Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 07:53 pm BST

PDB ID	:	9I33 / pdb_00009i33
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with butanoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	2.02 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:

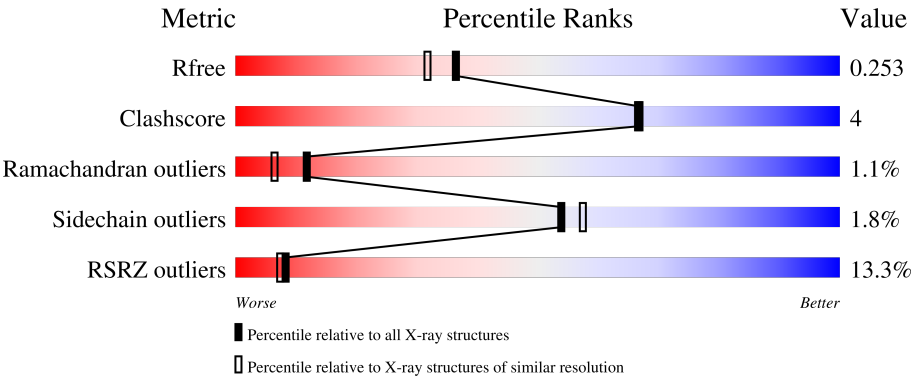
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	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 2.02 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	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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	6% 89% 9%
1	B	364	9% 88% 10%
1	C	364	23% 84% 13%
1	D	364	13% 85% 12%
1	E	364	15% 86% 12%

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Mol	Chain	Length	Quality of chain
1	F	364	23% 82% 15%
1	G	364	22% 87% 11%
1	H	364	12% 89% 9%
1	I	364	4% 93% 5%
1	J	364	8% 92% 7%
1	K	364	17% 89% 9%
1	L	364	5% 91% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 34718 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	2	0
			2722	1706	487	513	16			
1	B	360	Total	C	N	O	S	0	2	0
			2725	1709	488	512	16			
1	C	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	D	360	Total	C	N	O	S	0	1	0
			2719	1705	487	511	16			
1	E	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	F	360	Total	C	N	O	S	0	1	0
			2719	1705	487	511	16			
1	G	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	H	360	Total	C	N	O	S	0	1	0
			2719	1705	487	511	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	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
			2728	1710	488	514	16			
1	L	360	Total	C	N	O	S	0	1	0
			2719	1705	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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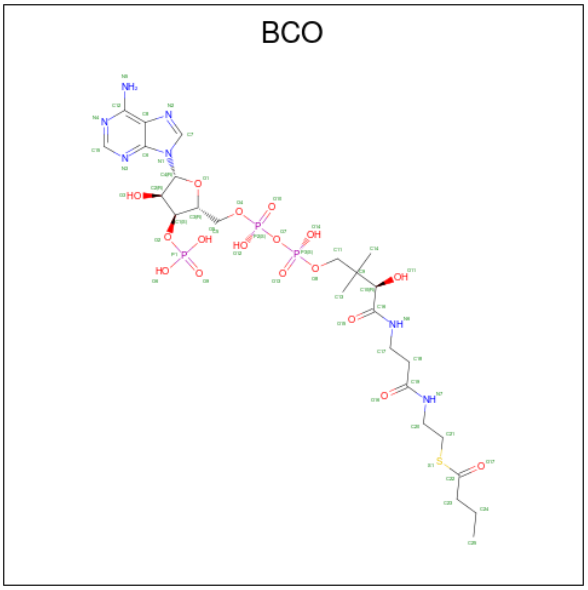
Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is Butyryl Coenzyme A (CCD ID: BCO) (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		

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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.

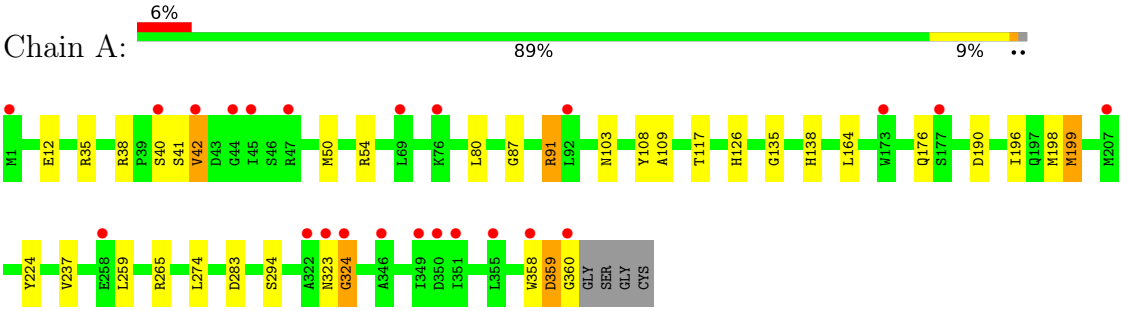
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	107	Total	O	0	0
			107	107		
3	C	113	Total	O	0	0
			113	113		
3	D	111	Total	O	0	0
			111	111		
3	E	114	Total	O	0	0
			114	114		
3	F	98	Total	O	0	0
			98	98		
3	G	99	Total	O	0	0
			99	99		
3	H	107	Total	O	0	0
			107	107		
3	I	141	Total	O	0	0
			141	141		
3	J	141	Total	O	0	0
			141	141		
3	K	142	Total	O	0	0
			142	142		
3	L	133	Total	O	0	0
			133	133		

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.

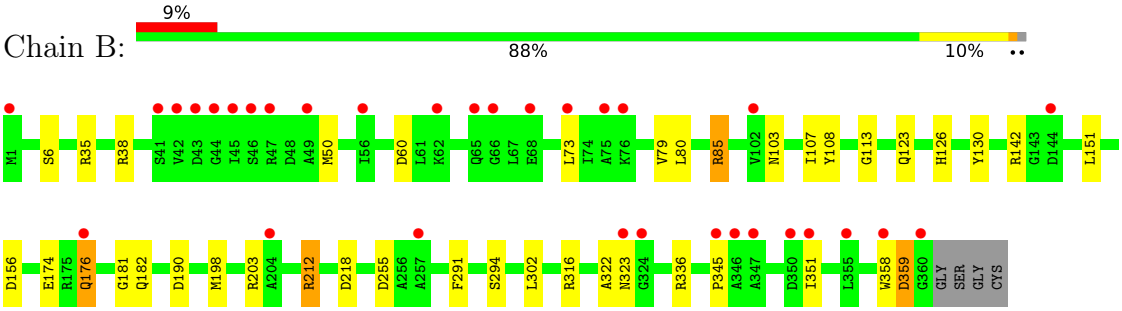
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



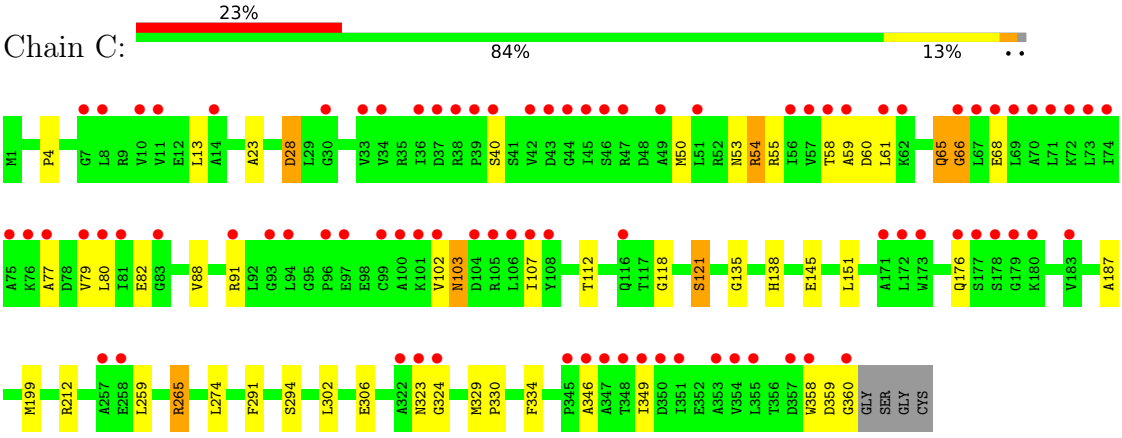
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain B:

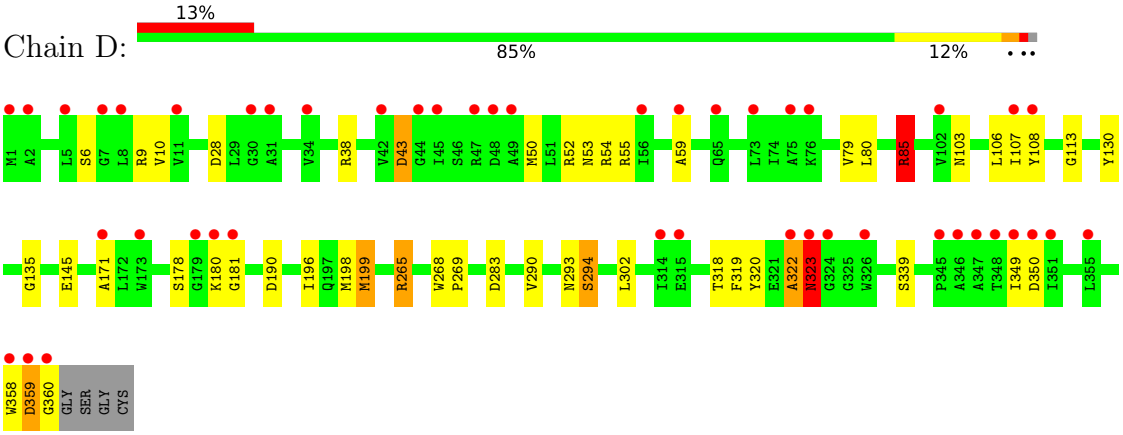


• Molecule 1: Alpha-methylacyl-CoA racemase

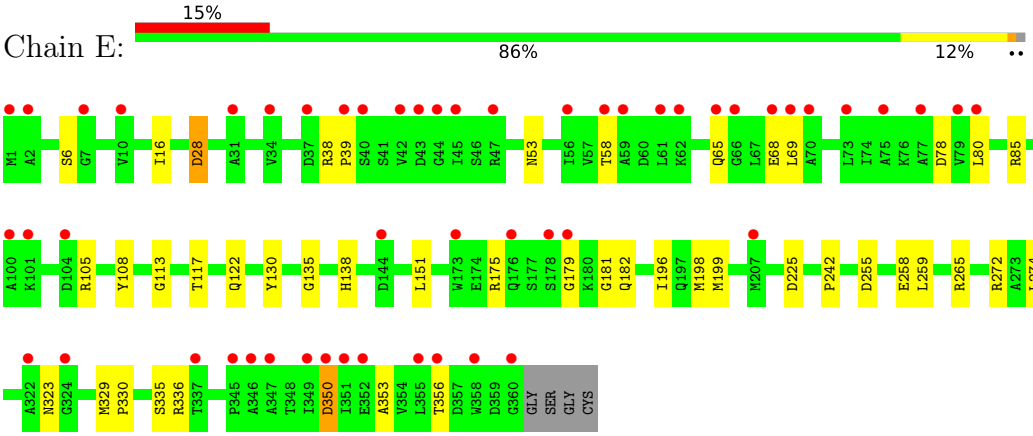
Chain C:



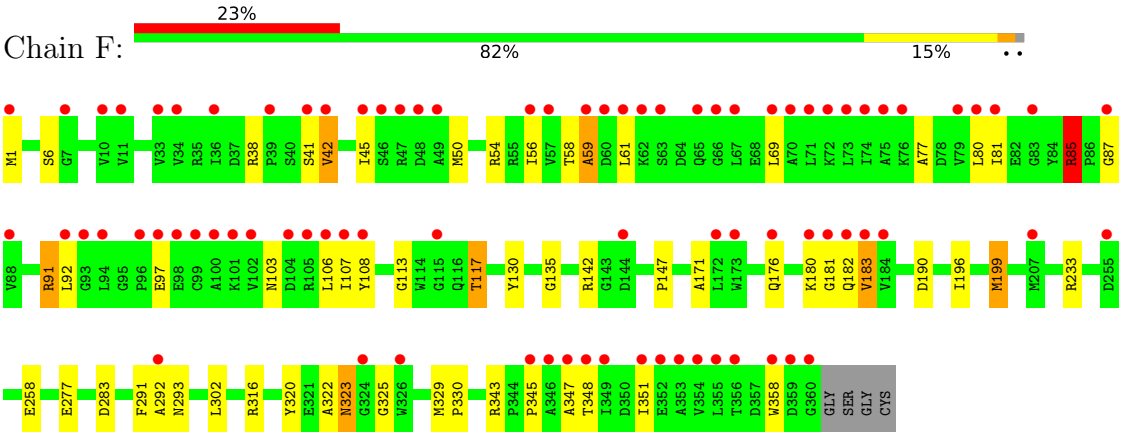
• Molecule 1: Alpha-methylacyl-CoA racemase



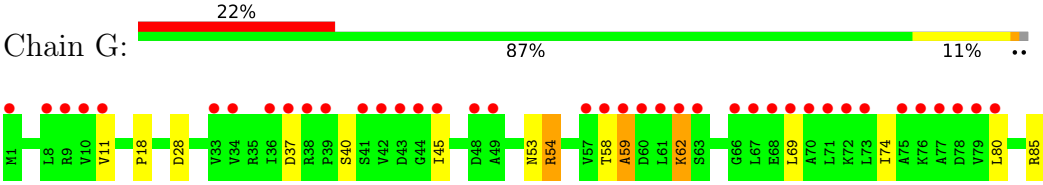
• Molecule 1: Alpha-methylacyl-CoA racemase

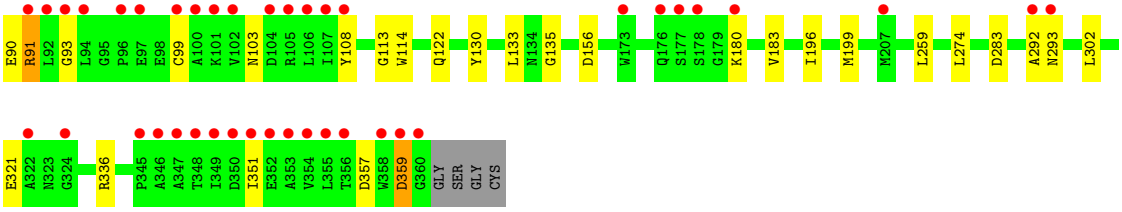


• Molecule 1: Alpha-methylacyl-CoA racemase



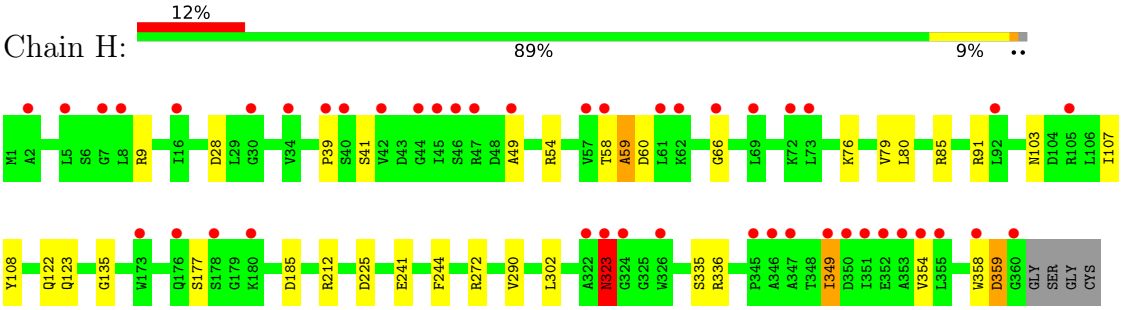
• Molecule 1: Alpha-methylacyl-CoA racemase





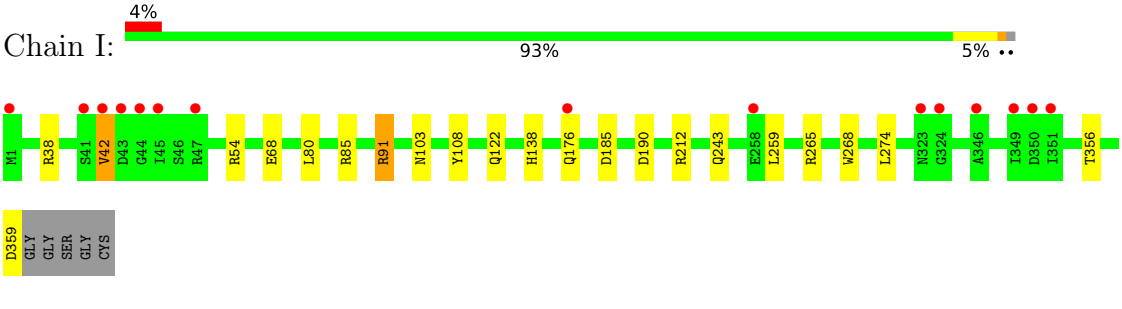
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain H:



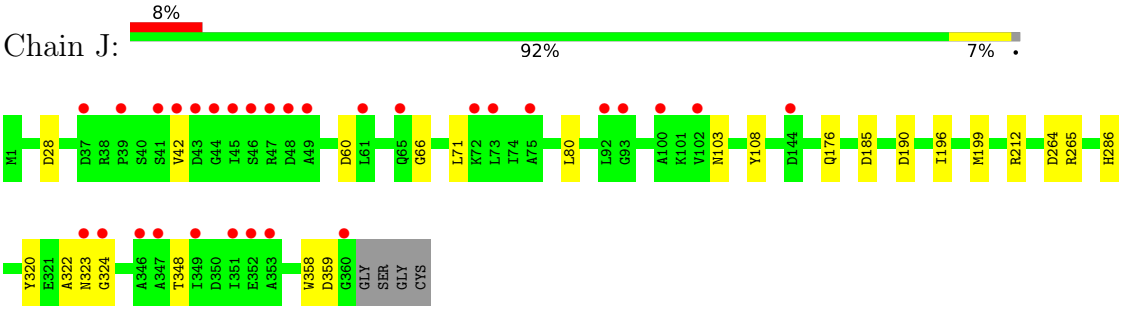
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain I:



