Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2025 – 08:02 pm BST

PDB ID	:	9I34 / pdb_00009i34
Title	:	Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis in complex with hexanoyl-CoA
Authors	:	Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on	:	2025-01-22
Resolution	:	1.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

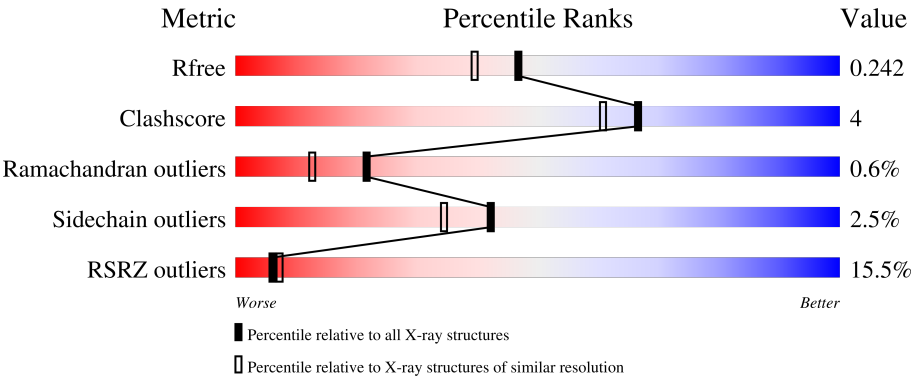
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	14% 87% 10%
1	B	364	12% 89% 8%
1	C	364	24% 87% 10%
1	D	364	11% 87% 10%
1	E	364	15% 85% 13%

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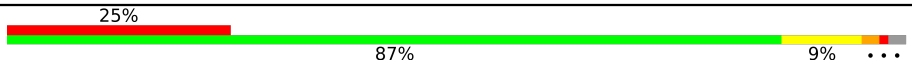
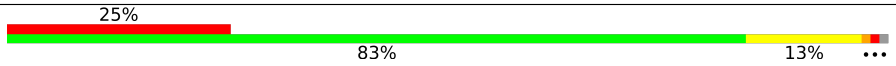
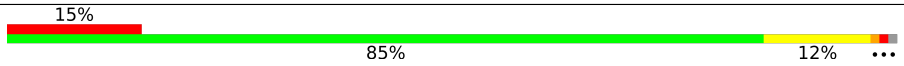
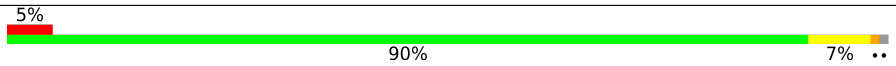
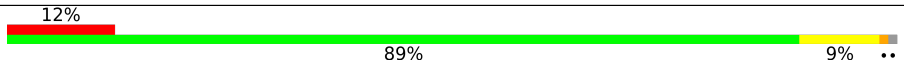
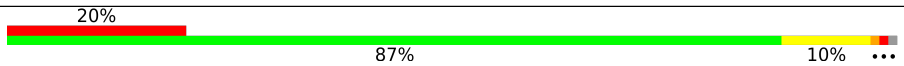
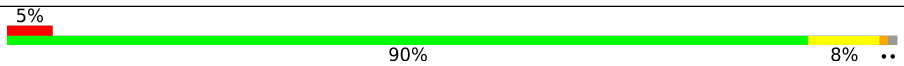
Mol	Chain	Length	Quality of chain
1	F	364	
1	G	364	
1	H	364	
1	I	364	
1	J	364	
1	K	364	
1	L	364	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35488 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	358	Total	C	N	O	S	0	1	0
			2707	1699	485	507	16			
1	B	359	Total	C	N	O	S	0	2	0
			2721	1707	487	511	16			
1	C	358	Total	C	N	O	S	0	2	0
			2714	1702	485	511	16			
1	D	359	Total	C	N	O	S	0	1	0
			2715	1703	486	510	16			
1	E	358	Total	C	N	O	S	0	2	0
			2710	1700	485	509	16			
1	F	358	Total	C	N	O	S	0	2	0
			2717	1705	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	360	Total	C	N	O	S	0	2	0
			2722	1706	487	513	16			
1	L	359	Total	C	N	O	S	0	2	0
			2721	1707	487	511	16			

There are 48 discrepancies between the modelled and reference sequences:

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

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

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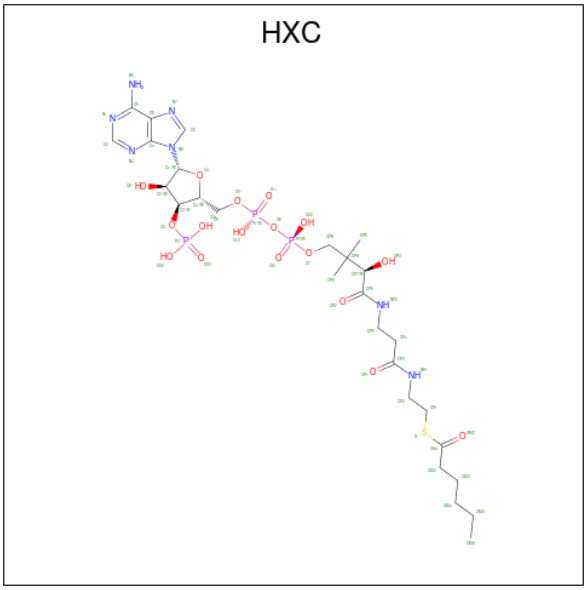
Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is HEXANOYL-COENZYME A (CCD ID: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			55	27	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
			55	27	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			55	27	7	17	3	1		

- Molecule 3 is water.

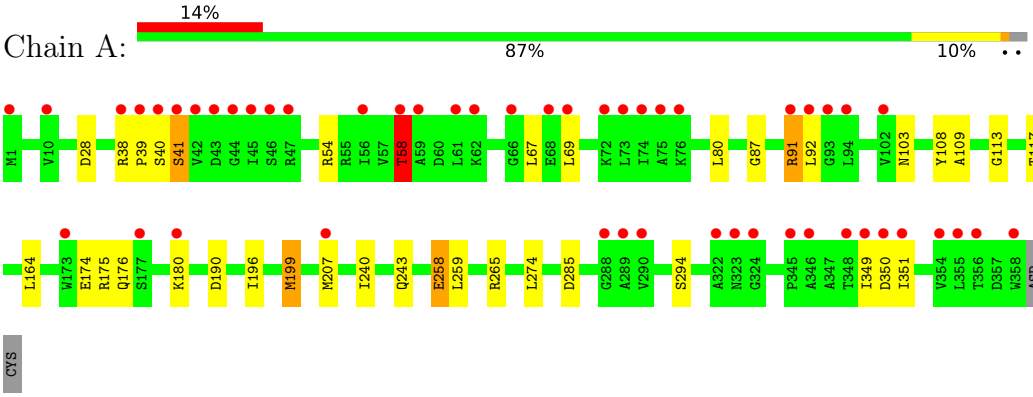
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total	O	0	0
			195	195		
3	B	161	Total	O	0	0
			161	161		
3	C	162	Total	O	0	0
			162	162		
3	D	194	Total	O	0	0
			194	194		
3	E	171	Total	O	0	0
			171	171		
3	F	173	Total	O	0	0
			173	173		
3	G	170	Total	O	0	0
			170	170		
3	H	178	Total	O	0	0
			178	178		
3	I	227	Total	O	0	0
			227	227		
3	J	203	Total	O	0	0
			203	203		
3	K	186	Total	O	0	0
			186	186		
3	L	215	Total	O	0	0
			215	215		

