



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:58 PM UTC

PDB ID : 9I2X / pdb_00009i2x
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with naproxenoyl-CoA
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on : 2025-01-22
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

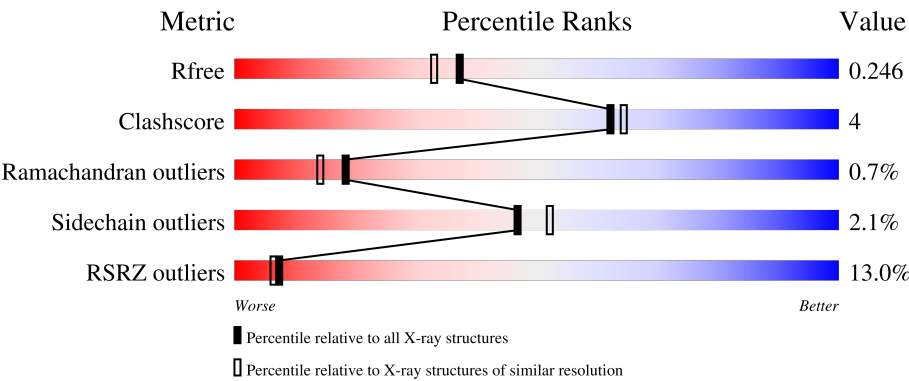
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	11% 88% 10% ..
1	B	364	9% 88% 9% ...
1	C	364	18% 84% 14% ..
1	D	364	12% 85% 12% ...
1	E	364	14% 88% 10% ..

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Mol	Chain	Length	Quality of chain
1	F	364	21%85%12%..
1	G	364	26%81%15%..
1	H	364	18%86%12%..
1	I	364	5%89%9%..
1	J	364	5%89%9%.
1	K	364	11%87%11%..
1	L	364	4%89%8%..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35168 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	B	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	C	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	F	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	G	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	H	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	I	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	J	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	K	359	Total	C	N	O	S	0	2	0
			2718	1704	486	512	16			
1	L	359	Total	C	N	O	S	0	2	0
			2724	1708	488	512	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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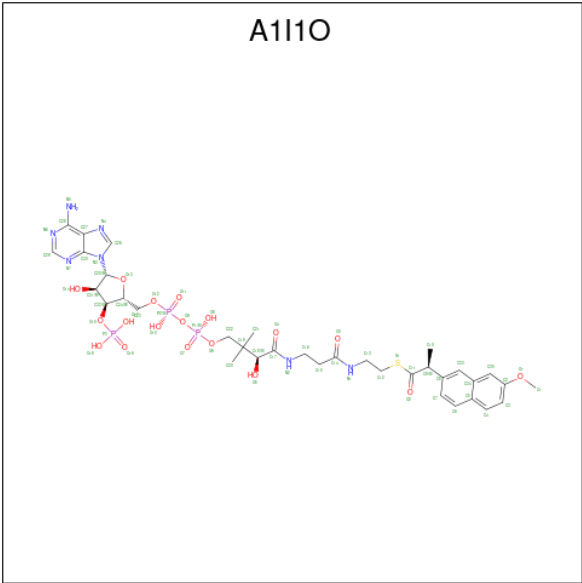
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	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 Naproxenoyl-CoA (CCD ID: A1I1O) (formula: C₃₅H₄₈N₇O₁₈P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	K	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			64	35	7	18	3	1		

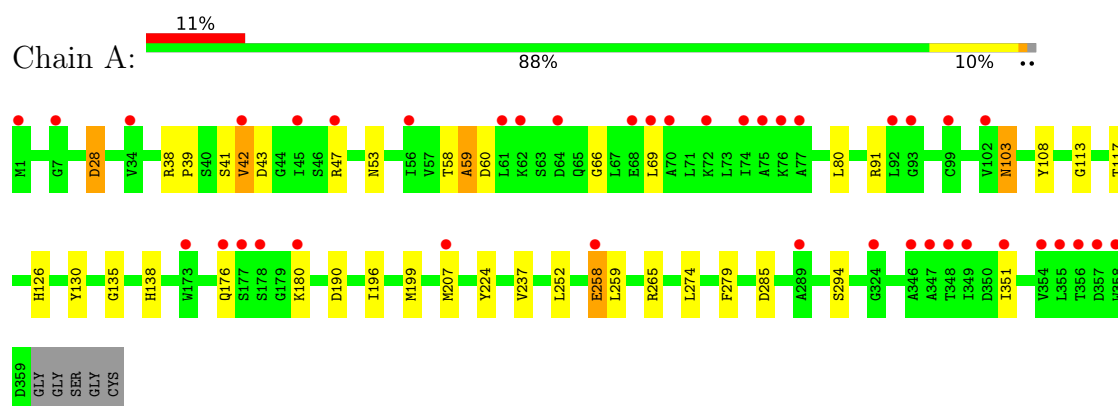
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	148	Total	O	0	0
			148	148		
3	C	150	Total	O	0	0
			150	150		
3	D	151	Total	O	0	0
			151	151		
3	E	132	Total	O	0	0
			132	132		
3	F	129	Total	O	0	0
			129	129		
3	G	124	Total	O	0	0
			124	124		
3	H	136	Total	O	0	0
			136	136		
3	I	179	Total	O	0	0
			179	179		
3	J	169	Total	O	0	0
			169	169		
3	K	159	Total	O	0	0
			159	159		
3	L	163	Total	O	0	0
			163	163		

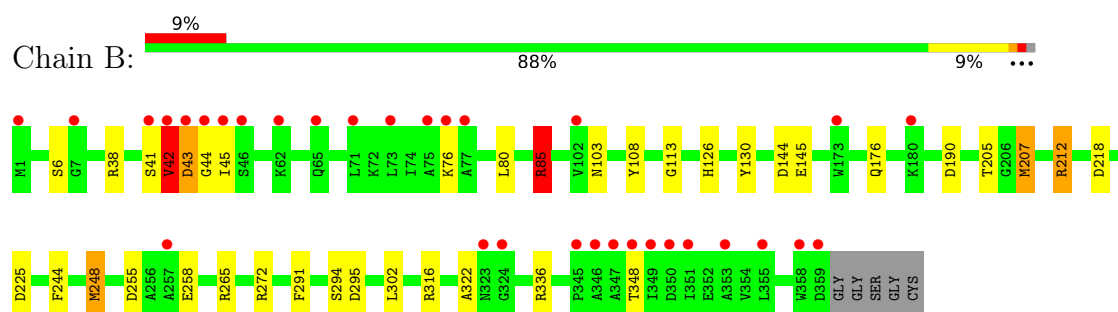
3 Residue-property plots

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

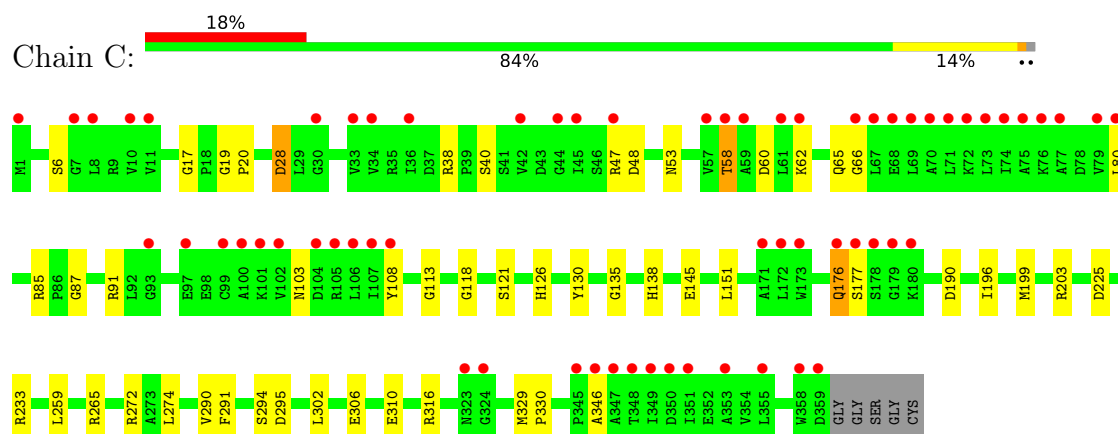
- Molecule 1: Alpha-methylacyl-CoA racemase



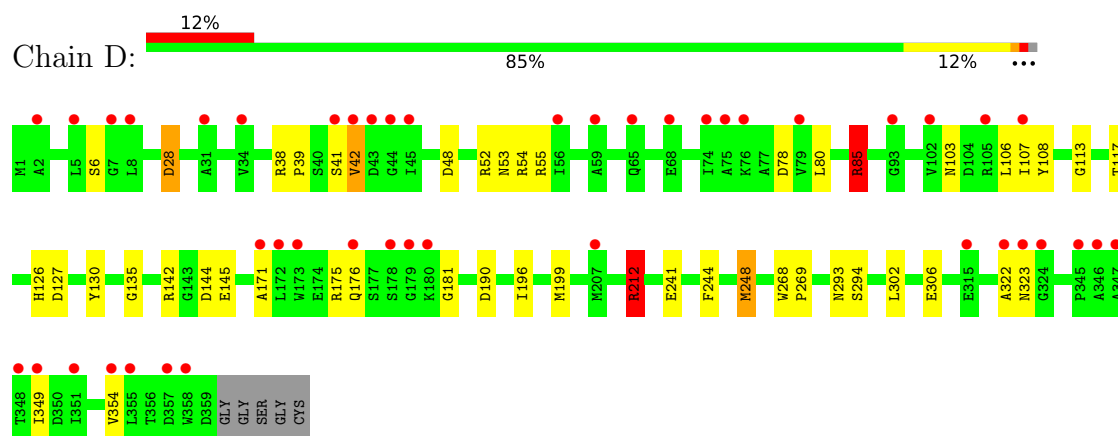
- Molecule 1: Alpha-methylacyl-CoA racemase



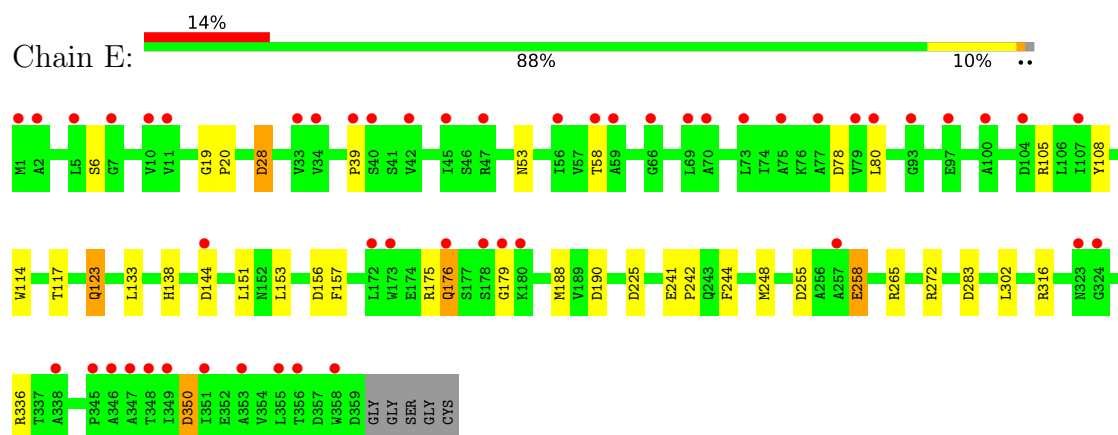
- Molecule 1: Alpha-methylacyl-CoA racemase



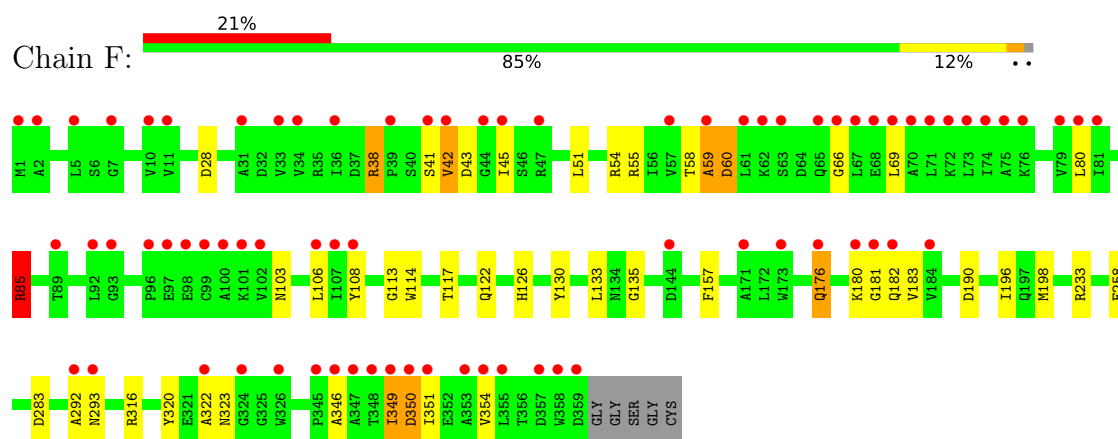
- Molecule 1: Alpha-methylacyl-CoA racemase



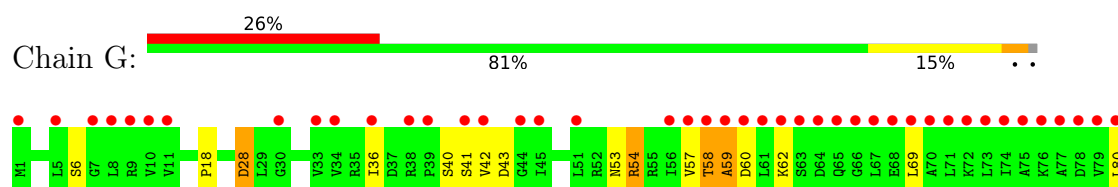
- Molecule 1: Alpha-methylacyl-CoA racemase

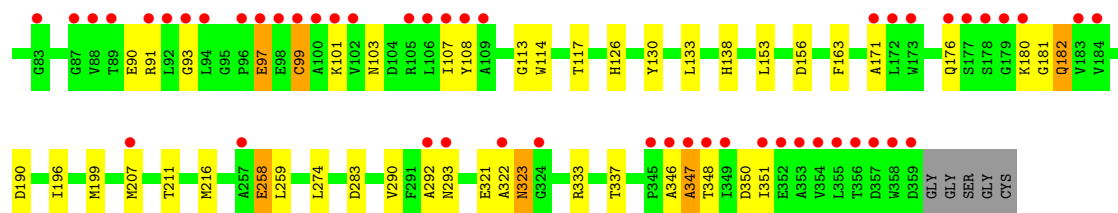


- Molecule 1: Alpha-methylacyl-CoA racemase

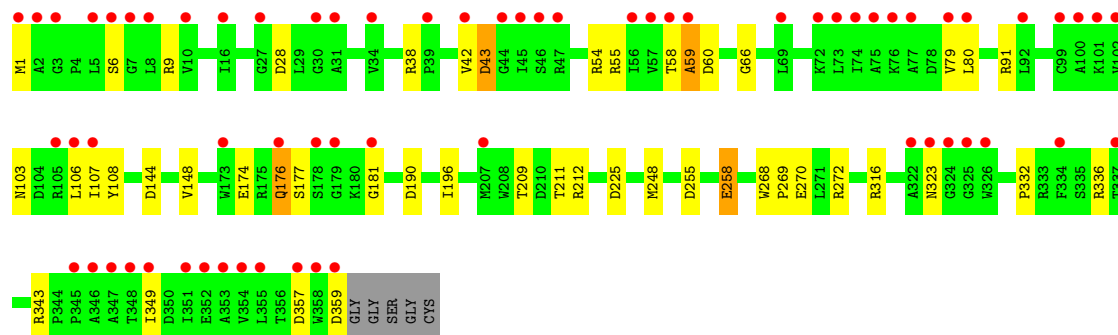
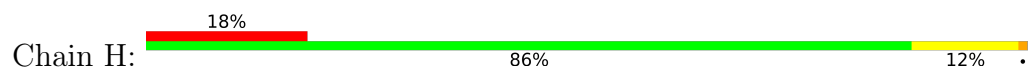


- Molecule 1: Alpha-methylacyl-CoA racemase

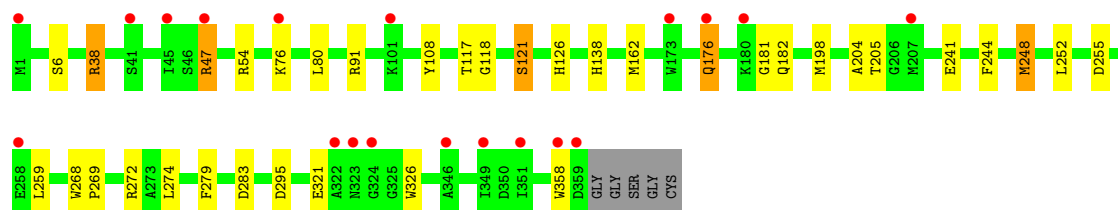
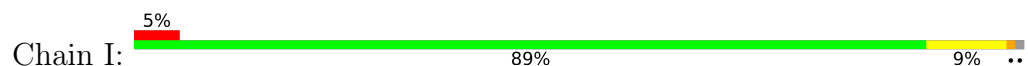




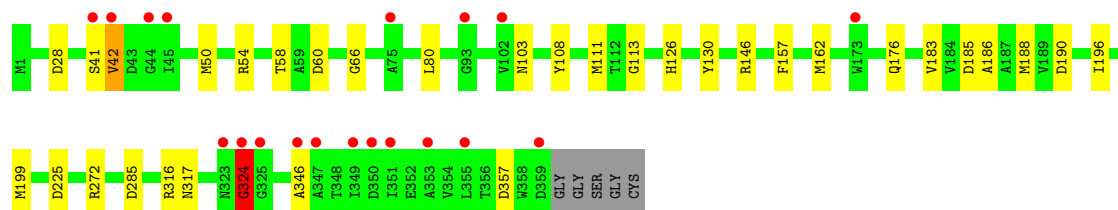
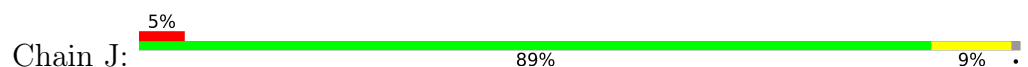
● Molecule 1: Alpha-methylacyl-CoA racemase



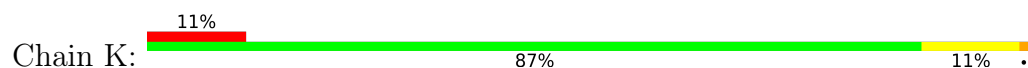
● Molecule 1: Alpha-methylacyl-CoA racemase

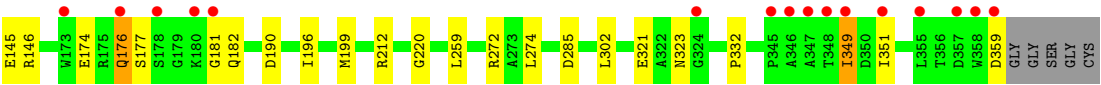


● Molecule 1: Alpha-methylacyl-CoA racemase

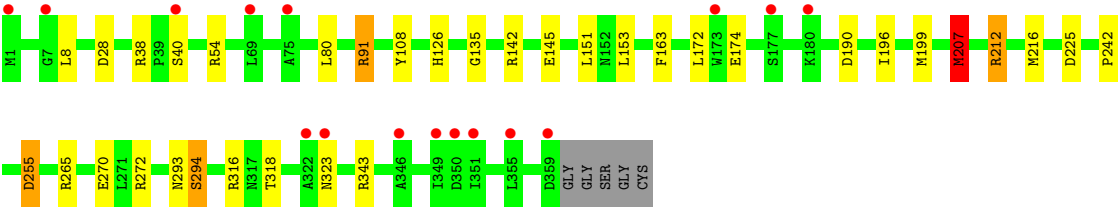
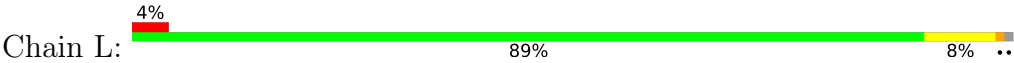


