



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:57 AM UTC

PDB ID : 9I2Z / pdb_00009i2z
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with 2-methyldecanoyl-CoA
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on : 2025-01-22
Resolution : 2.11 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:

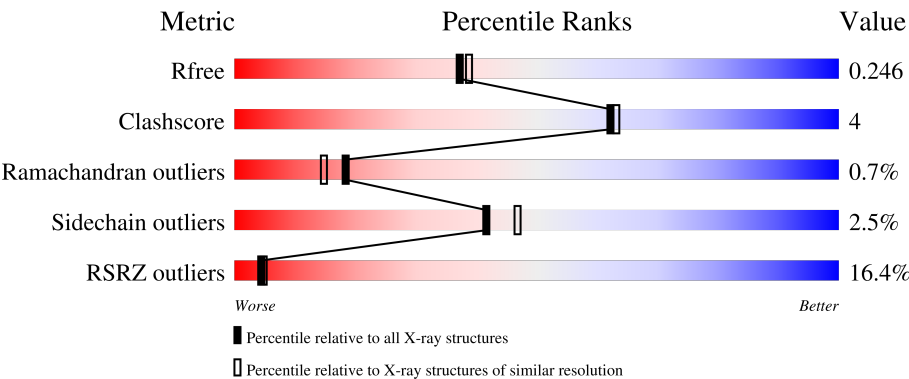
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.11 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	<div><div>20%</div><div><div></div><div>87%</div><div>10%</div><div>..</div></div></div>
1	B	364	<div><div>11%</div><div><div></div><div>91%</div><div>8%</div><div>.</div></div></div>
1	C	364	<div><div>15%</div><div><div></div><div>86%</div><div>11%</div><div>..</div></div></div>
1	D	364	<div><div>17%</div><div><div></div><div>86%</div><div>11%</div><div>..</div></div></div>
1	E	364	<div><div>19%</div><div><div></div><div>82%</div><div>15%</div><div>..</div></div></div>

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34951 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
			2714	1702	486	510	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	357	Total	C	N	O	S	0	1	0
			2703	1697	484	506	16			
1	G	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	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	1	0
			2715	1703	486	510	16			
1	J	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	K	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	L	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	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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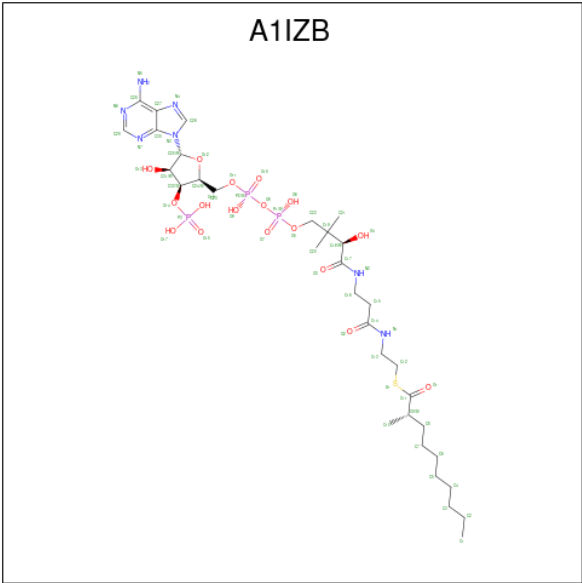
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	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 (S)-2-methyldecanoyl-CoA (CCD ID: A1IZB) (formula: C₃₂H₅₆N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	B	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	C	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	D	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	E	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	F	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	G	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	H	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	I	1	Total	C	N	O	P	S		0	0
			60	32	7	17	3	1			
2	J	1	Total	C	N	O	P	S		0	0
			60	32	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
			60	32	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			60	32	7	17	3	1		

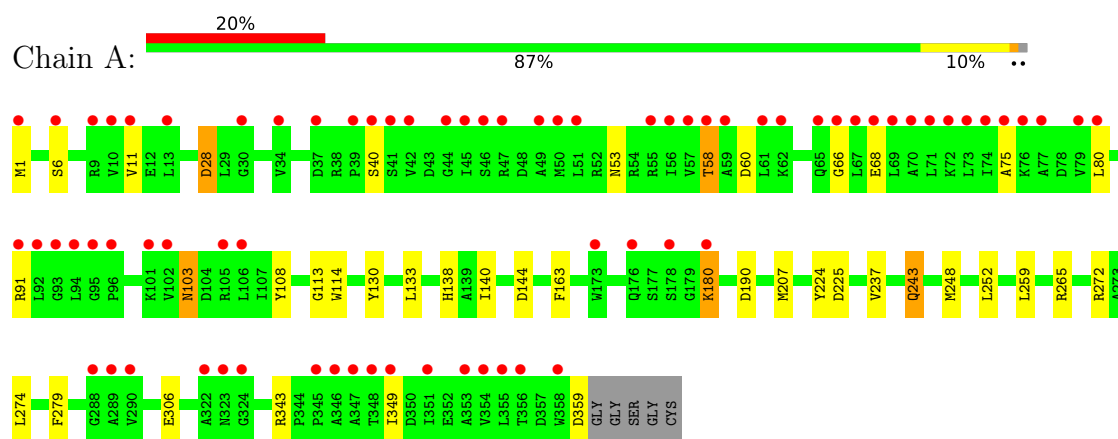
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	126	Total	O	0	0
			126	126		
3	C	130	Total	O	0	0
			130	130		
3	D	150	Total	O	0	0
			150	150		
3	E	131	Total	O	0	0
			131	131		
3	F	133	Total	O	0	0
			133	133		
3	G	122	Total	O	0	0
			122	122		
3	H	111	Total	O	0	0
			111	111		
3	I	160	Total	O	0	0
			160	160		
3	J	153	Total	O	0	0
			153	153		
3	K	153	Total	O	0	0
			153	153		
3	L	163	Total	O	0	0
			163	163		

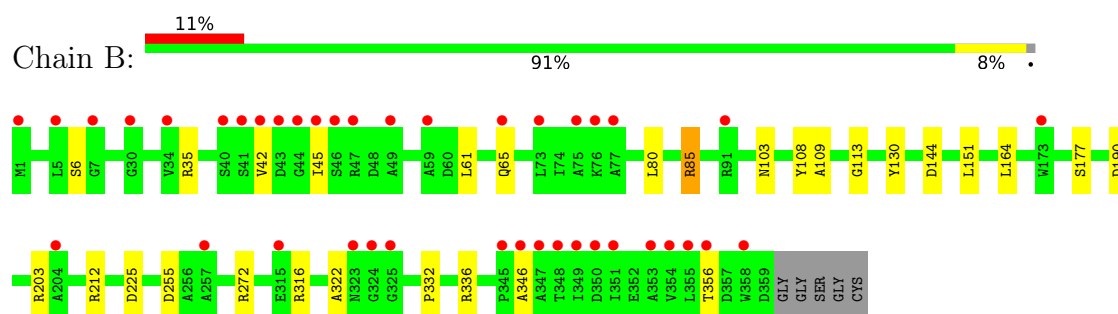
3 Residue-property plots [i](#)

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.

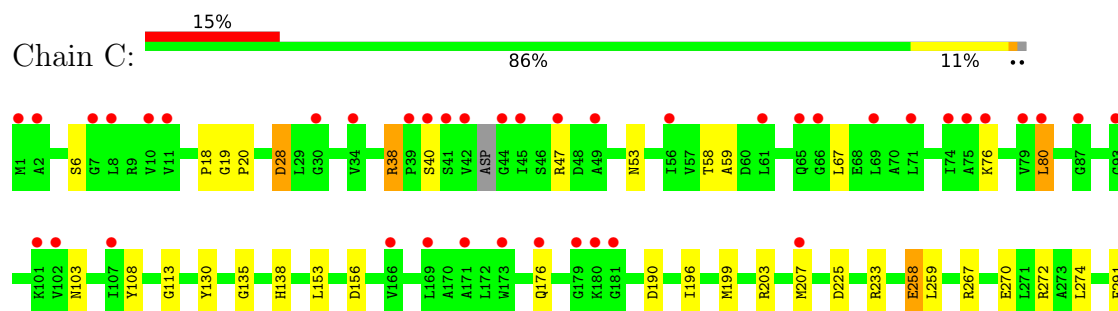
- Molecule 1: Alpha-methylacyl-CoA racemase



- Molecule 1: Alpha-methylacyl-CoA racemase

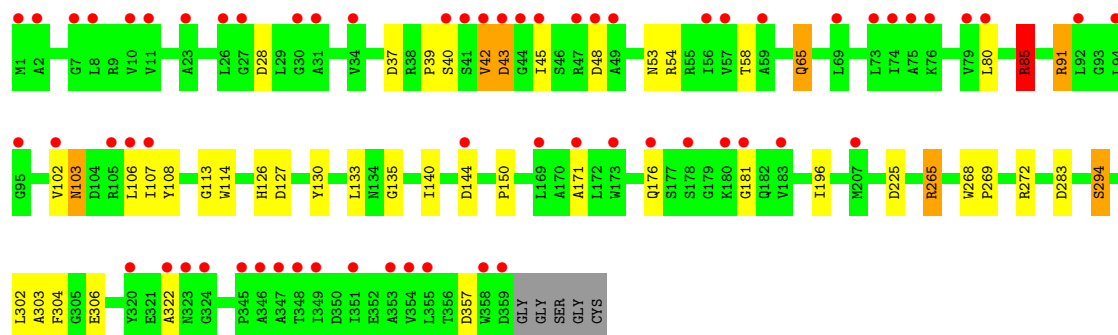
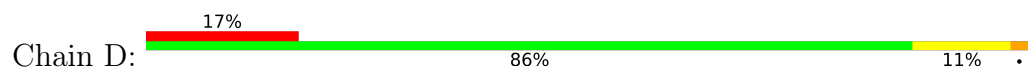


- Molecule 1: Alpha-methylacyl-CoA racemase

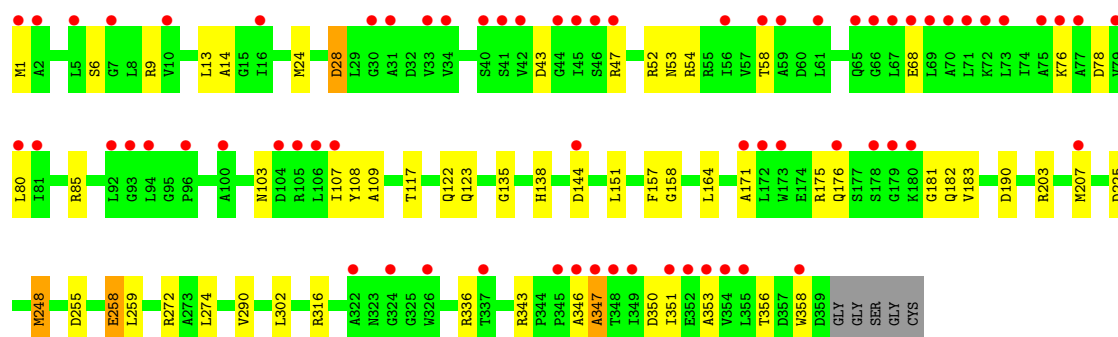
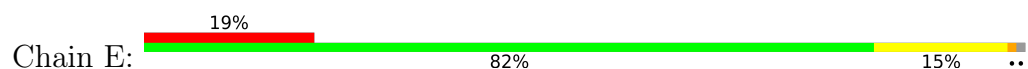




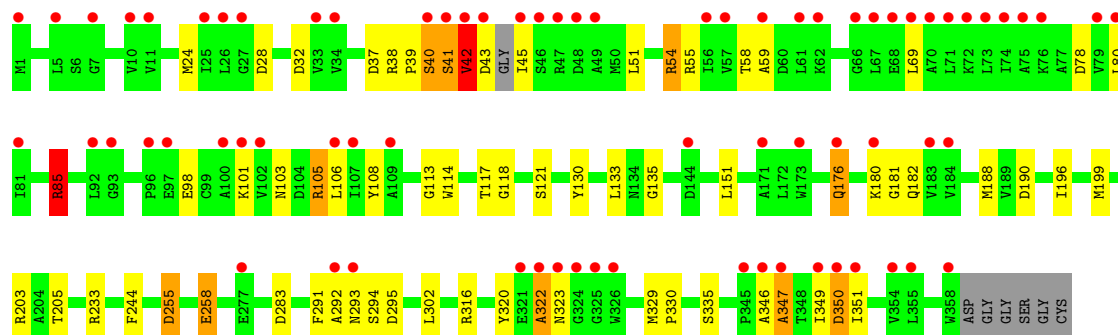
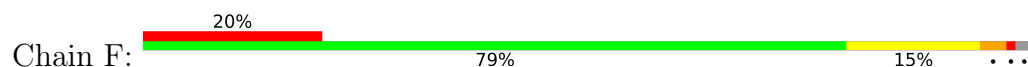
• Molecule 1: Alpha-methylacyl-CoA racemase



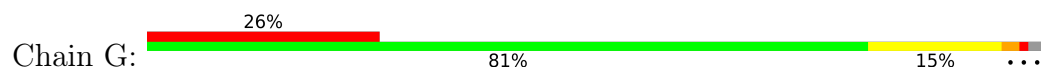
• Molecule 1: Alpha-methylacyl-CoA racemase

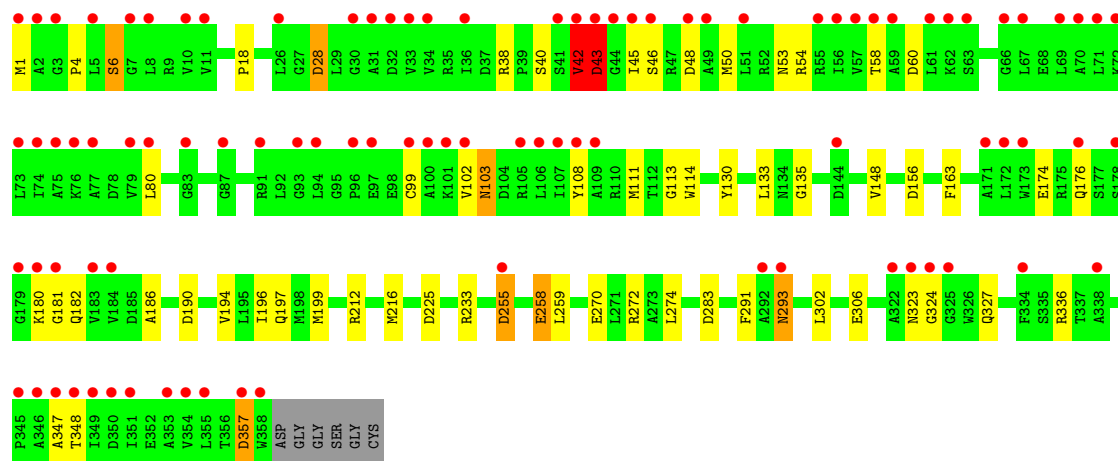


• Molecule 1: Alpha-methylacyl-CoA racemase

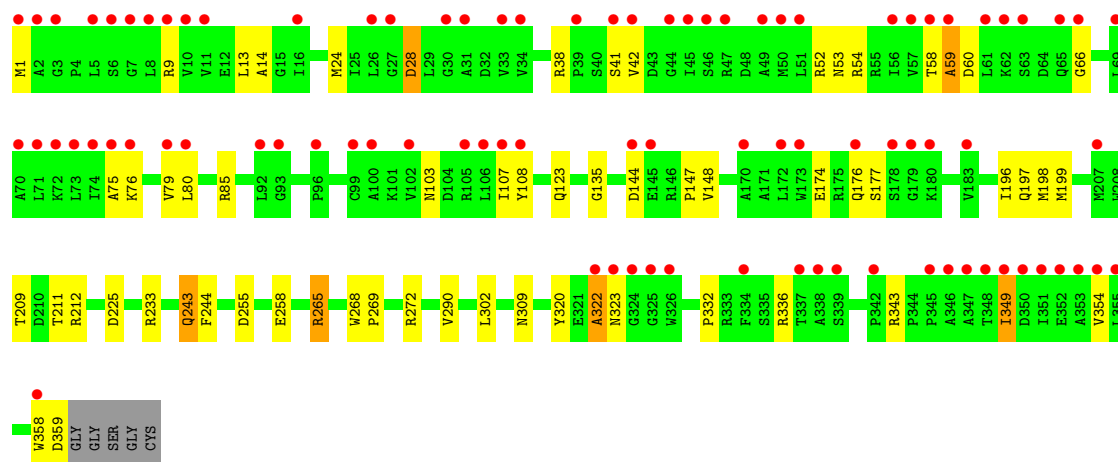
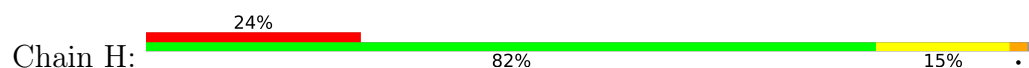


• Molecule 1: Alpha-methylacyl-CoA racemase

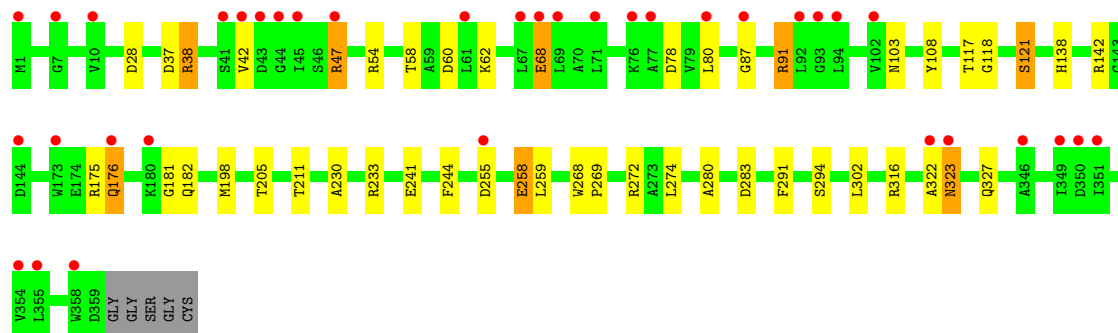
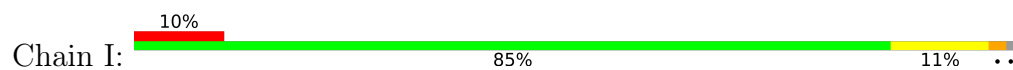




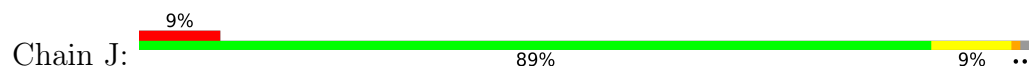
• Molecule 1: Alpha-methylacyl-CoA racemase

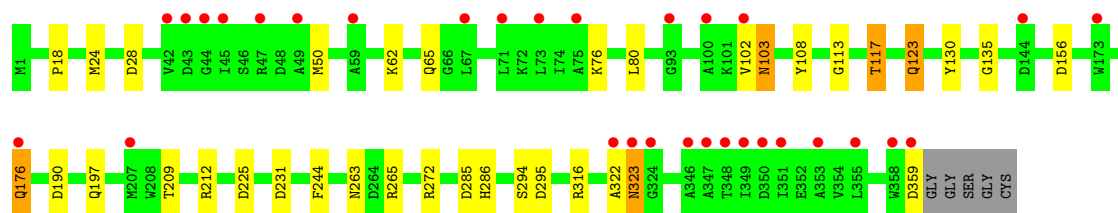


• Molecule 1: Alpha-methylacyl-CoA racemase

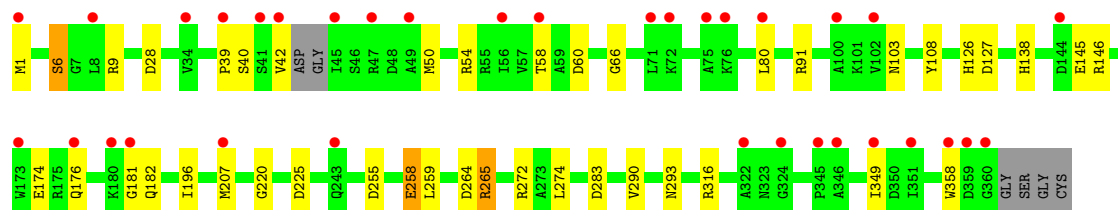
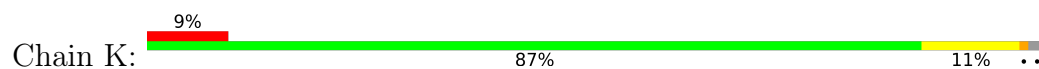