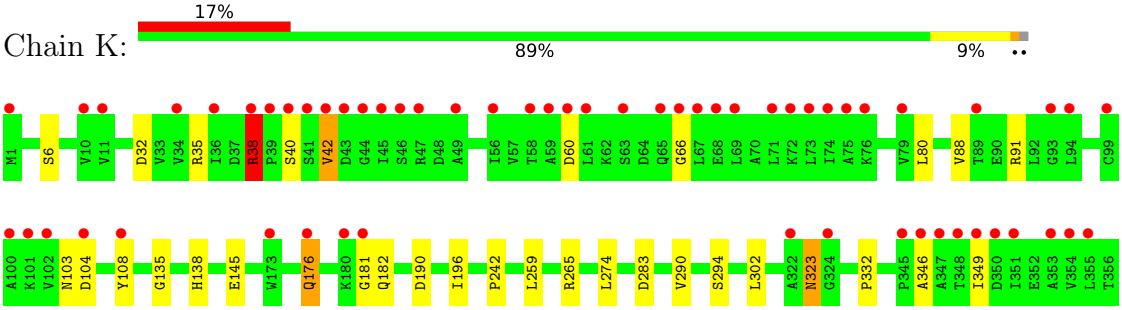
• Molecule 1: Alpha-methylacyl-CoA racemase

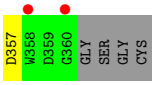
Chain J:



• Molecule 1: Alpha-methylacyl-CoA racemase

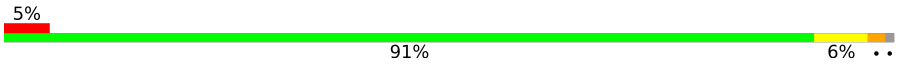
Chain K:

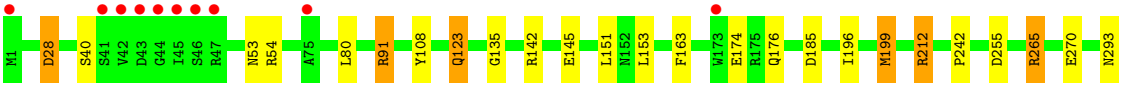


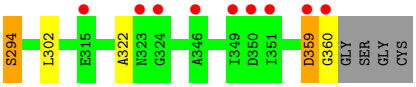


• Molecule 1: Alpha-methylacyl-CoA racemase

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	276.51Å 276.51Å 389.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.50 – 2.02 225.50 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.50-2.02) 99.9 (225.50-2.02)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.208 , 0.243 0.220 , 0.253	Depositor DCC
R_{free} test set	24519 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.006 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	34718	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: BCO

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	0/2795	1.03	3/3802 (0.1%)
1	B	0.66	0/2795	1.07	9/3802 (0.2%)
1	C	0.63	0/2795	1.08	3/3802 (0.1%)
1	D	0.65	0/2786	1.08	4/3790 (0.1%)
1	E	0.65	0/2795	1.04	2/3802 (0.1%)
1	F	0.64	0/2786	1.08	5/3790 (0.1%)
1	G	0.62	0/2795	1.07	3/3802 (0.1%)
1	H	0.63	0/2786	1.06	5/3790 (0.1%)
1	I	0.64	0/2791	1.06	7/3797 (0.2%)
1	J	0.65	0/2786	1.06	3/3790 (0.1%)
1	K	0.65	0/2804	1.09	4/3814 (0.1%)
1	L	0.65	0/2786	1.06	7/3790 (0.2%)
All	All	0.64	0/33500	1.06	55/45571 (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	C	0	1
1	D	0	4
1	E	0	1
1	F	0	4
1	G	0	2
1	H	0	4
1	I	0	1
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	34

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	28	ASP	CA-CB-CG	8.26	120.86	112.60
1	B	203	ARG	CB-CA-C	-7.34	98.37	110.85
1	I	91	ARG	CB-CA-C	-6.98	97.72	110.63
1	E	255	ASP	CA-CB-CG	6.97	119.57	112.60
1	J	28	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	156	ASP	CB-CA-C	-6.32	100.92	110.90
1	J	190	ASP	CA-CB-CG	6.27	118.87	112.60
1	G	293	ASN	CA-CB-CG	6.26	118.86	112.60
1	B	255	ASP	CB-CA-C	6.24	120.64	110.22
1	H	123	GLN	CB-CA-C	6.20	119.94	109.84
1	L	28	ASP	CA-CB-CG	5.86	118.46	112.60
1	G	283	ASP	CA-CB-CG	5.85	118.45	112.60
1	G	91	ARG	CB-CA-C	-5.80	99.20	110.46
1	L	255	ASP	CB-CA-C	-5.73	100.08	109.53
1	L	123	GLN	N-CA-CB	-5.71	101.09	109.95
1	C	28	ASP	CA-CB-CG	5.71	118.31	112.60
1	J	185	ASP	CA-CB-CG	5.70	118.30	112.60
1	L	91	ARG	CB-CA-C	-5.69	101.01	110.68
1	B	203	ARG	N-CA-CB	5.67	118.56	110.16
1	L	123	GLN	CB-CA-C	5.67	119.08	109.84
1	D	283	ASP	CA-CB-CG	5.61	118.21	112.60
1	K	32	ASP	CA-CB-CG	5.58	118.19	112.60
1	B	38	ARG	CB-CA-C	5.57	117.14	108.61
1	B	174	GLU	CA-C-N	5.51	127.66	120.28
1	B	174	GLU	C-N-CA	5.51	127.66	120.28
1	I	38	ARG	CB-CA-C	-5.50	100.42	109.27
1	K	38	ARG	N-CA-CB	5.49	117.98	110.03
1	A	91	ARG	CB-CA-C	-5.48	100.50	110.63
1	I	190	ASP	CA-CB-CG	5.42	118.02	112.60
1	H	323	ASN	CB-CA-C	-5.39	108.77	115.89
1	D	190	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	258	GLU	CB-CA-C	-5.35	99.30	109.95
1	K	283	ASP	CA-CB-CG	5.31	117.91	112.60
1	I	185	ASP	CA-CB-CG	5.26	117.86	112.60
1	L	185	ASP	CA-CB-CG	5.25	117.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	185	ASP	CA-CB-CG	5.23	117.83	112.60
1	F	283	ASP	CA-CB-CG	5.23	117.83	112.60
1	L	265	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	I	243	GLN	CB-CG-CD	5.23	121.49	112.60
1	D	265	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	38	ARG	CB-CA-C	5.19	116.55	108.61
1	H	28	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	306	GLU	CB-CA-C	-5.16	100.67	109.65
1	F	147	PRO	CA-C-N	-5.16	118.84	123.33
1	F	147	PRO	C-N-CA	-5.16	118.84	123.33
1	I	356	THR	CA-CB-OG1	-5.15	101.88	109.60
1	B	218	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	60	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	190	ASP	CA-CB-CG	5.09	117.69	112.60
1	F	190	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	283	ASP	CA-CB-CG	5.04	117.64	112.60
1	K	190	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	190	ASP	CA-CB-CG	5.03	117.62	112.60
1	H	39	PRO	N-CA-C	-5.02	106.99	113.57
1	I	91	ARG	N-CA-CB	5.00	117.93	110.22

There are no chirality outliers.

All (34) 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	322	ALA	Peptide
1	B	35	ARG	Sidechain
1	C	54	ARG	Peptide
1	D	322	ALA	Peptide
1	D	323	ASN	Peptide
1	D	54	ARG	Peptide
1	D	85	ARG	Sidechain
1	E	350	ASP	Peptide
1	F	233	ARG	Sidechain
1	F	54	ARG	Peptide
1	F	85	ARG	Sidechain
1	F	91	ARG	Sidechain
1	G	54	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	G	91	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	323	ASN	Peptide
1	H	54	ARG	Peptide
1	H	91	ARG	Sidechain
1	I	54	ARG	Peptide
1	J	212	ARG	Sidechain
1	J	265	ARG	Sidechain
1	K	265	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	2722	0	2661	22	0
1	B	2725	0	2671	21	0
1	C	2722	0	2661	35	0
1	D	2719	0	2663	30	0
1	E	2722	0	2661	28	0
1	F	2719	0	2663	34	0
1	G	2722	0	2661	25	0
1	H	2719	0	2663	18	0
1	I	2718	0	2658	10	0
1	J	2719	0	2663	11	0
1	K	2728	0	2669	18	0
1	L	2719	0	2663	18	0
2	A	53	0	40	2	0
2	B	53	0	40	3	0
2	C	53	0	40	2	0
2	D	53	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	53	0	40	1	0
2	F	53	0	40	3	0
2	G	53	0	40	0	0
2	H	53	0	40	0	0
2	I	53	0	40	0	0
2	J	53	0	40	0	0
2	K	53	0	40	1	0
2	L	53	0	40	0	0
3	A	122	0	0	1	0
3	B	107	0	0	1	0
3	C	113	0	0	4	0
3	D	111	0	0	0	0
3	E	114	0	0	3	0
3	F	98	0	0	5	0
3	G	99	0	0	2	0
3	H	107	0	0	0	0
3	I	141	0	0	1	0
3	J	141	0	0	1	0
3	K	142	0	0	2	0
3	L	133	0	0	1	0
All	All	34718	0	32437	235	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 (235) 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:BCO:O10	1.68	0.93
1:C:118:GLY:O	1:C:121:SER:OG	1.88	0.90
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.64	0.79
1:D:85:ARG:HD3	2:D:401:BCO:O12	1.86	0.75
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.73	0.70
1:B:85:ARG:HD2	2:B:401:BCO:O10	1.91	0.69
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.74	0.68
1:C:346:ALA:HB3	3:C:531:HOH:O	1.95	0.65
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.32	0.64
1:F:58:THR:O	1:F:59:ALA:HB2	1.97	0.63
1:B:358:TRP:O	1:B:359:ASP:HB2	1.99	0.62
1:F:80:LEU:HD22	1:F:108:TYR:CE1	2.34	0.62
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:346:ALA:HB3	3:K:547:HOH:O	2.00	0.61
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.35	0.61
1:G:80:LEU:HD23	1:G:108:TYR:CE1	2.36	0.61
1:K:176:GLN:HA	1:K:176:GLN:HE21	1.66	0.61
1:C:291:PHE:O	1:C:294:SER:HB3	2.00	0.61
1:D:85:ARG:CD	2:D:401:BCO:O12	2.48	0.61
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.83	0.61
1:K:80:LEU:HD23	1:K:108:TYR:CE1	2.36	0.60
1:F:85:ARG:CD	2:F:401:BCO:O10	2.49	0.59
1:A:87:GLY:O	1:A:91:ARG:HG3	2.03	0.59
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.17	0.58
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.37	0.58
1:K:138:HIS:HD2	3:K:564:HOH:O	1.85	0.58
1:E:85:ARG:NH1	1:E:122:GLN:O	2.35	0.58
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.86	0.57
1:J:322:ALA:O	1:J:324:GLY:N	2.37	0.57
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.37	0.57
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.40	0.57
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.40	0.56
1:E:336:ARG:HG2	1:E:336:ARG:HH11	1.70	0.56
1:K:294:SER:O	1:L:123:GLN:HG3	2.05	0.56
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.41	0.56
1:F:1:MET:HE2	1:F:343:ARG:NH2	2.21	0.56
1:H:9:ARG:NH2	1:H:358:TRP:HA	2.21	0.56
1:A:126:HIS:ND1	2:A:401:BCO:H33	2.20	0.55
1:G:85:ARG:NH1	1:G:122:GLN:O	2.39	0.55
1:D:28:ASP:HA	1:D:53:ASN:ND2	2.22	0.55
1:F:80:LEU:CD2	1:F:108:TYR:CE1	2.89	0.55
1:F:106:LEU:O	1:F:181:GLY:HA3	2.05	0.54
1:C:88:VAL:HG13	2:C:401:BCO:H3	1.89	0.54
1:G:11:VAL:HG12	1:G:80:LEU:HD12	1.89	0.54
1:H:58:THR:O	1:H:59:ALA:HB2	2.05	0.54
1:B:85:ARG:CD	2:B:401:BCO:O10	2.55	0.54
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.90	0.54
1:A:323:ASN:O	1:A:324:GLY:C	2.50	0.54
1:C:138:HIS:HD2	3:C:550:HOH:O	1.90	0.53
1:E:78:ASP:OD1	1:E:175:ARG:NH2	2.26	0.53
1:E:39:PRO:HA	1:E:58:THR:OG1	2.08	0.53
1:H:358:TRP:O	1:H:359:ASP:HB2	2.08	0.53
1:E:272:ARG:NH1	3:E:503:HOH:O	2.43	0.52
1:F:329:MET:HE3	1:F:330:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:C	1:C:80:LEU:HD13	2.34	0.52
1:C:265:ARG:HD2	3:C:544:HOH:O	2.09	0.52
1:D:28:ASP:HA	1:D:53:ASN:HD22	1.74	0.52
1:A:50:MET:HE1	1:B:198:MET:HB2	1.92	0.51
1:H:60:ASP:O	1:H:66:GLY:HA3	2.09	0.51
1:H:85:ARG:NH2	1:H:122:GLN:O	2.42	0.51
1:D:294:SER:HB2	1:L:293:ASN:O	2.10	0.51
1:C:65:GLN:O	1:C:68:GLU:N	2.42	0.51
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.26	0.51
1:F:87:GLY:O	1:F:91:ARG:HG3	2.10	0.51
1:D:107:ILE:HD12	1:D:171:ALA:HB1	1.92	0.51
1:K:323:ASN:OD1	1:K:323:ASN:N	2.43	0.50
1:E:259:LEU:HD22	1:E:274:LEU:HD13	1.93	0.50
1:H:358:TRP:O	1:H:359:ASP:CB	2.59	0.50
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.95	0.50
1:K:80:LEU:CD2	1:K:108:TYR:CE1	2.94	0.50
1:E:181:GLY:O	1:E:182:GLN:HB3	2.12	0.50
1:B:126:HIS:ND1	2:B:401:BCO:H33	2.26	0.50
1:E:138:HIS:HD2	3:E:559:HOH:O	1.94	0.50
1:A:359:ASP:O	1:A:360:GLY:C	2.55	0.49
1:G:58:THR:O	1:G:59:ALA:HB2	2.11	0.49
1:K:196:ILE:HG13	1:L:153:LEU:HD21	1.93	0.49
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.76	0.49
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.95	0.49
1:C:28:ASP:HA	1:C:53:ASN:HD22	1.78	0.49
1:C:88:VAL:CG1	2:C:401:BCO:H3	2.42	0.49
1:C:359:ASP:O	1:C:360:GLY:C	2.55	0.49
1:A:138:HIS:HD2	3:A:531:HOH:O	1.96	0.48
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.95	0.48
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.27	0.48
1:G:69:LEU:HD13	1:G:351:ILE:HG21	1.95	0.48
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.95	0.48
1:G:180:LYS:HB2	1:H:336:ARG:NH2	2.29	0.48
1:H:76:LYS:HB2	1:H:358:TRP:HE3	1.78	0.48
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.49	0.48
1:D:106:LEU:O	1:D:181:GLY:HA3	2.14	0.48
1:I:138:HIS:HD2	3:I:532:HOH:O	1.97	0.48
1:F:196:ILE:HG12	1:F:199:MET:HB2	1.96	0.48
1:E:135:GLY:HA2	1:F:302:LEU:O	2.13	0.48
1:F:291:PHE:O	1:F:293:ASN:N	2.47	0.48
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:GLN:HE21	1:E:69:LEU:HD12	1.80	0.47
1:E:105:ARG:HG2	1:E:179:GLY:O	2.13	0.47
1:I:85:ARG:NH1	1:I:122:GLN:O	2.44	0.47
1:K:302:LEU:O	1:L:135:GLY:HA2	2.14	0.47
1:F:345:PRO:HA	3:F:532:HOH:O	2.14	0.47
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.50	0.47
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.29	0.47
1:C:135:GLY:HA2	1:D:302:LEU:O	2.15	0.47
1:G:45:ILE:HA	3:G:511:HOH:O	2.15	0.47
1:H:241:GLU:HB2	1:H:244:PHE:CD2	2.50	0.46
1:F:293:ASN:ND2	3:F:503:HOH:O	2.38	0.46
1:G:114:TRP:CZ3	1:G:133:LEU:HD22	2.49	0.46
1:C:112:THR:O	1:C:187:ALA:HA	2.15	0.46
1:K:176:GLN:CD	1:L:176:GLN:HG2	2.40	0.46
1:G:302:LEU:O	1:H:135:GLY:HA2	2.15	0.46
1:E:28:ASP:HA	1:E:53:ASN:ND2	2.30	0.46
1:F:322:ALA:O	1:F:323:ASN:C	2.59	0.46
1:J:60:ASP:O	1:J:66:GLY:HA3	2.16	0.46
1:C:77:ALA:HB2	1:C:358:TRP:HZ3	1.80	0.46
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.97	0.46
1:B:291:PHE:O	1:B:294:SER:HB3	2.16	0.46
1:C:102:VAL:O	1:C:103:ASN:HB2	2.16	0.46
1:E:302:LEU:O	1:F:135:GLY:HA2	2.15	0.46
1:G:87:GLY:N	3:G:513:HOH:O	2.49	0.46
1:L:359:ASP:O	1:L:360:GLY:C	2.59	0.46
1:C:50:MET:HE1	1:D:198:MET:HB2	1.98	0.46
1:G:80:LEU:CD2	1:G:108:TYR:CE1	2.99	0.46
1:F:181:GLY:O	1:F:182:GLN:HB3	2.16	0.45
1:H:49:ALA:HB2	1:H:323:ASN:HD21	1.80	0.45
1:K:181:GLY:O	1:K:182:GLN:HB3	2.15	0.45
1:D:358:TRP:O	1:D:359:ASP:HB2	2.15	0.45
1:F:142:ARG:NH1	3:F:508:HOH:O	2.48	0.45
1:L:270:GLU:HG3	3:L:518:HOH:O	2.16	0.45
1:B:142:ARG:O	1:B:212:ARG:HD2	2.17	0.45
1:F:38:ARG:HG2	3:F:527:HOH:O	2.16	0.45
1:J:320:TYR:CE2	1:J:322:ALA:HB2	2.52	0.45
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.97	0.45
1:A:91:ARG:HD2	1:E:242:PRO:HB3	1.99	0.45
1:D:293:ASN:O	1:L:294:SER:HB2	2.17	0.45
1:E:117:THR:O	1:F:316:ARG:HD2	2.17	0.45
1:G:90:GLU:O	1:G:93:GLY:N	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:ARG:O	1:L:212:ARG:HD2	2.17	0.45
1:J:196:ILE:HG12	1:J:199:MET:HB2	1.98	0.45
1:C:61:LEU:O	3:C:501:HOH:O	2.21	0.45
1:A:135:GLY:HA2	1:B:302:LEU:O	2.17	0.44
1:C:55:ARG:HG2	1:C:349:ILE:CD1	2.48	0.44
1:L:174:GLU:OE1	1:L:174:GLU:C	2.60	0.44
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.53	0.44
1:I:176:GLN:HE21	1:I:176:GLN:HA	1.82	0.44
1:J:286:HIS:HD2	3:J:635:HOH:O	1.98	0.44
1:E:353:ALA:O	1:E:356:THR:HB	2.16	0.44
1:F:113:GLY:HA3	1:F:130:TYR:CE1	2.52	0.44
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.47	0.44
1:F:320:TYR:CE2	1:F:322:ALA:HB2	2.52	0.44
1:D:318:THR:HG22	1:D:319:PHE:CE1	2.52	0.44
1:F:61:LEU:HB2	1:F:92:LEU:HD22	2.00	0.44
1:C:323:ASN:O	1:C:324:GLY:C	2.61	0.43
1:D:9:ARG:NH2	1:D:358:TRP:HA	2.33	0.43
1:F:107:ILE:HD12	1:F:171:ALA:HB1	1.99	0.43
1:D:265:ARG:HG2	1:D:268:TRP:CH2	2.53	0.43
1:G:54:ARG:HG2	1:G:54:ARG:HH11	1.82	0.43
1:J:264:ASP:C	1:J:264:ASP:OD1	2.61	0.43
1:E:198:MET:HB2	1:F:50:MET:HE1	1.99	0.43
1:K:88:VAL:CG1	2:K:401:BCO:H3	2.49	0.43
1:K:135:GLY:HA2	1:L:302:LEU:O	2.18	0.43
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.54	0.43
1:E:316:ARG:HD2	1:F:117:THR:O	2.19	0.43
1:A:80:LEU:CD2	1:A:108:TYR:CE2	3.02	0.43
1:A:117:THR:O	1:B:316:ARG:HD2	2.18	0.43
1:A:198:MET:HB2	1:B:50:MET:HE1	2.01	0.43
1:C:302:LEU:O	1:D:135:GLY:HA2	2.18	0.43
1:D:323:ASN:HD22	1:D:323:ASN:HA	1.67	0.43
1:E:258:GLU:HG3	3:E:562:HOH:O	2.18	0.43
1:B:80:LEU:CD2	1:B:108:TYR:CE2	3.02	0.43
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.36	0.43
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.44	0.42
1:C:77:ALA:HB2	1:C:358:TRP:CZ3	2.55	0.42
1:F:58:THR:O	1:F:59:ALA:CB	2.63	0.42
1:G:62:LYS:HB2	1:G:62:LYS:HE2	1.71	0.42
1:H:349:ILE:HD11	1:H:354:VAL:HG22	2.00	0.42
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.90	0.42
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD12	1:C:82:GLU:HB3	2.01	0.42
1:G:11:VAL:HG12	1:G:80:LEU:CD1	2.48	0.42
1:G:336:ARG:HG2	1:G:336:ARG:HH11	1.84	0.42
1:E:69:LEU:HD23	1:E:69:LEU:HA	1.92	0.42
1:K:60:ASP:O	1:K:66:GLY:HA3	2.18	0.42
1:G:74:ILE:HG21	1:G:99:CYS:SG	2.59	0.42
1:G:183:VAL:H	1:H:335:SER:HG	1.66	0.42
1:K:145:GLU:OE2	1:L:145:GLU:OE1	2.38	0.42
1:F:77:ALA:HB2	1:F:358:TRP:CZ3	2.54	0.42
1:A:126:HIS:HA	2:A:401:BCO:H32	2.01	0.42
1:D:320:TYR:CE2	1:D:322:ALA:HB2	2.55	0.42
1:G:135:GLY:HA2	1:H:302:LEU:O	2.19	0.42
1:D:359:ASP:HB3	1:D:360:GLY:H	1.75	0.42
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.50	0.42
1:E:335:SER:HG	1:F:183:VAL:H	1.67	0.42
1:F:80:LEU:HG	1:F:81:ILE:N	2.35	0.42
1:G:196:ILE:HG12	1:G:199:MET:HB2	2.02	0.42
1:G:18:PRO:HB3	1:G:156:ASP:O	2.20	0.42
1:C:4:PRO:HG3	1:C:334:PHE:CZ	2.55	0.41
1:C:79:VAL:HG22	1:C:107:ILE:HB	2.00	0.41
1:D:268:TRP:N	1:D:269:PRO:CD	2.82	0.41
2:F:401:BCO:O15	2:F:401:BCO:H18	2.19	0.41
1:A:358:TRP:O	1:A:359:ASP:CB	2.68	0.41
1:C:65:GLN:O	1:C:66:GLY:C	2.63	0.41
1:E:196:ILE:HG12	1:E:199:MET:HB2	2.03	0.41
1:F:325:GLY:HA2	3:F:577:HOH:O	2.19	0.41
1:L:28:ASP:HA	1:L:53:ASN:ND2	2.35	0.41
1:B:79:VAL:HG22	1:B:107:ILE:HB	2.02	0.41
1:D:10:VAL:HG22	1:D:79:VAL:HB	2.01	0.41
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.45	0.41
1:B:181:GLY:O	1:B:182:GLN:HB3	2.21	0.41
1:C:91:ARG:HD3	1:L:242:PRO:HB3	2.03	0.41
1:K:332:PRO:HG3	1:L:163:PHE:O	2.21	0.41
1:A:224:TYR:HA	1:A:237:VAL:O	2.21	0.41
1:C:138:HIS:O	1:C:212:ARG:HD3	2.20	0.41
1:D:50:MET:O	1:D:50:MET:HG2	2.21	0.41
1:A:109:ALA:HB1	1:A:164:LEU:HD11	2.03	0.41
1:I:265:ARG:HG2	1:I:268:TRP:CZ3	2.56	0.41
1:B:345:PRO:HB3	3:B:568:HOH:O	2.20	0.41
1:C:91:ARG:CD	1:L:242:PRO:HB3	2.51	0.41
1:D:28:ASP:CG	1:D:52:ARG:HH21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:SER:O	1:D:180:LYS:HG2	2.21	0.41
1:J:71:LEU:HD23	1:J:71:LEU:HA	1.95	0.41
1:I:91:ARG:CD	1:K:242:PRO:HB3	2.51	0.41
1:I:138:HIS:O	1:I:212:ARG:HD3	2.21	0.40
1:A:294:SER:O	1:B:123:GLN:HG3	2.22	0.40
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.85	0.40
1:D:55:ARG:HD2	1:D:349:ILE:HD11	2.03	0.40
1:E:113:GLY:HA3	1:E:130:TYR:CZ	2.57	0.40
1:C:23:ALA:HB3	1:C:54:ARG:NH2	2.36	0.40
1:G:259:LEU:CD2	1:G:274:LEU:HD13	2.44	0.40
1:J:358:TRP:O	1:J:359:ASP:HB3	2.22	0.40
1:A:12:GLU:OE2	1:A:35:ARG:NH1	2.49	0.40
1:D:318:THR:HG22	1:D:319:PHE:CD1	2.57	0.40
1:E:38:ARG:NH2	2:E:401:BCO:O1	2.55	0.40
1:E:329:MET:HE3	1:E:330:PRO:HD2	2.04	0.40
1:F:77:ALA:HB2	1:F:358:TRP:HZ3	1.87	0.40
1:J:42:VAL:HG11	1:J:348:THR:OG1	2.21	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	360/364 (99%)	337 (94%)	17 (5%)	6 (2%)	7 3
1	B	360/364 (99%)	346 (96%)	9 (2%)	5 (1%)	9 4
1	C	360/364 (99%)	332 (92%)	23 (6%)	5 (1%)	9 4
1	D	359/364 (99%)	338 (94%)	16 (4%)	5 (1%)	9 4
1	E	360/364 (99%)	338 (94%)	20 (6%)	2 (1%)	22 16
1	F	359/364 (99%)	331 (92%)	21 (6%)	7 (2%)	6 2
1	G	360/364 (99%)	328 (91%)	28 (8%)	4 (1%)	12 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	359/364 (99%)	341 (95%)	14 (4%)	4 (1%)	12 6
1	I	359/364 (99%)	348 (97%)	9 (2%)	2 (1%)	22 16
1	J	359/364 (99%)	343 (96%)	14 (4%)	2 (1%)	22 16
1	K	361/364 (99%)	344 (95%)	15 (4%)	2 (1%)	22 16
1	L	359/364 (99%)	342 (95%)	15 (4%)	2 (1%)	22 16
All	All	4315/4368 (99%)	4068 (94%)	201 (5%)	46 (1%)	12 6