● Molecule 1: Alpha-methylacyl-CoA racemase





● Molecule 1: Alpha-methylacyl-CoA racemase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	276.28Å 276.28Å 389.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.29 – 2.00 225.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.29-2.00) 99.9 (225.29-2.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.206 , 0.239 0.214 , 0.246	Depositor DCC
R_{free} test set	24761 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 0.009 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	35168	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1I1O

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.65	0/2791	1.15	7/3797 (0.2%)
1	B	0.67	0/2782	1.12	7/3785 (0.2%)
1	C	0.65	0/2791	1.17	11/3797 (0.3%)
1	D	0.66	0/2782	1.15	8/3785 (0.2%)
1	E	0.66	0/2791	1.13	5/3797 (0.1%)
1	F	0.66	0/2782	1.14	9/3785 (0.2%)
1	G	0.63	0/2791	1.18	12/3797 (0.3%)
1	H	0.65	0/2782	1.16	8/3785 (0.2%)
1	I	0.66	0/2791	1.14	9/3797 (0.2%)
1	J	0.66	0/2782	1.13	7/3785 (0.2%)
1	K	0.66	0/2791	1.13	9/3797 (0.2%)
1	L	0.66	0/2791	1.15	8/3797 (0.2%)
All	All	0.66	0/33447	1.15	100/45504 (0.2%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	4
All	All	0	28

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	38	ARG	N-CA-CB	-9.89	96.94	110.29
1	L	38	ARG	CB-CA-C	8.72	121.17	108.87
1	G	207	MET	CG-SD-CE	8.53	119.66	100.90
1	I	255	ASP	CB-CA-C	8.48	124.38	110.22
1	E	28	ASP	CA-CB-CG	8.15	120.75	112.60
1	H	28	ASP	CA-CB-CG	8.00	120.60	112.60
1	H	211	THR	CA-CB-OG1	-7.56	98.26	109.60
1	A	258	GLU	N-CA-CB	7.49	122.22	110.46
1	A	28	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	47	ARG	CB-CA-C	7.22	122.76	110.56
1	L	207	MET	CG-SD-CE	7.20	116.74	100.90
1	K	28	ASP	CA-CB-CG	7.14	119.74	112.60
1	A	207	MET	CG-SD-CE	7.12	116.56	100.90
1	C	28	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	190	ASP	CA-CB-CG	6.88	119.48	112.60
1	L	28	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	258	GLU	CB-CA-C	-6.73	96.80	109.72
1	B	255	ASP	CB-CA-C	6.72	121.44	110.22
1	D	248	MET	CG-SD-CE	6.62	115.46	100.90
1	G	190	ASP	CA-CB-CG	6.57	119.17	112.60
1	G	283	ASP	CA-CB-CG	6.55	119.15	112.60
1	G	28	ASP	CA-CB-CG	6.52	119.12	112.60
1	F	190	ASP	CA-CB-CG	6.42	119.02	112.60
1	F	258	GLU	CB-CA-C	-6.40	98.49	110.01
1	I	91	ARG	CB-CA-C	-6.32	98.94	110.63
1	B	38	ARG	CB-CA-C	6.31	117.77	108.87
1	J	190	ASP	CA-CB-CG	6.28	118.88	112.60
1	G	258	GLU	CB-CA-C	-6.25	98.77	110.01
1	E	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	144	ASP	CA-CB-CG	6.20	118.80	112.60
1	C	47	ARG	N-CA-CB	-6.19	101.52	110.56
1	J	28	ASP	CA-CB-CG	6.18	118.78	112.60
1	I	38	ARG	CB-CA-C	-6.15	99.89	109.11
1	I	321	GLU	CB-CA-C	-6.09	99.48	109.53
1	C	190	ASP	CA-CB-CG	6.08	118.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	255	ASP	CA-CB-CG	6.08	118.67	112.60
1	H	190	ASP	CA-CB-CG	6.06	118.66	112.60
1	G	216	MET	CG-SD-CE	6.03	114.17	100.90
1	I	176	GLN	N-CA-CB	6.02	118.97	110.12
1	G	350	ASP	CB-CA-C	5.98	119.73	109.51
1	L	190	ASP	CA-CB-CG	5.95	118.55	112.60
1	D	28	ASP	CA-CB-CG	5.90	118.50	112.60
1	D	38	ARG	CB-CA-C	5.86	116.82	108.68
1	A	190	ASP	CA-CB-CG	5.84	118.44	112.60
1	G	99	CYS	CB-CA-C	5.83	121.36	110.70
1	F	38	ARG	N-CA-CB	-5.82	101.93	110.14
1	C	58	THR	CA-CB-OG1	-5.82	100.87	109.60
1	L	318	THR	CA-CB-OG1	-5.79	100.91	109.60
1	E	123	GLN	CB-CA-C	-5.74	100.70	109.89
1	K	212	ARG	CB-CA-C	5.71	119.42	109.65
1	A	285	ASP	CB-CA-C	5.71	120.56	110.85
1	K	321	GLU	CB-CA-C	-5.69	100.15	109.53
1	C	290	VAL	N-CA-CB	-5.65	103.40	110.47
1	I	283	ASP	CA-CB-CG	5.61	118.21	112.60
1	B	258	GLU	CB-CA-C	-5.61	98.79	109.95
1	G	58	THR	CA-CB-OG1	-5.60	101.19	109.60
1	E	283	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	38	ARG	CB-CA-C	5.55	117.41	109.26
1	D	144	ASP	CA-CB-CG	5.54	118.14	112.60
1	F	350	ASP	CB-CA-C	5.54	119.65	109.46
1	K	38	ARG	N-CA-CB	5.51	118.16	110.11
1	K	32	ASP	CA-CB-CG	5.50	118.10	112.60
1	J	157	PHE	CB-CA-C	5.47	119.53	111.65
1	C	265	ARG	CD-NE-CZ	5.39	131.94	124.40
1	K	190	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	48	ASP	CA-CB-CG	5.36	117.96	112.60
1	D	190	ASP	CA-CB-CG	5.36	117.95	112.60
1	K	146	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	I	205	THR	CA-CB-OG1	-5.34	101.58	109.60
1	H	357	ASP	CA-CB-CG	5.32	117.92	112.60
1	F	28	ASP	CA-CB-CG	5.31	117.91	112.60
1	F	55	ARG	CB-CA-C	5.31	118.91	109.72
1	B	207	MET	CG-SD-CE	5.29	112.55	100.90
1	C	62	LYS	CB-CA-C	5.29	120.11	110.11
1	C	306	GLU	CB-CA-C	-5.29	100.45	109.65
1	H	270	GLU	N-CA-CB	-5.28	102.35	110.01
1	D	48	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	60	ASP	CA-CB-CG	5.27	117.87	112.60
1	H	258	GLU	CB-CA-C	-5.26	100.54	110.01
1	L	255	ASP	CB-CA-C	-5.26	101.27	109.84
1	I	248	MET	CG-SD-CE	5.25	112.45	100.90
1	D	306	GLU	CB-CA-C	-5.25	100.74	109.55
1	J	285	ASP	CB-CA-C	5.24	120.32	110.63
1	G	60	ASP	CA-CB-CG	5.20	117.80	112.60
1	J	54	ARG	CB-CA-C	-5.16	98.11	109.56
1	J	146	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	J	185	ASP	CA-CB-CG	5.14	117.74	112.60
1	L	91	ARG	CB-CA-C	-5.14	102.25	110.79
1	H	323	ASN	CB-CA-C	-5.13	109.12	115.89
1	H	144	ASP	CA-CB-CG	5.12	117.72	112.60
1	K	58	THR	CA-CB-OG1	5.10	117.24	109.60
1	C	310	GLU	CB-CG-CD	5.09	121.25	112.60
1	G	290	VAL	N-CA-CB	5.09	116.16	110.51
1	D	54	ARG	CB-CA-C	-5.08	98.27	109.56
1	B	85	ARG	N-CA-CB	5.08	117.70	110.03
1	K	285	ASP	CB-CA-C	5.06	120.39	110.67
1	F	157	PHE	CB-CA-C	5.06	118.93	111.65
1	B	218	ASP	CA-CB-CG	5.05	117.66	112.60
1	G	211	THR	CA-CB-OG1	-5.04	102.04	109.60
1	F	283	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	322	ALA	Peptide
1	B	85	ARG	Sidechain
1	C	203	ARG	Sidechain
1	C	233	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	42	VAL	Peptide
1	D	85	ARG	Sidechain
1	E	265	ARG	Sidechain
1	E	350	ASP	Peptide
1	F	233	ARG	Sidechain
1	F	85	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	333	ARG	Sidechain
1	G	54	ARG	Peptide
1	G	91	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	54	ARG	Peptide
1	H	91	ARG	Sidechain
1	I	54	ARG	Peptide
1	J	324	GLY	Peptide
1	K	35	ARG	Sidechain
1	K	38	ARG	Sidechain
1	L	212	ARG	Sidechain
1	L	265	ARG	Sidechain
1	L	54	ARG	Peptide
1	L	91	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2718	0	2658	25	0
1	B	2715	0	2660	21	0
1	C	2718	0	2658	30	0
1	D	2715	0	2660	32	0
1	E	2718	0	2658	24	0
1	F	2715	0	2660	34	0
1	G	2718	0	2658	32	0
1	H	2715	0	2660	22	0
1	I	2718	0	2658	22	0
1	J	2715	0	2660	19	0
1	K	2718	0	2658	24	0
1	L	2724	0	2667	20	0
2	A	64	0	0	4	0
2	B	64	0	0	3	0
2	C	64	0	0	6	0
2	D	64	0	0	5	0
2	E	64	0	0	0	0
2	F	64	0	0	5	0
2	G	64	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	64	0	0	2	0
2	I	64	0	0	4	0
2	J	64	0	0	2	0
2	K	64	0	0	4	0
2	L	64	0	0	2	0
3	A	153	0	0	1	0
3	B	148	0	0	0	0
3	C	150	0	0	2	0
3	D	151	0	0	0	0
3	E	132	0	0	1	0
3	F	129	0	0	3	0
3	G	124	0	0	1	0
3	H	136	0	0	0	0
3	I	179	0	0	3	0
3	J	169	0	0	1	0
3	K	159	0	0	4	0
3	L	163	0	0	2	0
All	All	35168	0	31915	269	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 (269) 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:D:85:ARG:HD3	2:D:401:A1I1O:O10	1.74	0.88
1:F:85:ARG:HD3	2:F:401:A1I1O:O11	1.76	0.86
1:A:126:HIS:ND1	2:A:401:A1I1O:C11	2.41	0.82
1:D:126:HIS:ND1	2:D:401:A1I1O:C11	2.43	0.81
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.60	0.81
1:D:126:HIS:ND1	2:D:401:A1I1O:C9	2.45	0.79
1:I:126:HIS:ND1	2:I:401:A1I1O:C11	2.46	0.79
1:L:126:HIS:ND1	2:L:401:A1I1O:C11	2.46	0.79
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.21	0.76
1:B:85:ARG:HD3	2:B:401:A1I1O:O10	1.86	0.75
1:G:80:LEU:HD23	1:G:108:TYR:CE1	2.24	0.73
1:K:126:HIS:ND1	2:K:401:A1I1O:C11	2.53	0.71
1:F:126:HIS:ND1	2:F:401:A1I1O:C11	2.56	0.69
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.26	0.69
1:F:126:HIS:ND1	2:F:401:A1I1O:C9	2.55	0.69
1:K:126:HIS:ND1	2:K:401:A1I1O:C9	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:A1I1O:C7	2:D:401:A1I1O:S1	2.81	0.68
1:G:126:HIS:ND1	2:G:401:A1I1O:C9	2.57	0.68
1:I:76:LYS:HE3	1:I:358:TRP:O	1.95	0.67
1:B:41:SER:O	1:B:42:VAL:HG23	1.96	0.66
1:G:90:GLU:O	1:G:93:GLY:N	2.25	0.65
1:A:126:HIS:ND1	2:A:401:A1I1O:O2	2.29	0.65
1:G:69:LEU:HB3	1:G:351:ILE:HD13	1.79	0.65
1:J:41:SER:O	1:J:42:VAL:HG13	1.97	0.64
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.82	0.63
1:I:126:HIS:ND1	2:I:401:A1I1O:C9	2.61	0.63
1:G:80:LEU:CD2	1:G:108:TYR:CE1	2.82	0.62
1:I:38:ARG:HH21	1:I:38:ARG:HG3	1.64	0.62
1:G:126:HIS:ND1	2:G:401:A1I1O:C11	2.63	0.61
1:K:138:HIS:HD2	3:K:577:HOH:O	1.83	0.60
1:L:270:GLU:HG3	3:L:526:HOH:O	1.99	0.60
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.37	0.60
1:C:138:HIS:HD2	3:C:567:HOH:O	1.84	0.59
1:K:91:ARG:NH1	3:K:505:HOH:O	2.33	0.59
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.17	0.59
1:J:126:HIS:ND1	2:J:401:A1I1O:C11	2.65	0.59
1:C:346:ALA:HB3	3:C:548:HOH:O	2.03	0.59
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.37	0.59
1:A:138:HIS:HD2	3:A:538:HOH:O	1.86	0.59
1:A:80:LEU:CD2	1:A:108:TYR:CE2	2.86	0.58
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.38	0.58
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.85	0.58
1:D:78:ASP:OD1	1:D:175:ARG:NH2	2.18	0.58
1:E:105:ARG:HG2	1:E:179:GLY:O	2.03	0.58
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.85	0.57
1:C:291:PHE:O	1:C:294:SER:HB3	2.05	0.57
1:J:126:HIS:ND1	2:J:401:A1I1O:C9	2.68	0.57
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.88	0.57
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.37	0.56
1:C:80:LEU:HD23	1:C:108:TYR:CE2	2.39	0.56
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.38	0.56
1:F:85:ARG:NH1	2:F:401:A1I1O:O8	2.39	0.56
1:C:126:HIS:ND1	2:C:401:A1I1O:C9	2.69	0.55
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.38	0.55
1:K:176:GLN:HA	1:K:176:GLN:HE21	1.71	0.55
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.21	0.55
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:VAL:HG12	1:F:43:ASP:N	2.21	0.55
1:A:126:HIS:ND1	2:A:401:A1I1O:C9	2.70	0.55
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.39	0.55
1:C:17:GLY:O	1:C:20:PRO:HD2	2.07	0.54
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.38	0.54
1:I:126:HIS:ND1	2:I:401:A1I1O:O2	2.39	0.54
1:L:126:HIS:ND1	2:L:401:A1I1O:C9	2.71	0.54
1:K:332:PRO:HG3	1:L:163:PHE:O	2.08	0.54
1:D:28:ASP:HA	1:D:53:ASN:ND2	2.23	0.54
1:C:19:GLY:N	1:C:20:PRO:CD	2.71	0.53
1:A:41:SER:O	1:A:42:VAL:C	2.52	0.53
1:B:291:PHE:O	1:B:294:SER:HB3	2.09	0.53
1:C:28:ASP:HA	1:C:53:ASN:HD22	1.72	0.53
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.91	0.53
1:F:38:ARG:HG2	3:F:515:HOH:O	2.09	0.52
1:I:138:HIS:HD2	3:I:556:HOH:O	1.92	0.52
1:G:337:THR:HG21	1:H:174:GLU:OE2	2.10	0.52
1:I:272:ARG:NH1	3:I:508:HOH:O	2.42	0.52
1:J:42:VAL:HG21	1:J:58:THR:HG21	1.91	0.52
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.92	0.52
1:H:60:ASP:O	1:H:66:GLY:HA3	2.08	0.52
1:H:255:ASP:HB3	1:H:258:GLU:HG3	1.92	0.52
1:K:91:ARG:NH2	2:K:401:A1I1O:O18	2.43	0.52
1:K:145:GLU:OE1	1:L:145:GLU:OE1	2.28	0.52
1:H:58:THR:O	1:H:59:ALA:HB2	2.10	0.52
1:D:85:ARG:CD	2:D:401:A1I1O:O10	2.52	0.52
1:J:60:ASP:O	1:J:66:GLY:HA3	2.10	0.52
1:D:28:ASP:HA	1:D:53:ASN:HD22	1.75	0.52
1:K:55:ARG:HD2	1:K:349:ILE:HD12	1.92	0.52
1:C:91:ARG:NH2	2:C:401:A1I1O:O17	2.43	0.51
1:K:80:LEU:HD23	1:K:108:TYR:CE2	2.45	0.51
1:H:255:ASP:HB3	1:H:258:GLU:CG	2.40	0.51
1:K:220:GLY:O	1:K:272:ARG:NH2	2.43	0.51
1:E:138:HIS:HD2	3:E:580:HOH:O	1.93	0.51
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.25	0.51
1:H:42:VAL:O	1:H:43:ASP:C	2.54	0.51
1:C:91:ARG:HD2	1:L:242:PRO:HB3	1.93	0.50
1:F:85:ARG:CD	2:F:401:A1I1O:O11	2.56	0.50
1:I:204:ALA:HB1	1:J:324:GLY:HA3	1.93	0.50
1:H:106:LEU:O	1:H:181:GLY:HA3	2.12	0.49
1:C:126:HIS:ND1	2:C:401:A1I1O:C11	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ASP:OD1	1:E:175:ARG:NH2	2.20	0.49
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.38	0.49
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.95	0.49
2:C:401:A1I1O:C7	2:C:401:A1I1O:S1	2.99	0.49
1:G:322:ALA:C	1:G:323:ASN:HD22	2.21	0.49
1:E:255:ASP:HB3	1:E:258:GLU:HG3	1.93	0.49
1:F:320:TYR:CE2	1:F:322:ALA:HB2	2.47	0.49
1:A:180:LYS:O	1:B:336:ARG:NH2	2.46	0.48
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.30	0.48
1:K:39:PRO:O	1:K:42:VAL:HG23	2.12	0.48
1:D:42:VAL:O	1:D:42:VAL:HG13	2.13	0.48
1:E:117:THR:O	1:F:316:ARG:HD2	2.13	0.48
1:G:163:PHE:O	1:H:332:PRO:HG3	2.13	0.48
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.94	0.48
1:G:36:ILE:HA	1:G:57:VAL:O	2.14	0.48
1:G:176:GLN:HG3	1:H:176:GLN:HE21	1.78	0.48
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.94	0.48
1:B:144:ASP:OD1	1:B:145:GLU:HG3	2.13	0.48
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.96	0.48
1:F:122:GLN:HG2	3:F:502:HOH:O	2.13	0.48
2:H:401:A1I1O:O4	2:H:401:A1I1O:C20	2.62	0.48
1:G:28:ASP:HA	1:G:53:ASN:HD22	1.79	0.48
1:I:118:GLY:O	1:I:121:SER:OG	2.26	0.48
1:D:142:ARG:O	1:D:212:ARG:HD2	2.13	0.48
1:F:69:LEU:HD13	1:F:351:ILE:HG23	1.96	0.47
1:G:113:GLY:HA3	1:G:130:TYR:CE1	2.49	0.47
1:E:39:PRO:HB3	1:E:58:THR:CG2	2.44	0.47
1:C:118:GLY:O	1:C:121:SER:OG	2.28	0.47
1:E:114:TRP:CZ3	1:E:133:LEU:HD22	2.50	0.47
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.50	0.47
1:J:111:MET:HE3	1:J:186:ALA:O	2.15	0.47
1:B:244:PHE:HB3	1:B:295:ASP:O	2.15	0.47
1:H:55:ARG:HG2	1:H:349:ILE:HD12	1.97	0.46
1:A:176:GLN:NE2	1:B:176:GLN:HG2	2.30	0.46
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.40	0.46
1:K:42:VAL:HG12	1:K:43:ASP:O	2.15	0.46
2:K:401:A1I1O:C7	2:K:401:A1I1O:S1	3.03	0.46
1:E:39:PRO:CA	1:E:58:THR:HG23	2.46	0.46
1:E:153:LEU:HD21	1:F:196:ILE:HG13	1.97	0.46
1:F:58:THR:O	1:F:59:ALA:HB2	2.14	0.46
1:A:117:THR:O	1:B:316:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ILE:HD11	1:D:354:VAL:HG22	1.97	0.46
1:L:174:GLU:OE1	1:L:174:GLU:C	2.59	0.46
1:D:106:LEU:O	1:D:181:GLY:HA3	2.16	0.46
1:G:58:THR:O	1:G:59:ALA:HB2	2.15	0.46
1:B:126:HIS:ND1	2:B:401:A1I1O:C9	2.79	0.46
1:C:87:GLY:O	1:C:91:ARG:HG3	2.15	0.46
1:G:97:GLU:HA	1:G:97:GLU:OE2	2.16	0.46
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.99	0.45
1:K:351:ILE:HG23	3:K:524:HOH:O	2.15	0.45
1:L:343:ARG:NH2	3:L:510:HOH:O	2.43	0.45
1:A:69:LEU:HD13	1:A:351:ILE:CG2	2.47	0.45
1:D:39:PRO:O	1:D:42:VAL:HG12	2.15	0.45
1:E:28:ASP:HA	1:E:53:ASN:ND2	2.31	0.45
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.97	0.45
1:D:349:ILE:HD11	1:D:354:VAL:CG2	2.47	0.45
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.52	0.45
1:I:268:TRP:N	1:I:269:PRO:CD	2.79	0.45
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.52	0.45
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.81	0.45
1:G:176:GLN:HG3	1:H:176:GLN:NE2	2.31	0.45
1:A:224:TYR:HA	1:A:237:VAL:O	2.17	0.44
1:G:346:ALA:O	1:G:347:ALA:O	2.34	0.44
1:G:117:THR:O	1:H:316:ARG:HD2	2.17	0.44
1:G:180:LYS:HB2	1:H:336:ARG:NH2	2.32	0.44
1:G:18:PRO:HB3	1:G:156:ASP:O	2.16	0.44
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.52	0.44
1:E:316:ARG:HD2	1:F:117:THR:O	2.18	0.44
1:F:80:LEU:HD23	1:F:108:TYR:CE2	2.52	0.44
1:F:108:TYR:HB3	1:F:183:VAL:HG22	2.00	0.44
1:E:302:LEU:O	1:F:135:GLY:HA2	2.17	0.44
2:I:401:A1I1O:C7	2:I:401:A1I1O:S1	3.06	0.44
1:K:117:THR:O	1:L:316:ARG:HD2	2.18	0.44
1:D:55:ARG:HD2	1:D:349:ILE:CD1	2.48	0.44
1:D:107:ILE:HD12	1:D:171:ALA:HB1	1.99	0.44
1:G:138:HIS:HD2	3:G:530:HOH:O	2.00	0.44
1:I:162:MET:HB3	1:J:162:MET:HB3	2.00	0.44
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.52	0.44
1:C:196:ILE:HG12	1:C:199:MET:HB2	2.00	0.43
1:E:176:GLN:HG3	1:F:176:GLN:NE2	2.32	0.43
1:G:114:TRP:CZ3	1:G:133:LEU:HD22	2.52	0.43
1:G:181:GLY:O	1:G:182:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:GLU:HB2	1:E:244:PHE:CD2	2.52	0.43
1:C:176:GLN:NE2	1:D:176:GLN:HG2	2.34	0.43
1:L:225:ASP:OD2	1:L:272:ARG:NH1	2.51	0.43
1:A:47:ARG:HD2	1:B:205:THR:HG22	2.01	0.43
1:C:38:ARG:NH2	2:C:401:A1I1O:O13	2.50	0.43
1:F:113:GLY:HA3	1:F:130:TYR:CE1	2.54	0.43
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.53	0.43
1:J:108:TYR:HB3	1:J:183:VAL:HG22	2.01	0.43
1:K:19:GLY:N	1:K:20:PRO:HD2	2.34	0.43
1:F:60:ASP:O	1:F:66:GLY:HA3	2.18	0.43
1:D:55:ARG:HD2	1:D:349:ILE:HD13	2.01	0.43
1:D:294:SER:HB2	1:L:293:ASN:O	2.19	0.43
1:I:244:PHE:HB3	1:I:295:ASP:O	2.19	0.43
1:L:142:ARG:O	1:L:212:ARG:HD2	2.19	0.43
1:B:42:VAL:HG11	1:B:348:THR:HG21	2.01	0.43
1:C:316:ARG:HD2	1:D:117:THR:O	2.19	0.43
1:D:28:ASP:CG	1:D:52:ARG:HH21	2.27	0.43
1:C:85:ARG:NH2	2:C:401:A1I1O:O7	2.37	0.42
1:I:181:GLY:O	1:I:182:GLN:HB3	2.18	0.42
1:C:302:LEU:O	1:D:135:GLY:HA2	2.19	0.42
1:E:19:GLY:N	1:E:20:PRO:HD2	2.34	0.42
1:F:106:LEU:O	1:F:181:GLY:HA3	2.18	0.42
1:A:103:ASN:OD1	1:A:103:ASN:C	2.61	0.42
1:E:157:PHE:HZ	1:F:198:MET:HE3	1.85	0.42
1:I:241:GLU:HB2	1:I:244:PHE:CD2	2.54	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.81	0.42
1:J:346:ALA:HB3	3:J:565:HOH:O	2.19	0.42
1:K:351:ILE:CG2	3:K:524:HOH:O	2.66	0.42
1:B:126:HIS:ND1	2:B:401:A1I1O:C11	2.83	0.42
1:E:156:ASP:HA	1:E:188:MET:SD	2.58	0.42
1:F:114:TRP:CZ3	1:F:133:LEU:HD22	2.55	0.42
1:J:113:GLY:HA2	1:J:188:MET:HB2	2.01	0.42
1:A:252:LEU:HD21	1:A:279:PHE:CE1	2.55	0.42
1:G:54:ARG:HG2	1:G:54:ARG:HH11	1.83	0.42
1:A:58:THR:O	1:A:59:ALA:HB2	2.18	0.42
1:B:248:MET:HE3	1:B:248:MET:HB3	2.01	0.42
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.55	0.42
1:G:107:ILE:HD12	1:G:171:ALA:HB1	2.01	0.42
1:G:196:ILE:HG12	1:G:199:MET:HB2	2.02	0.42
1:C:176:GLN:HA	1:C:176:GLN:HE21	1.84	0.42
1:F:69:LEU:HD13	1:F:351:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:LEU:O	1:L:135:GLY:HA2	2.19	0.42
1:E:176:GLN:CD	1:F:176:GLN:HG2	2.45	0.41
1:H:38:ARG:NH1	2:H:401:A1I1O:O13	2.51	0.41
1:D:241:GLU:HB2	1:D:244:PHE:CD2	2.56	0.41
1:I:47:ARG:CB	1:I:47:ARG:HH11	2.33	0.41
1:J:196:ILE:HG12	1:J:199:MET:HB2	2.02	0.41
1:A:91:ARG:HD2	1:E:242:PRO:HB3	2.02	0.41
1:B:43:ASP:HB2	1:B:44:GLY:H	1.79	0.41
1:F:51:LEU:HA	1:F:54:ARG:NH1	2.35	0.41
1:L:216:MET:HE3	1:L:216:MET:HB2	1.89	0.41
1:C:295:ASP:CG	1:D:85:ARG:HH22	2.28	0.41
1:L:8:LEU:HD11	1:L:172:LEU:HD11	2.02	0.41
1:A:28:ASP:HA	1:A:53:ASN:ND2	2.36	0.41
1:A:60:ASP:O	1:A:66:GLY:HA3	2.20	0.41
1:C:135:GLY:HA2	1:D:302:LEU:O	2.20	0.41
1:D:126:HIS:O	1:D:127:ASP:C	2.63	0.41
1:I:252:LEU:HD21	1:I:279:PHE:CE1	2.55	0.41
1:B:80:LEU:CD2	1:B:108:TYR:CE2	3.03	0.41
1:F:181:GLY:O	1:F:182:GLN:HB3	2.20	0.41
1:K:181:GLY:O	1:K:182:GLN:HB3	2.21	0.41
1:H:268:TRP:N	1:H:269:PRO:CD	2.83	0.41
1:K:196:ILE:HG13	1:L:153:LEU:HD21	2.03	0.41
1:A:196:ILE:HG12	1:A:199:MET:HB2	2.02	0.41
2:A:401:A1I1O:O4	2:A:401:A1I1O:C21	2.69	0.41
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.56	0.41
1:C:60:ASP:O	1:C:66:GLY:HA3	2.20	0.41
1:F:346:ALA:HB3	3:F:537:HOH:O	2.21	0.41
1:K:80:LEU:CD2	1:K:108:TYR:CE2	3.04	0.41
1:A:135:GLY:HA2	1:B:302:LEU:O	2.21	0.41
1:G:80:LEU:HD23	1:G:108:TYR:CD1	2.55	0.41
1:G:99:CYS:C	1:G:101:LYS:H	2.29	0.41
1:J:316:ARG:O	1:J:317:ASN:C	2.63	0.41
1:B:45:ILE:HD12	1:B:45:ILE:H	1.85	0.41
1:H:1:MET:HE2	1:H:343:ARG:CZ	2.51	0.41
1:D:293:ASN:O	1:L:294:SER:HB2	2.21	0.40
1:E:123:GLN:HE21	1:F:293:ASN:HA	1.86	0.40
1:K:174:GLU:C	1:K:174:GLU:OE1	2.64	0.40
1:K:196:ILE:HG12	1:K:199:MET:HB2	2.03	0.40
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.57	0.40
1:G:153:LEU:HD21	1:H:196:ILE:HG13	2.03	0.40
1:I:117:THR:O	1:J:316:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:PRO:HA	1:E:58:THR:HG23	2.02	0.40
1:F:349:ILE:HD11	1:F:354:VAL:HG22	2.04	0.40
1:L:207:MET:HA	1:L:207:MET:CE	2.50	0.40
1:A:39:PRO:CA	1:A:58:THR:HG23	2.52	0.40
1:F:42:VAL:HG21	1:F:58:THR:CG2	2.52	0.40
1:I:198:MET:HB2	1:J:50:MET:HE1	2.03	0.40
1:I:326:TRP:HD1	3:I:617:HOH:O	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/364 (99%)	341 (95%)	14 (4%)	4 (1%)	11	7
1	B	358/364 (98%)	340 (95%)	16 (4%)	2 (1%)	21	17
1	C	359/364 (99%)	342 (95%)	14 (4%)	3 (1%)	16	11
1	D	358/364 (98%)	342 (96%)	14 (4%)	2 (1%)	21	17
1	E	359/364 (99%)	342 (95%)	16 (4%)	1 (0%)	36	35
1	F	358/364 (98%)	334 (93%)	19 (5%)	5 (1%)	9	4
1	G	359/364 (99%)	328 (91%)	24 (7%)	7 (2%)	6	3
1	H	358/364 (98%)	341 (95%)	14 (4%)	3 (1%)	16	11
1	I	359/364 (99%)	344 (96%)	15 (4%)	0	100	100
1	J	358/364 (98%)	341 (95%)	15 (4%)	2 (1%)	21	17
1	K	359/364 (99%)	342 (95%)	15 (4%)	2 (1%)	21	17
1	L	359/364 (99%)	344 (96%)	14 (4%)	1 (0%)	36	35
All	All	4303/4368 (98%)	4081 (95%)	190 (4%)	32 (1%)	18	14