• Molecule 1: Alpha-methylacyl-CoA racemase

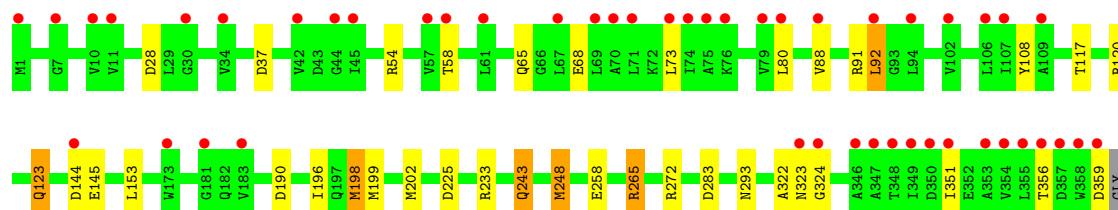
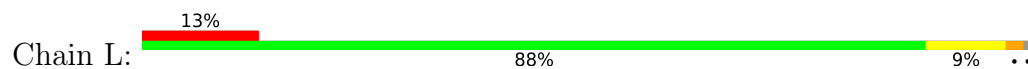




● Molecule 1: Alpha-methylacyl-CoA racemase



● Molecule 1: Alpha-methylacyl-CoA racemase



GLY
SER
GLY
CYS

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	277.03Å 277.03Å 390.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	226.02 – 2.11 226.02 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (226.02-2.11) 99.9 (226.02-2.11)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.201 , 0.239 0.208 , 0.246	Depositor DCC
R_{free} test set	21368 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.004 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	34951	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 3.27% 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: A1IZB

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	10/3797 (0.3%)
1	B	0.66	0/2782	1.17	7/3785 (0.2%)
1	C	0.66	0/2786	1.19	10/3788 (0.3%)
1	D	0.66	0/2782	1.19	10/3785 (0.3%)
1	E	0.65	0/2791	1.16	8/3797 (0.2%)
1	F	0.65	0/2769	1.18	10/3766 (0.3%)
1	G	0.63	0/2783	1.19	12/3786 (0.3%)
1	H	0.66	0/2782	1.21	15/3785 (0.4%)
1	I	0.66	0/2782	1.15	10/3785 (0.3%)
1	J	0.66	0/2782	1.19	10/3785 (0.3%)
1	K	0.65	0/2782	1.14	7/3783 (0.2%)
1	L	0.66	0/2782	1.19	14/3785 (0.4%)
All	All	0.65	0/33394	1.18	123/45427 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	4
1	G	0	3
1	H	0	5
1	I	0	3
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	5
All	All	0	32

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ARG	N-CA-CB	10.55	126.55	110.30
1	B	203	ARG	CB-CA-C	-10.07	91.34	110.67
1	L	123	GLN	CB-CA-C	10.05	125.96	109.89
1	L	123	GLN	N-CA-CB	-9.65	95.47	109.85
1	B	203	ARG	N-CA-CB	9.62	125.19	110.28
1	B	255	ASP	CB-CA-C	9.48	125.84	110.29
1	G	255	ASP	CB-CA-C	8.94	124.47	109.80
1	H	28	ASP	CA-CB-CG	8.44	121.04	112.60
1	C	258	GLU	CB-CA-C	-8.05	96.95	110.56
1	F	190	ASP	CA-CB-CG	8.05	120.65	112.60
1	F	258	GLU	CB-CA-C	-7.62	97.69	110.56
1	J	123	GLN	CB-CA-C	7.61	122.06	109.89
1	G	190	ASP	CA-CB-CG	7.58	120.17	112.60
1	K	258	GLU	CB-CA-C	-7.57	97.77	110.56
1	E	28	ASP	CA-CB-CG	7.54	120.14	112.60
1	F	38	ARG	N-CA-CB	-7.43	98.28	110.02
1	J	190	ASP	CA-CB-CG	7.34	119.94	112.60
1	F	255	ASP	CB-CA-C	7.31	121.75	109.84
1	H	148	VAL	CB-CA-C	7.18	117.09	110.13
1	E	203	ARG	CB-CA-C	-7.09	98.80	110.85
1	B	190	ASP	CA-CB-CG	7.00	119.59	112.60
1	E	123	GLN	CB-CA-C	-6.95	97.76	109.65
1	A	28	ASP	CA-CB-CG	6.94	119.54	112.60
1	I	211	THR	CA-CB-OG1	-6.94	99.19	109.60
1	B	65	GLN	N-CA-CB	-6.93	99.94	109.98
1	J	123	GLN	N-CA-CB	-6.91	99.56	109.85
1	C	203	ARG	CB-CA-C	-6.89	96.33	110.38
1	L	190	ASP	CA-CB-CG	6.82	119.42	112.60
1	L	28	ASP	CA-CB-CG	6.81	119.41	112.60
1	G	283	ASP	CA-CB-CG	6.77	119.37	112.60
1	D	65	GLN	N-CA-CB	-6.73	100.22	109.98
1	H	211	THR	CA-CB-OG1	-6.73	99.51	109.60
1	E	190	ASP	CA-CB-CG	6.68	119.28	112.60
1	K	207	MET	CG-SD-CE	6.58	115.38	100.90
1	B	144	ASP	CA-CB-CG	6.55	119.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	38	ARG	CB-CA-C	-6.49	99.37	109.11
1	L	243	GLN	N-CA-CB	6.49	119.66	110.12
1	D	144	ASP	CA-CB-CG	6.45	119.05	112.60
1	J	65	GLN	N-CA-CB	-6.43	100.68	110.33
1	A	207	MET	CG-SD-CE	6.42	115.02	100.90
1	C	207	MET	CG-SD-CE	6.40	114.99	100.90
1	D	306	GLU	CB-CA-C	-6.38	98.54	109.65
1	E	248	MET	CG-SD-CE	6.26	114.67	100.90
1	L	265	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	C	306	GLU	CB-CA-C	-6.25	98.77	109.65
1	C	28	ASP	CA-CB-CG	6.21	118.81	112.60
1	L	248	MET	CG-SD-CE	6.18	114.50	100.90
1	H	148	VAL	CA-C-O	6.17	123.33	119.51
1	D	283	ASP	CA-CB-CG	6.08	118.68	112.60
1	I	28	ASP	CA-CB-CG	6.06	118.66	112.60
1	J	117	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	190	ASP	CA-CB-CG	6.01	118.61	112.60
1	J	28	ASP	CA-CB-CG	6.00	118.60	112.60
1	L	243	GLN	CB-CA-C	-5.99	100.85	110.79
1	G	99	CYS	CB-CA-C	5.92	121.38	110.56
1	A	144	ASP	CA-CB-CG	5.90	118.50	112.60
1	G	60	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	58	THR	CA-CB-OG1	-5.89	100.77	109.60
1	G	258	GLU	CB-CA-C	-5.88	99.42	110.01
1	L	144	ASP	CA-CB-CG	5.88	118.48	112.60
1	G	28	ASP	CA-CB-CG	5.78	118.38	112.60
1	G	306	GLU	CB-CA-C	-5.77	99.86	109.55
1	H	144	ASP	CA-CB-CG	5.75	118.35	112.60
1	I	91	ARG	CB-CA-C	-5.72	100.05	110.63
1	C	38	ARG	CB-CA-C	-5.70	100.10	109.27
1	I	258	GLU	CB-CA-C	-5.67	98.66	109.95
1	D	54	ARG	CB-CA-C	-5.66	97.00	109.56
1	E	207	MET	CG-SD-CE	5.65	113.32	100.90
1	A	243	GLN	N-CA-CB	5.62	118.48	110.16
1	A	68	GLU	CB-CA-C	5.61	120.97	110.70
1	G	357	ASP	CA-CB-CG	5.61	118.21	112.60
1	F	28	ASP	CA-CB-CG	5.59	118.19	112.60
1	L	65	GLN	N-CA-CB	-5.59	101.96	110.07
1	I	176	GLN	N-CA-CB	5.59	118.33	110.12
1	D	91	ARG	N-CA-CB	5.58	119.81	110.32
1	C	190	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	265	ARG	NE-CZ-NH2	5.55	124.20	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	65	GLN	CB-CA-C	5.54	120.82	109.67
1	B	65	GLN	CB-CA-C	5.54	119.54	110.95
1	A	243	GLN	CB-CA-C	-5.51	101.48	110.85
1	D	48	ASP	CA-CB-CG	5.51	118.11	112.60
1	H	258	GLU	CB-CA-C	-5.48	100.15	110.01
1	I	205	THR	CA-CB-OG1	-5.48	101.39	109.60
1	K	283	ASP	CB-CA-C	5.47	120.86	110.51
1	I	283	ASP	CA-CB-CG	5.47	118.07	112.60
1	K	255	ASP	CB-CA-C	5.47	119.05	110.19
1	K	146	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	L	283	ASP	CB-CA-C	5.40	119.28	109.83
1	F	350	ASP	CB-CA-C	5.39	118.65	109.53
1	K	28	ASP	CA-CB-CG	5.39	117.99	112.60
1	F	32	ASP	CA-CB-CG	5.37	117.97	112.60
1	I	68	GLU	CB-CA-C	5.35	120.43	109.67
1	J	285	ASP	CB-CA-C	5.33	120.90	110.67
1	C	327	GLN	CB-CA-C	-5.32	101.73	109.45
1	A	306	GLU	CB-CA-C	-5.31	100.40	109.65
1	C	330	PRO	CB-CA-C	-5.30	104.61	111.39
1	L	359	ASP	CA-CB-CG	5.30	117.90	112.60
1	E	203	ARG	N-CA-CB	5.29	117.98	110.16
1	E	144	ASP	CA-CB-CG	5.28	117.88	112.60
1	F	54	ARG	CB-CA-C	-5.26	97.87	109.56
1	F	78	ASP	CB-CA-C	-5.26	100.04	109.24
1	H	85	ARG	N-CA-CB	5.24	117.94	110.03
1	G	148	VAL	CB-CA-C	5.23	115.20	110.13
1	D	357	ASP	CA-CB-CG	5.23	117.83	112.60
1	J	231	ASP	CA-CB-CG	5.21	117.81	112.60
1	H	123	GLN	CB-CA-C	5.21	118.34	109.84
1	G	212	ARG	CB-CA-C	5.21	118.56	109.65
1	J	263	ASN	CA-CB-CG	-5.19	107.41	112.60
1	I	283	ASP	CB-CA-C	5.18	120.07	109.76
1	D	283	ASP	CB-CA-C	5.17	120.29	110.51
1	A	248	MET	CG-SD-CE	5.15	112.23	100.90
1	H	243	GLN	N-CA-CB	5.14	117.76	110.16
1	L	356	THR	CA-CB-OG1	-5.12	101.92	109.60
1	F	283	ASP	CA-CB-CG	5.11	117.71	112.60
1	L	198	MET	CG-SD-CE	-5.09	89.69	100.90
1	H	147	PRO	CA-C-N	-5.07	118.92	123.33
1	H	147	PRO	C-N-CA	-5.07	118.92	123.33
1	H	309	ASN	CB-CA-C	-5.07	102.04	110.81
1	H	255	ASP	CB-CA-C	5.06	118.11	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	244	PHE	CA-CB-CG	5.05	118.86	113.80
1	G	48	ASP	CA-CB-CG	5.04	117.64	112.60
1	K	283	ASP	CA-CB-CG	5.02	117.62	112.60
1	H	265	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	B	322	ALA	Peptide
1	B	35	ARG	Sidechain
1	C	233	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	85	ARG	Sidechain
1	E	350	ASP	Peptide
1	E	54	ARG	Peptide
1	F	105	ARG	Sidechain
1	F	233	ARG	Sidechain
1	F	322	ALA	Peptide
1	F	85	ARG	Sidechain
1	G	233	ARG	Sidechain
1	G	291	PHE	Peptide
1	G	38	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	233	ARG	Sidechain
1	H	265	ARG	Sidechain
1	H	322	ALA	Peptide
1	H	54	ARG	Peptide
1	I	142	ARG	Sidechain
1	I	233	ARG	Sidechain
1	I	322	ALA	Peptide
1	J	212	ARG	Sidechain
1	J	265	ARG	Sidechain
1	K	265	ARG	Sidechain
1	K	54	ARG	Peptide
1	L	233	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 ⓘ