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	103	ASN
1	B	359	ASP
1	C	103	ASN
1	D	103	ASN
1	D	359	ASP
1	F	41	SER
1	F	103	ASN
1	G	103	ASN
1	H	59	ALA
1	K	42	VAL
1	A	41	SER
1	A	359	ASP
1	C	66	GLY
1	F	59	ALA
1	F	292	ALA
1	F	347	ALA
1	G	59	ALA
1	H	359	ASP
1	K	103	ASN
1	B	103	ASN
1	B	151	LEU
1	B	323	ASN
1	D	339	SER
1	E	151	LEU
1	E	323	ASN
1	F	323	ASN
1	I	103	ASN
1	J	323	ASN
1	L	359	ASP

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Mol	Chain	Res	Type
1	C	65	GLN
1	D	43	ASP
1	F	42	VAL
1	G	292	ALA
1	G	359	ASP
1	H	41	SER
1	J	103	ASN
1	L	151	LEU
1	A	40	SER
1	B	60	ASP
1	D	59	ALA
1	H	103	ASN
1	C	59	ALA
1	C	151	LEU
1	A	324	GLY
1	I	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	277/277 (100%)	275 (99%)	2 (1%)	81 85
1	B	277/277 (100%)	273 (99%)	4 (1%)	62 67
1	C	277/277 (100%)	272 (98%)	5 (2%)	54 57
1	D	276/277 (100%)	268 (97%)	8 (3%)	37 37
1	E	277/277 (100%)	272 (98%)	5 (2%)	54 57
1	F	276/277 (100%)	264 (96%)	12 (4%)	25 22
1	G	277/277 (100%)	271 (98%)	6 (2%)	47 49
1	H	276/277 (100%)	273 (99%)	3 (1%)	70 75
1	I	277/277 (100%)	274 (99%)	3 (1%)	70 75
1	J	276/277 (100%)	276 (100%)	0	100 100
1	K	278/277 (100%)	268 (96%)	10 (4%)	30 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	276/277 (100%)	273 (99%)	3 (1%)	70 75
All	All	3320/3324 (100%)	3259 (98%)	61 (2%)	54 57

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	199	MET
1	B	6	SER
1	B	85	ARG
1	B	176	GLN
1	B	351	ILE
1	C	40	SER
1	C	58	THR
1	C	121	SER
1	C	199	MET
1	C	265	ARG
1	D	6	SER
1	D	43	ASP
1	D	85	ARG
1	D	199	MET
1	D	290	VAL
1	D	294	SER
1	D	323	ASN
1	D	350	ASP
1	E	6	SER
1	E	16	ILE
1	E	68	GLU
1	E	265	ARG
1	E	350	ASP
1	F	6	SER
1	F	42	VAL
1	F	45	ILE
1	F	56	ILE
1	F	85	ARG
1	F	97	GLU
1	F	117	THR
1	F	176	GLN
1	F	183	VAL
1	F	199	MET
1	F	277	GLU
1	F	348	THR

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Mol	Chain	Res	Type
1	G	37	ASP
1	G	40	SER
1	G	62	LYS
1	G	321	GLU
1	G	357	ASP
1	G	359	ASP
1	H	177	SER
1	H	290	VAL
1	H	349	ILE
1	I	42	VAL
1	I	68	GLU
1	I	359	ASP
1	K	6	SER
1	K	38	ARG
1	K	40	SER
1	K	42	VAL
1	K	104	ASP
1	K	176	GLN
1	K	290	VAL
1	K	323	ASN
1	K	349	ILE
1	K	357	ASP
1	L	40	SER
1	L	199	MET
1	L	294	SER

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	263	ASN
1	A	309	ASN
1	A	327	GLN
1	B	176	GLN
1	B	282	HIS
1	B	286	HIS
1	B	293	ASN
1	B	323	ASN
1	C	116	GLN
1	C	138	HIS
1	C	176	GLN

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Mol	Chain	Res	Type
1	C	263	ASN
1	C	282	HIS
1	C	327	GLN
1	D	286	HIS
1	D	308	HIS
1	E	65	GLN
1	E	116	GLN
1	E	138	HIS
1	E	263	ASN
1	E	327	GLN
1	F	116	GLN
1	F	122	GLN
1	F	282	HIS
1	F	286	HIS
1	G	138	HIS
1	G	176	GLN
1	G	263	ASN
1	G	286	HIS
1	G	327	GLN
1	H	286	HIS
1	H	323	ASN
1	I	138	HIS
1	I	176	GLN
1	I	263	ASN
1	I	327	GLN
1	J	116	GLN
1	J	134	ASN
1	J	286	HIS
1	J	308	HIS
1	K	134	ASN
1	K	138	HIS
1	K	176	GLN
1	K	282	HIS
1	K	327	GLN
1	L	122	GLN
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 (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	BCO	K	401	-	47,55,55	1.06	3 (6%)	58,81,81	1.89	9 (15%)
2	BCO	H	401	-	47,55,55	0.82	1 (2%)	58,81,81	1.69	11 (18%)
2	BCO	I	401	-	47,55,55	1.14	4 (8%)	58,81,81	1.78	5 (8%)
2	BCO	E	401	-	47,55,55	0.99	4 (8%)	58,81,81	1.56	7 (12%)
2	BCO	L	401	-	47,55,55	1.83	3 (6%)	58,81,81	1.41	4 (6%)
2	BCO	J	401	-	47,55,55	1.63	3 (6%)	58,81,81	1.51	7 (12%)
2	BCO	G	401	-	47,55,55	1.43	3 (6%)	58,81,81	1.59	9 (15%)
2	BCO	D	401	-	47,55,55	1.52	4 (8%)	58,81,81	1.38	6 (10%)
2	BCO	C	401	-	47,55,55	1.43	3 (6%)	58,81,81	1.77	12 (20%)
2	BCO	B	401	-	47,55,55	1.58	3 (6%)	58,81,81	1.71	13 (22%)
2	BCO	A	401	-	47,55,55	1.64	3 (6%)	58,81,81	1.81	11 (18%)
2	BCO	F	401	-	47,55,55	1.54	3 (6%)	58,81,81	1.31	6 (10%)

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	BCO	K	401	-	-	11/50/70/70	0/3/3/3
2	BCO	H	401	-	-	19/50/70/70	0/3/3/3
2	BCO	I	401	-	-	8/50/70/70	0/3/3/3
2	BCO	E	401	-	-	9/50/70/70	0/3/3/3
2	BCO	L	401	-	-	6/50/70/70	0/3/3/3
2	BCO	J	401	-	-	6/50/70/70	0/3/3/3
2	BCO	G	401	-	-	7/50/70/70	0/3/3/3
2	BCO	D	401	-	-	7/50/70/70	0/3/3/3
2	BCO	C	401	-	-	11/50/70/70	0/3/3/3
2	BCO	B	401	-	-	15/50/70/70	0/3/3/3
2	BCO	A	401	-	-	11/50/70/70	0/3/3/3
2	BCO	F	401	-	-	7/50/70/70	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	BCO	C22-S1	9.59	1.99	1.76
2	J	401	BCO	C22-S1	8.19	1.96	1.76
2	A	401	BCO	C22-S1	7.57	1.94	1.76
2	B	401	BCO	C22-S1	7.40	1.94	1.76
2	F	401	BCO	C22-S1	7.39	1.94	1.76
2	D	401	BCO	C22-S1	7.23	1.93	1.76
2	G	401	BCO	C22-S1	7.18	1.93	1.76
2	C	401	BCO	C22-S1	6.29	1.91	1.76
2	A	401	BCO	O17-C22	5.90	1.30	1.21
2	L	401	BCO	O17-C22	5.11	1.29	1.21
2	B	401	BCO	O17-C22	4.91	1.29	1.21
2	D	401	BCO	O17-C22	4.87	1.28	1.21
2	J	401	BCO	O17-C22	4.78	1.28	1.21
2	C	401	BCO	O17-C22	4.76	1.28	1.21
2	F	401	BCO	O17-C22	4.73	1.28	1.21
2	I	401	BCO	C22-S1	4.42	1.86	1.76
2	G	401	BCO	O17-C22	4.19	1.27	1.21
2	K	401	BCO	C22-S1	4.04	1.85	1.76
2	A	401	BCO	C23-C22	3.06	1.54	1.50
2	L	401	BCO	C23-C22	3.06	1.54	1.50
2	I	401	BCO	O17-C22	3.01	1.25	1.21
2	F	401	BCO	C23-C22	2.96	1.53	1.50
2	J	401	BCO	C23-C22	2.90	1.53	1.50
2	E	401	BCO	C22-S1	2.86	1.83	1.76
2	I	401	BCO	C23-C22	2.81	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	BCO	C23-C22	2.76	1.53	1.50
2	E	401	BCO	O17-C22	2.73	1.25	1.21
2	C	401	BCO	C23-C22	2.67	1.53	1.50
2	E	401	BCO	C23-C22	2.61	1.53	1.50
2	K	401	BCO	O17-C22	2.53	1.25	1.21
2	D	401	BCO	C23-C22	2.47	1.53	1.50
2	K	401	BCO	C23-C22	2.45	1.53	1.50
2	D	401	BCO	P1-O2	2.31	1.63	1.59
2	G	401	BCO	C23-C22	2.26	1.53	1.50
2	H	401	BCO	C23-C22	2.13	1.53	1.50
2	I	401	BCO	C21-C20	2.10	1.59	1.51
2	E	401	BCO	P1-O2	2.01	1.63	1.59