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	103	ASN
1	B	42	VAL
1	C	103	ASN
1	F	41	SER
1	F	103	ASN
1	G	59	ALA
1	G	97	GLU
1	G	103	ASN
1	G	347	ALA
1	H	59	ALA
1	K	103	ASN
1	D	103	ASN
1	F	59	ALA
1	G	292	ALA
1	H	43	ASP
1	J	324	GLY
1	B	103	ASN
1	C	151	LEU
1	F	42	VAL
1	F	292	ALA
1	G	182	GLN
1	H	103	ASN
1	A	43	ASP
1	A	59	ALA
1	E	151	LEU
1	J	103	ASN
1	L	151	LEU
1	C	65	GLN
1	D	323	ASN
1	G	42	VAL
1	K	42	VAL

5.3.2 Protein sidechains ⓘ

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%)	76	82
1	B	276/277 (100%)	267 (97%)	9 (3%)	33	34
1	C	277/277 (100%)	272 (98%)	5 (2%)	51	58
1	D	276/277 (100%)	271 (98%)	5 (2%)	51	58
1	E	277/277 (100%)	272 (98%)	5 (2%)	51	58
1	F	276/277 (100%)	270 (98%)	6 (2%)	45	50
1	G	277/277 (100%)	267 (96%)	10 (4%)	31	31
1	H	276/277 (100%)	268 (97%)	8 (3%)	37	40
1	I	277/277 (100%)	273 (99%)	4 (1%)	59	66
1	J	276/277 (100%)	274 (99%)	2 (1%)	76	82
1	K	277/277 (100%)	269 (97%)	8 (3%)	37	40
1	L	277/277 (100%)	272 (98%)	5 (2%)	51	58
All	All	3319/3324 (100%)	3250 (98%)	69 (2%)	47	52

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

Mol	Chain	Res	Type
1	A	258	GLU
1	A	294	SER
1	B	6	SER
1	B	42	VAL
1	B	43	ASP
1	B	76	LYS
1	B	85	ARG
1	B	207	MET
1	B	212	ARG
1	B	248	MET
1	B	265	ARG
1	C	6	SER
1	C	40	SER
1	C	58	THR
1	C	176	GLN
1	C	177	SER
1	D	6	SER
1	D	41	SER
1	D	85	ARG
1	D	212	ARG
1	D	248	MET
1	E	6	SER

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Mol	Chain	Res	Type
1	E	176	GLN
1	E	248	MET
1	E	258	GLU
1	E	350	ASP
1	F	45	ILE
1	F	85	ARG
1	F	176	GLN
1	F	323	ASN
1	F	349	ILE
1	F	350	ASP
1	G	6	SER
1	G	40	SER
1	G	41	SER
1	G	43	ASP
1	G	62	LYS
1	G	258	GLU
1	G	293	ASN
1	G	321	GLU
1	G	323	ASN
1	G	348	THR
1	H	6	SER
1	H	9	ARG
1	H	148	VAL
1	H	176	GLN
1	H	177	SER
1	H	209	THR
1	H	248	MET
1	H	359	ASP
1	I	6	SER
1	I	47	ARG
1	I	121	SER
1	I	248	MET
1	J	42	VAL
1	J	357	ASP
1	K	38	ARG
1	K	40	SER
1	K	41	SER
1	K	176	GLN
1	K	177	SER
1	K	323	ASN
1	K	349	ILE
1	K	359	ASP

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Mol	Chain	Res	Type
1	L	40	SER
1	L	207	MET
1	L	255	ASP
1	L	294	SER
1	L	323	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	176	GLN
1	A	263	ASN
1	A	327	GLN
1	B	286	HIS
1	B	293	ASN
1	B	323	ASN
1	C	116	GLN
1	C	138	HIS
1	C	176	GLN
1	C	263	ASN
1	C	282	HIS
1	C	327	GLN
1	D	308	HIS
1	D	323	ASN
1	E	138	HIS
1	E	176	GLN
1	E	263	ASN
1	E	293	ASN
1	F	176	GLN
1	F	197	GLN
1	F	286	HIS
1	F	293	ASN
1	G	138	HIS
1	G	176	GLN
1	G	282	HIS
1	G	286	HIS
1	G	293	ASN
1	G	323	ASN
1	G	327	GLN
1	H	176	GLN
1	H	286	HIS
1	H	323	ASN

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Mol	Chain	Res	Type
1	I	138	HIS
1	I	176	GLN
1	I	323	ASN
1	I	327	GLN
1	J	134	ASN
1	J	282	HIS
1	J	286	HIS
1	K	138	HIS
1	K	176	GLN
1	K	323	ASN
1	K	327	GLN
1	L	122	GLN
1	L	176	GLN
1	L	293	ASN

5.3.3 RNA [i](#)

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	A1I1O	I	401	-	66,68,68	3.40	5 (7%)	94,101,101	2.36	17 (18%)
2	A1I1O	D	401	-	66,68,68	3.49	2 (3%)	94,101,101	1.91	12 (12%)
2	A1I1O	G	401	-	66,68,68	2.08	3 (4%)	94,101,101	2.06	18 (19%)
2	A1I1O	A	401	-	66,68,68	2.21	4 (6%)	94,101,101	2.28	19 (20%)
2	A1I1O	H	401	-	66,68,68	0.87	3 (4%)	94,101,101	1.23	9 (9%)
2	A1I1O	F	401	-	66,68,68	1.94	2 (3%)	94,101,101	1.84	15 (15%)
2	A1I1O	B	401	-	66,68,68	1.31	2 (3%)	94,101,101	1.68	16 (17%)
2	A1I1O	E	401	-	66,68,68	1.07	6 (9%)	94,101,101	1.37	13 (13%)
2	A1I1O	J	401	-	66,68,68	1.90	3 (4%)	94,101,101	1.53	12 (12%)
2	A1I1O	L	401	-	66,68,68	2.57	6 (9%)	94,101,101	2.25	16 (17%)
2	A1I1O	K	401	-	66,68,68	1.29	3 (4%)	94,101,101	1.88	19 (20%)
2	A1I1O	C	401	-	66,68,68	1.54	3 (4%)	94,101,101	1.34	10 (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	A1I1O	I	401	-	-	18/61/77/77	0/5/5/5
2	A1I1O	D	401	-	-	20/61/77/77	0/5/5/5
2	A1I1O	G	401	-	-	20/61/77/77	0/5/5/5
2	A1I1O	A	401	-	-	21/61/77/77	0/5/5/5
2	A1I1O	H	401	-	-	21/61/77/77	0/5/5/5
2	A1I1O	F	401	-	-	19/61/77/77	0/5/5/5
2	A1I1O	B	401	-	-	24/61/77/77	0/5/5/5
2	A1I1O	E	401	-	-	20/61/77/77	0/5/5/5
2	A1I1O	J	401	-	-	24/61/77/77	0/5/5/5
2	A1I1O	L	401	-	-	18/61/77/77	0/5/5/5
2	A1I1O	K	401	-	-	21/61/77/77	0/5/5/5
2	A1I1O	C	401	-	-	24/61/77/77	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	A1I1O	C9-C11	-27.75	1.30	1.53
2	I	401	A1I1O	C9-C11	-26.68	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	A1I1O	C9-C11	-19.76	1.37	1.53
2	A	401	A1I1O	C9-C11	-16.96	1.39	1.53
2	G	401	A1I1O	C9-C11	-15.84	1.40	1.53
2	J	401	A1I1O	C9-C11	-14.39	1.41	1.53
2	F	401	A1I1O	C9-C11	-14.34	1.41	1.53
2	C	401	A1I1O	C9-C11	-10.89	1.44	1.53
2	B	401	A1I1O	C9-C11	-9.02	1.46	1.53
2	K	401	A1I1O	C9-C11	-8.32	1.46	1.53
2	E	401	A1I1O	P1-O9	4.91	1.64	1.59
2	I	401	A1I1O	C10-C9	3.14	1.62	1.52
2	E	401	A1I1O	P2-O9	3.13	1.62	1.59
2	I	401	A1I1O	C11-S1	3.04	1.85	1.75
2	H	401	A1I1O	O2-C11	3.04	1.25	1.20
2	H	401	A1I1O	P1-O9	3.00	1.62	1.59
2	J	401	A1I1O	P1-O9	2.57	1.62	1.59
2	K	401	A1I1O	O2-C11	2.55	1.24	1.20
2	C	401	A1I1O	O4-C17	2.55	1.28	1.23
2	H	401	A1I1O	C11-S1	2.53	1.83	1.75
2	E	401	A1I1O	C9-C11	-2.49	1.51	1.53
2	K	401	A1I1O	P2-O9	-2.47	1.56	1.59
2	I	401	A1I1O	P1-O9	2.44	1.62	1.59
2	E	401	A1I1O	C11-S1	2.44	1.83	1.75
2	D	401	A1I1O	C10-C9	2.38	1.60	1.52
2	F	401	A1I1O	P3-O15	2.34	1.63	1.59
2	C	401	A1I1O	P1-O9	2.32	1.62	1.59
2	E	401	A1I1O	O2-C11	2.28	1.24	1.20
2	L	401	A1I1O	C22-C19	2.26	1.56	1.52
2	E	401	A1I1O	C3-C2	2.25	1.43	1.38
2	A	401	A1I1O	C11-S1	2.23	1.82	1.75
2	A	401	A1I1O	C10-C9	2.20	1.59	1.52
2	L	401	A1I1O	C11-S1	2.20	1.82	1.75
2	I	401	A1I1O	C3-C2	2.12	1.42	1.38
2	L	401	A1I1O	P1-O9	2.11	1.61	1.59
2	L	401	A1I1O	C3-C2	2.10	1.42	1.38
2	G	401	A1I1O	C3-C2	2.10	1.42	1.38
2	L	401	A1I1O	C10-C9	2.04	1.59	1.52
2	J	401	A1I1O	C3-C2	2.03	1.42	1.38
2	A	401	A1I1O	C3-C2	2.03	1.42	1.38
2	B	401	A1I1O	O2-C11	2.03	1.23	1.20
2	G	401	A1I1O	C10-C9	2.01	1.59	1.52