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	20	0
1	B	2715	0	2660	13	0
1	C	2714	0	2656	22	0
1	D	2715	0	2660	24	0
1	E	2718	0	2658	28	0
1	F	2703	0	2652	43	0
1	G	2710	0	2654	34	0
1	H	2715	0	2660	33	0
1	I	2715	0	2660	30	0
1	J	2715	0	2660	21	0
1	K	2710	0	2653	21	0
1	L	2715	0	2660	16	0
2	A	60	0	0	1	0
2	B	60	0	0	3	0
2	C	60	0	0	1	0
2	D	60	0	0	1	0
2	E	60	0	0	0	0
2	F	60	0	0	2	0
2	G	60	0	0	0	0
2	H	60	0	0	2	0
2	I	60	0	0	0	0
2	J	60	0	0	1	0
2	K	60	0	0	1	0
2	L	60	0	0	0	0
3	A	136	0	0	1	0
3	B	126	0	0	0	0
3	C	130	0	0	1	0
3	D	150	0	0	1	0
3	E	131	0	0	1	0
3	F	133	0	0	2	0
3	G	122	0	0	2	0
3	H	111	0	0	0	0
3	I	160	0	0	2	0
3	J	153	0	0	1	0
3	K	153	0	0	1	0
3	L	163	0	0	2	0
All	All	34951	0	31891	267	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 (267) 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:B:85:ARG:HD2	2:B:401:A1IZB:O9	1.83	0.79
1:F:85:ARG:HD3	2:F:401:A1IZB:O10	1.84	0.77
1:C:80:LEU:HD22	1:C:108:TYR:CE2	2.22	0.74
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.70	0.72
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.29	0.67
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.30	0.67
1:I:47:ARG:HH11	1:I:47:ARG:HB3	1.60	0.67
1:H:75:ALA:O	1:H:76:LYS:HB2	1.94	0.66
1:D:294:SER:HB2	1:L:293:ASN:O	1.97	0.65
1:F:85:ARG:CD	2:F:401:A1IZB:O10	2.45	0.65
1:G:80:LEU:CD2	1:G:108:TYR:CE2	2.79	0.65
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.77	0.64
1:F:39:PRO:C	1:F:41:SER:H	2.06	0.63
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.32	0.63
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.34	0.63
1:I:118:GLY:O	1:I:121:SER:OG	2.17	0.63
1:G:1:MET:O	1:G:6:SER:OG	2.12	0.62
1:E:255:ASP:HB3	1:E:258:GLU:HG2	1.81	0.62
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.35	0.61
1:E:85:ARG:NH1	1:E:122:GLN:O	2.34	0.60
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.84	0.60
1:K:138:HIS:HD2	3:K:568:HOH:O	1.84	0.60
1:F:98:GLU:OE2	1:F:101:LYS:HE2	2.01	0.59
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.37	0.59
1:C:28:ASP:HA	1:C:53:ASN:HD22	1.68	0.58
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.35	0.58
1:I:80:LEU:HD23	1:I:108:TYR:CE2	2.38	0.57
1:A:11:VAL:HG12	1:A:80:LEU:HD12	1.86	0.57
1:G:194:VAL:O	1:G:197:GLN:HB2	2.04	0.57
1:L:37:ASP:O	1:L:58:THR:HA	2.04	0.57
1:F:41:SER:O	1:F:42:VAL:HG23	2.04	0.57
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.40	0.57
1:A:163:PHE:O	1:B:332:PRO:HG3	2.05	0.56
1:C:291:PHE:O	1:C:294:SER:HB3	2.05	0.56
1:J:322:ALA:O	1:J:323:ASN:C	2.49	0.56
1:H:38:ARG:NH1	2:H:401:A1IZB:O12	2.39	0.56
1:H:28:ASP:HA	1:H:53:ASN:HD22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:HIS:HD2	3:A:542:HOH:O	1.89	0.55
1:H:28:ASP:HA	1:H:53:ASN:ND2	2.21	0.55
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.90	0.55
1:F:51:LEU:HA	1:F:54:ARG:NH1	2.22	0.55
1:D:80:LEU:CD2	1:D:108:TYR:CE2	2.90	0.55
1:I:294:SER:O	1:J:123:GLN:HG3	2.07	0.55
1:A:80:LEU:CD2	1:A:108:TYR:CE2	2.90	0.55
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.39	0.55
1:F:54:ARG:O	1:F:346:ALA:HB3	2.08	0.54
1:E:138:HIS:HD2	3:E:543:HOH:O	1.91	0.54
1:F:291:PHE:O	1:F:293:ASN:N	2.41	0.54
1:G:196:ILE:HG12	1:G:199:MET:HB2	1.89	0.54
1:H:60:ASP:O	1:H:66:GLY:HA3	2.07	0.54
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.90	0.53
1:C:135:GLY:HA2	1:D:302:LEU:O	2.07	0.53
1:G:80:LEU:HD23	1:G:108:TYR:CE2	2.43	0.53
1:C:138:HIS:HD2	3:C:578:HOH:O	1.91	0.53
1:G:28:ASP:HA	1:G:53:ASN:HD22	1.73	0.53
1:E:78:ASP:OD1	1:E:175:ARG:NH2	2.24	0.53
1:I:272:ARG:NH1	3:I:505:HOH:O	2.40	0.53
1:G:102:VAL:O	1:G:103:ASN:HB2	2.07	0.52
1:H:75:ALA:O	1:H:76:LYS:CB	2.57	0.52
1:L:198:MET:HE2	1:L:202:MET:SD	2.49	0.52
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.24	0.52
1:C:346:ALA:O	1:C:347:ALA:O	2.28	0.52
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.25	0.52
1:I:176:GLN:HG3	1:J:176:GLN:NE2	2.24	0.52
1:J:76:LYS:HE2	1:J:359:ASP:C	2.35	0.51
1:C:38:ARG:NH2	2:C:401:A1IZB:O12	2.43	0.51
1:L:88:VAL:O	1:L:92:LEU:HD12	2.09	0.51
1:G:302:LEU:O	1:H:135:GLY:HA2	2.11	0.51
1:G:28:ASP:HA	1:G:53:ASN:ND2	2.26	0.51
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.93	0.50
1:C:176:GLN:CD	1:D:176:GLN:HG2	2.36	0.50
1:F:39:PRO:O	1:F:41:SER:N	2.44	0.50
1:G:272:ARG:NH1	3:G:511:HOH:O	2.44	0.50
1:D:265:ARG:HD2	3:D:587:HOH:O	2.10	0.50
1:G:180:LYS:HB2	1:H:336:ARG:NH2	2.26	0.50
1:G:216:MET:HE1	2:H:401:A1IZB:C1	2.41	0.50
1:H:58:THR:O	1:H:59:ALA:HB2	2.11	0.50
1:K:39:PRO:HA	1:K:58:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.95	0.50
1:K:145:GLU:OE1	1:L:145:GLU:OE1	2.29	0.49
1:A:91:ARG:NH2	2:A:401:A1IZB:O17	2.45	0.49
1:I:323:ASN:OD1	1:I:323:ASN:N	2.44	0.49
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.48	0.49
1:I:60:ASP:OD1	1:I:62:LYS:HB2	2.13	0.49
1:C:19:GLY:N	1:C:20:PRO:CD	2.76	0.49
1:F:181:GLY:O	1:F:182:GLN:HB3	2.12	0.49
1:I:255:ASP:HB3	1:I:258:GLU:HG2	1.93	0.49
1:E:316:ARG:HD2	1:F:117:THR:O	2.13	0.49
1:I:38:ARG:HH21	1:I:38:ARG:HG3	1.77	0.49
1:G:336:ARG:HG2	1:G:336:ARG:HH11	1.76	0.49
1:I:54:ARG:HG2	1:I:54:ARG:HH11	1.78	0.48
1:D:85:ARG:HD3	2:D:401:A1IZB:O9	2.12	0.48
1:F:322:ALA:O	1:F:323:ASN:C	2.56	0.48
1:J:294:SER:HB2	1:K:293:ASN:O	2.14	0.48
1:E:255:ASP:HB3	1:E:258:GLU:CG	2.42	0.48
1:F:320:TYR:CE2	1:F:322:ALA:HB2	2.48	0.48
1:B:85:ARG:CD	2:B:401:A1IZB:O9	2.58	0.48
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.47	0.48
1:K:220:GLY:O	1:K:272:ARG:NH2	2.47	0.48
1:K:196:ILE:HG13	1:L:153:LEU:HD21	1.95	0.48
1:L:323:ASN:CG	1:L:324:GLY:H	2.22	0.48
1:G:4:PRO:O	1:H:174:GLU:HB2	2.14	0.47
1:F:118:GLY:O	1:F:121:SER:OG	2.29	0.47
1:H:320:TYR:HE2	1:H:322:ALA:HB2	1.78	0.47
1:F:37:ASP:O	1:F:58:THR:HA	2.14	0.47
1:F:293:ASN:ND2	3:F:503:HOH:O	2.26	0.47
1:E:107:ILE:HD12	1:E:171:ALA:HB1	1.95	0.47
1:A:225:ASP:OD2	1:A:272:ARG:NH1	2.47	0.47
1:F:244:PHE:HB3	1:F:295:ASP:O	2.15	0.47
1:H:1:MET:HE2	1:H:343:ARG:CZ	2.45	0.47
1:H:358:TRP:O	1:H:359:ASP:HB2	2.15	0.47
1:I:47:ARG:HB3	1:I:47:ARG:NH1	2.29	0.47
1:D:37:ASP:O	1:D:58:THR:HA	2.15	0.47
1:I:87:GLY:O	1:I:91:ARG:HG3	2.16	0.47
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.80	0.46
1:G:163:PHE:O	1:H:332:PRO:HG3	2.15	0.46
1:J:18:PRO:HB3	1:J:156:ASP:O	2.14	0.46
1:E:346:ALA:O	1:E:347:ALA:O	2.33	0.46
1:K:50:MET:HE1	1:L:198:MET:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:PRO:C	1:F:41:SER:N	2.72	0.46
1:G:18:PRO:HB3	1:G:156:ASP:O	2.14	0.46
1:G:111:MET:HE3	1:G:186:ALA:O	2.15	0.46
1:L:120:ARG:HD3	3:L:514:HOH:O	2.15	0.46
1:A:1:MET:HE2	1:A:343:ARG:NH2	2.29	0.46
1:E:47:ARG:HD2	1:F:205:THR:HG22	1.97	0.46
1:H:42:VAL:HG23	1:H:42:VAL:O	2.16	0.46
1:J:102:VAL:O	1:J:103:ASN:HB2	2.16	0.46
1:I:37:ASP:O	1:I:58:THR:HA	2.16	0.46
1:F:55:ARG:HD2	1:F:349:ILE:CD1	2.45	0.46
1:E:176:GLN:CD	1:F:176:GLN:HG2	2.40	0.46
1:E:353:ALA:O	1:E:356:THR:HB	2.15	0.46
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.51	0.45
1:D:107:ILE:HD12	1:D:171:ALA:HB1	1.97	0.45
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.99	0.45
1:I:198:MET:HB2	1:J:50:MET:HE1	1.97	0.45
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.51	0.45
1:E:117:THR:O	1:F:316:ARG:HD2	2.17	0.45
1:J:244:PHE:HB3	1:J:295:ASP:O	2.17	0.45
1:K:60:ASP:O	1:K:66:GLY:HA3	2.17	0.45
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.81	0.45
1:C:153:LEU:HD21	1:D:196:ILE:HG13	1.98	0.45
1:F:55:ARG:HD2	1:F:349:ILE:HD11	1.99	0.45
1:F:106:LEU:O	1:F:181:GLY:HA3	2.16	0.45
1:G:327:GLN:NE2	1:H:197:GLN:HE21	2.14	0.45
1:K:181:GLY:O	1:K:182:GLN:HB3	2.16	0.45
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.97	0.45
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.52	0.44
1:G:50:MET:O	1:G:50:MET:HG2	2.17	0.44
1:G:114:TRP:CZ3	1:G:133:LEU:HD22	2.53	0.44
1:L:73:LEU:HD11	1:L:351:ILE:HG13	1.99	0.44
1:F:329:MET:HE3	1:F:330:PRO:HD2	1.98	0.44
1:I:181:GLY:O	1:I:182:GLN:HB3	2.17	0.44
1:L:225:ASP:OD2	1:L:272:ARG:NH1	2.49	0.44
1:G:176:GLN:CD	1:H:176:GLN:HG2	2.42	0.44
1:I:117:THR:O	1:J:316:ARG:HD2	2.17	0.44
1:F:24:MET:HB3	1:F:24:MET:HE2	1.73	0.44
1:F:42:VAL:HG12	1:F:43:ASP:N	2.31	0.44
1:F:294:SER:HB3	1:G:293:ASN:HB3	1.99	0.44
1:I:268:TRP:N	1:I:269:PRO:CD	2.80	0.44
1:I:176:GLN:HG3	1:J:176:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LEU:HD12	1:C:67:LEU:O	2.17	0.44
1:F:346:ALA:O	1:F:347:ALA:O	2.35	0.44
1:J:62:LYS:NZ	2:J:401:A1IZB:O16	2.51	0.44
1:K:9:ARG:NH2	1:K:358:TRP:HA	2.33	0.44
1:L:80:LEU:CD2	1:L:108:TYR:CE2	3.00	0.44
1:F:54:ARG:O	1:F:346:ALA:CB	2.65	0.44
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.51	0.44
1:E:109:ALA:HB1	1:E:164:LEU:HD11	2.00	0.44
1:D:126:HIS:O	1:D:127:ASP:C	2.60	0.43
1:E:28:ASP:CG	1:E:52:ARG:HH21	2.26	0.43
1:E:135:GLY:HA2	1:F:302:LEU:O	2.17	0.43
1:A:140:ILE:CD1	1:B:151:LEU:HG	2.48	0.43
1:C:302:LEU:O	1:D:135:GLY:HA2	2.18	0.43
1:G:113:GLY:HA3	1:G:130:TYR:CZ	2.53	0.43
1:E:183:VAL:H	1:F:335:SER:HG	1.65	0.43
1:G:80:LEU:HD23	1:G:108:TYR:CD2	2.53	0.43
1:K:39:PRO:CA	1:K:58:THR:CG2	2.97	0.43
1:K:264:ASP:OD1	1:K:264:ASP:C	2.62	0.43
1:A:75:ALA:HA	1:A:103:ASN:HB2	2.01	0.43
1:D:140:ILE:HD13	1:D:150:PRO:HG3	1.99	0.43
1:H:9:ARG:NH2	1:H:358:TRP:HA	2.33	0.43
1:F:113:GLY:HA3	1:F:130:TYR:CZ	2.54	0.43
1:G:54:ARG:HG2	1:G:54:ARG:HH11	1.83	0.43
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.99	0.43
1:F:42:VAL:HG21	1:F:58:THR:HG22	2.00	0.43
1:F:114:TRP:CZ3	1:F:133:LEU:HD22	2.54	0.43
1:G:135:GLY:HA2	1:H:302:LEU:O	2.18	0.43
1:G:42:VAL:O	1:G:43:ASP:C	2.61	0.43
1:H:28:ASP:CG	1:H:52:ARG:HH21	2.27	0.43
1:I:241:GLU:HB2	1:I:244:PHE:CD2	2.54	0.43
1:K:91:ARG:NH2	2:K:401:A1IZB:O16	2.42	0.43
1:K:225:ASP:OD2	1:K:272:ARG:NH1	2.51	0.43
1:C:19:GLY:N	1:C:20:PRO:HD2	2.34	0.43
1:D:39:PRO:O	1:D:42:VAL:HG12	2.18	0.43
1:G:270:GLU:HG3	3:G:560:HOH:O	2.19	0.43
1:I:78:ASP:OD1	1:I:175:ARG:NH2	2.39	0.43
1:D:225:ASP:OD2	1:D:272:ARG:NH1	2.52	0.43
1:G:50:MET:HE1	1:H:198:MET:HB2	2.00	0.43
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.98	0.42
1:F:196:ILE:HG12	1:F:199:MET:HB2	2.01	0.42
1:G:181:GLY:O	1:G:182:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:HIS:HE1	3:J:633:HOH:O	2.00	0.42
1:F:113:GLY:HA2	1:F:188:MET:HB2	2.01	0.42
1:I:47:ARG:HH11	1:I:47:ARG:CB	2.30	0.42
1:C:18:PRO:HB3	1:C:156:ASP:O	2.19	0.42
1:E:302:LEU:O	1:F:135:GLY:HA2	2.19	0.42
1:G:323:ASN:O	1:G:324:GLY:C	2.63	0.42
1:A:180:LYS:O	1:B:336:ARG:NH2	2.53	0.42
1:C:336:ARG:HG2	1:C:336:ARG:HH11	1.84	0.42
1:D:106:LEU:O	1:D:181:GLY:HA3	2.20	0.42
1:A:224:TYR:HA	1:A:237:VAL:O	2.20	0.42
1:E:259:LEU:HD22	1:E:274:LEU:HD13	2.02	0.42
1:K:80:LEU:HD23	1:K:108:TYR:CE2	2.53	0.42
1:I:316:ARG:HD2	1:J:117:THR:O	2.20	0.42
1:A:28:ASP:HA	1:A:53:ASN:ND2	2.35	0.42
1:A:252:LEU:HD21	1:A:279:PHE:CE1	2.55	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.82	0.42
1:H:24:MET:HE2	1:H:24:MET:HB3	1.92	0.42
1:B:316:ARG:HB3	1:B:316:ARG:NH1	2.34	0.42
1:G:225:ASP:OD2	1:G:272:ARG:NH1	2.52	0.42
1:J:80:LEU:CD2	1:J:108:TYR:CE2	2.99	0.42
1:D:28:ASP:HA	1:D:53:ASN:ND2	2.35	0.41
1:E:13:LEU:O	1:E:14:ALA:C	2.62	0.41
1:I:138:HIS:HD2	3:I:532:HOH:O	2.04	0.41
1:E:24:MET:HE2	1:E:24:MET:HB3	1.95	0.41
1:K:1:MET:O	1:K:6:SER:OG	2.32	0.41
1:B:61:LEU:HG	2:B:401:A1IZB:N5	2.35	0.41
1:C:267:ARG:HH21	1:C:270:GLU:CD	2.29	0.41
1:K:126:HIS:O	1:K:127:ASP:C	2.63	0.41
1:I:327:GLN:NE2	1:J:197:GLN:HE21	2.18	0.41
1:A:114:TRP:CZ3	1:A:133:LEU:HD22	2.55	0.41
1:D:102:VAL:O	1:D:103:ASN:HB2	2.20	0.41
1:J:24:MET:HE2	1:J:24:MET:HB3	1.96	0.41
1:D:28:ASP:HA	1:D:53:ASN:HD22	1.85	0.41
1:E:28:ASP:HA	1:E:53:ASN:ND2	2.36	0.41
1:E:181:GLY:O	1:E:182:GLN:HB3	2.21	0.41
1:H:13:LEU:O	1:H:14:ALA:C	2.62	0.41
1:H:268:TRP:N	1:H:269:PRO:CD	2.83	0.41
1:I:230:ALA:HB2	1:I:280:ALA:O	2.20	0.41
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.56	0.41
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.55	0.41
1:D:303:ALA:O	1:D:304:PHE:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HE2	1:E:343:ARG:NH2	2.36	0.41
1:E:9:ARG:NH2	1:E:358:TRP:HA	2.36	0.41
1:F:80:LEU:HD23	1:F:108:TYR:CE2	2.56	0.41
1:I:291:PHE:O	1:I:294:SER:HB3	2.21	0.41
1:L:123:GLN:CD	3:L:514:HOH:O	2.63	0.41
1:K:39:PRO:HA	1:K:58:THR:HG21	2.03	0.41
1:K:174:GLU:OE1	1:K:174:GLU:C	2.64	0.41
1:A:60:ASP:O	1:A:66:GLY:HA3	2.21	0.40
1:D:114:TRP:CZ3	1:D:133:LEU:HD22	2.56	0.40
1:E:157:PHE:O	1:E:158:GLY:C	2.63	0.40
1:F:69:LEU:HD13	1:F:351:ILE:CG2	2.50	0.40
1:H:1:MET:HE2	1:H:343:ARG:NH2	2.36	0.40
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.55	0.40
1:F:105:ARG:HD2	3:F:513:HOH:O	2.21	0.40
1:H:174:GLU:OE1	1:H:174:GLU:C	2.64	0.40
1:I:302:LEU:O	1:J:135:GLY:HA2	2.21	0.40
1:B:45:ILE:HG23	1:B:346:ALA:O	2.21	0.40
1:H:196:ILE:HG12	1:H:199:MET:HB2	2.03	0.40
1:K:316:ARG:HD2	1:L:117:THR:O	2.21	0.40
1:C:196:ILE:HG12	1:C:199:MET:HB2	2.04	0.40
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.57	0.40
1:G:174:GLU:C	1:G:174:GLU:OE1	2.64	0.40
1:H:349:ILE:HD11	1:H:354:VAL:HG22	2.03	0.40
1:A:11:VAL:HG12	1:A:80:LEU:CD1	2.51	0.40
1:B:109:ALA:HB1	1:B:164:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	334 (93%)	23 (6%)	2 (1%)	21 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/364 (98%)	341 (95%)	16 (4%)	1 (0%)	36	36
1	C	357/364 (98%)	342 (96%)	12 (3%)	3 (1%)	16	12
1	D	358/364 (98%)	341 (95%)	15 (4%)	2 (1%)	21	18
1	E	359/364 (99%)	341 (95%)	15 (4%)	3 (1%)	16	12
1	F	354/364 (97%)	331 (94%)	15 (4%)	8 (2%)	5	2
1	G	358/364 (98%)	333 (93%)	20 (6%)	5 (1%)	9	5
1	H	358/364 (98%)	335 (94%)	21 (6%)	2 (1%)	21	18
1	I	358/364 (98%)	339 (95%)	18 (5%)	1 (0%)	36	36
1	J	358/364 (98%)	342 (96%)	14 (4%)	2 (1%)	21	18
1	K	356/364 (98%)	340 (96%)	15 (4%)	1 (0%)	36	36
1	L	358/364 (98%)	341 (95%)	17 (5%)	0	100	100
All	All	4291/4368 (98%)	4060 (95%)	201 (5%)	30 (1%)	18	15

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	C	103	ASN
1	C	347	ALA
1	D	103	ASN
1	E	347	ALA
1	F	40	SER
1	F	42	VAL
1	F	347	ALA
1	G	43	ASP
1	G	103	ASN
1	H	59	ALA
1	A	40	SER
1	B	103	ASN
1	F	41	SER
1	F	103	ASN
1	F	292	ALA
1	G	46	SER
1	G	347	ALA
1	I	103	ASN
1	J	103	ASN
1	H	103	ASN
1	K	103	ASN

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Mol	Chain	Res	Type
1	D	43	ASP
1	E	103	ASN
1	E	151	LEU
1	F	151	LEU
1	C	59	ALA
1	F	59	ALA
1	G	42	VAL
1	J	323	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/277 (100%)	271 (98%)	6 (2%)	45	52
1	B	276/277 (100%)	270 (98%)	6 (2%)	45	52
1	C	276/277 (100%)	268 (97%)	8 (3%)	37	41
1	D	276/277 (100%)	268 (97%)	8 (3%)	37	41
1	E	277/277 (100%)	268 (97%)	9 (3%)	34	37
1	F	275/277 (99%)	266 (97%)	9 (3%)	33	36
1	G	276/277 (100%)	265 (96%)	11 (4%)	28	28
1	H	276/277 (100%)	269 (98%)	7 (2%)	42	47
1	I	276/277 (100%)	271 (98%)	5 (2%)	51	59
1	J	276/277 (100%)	274 (99%)	2 (1%)	76	83
1	K	276/277 (100%)	268 (97%)	8 (3%)	37	41
1	L	276/277 (100%)	271 (98%)	5 (2%)	51	59
All	All	3313/3324 (100%)	3229 (98%)	84 (2%)	42	47

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	58	THR

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Mol	Chain	Res	Type
1	A	180	LYS
1	A	243	GLN
1	A	349	ILE
1	A	359	ASP
1	B	6	SER
1	B	42	VAL
1	B	85	ARG
1	B	177	SER
1	B	212	ARG
1	B	356	THR
1	C	6	SER
1	C	40	SER
1	C	47	ARG
1	C	58	THR
1	C	76	LYS
1	C	80	LEU
1	C	258	GLU
1	C	351	ILE
1	D	40	SER
1	D	42	VAL
1	D	43	ASP
1	D	45	ILE
1	D	65	GLN
1	D	85	ARG
1	D	91	ARG
1	D	294	SER
1	E	6	SER
1	E	43	ASP
1	E	58	THR
1	E	68	GLU
1	E	76	LYS
1	E	248	MET
1	E	258	GLU
1	E	290	VAL
1	E	351	ILE
1	F	40	SER
1	F	42	VAL
1	F	45	ILE
1	F	85	ARG
1	F	176	GLN
1	F	203	ARG
1	F	255	ASP