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	401	BCO	C21-S1-C22	9.63	131.86	101.87
2	E	401	BCO	C21-S1-C22	8.44	128.14	101.87
2	K	401	BCO	C21-S1-C22	8.36	127.91	101.87
2	A	401	BCO	O17-C22-S1	7.21	131.98	122.61
2	L	401	BCO	O17-C22-C23	-6.26	116.59	123.99
2	B	401	BCO	O17-C22-S1	6.23	130.70	122.61
2	D	401	BCO	O17-C22-S1	6.02	130.43	122.61
2	C	401	BCO	O17-C22-S1	5.74	130.07	122.61
2	L	401	BCO	O17-C22-S1	5.43	129.66	122.61
2	A	401	BCO	C23-C22-S1	-5.32	107.26	113.46
2	H	401	BCO	C21-S1-C22	5.23	118.14	101.87
2	C	401	BCO	O14-P3-O13	5.17	137.79	112.24
2	G	401	BCO	O14-P3-O13	5.05	137.21	112.24
2	G	401	BCO	O17-C22-C23	-4.94	118.16	123.99
2	J	401	BCO	O17-C22-S1	4.78	128.82	122.61
2	H	401	BCO	C13-C9-C11	-4.74	100.50	108.23
2	J	401	BCO	O17-C22-C23	-4.61	118.54	123.99
2	J	401	BCO	O14-P3-O13	4.60	134.98	112.24
2	G	401	BCO	O17-C22-S1	4.59	128.57	122.61
2	K	401	BCO	O14-P3-O13	4.41	134.04	112.24
2	C	401	BCO	C23-C22-S1	-4.31	108.44	113.46
2	D	401	BCO	O17-C22-C23	-4.30	118.92	123.99
2	A	401	BCO	C20-N7-C19	-4.27	114.91	122.84
2	K	401	BCO	C18-C19-N7	4.22	123.52	116.42
2	H	401	BCO	C23-C22-S1	4.19	118.34	113.46
2	F	401	BCO	O17-C22-C23	-4.11	119.14	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	BCO	O14-P3-O13	4.08	132.41	112.24
2	H	401	BCO	C14-C9-C11	4.04	114.82	108.23
2	F	401	BCO	O17-C22-S1	4.02	127.83	122.61
2	B	401	BCO	O2-P1-O9	-3.94	94.20	109.39
2	F	401	BCO	O14-P3-O13	3.86	131.30	112.24
2	I	401	BCO	O14-P3-O13	3.82	131.13	112.24
2	G	401	BCO	O8-P3-O13	-3.76	94.39	109.07
2	B	401	BCO	O17-C22-C23	-3.75	119.56	123.99
2	I	401	BCO	O17-C22-C23	-3.64	119.69	123.99
2	C	401	BCO	O8-P3-O13	-3.55	95.20	109.07
2	K	401	BCO	O17-C22-C23	-3.46	119.90	123.99
2	J	401	BCO	O8-P3-O13	-3.37	95.91	109.07
2	H	401	BCO	O14-P3-O13	3.34	128.78	112.24
2	C	401	BCO	C20-N7-C19	-3.24	116.83	122.84
2	B	401	BCO	C23-C22-S1	-3.20	109.74	113.46
2	C	401	BCO	C21-C20-N7	-3.17	105.76	112.42
2	B	401	BCO	O14-P3-O13	3.10	127.56	112.24
2	E	401	BCO	O3-C2-C1	3.06	119.87	111.17
2	B	401	BCO	O6-P1-O2	3.04	119.61	105.99
2	H	401	BCO	O17-C22-S1	-3.02	118.69	122.61
2	C	401	BCO	O2-P1-O9	-3.00	97.81	109.39
2	K	401	BCO	O16-C19-C18	-2.96	116.60	122.02
2	L	401	BCO	O14-P3-O13	2.93	126.72	112.24
2	K	401	BCO	C8-C12-N5	2.87	124.71	120.35
2	F	401	BCO	C8-C12-N5	2.83	124.66	120.35
2	I	401	BCO	O2-P1-O9	-2.80	98.57	109.39
2	E	401	BCO	O3-C2-C4	-2.79	100.54	110.85
2	B	401	BCO	C21-C20-N7	-2.79	106.55	112.42
2	G	401	BCO	O3-C2-C1	-2.74	103.39	111.17
2	A	401	BCO	O17-C22-C23	-2.73	120.77	123.99
2	E	401	BCO	C8-C12-N5	2.73	124.50	120.35
2	C	401	BCO	C8-C12-N5	2.73	124.49	120.35
2	G	401	BCO	C8-C12-N5	2.73	124.49	120.35
2	L	401	BCO	O6-P1-O9	2.67	121.14	110.68
2	J	401	BCO	C8-C12-N5	2.67	124.40	120.35
2	C	401	BCO	O2-C1-C2	2.64	121.26	111.68
2	H	401	BCO	C8-C12-N5	2.63	124.35	120.35
2	K	401	BCO	O14-P3-O8	-2.55	95.88	107.75
2	G	401	BCO	O2-P1-O9	-2.54	99.59	109.39
2	A	401	BCO	O8-P3-O13	-2.54	99.15	109.07
2	B	401	BCO	O8-P3-O13	-2.48	99.38	109.07
2	B	401	BCO	O3-C2-C1	2.47	118.17	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	BCO	C23-C22-S1	-2.43	110.63	113.46
2	D	401	BCO	O2-P1-O9	-2.37	100.24	109.39
2	A	401	BCO	O3-C2-C4	-2.36	102.13	110.85
2	H	401	BCO	O6-P1-O5	2.33	116.53	107.64
2	H	401	BCO	C13-C9-C10	2.32	112.84	108.82
2	E	401	BCO	C13-C9-C10	2.31	112.83	108.82
2	F	401	BCO	O11-C10-C9	-2.28	104.88	110.25
2	B	401	BCO	C8-C12-N5	2.26	123.79	120.35
2	A	401	BCO	O2-P1-O9	-2.25	100.71	109.39
2	G	401	BCO	O2-C1-C2	2.24	119.80	111.68
2	B	401	BCO	C20-N7-C19	-2.23	118.69	122.84
2	A	401	BCO	O11-C10-C9	-2.22	105.03	110.25
2	K	401	BCO	O3-C2-C1	2.22	117.46	111.17
2	J	401	BCO	O2-C1-C3	2.21	118.07	110.08
2	B	401	BCO	O5-P1-O9	2.20	119.31	110.68
2	F	401	BCO	O8-C11-C9	-2.19	107.03	110.55
2	C	401	BCO	O5-P1-O9	2.17	119.17	110.68
2	A	401	BCO	O6-P1-O5	2.15	115.85	107.64
2	D	401	BCO	O14-P3-O13	2.15	122.86	112.24
2	C	401	BCO	O17-C22-C23	-2.14	121.46	123.99
2	H	401	BCO	C17-C18-C19	2.11	115.88	112.36
2	K	401	BCO	O6-P1-O9	2.11	118.94	110.68
2	E	401	BCO	C18-C19-N7	2.10	119.97	116.42
2	A	401	BCO	C8-C12-N5	2.07	123.50	120.35
2	C	401	BCO	O8-C11-C9	-2.06	107.24	110.55
2	E	401	BCO	O14-P3-O13	2.05	122.36	112.24
2	H	401	BCO	C1-C2-C4	2.04	104.42	99.89
2	J	401	BCO	O8-C11-C9	-2.04	107.26	110.55
2	B	401	BCO	O6-P1-O9	-2.04	102.69	110.68
2	I	401	BCO	C8-C12-N5	2.04	123.45	120.35
2	D	401	BCO	C8-C12-N5	2.02	123.42	120.35
2	G	401	BCO	O6-P1-O9	2.01	118.54	110.68

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	BCO	C5-O4-P2-O10
2	A	401	BCO	N6-C17-C18-C19
2	A	401	BCO	N7-C20-C21-S1
2	A	401	BCO	C20-C21-S1-C22
2	A	401	BCO	O17-C22-S1-C21

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Mol	Chain	Res	Type	Atoms
2	A	401	BCO	C23-C22-S1-C21
2	A	401	BCO	C22-C23-C24-C25
2	B	401	BCO	C1-O2-P1-O9
2	B	401	BCO	C3-C1-O2-P1
2	B	401	BCO	C5-O4-P2-O12
2	B	401	BCO	C5-O4-P2-O10
2	B	401	BCO	C5-O4-P2-O7
2	B	401	BCO	N6-C17-C18-C19
2	B	401	BCO	N7-C20-C21-S1
2	B	401	BCO	O17-C22-S1-C21
2	B	401	BCO	C23-C22-S1-C21
2	B	401	BCO	C22-C23-C24-C25
2	C	401	BCO	C11-O8-P3-O14
2	C	401	BCO	N6-C17-C18-C19
2	C	401	BCO	N7-C20-C21-S1
2	C	401	BCO	O17-C22-S1-C21
2	C	401	BCO	C23-C22-S1-C21
2	D	401	BCO	C5-O4-P2-O10
2	D	401	BCO	O17-C22-S1-C21
2	D	401	BCO	C23-C22-S1-C21
2	E	401	BCO	O17-C22-S1-C21
2	E	401	BCO	C23-C22-S1-C21
2	F	401	BCO	C1-O2-P1-O6
2	F	401	BCO	C5-O4-P2-O7
2	F	401	BCO	N6-C17-C18-C19
2	F	401	BCO	O17-C22-S1-C21
2	F	401	BCO	C23-C22-S1-C21
2	G	401	BCO	C5-O4-P2-O10
2	G	401	BCO	C5-O4-P2-O7
2	G	401	BCO	O17-C22-S1-C21
2	G	401	BCO	C23-C22-S1-C21
2	H	401	BCO	C1-O2-P1-O9
2	H	401	BCO	O1-C3-C5-O4
2	H	401	BCO	C5-O4-P2-O7
2	H	401	BCO	C11-O8-P3-O7
2	H	401	BCO	C16-C10-C9-C11
2	H	401	BCO	N7-C20-C21-S1
2	H	401	BCO	C20-C21-S1-C22
2	H	401	BCO	O17-C22-S1-C21
2	H	401	BCO	C23-C22-S1-C21
2	I	401	BCO	O17-C22-S1-C21
2	I	401	BCO	C23-C22-S1-C21

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Mol	Chain	Res	Type	Atoms
2	J	401	BCO	C3-C1-O2-P1
2	J	401	BCO	C5-O4-P2-O7
2	J	401	BCO	O17-C22-S1-C21
2	J	401	BCO	C23-C22-S1-C21
2	K	401	BCO	C3-C1-O2-P1
2	K	401	BCO	C5-O4-P2-O10
2	K	401	BCO	C5-O4-P2-O7
2	K	401	BCO	C18-C19-N7-C20
2	K	401	BCO	O16-C19-N7-C20
2	L	401	BCO	O17-C22-S1-C21
2	L	401	BCO	C23-C22-S1-C21
2	H	401	BCO	C18-C19-N7-C20
2	B	401	BCO	O1-C3-C5-O4
2	F	401	BCO	O1-C3-C5-O4
2	J	401	BCO	O1-C3-C5-O4
2	C	401	BCO	C2-C1-O2-P1
2	G	401	BCO	C2-C1-O2-P1
2	H	401	BCO	C3-C1-O2-P1
2	G	401	BCO	O1-C3-C5-O4
2	I	401	BCO	C22-C23-C24-C25
2	K	401	BCO	C22-C23-C24-C25
2	H	401	BCO	O16-C19-N7-C20
2	H	401	BCO	C2-C1-O2-P1
2	H	401	BCO	C18-C17-N6-C16
2	H	401	BCO	C22-C23-C24-C25
2	D	401	BCO	N6-C17-C18-C19
2	E	401	BCO	N6-C17-C18-C19
2	J	401	BCO	N6-C17-C18-C19
2	L	401	BCO	N6-C17-C18-C19
2	B	401	BCO	C1-C3-C5-O4
2	C	401	BCO	C20-C21-S1-C22
2	E	401	BCO	S1-C22-C23-C24
2	I	401	BCO	S1-C22-C23-C24
2	I	401	BCO	O17-C22-C23-C24
2	K	401	BCO	S1-C22-C23-C24
2	K	401	BCO	O17-C22-C23-C24
2	K	401	BCO	O1-C3-C5-O4
2	F	401	BCO	C1-O2-P1-O9
2	A	401	BCO	C5-O4-P2-O7
2	C	401	BCO	C5-O4-P2-O7
2	D	401	BCO	C5-O4-P2-O7
2	H	401	BCO	C5-O4-P2-O12

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Mol	Chain	Res	Type	Atoms
2	H	401	BCO	C5-O4-P2-O10
2	H	401	BCO	C11-O8-P3-O13
2	I	401	BCO	C11-O8-P3-O13
2	A	401	BCO	O1-C3-C5-O4
2	D	401	BCO	O1-C3-C5-O4
2	K	401	BCO	P3-O7-P2-O12
2	G	401	BCO	N6-C17-C18-C19
2	C	401	BCO	O1-C3-C5-O4
2	B	401	BCO	C20-C21-S1-C22
2	E	401	BCO	C20-C21-S1-C22
2	K	401	BCO	C20-C21-S1-C22
2	E	401	BCO	O17-C22-C23-C24
2	B	401	BCO	C1-O2-P1-O5
2	H	401	BCO	C1-O2-P1-O5
2	E	401	BCO	O1-C3-C5-O4
2	A	401	BCO	P3-O7-P2-O12
2	A	401	BCO	P3-O7-P2-O10
2	B	401	BCO	P3-O7-P2-O12
2	C	401	BCO	P3-O7-P2-O12
2	D	401	BCO	P3-O7-P2-O10
2	E	401	BCO	P3-O7-P2-O12
2	E	401	BCO	P3-O7-P2-O10
2	I	401	BCO	P3-O7-P2-O12
2	L	401	BCO	P3-O7-P2-O12
2	L	401	BCO	C5-O4-P2-O10
2	I	401	BCO	O1-C3-C5-O4
2	L	401	BCO	O1-C3-C5-O4
2	C	401	BCO	C3-C1-O2-P1

There are no ring outliers.

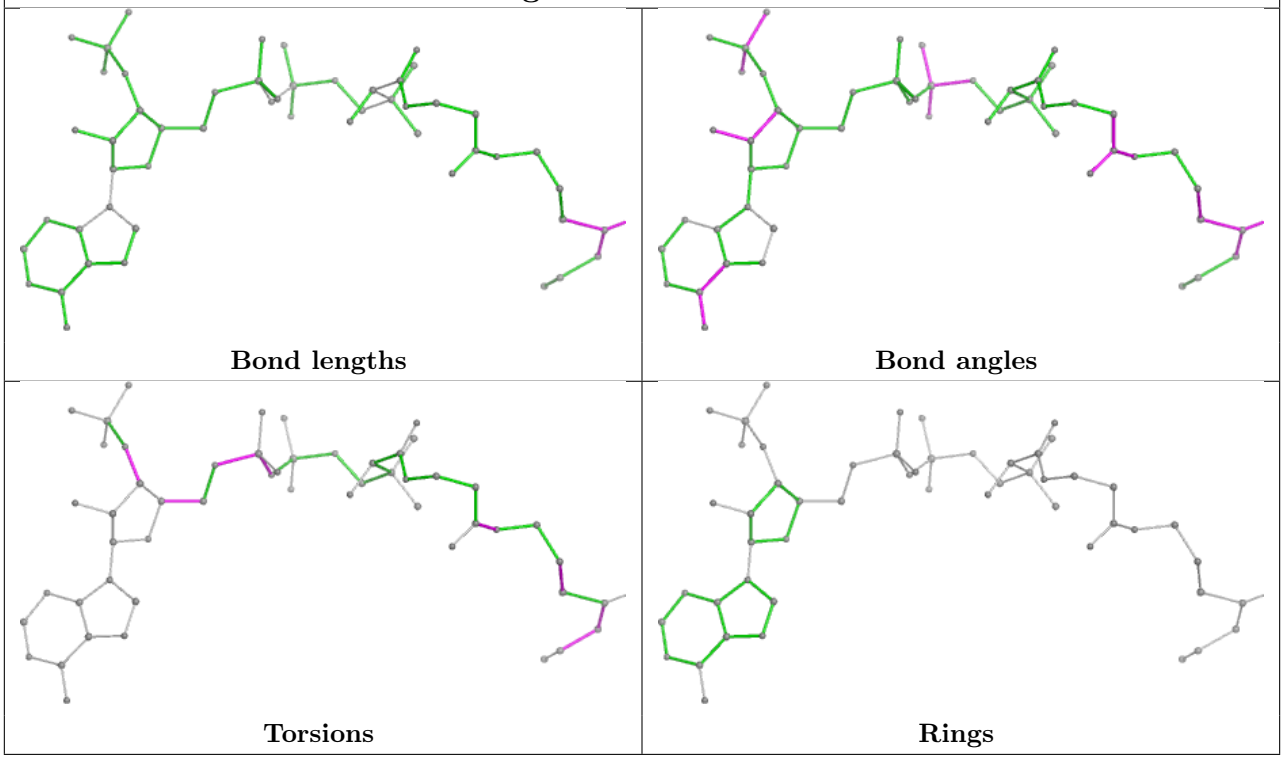
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	401	BCO	1	0
2	E	401	BCO	1	0
2	D	401	BCO	2	0
2	C	401	BCO	2	0
2	B	401	BCO	3	0
2	A	401	BCO	2	0
2	F	401	BCO	3	0

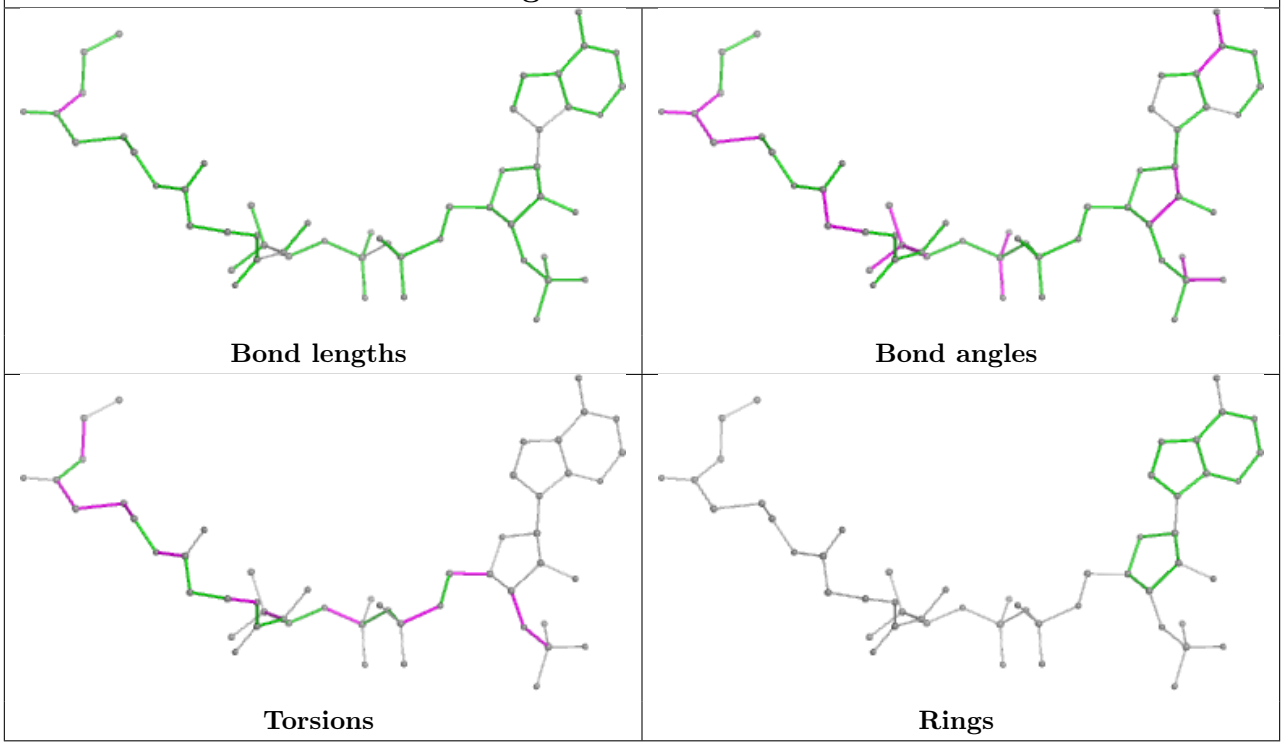
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