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	A1I1O	O2-C11-C9	-15.41	99.88	124.11
2	L	401	A1I1O	O2-C11-C9	-14.42	101.43	124.11
2	A	401	A1I1O	O2-C11-C9	-13.40	103.04	124.11
2	D	401	A1I1O	O2-C11-C9	-10.15	108.15	124.11
2	G	401	A1I1O	O2-C11-C9	-9.60	109.01	124.11
2	F	401	A1I1O	O2-C11-C9	-9.43	109.28	124.11
2	I	401	A1I1O	C20-C19-C18	-7.88	95.33	108.77
2	K	401	A1I1O	C20-C19-C18	-7.78	95.51	108.77
2	A	401	A1I1O	C10-C9-C8	7.67	132.14	112.92
2	G	401	A1I1O	O2-C11-S1	-7.56	113.63	123.80
2	B	401	A1I1O	O2-C11-C9	-7.11	112.93	124.11
2	L	401	A1I1O	C21-C19-C18	-7.09	96.68	108.77
2	E	401	A1I1O	O2-C11-C9	-6.93	113.20	124.11
2	D	401	A1I1O	C21-C19-C18	-6.73	97.30	108.77
2	B	401	A1I1O	C21-C19-C22	6.66	119.22	108.22
2	L	401	A1I1O	C10-C9-C8	6.38	128.91	112.92
2	C	401	A1I1O	O2-C11-C9	-6.34	114.14	124.11
2	J	401	A1I1O	C20-C19-C18	6.05	119.09	108.77
2	A	401	A1I1O	O2-C11-S1	-6.00	115.73	123.80
2	D	401	A1I1O	O2-C11-S1	-5.87	115.91	123.80
2	J	401	A1I1O	O2-C11-C9	-5.86	114.89	124.11
2	G	401	A1I1O	O8-P1-O7	5.77	139.28	112.44
2	D	401	A1I1O	C20-C19-C18	5.56	118.24	108.77
2	K	401	A1I1O	O2-C11-S1	-5.52	116.37	123.80
2	G	401	A1I1O	C21-C19-C18	5.46	118.08	108.77
2	F	401	A1I1O	C21-C19-C18	-5.33	99.67	108.77
2	L	401	A1I1O	O2-C11-S1	-5.26	116.73	123.80
2	K	401	A1I1O	C21-C19-C18	5.19	117.62	108.77
2	I	401	A1I1O	C10-C9-C8	5.15	125.82	112.92
2	A	401	A1I1O	C20-C19-C18	-5.14	100.01	108.77
2	K	401	A1I1O	C10-C9-C11	-5.05	96.54	111.72
2	G	401	A1I1O	C20-C19-C18	-5.02	100.22	108.77
2	F	401	A1I1O	O9-P1-O7	-4.96	95.80	110.70
2	I	401	A1I1O	O2-C11-S1	-4.91	117.20	123.80
2	K	401	A1I1O	O2-C11-C9	-4.90	116.41	124.11
2	A	401	A1I1O	C20-C19-C22	4.82	116.18	108.22
2	D	401	A1I1O	C10-C9-C11	-4.81	97.27	111.72
2	F	401	A1I1O	C10-C9-C11	-4.81	97.28	111.72
2	D	401	A1I1O	C10-C9-C8	4.80	124.96	112.92
2	H	401	A1I1O	O2-C11-C9	-4.76	116.63	124.11
2	C	401	A1I1O	C10-C9-C11	-4.65	97.74	111.72
2	A	401	A1I1O	O10-P2-O9	4.65	119.85	107.27
2	L	401	A1I1O	C10-C9-C11	-4.54	98.09	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	A1I1O	C10-C9-C11	-4.51	98.18	111.72
2	F	401	A1I1O	O8-P1-O7	4.50	133.39	112.44
2	G	401	A1I1O	C10-C9-C11	-4.45	98.34	111.72
2	A	401	A1I1O	C10-C9-C11	-4.44	98.39	111.72
2	H	401	A1I1O	C20-C19-C18	4.19	115.92	108.77
2	F	401	A1I1O	C10-C9-C8	4.17	123.38	112.92
2	L	401	A1I1O	O8-P1-O7	4.15	131.75	112.44
2	I	401	A1I1O	C21-C19-C18	4.11	115.77	108.77
2	K	401	A1I1O	O10-P2-O9	4.08	118.31	107.27
2	G	401	A1I1O	O10-P2-O9	4.05	118.23	107.27
2	A	401	A1I1O	O8-P1-O7	3.98	130.95	112.44
2	G	401	A1I1O	O9-P1-O7	-3.93	98.89	110.70
2	I	401	A1I1O	C10-C9-C11	-3.90	100.00	111.72
2	I	401	A1I1O	C8-C9-C11	-3.90	101.18	109.92
2	J	401	A1I1O	O8-P1-O7	3.89	130.53	112.44
2	B	401	A1I1O	C18-C17-N2	-3.87	109.14	116.48
2	B	401	A1I1O	O2-C11-S1	-3.86	118.61	123.80
2	B	401	A1I1O	C21-C19-C18	-3.86	102.19	108.77
2	I	401	A1I1O	O9-P1-O7	-3.82	99.22	110.70
2	K	401	A1I1O	C18-C17-N2	-3.77	109.33	116.48
2	J	401	A1I1O	C10-C9-C8	3.75	122.31	112.92
2	C	401	A1I1O	C18-C17-N2	-3.70	109.47	116.48
2	C	401	A1I1O	C20-C19-C22	3.69	114.31	108.22
2	I	401	A1I1O	O8-P1-O7	3.68	129.54	112.44
2	B	401	A1I1O	C10-C9-C8	3.63	122.03	112.92
2	C	401	A1I1O	O8-P1-O7	3.63	129.34	112.44
2	I	401	A1I1O	O10-P2-O9	3.63	117.07	107.27
2	B	401	A1I1O	C10-C9-C11	-3.59	100.93	111.72
2	A	401	A1I1O	C8-C9-C11	-3.57	101.93	109.92
2	C	401	A1I1O	C21-C19-C18	3.56	114.83	108.77
2	L	401	A1I1O	C20-C19-C18	3.54	114.81	108.77
2	F	401	A1I1O	C21-C19-C22	-3.50	102.45	108.22
2	K	401	A1I1O	C10-C9-C8	3.50	121.68	112.92
2	J	401	A1I1O	O2-C11-S1	-3.48	119.11	123.80
2	I	401	A1I1O	C18-C17-N2	-3.48	109.89	116.48
2	G	401	A1I1O	O5-C18-C19	3.46	118.20	110.18
2	K	401	A1I1O	C20-C19-C22	-3.45	102.53	108.22
2	E	401	A1I1O	O14-C31-C32	3.43	120.78	111.19
2	J	401	A1I1O	O6-C22-C19	-3.42	105.05	110.55
2	F	401	A1I1O	O14-C31-C32	3.38	120.64	111.19
2	D	401	A1I1O	C18-C17-N2	-3.37	110.08	116.48
2	H	401	A1I1O	C21-C19-C22	3.37	113.79	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	A1I1O	O2-C11-S1	-3.36	119.28	123.80
2	G	401	A1I1O	C21-C19-C20	-3.34	102.54	109.20
2	K	401	A1I1O	O17-P3-O15	-3.30	93.00	105.85
2	H	401	A1I1O	C21-C19-C18	-3.28	103.17	108.77
2	G	401	A1I1O	C18-C17-N2	-3.25	110.31	116.48
2	L	401	A1I1O	C18-C17-N2	-3.23	110.35	116.48
2	I	401	A1I1O	C21-C19-C22	3.21	113.52	108.22
2	A	401	A1I1O	O6-P1-O7	-3.20	96.24	108.94
2	B	401	A1I1O	O18-P3-O16	-3.11	98.74	110.83
2	K	401	A1I1O	O8-P1-O7	3.11	126.89	112.44
2	A	401	A1I1O	C18-C17-N2	-3.10	110.60	116.48
2	E	401	A1I1O	O14-C31-C25	-3.09	99.45	110.10
2	H	401	A1I1O	O5-C18-C19	3.07	117.29	110.18
2	F	401	A1I1O	C20-C19-C22	3.06	113.28	108.22
2	K	401	A1I1O	O17-P3-O16	3.05	122.72	110.83
2	J	401	A1I1O	O18-P3-O17	3.00	119.06	107.80
2	B	401	A1I1O	O18-P3-O17	2.99	119.01	107.80
2	G	401	A1I1O	C10-C9-C8	2.96	120.33	112.92
2	F	401	A1I1O	C18-C17-N2	-2.95	110.88	116.48
2	E	401	A1I1O	C20-C19-C18	2.94	113.78	108.77
2	F	401	A1I1O	C16-C15-C14	2.91	117.24	112.39
2	G	401	A1I1O	C21-C19-C22	2.89	113.00	108.22
2	G	401	A1I1O	O9-P2-O11	-2.88	102.03	110.70
2	K	401	A1I1O	O18-P3-O17	2.87	118.57	107.80
2	J	401	A1I1O	O8-P1-O6	-2.80	94.85	107.57
2	K	401	A1I1O	C21-C19-C22	2.79	112.84	108.22
2	A	401	A1I1O	O18-P3-O16	2.77	121.63	110.83
2	A	401	A1I1O	C16-C15-C14	2.74	116.96	112.39
2	A	401	A1I1O	C21-C19-C18	2.73	113.42	108.77
2	L	401	A1I1O	O8-P1-O6	-2.70	95.32	107.57
2	H	401	A1I1O	O8-P1-O7	2.70	125.01	112.44
2	A	401	A1I1O	O14-C31-C32	2.69	118.72	111.19
2	K	401	A1I1O	O6-P1-O7	-2.68	98.30	108.94
2	I	401	A1I1O	O5-C18-C19	2.68	116.39	110.18
2	B	401	A1I1O	O8-P1-O6	-2.67	95.48	107.57
2	L	401	A1I1O	O5-C18-C19	2.64	116.29	110.18
2	J	401	A1I1O	C18-C17-N2	-2.63	111.50	116.48
2	J	401	A1I1O	C21-C19-C18	-2.62	104.30	108.77
2	E	401	A1I1O	O5-C18-C19	2.60	116.20	110.18
2	I	401	A1I1O	O18-P3-O15	-2.60	95.72	105.85
2	B	401	A1I1O	O8-P1-O7	2.59	124.52	112.44
2	D	401	A1I1O	O5-C18-C19	2.57	116.14	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	A1I1O	O8-P1-O6	-2.57	95.91	107.57
2	K	401	A1I1O	O18-P3-O16	-2.56	100.85	110.83
2	I	401	A1I1O	O18-P3-O17	2.54	117.32	107.80
2	E	401	A1I1O	C18-C17-N2	-2.53	111.69	116.48
2	F	401	A1I1O	O14-C31-C25	-2.52	101.41	110.10
2	L	401	A1I1O	O10-P2-O9	2.48	113.99	107.27
2	L	401	A1I1O	O18-P3-O17	2.48	117.11	107.80
2	D	401	A1I1O	O8-P1-O7	2.48	123.99	112.44
2	C	401	A1I1O	O8-P1-O6	-2.47	96.35	107.57
2	C	401	A1I1O	C10-C9-C8	2.46	119.09	112.92
2	L	401	A1I1O	O8-P1-O9	2.46	113.92	107.27
2	D	401	A1I1O	O15-P3-O16	-2.45	100.62	109.33
2	C	401	A1I1O	O10-P2-O9	2.43	113.85	107.27
2	G	401	A1I1O	O14-C31-C32	2.40	117.89	111.19
2	A	401	A1I1O	O9-P1-O7	-2.38	103.55	110.70
2	B	401	A1I1O	O8-P1-O9	-2.37	100.88	107.27
2	E	401	A1I1O	C12-S1-C11	-2.33	95.03	101.73
2	J	401	A1I1O	C21-C19-C20	-2.33	104.56	109.20
2	H	401	A1I1O	O9-P1-O7	-2.32	103.73	110.70
2	E	401	A1I1O	C21-C19-C22	2.30	112.03	108.22
2	B	401	A1I1O	C20-C19-C18	2.29	112.68	108.77
2	E	401	A1I1O	O8-P1-O7	2.29	123.10	112.44
2	E	401	A1I1O	O17-P3-O16	-2.28	101.95	110.83
2	E	401	A1I1O	C10-C9-C8	2.27	118.62	112.92
2	K	401	A1I1O	C7-C8-C9	-2.27	115.05	120.76
2	D	401	A1I1O	O8-P1-O9	2.27	113.40	107.27
2	G	401	A1I1O	O14-C31-C25	-2.25	102.35	110.10
2	A	401	A1I1O	O17-P3-O15	2.24	114.58	105.85
2	L	401	A1I1O	O9-P2-O11	2.23	117.42	110.70
2	E	401	A1I1O	C10-C9-C11	-2.22	105.06	111.72
2	K	401	A1I1O	C16-C15-C14	2.20	116.06	112.39
2	A	401	A1I1O	O15-P3-O16	-2.20	101.49	109.33
2	L	401	A1I1O	C20-C19-C22	2.18	111.82	108.22
2	F	401	A1I1O	C20-C19-C18	2.18	112.48	108.77
2	G	401	A1I1O	O15-P3-O16	-2.17	101.60	109.33
2	B	401	A1I1O	O18-P3-O15	2.17	114.30	105.85
2	E	401	A1I1O	C21-C19-C18	-2.16	105.09	108.77
2	H	401	A1I1O	C20-C19-C22	-2.15	104.68	108.22
2	C	401	A1I1O	O5-C18-C19	2.14	115.15	110.18
2	F	401	A1I1O	C12-S1-C11	-2.13	95.62	101.73
2	K	401	A1I1O	O4-C17-C18	2.13	126.83	120.89
2	B	401	A1I1O	O14-C31-C32	2.11	117.09	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	A1I1O	C13-N1-C14	-2.09	118.94	122.82
2	H	401	A1I1O	O18-P3-O17	2.08	115.59	107.80
2	I	401	A1I1O	O8-P1-O9	2.06	112.85	107.27
2	D	401	A1I1O	O18-P3-O16	2.06	118.86	110.83
2	A	401	A1I1O	C21-C19-C22	-2.04	104.85	108.22
2	L	401	A1I1O	P3-O15-C32	2.02	128.83	123.43
2	B	401	A1I1O	O17-P3-O16	2.01	118.68	110.83

There are no chirality outliers.

All (250) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1I1O	C14-C15-C16-N2
2	A	401	A1I1O	N2-C17-C18-O5
2	A	401	A1I1O	C17-C18-C19-C20
2	A	401	A1I1O	C17-C18-C19-C21
2	A	401	A1I1O	C17-C18-C19-C22
2	A	401	A1I1O	O5-C18-C19-C20
2	A	401	A1I1O	O5-C18-C19-C22
2	A	401	A1I1O	C18-C19-C22-O6
2	A	401	A1I1O	C20-C19-C22-O6
2	A	401	A1I1O	C21-C19-C22-O6
2	B	401	A1I1O	S1-C11-C9-C8
2	B	401	A1I1O	C14-C15-C16-N2
2	B	401	A1I1O	N2-C17-C18-O5
2	B	401	A1I1O	N2-C17-C18-C19
2	B	401	A1I1O	O4-C17-C18-O5
2	B	401	A1I1O	C17-C18-C19-C20
2	B	401	A1I1O	C17-C18-C19-C21
2	B	401	A1I1O	C17-C18-C19-C22
2	B	401	A1I1O	O5-C18-C19-C21
2	B	401	A1I1O	O5-C18-C19-C22
2	B	401	A1I1O	C18-C19-C22-O6
2	B	401	A1I1O	C20-C19-C22-O6
2	B	401	A1I1O	C21-C19-C22-O6
2	B	401	A1I1O	C23-O12-P2-O11
2	C	401	A1I1O	S1-C11-C9-C8
2	C	401	A1I1O	C14-C15-C16-N2
2	C	401	A1I1O	N2-C17-C18-O5
2	C	401	A1I1O	C17-C18-C19-C20
2	C	401	A1I1O	C17-C18-C19-C21
2	C	401	A1I1O	C17-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
2	C	401	A1I1O	O5-C18-C19-C20
2	C	401	A1I1O	O5-C18-C19-C22
2	C	401	A1I1O	C18-C19-C22-O6
2	C	401	A1I1O	C20-C19-C22-O6
2	C	401	A1I1O	C21-C19-C22-O6
2	D	401	A1I1O	S1-C11-C9-C8
2	D	401	A1I1O	C14-C15-C16-N2
2	D	401	A1I1O	N2-C17-C18-O5
2	D	401	A1I1O	O4-C17-C18-O5
2	D	401	A1I1O	C17-C18-C19-C20
2	D	401	A1I1O	C17-C18-C19-C21
2	D	401	A1I1O	C17-C18-C19-C22
2	D	401	A1I1O	O5-C18-C19-C20
2	D	401	A1I1O	O5-C18-C19-C21
2	D	401	A1I1O	O5-C18-C19-C22
2	D	401	A1I1O	C23-O12-P2-O11
2	E	401	A1I1O	C14-C15-C16-N2
2	E	401	A1I1O	N2-C17-C18-O5
2	E	401	A1I1O	O4-C17-C18-O5
2	E	401	A1I1O	C17-C18-C19-C20
2	E	401	A1I1O	C17-C18-C19-C21
2	E	401	A1I1O	C17-C18-C19-C22
2	E	401	A1I1O	O5-C18-C19-C20
2	E	401	A1I1O	O5-C18-C19-C21
2	E	401	A1I1O	O5-C18-C19-C22
2	E	401	A1I1O	C18-C19-C22-O6
2	E	401	A1I1O	C20-C19-C22-O6
2	E	401	A1I1O	C21-C19-C22-O6
2	F	401	A1I1O	S1-C11-C9-C8
2	F	401	A1I1O	C14-C15-C16-N2
2	F	401	A1I1O	N2-C17-C18-O5
2	F	401	A1I1O	O4-C17-C18-O5
2	F	401	A1I1O	C17-C18-C19-C20
2	F	401	A1I1O	C17-C18-C19-C21
2	F	401	A1I1O	C17-C18-C19-C22
2	F	401	A1I1O	O5-C18-C19-C20
2	F	401	A1I1O	O5-C18-C19-C21
2	F	401	A1I1O	O5-C18-C19-C22
2	F	401	A1I1O	C22-O6-P1-O7
2	G	401	A1I1O	S1-C11-C9-C8
2	G	401	A1I1O	O2-C11-S1-C12
2	G	401	A1I1O	C14-C15-C16-N2