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Mol	Chain	Res	Type
1	F	258	GLU
1	F	350	ASP
1	G	6	SER
1	G	40	SER
1	G	42	VAL
1	G	43	ASP
1	G	45	ILE
1	G	58	THR
1	G	255	ASP
1	G	258	GLU
1	G	293	ASN
1	G	348	THR
1	G	357	ASP
1	H	41	SER
1	H	177	SER
1	H	209	THR
1	H	243	GLN
1	H	290	VAL
1	H	323	ASN
1	H	349	ILE
1	I	42	VAL
1	I	47	ARG
1	I	68	GLU
1	I	121	SER
1	I	323	ASN
1	J	176	GLN
1	J	209	THR
1	K	6	SER
1	K	40	SER
1	K	42	VAL
1	K	176	GLN
1	K	258	GLU
1	K	265	ARG
1	K	290	VAL
1	K	349	ILE
1	L	68	GLU
1	L	92	LEU
1	L	243	GLN
1	L	248	MET
1	L	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1IZB	F	401	-	59,62,62	0.88	3 (5%)	81,89,89	1.17	6 (7%)
2	A1IZB	I	401	-	59,62,62	0.91	4 (6%)	81,89,89	1.34	10 (12%)
2	A1IZB	L	401	-	59,62,62	0.98	4 (6%)	81,89,89	1.28	5 (6%)
2	A1IZB	J	401	-	59,62,62	0.90	4 (6%)	81,89,89	1.26	10 (12%)
2	A1IZB	B	401	-	59,62,62	0.88	3 (5%)	81,89,89	1.18	9 (11%)
2	A1IZB	D	401	-	59,62,62	0.82	2 (3%)	81,89,89	1.19	6 (7%)
2	A1IZB	A	401	-	59,62,62	0.85	3 (5%)	81,89,89	1.26	10 (12%)
2	A1IZB	H	401	-	59,62,62	1.14	4 (6%)	81,89,89	1.24	8 (9%)
2	A1IZB	E	401	-	59,62,62	0.86	4 (6%)	81,89,89	1.20	6 (7%)
2	A1IZB	C	401	-	59,62,62	0.91	3 (5%)	81,89,89	1.07	7 (8%)
2	A1IZB	K	401	-	59,62,62	0.79	2 (3%)	81,89,89	1.18	7 (8%)
2	A1IZB	G	401	-	59,62,62	0.90	3 (5%)	81,89,89	1.44	13 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IZB	F	401	-	-	13/62/79/79	0/3/3/3
2	A1IZB	I	401	-	-	13/62/79/79	0/3/3/3
2	A1IZB	L	401	-	-	18/62/79/79	0/3/3/3
2	A1IZB	J	401	-	-	9/62/79/79	0/3/3/3
2	A1IZB	B	401	-	-	13/62/79/79	0/3/3/3
2	A1IZB	D	401	-	-	7/62/79/79	0/3/3/3
2	A1IZB	A	401	-	-	11/62/79/79	0/3/3/3
2	A1IZB	H	401	-	-	18/62/79/79	0/3/3/3
2	A1IZB	E	401	-	-	17/62/79/79	0/3/3/3
2	A1IZB	C	401	-	-	12/62/79/79	0/3/3/3
2	A1IZB	K	401	-	-	11/62/79/79	0/3/3/3
2	A1IZB	G	401	-	-	11/62/79/79	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	A1IZB	P1-O8	4.61	1.64	1.59
2	H	401	A1IZB	O1-C11	4.10	1.26	1.20
2	G	401	A1IZB	O1-C11	3.89	1.26	1.20
2	I	401	A1IZB	O1-C11	3.87	1.26	1.20
2	L	401	A1IZB	O1-C11	3.60	1.25	1.20
2	C	401	A1IZB	P1-O8	3.40	1.63	1.59
2	H	401	A1IZB	P2-O8	3.38	1.63	1.59
2	E	401	A1IZB	O1-C11	3.25	1.25	1.20
2	B	401	A1IZB	O1-C11	3.17	1.25	1.20
2	F	401	A1IZB	P2-O8	3.13	1.62	1.59
2	L	401	A1IZB	P1-O8	3.12	1.62	1.59
2	L	401	A1IZB	P2-O8	3.12	1.62	1.59
2	C	401	A1IZB	O1-C11	3.11	1.25	1.20
2	D	401	A1IZB	O1-C11	2.93	1.25	1.20
2	D	401	A1IZB	P3-O14	2.87	1.64	1.59
2	F	401	A1IZB	O1-C11	2.85	1.24	1.20
2	A	401	A1IZB	P3-O14	2.84	1.64	1.59
2	L	401	A1IZB	P3-O14	2.80	1.64	1.59
2	A	401	A1IZB	P2-O8	2.77	1.62	1.59
2	E	401	A1IZB	P1-O8	2.76	1.62	1.59
2	F	401	A1IZB	O2-C14	2.75	1.28	1.23
2	G	401	A1IZB	P3-O14	2.73	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	A1IZB	O1-C11	2.72	1.24	1.20
2	A	401	A1IZB	O1-C11	2.65	1.24	1.20
2	B	401	A1IZB	P3-O14	2.64	1.64	1.59
2	J	401	A1IZB	O1-C11	2.59	1.24	1.20
2	J	401	A1IZB	P3-O14	2.43	1.63	1.59
2	B	401	A1IZB	C11-S1	2.31	1.82	1.75
2	I	401	A1IZB	C22-C19	2.26	1.56	1.52
2	H	401	A1IZB	C11-S1	2.22	1.82	1.75
2	E	401	A1IZB	P3-O14	2.21	1.63	1.59
2	K	401	A1IZB	P3-O14	2.17	1.63	1.59
2	J	401	A1IZB	P3-O17	-2.13	1.46	1.54
2	J	401	A1IZB	C22-C19	2.13	1.56	1.52
2	E	401	A1IZB	P2-O8	2.09	1.61	1.59
2	I	401	A1IZB	P3-O14	2.07	1.63	1.59
2	G	401	A1IZB	O2-C14	2.05	1.27	1.23
2	I	401	A1IZB	P2-O8	2.05	1.61	1.59
2	C	401	A1IZB	O2-C14	2.01	1.27	1.23

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	A1IZB	C31-C32-C24	-5.33	93.91	103.24
2	L	401	A1IZB	C31-C32-C24	-4.91	94.65	103.24
2	G	401	A1IZB	O6-P1-O7	4.78	134.68	112.44
2	H	401	A1IZB	O14-P3-O15	-4.76	92.35	109.33
2	I	401	A1IZB	C31-C32-C24	-4.41	95.52	103.24
2	E	401	A1IZB	O14-P3-O15	-4.29	94.03	109.33
2	L	401	A1IZB	C12-S1-C11	4.11	113.53	101.73
2	F	401	A1IZB	C31-C32-C24	-4.09	96.07	103.24
2	F	401	A1IZB	O14-P3-O15	-4.09	94.75	109.33
2	J	401	A1IZB	O16-P3-O14	-4.01	90.22	105.85
2	K	401	A1IZB	C31-C32-C24	-3.98	96.28	103.24
2	B	401	A1IZB	C31-C32-C24	-3.77	96.63	103.24
2	A	401	A1IZB	C31-C32-C24	-3.67	96.82	103.24
2	G	401	A1IZB	C31-C32-C24	-3.63	96.88	103.24
2	I	401	A1IZB	O6-P1-O7	3.63	129.34	112.44
2	E	401	A1IZB	O13-C31-C32	3.62	121.33	111.19
2	G	401	A1IZB	O14-P3-O15	-3.60	96.49	109.33
2	H	401	A1IZB	C16-C15-C14	3.56	118.33	112.39
2	I	401	A1IZB	O14-P3-O15	-3.51	96.81	109.33
2	L	401	A1IZB	C24-O12-C25	-3.48	101.77	109.47
2	K	401	A1IZB	O14-P3-O15	-3.47	96.96	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	401	A1IZB	C31-C32-C24	-3.46	97.19	103.24
2	E	401	A1IZB	C31-C32-C24	-3.45	97.19	103.24
2	B	401	A1IZB	O16-P3-O14	3.41	119.14	105.85
2	G	401	A1IZB	O16-P3-O14	3.40	119.08	105.85
2	G	401	A1IZB	O13-C31-C32	3.39	120.68	111.19
2	A	401	A1IZB	O9-P2-O8	3.30	116.19	107.27
2	D	401	A1IZB	C24-O12-C25	-3.29	102.19	109.47
2	G	401	A1IZB	O13-C31-C25	-3.27	98.85	110.10
2	J	401	A1IZB	O6-P1-O7	3.27	127.64	112.44
2	A	401	A1IZB	C21-C19-C22	-3.26	102.84	108.22
2	H	401	A1IZB	P3-O14-C32	3.25	132.10	123.43
2	J	401	A1IZB	O16-P3-O15	3.21	123.33	110.83
2	I	401	A1IZB	C24-O12-C25	-3.20	102.41	109.47
2	E	401	A1IZB	P3-O14-C32	3.19	131.96	123.43
2	G	401	A1IZB	P3-O14-C32	3.18	131.93	123.43
2	L	401	A1IZB	C8-C9-C11	3.18	120.39	110.10
2	K	401	A1IZB	O5-P1-O7	-3.15	96.45	108.94
2	G	401	A1IZB	O8-P1-O7	-3.12	101.31	110.70
2	C	401	A1IZB	C31-C32-C24	-3.12	97.78	103.24
2	I	401	A1IZB	O9-P2-O8	3.10	115.66	107.27
2	A	401	A1IZB	O6-P1-O7	3.06	126.70	112.44
2	J	401	A1IZB	O14-P3-O15	3.06	120.24	109.33
2	H	401	A1IZB	C31-C32-C24	-2.99	98.00	103.24
2	F	401	A1IZB	O6-P1-O7	2.96	126.23	112.44
2	L	401	A1IZB	O6-P1-O7	2.96	126.23	112.44
2	H	401	A1IZB	O17-P3-O15	2.96	122.38	110.83
2	K	401	A1IZB	P3-O14-C32	2.90	131.17	123.43
2	G	401	A1IZB	O5-P1-O7	-2.86	97.61	108.94
2	A	401	A1IZB	O17-P3-O15	-2.81	99.88	110.83
2	B	401	A1IZB	O17-P3-O14	-2.81	94.90	105.85
2	B	401	A1IZB	C31-C25-N3	-2.81	106.33	113.30
2	D	401	A1IZB	O6-P1-O7	2.80	125.45	112.44
2	I	401	A1IZB	O17-P3-O15	2.73	121.46	110.83
2	J	401	A1IZB	O5-P1-O7	-2.70	98.24	108.94
2	D	401	A1IZB	C21-C19-C18	2.67	113.32	108.77
2	C	401	A1IZB	P3-O14-C32	2.67	130.56	123.43
2	I	401	A1IZB	C10-C9-C8	2.59	117.83	111.29
2	I	401	A1IZB	C13-N1-C14	-2.58	118.03	122.82
2	K	401	A1IZB	C24-O12-C25	-2.54	103.86	109.47
2	A	401	A1IZB	O6-P1-O5	-2.51	96.18	107.57
2	B	401	A1IZB	O17-P3-O16	2.51	117.20	107.80
2	C	401	A1IZB	O17-P3-O14	-2.50	96.09	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	A1IZB	O16-P3-O15	2.50	120.57	110.83
2	G	401	A1IZB	C12-S1-C11	-2.48	94.62	101.73
2	B	401	A1IZB	O16-P3-O15	-2.47	101.20	110.83
2	G	401	A1IZB	O17-P3-O16	-2.47	98.53	107.80
2	K	401	A1IZB	O6-P1-O7	2.46	123.89	112.44
2	J	401	A1IZB	P3-O14-C32	2.42	129.89	123.43
2	C	401	A1IZB	O17-P3-O15	2.41	120.22	110.83
2	I	401	A1IZB	O5-P1-O7	-2.41	99.39	108.94
2	B	401	A1IZB	C24-O12-C25	-2.41	104.16	109.47
2	J	401	A1IZB	C24-O12-C25	-2.39	104.19	109.47
2	A	401	A1IZB	C16-C15-C14	2.36	116.32	112.39
2	J	401	A1IZB	O9-P2-O8	2.35	113.62	107.27
2	I	401	A1IZB	C21-C19-C22	2.32	112.05	108.22
2	E	401	A1IZB	O16-P3-O14	2.31	114.85	105.85
2	A	401	A1IZB	C23-C24-C32	2.30	122.02	114.38
2	E	401	A1IZB	O1-C11-S1	-2.27	120.74	123.80
2	C	401	A1IZB	O16-P3-O14	2.25	114.61	105.85
2	F	401	A1IZB	O16-P3-O14	2.24	114.60	105.85
2	H	401	A1IZB	C16-N2-C17	2.23	126.55	122.55
2	F	401	A1IZB	O8-P1-O7	-2.21	104.05	110.70
2	D	401	A1IZB	O9-P2-O8	2.19	113.20	107.27
2	H	401	A1IZB	O16-P3-O14	2.19	114.39	105.85
2	A	401	A1IZB	O17-P3-O14	2.18	114.34	105.85
2	A	401	A1IZB	C24-O12-C25	-2.17	104.67	109.47
2	B	401	A1IZB	O13-C31-C32	2.15	117.22	111.19
2	G	401	A1IZB	O17-P3-O15	2.15	119.20	110.83
2	B	401	A1IZB	C12-S1-C11	-2.11	95.66	101.73
2	F	401	A1IZB	C24-O12-C25	-2.10	104.83	109.47
2	C	401	A1IZB	O5-P1-O7	-2.10	100.61	108.94
2	C	401	A1IZB	O6-P1-O7	2.08	122.11	112.44
2	G	401	A1IZB	C24-O12-C25	-2.05	104.94	109.47
2	J	401	A1IZB	C13-N1-C14	-2.05	119.01	122.82
2	H	401	A1IZB	O12-C24-C32	-2.04	100.61	104.92
2	D	401	A1IZB	O13-C31-C25	2.00	116.99	110.10

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1IZB	S1-C11-C9-C10
2	A	401	A1IZB	C14-C15-C16-N2
2	B	401	A1IZB	S1-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
2	B	401	A1IZB	C7-C8-C9-C11
2	B	401	A1IZB	C7-C8-C9-C10
2	B	401	A1IZB	C23-O11-P2-O9
2	C	401	A1IZB	C7-C8-C9-C11
2	C	401	A1IZB	C7-C8-C9-C10
2	C	401	A1IZB	C14-C15-C16-N2
2	C	401	A1IZB	C23-O11-P2-O9
2	D	401	A1IZB	S1-C11-C9-C10
2	D	401	A1IZB	C14-C15-C16-N2
2	D	401	A1IZB	C23-O11-P2-O8
2	D	401	A1IZB	C23-O11-P2-O9
2	D	401	A1IZB	C23-O11-P2-O10
2	E	401	A1IZB	C7-C8-C9-C11
2	E	401	A1IZB	C7-C8-C9-C10
2	E	401	A1IZB	C12-C13-N1-C14
2	E	401	A1IZB	C14-C15-C16-N2
2	F	401	A1IZB	S1-C11-C9-C10
2	F	401	A1IZB	C14-C15-C16-N2
2	F	401	A1IZB	C23-O11-P2-O9
2	G	401	A1IZB	S1-C11-C9-C10
2	G	401	A1IZB	C14-C15-C16-N2
2	G	401	A1IZB	C23-O11-P2-O9
2	H	401	A1IZB	C7-C8-C9-C10
2	H	401	A1IZB	C14-C15-C16-N2
2	I	401	A1IZB	C14-C15-C16-N2
2	I	401	A1IZB	C22-O5-P1-O6
2	J	401	A1IZB	S1-C11-C9-C10
2	J	401	A1IZB	C23-O11-P2-O10
2	K	401	A1IZB	C14-C15-C16-N2
2	L	401	A1IZB	C9-C11-S1-C12
2	L	401	A1IZB	O1-C11-S1-C12
2	L	401	A1IZB	C7-C8-C9-C11
2	L	401	A1IZB	C7-C8-C9-C10
2	L	401	A1IZB	C13-C12-S1-C11
2	L	401	A1IZB	C22-O5-P1-O7
2	L	401	A1IZB	C23-O11-P2-O9
2	L	401	A1IZB	C23-O11-P2-O10
2	B	401	A1IZB	C6-C7-C8-C9
2	E	401	A1IZB	O11-C23-C24-O12
2	G	401	A1IZB	C6-C7-C8-C9
2	F	401	A1IZB	C6-C7-C8-C9
2	B	401	A1IZB	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	401	A1IZB	C6-C7-C8-C9
2	E	401	A1IZB	O11-C23-C24-C32
2	G	401	A1IZB	C2-C3-C4-C5
2	I	401	A1IZB	C6-C7-C8-C9
2	D	401	A1IZB	C7-C8-C9-C10
2	F	401	A1IZB	C7-C8-C9-C10
2	E	401	A1IZB	C6-C7-C8-C9
2	L	401	A1IZB	C3-C4-C5-C6
2	H	401	A1IZB	O11-C23-C24-O12
2	L	401	A1IZB	C5-C6-C7-C8
2	J	401	A1IZB	C2-C3-C4-C5
2	B	401	A1IZB	C1-C2-C3-C4
2	B	401	A1IZB	C14-C15-C16-N2
2	F	401	A1IZB	C7-C8-C9-C11
2	E	401	A1IZB	C3-C4-C5-C6
2	J	401	A1IZB	C5-C6-C7-C8
2	L	401	A1IZB	O2-C14-N1-C13
2	F	401	A1IZB	C2-C3-C4-C5
2	I	401	A1IZB	C5-C6-C7-C8
2	G	401	A1IZB	C7-C8-C9-C10
2	E	401	A1IZB	C2-C3-C4-C5
2	C	401	A1IZB	O1-C11-C9-C8
2	H	401	A1IZB	O1-C11-C9-C8
2	I	401	A1IZB	O1-C11-C9-C8
2	F	401	A1IZB	C1-C2-C3-C4
2	C	401	A1IZB	C1-C2-C3-C4
2	L	401	A1IZB	C15-C14-N1-C13
2	G	401	A1IZB	C5-C6-C7-C8
2	G	401	A1IZB	C3-C4-C5-C6
2	K	401	A1IZB	C5-C6-C7-C8
2	A	401	A1IZB	C7-C8-C9-C10
2	K	401	A1IZB	C7-C8-C9-C10
2	H	401	A1IZB	C5-C6-C7-C8
2	H	401	A1IZB	C1-C2-C3-C4
2	E	401	A1IZB	C1-C2-C3-C4
2	H	401	A1IZB	C7-C8-C9-C11
2	I	401	A1IZB	C7-C8-C9-C11
2	L	401	A1IZB	C6-C7-C8-C9
2	K	401	A1IZB	C9-C11-S1-C12
2	K	401	A1IZB	O1-C11-C9-C8
2	L	401	A1IZB	O1-C11-C9-C8
2	H	401	A1IZB	C21-C19-C22-O5

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Mol	Chain	Res	Type	Atoms
2	E	401	A1IZB	C5-C6-C7-C8
2	H	401	A1IZB	C18-C19-C22-O5
2	A	401	A1IZB	C23-O11-P2-O8
2	A	401	A1IZB	C23-O11-P2-O9
2	A	401	A1IZB	C23-O11-P2-O10
2	B	401	A1IZB	C23-O11-P2-O8
2	B	401	A1IZB	C23-O11-P2-O10
2	C	401	A1IZB	C23-O11-P2-O8
2	C	401	A1IZB	C23-O11-P2-O10
2	F	401	A1IZB	C23-O11-P2-O8
2	F	401	A1IZB	C23-O11-P2-O10
2	G	401	A1IZB	C23-O11-P2-O8
2	G	401	A1IZB	C23-O11-P2-O10
2	H	401	A1IZB	C23-O11-P2-O10
2	I	401	A1IZB	C23-O11-P2-O8
2	I	401	A1IZB	C23-O11-P2-O9
2	I	401	A1IZB	C23-O11-P2-O10
2	J	401	A1IZB	C23-O11-P2-O8
2	J	401	A1IZB	C23-O11-P2-O9
2	K	401	A1IZB	C23-O11-P2-O8
2	K	401	A1IZB	C23-O11-P2-O9
2	K	401	A1IZB	C23-O11-P2-O10
2	L	401	A1IZB	C23-O11-P2-O8
2	H	401	A1IZB	C24-C32-O14-P3
2	J	401	A1IZB	O11-C23-C24-O12
2	A	401	A1IZB	P1-O8-P2-O9
2	J	401	A1IZB	P1-O8-P2-O9
2	A	401	A1IZB	C7-C8-C9-C11
2	D	401	A1IZB	C7-C8-C9-C11
2	G	401	A1IZB	C7-C8-C9-C11
2	K	401	A1IZB	C7-C8-C9-C11
2	L	401	A1IZB	C32-O14-P3-O17
2	C	401	A1IZB	C3-C4-C5-C6
2	C	401	A1IZB	C5-C6-C7-C8
2	E	401	A1IZB	O1-C11-C9-C8
2	H	401	A1IZB	P1-O8-P2-O9
2	H	401	A1IZB	C6-C7-C8-C9
2	H	401	A1IZB	O11-C23-C24-C32
2	C	401	A1IZB	O11-C23-C24-O12
2	A	401	A1IZB	C4-C5-C6-C7
2	L	401	A1IZB	C15-C16-N2-C17
2	J	401	A1IZB	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	L	401	A1IZB	C24-C32-O14-P3
2	B	401	A1IZB	P1-O8-P2-O9
2	E	401	A1IZB	P2-O8-P1-O6
2	E	401	A1IZB	P1-O8-P2-O9
2	E	401	A1IZB	P1-O8-P2-O10
2	F	401	A1IZB	P1-O8-P2-O10
2	I	401	A1IZB	P1-O8-P2-O9
2	K	401	A1IZB	P1-O8-P2-O9
2	I	401	A1IZB	C9-C11-S1-C12
2	I	401	A1IZB	O11-C23-C24-O12
2	A	401	A1IZB	C32-O14-P3-O17
2	H	401	A1IZB	C32-O14-P3-O17
2	E	401	A1IZB	C21-C19-C22-O5
2	H	401	A1IZB	C20-C19-C22-O5
2	F	401	A1IZB	C4-C5-C6-C7
2	H	401	A1IZB	C3-C4-C5-C6
2	H	401	A1IZB	C32-O14-P3-O15
2	I	401	A1IZB	C7-C8-C9-C10
2	B	401	A1IZB	P1-O8-P2-O10
2	C	401	A1IZB	P1-O8-P2-O9
2	E	401	A1IZB	P2-O8-P1-O7
2	F	401	A1IZB	P1-O8-P2-O9
2	K	401	A1IZB	P1-O8-P2-O10
2	B	401	A1IZB	O11-C23-C24-O12