3 Residue-property plots (i)

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

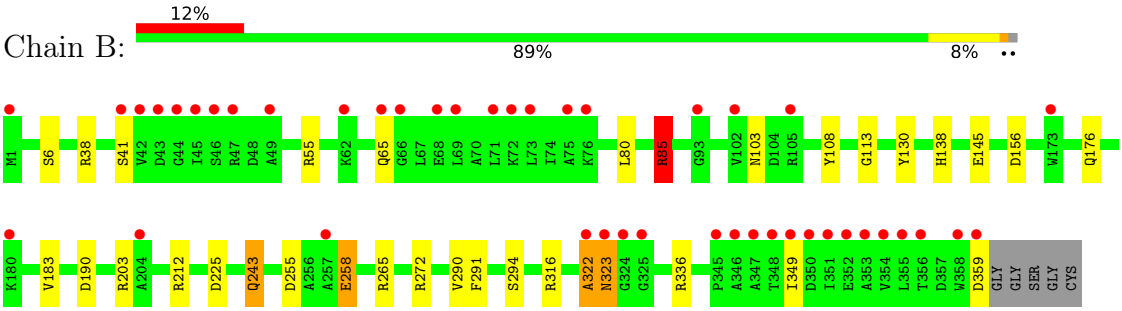
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain A:



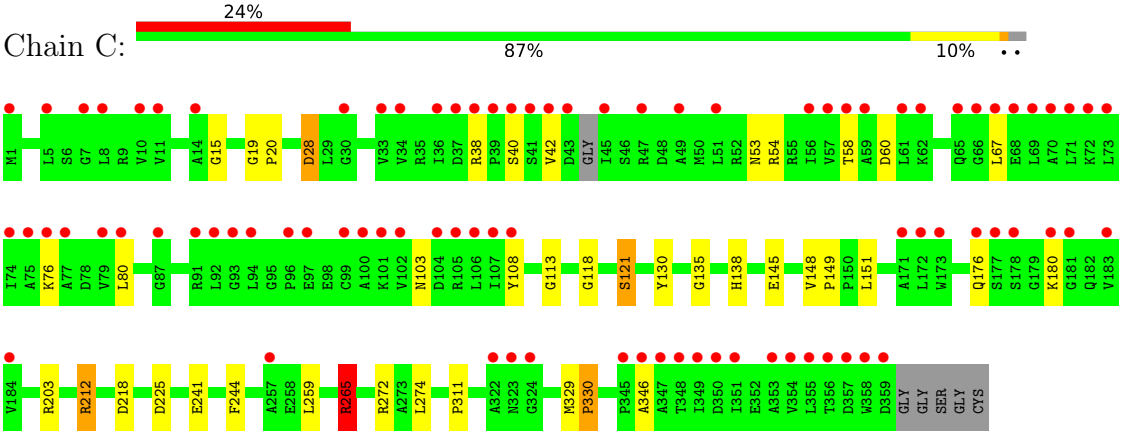
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain B:



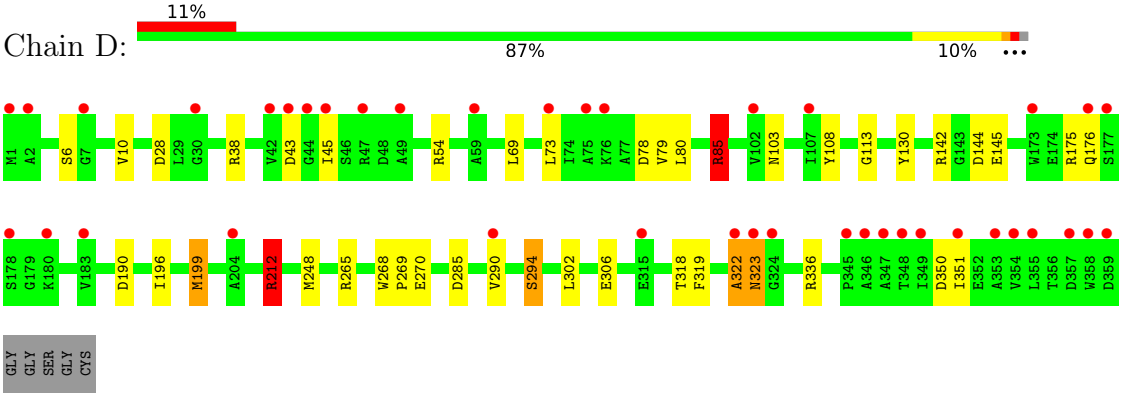
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain C:



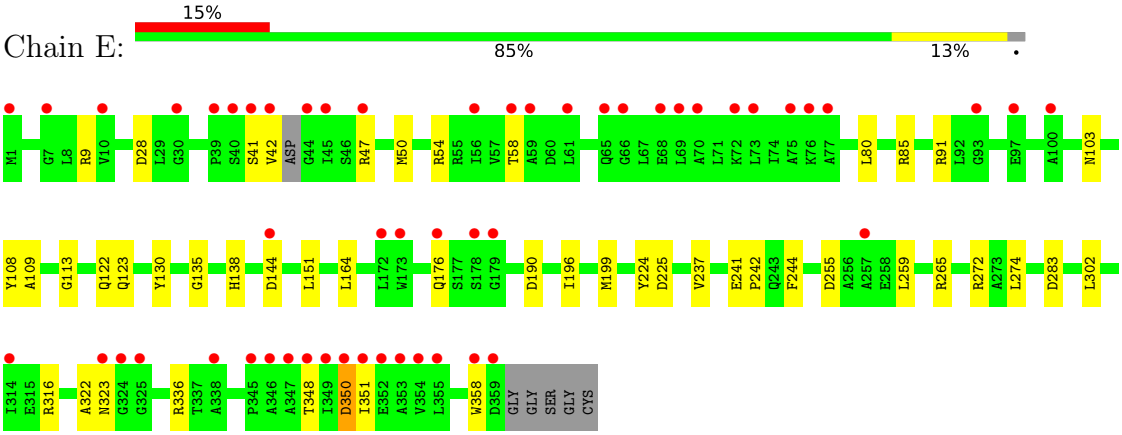
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain D:



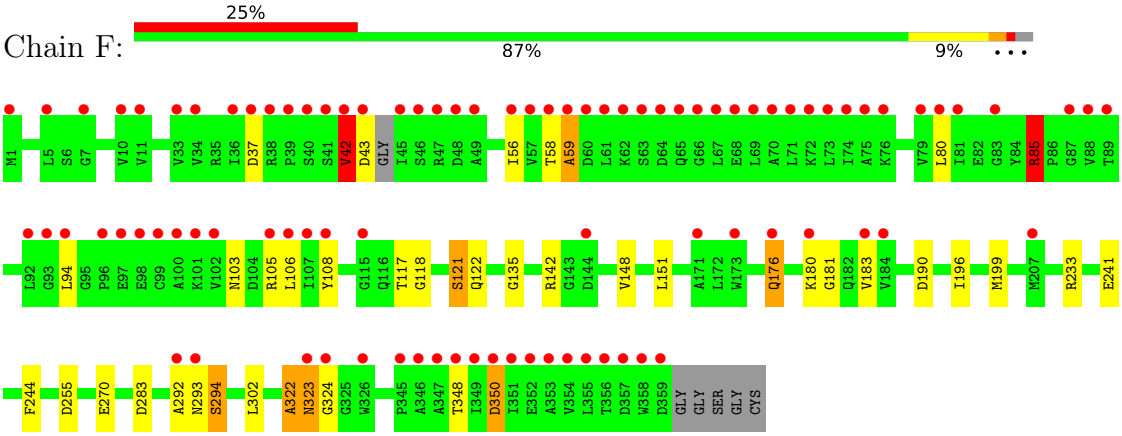
• Molecule 1: Alpha-methylacyl-CoA racemase

Chain E:



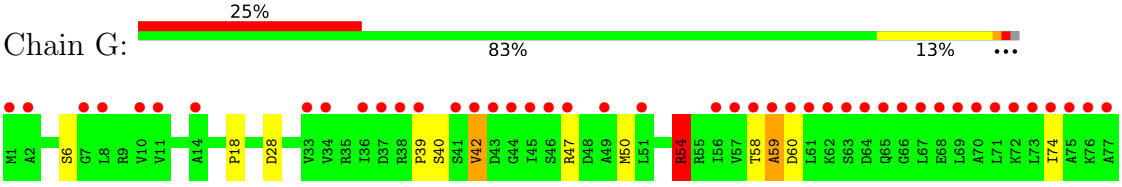
• Molecule 1: Alpha-methylacyl-CoA racemase

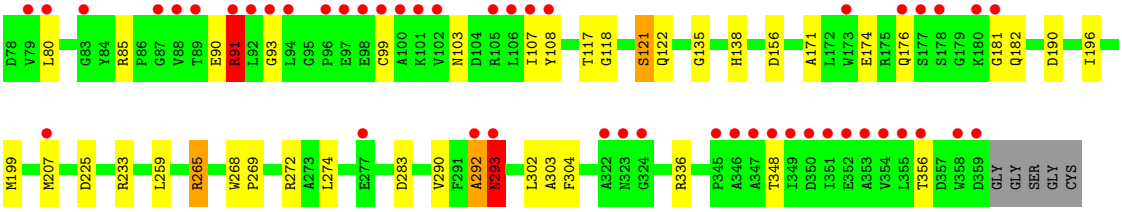
Chain F:



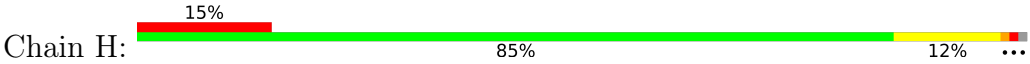
• Molecule 1: Alpha-methylacyl-CoA racemase

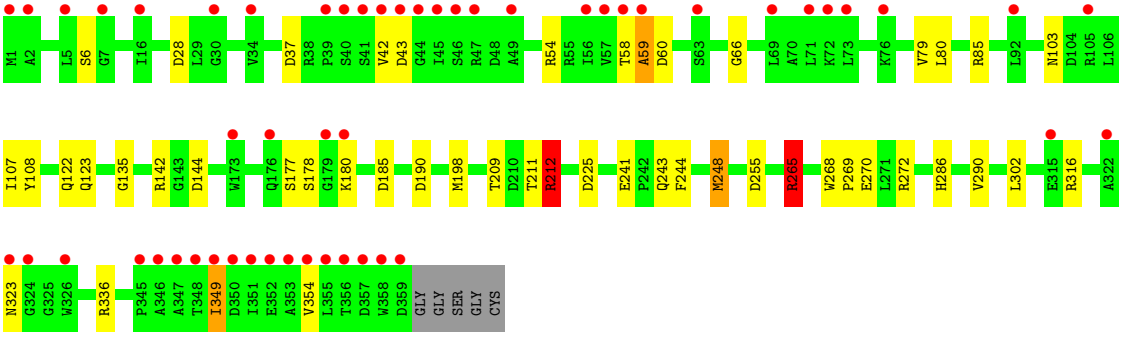
Chain G:



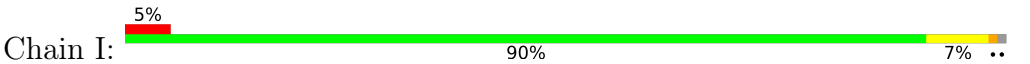


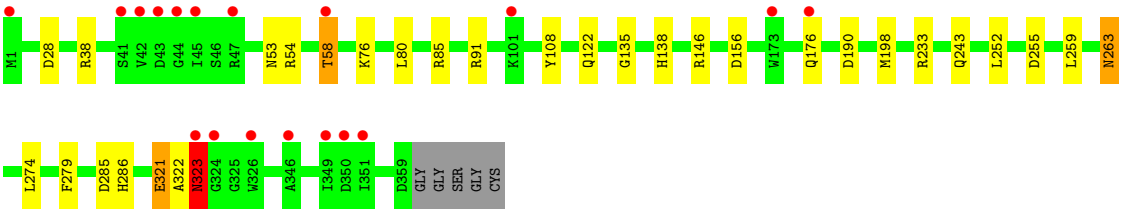
• Molecule 1: Alpha-methylacyl-CoA racemase