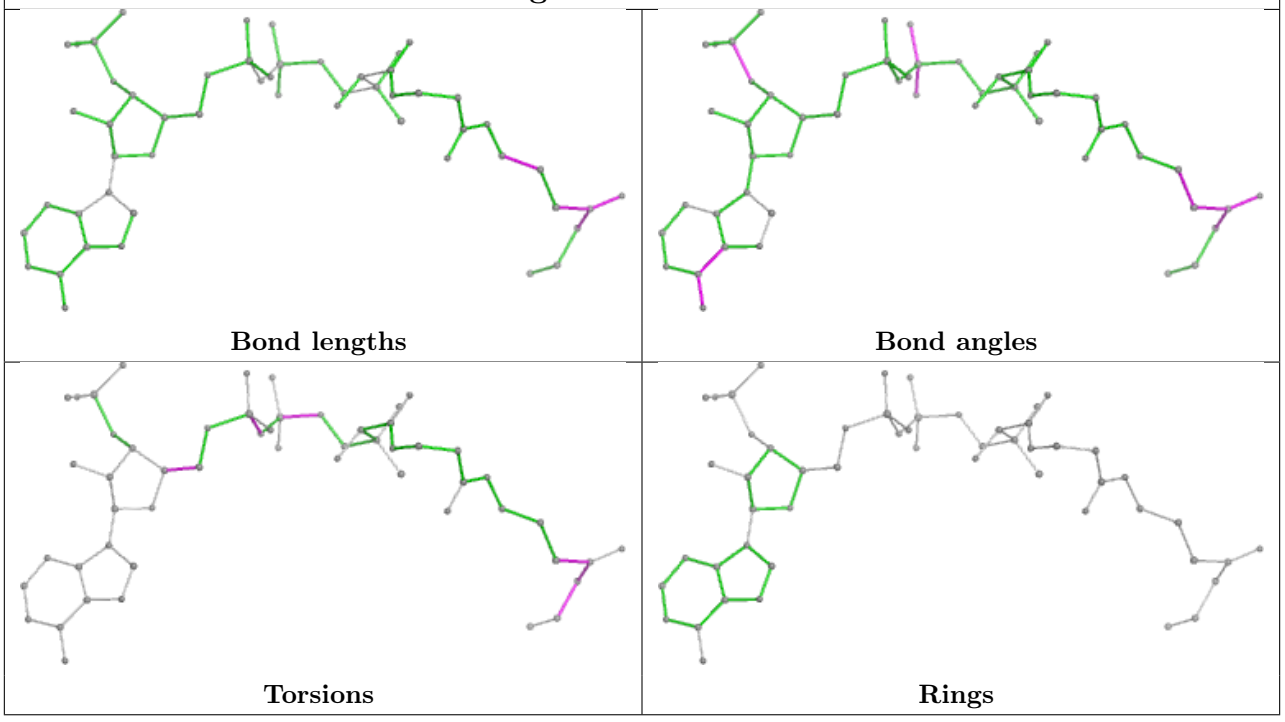
Ligand BCO K 401



Ligand BCO H 401



Ligand BCO I 401



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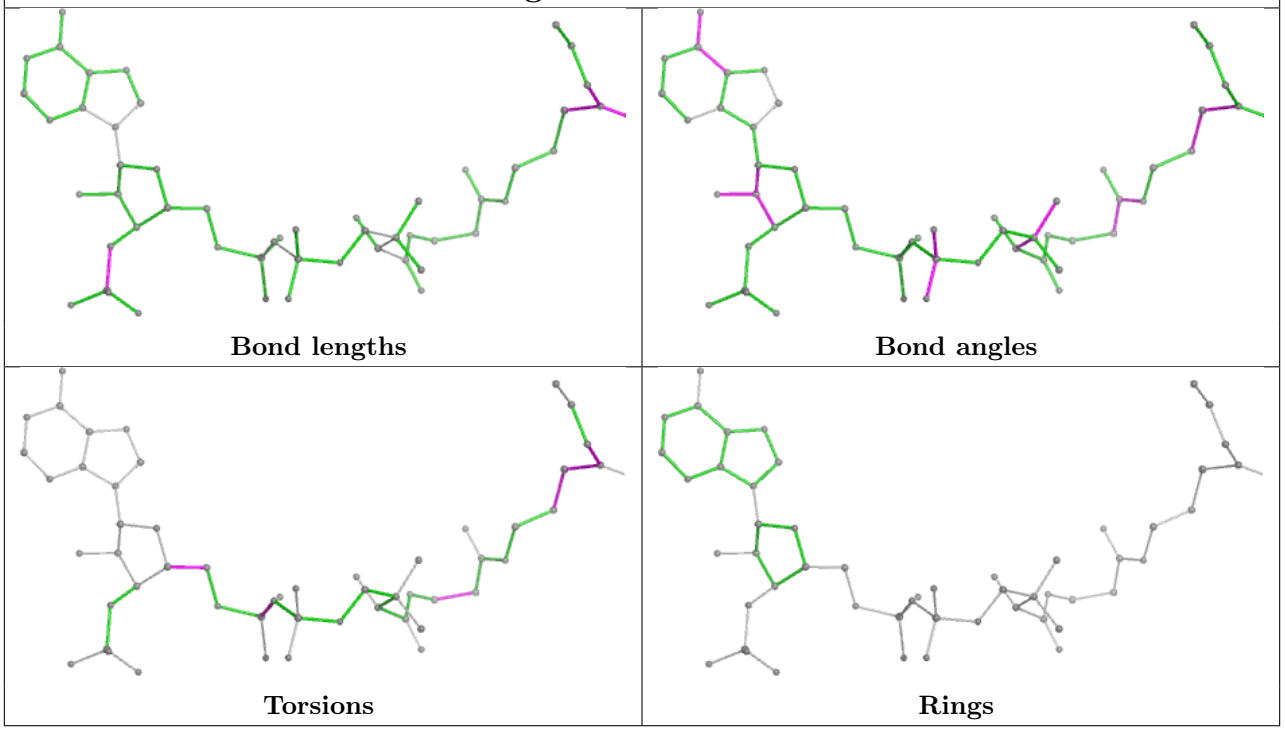

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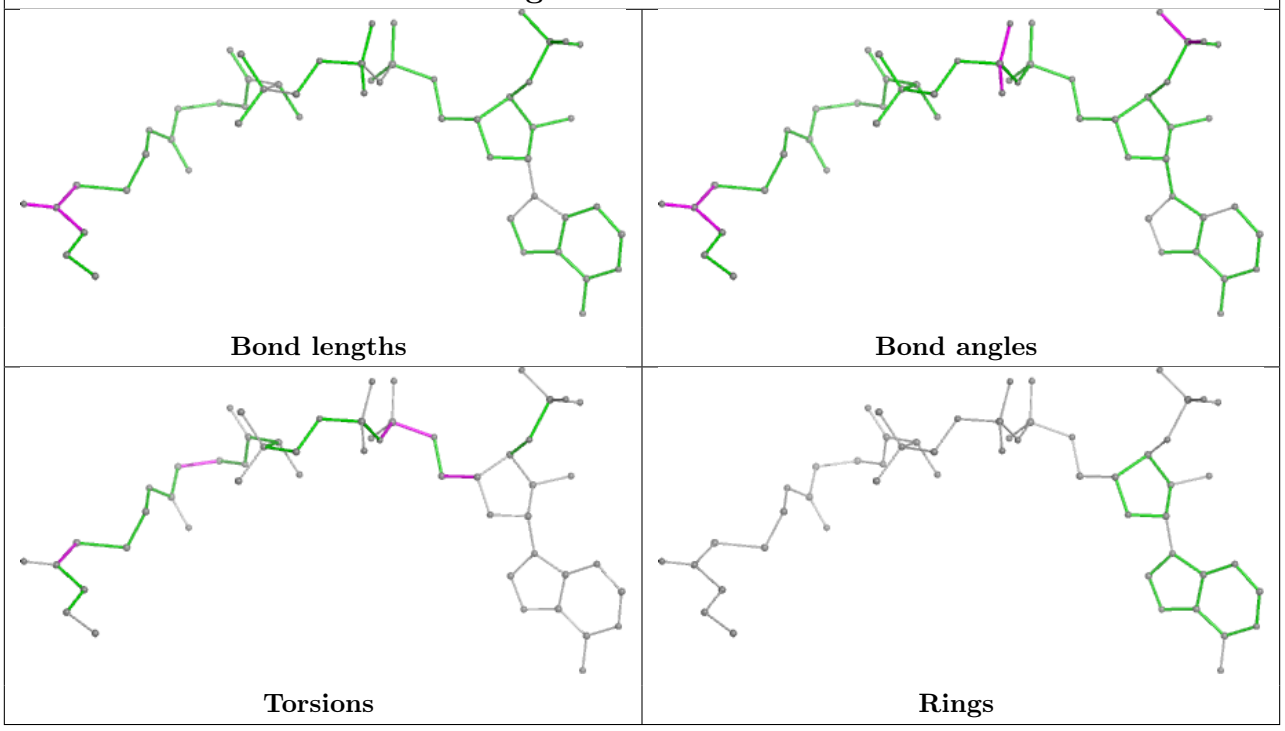

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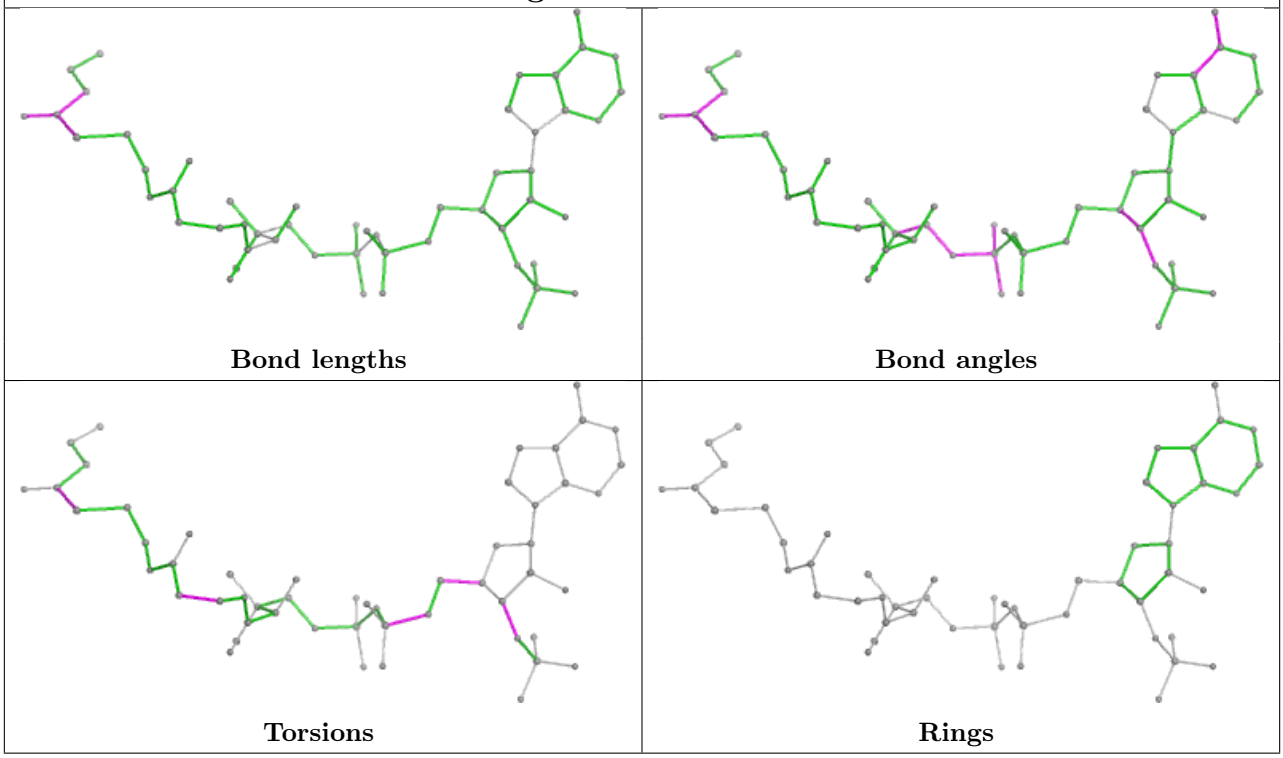

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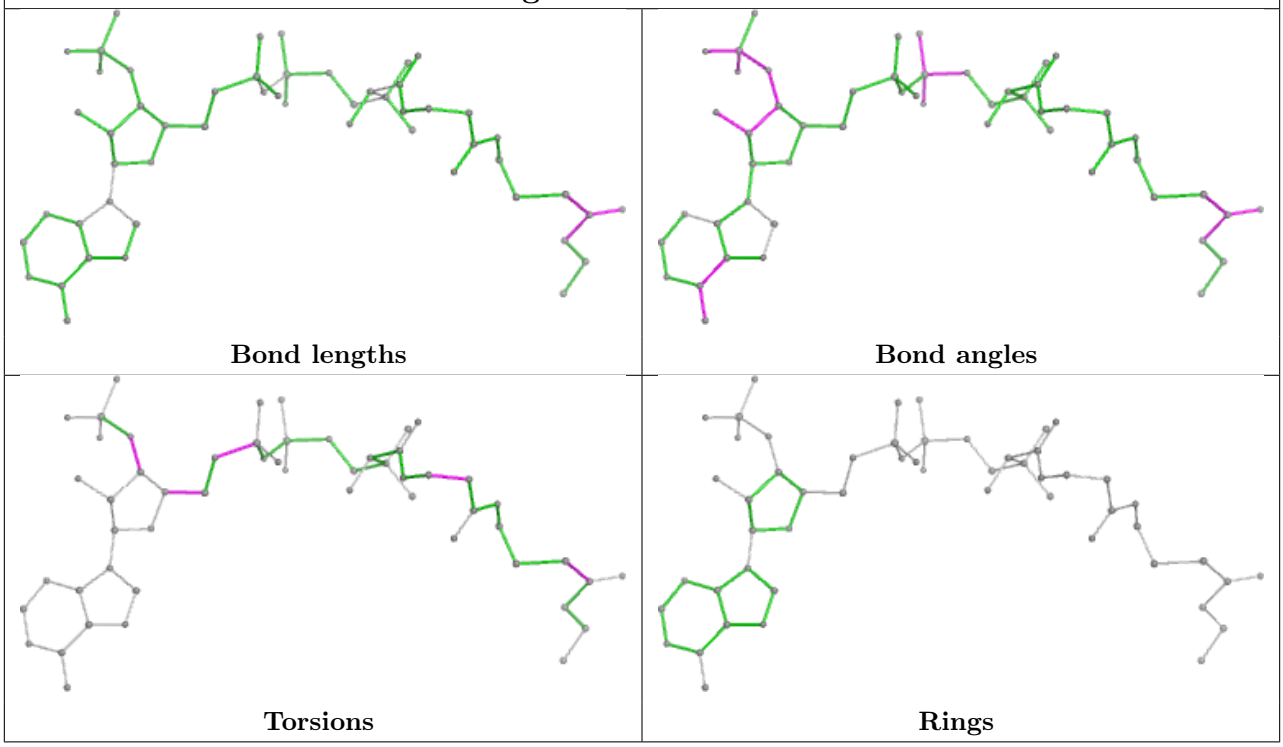
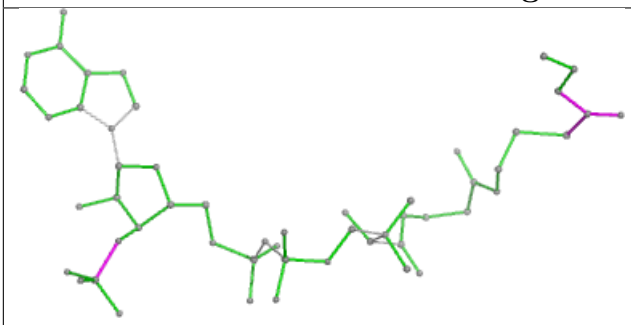
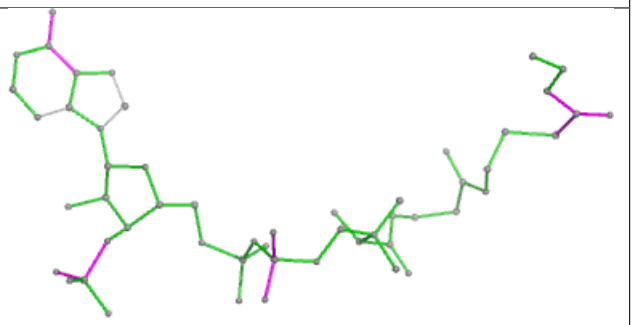