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Mol	Chain	Res	Type	Atoms
2	G	401	A1I1O	N2-C17-C18-O5
2	G	401	A1I1O	O4-C17-C18-O5
2	G	401	A1I1O	C17-C18-C19-C20
2	G	401	A1I1O	C17-C18-C19-C21
2	G	401	A1I1O	C17-C18-C19-C22
2	G	401	A1I1O	O5-C18-C19-C20
2	G	401	A1I1O	O5-C18-C19-C21
2	G	401	A1I1O	O5-C18-C19-C22
2	G	401	A1I1O	C22-O6-P1-O7
2	H	401	A1I1O	S1-C11-C9-C8
2	H	401	A1I1O	N2-C17-C18-O5
2	H	401	A1I1O	N2-C17-C18-C19
2	H	401	A1I1O	C17-C18-C19-C20
2	H	401	A1I1O	C17-C18-C19-C21
2	H	401	A1I1O	C17-C18-C19-C22
2	H	401	A1I1O	O5-C18-C19-C20
2	H	401	A1I1O	O5-C18-C19-C21
2	H	401	A1I1O	O5-C18-C19-C22
2	H	401	A1I1O	C22-O6-P1-O8
2	H	401	A1I1O	C22-O6-P1-O9
2	I	401	A1I1O	C14-C15-C16-N2
2	I	401	A1I1O	N2-C17-C18-O5
2	I	401	A1I1O	O4-C17-C18-O5
2	I	401	A1I1O	C17-C18-C19-C20
2	I	401	A1I1O	C17-C18-C19-C21
2	I	401	A1I1O	C17-C18-C19-C22
2	I	401	A1I1O	O5-C18-C19-C20
2	I	401	A1I1O	O5-C18-C19-C21
2	I	401	A1I1O	O5-C18-C19-C22
2	J	401	A1I1O	S1-C11-C9-C8
2	J	401	A1I1O	C18-C17-N2-C16
2	J	401	A1I1O	N2-C17-C18-O5
2	J	401	A1I1O	O4-C17-C18-C19
2	J	401	A1I1O	C17-C18-C19-C20
2	J	401	A1I1O	C17-C18-C19-C21
2	J	401	A1I1O	C17-C18-C19-C22
2	J	401	A1I1O	C18-C19-C22-O6
2	J	401	A1I1O	C20-C19-C22-O6
2	J	401	A1I1O	C21-C19-C22-O6
2	K	401	A1I1O	S1-C11-C9-C8
2	K	401	A1I1O	C14-C15-C16-N2
2	K	401	A1I1O	N2-C17-C18-O5

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Mol	Chain	Res	Type	Atoms
2	K	401	A1I1O	C17-C18-C19-C20
2	K	401	A1I1O	C17-C18-C19-C21
2	K	401	A1I1O	C17-C18-C19-C22
2	K	401	A1I1O	O5-C18-C19-C20
2	K	401	A1I1O	O5-C18-C19-C21
2	K	401	A1I1O	O5-C18-C19-C22
2	L	401	A1I1O	C14-C15-C16-N2
2	L	401	A1I1O	N2-C17-C18-O5
2	L	401	A1I1O	O4-C17-C18-O5
2	L	401	A1I1O	C17-C18-C19-C20
2	L	401	A1I1O	C17-C18-C19-C21
2	L	401	A1I1O	C17-C18-C19-C22
2	L	401	A1I1O	O5-C18-C19-C20
2	L	401	A1I1O	O5-C18-C19-C21
2	L	401	A1I1O	O5-C18-C19-C22
2	D	401	A1I1O	C3-C2-O1-C1
2	D	401	A1I1O	C35-C2-O1-C1
2	J	401	A1I1O	C3-C2-O1-C1
2	J	401	A1I1O	C35-C2-O1-C1
2	F	401	A1I1O	C35-C2-O1-C1
2	F	401	A1I1O	C3-C2-O1-C1
2	K	401	A1I1O	C35-C2-O1-C1
2	K	401	A1I1O	C3-C2-O1-C1
2	A	401	A1I1O	O2-C11-C9-C8
2	I	401	A1I1O	O2-C11-C9-C8
2	C	401	A1I1O	C3-C2-O1-C1
2	C	401	A1I1O	C35-C2-O1-C1
2	I	401	A1I1O	C35-C2-O1-C1
2	I	401	A1I1O	C3-C2-O1-C1
2	H	401	A1I1O	C14-C15-C16-N2
2	J	401	A1I1O	C14-C15-C16-N2
2	B	401	A1I1O	O2-C11-S1-C12
2	C	401	A1I1O	O2-C11-S1-C12
2	D	401	A1I1O	O2-C11-S1-C12
2	F	401	A1I1O	O2-C11-S1-C12
2	J	401	A1I1O	O2-C11-S1-C12
2	K	401	A1I1O	O2-C11-S1-C12
2	L	401	A1I1O	O2-C11-S1-C12
2	A	401	A1I1O	O4-C17-C18-O5
2	C	401	A1I1O	O4-C17-C18-O5
2	H	401	A1I1O	O4-C17-C18-O5
2	J	401	A1I1O	O4-C17-C18-O5

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Mol	Chain	Res	Type	Atoms
2	K	401	A1I1O	O4-C17-C18-O5
2	C	401	A1I1O	C32-O15-P3-O16
2	H	401	A1I1O	O2-C11-C9-C8
2	A	401	A1I1O	O5-C18-C19-C21
2	B	401	A1I1O	O5-C18-C19-C20
2	C	401	A1I1O	O5-C18-C19-C21
2	A	401	A1I1O	O4-C17-C18-C19
2	B	401	A1I1O	O4-C17-C18-C19
2	C	401	A1I1O	O4-C17-C18-C19
2	E	401	A1I1O	O4-C17-C18-C19
2	G	401	A1I1O	O4-C17-C18-C19
2	H	401	A1I1O	O4-C17-C18-C19
2	I	401	A1I1O	O4-C17-C18-C19
2	A	401	A1I1O	N2-C17-C18-C19
2	C	401	A1I1O	N2-C17-C18-C19
2	E	401	A1I1O	N2-C17-C18-C19
2	J	401	A1I1O	N2-C17-C18-C19
2	E	401	A1I1O	O2-C11-C9-C8
2	F	401	A1I1O	O2-C11-C9-C8
2	J	401	A1I1O	O2-C11-C9-C8
2	B	401	A1I1O	C35-C2-O1-C1
2	H	401	A1I1O	C18-C17-N2-C16
2	J	401	A1I1O	P1-O9-P2-O10
2	C	401	A1I1O	C9-C11-S1-C12
2	E	401	A1I1O	C9-C11-S1-C12
2	G	401	A1I1O	C9-C11-S1-C12
2	B	401	A1I1O	C3-C2-O1-C1
2	E	401	A1I1O	O2-C11-S1-C12
2	I	401	A1I1O	O2-C11-S1-C12
2	H	401	A1I1O	C20-C19-C22-O6
2	H	401	A1I1O	C21-C19-C22-O6
2	A	401	A1I1O	C32-O15-P3-O16
2	B	401	A1I1O	C32-O15-P3-O16
2	J	401	A1I1O	C32-O15-P3-O16
2	D	401	A1I1O	C23-O12-P2-O9
2	J	401	A1I1O	O5-C18-C19-C22
2	J	401	A1I1O	C23-O12-P2-O11
2	K	401	A1I1O	C23-O12-P2-O11
2	B	401	A1I1O	O2-C11-C9-C8
2	C	401	A1I1O	O2-C11-C9-C8
2	D	401	A1I1O	O2-C11-C9-C8
2	L	401	A1I1O	O2-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
2	A	401	A1I1O	C18-C17-N2-C16
2	F	401	A1I1O	C18-C17-N2-C16
2	A	401	A1I1O	P1-O9-P2-O10
2	B	401	A1I1O	P1-O9-P2-O10
2	C	401	A1I1O	P1-O9-P2-O10
2	E	401	A1I1O	P1-O9-P2-O10
2	G	401	A1I1O	P1-O9-P2-O10
2	H	401	A1I1O	P1-O9-P2-O10
2	I	401	A1I1O	P1-O9-P2-O10
2	K	401	A1I1O	P1-O9-P2-O10
2	D	401	A1I1O	O4-C17-C18-C19
2	F	401	A1I1O	O4-C17-C18-C19
2	K	401	A1I1O	O4-C17-C18-C19
2	L	401	A1I1O	O4-C17-C18-C19
2	L	401	A1I1O	C35-C2-O1-C1
2	H	401	A1I1O	C15-C16-N2-C17
2	D	401	A1I1O	N2-C17-C18-C19
2	F	401	A1I1O	N2-C17-C18-C19
2	G	401	A1I1O	N2-C17-C18-C19
2	I	401	A1I1O	N2-C17-C18-C19
2	K	401	A1I1O	N2-C17-C18-C19
2	L	401	A1I1O	N2-C17-C18-C19
2	L	401	A1I1O	C3-C2-O1-C1
2	A	401	A1I1O	S1-C11-C9-C8
2	E	401	A1I1O	S1-C11-C9-C8
2	I	401	A1I1O	S1-C11-C9-C8
2	L	401	A1I1O	S1-C11-C9-C8
2	K	401	A1I1O	C18-C17-N2-C16
2	F	401	A1I1O	P1-O9-P2-O11
2	C	401	A1I1O	O12-C23-C24-O13
2	A	401	A1I1O	P1-O9-P2-O11
2	C	401	A1I1O	P1-O9-P2-O11
2	D	401	A1I1O	P1-O9-P2-O11
2	J	401	A1I1O	P1-O9-P2-O11
2	L	401	A1I1O	P2-O9-P1-O8
2	B	401	A1I1O	C9-C11-S1-C12
2	J	401	A1I1O	C9-C11-S1-C12
2	K	401	A1I1O	C9-C11-S1-C12
2	G	401	A1I1O	C35-C2-O1-C1
2	A	401	A1I1O	O12-C23-C24-O13
2	D	401	A1I1O	O12-C23-C24-O13
2	I	401	A1I1O	C32-O15-P3-O17

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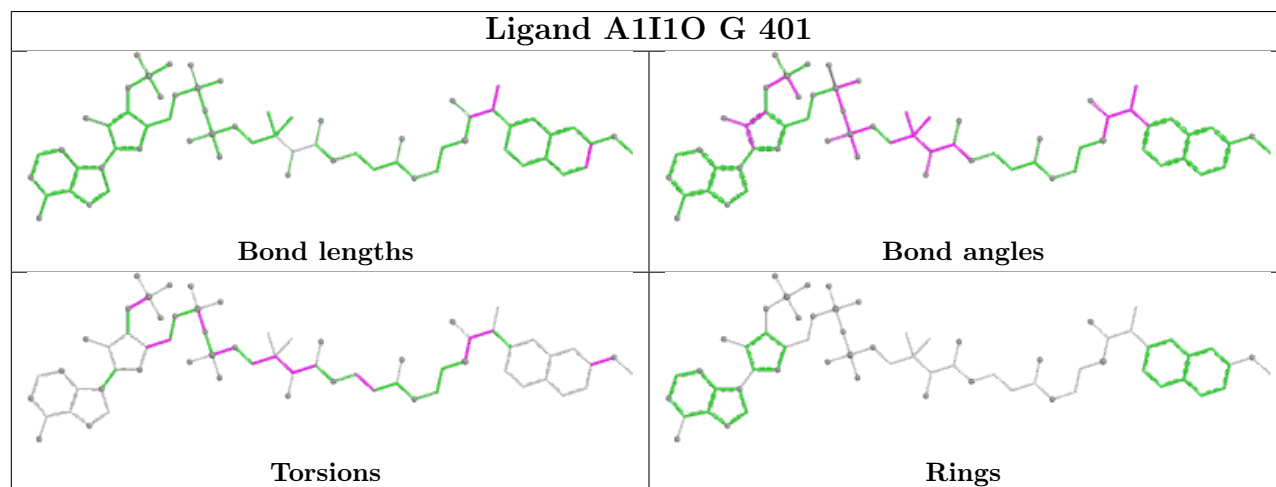
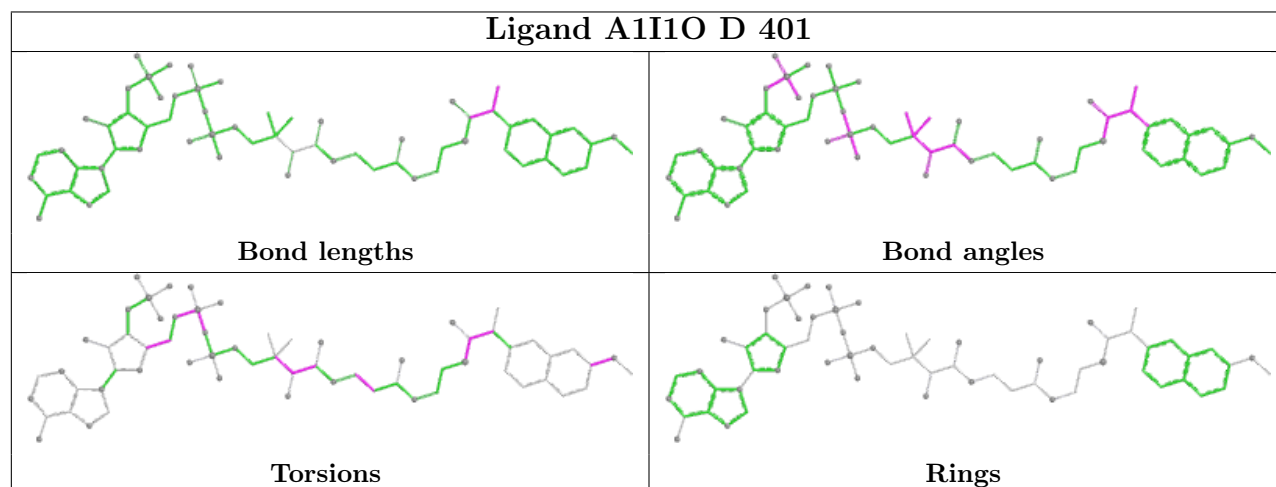
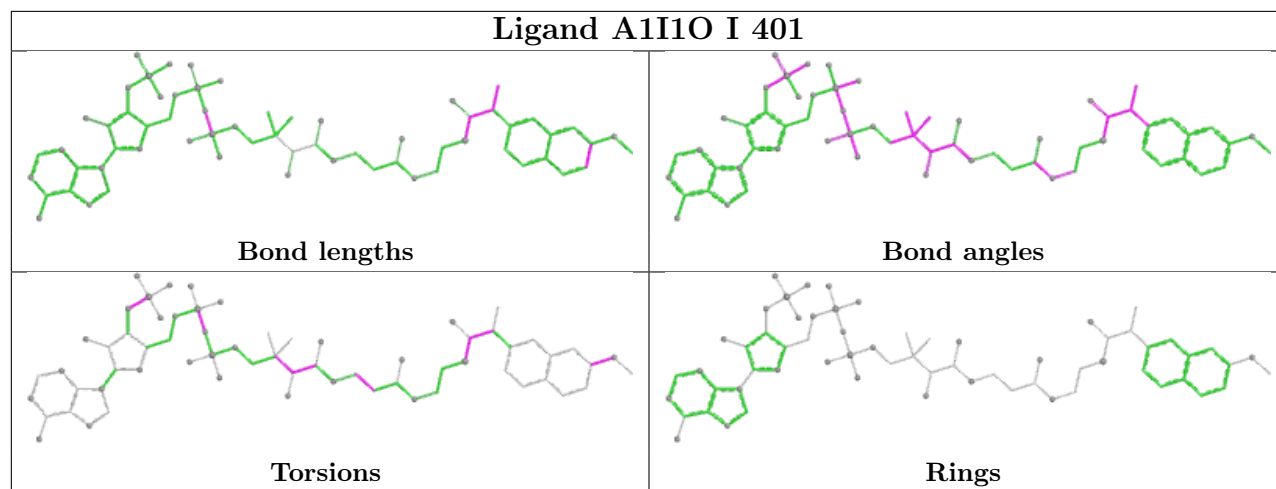
Mol	Chain	Res	Type	Atoms
2	J	401	A1I1O	C32-O15-P3-O17
2	K	401	A1I1O	O2-C11-C9-C8
2	G	401	A1I1O	O12-C23-C24-O13
2	E	401	A1I1O	C13-C12-S1-C11
2	G	401	A1I1O	C32-O15-P3-O16
2	G	401	A1I1O	C18-C19-C22-O6
2	L	401	A1I1O	P1-O9-P2-O10
2	B	401	A1I1O	O12-C23-C24-O13
2	H	401	A1I1O	O12-C23-C24-O13
2	K	401	A1I1O	O12-C23-C24-O13

There are no ring outliers.