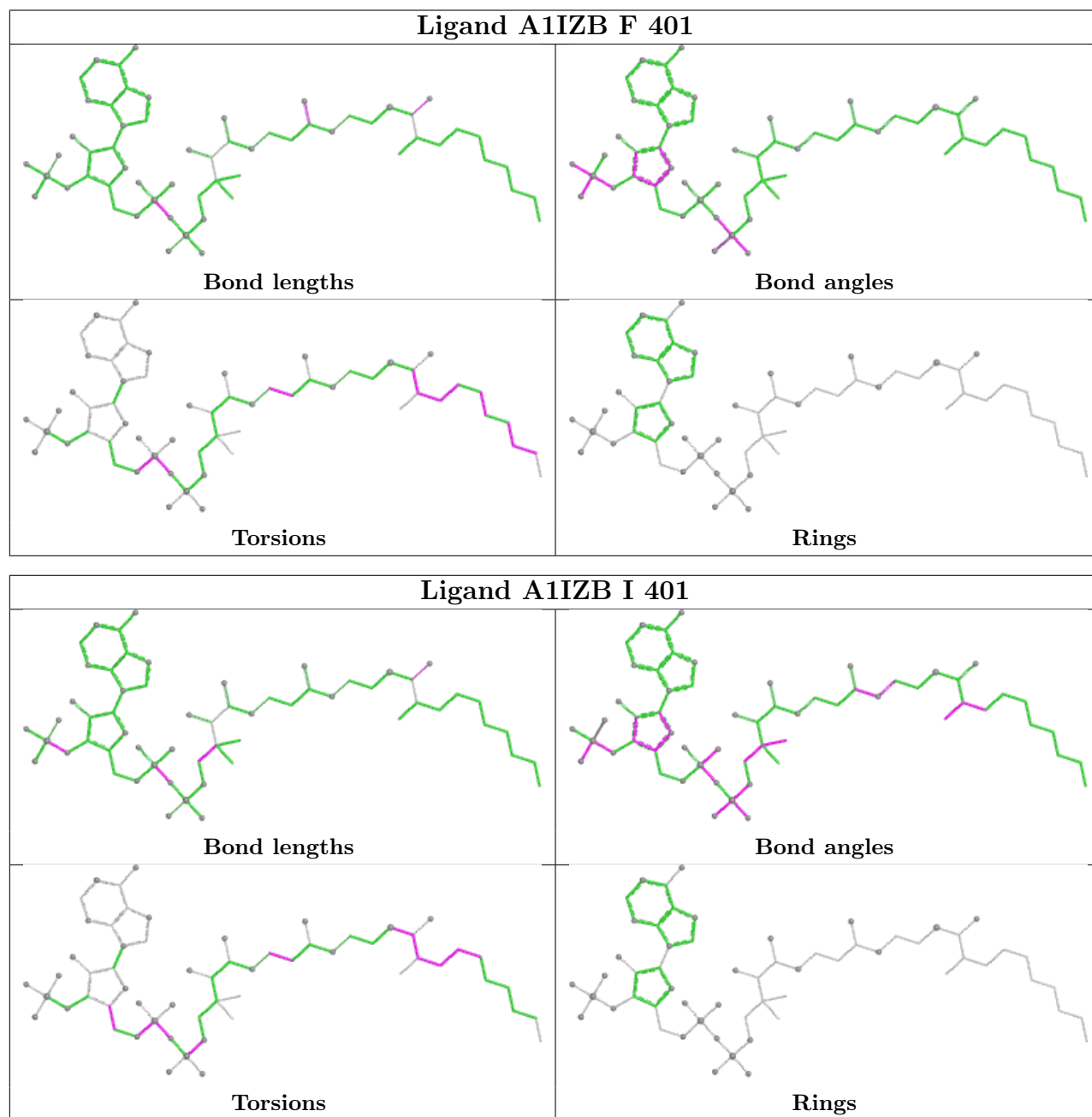
There are no ring outliers.

8 monomers are involved in 12 short contacts:

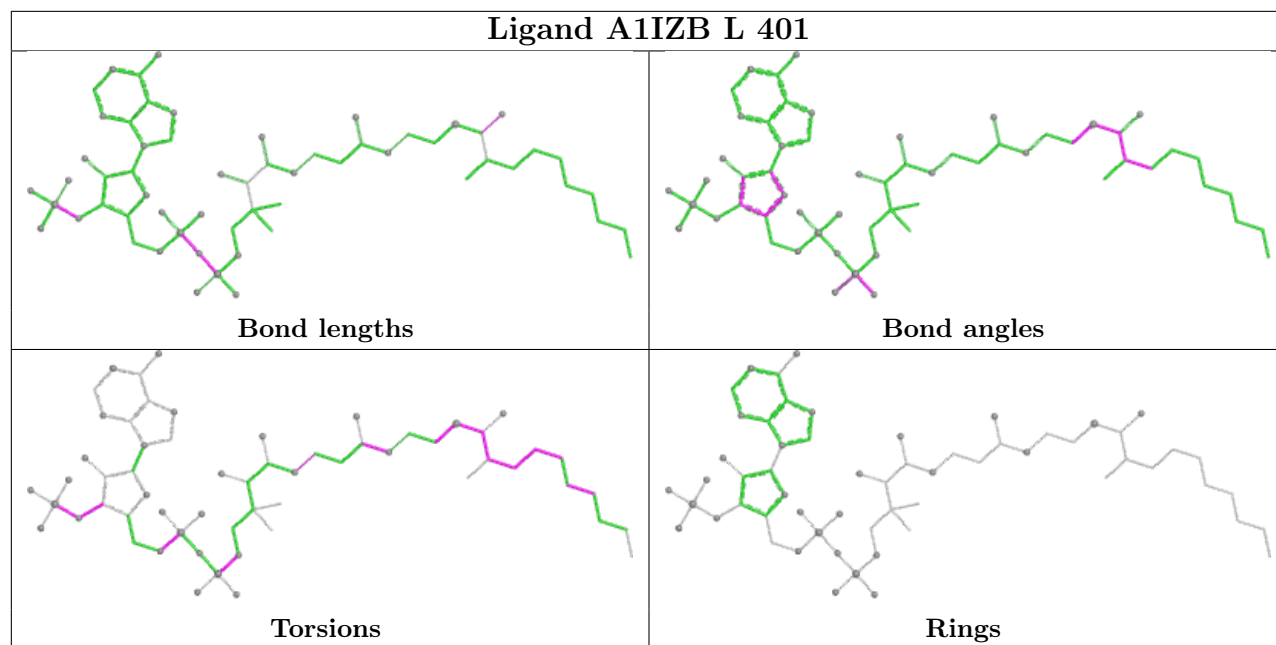
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	A1IZB	2	0
2	J	401	A1IZB	1	0
2	B	401	A1IZB	3	0
2	D	401	A1IZB	1	0
2	A	401	A1IZB	1	0
2	H	401	A1IZB	2	0
2	C	401	A1IZB	1	0
2	K	401	A1IZB	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

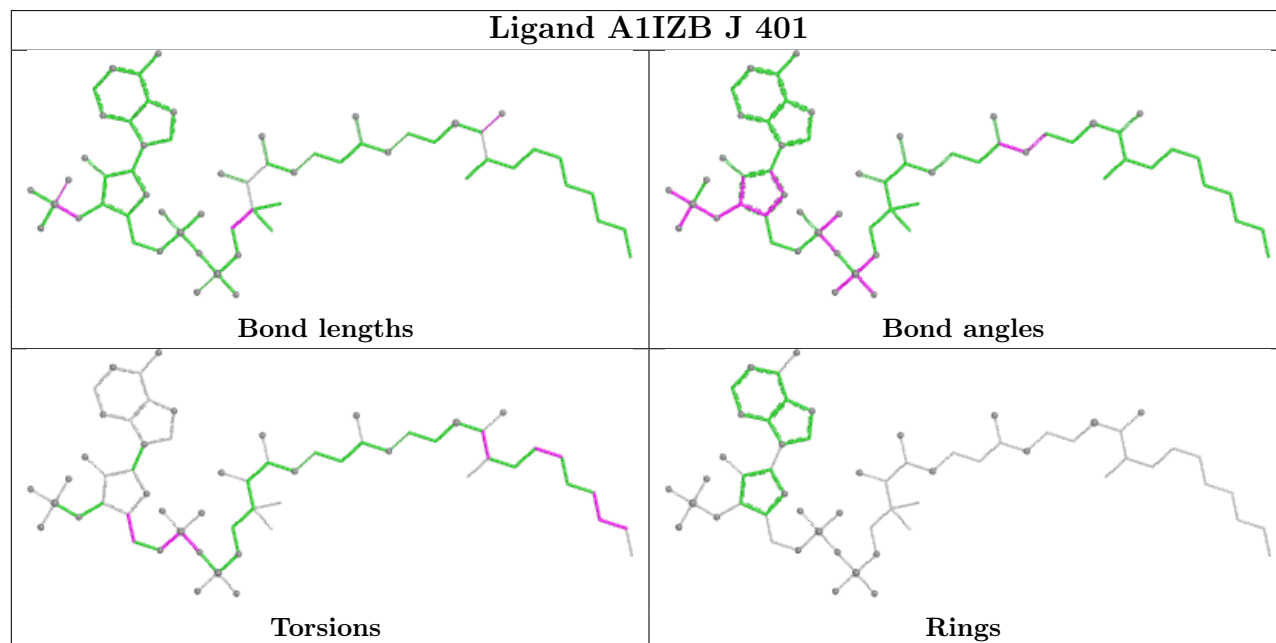
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