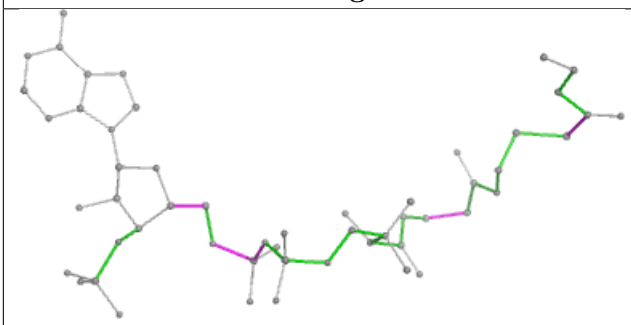
Ligand BCO D 401



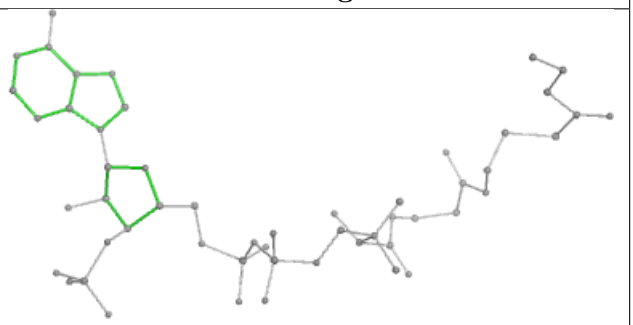
Bond lengths



Bond angles

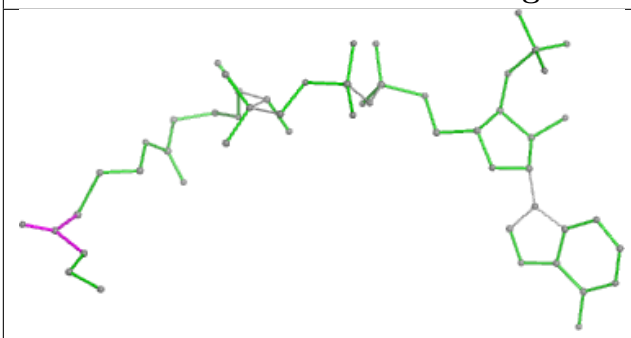


Torsions

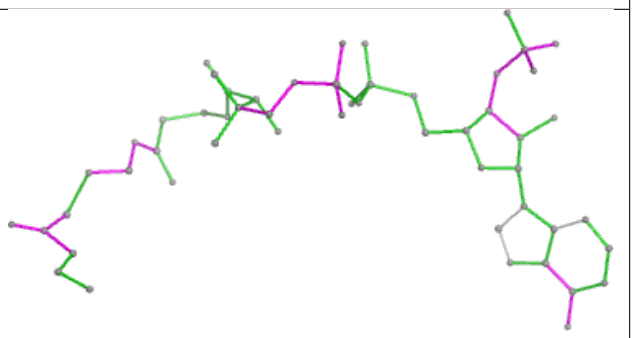


Rings

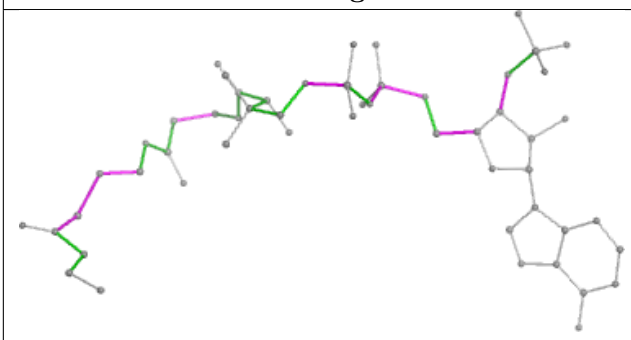
Ligand BCO C 401



Bond lengths



Bond angles



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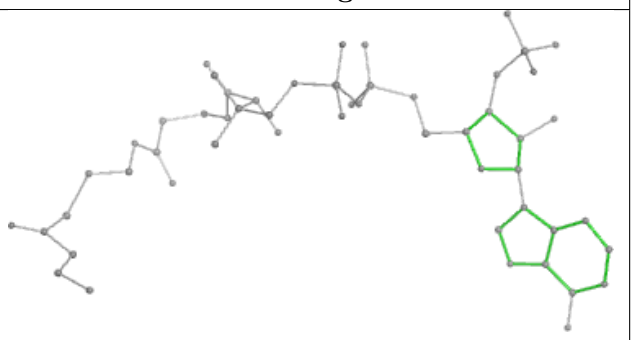
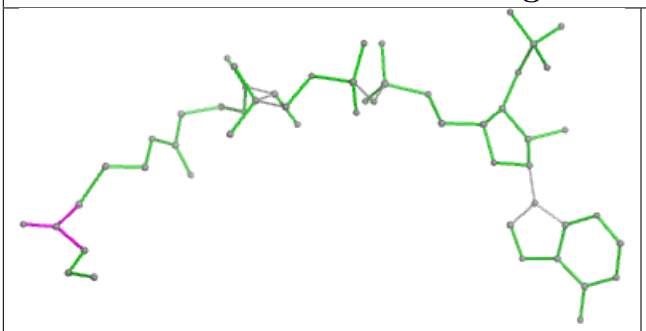
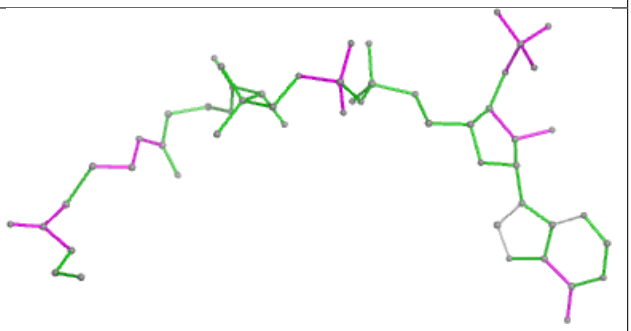


Rings

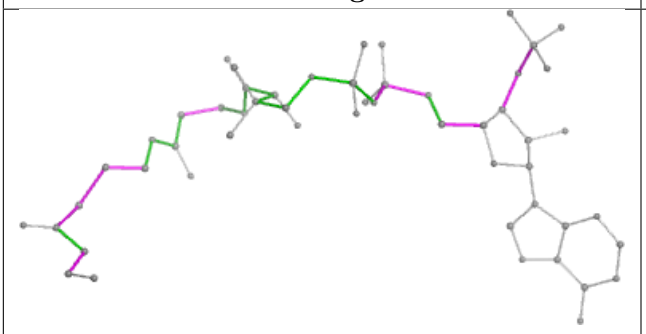
Ligand BCO B 401



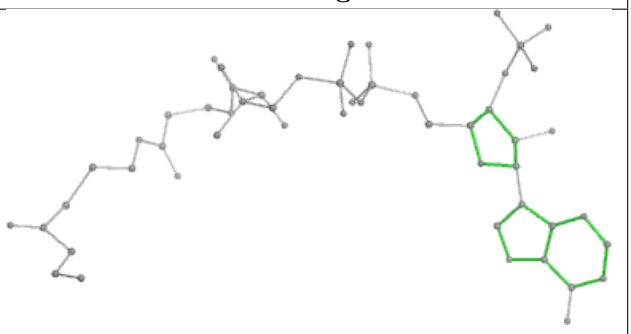
Bond lengths



Bond angles

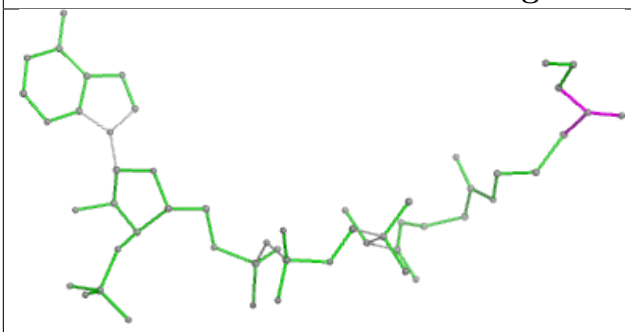


Torsions

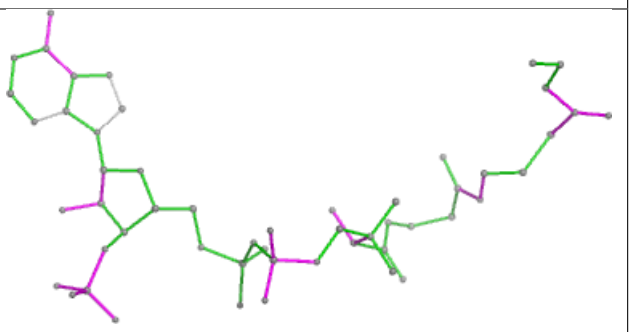


Rings

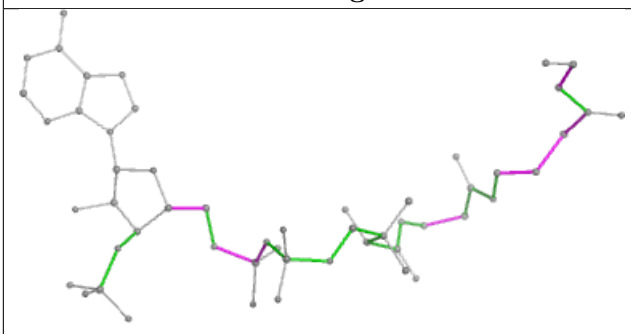
Ligand BCO A 401



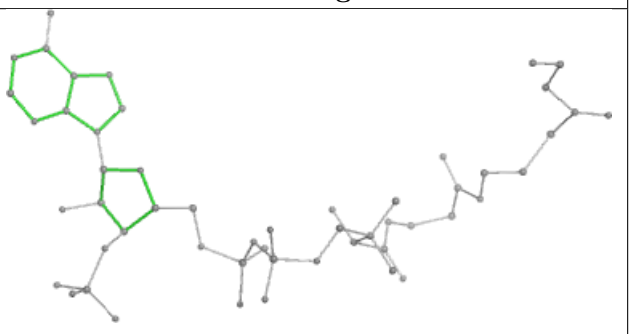
Bond lengths



Bond angles

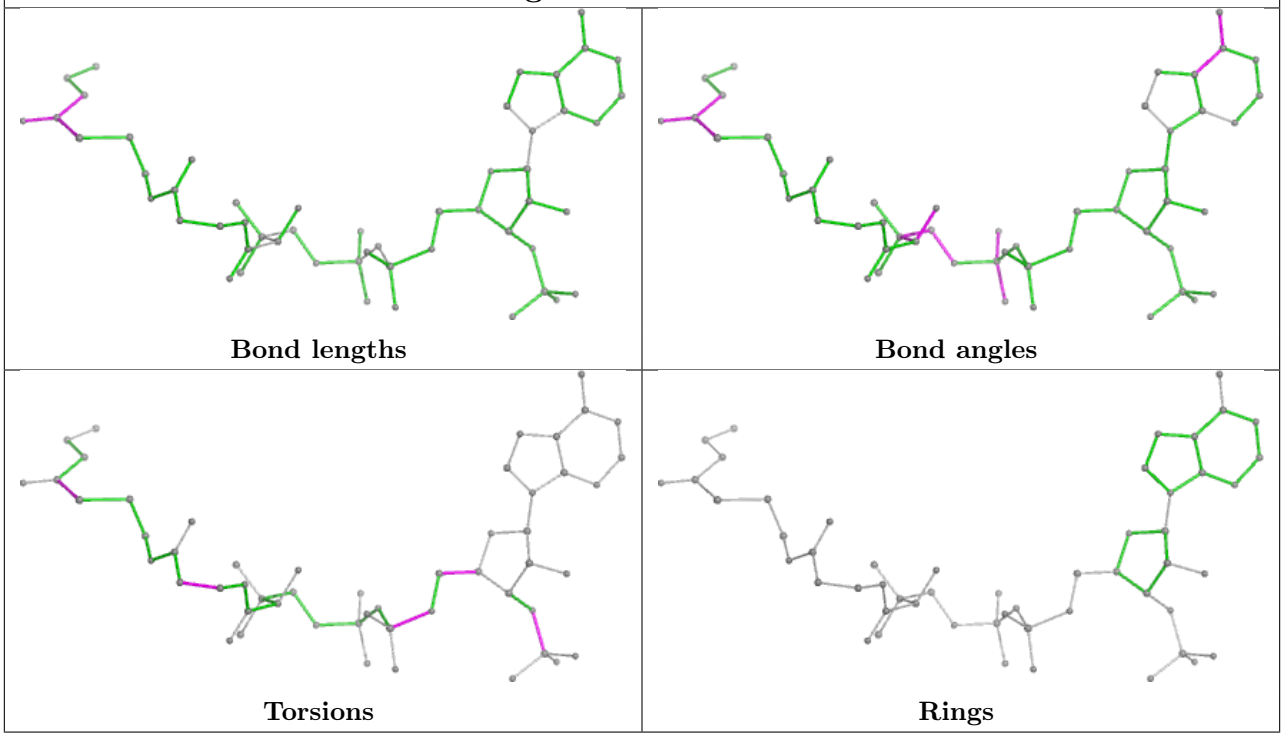


Torsions



Rings

Ligand BCO F 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%)	0.39	23 (6%) 27 25	25, 38, 77, 121	2 (0%)
1	B	360/364 (98%)	0.50	32 (8%) 17 16	19, 39, 78, 127	2 (0%)
1	C	360/364 (98%)	0.86	85 (23%) 2 2	24, 42, 82, 116	2 (0%)
1	D	360/364 (98%)	0.62	46 (12%) 9 8	24, 41, 77, 121	1 (0%)
1	E	360/364 (98%)	0.75	54 (15%) 6 6	24, 42, 91, 127	2 (0%)
1	F	360/364 (98%)	0.99	83 (23%) 2 2	24, 43, 85, 122	1 (0%)
1	G	360/364 (98%)	0.89	81 (22%) 3 2	24, 43, 86, 130	2 (0%)
1	H	360/364 (98%)	0.64	45 (12%) 9 8	25, 42, 89, 124	1 (0%)
1	I	359/364 (98%)	0.16	15 (4%) 41 40	23, 36, 66, 101	2 (0%)
1	J	360/364 (98%)	0.34	30 (8%) 19 18	25, 37, 75, 125	1 (0%)
1	K	360/364 (98%)	0.66	61 (16%) 5 4	16, 38, 82, 117	3 (0%)
1	L	360/364 (98%)	0.31	19 (5%) 33 32	24, 37, 68, 112	1 (0%)
All	All	4319/4368 (98%)	0.59	574 (13%) 8 7	16, 40, 81, 130	20 (0%)