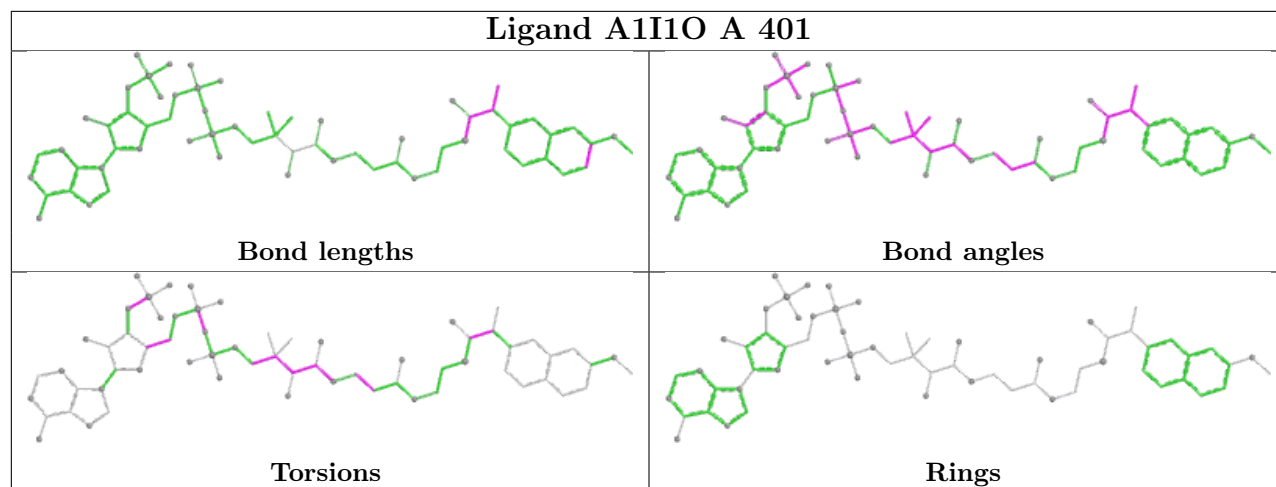
11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	A1I1O	4	0
2	D	401	A1I1O	5	0
2	G	401	A1I1O	2	0
2	A	401	A1I1O	4	0
2	H	401	A1I1O	2	0
2	F	401	A1I1O	5	0
2	B	401	A1I1O	3	0
2	J	401	A1I1O	2	0
2	L	401	A1I1O	2	0
2	K	401	A1I1O	4	0
2	C	401	A1I1O	6	0

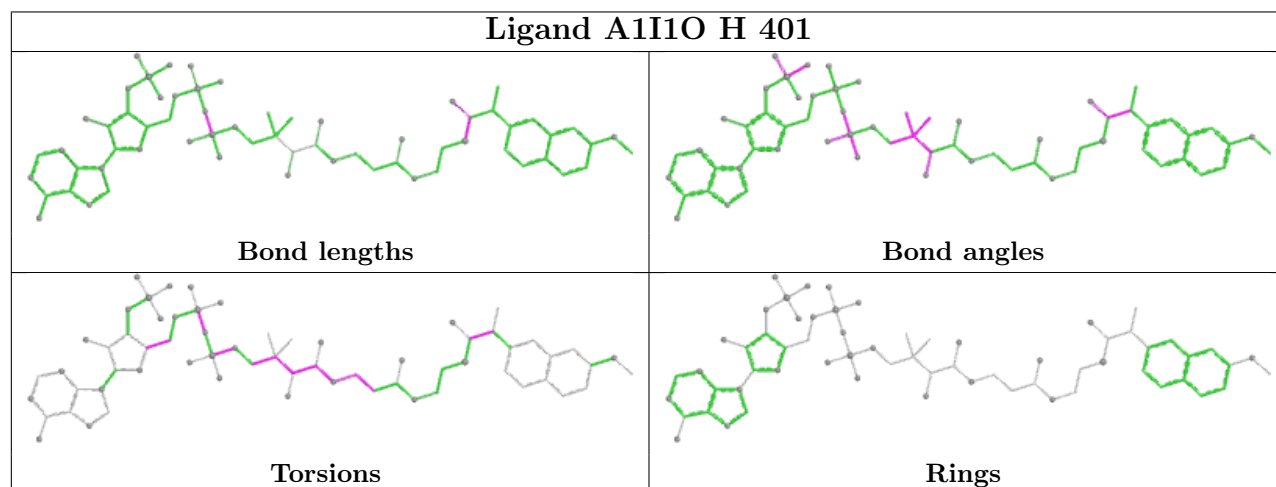
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



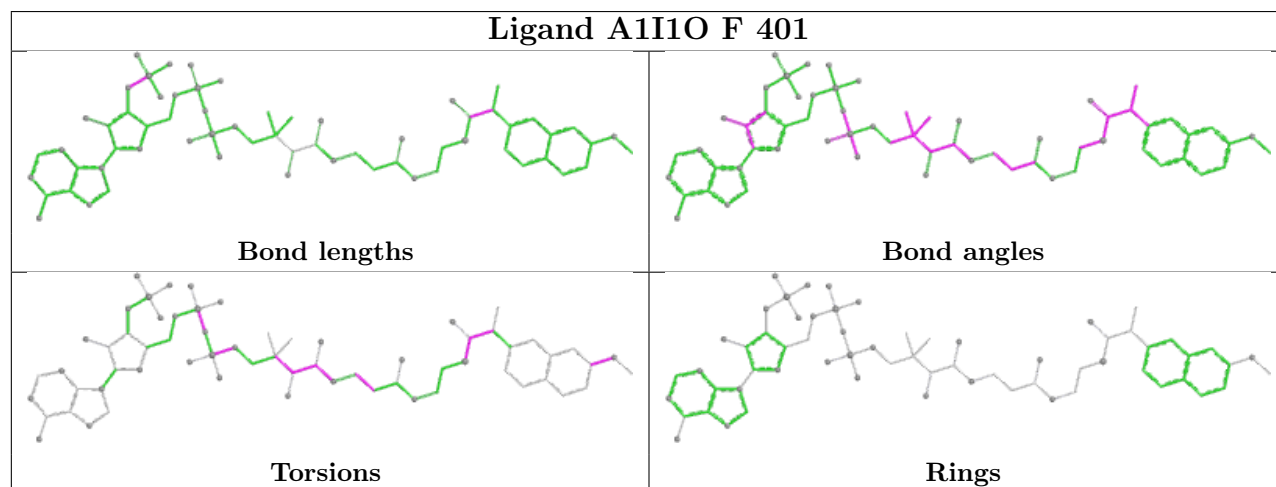
Ligand A1I1O A 401



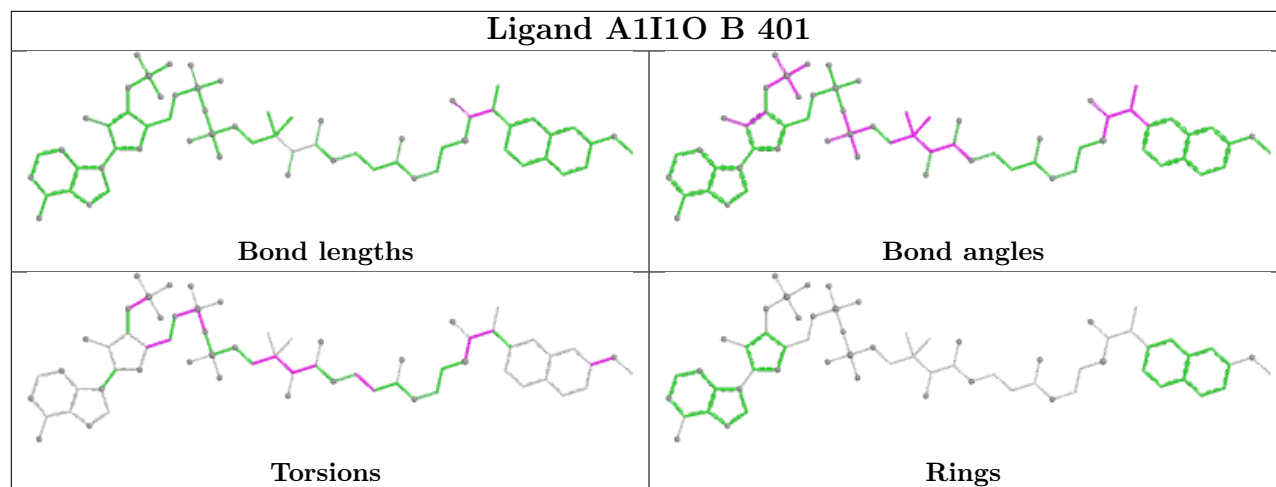
Ligand A1I1O H 401



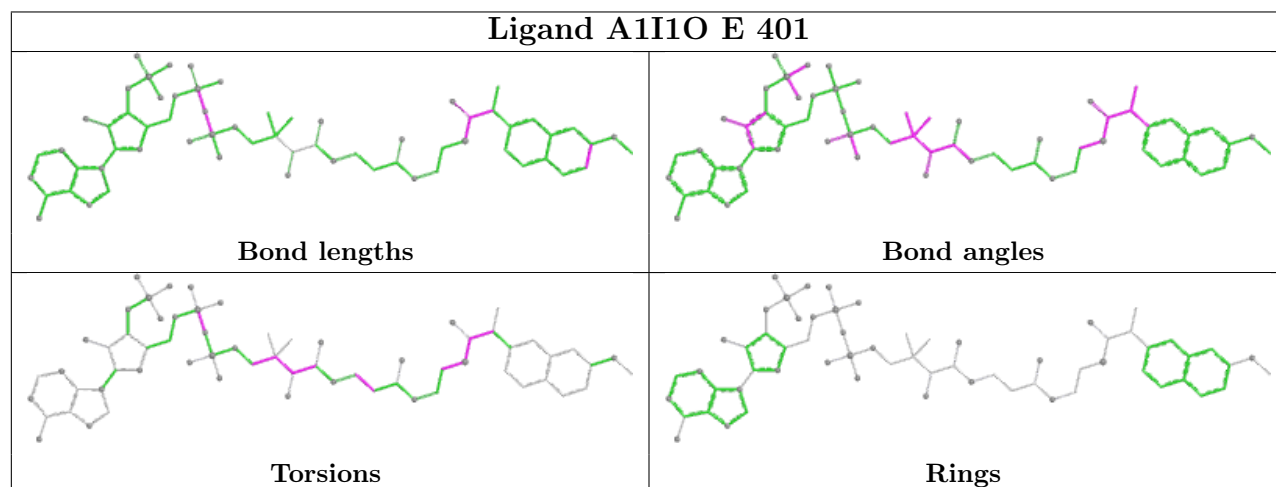
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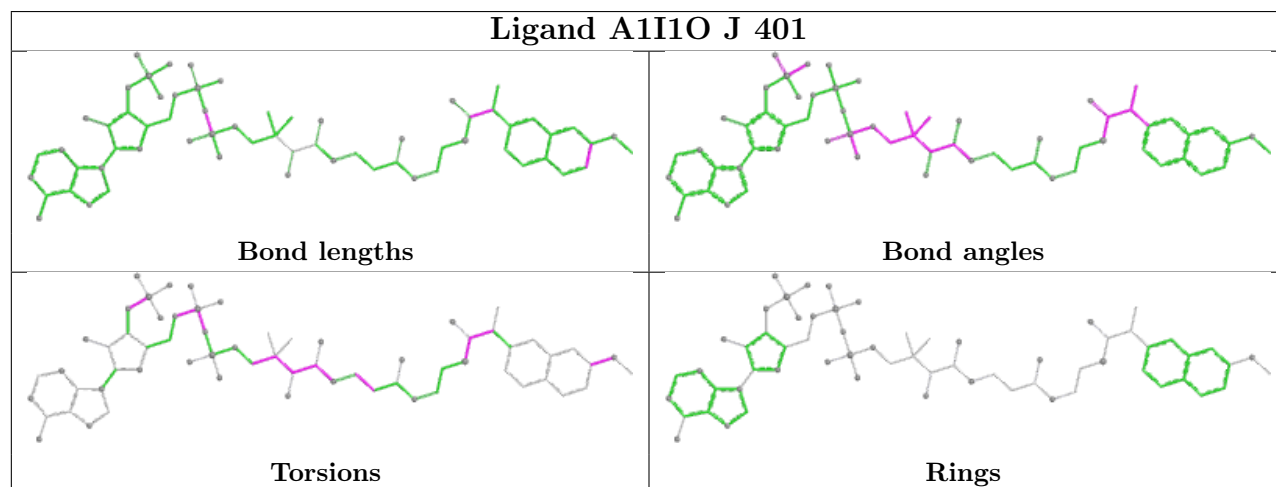
Ligand A1I1O B 401

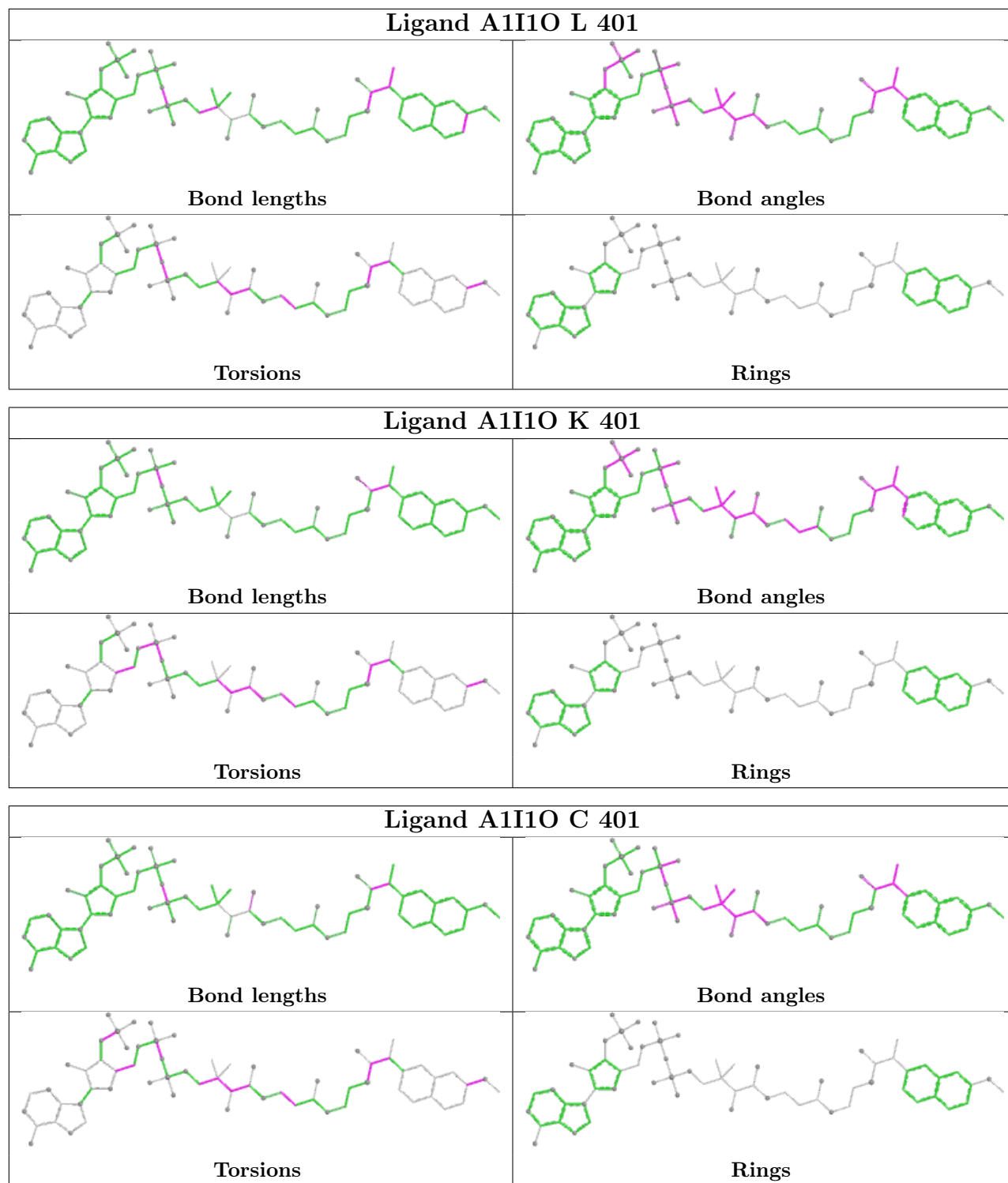


Ligand A1I1O E 401



Ligand A1I1O J 401





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/364 (98%)	0.63	41 (11%) 10 9	25, 40, 76, 128	2 (0%)
1	B	359/364 (98%)	0.53	32 (8%) 15 14	24, 40, 77, 108	1 (0%)
1	C	359/364 (98%)	0.80	64 (17%) 4 3	24, 42, 77, 108	2 (0%)
1	D	359/364 (98%)	0.71	45 (12%) 8 7	26, 41, 75, 121	1 (0%)
1	E	359/364 (98%)	0.75	50 (13%) 6 5	27, 42, 84, 121	2 (0%)
1	F	359/364 (98%)	0.91	75 (20%) 2 2	26, 44, 83, 115	1 (0%)
1	G	359/364 (98%)	1.13	93 (25%) 1 1	26, 44, 87, 121	2 (0%)
1	H	359/364 (98%)	0.86	66 (18%) 3 3	24, 43, 87, 124	1 (0%)
1	I	359/364 (98%)	0.39	19 (5%) 32 31	25, 38, 66, 100	2 (0%)
1	J	359/364 (98%)	0.38	19 (5%) 32 31	26, 38, 70, 104	1 (0%)
1	K	359/364 (98%)	0.53	40 (11%) 10 9	25, 39, 75, 124	2 (0%)
1	L	359/364 (98%)	0.39	16 (4%) 38 37	16, 39, 67, 104	2 (0%)
All	All	4308/4368 (98%)	0.67	560 (12%) 7 6	16, 40, 78, 128	19 (0%)

