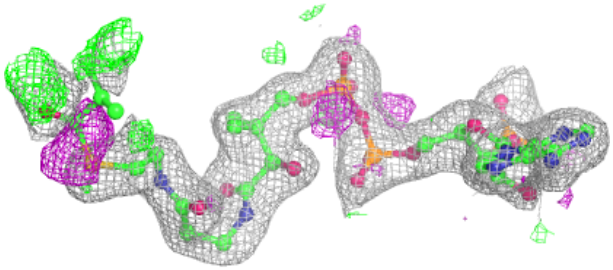


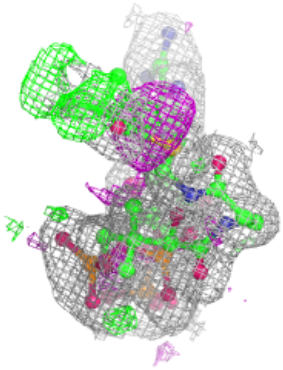


Electron density around CO6 H 401:

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

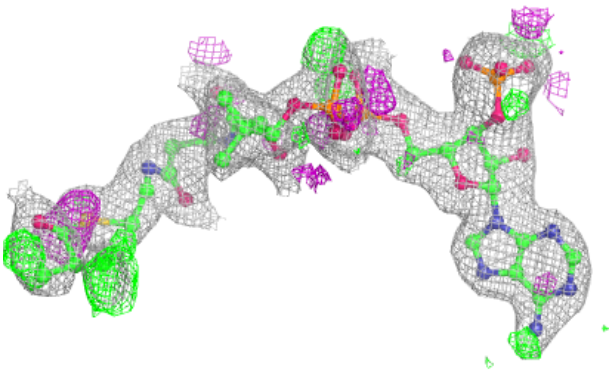


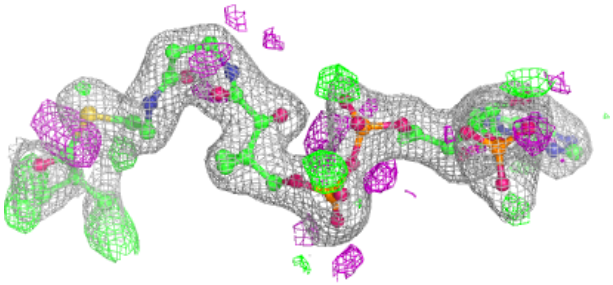


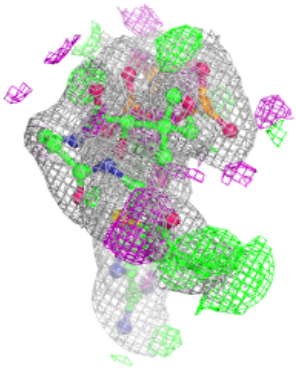


Electron density around CO6 C 401:

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

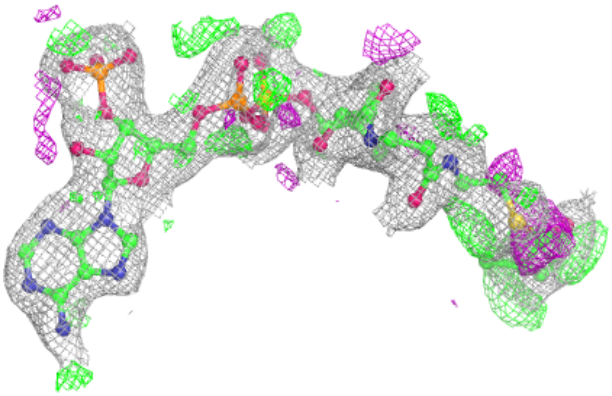


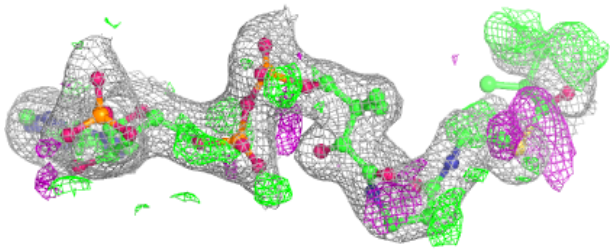




Electron density around CO6 G 401:

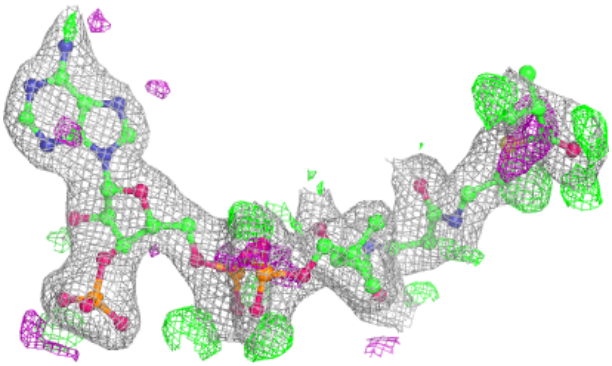
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

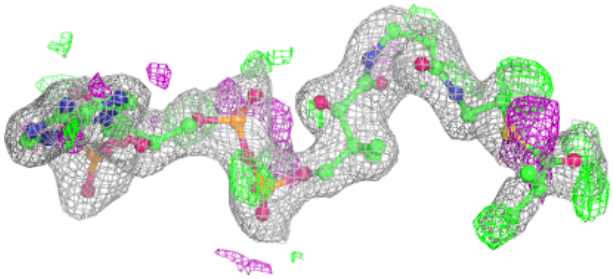


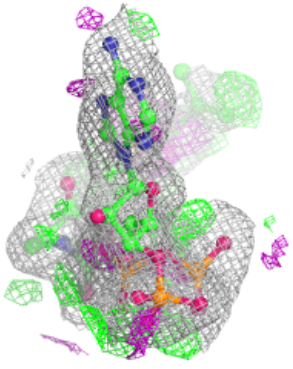


Electron density around CO6 A 401:

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

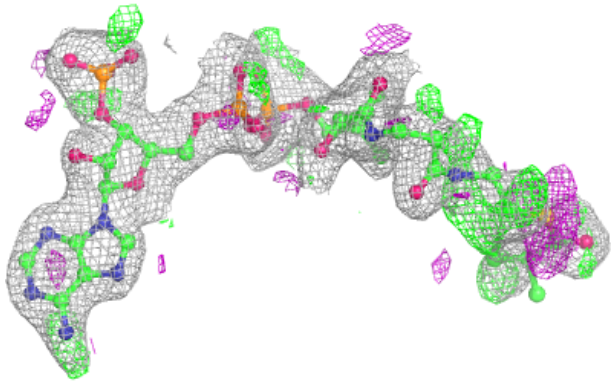


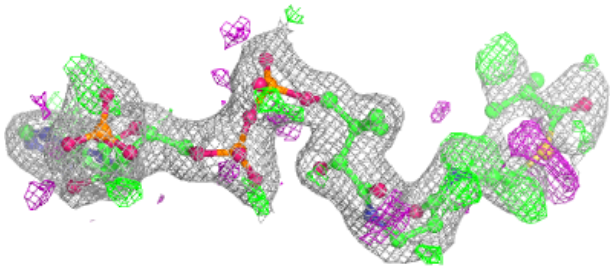


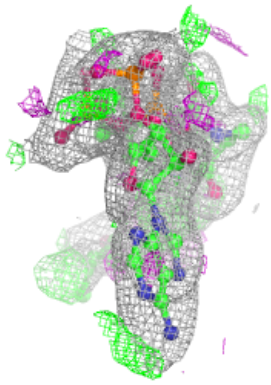


Electron density around CO6 K 401:

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

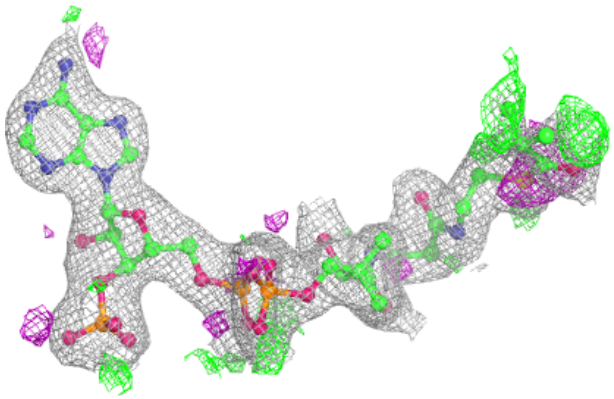


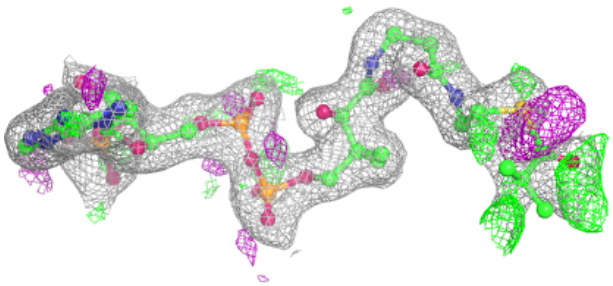


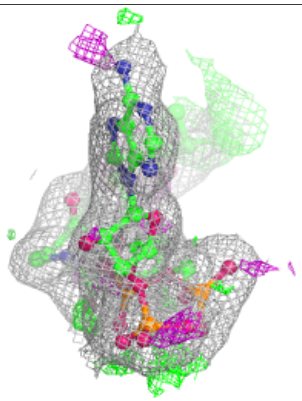


Electron density around CO6 J 401:

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

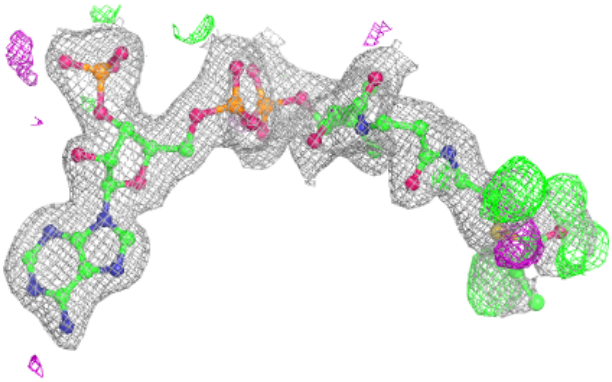


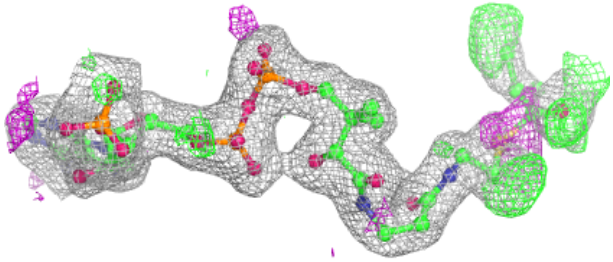


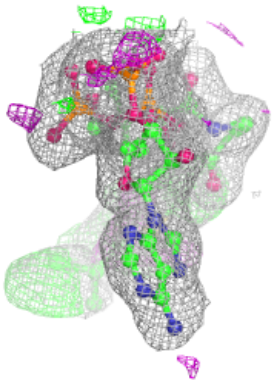


Electron density around CO6 B 401:

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

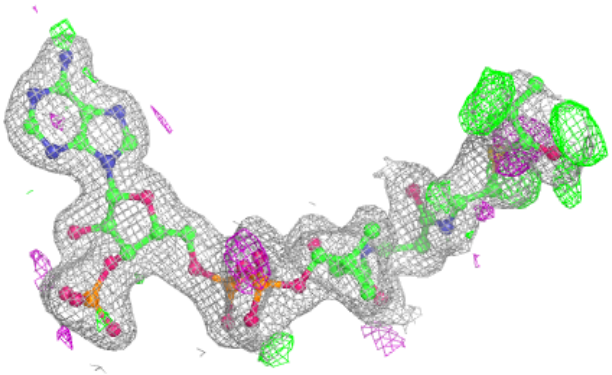


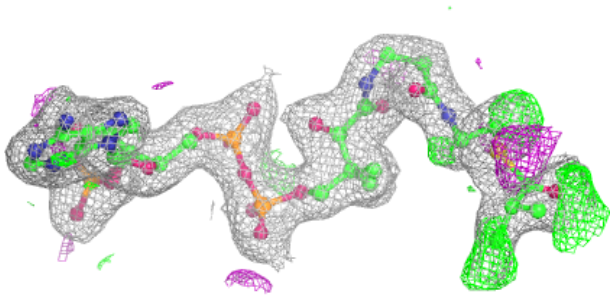


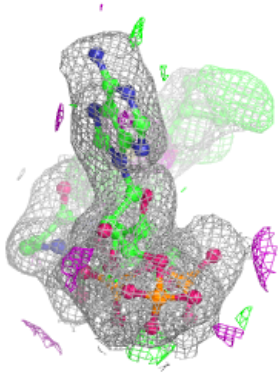


Electron density around CO6 D 401:

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

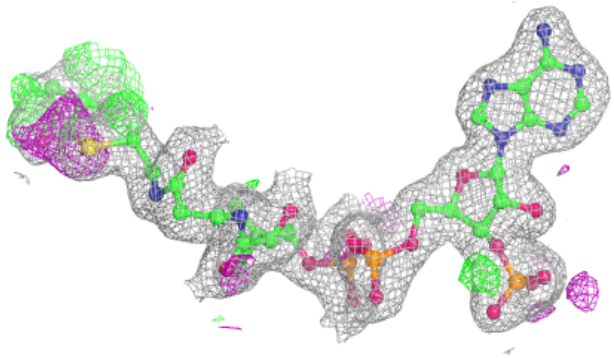


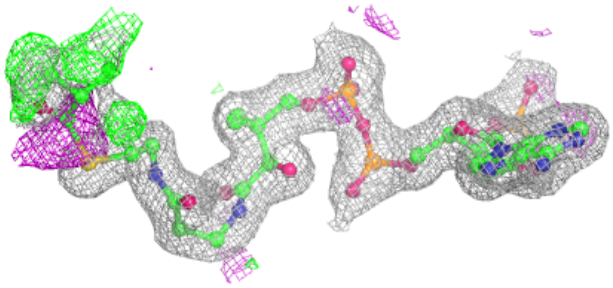


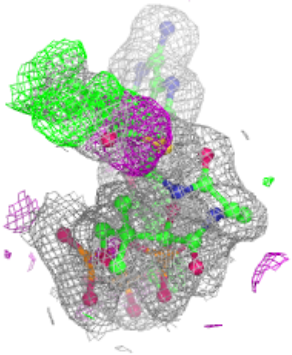


Electron density around CO6 L 401:

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

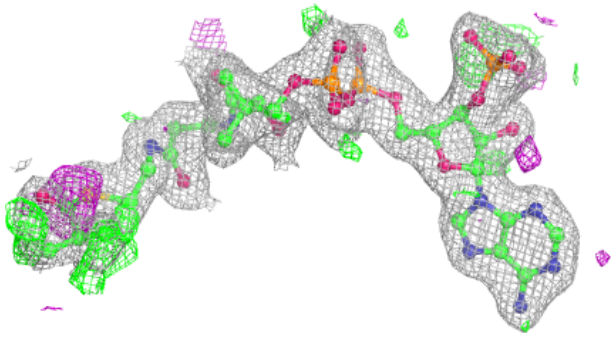


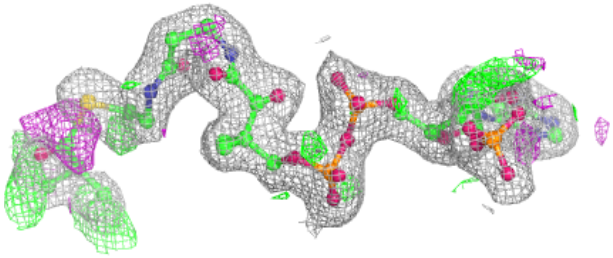


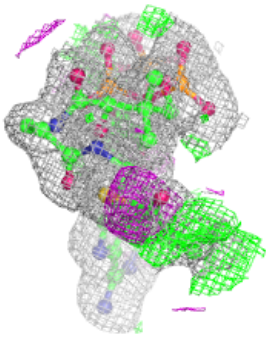


Electron density around CO6 I 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.