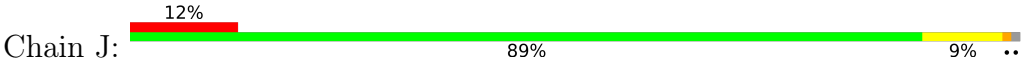


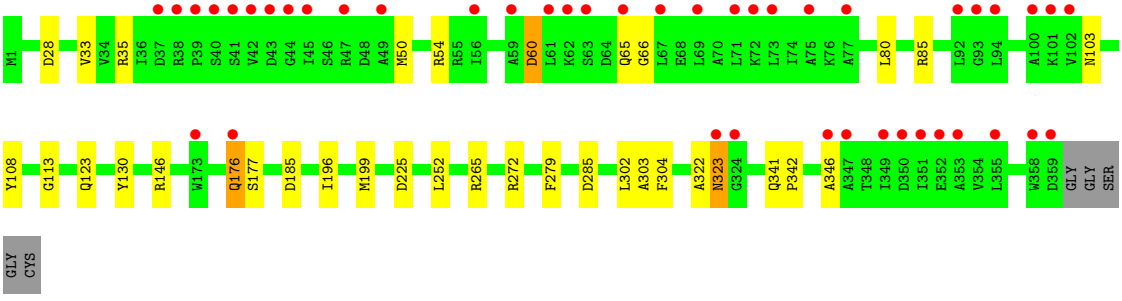
• Molecule 1: Alpha-methylacyl-CoA racemase



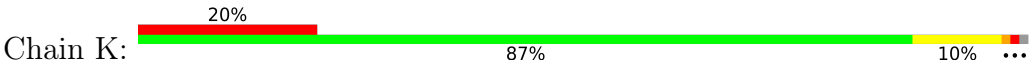


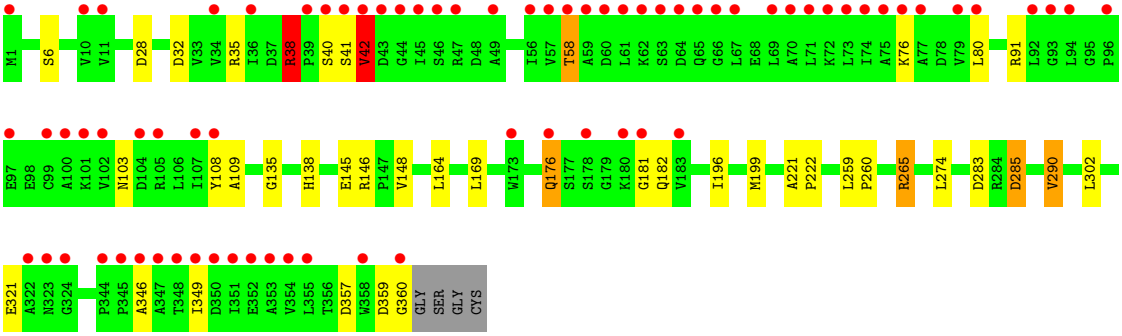
• Molecule 1: Alpha-methylacyl-CoA racemase





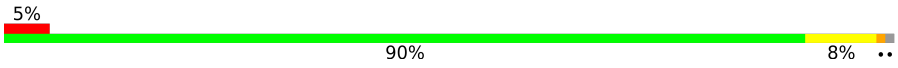
• Molecule 1: Alpha-methylacyl-CoA racemase

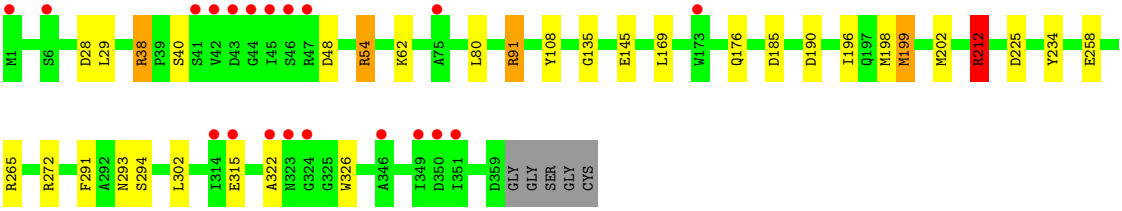




• Molecule 1: Alpha-methylacyl-CoA racemase

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	276.49Å 276.49Å 390.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	225.58 – 1.95 225.58 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (225.58-1.95) 99.9 (225.58-1.95)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.205 , 0.233 0.215 , 0.242	Depositor DCC
R_{free} test set	27062 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.007 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	35488	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/2774	1.17	10/3774 (0.3%)
1	B	0.69	0/2791	1.19	11/3797 (0.3%)
1	C	0.68	0/2786	1.21	10/3789 (0.3%)
1	D	0.69	0/2782	1.18	13/3785 (0.3%)
1	E	0.67	0/2782	1.14	8/3783 (0.2%)
1	F	0.67	0/2786	1.17	5/3789 (0.1%)
1	G	0.67	0/2791	1.20	10/3797 (0.3%)
1	H	0.67	0/2782	1.19	14/3785 (0.4%)
1	I	0.70	0/2791	1.17	12/3797 (0.3%)
1	J	0.69	0/2782	1.21	16/3785 (0.4%)
1	K	0.69	0/2795	1.21	13/3802 (0.3%)
1	L	0.67	0/2791	1.15	13/3797 (0.3%)
All	All	0.68	0/33433	1.18	135/45480 (0.3%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	33