All (560) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	346	ALA	7.4
1	A	42	VAL	6.7
1	D	42	VAL	6.4
1	D	346	ALA	6.4
1	H	346	ALA	5.9
1	E	346	ALA	5.8
1	K	42	VAL	5.7
1	F	346	ALA	5.7
1	H	42	VAL	5.6
1	B	346	ALA	5.5
1	H	349	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	97	GLU	5.3
1	E	349	ILE	5.2
1	G	42	VAL	5.2
1	G	93	GLY	5.0
1	E	351	ILE	5.0
1	F	351	ILE	4.9
1	H	45	ILE	4.8
1	J	346	ALA	4.8
1	B	45	ILE	4.7
1	K	324	GLY	4.6
1	C	45	ILE	4.6
1	G	178	SER	4.5
1	C	176	GLN	4.5
1	G	102	VAL	4.4
1	G	355	LEU	4.3
1	G	348	THR	4.3
1	C	75	ALA	4.3
1	A	346	ALA	4.2
1	G	69	LEU	4.2
1	F	42	VAL	4.2
1	G	44	GLY	4.2
1	J	351	ILE	4.2
1	E	347	ALA	4.2
1	K	45	ILE	4.1
1	C	180	LYS	4.0
1	G	101	LYS	4.0
1	K	349	ILE	4.0
1	F	324	GLY	4.0
1	G	347	ALA	3.9
1	G	10	VAL	3.9
1	G	354	VAL	3.9
1	F	45	ILE	3.9
1	G	94	LEU	3.9
1	G	358	TRP	3.9
1	C	346	ALA	3.9
1	E	42	VAL	3.9
1	A	351	ILE	3.9
1	H	351	ILE	3.9
1	G	75	ALA	3.9
1	G	59	ALA	3.8
1	G	346	ALA	3.8
1	G	99	CYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	61	LEU	3.8
1	G	79	VAL	3.8
1	A	349	ILE	3.7
1	F	57	VAL	3.7
1	G	207	MET	3.7
1	G	177	SER	3.7
1	G	351	ILE	3.7
1	D	347	ALA	3.7
1	E	355	LEU	3.7
1	C	42	VAL	3.7
1	G	293	ASN	3.7
1	G	92	LEU	3.7
1	D	323	ASN	3.7
1	H	34	VAL	3.7
1	B	351	ILE	3.7
1	G	100	ALA	3.7
1	H	347	ALA	3.7
1	G	11	VAL	3.6
1	C	349	ILE	3.6
1	G	349	ILE	3.6
1	C	347	ALA	3.6
1	F	93	GLY	3.6
1	L	346	ALA	3.6
1	B	42	VAL	3.5
1	G	1	MET	3.5
1	L	351	ILE	3.5
1	G	180	LYS	3.5
1	G	324	GLY	3.5
1	H	358	TRP	3.5
1	F	349	ILE	3.5
1	G	70	ALA	3.5
1	H	2	ALA	3.5
1	H	7	GLY	3.5
1	F	11	VAL	3.5
1	B	324	GLY	3.5
1	C	351	ILE	3.4
1	D	59	ALA	3.4
1	A	93	GLY	3.4
1	G	7	GLY	3.4
1	H	323	ASN	3.4
1	F	173	TRP	3.4
1	G	71	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	176	GLN	3.4
1	G	33	VAL	3.4
1	K	176	GLN	3.4
1	G	57	VAL	3.4
1	A	177	SER	3.4
1	F	101	LYS	3.4
1	C	171	ALA	3.4
1	D	349	ILE	3.4
1	G	173	TRP	3.3
1	I	207	MET	3.3
1	D	355	LEU	3.3
1	F	106	LEU	3.3
1	G	63	SER	3.3
1	A	324	GLY	3.3
1	G	66	GLY	3.3
1	J	324	GLY	3.3
1	F	79	VAL	3.3
1	G	107	ILE	3.3
1	J	45	ILE	3.3
1	F	359	ASP	3.3
1	J	42	VAL	3.3
1	D	76	LYS	3.3
1	B	257	ALA	3.2
1	G	36	ILE	3.2
1	G	87	GLY	3.2
1	C	173	TRP	3.2
1	G	34	VAL	3.2
1	A	62	LYS	3.2
1	H	73	LEU	3.2
1	C	66	GLY	3.2
1	H	179	GLY	3.2
1	F	354	VAL	3.2
1	D	45	ILE	3.2
1	E	45	ILE	3.2
1	G	73	LEU	3.2
1	E	345	PRO	3.2
1	A	173	TRP	3.1
1	D	358	TRP	3.1
1	F	33	VAL	3.1
1	H	75	ALA	3.1
1	G	359	ASP	3.1
1	E	178	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	353	ALA	3.1
1	K	100	ALA	3.1
1	I	41	SER	3.1
1	F	348	THR	3.1
1	H	105	ARG	3.1
1	F	347	ALA	3.1
1	I	351	ILE	3.1
1	C	358	TRP	3.1
1	D	173	TRP	3.1
1	G	76	LYS	3.1
1	H	173	TRP	3.1
1	B	41	SER	3.1
1	L	40	SER	3.1
1	E	7	GLY	3.1
1	E	93	GLY	3.1
1	E	324	GLY	3.1
1	L	359	ASP	3.1
1	A	75	ALA	3.1
1	H	322	ALA	3.1
1	D	102	VAL	3.1
1	G	45	ILE	3.1
1	L	349	ILE	3.1
1	D	178	SER	3.0
1	D	351	ILE	3.0
1	H	324	GLY	3.0
1	L	173	TRP	3.0
1	D	176	GLN	3.0
1	H	176	GLN	3.0
1	F	69	LEU	3.0
1	E	56	ILE	3.0
1	B	323	ASN	3.0
1	E	358	TRP	3.0
1	F	1	MET	3.0
1	C	105	ARG	3.0
1	D	41	SER	3.0
1	H	355	LEU	3.0
1	L	323	ASN	3.0
1	G	108	TYR	3.0
1	I	346	ALA	2.9
1	A	69	LEU	2.9
1	G	67	LEU	2.9
1	H	5	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	69	LEU	2.9
1	C	34	VAL	2.9
1	H	354	VAL	2.9
1	C	93	GLY	2.9
1	K	181	GLY	2.9
1	G	72	LYS	2.9
1	I	47	ARG	2.9
1	B	358	TRP	2.9
1	G	77	ALA	2.9
1	K	347	ALA	2.9
1	C	69	LEU	2.9
1	F	73	LEU	2.9
1	K	71	LEU	2.9
1	G	356	THR	2.9
1	F	358	TRP	2.9
1	B	75	ALA	2.9
1	F	355	LEU	2.9
1	G	357	ASP	2.9
1	K	102	VAL	2.9
1	A	45	ILE	2.9
1	B	349	ILE	2.9
1	I	176	GLN	2.9
1	K	345	PRO	2.9
1	F	180	LYS	2.9
1	G	62	LYS	2.9
1	I	180	LYS	2.9
1	F	176	GLN	2.8
1	A	348	THR	2.8
1	D	107	ILE	2.8
1	F	107	ILE	2.8
1	H	76	LYS	2.8
1	K	72	LYS	2.8
1	B	347	ALA	2.8
1	E	1	MET	2.8
1	F	66	GLY	2.8
1	I	322	ALA	2.8
1	I	324	GLY	2.8
1	G	8	LEU	2.8
1	A	68	GLU	2.8
1	G	88	VAL	2.8
1	G	39	PRO	2.8
1	H	16	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	144	ASP	2.8
1	H	44	GLY	2.8
1	H	353	ALA	2.8
1	A	355	LEU	2.8
1	A	102	VAL	2.8
1	G	183	VAL	2.8
1	A	76	LYS	2.8
1	D	56	ILE	2.8
1	F	293	ASN	2.8
1	E	176	GLN	2.8
1	C	30	GLY	2.8
1	D	44	GLY	2.8
1	K	93	GLY	2.8
1	E	77	ALA	2.8
1	H	8	LEU	2.8
1	F	39	PRO	2.8
1	G	96	PRO	2.8
1	A	354	VAL	2.8
1	F	10	VAL	2.8
1	A	358	TRP	2.8
1	I	323	ASN	2.7
1	D	43	ASP	2.7
1	K	359	ASP	2.7
1	D	324	GLY	2.7
1	J	75	ALA	2.7
1	C	61	LEU	2.7
1	B	348	THR	2.7
1	H	345	PRO	2.7
1	C	79	VAL	2.7
1	E	79	VAL	2.7
1	C	177	SER	2.7
1	G	68	GLU	2.7
1	G	98	GLU	2.7
1	L	350	ASP	2.7
1	E	66	GLY	2.7
1	C	76	LYS	2.7
1	E	58	THR	2.7
1	G	345	PRO	2.7
1	I	349	ILE	2.7
1	C	104	ASP	2.7
1	E	173	TRP	2.7
1	I	173	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	7	GLY	2.7
1	K	47	ARG	2.7
1	C	100	ALA	2.7
1	D	75	ALA	2.7
1	A	92	LEU	2.7
1	D	8	LEU	2.7
1	G	41	SER	2.7
1	A	74	ILE	2.7
1	G	56	ILE	2.7
1	H	57	VAL	2.7
1	H	102	VAL	2.7
1	K	351	ILE	2.7
1	F	99	CYS	2.7
1	A	180	LYS	2.7
1	F	62	LYS	2.7
1	H	326	TRP	2.7
1	B	350	ASP	2.6
1	C	102	VAL	2.6
1	K	180	LYS	2.6
1	H	107	ILE	2.6
1	C	47	ARG	2.6
1	H	30	GLY	2.6
1	F	97	GLU	2.6
1	I	1	MET	2.6
1	E	75	ALA	2.6
1	E	39	PRO	2.6
1	L	355	LEU	2.6
1	K	34	VAL	2.6
1	B	65	GLN	2.6
1	A	1	MET	2.6
1	G	292	ALA	2.6
1	J	347	ALA	2.6
1	C	8	LEU	2.6
1	C	101	LYS	2.6
1	E	180	LYS	2.6
1	A	47	ARG	2.6
1	C	107	ILE	2.6
1	A	207	MET	2.6
1	K	101	LYS	2.6
1	F	89	THR	2.6
1	F	292	ALA	2.6
1	B	345	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	345	PRO	2.6
1	G	105	ARG	2.6
1	H	337	THR	2.6
1	H	39	PRO	2.6
1	F	41	SER	2.6
1	H	334	PHE	2.5
1	C	68	GLU	2.5
1	C	1	MET	2.5
1	E	179	GLY	2.5
1	G	83	GLY	2.5
1	F	59	ALA	2.5
1	K	75	ALA	2.5
1	G	172	LEU	2.5
1	B	1	MET	2.5
1	F	36	ILE	2.5
1	K	44	GLY	2.5
1	F	76	LYS	2.5
1	B	43	ASP	2.5
1	A	347	ALA	2.5
1	C	353	ALA	2.5
1	E	70	ALA	2.5
1	C	67	LEU	2.5
1	B	7	GLY	2.5
1	D	7	GLY	2.5
1	C	11	VAL	2.5
1	C	74	ILE	2.5
1	F	184	VAL	2.5
1	C	99	CYS	2.5
1	A	178	SER	2.5
1	C	178	SER	2.5
1	C	345	PRO	2.5
1	D	345	PRO	2.5
1	F	171	ALA	2.5
1	G	257	ALA	2.5
1	H	31	ALA	2.5
1	C	71	LEU	2.5
1	F	71	LEU	2.5
1	G	5	LEU	2.5
1	H	47	ARG	2.5
1	F	44	GLY	2.5
1	G	179	GLY	2.5
1	I	359	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	359	ASP	2.4
1	A	99	CYS	2.4
1	F	63	SER	2.4
1	E	59	ALA	2.4
1	E	257	ALA	2.4
1	F	353	ALA	2.4
1	K	1	MET	2.4
1	C	323	ASN	2.4
1	G	65	GLN	2.4
1	E	10	VAL	2.4
1	F	34	VAL	2.4
1	G	74	ILE	2.4
1	H	178	SER	2.4
1	L	177	SER	2.4
1	A	356	THR	2.4
1	D	180	LYS	2.4
1	E	100	ALA	2.4
1	H	72	LYS	2.4
1	D	172	LEU	2.4
1	E	172	LEU	2.4
1	D	357	ASP	2.4
1	K	144	ASP	2.4
1	A	34	VAL	2.4
1	F	81	ILE	2.4
1	I	358	TRP	2.4
1	L	1	MET	2.4
1	A	77	ALA	2.4
1	B	77	ALA	2.4
1	D	2	ALA	2.4
1	F	70	ALA	2.4
1	J	353	ALA	2.4
1	B	73	LEU	2.4
1	E	73	LEU	2.4
1	J	355	LEU	2.4
1	C	179	GLY	2.4
1	C	324	GLY	2.4
1	J	325	GLY	2.4
1	L	7	GLY	2.4
1	A	56	ILE	2.4
1	C	10	VAL	2.4
1	K	107	ILE	2.4
1	B	76	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	6	SER	2.4
1	C	58	THR	2.4
1	G	58	THR	2.4
1	E	69	LEU	2.3
1	E	323	ASN	2.3
1	G	64	ASP	2.3
1	G	78	ASP	2.3
1	I	45	ILE	2.3
1	D	354	VAL	2.3
1	G	184	VAL	2.3
1	G	352	GLU	2.3
1	A	289	ALA	2.3
1	C	59	ALA	2.3
1	G	322	ALA	2.3
1	F	7	GLY	2.3
1	G	106	LEU	2.3
1	E	104	ASP	2.3
1	G	91	ARG	2.3
1	A	258	GLU	2.3
1	F	98	GLU	2.3
1	F	102	VAL	2.3
1	C	73	LEU	2.3
1	C	350	ASP	2.3
1	C	355	LEU	2.3
1	D	179	GLY	2.3
1	H	106	LEU	2.3
1	K	94	LEU	2.3
1	I	76	LYS	2.3
1	A	176	GLN	2.3
1	C	36	ILE	2.3
1	J	349	ILE	2.3
1	E	33	VAL	2.3
1	A	72	LYS	2.3
1	F	31	ALA	2.3
1	G	30	GLY	2.3
1	L	180	LYS	2.3
1	A	61	LEU	2.3
1	C	106	LEU	2.3
1	G	80	LEU	2.3
1	H	1	MET	2.3
1	B	46	SER	2.2
1	F	65	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	41	SER	2.2
1	E	11	VAL	2.2
1	J	323	ASN	2.2
1	F	75	ALA	2.2
1	F	322	ALA	2.2
1	H	100	ALA	2.2
1	F	61	LEU	2.2
1	K	80	LEU	2.2
1	C	108	TYR	2.2
1	D	315	GLU	2.2
1	E	40	SER	2.2
1	G	38	ARG	2.2
1	H	56	ILE	2.2
1	H	58	THR	2.2
1	B	102	VAL	2.2
1	D	34	VAL	2.2
1	F	72	LYS	2.2
1	H	10	VAL	2.2
1	K	39	PRO	2.2
1	H	207	MET	2.2
1	K	357	ASP	2.2
1	F	181	GLY	2.2
1	H	3	GLY	2.2
1	C	70	ALA	2.2
1	C	77	ALA	2.2
1	D	322	ALA	2.2
1	E	97	GLU	2.2
1	I	258	GLU	2.2
1	C	172	LEU	2.2
1	F	5	LEU	2.2
1	B	173	TRP	2.2
1	J	173	TRP	2.2
1	B	180	LYS	2.2
1	K	76	LYS	2.2
1	E	107	ILE	2.2
1	E	144	ASP	2.2
1	F	74	ILE	2.2
1	H	357	ASP	2.2
1	D	79	VAL	2.2
1	D	93	GLY	2.2
1	A	70	ALA	2.2
1	D	65	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	338	ALA	2.2
1	H	77	ALA	2.2
1	E	80	LEU	2.2
1	G	51	LEU	2.2
1	H	80	LEU	2.2
1	K	73	LEU	2.2
1	K	355	LEU	2.2
1	K	178	SER	2.2
1	B	62	LYS	2.2
1	H	101	LYS	2.2
1	A	357	ASP	2.2
1	E	356	THR	2.2
1	G	89	THR	2.2
1	H	359	ASP	2.2
1	D	74	ILE	2.1
1	E	2	ALA	2.1
1	F	2	ALA	2.1
1	L	75	ALA	2.1
1	B	355	LEU	2.1
1	E	47	ARG	2.1
1	K	63	SER	2.1
1	F	357	ASP	2.1
1	K	348	THR	2.1
1	K	358	TRP	2.1
1	F	182	GLN	2.1
1	B	44	GLY	2.1
1	H	27	GLY	2.1
1	H	79	VAL	2.1
1	J	93	GLY	2.1
1	B	353	ALA	2.1
1	E	353	ALA	2.1
1	E	5	LEU	2.1
1	F	80	LEU	2.1
1	F	92	LEU	2.1
1	H	92	LEU	2.1
1	K	58	THR	2.1
1	A	7	GLY	2.1
1	F	47	ARG	2.1
1	C	33	VAL	2.1
1	C	57	VAL	2.1
1	K	10	VAL	2.1
1	D	31	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	171	ALA	2.1
1	F	100	ALA	2.1
1	G	109	ALA	2.1
1	G	171	ALA	2.1
1	B	71	LEU	2.1
1	C	80	LEU	2.1
1	H	46	SER	2.1
1	L	69	LEU	2.1
1	D	68	GLU	2.1
1	B	359	ASP	2.1
1	F	350	ASP	2.1
1	J	350	ASP	2.1
1	F	108	TYR	2.1
1	H	348	THR	2.1
1	H	181	GLY	2.1
1	J	44	GLY	2.1
1	C	62	LYS	2.1
1	I	101	LYS	2.1
1	E	34	VAL	2.1
1	J	102	VAL	2.1
1	F	326	TRP	2.1
1	C	97	GLU	2.0
1	H	59	ALA	2.1
1	H	352	GLU	2.0
1	D	5	LEU	2.0
1	C	359	ASP	2.0
1	D	105	ARG	2.0
1	D	348	THR	2.0
1	E	348	THR	2.0
1	C	72	LYS	2.0
1	H	325	GLY	2.0
1	H	74	ILE	2.0
1	F	68	GLU	2.0
1	D	207	MET	2.0
1	K	40	SER	2.0
1	K	173	TRP	2.0
1	L	322	ALA	2.0
1	F	67	LEU	2.0
1	A	64	ASP	2.0
1	G	60	ASP	2.0
1	G	9	ARG	2.0
1	H	99	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	348	THR	2.0
1	F	96	PRO	2.0
1	C	44	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

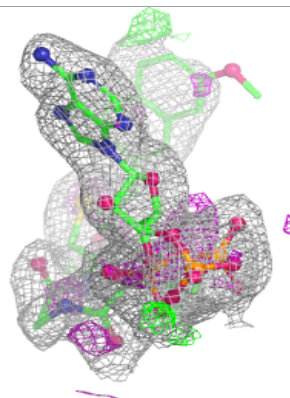
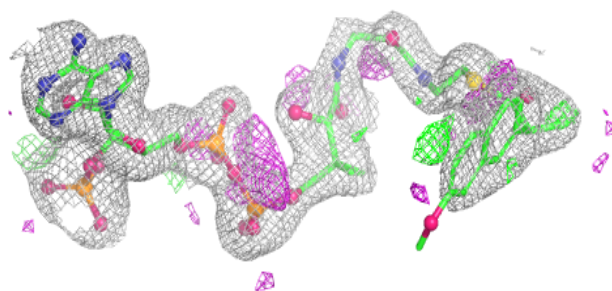
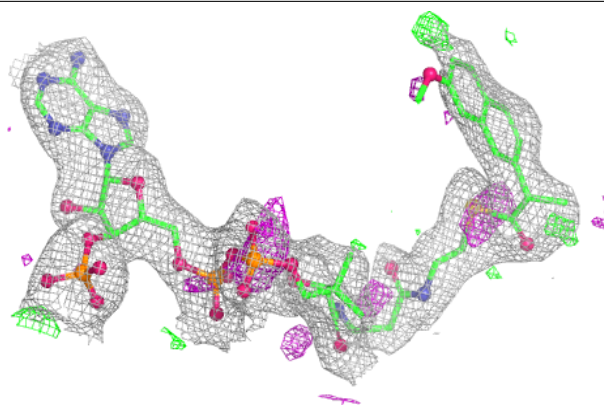
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1I1O	E	401	64/64	0.91	0.14	40,56,87,119	0
2	A1I1O	G	401	64/64	0.92	0.15	29,53,94,132	0
2	A1I1O	H	401	64/64	0.92	0.14	43,62,98,126	0
2	A1I1O	A	401	64/64	0.93	0.13	25,49,97,128	0
2	A1I1O	F	401	64/64	0.93	0.14	28,49,95,115	0
2	A1I1O	C	401	64/64	0.94	0.12	31,50,76,107	0
2	A1I1O	D	401	64/64	0.94	0.12	21,43,90,108	0
2	A1I1O	B	401	64/64	0.95	0.12	28,48,87,118	0
2	A1I1O	I	401	64/64	0.95	0.11	22,40,84,115	0
2	A1I1O	J	401	64/64	0.95	0.11	26,46,85,119	0
2	A1I1O	K	401	64/64	0.95	0.11	29,46,88,98	0
2	A1I1O	L	401	64/64	0.95	0.12	22,41,89,122	0

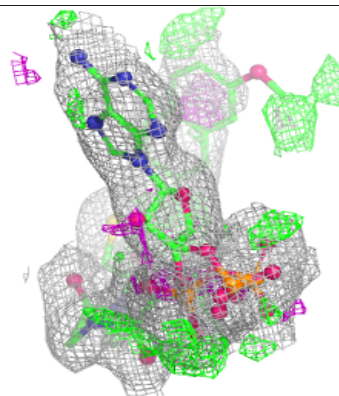
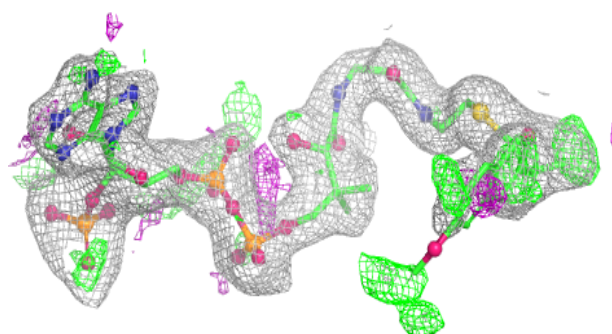
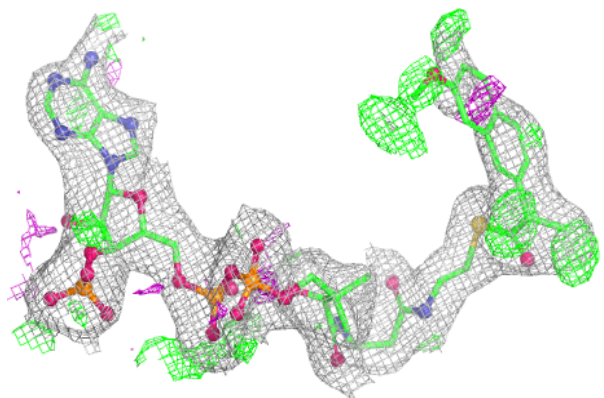
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1I1O 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)