All (574) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	7.8
1	E	346	ALA	7.4
1	H	360	GLY	7.4
1	C	42	VAL	6.6
1	K	45	ILE	5.9
1	F	42	VAL	5.8
1	G	360	GLY	5.7
1	J	360	GLY	5.7
1	K	360	GLY	5.5
1	F	346	ALA	5.4
1	B	42	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	L	360	GLY	5.3
1	B	45	ILE	5.3
1	A	42	VAL	5.2
1	E	42	VAL	5.1
1	C	45	ILE	5.1
1	F	351	ILE	5.1
1	H	42	VAL	5.0
1	D	346	ALA	5.0
1	K	346	ALA	5.0
1	E	349	ILE	4.9
1	F	360	GLY	4.7
1	D	360	GLY	4.7
1	K	72	LYS	4.7
1	J	45	ILE	4.6
1	J	351	ILE	4.6
1	F	45	ILE	4.5
1	E	360	GLY	4.4
1	G	61	LEU	4.4
1	C	75	ALA	4.3
1	G	351	ILE	4.3
1	B	346	ALA	4.3
1	H	45	ILE	4.3
1	K	42	VAL	4.2
1	C	346	ALA	4.2
1	E	351	ILE	4.2
1	I	47	ARG	4.2
1	C	69	LEU	4.2
1	K	75	ALA	4.1
1	H	39	PRO	4.1
1	A	351	ILE	4.1
1	F	180	LYS	4.1
1	F	34	VAL	4.1
1	H	351	ILE	4.1
1	F	101	LYS	4.0
1	G	346	ALA	4.0
1	A	324	GLY	4.0
1	F	347	ALA	3.9
1	J	346	ALA	3.9
1	E	39	PRO	3.9
1	G	178	SER	3.9
1	H	346	ALA	3.9
1	J	49	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	44	GLY	3.9
1	E	347	ALA	3.9
1	K	49	ALA	3.9
1	G	93	GLY	3.9
1	F	75	ALA	3.9
1	G	293	ASN	3.9
1	L	45	ILE	3.8
1	G	42	VAL	3.8
1	C	66	GLY	3.8
1	F	79	VAL	3.8
1	G	176	GLN	3.8
1	J	44	GLY	3.8
1	D	358	TRP	3.8
1	E	45	ILE	3.7
1	G	355	LEU	3.7
1	K	93	GLY	3.7
1	B	46	SER	3.7
1	F	49	ALA	3.7
1	G	349	ILE	3.6
1	C	70	ALA	3.6
1	G	358	TRP	3.6
1	A	360	GLY	3.6
1	F	61	LEU	3.6
1	H	349	ILE	3.6
1	C	171	ALA	3.6
1	G	100	ALA	3.6
1	F	57	VAL	3.6
1	F	176	GLN	3.5
1	F	1	MET	3.5
1	D	180	LYS	3.5
1	G	101	LYS	3.5
1	F	97	GLU	3.5
1	K	349	ILE	3.5
1	E	178	SER	3.5
1	C	176	GLN	3.5
1	F	93	GLY	3.5
1	G	324	GLY	3.5
1	F	73	LEU	3.5
1	F	106	LEU	3.5
1	C	93	GLY	3.5
1	F	99	CYS	3.5
1	F	358	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	45	ILE	3.5
1	G	102	VAL	3.4
1	G	354	VAL	3.4
1	C	349	ILE	3.4
1	K	40	SER	3.4
1	F	11	VAL	3.4
1	F	354	VAL	3.4
1	G	94	LEU	3.4
1	F	39	PRO	3.4
1	B	43	ASP	3.4
1	C	107	ILE	3.4
1	C	355	LEU	3.4
1	B	351	ILE	3.3
1	D	355	LEU	3.3
1	F	107	ILE	3.3
1	K	73	LEU	3.3
1	K	345	PRO	3.3
1	C	173	TRP	3.3
1	C	351	ILE	3.3
1	D	45	ILE	3.3
1	F	36	ILE	3.3
1	F	207	MET	3.3
1	I	351	ILE	3.3
1	C	324	GLY	3.3
1	H	34	VAL	3.3
1	F	349	ILE	3.3
1	L	351	ILE	3.3
1	J	75	ALA	3.3
1	E	324	GLY	3.3
1	F	33	VAL	3.3
1	C	74	ILE	3.2
1	C	99	CYS	3.2
1	L	359	ASP	3.2
1	D	324	GLY	3.2
1	I	42	VAL	3.2
1	E	355	LEU	3.2
1	G	177	SER	3.2
1	A	349	ILE	3.2
1	C	360	GLY	3.2
1	F	87	GLY	3.2
1	J	42	VAL	3.2
1	G	99	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	347	ALA	3.2
1	K	44	GLY	3.2
1	F	173	TRP	3.2
1	F	183	VAL	3.2
1	C	43	ASP	3.2
1	F	355	LEU	3.2
1	B	44	GLY	3.2
1	H	49	ALA	3.2
1	G	62	LYS	3.2
1	G	57	VAL	3.1
1	C	358	TRP	3.1
1	C	108	TYR	3.1
1	G	92	LEU	3.1
1	K	180	LYS	3.1
1	D	347	ALA	3.1
1	K	176	GLN	3.1
1	G	10	VAL	3.1
1	E	69	LEU	3.1
1	F	324	GLY	3.1
1	G	207	MET	3.1
1	D	323	ASN	3.1
1	K	351	ILE	3.1
1	G	34	VAL	3.1
1	C	180	LYS	3.1
1	E	345	PRO	3.1
1	G	97	GLU	3.1
1	K	66	GLY	3.1
1	D	59	ALA	3.1
1	D	75	ALA	3.1
1	G	75	ALA	3.1
1	D	102	VAL	3.1
1	K	102	VAL	3.1
1	G	39	PRO	3.0
1	F	94	LEU	3.0
1	F	62	LYS	3.0
1	G	1	MET	3.0
1	C	96	PRO	3.0
1	C	61	LEU	3.0
1	C	71	LEU	3.0
1	C	106	LEU	3.0
1	E	75	ALA	3.0
1	L	173	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	105	ARG	3.0
1	J	43	ASP	3.0
1	C	177	SER	3.0
1	I	45	ILE	3.0
1	G	359	ASP	3.0
1	K	1	MET	3.0
1	E	40	SER	3.0
1	F	63	SER	3.0
1	G	41	SER	3.0
1	C	10	VAL	3.0
1	K	94	LEU	3.0
1	C	49	ALA	3.0
1	F	59	ALA	3.0
1	F	359	ASP	2.9
1	H	323	ASN	2.9
1	K	47	ARG	2.9
1	K	71	LEU	2.9
1	G	353	ALA	2.9
1	E	1	MET	2.9
1	B	41	SER	2.9
1	I	41	SER	2.9
1	K	46	SER	2.9
1	C	79	VAL	2.9
1	F	10	VAL	2.9
1	G	72	LYS	2.9
1	C	77	ALA	2.9
1	K	347	ALA	2.9
1	E	173	TRP	2.9
1	K	324	GLY	2.9
1	K	39	PRO	2.9
1	E	10	VAL	2.9
1	G	79	VAL	2.9
1	H	69	LEU	2.9
1	K	350	ASP	2.9
1	B	257	ALA	2.9
1	F	70	ALA	2.9
1	G	59	ALA	2.9
1	G	76	LYS	2.9
1	E	207	MET	2.8
1	C	8	LEU	2.8
1	E	7	GLY	2.8
1	E	179	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	348	THR	2.8
1	H	5	LEU	2.8
1	C	11	VAL	2.8
1	F	46	SER	2.8
1	G	96	PRO	2.8
1	A	358	TRP	2.8
1	H	47	ARG	2.8
1	F	353	ALA	2.8
1	L	46	SER	2.8
1	C	76	LYS	2.8
1	C	101	LYS	2.8
1	D	1	MET	2.8
1	D	351	ILE	2.8
1	L	349	ILE	2.8
1	G	69	LEU	2.8
1	E	77	ALA	2.7
1	D	65	GLN	2.7
1	D	42	VAL	2.7
1	F	102	VAL	2.7
1	E	58	THR	2.7
1	H	8	LEU	2.7
1	C	102	VAL	2.7
1	B	347	ALA	2.7
1	G	292	ALA	2.7
1	G	322	ALA	2.7
1	H	2	ALA	2.7
1	C	44	GLY	2.7
1	D	7	GLY	2.7
1	J	349	ILE	2.7
1	K	56	ILE	2.7
1	I	43	ASP	2.7
1	C	68	GLU	2.7
1	C	51	LEU	2.7
1	C	80	LEU	2.7
1	F	69	LEU	2.7
1	F	108	TYR	2.7
1	G	71	LEU	2.7
1	K	67	LEU	2.7
1	L	323	ASN	2.7
1	A	346	ALA	2.7
1	G	347	ALA	2.7
1	K	353	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	7	GLY	2.7
1	G	44	GLY	2.7
1	B	345	PRO	2.6
1	H	355	LEU	2.6
1	K	41	SER	2.6
1	D	49	ALA	2.6
1	D	322	ALA	2.6
1	E	70	ALA	2.6
1	E	322	ALA	2.6
1	F	181	GLY	2.6
1	F	98	GLU	2.6
1	K	348	THR	2.6
1	C	104	ASP	2.6
1	D	173	TRP	2.6
1	H	358	TRP	2.6
1	G	107	ILE	2.6
1	F	47	ARG	2.6
1	B	324	GLY	2.6
1	D	2	ALA	2.6
1	D	30	GLY	2.6
1	I	324	GLY	2.6
1	L	346	ALA	2.6
1	B	350	ASP	2.6
1	G	350	ASP	2.6
1	A	45	ILE	2.6
1	D	107	ILE	2.6
1	F	81	ILE	2.6
1	F	96	PRO	2.6
1	G	345	PRO	2.6
1	G	173	TRP	2.6
1	A	92	LEU	2.6
1	B	73	LEU	2.6
1	G	73	LEU	2.6
1	E	97	GLU	2.6
1	I	44	GLY	2.6
1	J	324	GLY	2.6
1	L	324	GLY	2.6
1	B	75	ALA	2.6
1	J	347	ALA	2.6
1	K	10	VAL	2.6
1	L	42	VAL	2.6
1	J	48	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	43	ASP	2.6
1	C	58	THR	2.6
1	C	39	PRO	2.6
1	H	345	PRO	2.6
1	K	74	ILE	2.6
1	A	47	ARG	2.6
1	E	176	GLN	2.6
1	G	63	SER	2.6
1	G	106	LEU	2.6
1	B	62	LYS	2.5
1	C	59	ALA	2.5
1	C	353	ALA	2.5
1	D	76	LYS	2.5
1	F	76	LYS	2.5
1	K	59	ALA	2.5
1	K	100	ALA	2.5
1	G	43	ASP	2.5
1	B	68	GLU	2.5
1	H	173	TRP	2.5
1	D	8	LEU	2.5
1	H	92	LEU	2.5
1	K	355	LEU	2.5
1	C	100	ALA	2.5
1	F	292	ALA	2.5
1	G	77	ALA	2.5
1	A	207	MET	2.5
1	F	88	VAL	2.5
1	G	11	VAL	2.5
1	G	88	VAL	2.5
1	F	348	THR	2.5
1	K	36	ILE	2.5
1	F	72	LYS	2.5
1	K	101	LYS	2.5
1	A	44	GLY	2.5
1	F	66	GLY	2.5
1	F	92	LEU	2.5
1	L	350	ASP	2.5
1	A	322	ALA	2.5
1	F	100	ALA	2.5
1	G	49	ALA	2.5
1	B	47	ARG	2.5
1	C	33	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	47	ARG	2.5
1	C	46	SER	2.5
1	F	74	ILE	2.5
1	G	180	LYS	2.5
1	C	7	GLY	2.5
1	C	67	LEU	2.5
1	E	73	LEU	2.5
1	G	80	LEU	2.5
1	J	73	LEU	2.5
1	D	47	ARG	2.5
1	G	91	ARG	2.5
1	H	347	ALA	2.5
1	C	34	VAL	2.5
1	E	79	VAL	2.5
1	H	354	VAL	2.5
1	A	40	SER	2.4
1	C	178	SER	2.4
1	C	56	ILE	2.4
1	C	30	GLY	2.4
1	H	324	GLY	2.4
1	G	104	ASP	2.4
1	G	58	THR	2.4
1	I	323	ASN	2.4
1	K	354	VAL	2.4
1	F	41	SER	2.4
1	I	349	ILE	2.4
1	K	181	GLY	2.4
1	L	1	MET	2.4
1	L	44	GLY	2.4
1	B	355	LEU	2.4
1	F	352	GLU	2.4
1	H	322	ALA	2.4
1	A	173	TRP	2.4
1	D	326	TRP	2.4
1	E	358	TRP	2.4
1	K	173	TRP	2.4
1	E	34	VAL	2.4
1	C	40	SER	2.4
1	H	178	SER	2.4
1	F	144	ASP	2.4
1	C	94	LEU	2.4
1	D	73	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	92	LEU	2.4
1	K	58	THR	2.4
1	K	11	VAL	2.4
1	D	345	PRO	2.4
1	F	345	PRO	2.4
1	C	105	ARG	2.4
1	B	65	GLN	2.4
1	D	179	GLY	2.4
1	G	108	TYR	2.4
1	F	48	ASP	2.4
1	J	144	ASP	2.4
1	K	43	ASP	2.4
1	H	16	ILE	2.4
1	H	352	GLU	2.3
1	B	323	ASN	2.3
1	E	2	ALA	2.3
1	E	59	ALA	2.3
1	F	184	VAL	2.3
1	B	66	GLY	2.3
1	D	48	ASP	2.3
1	E	37	ASP	2.3
1	E	43	ASP	2.3
1	C	258	GLU	2.3
1	K	68	GLU	2.3
1	G	36	ILE	2.3
1	C	348	THR	2.3
1	F	326	TRP	2.3
1	B	76	LYS	2.3
1	E	56	ILE	2.3
1	K	61	LEU	2.3
1	F	356	THR	2.3
1	H	46	SER	2.3
1	G	33	VAL	2.3
1	C	350	ASP	2.3
1	E	104	ASP	2.3
1	J	37	ASP	2.3
1	D	181	GLY	2.3
1	E	93	GLY	2.3
1	C	81	ILE	2.3
1	D	314	ILE	2.3
1	G	38	ARG	2.3
1	F	80	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	337	THR	2.3
1	F	182	GLN	2.3
1	G	70	ALA	2.3
1	H	58	THR	2.3
1	H	176	GLN	2.3
1	H	353	ALA	2.3
1	I	176	GLN	2.3
1	L	75	ALA	2.3
1	A	177	SER	2.3
1	C	97	GLU	2.2
1	E	68	GLU	2.2
1	I	258	GLU	2.2
1	J	39	PRO	2.2
1	F	60	ASP	2.2
1	G	37	ASP	2.2
1	G	48	ASP	2.2
1	B	102	VAL	2.2
1	H	7	GLY	2.2
1	H	66	GLY	2.2
1	C	62	LYS	2.2
1	E	356	THR	2.2
1	B	49	ALA	2.2
1	C	14	ALA	2.2
1	F	255	ASP	2.2
1	C	83	GLY	2.2
1	G	66	GLY	2.2
1	G	87	GLY	2.2
1	C	183	VAL	2.2
1	C	354	VAL	2.2
1	H	57	VAL	2.2
1	E	47	ARG	2.2
1	G	105	ARG	2.2
1	B	176	GLN	2.2
1	K	65	GLN	2.2
1	C	73	LEU	2.2
1	J	100	ALA	2.2
1	G	60	ASP	2.2
1	K	99	CYS	2.2
1	F	105	ARG	2.2
1	B	1	MET	2.2
1	I	1	MET	2.2
1	D	56	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	315	GLU	2.2
1	J	61	LEU	2.2
1	D	348	THR	2.2
1	B	204	ALA	2.2
1	C	257	ALA	2.2
1	E	31	ALA	2.2
1	J	41	SER	2.2
1	J	46	SER	2.2
1	C	345	PRO	2.2
1	F	83	GLY	2.2
1	G	9	ARG	2.2
1	H	44	GLY	2.2
1	A	323	ASN	2.2
1	A	1	MET	2.2
1	G	68	GLU	2.1
1	A	69	LEU	2.1
1	B	56	ILE	2.1
1	C	36	ILE	2.1
1	D	349	ILE	2.1
1	F	56	ILE	2.1
1	F	67	LEU	2.1
1	F	71	LEU	2.1
1	H	73	LEU	2.1
1	B	144	ASP	2.1
1	B	358	TRP	2.1
1	J	72	LYS	2.1
1	K	76	LYS	2.1
1	L	41	SER	2.1
1	D	359	ASP	2.1
1	K	108	TYR	2.1
1	E	66	GLY	2.1
1	C	57	VAL	2.1
1	D	11	VAL	2.1
1	J	102	VAL	2.1
1	K	34	VAL	2.1
1	A	355	LEU	2.1
1	D	5	LEU	2.1
1	E	62	LYS	2.1
1	F	172	LEU	2.1
1	K	69	LEU	2.1
1	C	91	ARG	2.1
1	C	357	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	350	ASP	2.1
1	G	356	THR	2.1
1	H	350	ASP	2.1
1	K	63	SER	2.1
1	K	104	ASP	2.1
1	J	353	ALA	2.1
1	J	323	ASN	2.1
1	G	352	GLU	2.1
1	E	101	LYS	2.1
1	H	180	LYS	2.1
1	J	47	ARG	2.1
1	L	47	ARG	2.1
1	A	350	ASP	2.1
1	E	350	ASP	2.1
1	F	104	ASP	2.1
1	G	8	LEU	2.1
1	G	78	ASP	2.1
1	H	40	SER	2.1
1	D	31	ALA	2.1
1	D	171	ALA	2.1
1	E	100	ALA	2.1
1	I	346	ALA	2.1
1	C	179	GLY	2.1
1	J	65	GLN	2.1
1	A	258	GLU	2.1
1	D	34	VAL	2.1
1	H	72	LYS	2.1
1	K	38	ARG	2.1
1	C	37	ASP	2.1
1	E	144	ASP	2.1
1	K	60	ASP	2.1
1	C	172	LEU	2.1
1	E	80	LEU	2.1
1	K	89	THR	2.1
1	C	116	GLN	2.1
1	D	44	GLY	2.0
1	E	65	GLN	2.1
1	F	115	GLY	2.0
1	C	323	ASN	2.0
1	C	38	ARG	2.0
1	C	72	LYS	2.0
1	K	79	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	350	ASP	2.0
1	E	61	LEU	2.0
1	F	65	GLN	2.0
1	G	67	LEU	2.0
1	H	61	LEU	2.0
1	D	315	GLU	2.0
1	E	352	GLU	2.0
1	H	30	GLY	2.0
1	J	93	GLY	2.0
1	J	352	GLU	2.0
1	C	322	ALA	2.0
1	K	322	ALA	2.0
1	A	76	LYS	2.0
1	D	108	TYR	2.0
1	H	62	LYS	2.0
1	H	326	TRP	2.0
1	K	358	TRP	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	BCO	E	401	53/53	0.88	0.15	42,60,87,128	0
2	BCO	H	401	53/53	0.89	0.16	46,61,93,129	0
2	BCO	C	401	53/53	0.90	0.14	35,49,74,90	0
2	BCO	F	401	53/53	0.91	0.14	33,52,72,92	0
2	BCO	G	401	53/53	0.92	0.13	28,49,79,84	0
2	BCO	A	401	53/53	0.92	0.13	33,49,65,91	0

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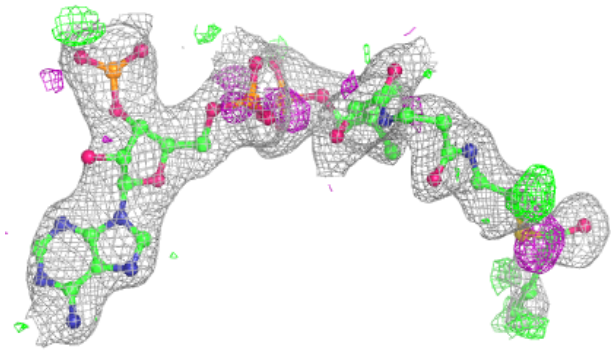
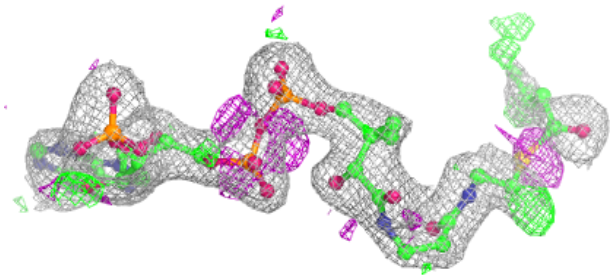
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BCO	J	401	53/53	0.92	0.12	32,43,67,77	0
2	BCO	K	401	53/53	0.92	0.14	32,51,84,106	0
2	BCO	B	401	53/53	0.93	0.13	30,47,72,91	0
2	BCO	L	401	53/53	0.93	0.11	26,37,63,85	0
2	BCO	I	401	53/53	0.95	0.10	25,37,88,102	0
2	BCO	D	401	53/53	0.95	0.10	26,41,68,89	0

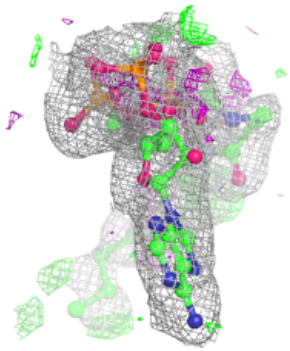
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCO 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)

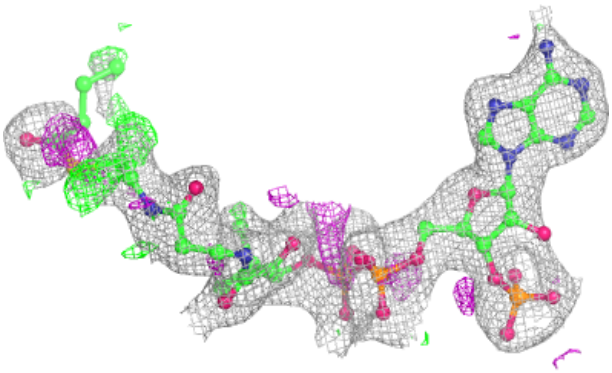


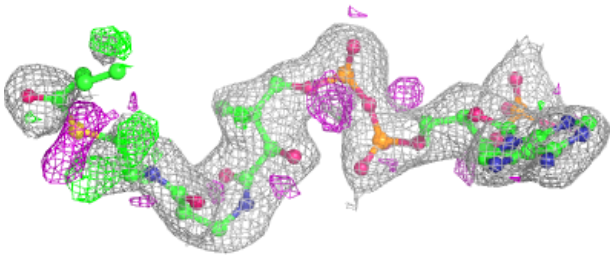


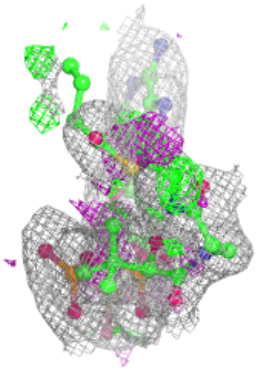


Electron density around BCO H 401:

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

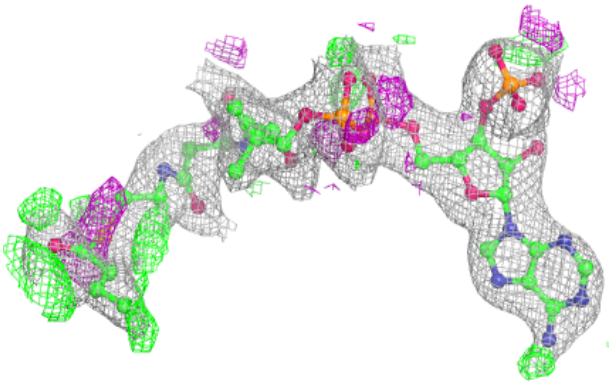


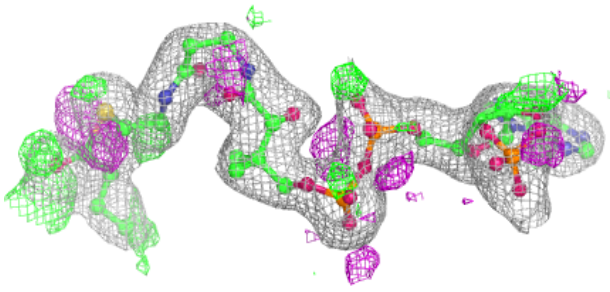


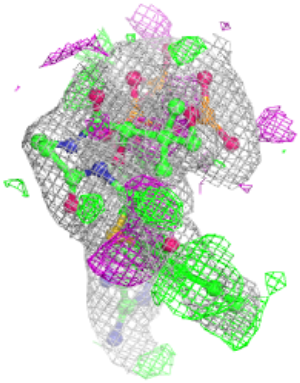


Electron density around BCO C 401:

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

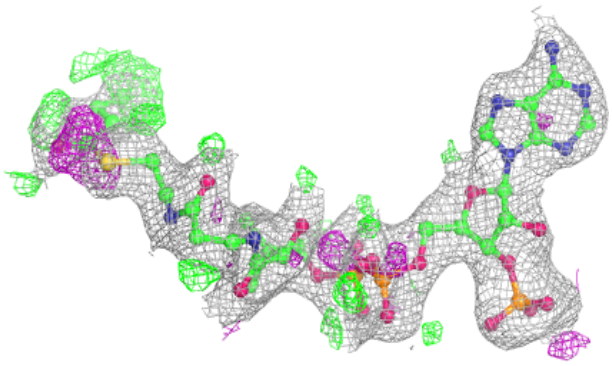


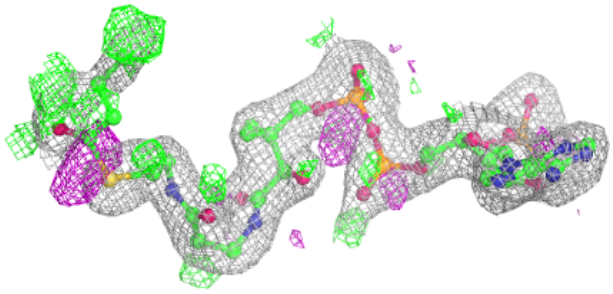


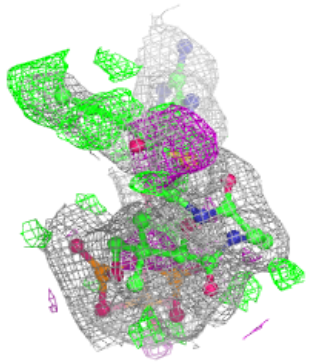


Electron density around BCO F 401:

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

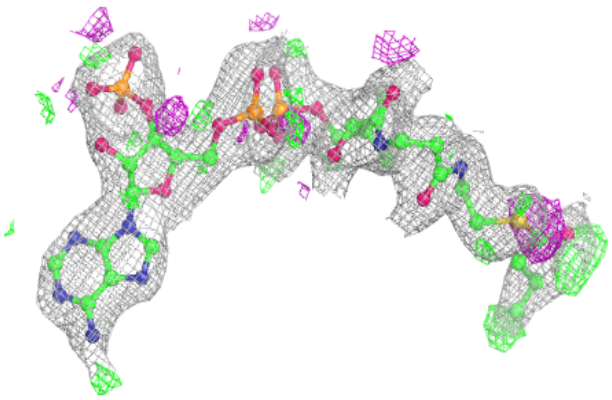


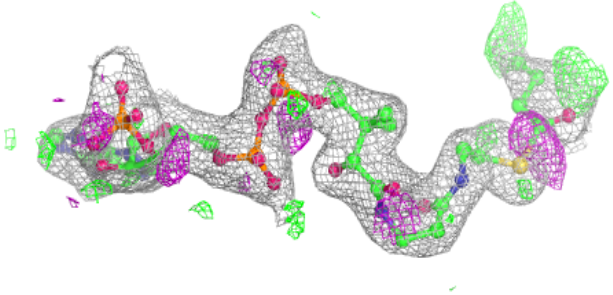


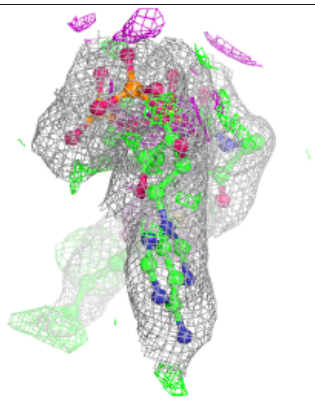


Electron density around BCO G 401:

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

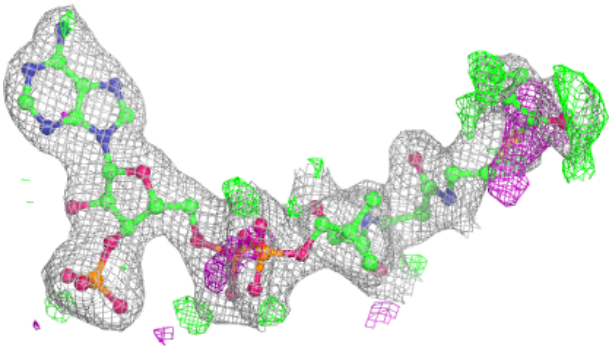


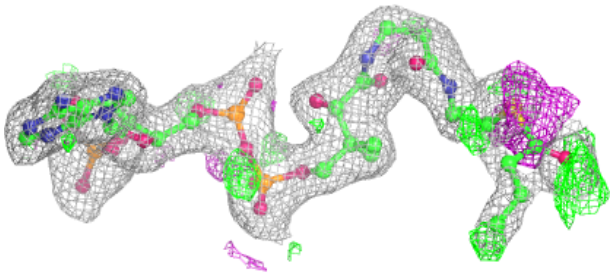


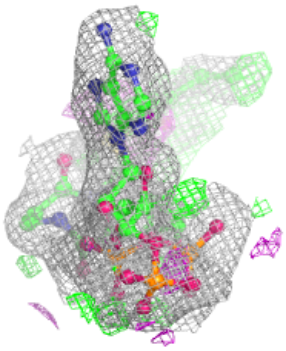


Electron density around BCO A 401:

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

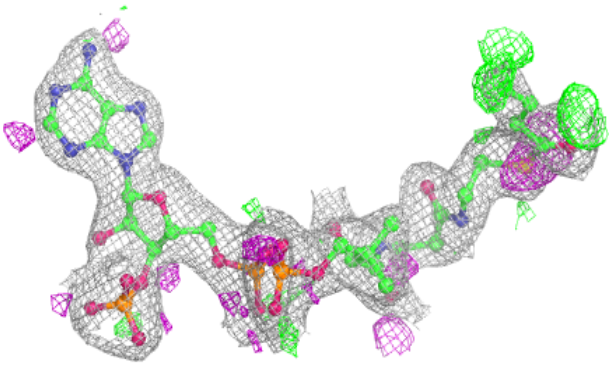


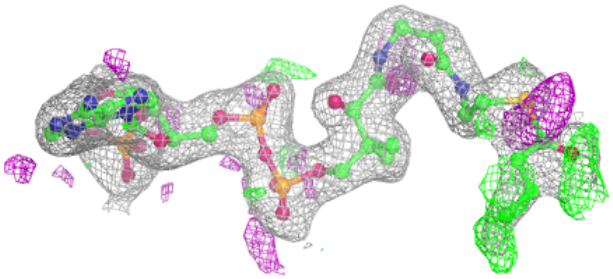


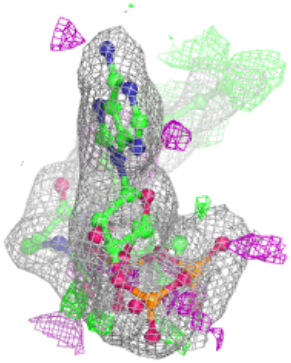


Electron density around BCO J 401:

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

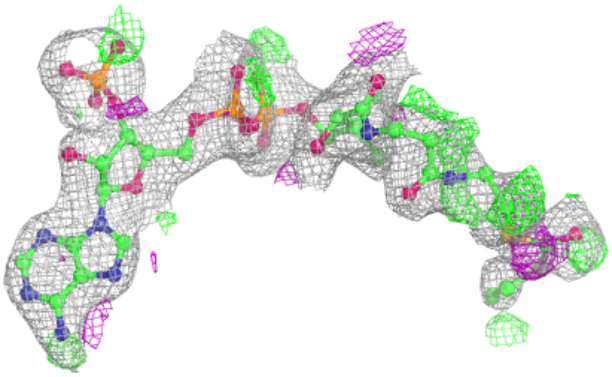


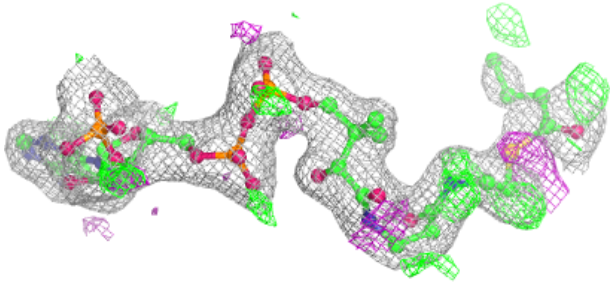


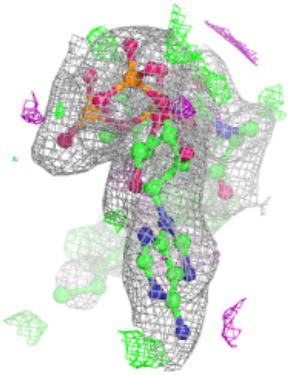


Electron density around BCO K 401:

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

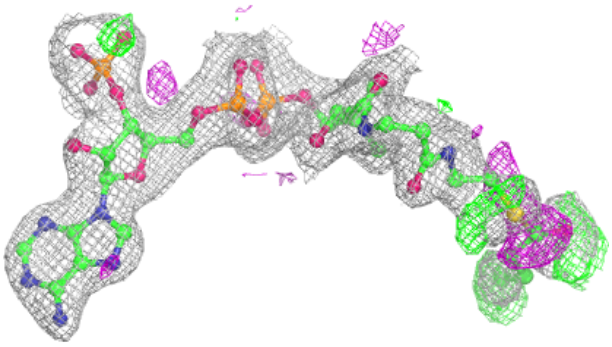


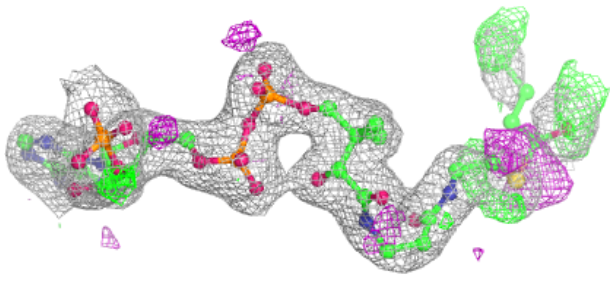


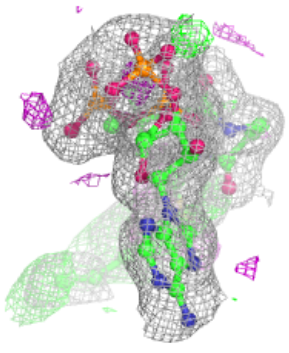


Electron density around BCO B 401:

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

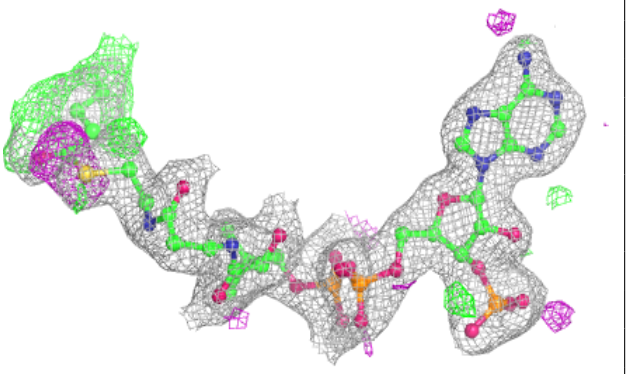


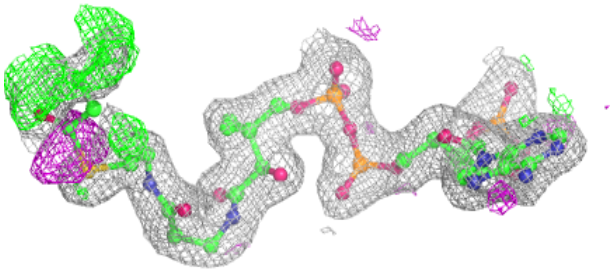


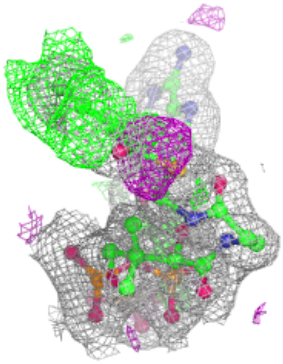


Electron density around BCO L 401:

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

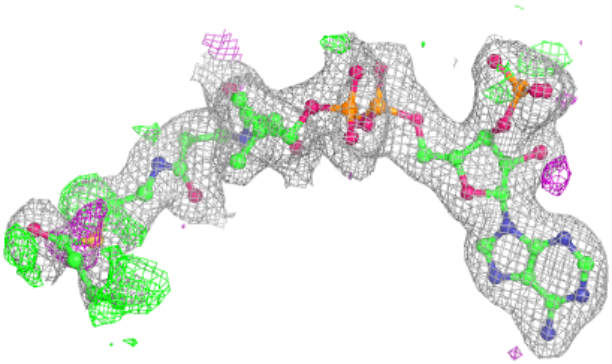


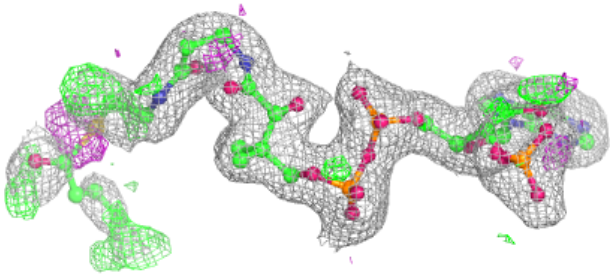


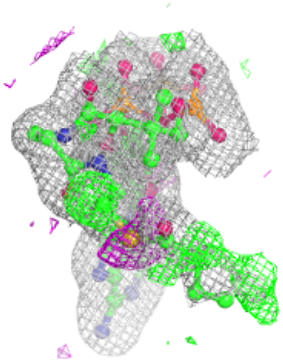


Electron density around BCO I 401:

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

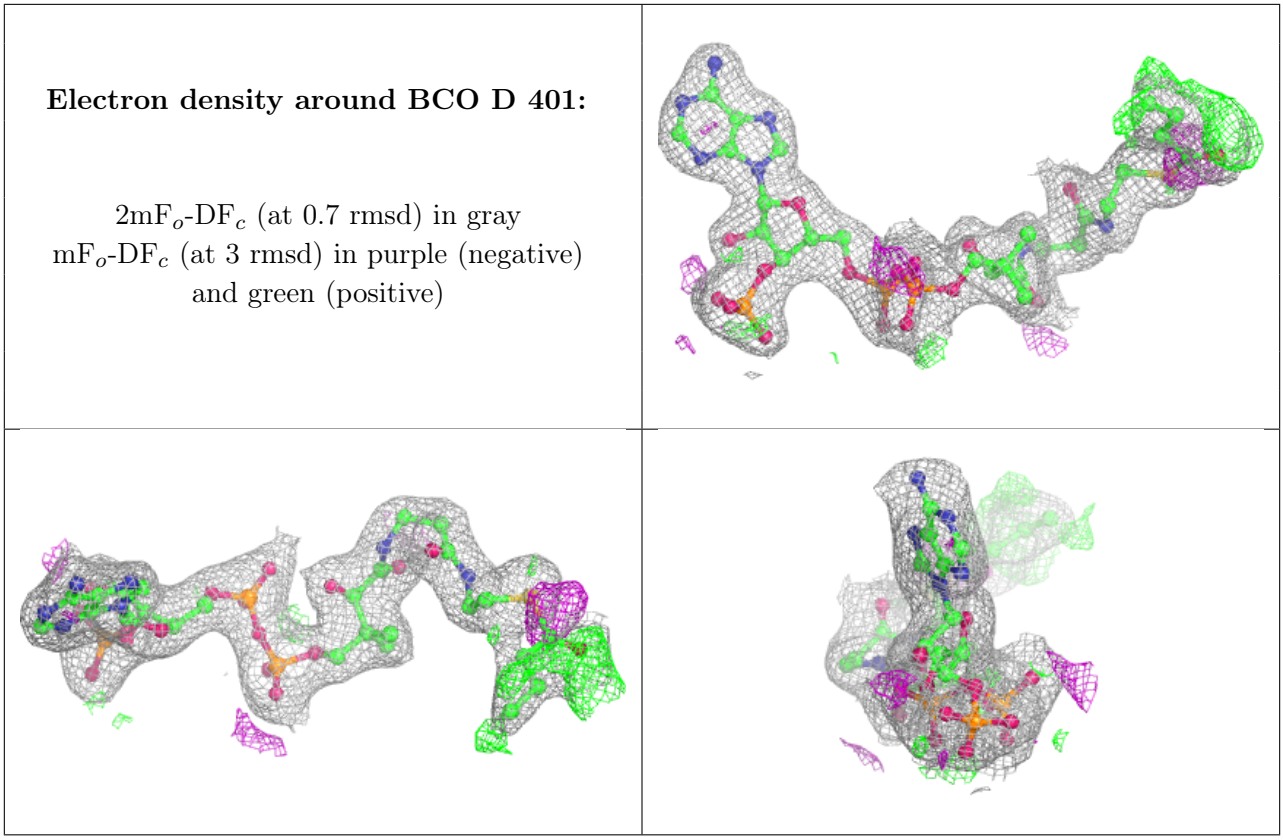






Electron density around BCO D 401:

$2mF_o$-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.