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	ARG	N-CA-CB	11.00	126.44	110.16
1	J	123	GLN	CB-CA-C	10.89	127.59	109.84
1	L	38	ARG	N-CA-CB	-9.86	96.98	110.29
1	I	255	ASP	CB-CA-C	9.85	126.14	110.19
1	B	203	ARG	CB-CA-C	-9.45	94.78	110.85
1	C	203	ARG	N-CA-CB	9.27	123.88	110.16
1	D	265	ARG	CD-NE-CZ	8.56	136.38	124.40
1	D	265	ARG	NE-CZ-NH2	8.52	126.87	119.20
1	B	255	ASP	CB-CA-C	8.48	124.39	110.22
1	C	203	ARG	CB-CA-C	-8.41	96.56	110.85
1	H	265	ARG	NE-CZ-NH2	8.36	126.73	119.20
1	L	38	ARG	CB-CA-C	8.13	120.34	108.87
1	K	38	ARG	N-CA-CB	7.93	121.69	110.11
1	J	123	GLN	N-CA-CB	-7.92	97.68	109.95
1	H	123	GLN	CB-CA-C	7.69	122.37	109.84
1	L	265	ARG	NE-CZ-NH2	7.54	125.99	119.20
1	J	265	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	K	38	ARG	CB-CA-C	-7.47	97.24	109.27
1	G	91	ARG	CB-CA-C	-7.45	96.85	110.63
1	F	350	ASP	CB-CA-C	6.98	121.32	109.53
1	B	258	GLU	CB-CA-C	-6.97	96.87	110.11
1	A	207	MET	CG-SD-CE	6.92	116.11	100.90
1	I	91	ARG	CB-CA-C	-6.89	97.45	110.67
1	E	28	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	190	ASP	CA-CB-CG	6.85	119.45	112.60
1	H	265	ARG	CD-NE-CZ	6.84	133.98	124.40
1	K	283	ASP	CA-CB-CG	6.82	119.42	112.60
1	D	265	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	J	265	ARG	CD-NE-CZ	6.74	133.84	124.40
1	L	28	ASP	CA-CB-CG	6.74	119.33	112.60
1	L	91	ARG	CB-CA-C	-6.68	99.33	110.68
1	A	58	THR	CA-CB-OG1	-6.66	99.61	109.60
1	K	265	ARG	CD-NE-CZ	6.64	133.70	124.40
1	J	265	ARG	NE-CZ-NH1	-6.56	114.94	121.50
1	B	156	ASP	CB-CA-C	-6.51	100.61	110.90
1	J	185	ASP	CA-CB-CG	6.47	119.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	265	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	G	91	ARG	N-CA-CB	6.42	120.11	110.22
1	A	28	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	91	ARG	CB-CA-C	-6.33	98.17	110.46
1	J	28	ASP	CA-CB-CG	6.31	118.91	112.60
1	D	248	MET	CG-SD-CE	6.30	114.76	100.90
1	J	285	ASP	CB-CA-C	6.30	122.77	110.67
1	A	38	ARG	CB-CA-C	6.29	118.54	109.11
1	I	91	ARG	N-CA-CB	6.26	119.98	110.28
1	K	265	ARG	NE-CZ-NH1	6.25	127.75	121.50
1	D	28	ASP	CA-CB-CG	6.22	118.82	112.60
1	C	265	ARG	CD-NE-CZ	6.19	133.07	124.40
1	A	258	GLU	N-CA-CB	6.03	119.66	110.44
1	K	28	ASP	CA-CB-CG	6.01	118.61	112.60
1	L	190	ASP	CA-CB-CG	5.99	118.59	112.60
1	G	283	ASP	CA-CB-CG	5.98	118.58	112.60
1	H	248	MET	CG-SD-CE	5.97	114.05	100.90
1	A	91	ARG	N-CA-CB	5.97	119.58	110.14
1	H	265	ARG	NE-CZ-NH1	-5.97	115.53	121.50
1	G	54	ARG	N-CA-CB	-5.94	100.48	111.53
1	G	60	ASP	CA-CB-CG	5.92	118.52	112.60
1	F	190	ASP	CA-CB-CG	5.91	118.51	112.60
1	I	156	ASP	CA-CB-CG	5.89	118.49	112.60
1	E	190	ASP	CA-CB-CG	5.88	118.48	112.60
1	I	190	ASP	CA-CB-CG	5.86	118.46	112.60
1	E	265	ARG	CA-CB-CG	-5.85	102.40	114.10
1	I	285	ASP	CB-CA-C	5.85	121.44	110.63
1	I	156	ASP	CB-CA-C	-5.84	101.71	110.88
1	D	144	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	38	ARG	CB-CA-C	5.83	117.08	108.87
1	G	28	ASP	CA-CB-CG	5.82	118.42	112.60
1	J	54	ARG	CB-CA-C	-5.78	97.64	109.94
1	B	190	ASP	CA-CB-CG	5.74	118.34	112.60
1	E	50	MET	CG-SD-CE	5.72	113.48	100.90
1	H	123	GLN	N-CA-CB	-5.65	101.19	109.95
1	C	28	ASP	CA-CB-CG	5.65	118.25	112.60
1	K	285	ASP	CB-CA-C	5.63	121.49	110.67
1	E	123	GLN	CB-CA-C	-5.62	100.91	109.89
1	K	32	ASP	CA-CB-CG	5.61	118.21	112.60
1	G	190	ASP	CA-CB-CG	5.59	118.19	112.60
1	L	185	ASP	CA-CB-CG	5.57	118.17	112.60
1	J	33	VAL	N-CA-CB	5.57	118.48	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	85	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	G	91	ARG	CG-CD-NE	5.55	124.20	112.00
1	D	323	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	60	ASP	CA-CB-CG	5.48	118.08	112.60
1	I	146	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	I	321	GLU	CB-CA-C	-5.46	101.10	110.22
1	B	156	ASP	CA-CB-CG	5.46	118.06	112.60
1	E	144	ASP	CA-CB-CG	5.44	118.04	112.60
1	E	255	ASP	CA-CB-CG	5.43	118.03	112.60
1	H	28	ASP	CA-CB-CG	5.43	118.03	112.60
1	L	29	LEU	N-CA-CB	-5.42	103.08	110.56
1	J	60	ASP	CA-CB-CG	5.42	118.02	112.60
1	K	58	THR	CA-CB-OG1	-5.42	101.48	109.60
1	H	42	VAL	N-CA-CB	5.41	120.16	111.23
1	A	258	GLU	CB-CA-C	-5.40	100.29	110.01
1	K	148	VAL	CA-C-O	5.39	122.85	119.51