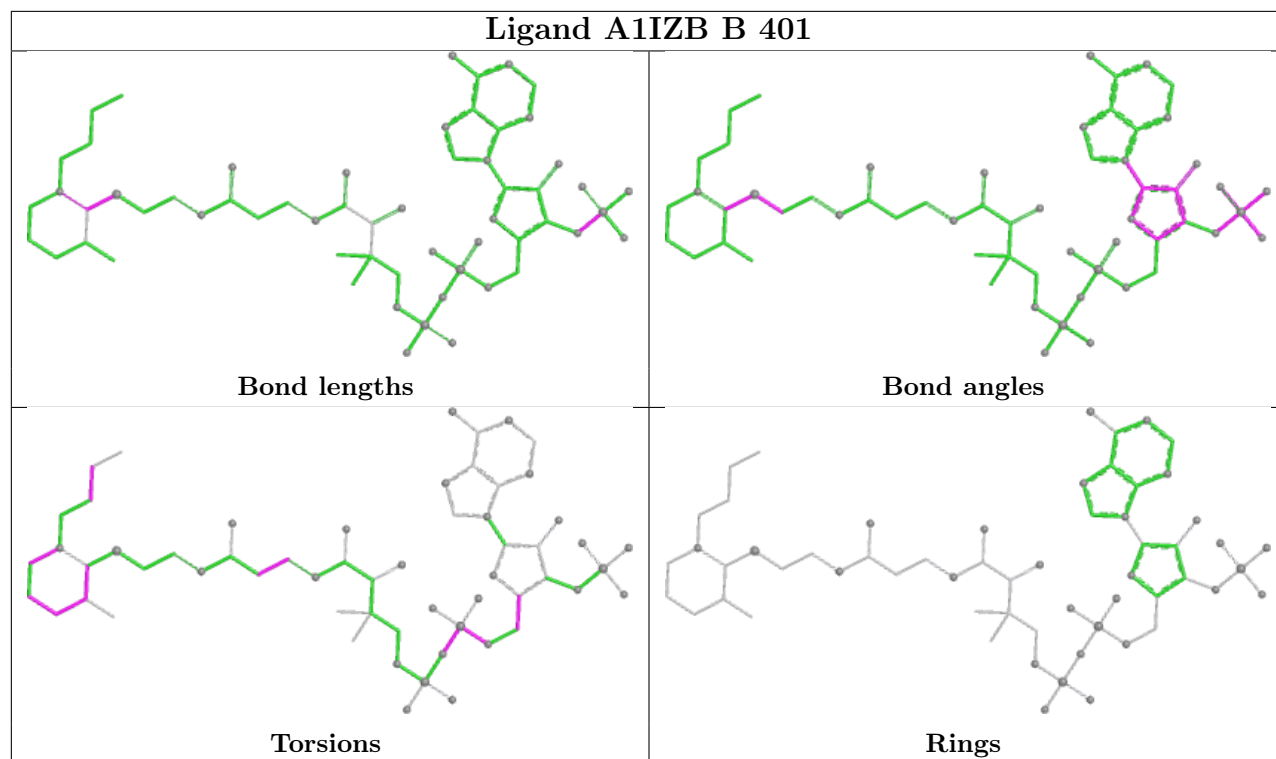
Ligand A1IZB L 401



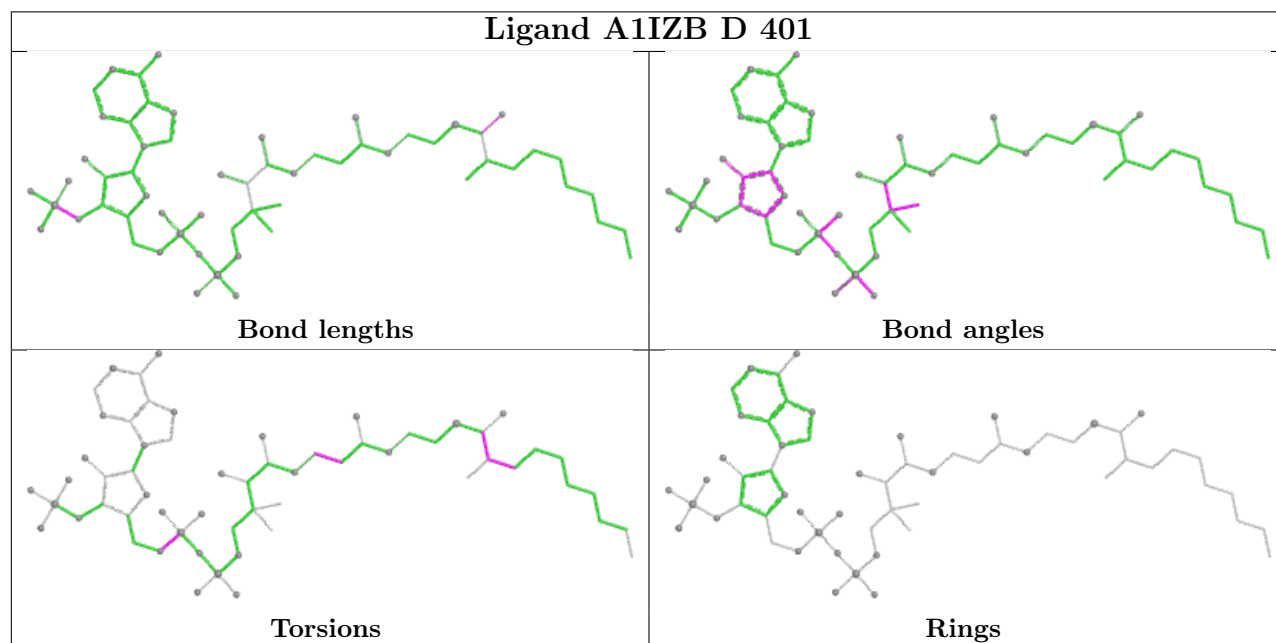
Ligand A1IZB J 401



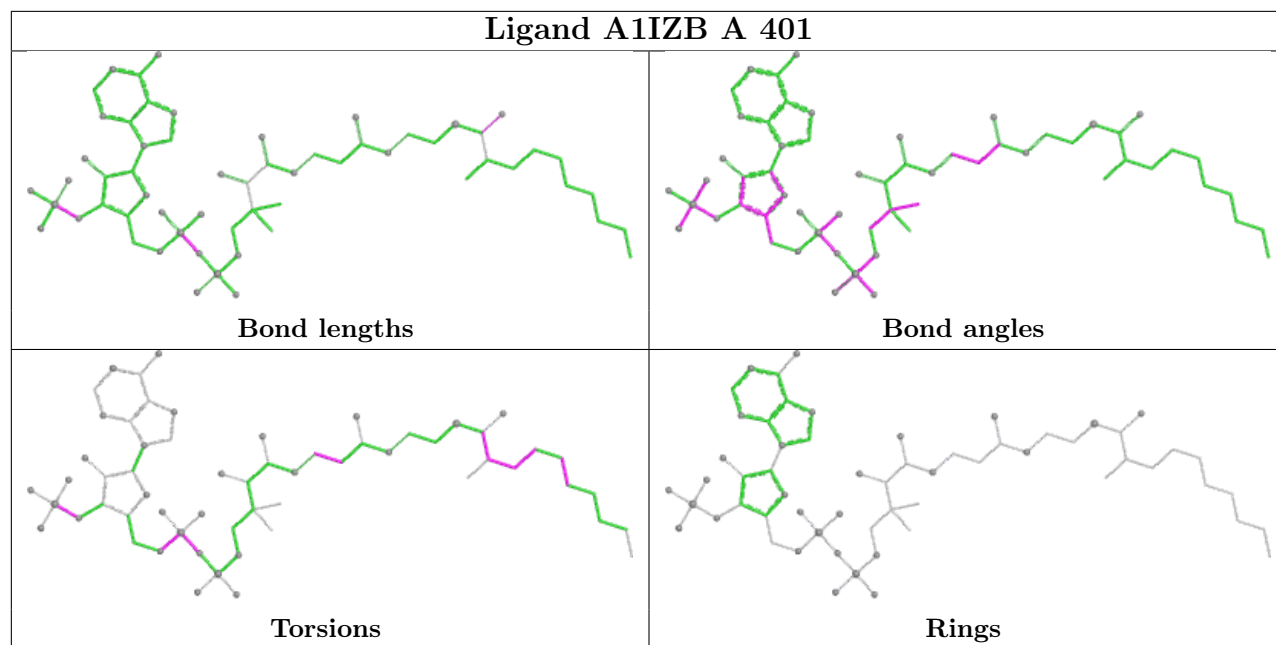
Ligand A1IZB B 401



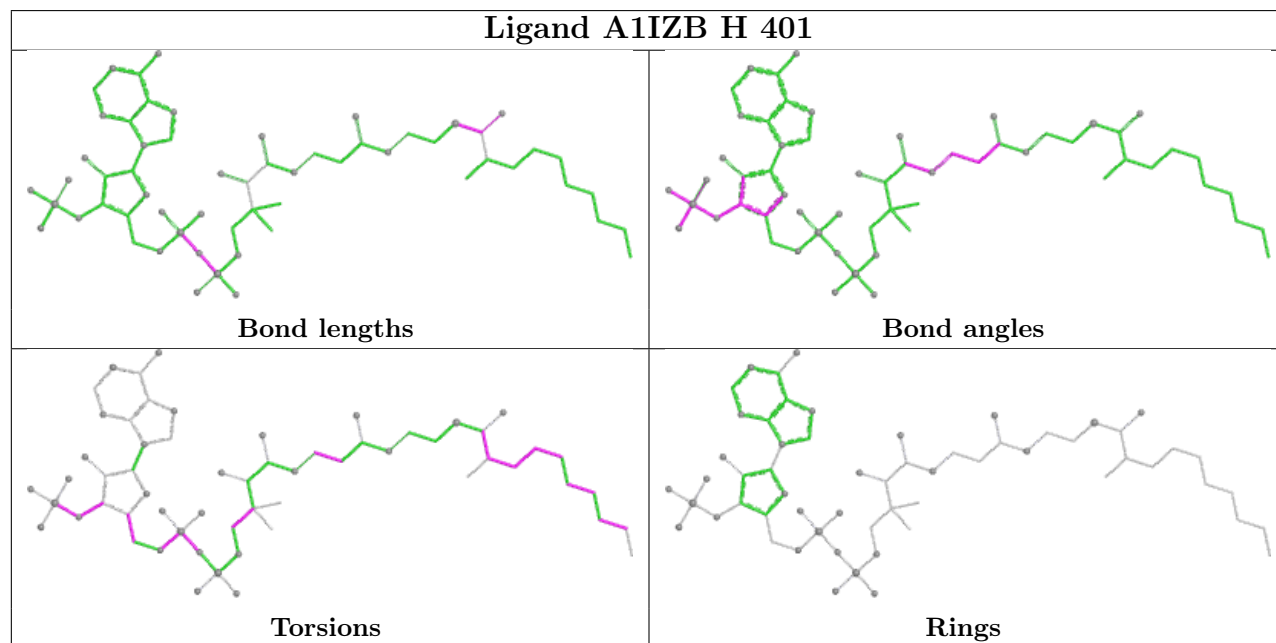
Ligand A1IZB D 401



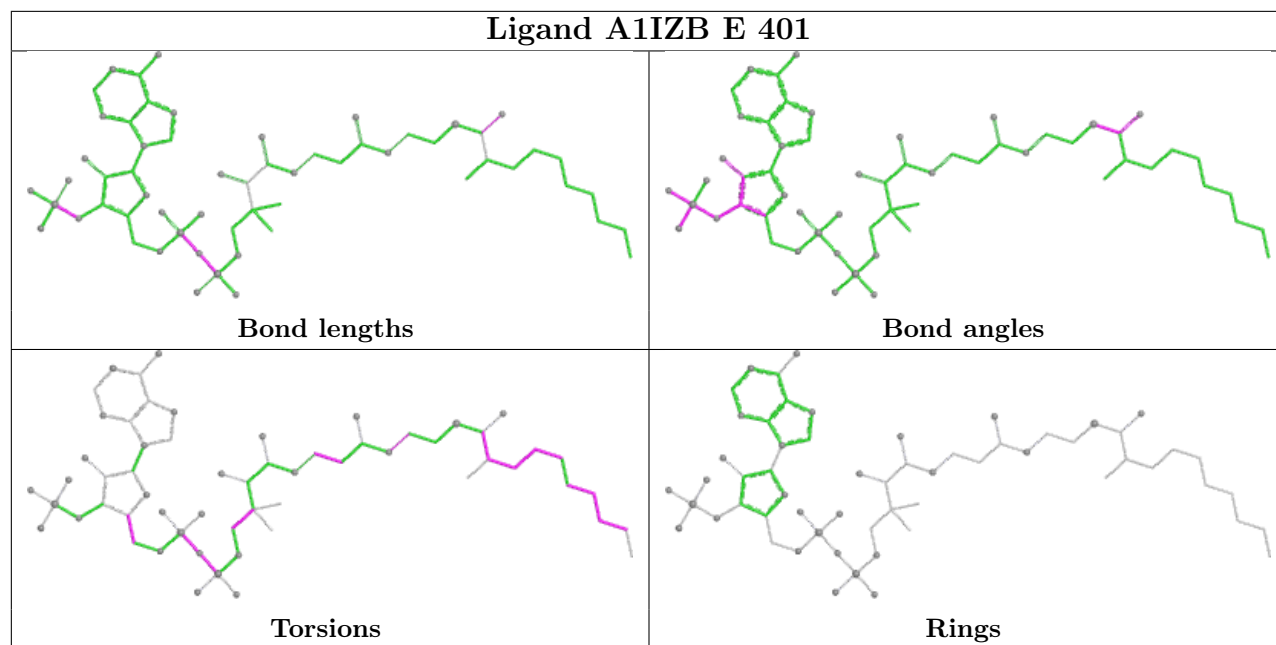
Ligand A1IZB A 401



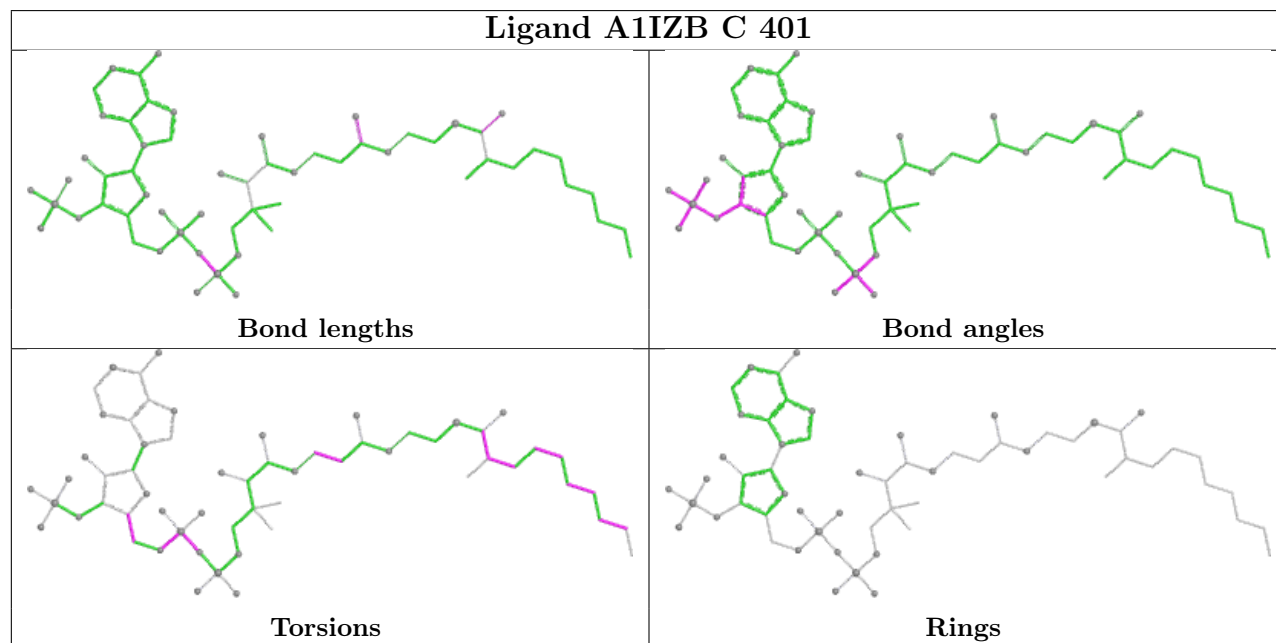
Ligand A1IZB H 401

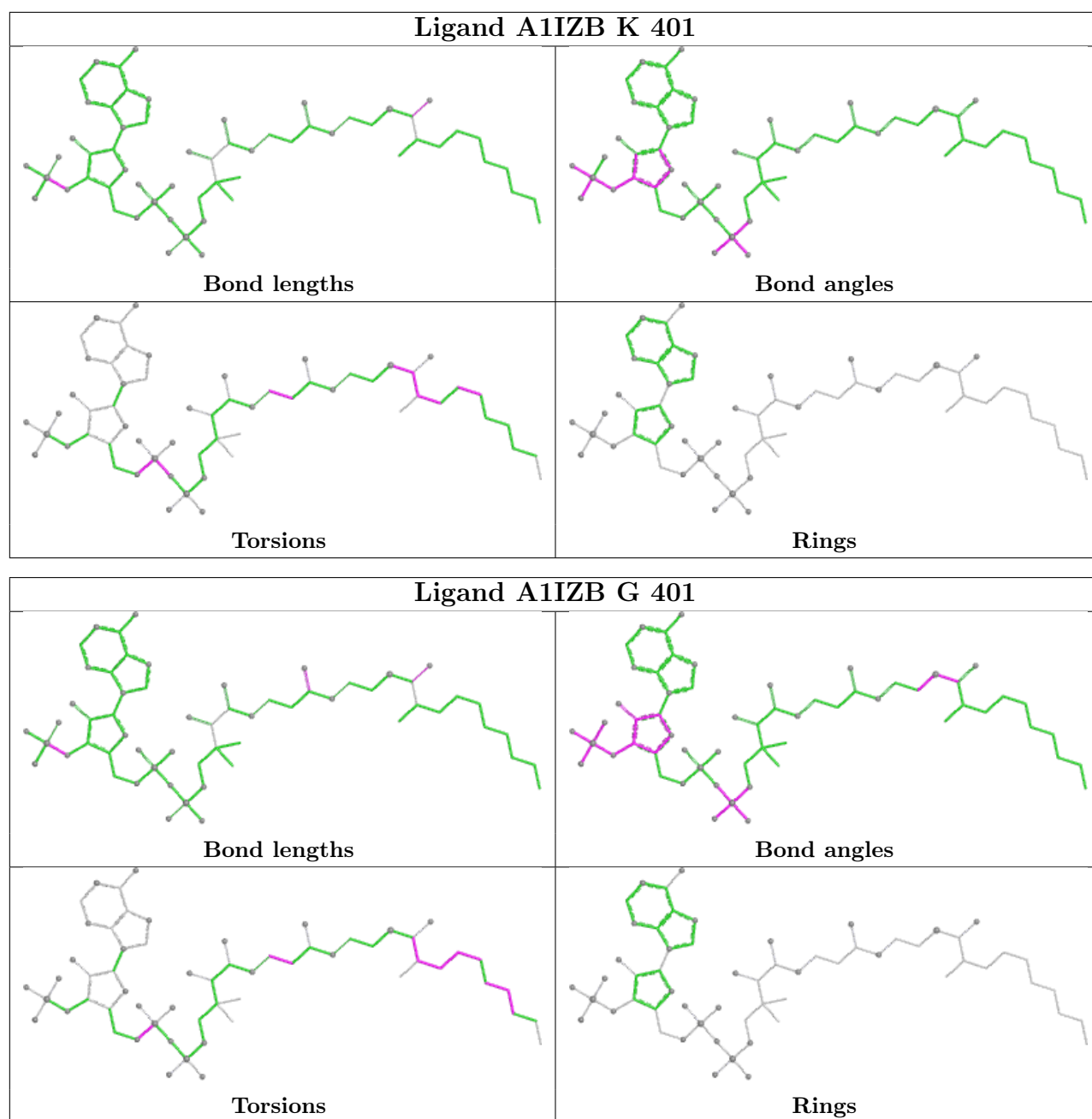


Ligand A1IZB E 401



Ligand A1IZB C 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, 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%)	0.88	73 (20%) 3 3	24, 40, 82, 107	2 (0%)
1	B	359/364 (98%)	0.70	40 (11%) 10 11	23, 40, 80, 118	1 (0%)
1	C	359/364 (98%)	0.78	55 (15%) 5 5	22, 40, 82, 111	2 (0%)
1	D	359/364 (98%)	0.83	63 (17%) 4 4	24, 40, 74, 128	1 (0%)
1	E	359/364 (98%)	0.95	69 (19%) 3 3	25, 42, 82, 122	2 (0%)
1	F	357/364 (98%)	1.04	73 (20%) 3 3	24, 43, 81, 120	1 (0%)
1	G	358/364 (98%)	1.22	93 (25%) 1 2	25, 44, 87, 131	2 (0%)
1	H	359/364 (98%)	1.10	89 (24%) 2 2	25, 43, 90, 117	1 (0%)
1	I	359/364 (98%)	0.68	36 (10%) 12 14	25, 38, 72, 101	1 (0%)
1	J	359/364 (98%)	0.56	31 (8%) 16 17	24, 37, 73, 112	1 (0%)
1	K	358/364 (98%)	0.63	34 (9%) 14 15	23, 39, 75, 111	2 (0%)
1	L	359/364 (98%)	0.78	48 (13%) 7 7	24, 40, 74, 103	1 (0%)
All	All	4304/4368 (98%)	0.85	704 (16%) 4 5	22, 40, 81, 131	17 (0%)