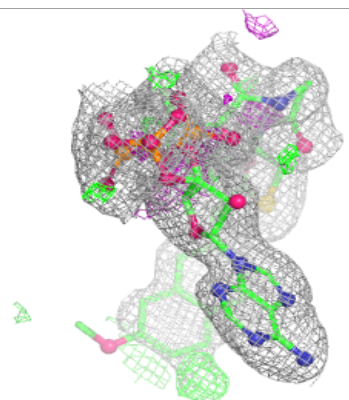
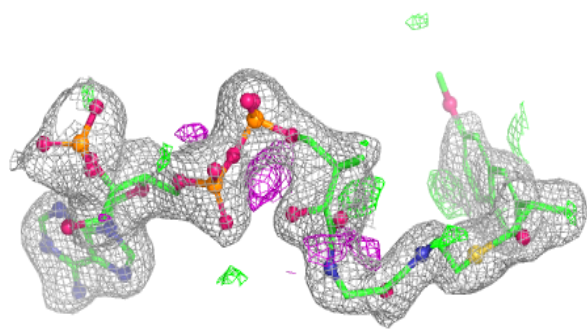
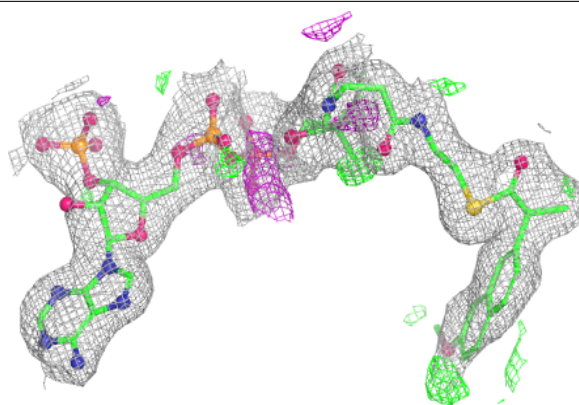
**Electron density around A1I1O G 401:**

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

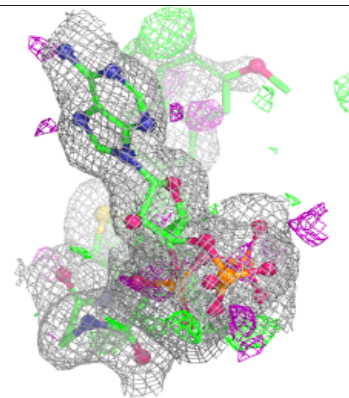
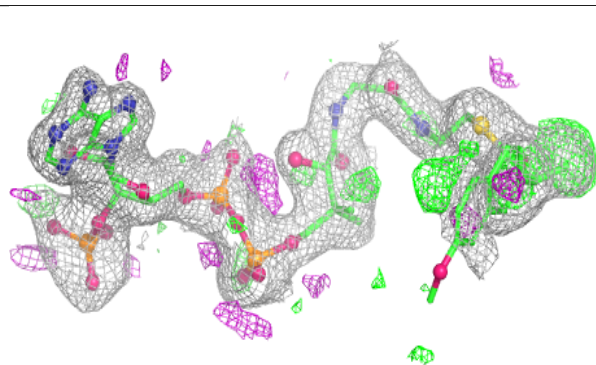
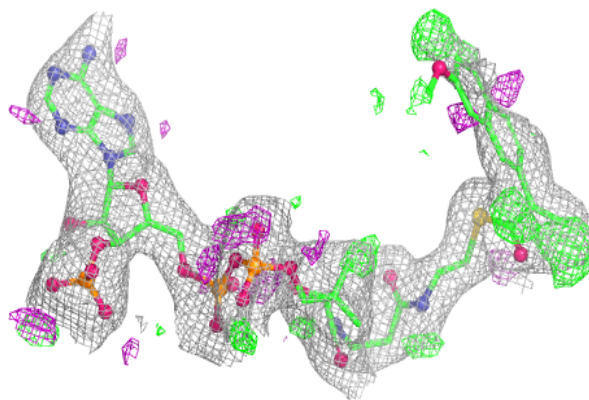


Electron density around A1I1O H 401:

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

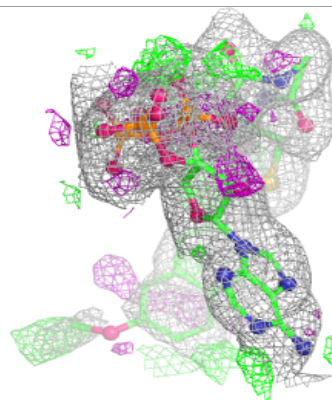
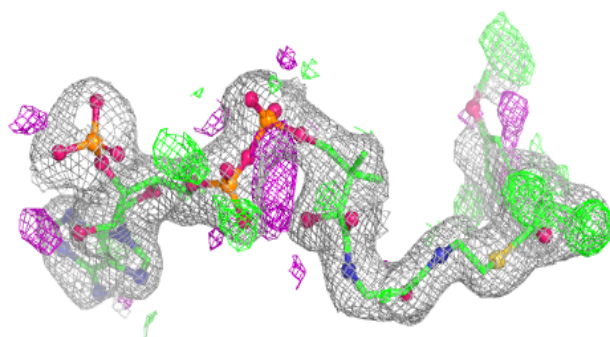
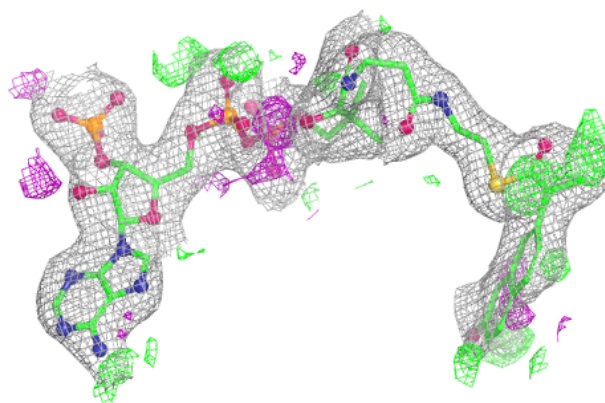
**Electron density around A1I1O A 401:**

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

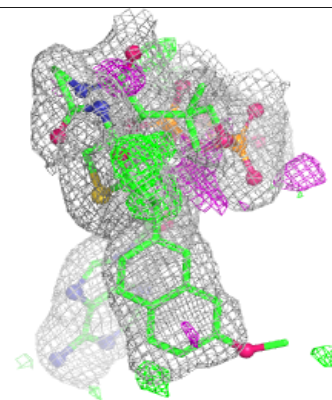
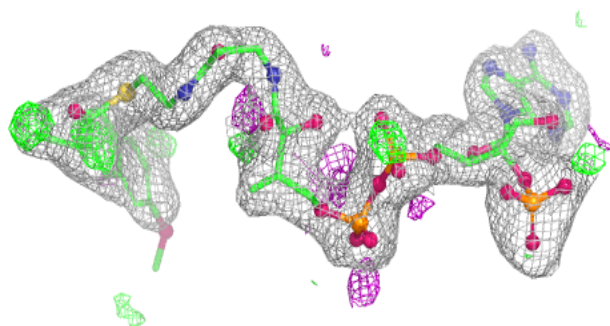
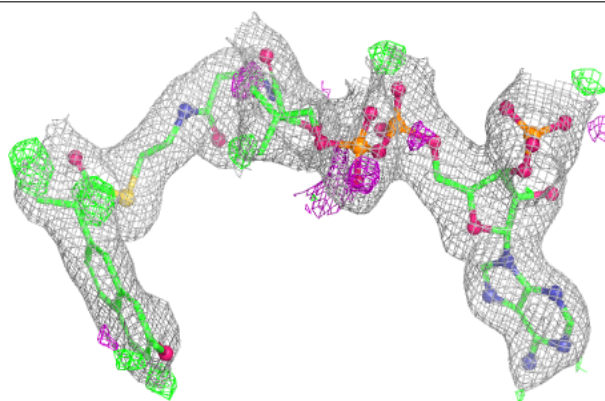


Electron density around A1I1O F 401:

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

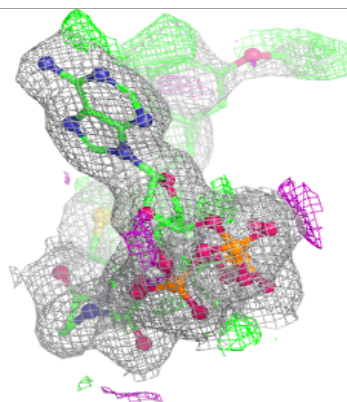
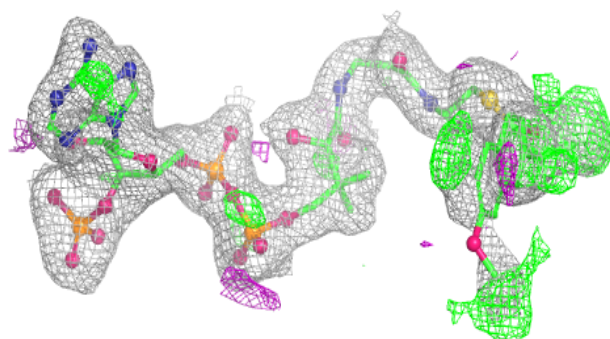
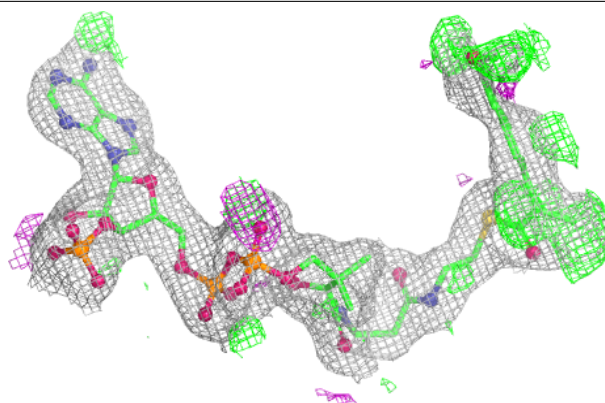
**Electron density around A1I1O C 401:**

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

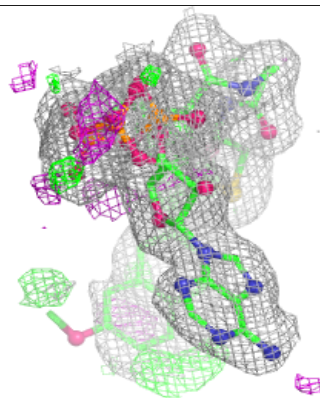
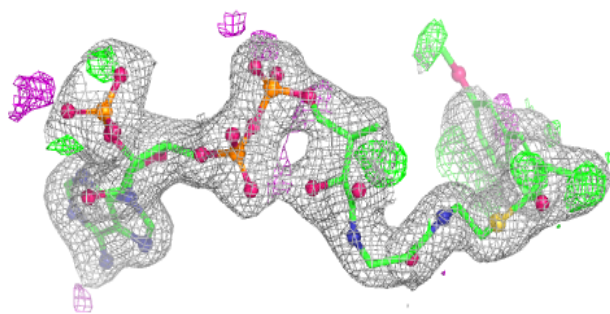
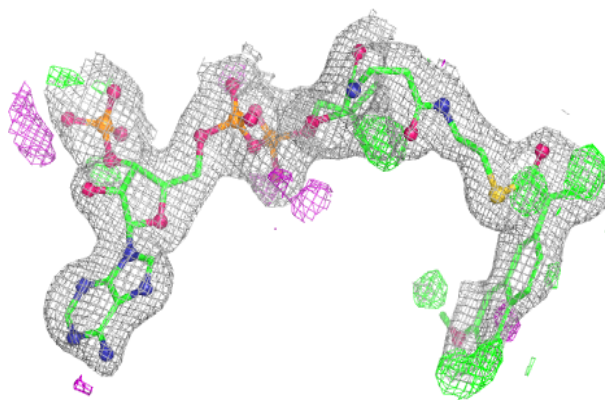


Electron density around A1I1O D 401:

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

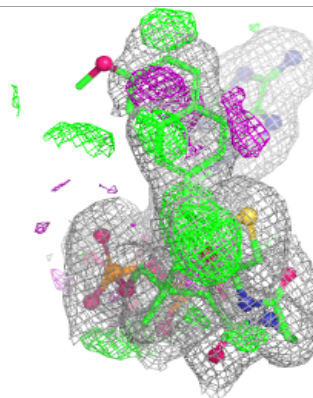
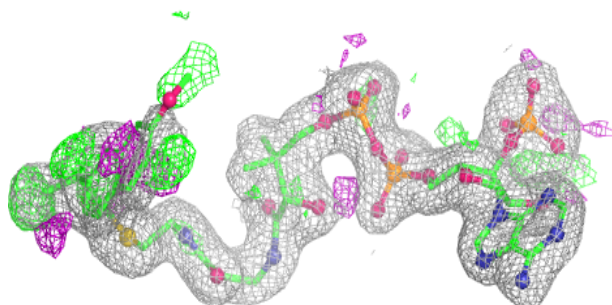
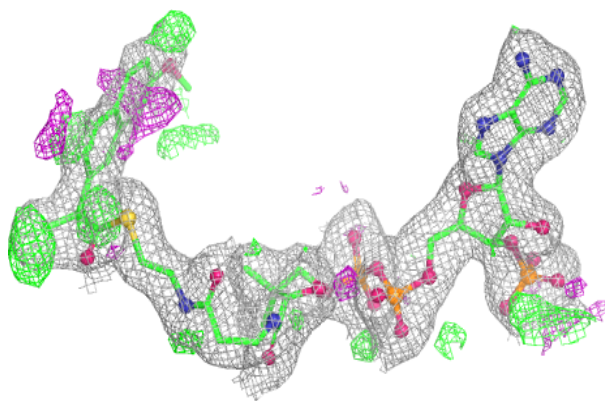
**Electron density around A1I1O B 401:**

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

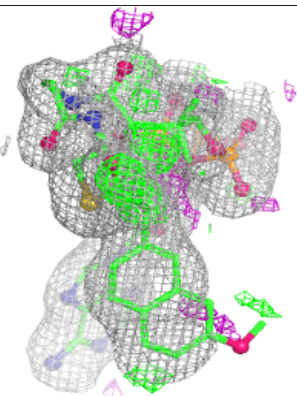
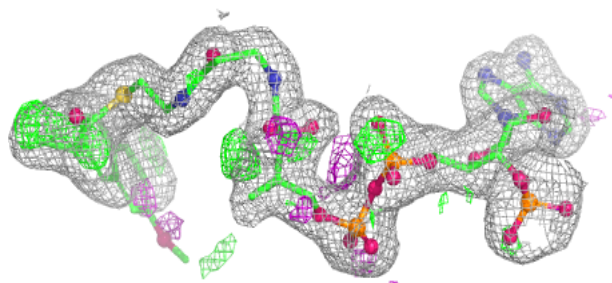
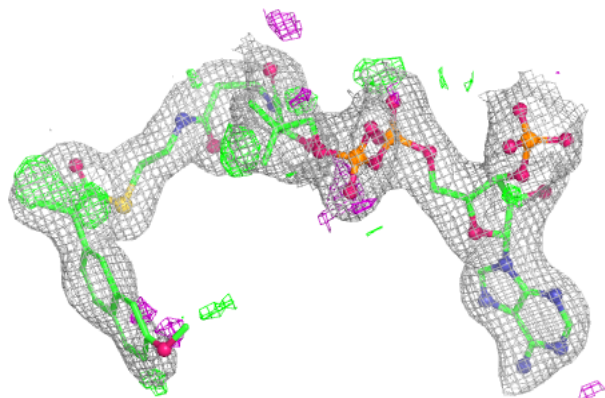


Electron density around A1I1O I 401:

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

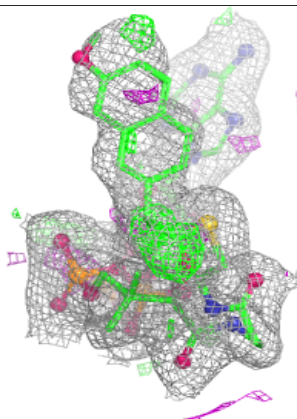
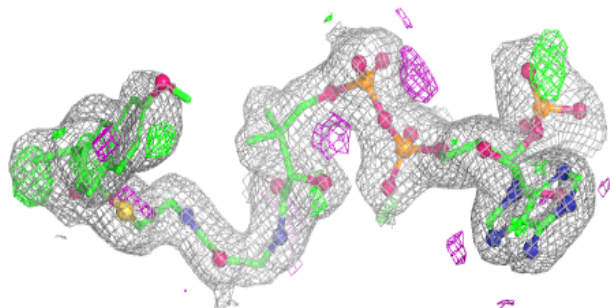
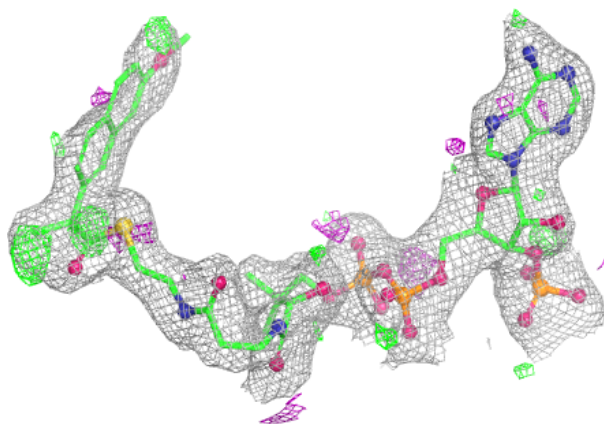
**Electron density around A1I1O J 401:**

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

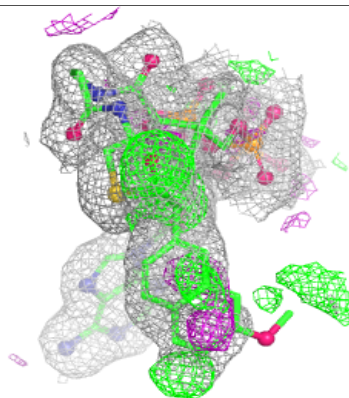
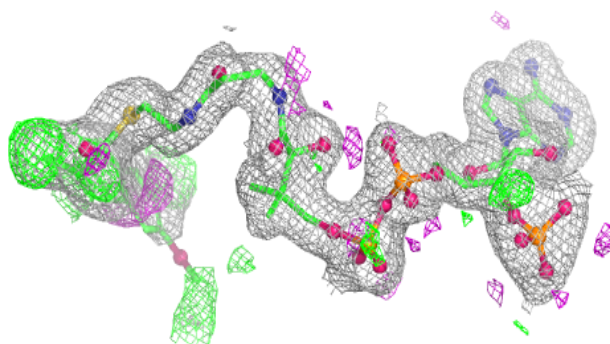
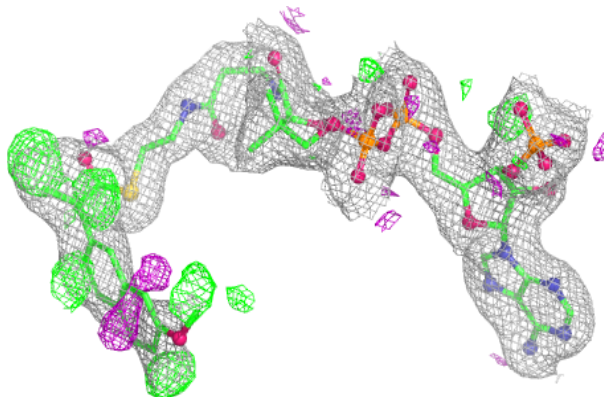


Electron density around A1I1O K 401:

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

**Electron density around A1I1O 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.