1	J	265	ARG	CA-CB-CG	-5.37	103.36	114.10
1	A	175	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	G	348	THR	CA-CB-OG1	-5.31	101.64	109.60
1	L	38	ARG	CA-CB-CG	5.30	124.70	114.10
1	D	38	ARG	CB-CA-C	5.28	116.47	108.86
1	D	306	GLU	CB-CA-C	-5.28	100.47	109.65
1	D	190	ASP	CA-CB-CG	5.27	117.87	112.60
1	I	263	ASN	CA-CB-CG	-5.25	107.35	112.60
1	C	38	ARG	CB-CA-C	-5.24	101.26	109.11
1	J	146	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	B	145	GLU	CB-CG-CD	-5.23	103.70	112.60
1	L	54	ARG	CB-CA-C	-5.23	99.07	109.79
1	F	283	ASP	CA-CB-CG	5.22	117.82	112.60
1	H	255	ASP	CB-CA-C	5.21	118.92	110.22
1	H	185	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	85	ARG	CD-NE-CZ	5.18	131.65	124.40
1	H	190	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	283	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	76	LYS	N-CA-CB	-5.17	103.43	110.56
1	J	65	GLN	CB-CA-C	5.16	119.62	110.85
1	K	321	GLU	CB-CA-C	-5.16	101.34	109.80
1	K	290	VAL	N-CA-CB	-5.12	103.58	110.54
1	B	65	GLN	N-CA-CB	-5.12	102.57	110.20
1	C	330	PRO	CB-CA-C	-5.10	104.86	111.39
1	I	58	THR	CA-CB-OG1	-5.10	101.95	109.60
1	B	265	ARG	NE-CZ-NH2	5.09	123.79	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	94	LEU	N-CA-C	-5.09	106.38	112.59
1	L	258	GLU	CB-CA-C	-5.09	100.85	110.01
1	H	144	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	218	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	212	ARG	CB-CA-C	5.08	118.11	109.53
1	L	91	ARG	CG-CD-NE	5.08	123.17	112.00
1	H	270	GLU	N-CA-CB	-5.07	102.72	110.07
1	D	350	ASP	CB-CA-C	-5.06	101.00	109.65
1	K	146	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	D	285	ASP	CB-CA-C	5.04	120.35	110.67
1	F	148	VAL	CA-C-O	5.04	122.63	119.51
1	J	54	ARG	CA-CB-CG	5.03	124.16	114.10
1	I	255	ASP	CA-CB-CG	5.03	117.63	112.60
1	G	293	ASN	CA-CB-CG	5.02	117.62	112.60
1	H	211	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	54	ARG	Peptide
1	B	322	ALA	Peptide
1	B	85	ARG	Sidechain
1	D	212	ARG	Sidechain
1	D	322	ALA	Peptide
1	D	54	ARG	Peptide
1	D	85	ARG	Sidechain
1	E	348	THR	Peptide
1	E	350	ASP	Peptide
1	E	54	ARG	Peptide
1	F	233	ARG	Sidechain
1	F	322	ALA	Peptide
1	F	85	ARG	Sidechain
1	G	233	ARG	Sidechain
1	G	265	ARG	Sidechain
1	G	47	ARG	Sidechain
1	G	54	ARG	Peptide
1	G	91	ARG	Sidechain
1	H	212	ARG	Sidechain
1	H	54	ARG	Peptide
1	I	233	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	54	ARG	Peptide
1	J	35	ARG	Sidechain
1	K	265	ARG	Sidechain
1	K	35	ARG	Sidechain
1	K	38	ARG	Sidechain
1	K	91	ARG	Sidechain
1	L	212	ARG	Sidechain
1	L	322	ALA	Peptide
1	L	38	ARG	Sidechain
1	L	54	ARG	Peptide
1	L	91	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2707	0	2656	23	0
1	B	2721	0	2668	20	0
1	C	2714	0	2654	24	0
1	D	2715	0	2660	25	0
1	E	2710	0	2653	21	0
1	F	2717	0	2664	30	0
1	G	2718	0	2658	30	0
1	H	2715	0	2660	24	0
1	I	2718	0	2658	15	0
1	J	2715	0	2660	14	0
1	K	2722	0	2661	19	0
1	L	2721	0	2668	17	0
2	A	55	0	42	2	0
2	B	55	0	42	3	0
2	C	55	0	42	0	0
2	D	55	0	42	2	0
2	E	55	0	42	1	0
2	F	55	0	42	2	0
2	G	55	0	42	3	0
2	H	55	0	42	1	0
2	I	55	0	42	1	0
2	J	55	0	42	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	55	0	42	0	0
2	L	55	0	42	0	0
3	A	195	0	0	6	0
3	B	161	0	0	2	0
3	C	162	0	0	5	0
3	D	194	0	0	2	0
3	E	171	0	0	1	0
3	F	173	0	0	7	0
3	G	170	0	0	4	0
3	H	178	0	0	5	0
3	I	227	0	0	3	0
3	J	203	0	0	1	0
3	K	186	0	0	4	0
3	L	215	0	0	6	0
All	All	35488	0	32424	233	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 (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ARG:HD3	2:F:401:HXC:O11	1.52	1.09
1:H:243:GLN:HB2	3:H:642:HOH:O	1.65	0.96
1:D:85:ARG:HD3	2:D:401:HXC:O11	1.71	0.91
1:E:176:GLN:CD	1:F:176:GLN:HG3	2.00	0.86
1:C:118:GLY:O	1:C:121:SER:OG	2.00	0.78
1:B:85:ARG:HD3	2:B:401:HXC:O11	1.85	0.76
2:A:401:HXC:OP3	3:A:501:HOH:O	2.04	0.75
1:K:80:LEU:HD23	1:K:108:TYR:CE1	2.23	0.74
1:F:85:ARG:CD	2:F:401:HXC:O11	2.35	0.73
1:G:80:LEU:HD23	1:G:108:TYR:CE2	2.25	0.71
1:I:176:GLN:HG3	1:J:176:GLN:HE21	1.58	0.69
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.76	0.68
1:E:85:ARG:NH1	1:E:122:GLN:O	2.26	0.68
1:K:138:HIS:HD2	3:K:587:HOH:O	1.77	0.67
1:D:351:ILE:HG22	3:D:581:HOH:O	1.94	0.66
1:H:80:LEU:HD23	1:H:108:TYR:CE2	2.31	0.65