All (704) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	346	ALA	8.0
1	D	42	VAL	7.6
1	G	346	ALA	7.5
1	F	346	ALA	7.1
1	B	346	ALA	7.1
1	K	346	ALA	6.9
1	K	42	VAL	6.5
1	E	42	VAL	6.2
1	H	42	VAL	6.1
1	G	45	ILE	6.1
1	J	346	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	G	42	VAL	5.9
1	B	45	ILE	5.8
1	H	355	LEU	5.8
1	C	349	ILE	5.5
1	F	351	ILE	5.3
1	B	42	VAL	5.1
1	A	351	ILE	5.0
1	H	34	VAL	4.9
1	E	349	ILE	4.9
1	H	349	ILE	4.9
1	F	42	VAL	4.8
1	G	293	ASN	4.7
1	H	351	ILE	4.7
1	K	45	ILE	4.7
1	L	351	ILE	4.7
1	A	346	ALA	4.6
1	I	346	ALA	4.5
1	G	324	GLY	4.5
1	G	33	VAL	4.5
1	G	347	ALA	4.5
1	F	347	ALA	4.4
1	D	45	ILE	4.4
1	G	358	TRP	4.3
1	G	292	ALA	4.3
1	H	75	ALA	4.3
1	G	11	VAL	4.3
1	C	45	ILE	4.3
1	G	56	ILE	4.3
1	G	355	LEU	4.2
1	G	10	VAL	4.2
1	K	349	ILE	4.2
1	F	45	ILE	4.2
1	B	351	ILE	4.1
1	C	347	ALA	4.1
1	A	69	LEU	4.1
1	F	355	LEU	4.1
1	G	348	THR	4.1
1	G	351	ILE	4.1
1	H	45	ILE	4.1
1	H	105	ARG	4.1
1	L	80	LEU	4.1
1	G	102	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	7	GLY	4.0
1	E	351	ILE	4.0
1	H	346	ALA	4.0
1	J	351	ILE	4.0
1	A	324	GLY	4.0
1	L	30	GLY	4.0
1	G	49	ALA	3.9
1	H	178	SER	3.9
1	G	101	LYS	3.9
1	H	72	LYS	3.9
1	G	59	ALA	3.9
1	H	59	ALA	3.9
1	H	8	LEU	3.9
1	A	349	ILE	3.9
1	D	44	GLY	3.9
1	D	346	ALA	3.9
1	A	355	LEU	3.9
1	G	1	MET	3.9
1	G	57	VAL	3.8
1	C	351	ILE	3.8
1	J	45	ILE	3.8
1	C	323	ASN	3.8
1	L	323	ASN	3.8
1	D	102	VAL	3.8
1	H	30	GLY	3.8
1	G	107	ILE	3.8
1	I	351	ILE	3.8
1	H	57	VAL	3.8
1	K	207	MET	3.8
1	H	106	LEU	3.8
1	A	102	VAL	3.8
1	G	79	VAL	3.8
1	G	178	SER	3.7
1	G	69	LEU	3.7
1	H	345	PRO	3.7
1	F	324	GLY	3.7
1	G	34	VAL	3.7
1	E	45	ILE	3.7
1	A	358	TRP	3.7
1	G	76	LYS	3.7
1	H	47	ARG	3.7
1	I	42	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	358	TRP	3.7
1	E	355	LEU	3.7
1	B	324	GLY	3.7
1	G	93	GLY	3.7
1	D	40	SER	3.7
1	E	79	VAL	3.7
1	A	45	ILE	3.7
1	F	180	LYS	3.7
1	I	180	LYS	3.7
1	G	100	ALA	3.7
1	L	75	ALA	3.7
1	F	69	LEU	3.6
1	F	358	TRP	3.6
1	C	76	LYS	3.6
1	G	180	LYS	3.6
1	F	59	ALA	3.6
1	E	44	GLY	3.6
1	G	41	SER	3.6
1	G	72	LYS	3.6
1	H	173	TRP	3.6
1	G	354	VAL	3.6
1	H	74	ILE	3.6
1	A	93	GLY	3.6
1	A	34	VAL	3.5
1	C	42	VAL	3.5
1	I	45	ILE	3.5
1	F	49	ALA	3.5
1	H	2	ALA	3.5
1	G	94	LEU	3.5
1	H	69	LEU	3.5
1	H	80	LEU	3.5
1	L	71	LEU	3.5
1	J	324	GLY	3.5
1	E	173	TRP	3.5
1	A	180	LYS	3.5
1	F	76	LYS	3.5
1	F	173	TRP	3.5
1	F	71	LEU	3.5
1	I	41	SER	3.5
1	J	323	ASN	3.5
1	A	56	ILE	3.4
1	D	107	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	74	ILE	3.4
1	K	360	GLY	3.4
1	D	76	LYS	3.4
1	B	7	GLY	3.4
1	I	47	ARG	3.4
1	E	10	VAL	3.4
1	G	183	VAL	3.4
1	C	171	ALA	3.4
1	L	69	LEU	3.4
1	L	94	LEU	3.4
1	L	355	LEU	3.4
1	B	323	ASN	3.4
1	B	46	SER	3.4
1	G	179	GLY	3.4
1	H	76	LYS	3.4
1	B	347	ALA	3.4
1	B	358	TRP	3.3
1	H	323	ASN	3.3
1	D	351	ILE	3.3
1	E	56	ILE	3.3
1	I	349	ILE	3.3
1	L	346	ALA	3.3
1	F	106	LEU	3.3
1	C	173	TRP	3.3
1	E	358	TRP	3.3
1	H	1	MET	3.3
1	A	40	SER	3.3
1	B	44	GLY	3.3
1	I	44	GLY	3.3
1	H	16	ILE	3.3
1	J	347	ALA	3.3
1	H	71	LEU	3.3
1	H	73	LEU	3.3
1	C	207	MET	3.3
1	G	61	LEU	3.3
1	H	92	LEU	3.3
1	J	207	MET	3.3
1	G	63	SER	3.2
1	A	30	GLY	3.2
1	D	322	ALA	3.2
1	A	74	ILE	3.2
1	E	1	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	67	LEU	3.2
1	F	323	ASN	3.2
1	L	92	LEU	3.2
1	A	58	THR	3.2
1	C	40	SER	3.2
1	D	324	GLY	3.2
1	H	352	GLU	3.2
1	E	59	ALA	3.2
1	G	70	ALA	3.2
1	G	73	LEU	3.2
1	I	69	LEU	3.2
1	F	176	GLN	3.2
1	A	345	PRO	3.2
1	C	358	TRP	3.2
1	A	354	VAL	3.2
1	H	354	VAL	3.2
1	E	75	ALA	3.2
1	G	71	LEU	3.2
1	H	5	LEU	3.2
1	K	39	PRO	3.2
1	A	59	ALA	3.1
1	D	59	ALA	3.1
1	E	34	VAL	3.1
1	G	349	ILE	3.1
1	A	62	LYS	3.1
1	E	66	GLY	3.1
1	E	93	GLY	3.1
1	G	7	GLY	3.1
1	H	180	LYS	3.1
1	C	176	GLN	3.1
1	G	2	ALA	3.1
1	D	355	LEU	3.1
1	G	80	LEU	3.1
1	L	74	ILE	3.1
1	A	39	PRO	3.1
1	G	96	PRO	3.1
1	G	357	ASP	3.1
1	F	354	VAL	3.1
1	G	8	LEU	3.1
1	L	349	ILE	3.1
1	H	324	GLY	3.1
1	D	323	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	10	VAL	3.1
1	A	67	LEU	3.1
1	G	5	LEU	3.1
1	G	67	LEU	3.1
1	F	81	ILE	3.1
1	A	173	TRP	3.0
1	L	173	TRP	3.0
1	A	66	GLY	3.0
1	C	44	GLY	3.0
1	E	7	GLY	3.0
1	E	58	THR	3.0
1	G	345	PRO	3.0
1	F	350	ASP	3.0
1	L	359	ASP	3.0
1	A	71	LEU	3.0
1	B	41	SER	3.0
1	J	44	GLY	3.0
1	K	324	GLY	3.0
1	F	57	VAL	3.0
1	H	56	ILE	3.0
1	K	351	ILE	3.0
1	A	323	ASN	3.0
1	G	44	GLY	3.0
1	H	66	GLY	3.0
1	L	7	GLY	3.0
1	A	1	MET	3.0
1	I	1	MET	3.0
1	B	40	SER	3.0
1	H	347	ALA	3.0
1	K	49	ALA	3.0
1	D	354	VAL	3.0
1	E	47	ARG	2.9
1	E	353	ALA	2.9
1	G	75	ALA	2.9
1	G	77	ALA	2.9
1	A	92	LEU	2.9
1	C	71	LEU	2.9
1	E	106	LEU	2.9
1	G	30	GLY	2.9
1	K	76	LYS	2.9
1	D	359	ASP	2.9
1	I	358	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	2.9
1	F	293	ASN	2.9
1	H	353	ALA	2.9
1	A	73	LEU	2.9
1	A	76	LYS	2.9
1	C	360	GLY	2.9
1	H	79	VAL	2.9
1	H	102	VAL	2.9
1	D	74	ILE	2.9
1	F	56	ILE	2.9
1	G	43	ASP	2.9
1	B	65	GLN	2.9
1	I	323	ASN	2.9
1	B	76	LYS	2.9
1	K	180	LYS	2.9
1	A	322	ALA	2.9
1	E	69	LEU	2.9
1	E	80	LEU	2.9
1	G	66	GLY	2.9
1	G	106	LEU	2.9
1	I	94	LEU	2.9
1	E	144	ASP	2.9
1	F	11	VAL	2.9
1	L	79	VAL	2.9
1	F	47	ARG	2.9
1	G	171	ALA	2.9
1	C	93	GLY	2.9
1	D	358	TRP	2.9
1	F	27	GLY	2.9
1	F	5	LEU	2.8
1	D	92	LEU	2.8
1	H	61	LEU	2.8
1	F	33	VAL	2.8
1	F	79	VAL	2.8
1	J	42	VAL	2.8
1	L	102	VAL	2.8
1	C	74	ILE	2.8
1	A	41	SER	2.8
1	E	207	MET	2.8
1	H	350	ASP	2.8
1	E	324	GLY	2.8
1	G	181	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	355	LEU	2.8
1	A	356	THR	2.8
1	I	173	TRP	2.8
1	C	180	LYS	2.8
1	H	107	ILE	2.8
1	H	27	GLY	2.8
1	H	179	GLY	2.8
1	B	75	ALA	2.8
1	E	77	ALA	2.8
1	F	75	ALA	2.8
1	F	109	ALA	2.8
1	D	94	LEU	2.8
1	K	71	LEU	2.8
1	L	106	LEU	2.8
1	D	180	LYS	2.8
1	H	348	THR	2.8
1	E	105	ARG	2.7
1	L	1	MET	2.7
1	B	350	ASP	2.7
1	E	30	GLY	2.7
1	F	66	GLY	2.7
1	D	347	ALA	2.7
1	E	72	LYS	2.7
1	H	70	ALA	2.7
1	E	73	LEU	2.7
1	K	102	VAL	2.7
1	F	25	ILE	2.7
1	D	207	MET	2.7
1	F	1	MET	2.7
1	K	41	SER	2.7
1	G	173	TRP	2.7
1	J	144	ASP	2.7
1	G	83	GLY	2.7
1	H	44	GLY	2.7
1	C	353	ALA	2.7
1	G	353	ALA	2.7
1	J	49	ALA	2.7
1	D	80	LEU	2.7
1	H	58	THR	2.7
1	H	176	GLN	2.7
1	H	33	VAL	2.7
1	I	354	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	63	SER	2.7
1	B	43	ASP	2.7
1	D	43	ASP	2.7
1	F	144	ASP	2.7
1	I	144	ASP	2.7
1	A	72	LYS	2.7
1	C	324	GLY	2.7
1	G	105	ARG	2.7
1	D	2	ALA	2.7
1	F	70	ALA	2.7
1	D	348	THR	2.7
1	F	96	PRO	2.7
1	H	108	TYR	2.7
1	E	178	SER	2.7
1	G	99	CYS	2.7
1	J	43	ASP	2.7
1	J	349	ILE	2.7
1	C	30	GLY	2.7
1	D	7	GLY	2.7
1	F	93	GLY	2.7
1	C	75	ALA	2.6
1	G	109	ALA	2.6
1	A	61	LEU	2.6
1	B	356	THR	2.6
1	G	172	LEU	2.6
1	H	39	PRO	2.6
1	K	345	PRO	2.6
1	J	359	ASP	2.6
1	E	33	VAL	2.6
1	F	74	ILE	2.6
1	D	173	TRP	2.6
1	E	346	ALA	2.6
1	A	80	LEU	2.6
1	A	94	LEU	2.6
1	C	345	PRO	2.6
1	A	6	SER	2.6
1	E	40	SER	2.6
1	E	180	LYS	2.6
1	H	41	SER	2.6
1	F	107	ILE	2.6
1	L	324	GLY	2.6
1	A	353	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	345	PRO	2.6
1	F	61	LEU	2.6
1	G	26	LEU	2.6
1	G	144	ASP	2.6
1	I	92	LEU	2.6
1	B	47	ARG	2.6
1	I	102	VAL	2.6
1	L	183	VAL	2.6
1	E	179	GLY	2.6
1	E	100	ALA	2.6
1	H	49	ALA	2.6
1	H	322	ALA	2.6
1	G	350	ASP	2.6
1	H	144	ASP	2.6
1	A	178	SER	2.6
1	G	51	LEU	2.6
1	H	326	TRP	2.6
1	I	67	LEU	2.6
1	K	358	TRP	2.6
1	L	67	LEU	2.6
1	A	79	VAL	2.5
1	D	183	VAL	2.5
1	E	354	VAL	2.5
1	F	34	VAL	2.5
1	L	88	VAL	2.5
1	A	75	ALA	2.5
1	A	289	ALA	2.5
1	E	70	ALA	2.5
1	E	347	ALA	2.5
1	L	348	THR	2.5
1	F	345	PRO	2.5
1	C	65	GLN	2.5
1	A	10	VAL	2.5
1	G	184	VAL	2.5
1	H	183	VAL	2.5
1	L	34	VAL	2.5
1	L	354	VAL	2.5
1	F	72	LYS	2.5
1	L	350	ASP	2.5
1	G	58	THR	2.5
1	H	337	THR	2.5
1	F	80	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	61	LEU	2.5
1	J	71	LEU	2.5
1	B	1	MET	2.5
1	B	173	TRP	2.5
1	C	66	GLY	2.5
1	C	181	GLY	2.5
1	D	30	GLY	2.5
1	H	62	LYS	2.5
1	L	76	LYS	2.5
1	C	102	VAL	2.5
1	G	36	ILE	2.5
1	C	350	ASP	2.5
1	G	176	GLN	2.5
1	F	100	ALA	2.5
1	F	322	ALA	2.5
1	H	31	ALA	2.5
1	H	170	ALA	2.5
1	A	106	LEU	2.5
1	E	172	LEU	2.5
1	H	51	LEU	2.5
1	I	80	LEU	2.5
1	C	1	MET	2.5
1	D	1	MET	2.5
1	G	62	LYS	2.5
1	K	47	ARG	2.5
1	I	87	GLY	2.5
1	L	44	GLY	2.5
1	F	349	ILE	2.5
1	H	10	VAL	2.4
1	F	43	ASP	2.4
1	F	46	SER	2.4
1	B	353	ALA	2.4
1	C	8	LEU	2.4
1	F	73	LEU	2.4
1	L	61	LEU	2.4
1	G	91	ARG	2.4
1	C	10	VAL	2.4
1	F	326	TRP	2.4
1	L	144	ASP	2.4
1	G	108	TYR	2.4
1	K	58	THR	2.4
1	D	345	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	49	ALA	2.4
1	D	75	ALA	2.4
1	K	100	ALA	2.4
1	E	71	LEU	2.4
1	J	355	LEU	2.4
1	A	95	GLY	2.4
1	A	68	GLU	2.4
1	E	176	GLN	2.4
1	G	334	PHE	2.4
1	I	176	GLN	2.4
1	B	354	VAL	2.4
1	L	10	VAL	2.4
1	A	101	LYS	2.4
1	B	348	THR	2.4
1	F	62	LYS	2.4
1	I	322	ALA	2.4
1	C	61	LEU	2.4
1	C	355	LEU	2.4
1	H	172	LEU	2.4
1	G	97	GLU	2.4
1	A	288	GLY	2.4
1	B	30	GLY	2.4
1	G	323	ASN	2.4
1	C	359	ASP	2.4
1	B	349	ILE	2.4
1	C	47	ARG	2.4
1	D	10	VAL	2.4
1	D	34	VAL	2.4
1	F	102	VAL	2.4
1	L	42	VAL	2.4
1	K	72	LYS	2.4
1	J	173	TRP	2.4
1	L	358	TRP	2.4
1	B	49	ALA	2.3
1	D	171	ALA	2.3
1	G	31	ALA	2.3
1	G	55	ARG	2.3
1	K	1	MET	2.3
1	A	46	SER	2.3
1	F	41	SER	2.3
1	G	46	SER	2.3
1	H	342	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	176	GLN	2.3
1	B	59	ALA	2.3
1	D	49	ALA	2.3
1	F	171	ALA	2.3
1	A	13	LEU	2.3
1	E	67	LEU	2.3
1	H	3	GLY	2.3
1	C	56	ILE	2.3
1	E	16	ILE	2.3
1	L	45	ILE	2.3
1	C	11	VAL	2.3
1	A	348	THR	2.3
1	H	96	PRO	2.3
1	L	58	THR	2.3
1	A	347	ALA	2.3
1	L	347	ALA	2.3
1	A	47	ARG	2.3
1	B	73	LEU	2.3
1	C	69	LEU	2.3
1	D	106	LEU	2.3
1	F	26	LEU	2.3
1	I	355	LEU	2.3
1	J	93	GLY	2.3
1	J	350	ASP	2.3
1	J	358	TRP	2.3
1	E	76	LYS	2.3
1	F	97	GLU	2.3
1	H	334	PHE	2.3
1	D	56	ILE	2.3
1	K	176	GLN	2.3
1	D	79	VAL	2.3
1	E	345	PRO	2.3
1	E	348	THR	2.3
1	D	353	ALA	2.3
1	J	75	ALA	2.3
1	J	353	ALA	2.3
1	K	144	ASP	2.3
1	H	93	GLY	2.3
1	I	93	GLY	2.3
1	D	8	LEU	2.3
1	D	169	LEU	2.3
1	E	94	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	92	LEU	2.3
1	I	71	LEU	2.3
1	D	176	GLN	2.2
1	F	40	SER	2.2
1	C	107	ILE	2.2
1	E	107	ILE	2.2
1	L	107	ILE	2.2
1	A	11	VAL	2.2
1	A	42	VAL	2.2
1	C	166	VAL	2.2
1	K	34	VAL	2.2
1	L	11	VAL	2.2
1	F	101	LYS	2.2
1	A	37	ASP	2.2
1	E	104	ASP	2.2
1	G	48	ASP	2.2
1	B	204	ALA	2.2
1	D	181	GLY	2.2
1	E	322	ALA	2.2
1	F	7	GLY	2.2
1	H	325	GLY	2.2
1	H	338	ALA	2.2
1	K	75	ALA	2.2
1	K	8	LEU	2.2
1	A	176	GLN	2.2
1	E	46	SER	2.2
1	A	55	ARG	2.2
1	J	47	ARG	2.2
1	D	349	ILE	2.2
1	C	79	VAL	2.2
1	F	184	VAL	2.2
1	J	102	VAL	2.2
1	D	48	ASP	2.2
1	H	207	MET	2.2
1	C	87	GLY	2.2
1	G	3	GLY	2.2
1	A	70	ALA	2.2
1	B	77	ALA	2.2
1	D	31	ALA	2.2
1	F	292	ALA	2.2
1	H	100	ALA	2.2
1	H	145	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	2.2
1	E	5	LEU	2.2
1	L	73	LEU	2.2
1	H	65	GLN	2.2
1	D	178	SER	2.2
1	H	46	SER	2.2
1	A	96	PRO	2.2
1	I	350	ASP	2.2
1	L	357	ASP	2.2
1	H	11	VAL	2.2
1	B	315	GLU	2.2
1	F	277	GLU	2.2
1	E	31	ALA	2.2
1	E	65	GLN	2.2
1	G	338	ALA	2.2
1	J	322	ALA	2.2
1	C	169	LEU	2.2
1	H	26	LEU	2.2
1	H	99	CYS	2.2
1	E	41	SER	2.2
1	C	101	LYS	2.2
1	H	50	MET	2.2
1	C	39	PRO	2.1
1	E	337	THR	2.2
1	K	359	ASP	2.2
1	E	352	GLU	2.1
1	A	57	VAL	2.1
1	A	290	VAL	2.1
1	I	10	VAL	2.1
1	L	57	VAL	2.1
1	G	325	GLY	2.1
1	C	2	ALA	2.1
1	G	322	ALA	2.1
1	J	100	ALA	2.1
1	L	109	ALA	2.1
1	H	9	ARG	2.1
1	J	67	LEU	2.1
1	D	41	SER	2.1
1	H	6	SER	2.1
1	K	173	TRP	2.1
1	K	243	GLN	2.1
1	C	34	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	2.1
1	D	47	ARG	2.1
1	E	2	ALA	2.1
1	L	353	ALA	2.1
1	F	68	GLU	2.1
1	I	68	GLU	2.1
1	B	91	ARG	2.1
1	F	325	GLY	2.1
1	L	181	GLY	2.1
1	B	34	VAL	2.1
1	D	11	VAL	2.1
1	D	57	VAL	2.1
1	F	183	VAL	2.1
1	A	77	ALA	2.1
1	B	257	ALA	2.1
1	J	59	ALA	2.1
1	L	70	ALA	2.1
1	C	41	SER	2.1
1	D	26	LEU	2.1
1	D	73	LEU	2.1
1	K	80	LEU	2.1
1	C	352	GLU	2.1
1	F	48	ASP	2.1
1	D	320	TYR	2.1
1	E	96	PRO	2.1
1	J	348	THR	2.1
1	A	44	GLY	2.1
1	C	7	GLY	2.1
1	C	179	GLY	2.1
1	K	181	GLY	2.1
1	E	81	ILE	2.1
1	E	68	GLU	2.0
1	F	321	GLU	2.0
1	H	339	SER	2.1
1	I	77	ALA	2.1
1	K	322	ALA	2.1
1	B	5	LEU	2.0
1	J	73	LEU	2.0
1	A	65	GLN	2.0
1	G	255	ASP	2.0
1	A	91	ARG	2.0
1	D	105	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	356	THR	2.0
1	I	76	LYS	2.0
1	B	325	GLY	2.0
1	D	95	GLY	2.0
1	I	7	GLY	2.0
1	K	56	ILE	2.0
1	A	50	MET	2.0
1	D	23	ALA	2.0
1	E	171	ALA	2.0
1	E	326	TRP	2.0
1	A	51	LEU	2.0
1	C	80	LEU	2.0
1	E	61	LEU	2.0
1	E	92	LEU	2.0
1	D	144	ASP	2.0
1	G	32	ASP	2.0
1	I	43	ASP	2.0
1	I	255	ASP	2.0
1	A	9	ARG	2.0
1	A	105	ARG	2.0
1	G	87	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(\AA^2)	Q<0.9
2	A1IZB	E	401	60/60	0.88	0.18	54,74,98,106	0
2	A1IZB	H	401	60/60	0.88	0.18	52,74,88,92	0

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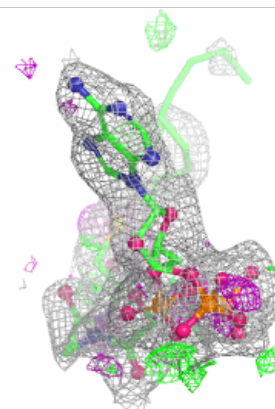
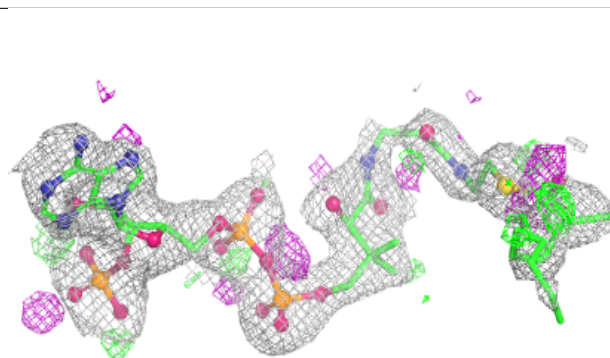
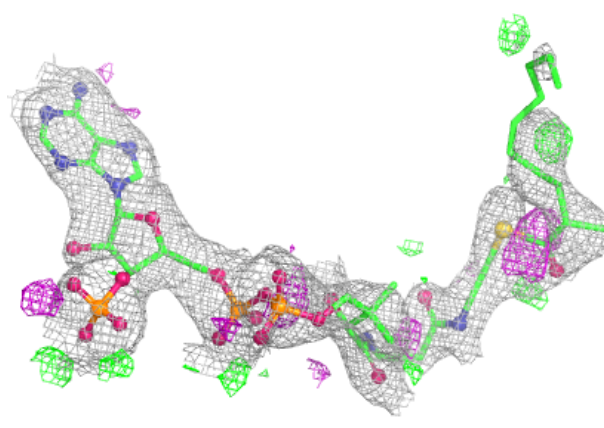
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	A1IZB	A	401	60/60	0.91	0.15	41,57,93,99	0
2	A1IZB	F	401	60/60	0.92	0.15	35,57,86,98	0
2	A1IZB	C	401	60/60	0.92	0.14	39,55,89,103	0
2	A1IZB	I	401	60/60	0.92	0.14	36,51,77,92	0
2	A1IZB	J	401	60/60	0.92	0.14	36,47,77,88	0
2	A1IZB	L	401	60/60	0.92	0.15	31,53,93,108	0
2	A1IZB	G	401	60/60	0.93	0.14	36,54,87,98	0
2	A1IZB	B	401	60/60	0.94	0.13	32,50,89,104	0
2	A1IZB	K	401	60/60	0.95	0.12	31,48,104,112	0
2	A1IZB	D	401	60/60	0.95	0.12	30,49,78,89	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.

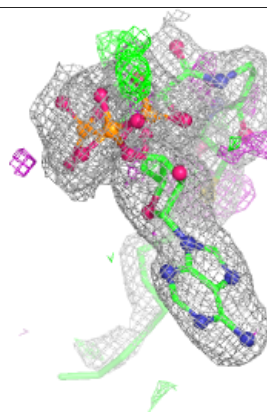
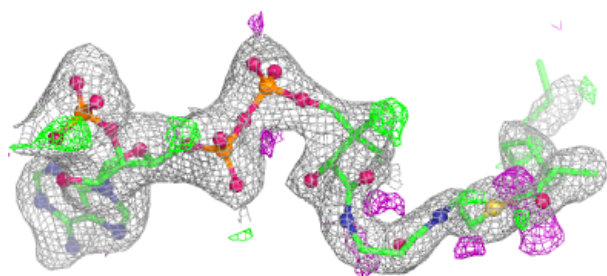
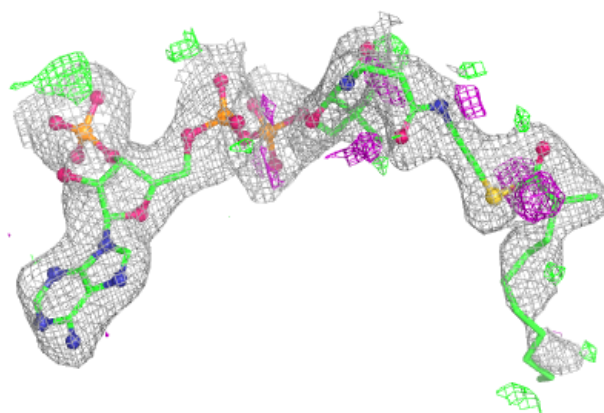
Electron density around A1IZB E 401:

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

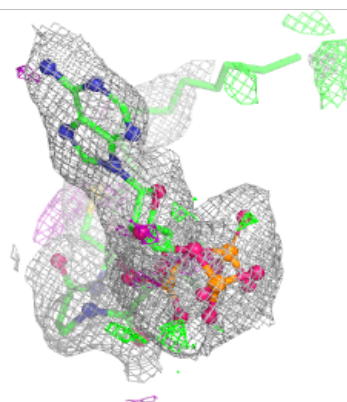
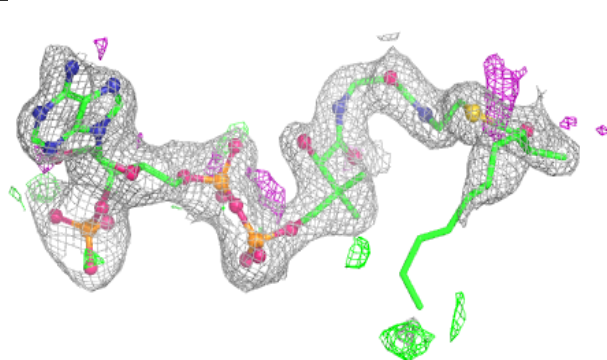
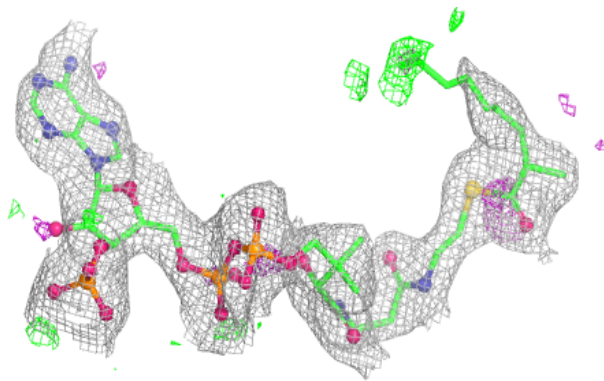


Electron density around A1IZB H 401:

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

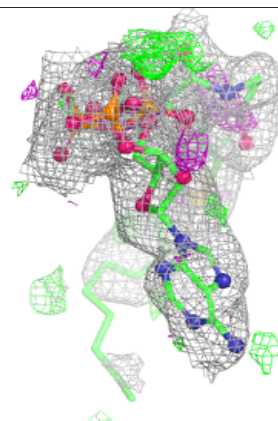
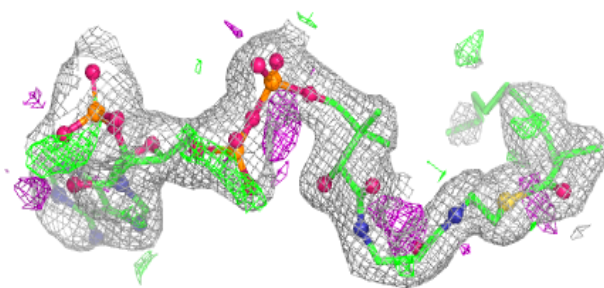
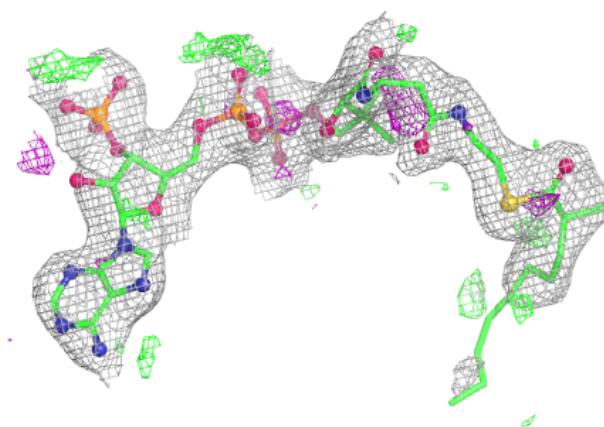
**Electron density around A1IZB A 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



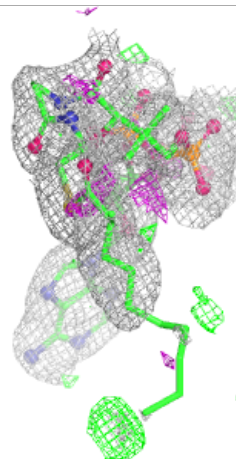
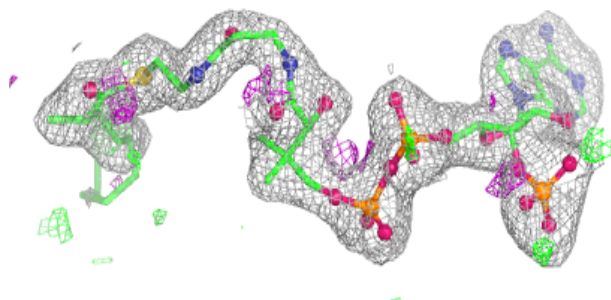
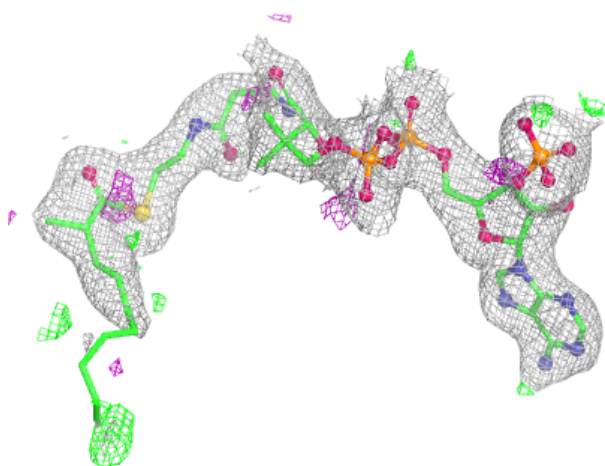
Electron density around A1IZB F 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



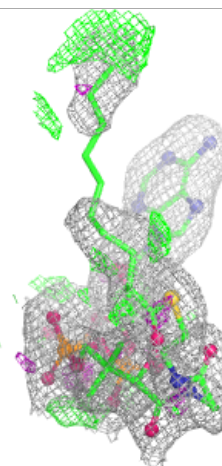
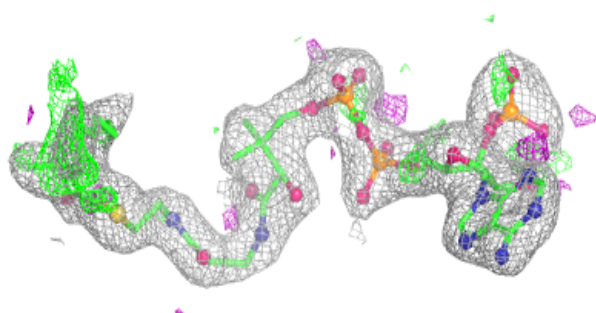
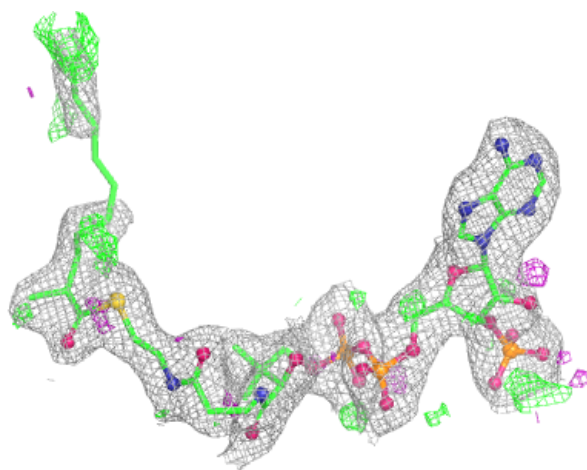
Electron density around A1IZB C 401:

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



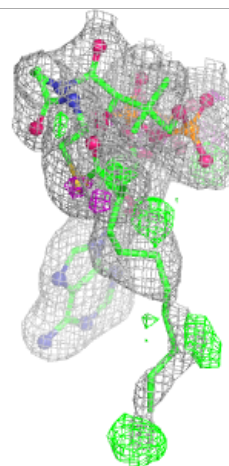
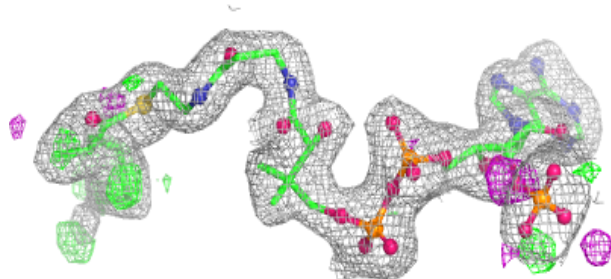
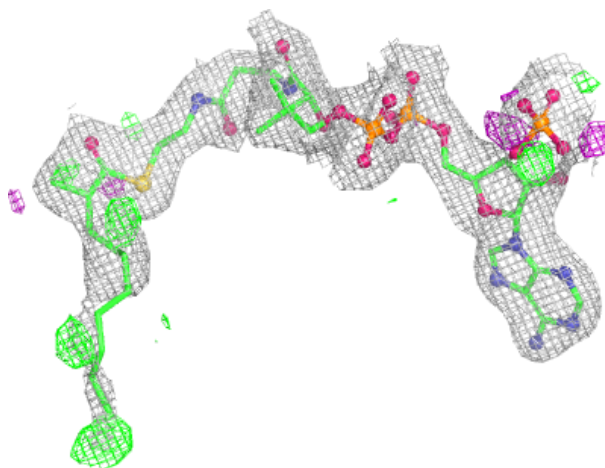
Electron density around A1IZB I 401:

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



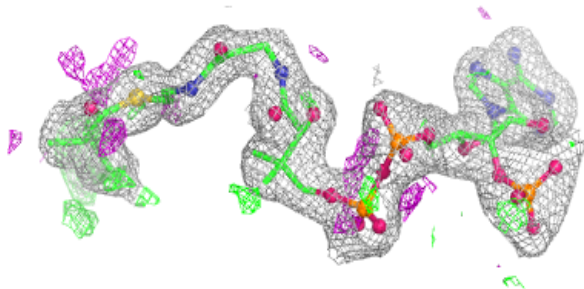
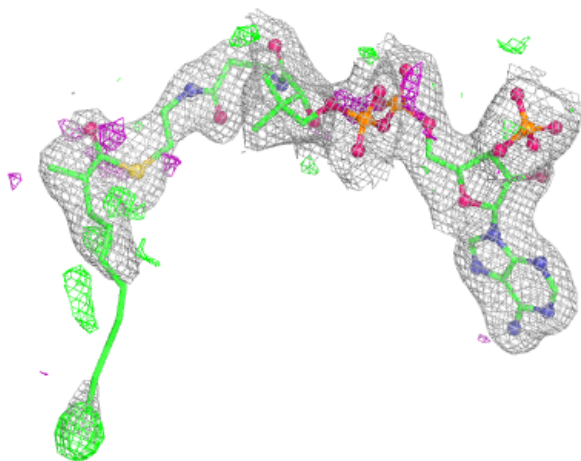
Electron density around A1IZB J 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



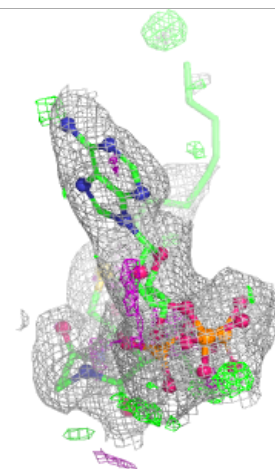
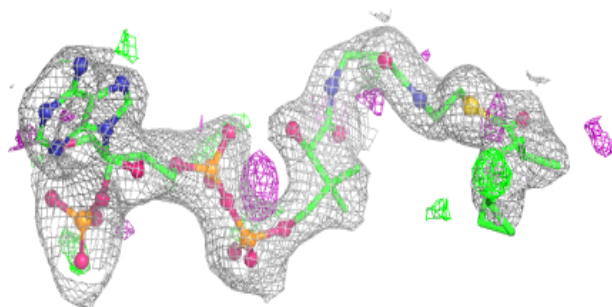
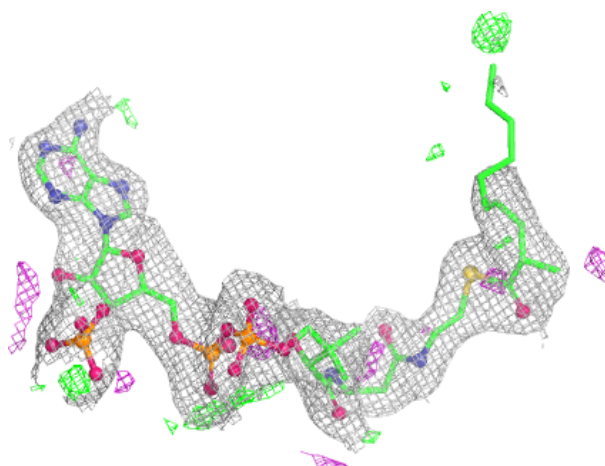
Electron density around A1IZB L 401:

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and green (positive)



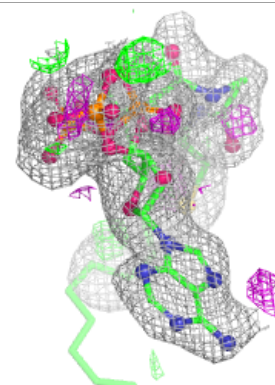
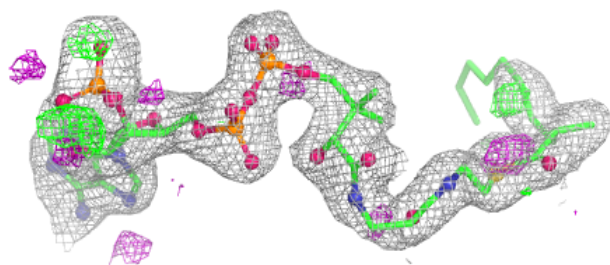
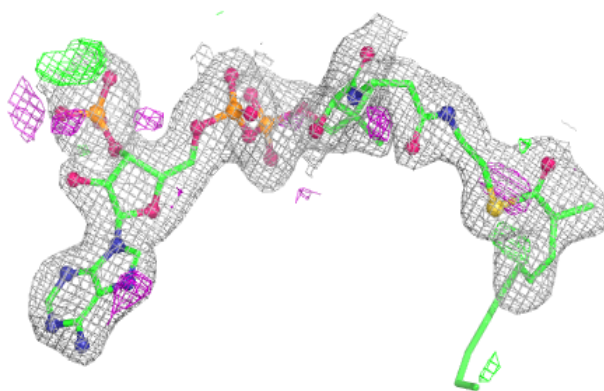
Electron density around A1IZB G 401:

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

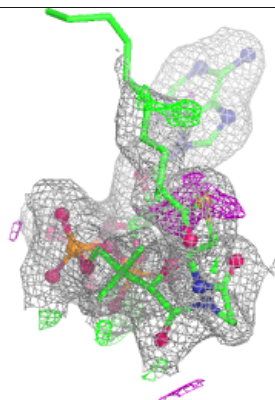
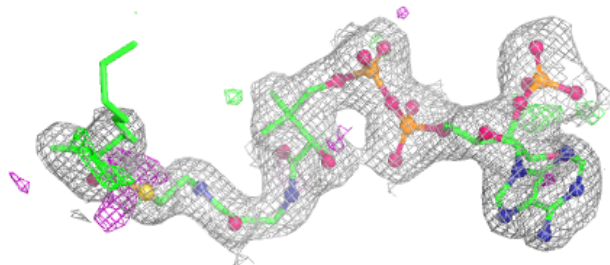
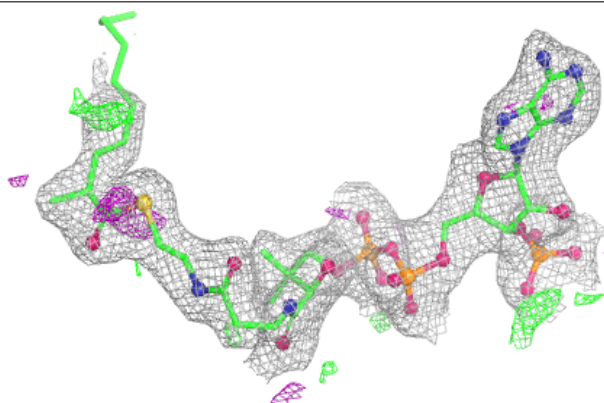


Electron density around A1IZB B 401:

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

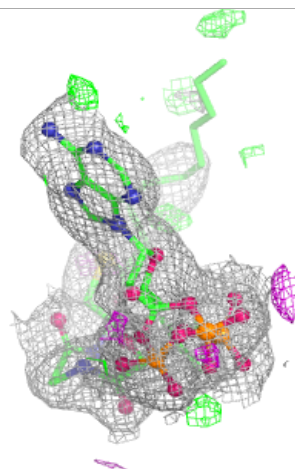
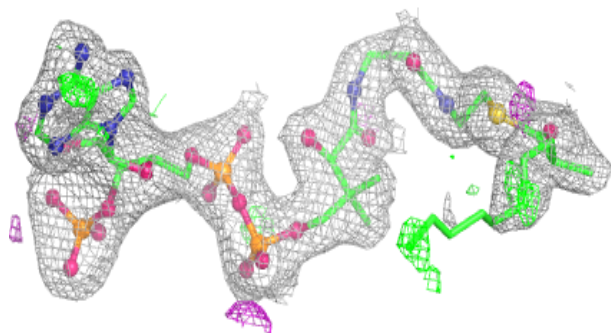
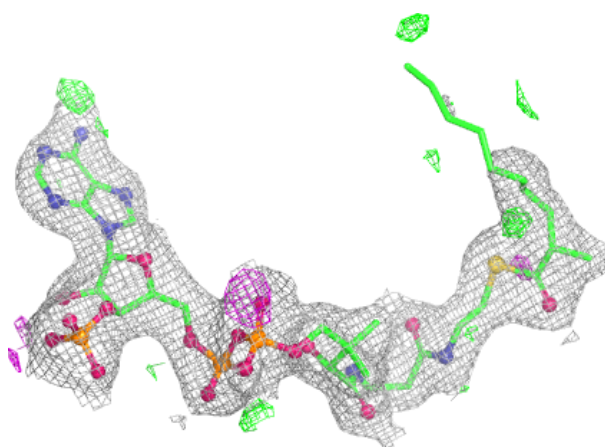
**Electron density around A1IZB K 401:**

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



Electron density around A1IZB 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.