1:A:40:SER:OG	3:A:502:HOH:O	2.15	0.63
1:L:326:TRP:CD1	3:L:689:HOH:O	2.50	0.63
1:F:80:LEU:CD2	1:F:108:TYR:CE2	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:THR:O	1:F:59:ALA:HB2	1.99	0.63
1:B:291:PHE:O	1:B:294:SER:HB3	1.99	0.62
1:G:85:ARG:NH1	1:G:122:GLN:O	2.31	0.62
1:J:322:ALA:O	1:J:323:ASN:C	2.42	0.62
1:C:145:GLU:OE2	1:D:145:GLU:OE1	2.18	0.62
1:D:69:LEU:HD13	1:D:351:ILE:HG21	1.82	0.61
1:G:259:LEU:HD22	1:G:274:LEU:HD13	1.83	0.61
1:I:322:ALA:HB1	1:I:323:ASN:HD22	1.67	0.60
1:D:80:LEU:HD23	1:D:108:TYR:CE2	2.36	0.60
1:G:118:GLY:O	1:G:121:SER:OG	2.19	0.59
1:D:294:SER:HB2	1:L:293:ASN:O	2.02	0.59
1:C:80:LEU:CD2	1:C:108:TYR:CE2	2.86	0.59
1:K:346:ALA:HB3	3:K:531:HOH:O	2.03	0.59
1:C:15:GLY:O	3:C:501:HOH:O	2.17	0.58
1:L:80:LEU:HD23	1:L:108:TYR:CE2	2.39	0.58
1:J:225:ASP:OD2	1:J:272:ARG:NH1	2.36	0.58
1:H:58:THR:O	1:H:59:ALA:HB2	2.03	0.57
1:K:145:GLU:OE1	1:L:145:GLU:OE1	2.21	0.57
1:A:87:GLY:O	1:A:91:ARG:HG3	2.05	0.57
1:E:336:ARG:NH2	1:F:180:LYS:HB2	2.20	0.57
1:L:315:GLU:OE1	3:L:502:HOH:O	2.17	0.57
1:D:85:ARG:CD	2:D:401:HXC:O11	2.49	0.57
1:E:176:GLN:NE2	1:F:176:GLN:HG3	2.19	0.57
1:F:292:ALA:HB3	1:G:292:ALA:HB3	1.86	0.56
1:L:234:TYR:OH	3:L:501:HOH:O	2.17	0.56
1:I:259:LEU:HD22	1:I:274:LEU:HD13	1.87	0.56
1:B:85:ARG:HD2	2:B:401:HXC:HP7	1.88	0.55
1:H:349:ILE:HD11	1:H:354:VAL:HG22	1.87	0.55
1:K:41:SER:O	1:K:42:VAL:HG13	2.06	0.55
1:K:80:LEU:CD2	1:K:108:TYR:CE1	2.90	0.55
1:C:138:HIS:HD2	3:C:544:HOH:O	1.88	0.55
1:I:322:ALA:O	1:I:323:ASN:C	2.49	0.55
1:A:138:HIS:HD2	3:A:541:HOH:O	1.90	0.54
1:C:265:ARG:HD2	3:C:606:HOH:O	2.07	0.54
1:H:286:HIS:HE1	3:H:636:HOH:O	1.90	0.54
1:F:105:ARG:NH1	3:F:508:HOH:O	2.38	0.54
1:A:243:GLN:HB2	3:A:663:HOH:O	2.07	0.54
1:J:80:LEU:HD23	1:J:108:TYR:CE2	2.42	0.54
1:B:322:ALA:CB	1:B:323:ASN:HB2	2.38	0.54
1:H:80:LEU:CD2	1:H:108:TYR:CE2	2.90	0.54
1:A:180:LYS:O	1:B:336:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ASP:OD1	1:D:175:ARG:NH2	2.37	0.53
1:G:58:THR:O	1:G:59:ALA:HB2	2.07	0.53
1:F:293:ASN:ND2	1:G:290:VAL:O	2.42	0.53
1:F:106:LEU:O	1:F:181:GLY:HA3	2.09	0.53
1:F:42:VAL:O	1:F:43:ASP:HB2	2.07	0.53
1:E:80:LEU:HD23	1:E:108:TYR:CE2	2.43	0.53
1:F:122:GLN:HG2	3:F:501:HOH:O	2.07	0.53
1:E:109:ALA:HB1	1:E:164:LEU:HD11	1.90	0.52
1:D:270:GLU:HG3	3:D:611:HOH:O	2.08	0.52
1:E:316:ARG:HD2	1:F:117:THR:O	2.10	0.52
1:K:176:GLN:OE1	1:L:176:GLN:HG2	2.10	0.52
1:I:138:HIS:HD2	3:I:522:HOH:O	1.93	0.52
1:H:265:ARG:HD2	3:H:520:HOH:O	2.09	0.52
1:G:39:PRO:HD2	3:G:538:HOH:O	2.09	0.51
1:H:80:LEU:HD23	1:H:108:TYR:CD2	2.46	0.51
1:D:142:ARG:O	1:D:212:ARG:HD2	2.10	0.51
1:D:318:THR:HG22	1:D:319:PHE:CE1	2.45	0.51
1:D:69:LEU:HD13	1:D:351:ILE:CG2	2.40	0.51
1:C:138:HIS:O	1:C:212:ARG:HD3	2.10	0.51
1:F:108:TYR:HB3	1:F:183:VAL:HG22	1.93	0.50
1:J:346:ALA:HB3	3:J:1385:HOH:O	2.11	0.50
1:C:176:GLN:CD	1:D:176:GLN:HG2	2.37	0.50
1:G:181:GLY:O	1:G:182:GLN:HB3	2.12	0.50
1:C:67:LEU:HD12	1:C:67:LEU:O	2.11	0.50
1:E:225:ASP:OD2	1:E:272:ARG:NH1	2.44	0.50
1:J:60:ASP:O	1:J:66:GLY:HA3	2.12	0.50
1:B:243[B]:GLN:HG2	3:F:606:HOH:O	2.10	0.50
1:G:80:LEU:CD2	1:G:108:TYR:CE2	2.93	0.50
1:B:322:ALA:HB1	1:B:323:ASN:HB2	1.93	0.49
1:G:18:PRO:HB3	1:G:156:ASP:O	2.12	0.49
1:D:318:THR:HG22	1:D:319:PHE:CD1	2.48	0.49
1:I:80:LEU:CD2	1:I:108:TYR:CE2	2.96	0.49
1:A:91:ARG:NH2	2:A:401:HXC:O33	2.46	0.49
1:L:48:ASP:HB2	3:L:644:HOH:O	2.13	0.49
1:K:285:ASP:HB2	3:K:505:HOH:O	2.11	0.49
1:E:138:HIS:HD2	3:E:579:HOH:O	1.96	0.49
1:F:80:LEU:HD22	1:F:108:TYR:CE2	2.48	0.48
1:A:80:LEU:HD23	1:A:108:TYR:CE2	2.49	0.48
1:B:243[B]:GLN:CG	3:F:606:HOH:O	2.62	0.48
1:F:270:GLU:HG3	3:F:588:HOH:O	2.12	0.48
1:D:10:VAL:HG22	1:D:79:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASP:HA	1:C:53:ASN:ND2	2.29	0.48
1:K:259:LEU:HD22	1:K:274:LEU:HD13	1.94	0.48
1:F:294:SER:HB2	1:G:293:ASN:HB3	1.95	0.48
1:I:286:HIS:ND1	3:I:504:HOH:O	2.35	0.48
1:C:19:GLY:N	1:C:20:PRO:CD	2.77	0.48
1:G:265:ARG:NH2	3:G:510:HOH:O	2.42	0.48
1:C:329:MET:HE3	1:C:330:PRO:HD2	1.95	0.48
1:E:9:ARG:NH2	1:E:358:TRP:HA	2.28	0.47
2:H:401:HXC:HP81	2:H:401:HXC:OP2	2.14	0.47
1:A:91:ARG:NH1	3:A:504:HOH:O	2.31	0.47
1:I:263:ASN:HB2	3:I:601:HOH:O	2.14	0.47
1:G:90:GLU:OE1	1:G:90:GLU:N	2.37	0.47
1:K:181:GLY:O	1:K:182:GLN:HB3	2.15	0.47
1:K:285:ASP:CB	3:K:505:HOH:O	2.63	0.47
1:F:255:ASP:HB2	3:F:648:HOH:O	2.15	0.47
1:G:225:ASP:OD2	1:G:272:ARG:NH1	2.46	0.47
1:A:109:ALA:HB1	1:A:164:LEU:HD11	1.96	0.46
1:K:109:ALA:HB1	1:K:164:LEU:HD11	1.98	0.46
1:L:291:PHE:O	1:L:294:SER:HB3	2.16	0.46
1:A:80:LEU:CD2	1:A:108:TYR:CE2	2.98	0.46
1:H:85:ARG:NH2	1:H:122:GLN:O	2.48	0.46
1:H:241:GLU:HB2	1:H:244:PHE:CD2	2.50	0.46
1:B:80:LEU:HD23	1:B:108:TYR:CE2	2.50	0.46
1:A:176:GLN:HG3	1:B:176:GLN:NE2	2.31	0.46
1:C:148:VAL:HG23	1:C:149:PRO:HD2	1.96	0.46
1:C:346:ALA:HB3	3:C:598:HOH:O	2.15	0.46
1:F:323:ASN:CG	1:F:324:GLY:N	2.72	0.46
1:G:50:MET:HE1	1:H:198:MET:HB2	1.96	0.46
1:F:196:ILE:HG12	1:F:199:MET:HB2	1.98	0.46
1:G:90:GLU:O	1:G:93:GLY:N	2.38	0.46
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.80	0.46
1:C:272:ARG:NH1	3:C:513:HOH:O	2.49	0.45
1:D:73:LEU:HD11	1:D:351:ILE:HG13	1.98	0.45
2:G:401:HXC:HM21	2:G:401:HXC:HP11	1.84	0.45
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.98	0.45
1:F:118:GLY:O	1:F:121:SER:OG	2.28	0.45
1:A:117:THR:O	1:B:316:ARG:HD2	2.16	0.45
1:G:74:ILE:HG21	1:G:99:CYS:SG	2.55	0.45
1:H:225:ASP:OD2	1:H:272:ARG:NH1	2.45	0.45
1:A:39:PRO:HG3	1:A:58:THR:HG23	1.97	0.45
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ARG:NH1	3:F:514:HOH:O	2.47	0.45
1:I:85:ARG:NH1	1:I:122:GLN:O	2.48	0.45
1:F:322:ALA:O	1:F:323:ASN:C	2.59	0.45
1:L:196:ILE:HG12	1:L:199:MET:HB2	1.98	0.45
1:C:145:GLU:CD	1:D:145:GLU:OE1	2.60	0.44
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.52	0.44
1:I:198:MET:HB2	1:J:50:MET:HE1	1.99	0.44
1:B:138:HIS:O	1:B:212:ARG:HD3	2.16	0.44
1:A:176:GLN:CD	1:B:176:GLN:HG2	2.42	0.44
1:G:138:HIS:HD2	3:G:565:HOH:O	2.00	0.44
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.53	0.44
1:A:196:ILE:HG12	1:A:199:MET:HB2	2.00	0.44
1:E:259:LEU:HD22	1:E:274:LEU:HD13	2.00	0.44
1:C:180:LYS:O	1:D:336:ARG:NH2	2.51	0.44
1:E:322:ALA:O	1:E:323:ASN:C	2.61	0.44
1:A:91:ARG:HD2	1:E:242:PRO:HB3	2.00	0.44
1:I:28:ASP:HA	1:I:53:ASN:ND2	2.32	0.44
1:B:272:ARG:NH1	3:B:514:HOH:O	2.50	0.44
1:C:225:ASP:OD2	1:C:272:ARG:NH1	2.51	0.44
1:I:252:LEU:HD21	1:I:279:PHE:CE1	2.53	0.44
1:K:76:LYS:HE2	1:K:360:GLY:HA2	2.00	0.44
1:C:80:LEU:HD23	1:C:108:TYR:CE2	2.52	0.43
1:H:60:ASP:O	1:H:66:GLY:HA3	2.18	0.43
1:G:196:ILE:HG12	1:G:199:MET:HB2	2.01	0.43
1:H:79:VAL:HG22	1:H:107:ILE:HB	1.99	0.43
1:B:225:ASP:OD2	1:B:272:ARG:NH1	2.49	0.43
1:E:241:GLU:HB2	1:E:244:PHE:CD2	2.52	0.43
1:K:135:GLY:HA2	1:L:302:LEU:O	2.19	0.43
1:F:323:ASN:CG	1:F:324:GLY:H	2.27	0.43
1:B:55:ARG:HD2	1:B:349:ILE:CD1	2.49	0.43
1:E:196:ILE:HG12	1:E:199:MET:HB2	2.00	0.43
1:J:113:GLY:HA3	1:J:130:TYR:CE1	2.52	0.43
1:E:47:ARG:HH21	1:E:47:ARG:HG3	1.84	0.43
1:G:174:GLU:OE1	1:G:174:GLU:C	2.61	0.43
1:H:142:ARG:O	1:H:212:ARG:HD2	2.19	0.43
1:I:176:GLN:CD	1:J:176:GLN:HG2	2.44	0.43
1:K:259:LEU:HB3	1:K:260:PRO:HD2	2.01	0.43
1:B:212:ARG:HG3	3:B:530:HOH:O	2.19	0.43
1:A:69:LEU:HD13	1:A:351:ILE:HG21	2.01	0.42
1:L:198:MET:HE2	1:L:202:MET:SD	2.58	0.42
1:C:135:GLY:HA2	1:D:302:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD13	1:A:92:LEU:O	2.19	0.42
1:A:240:ILE:HD13	2:B:401:HXC:HM63	2.01	0.42
1:A:285:ASP:HB2	3:A:660:HOH:O	2.18	0.42
1:D:196:ILE:HG12	1:D:199:MET:HB2	2.01	0.42
1:G:91:ARG:NH2	2:G:401:HXC:O32	2.52	0.42
1:G:302:LEU:O	1:H:135:GLY:HA2	2.19	0.42
1:I:135:GLY:HA2	1:J:302:LEU:O	2.19	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.81	0.42
1:F:37:ASP:O	1:F:58:THR:HA	2.19	0.42
1:K:196:ILE:HG12	1:K:199:MET:HB2	2.02	0.42
1:J:341:GLN:HA	1:J:342:PRO:HD3	1.95	0.42
1:L:225:ASP:OD2	1:L:272:ARG:NH1	2.52	0.42
1:F:80:LEU:HD23	1:F:108:TYR:CE2	2.53	0.42
1:J:252:LEU:HD21	1:J:279:PHE:CE1	2.55	0.42
2:G:401:HXC:OP3	3:G:501:HOH:O	2.22	0.42
1:B:108:TYR:HB3	1:B:183:VAL:HG22	2.02	0.41
1:G:107:ILE:HD12	1:G:171:ALA:HB1	2.01	0.41
1:H:37:ASP:O	1:H:58:THR:HA	2.20	0.41
1:B:80:LEU:CD2	1:B:108:TYR:CE2	3.02	0.41
1:E:135:GLY:HA2	1:F:302:LEU:O	2.19	0.41
1:E:224:TYR:HA	1:E:237:VAL:O	2.19	0.41
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.56	0.41
1:C:241:GLU:HB2	1:C:244:PHE:CD2	2.54	0.41
1:L:62:LYS:HE3	3:L:610:HOH:O	2.19	0.41
1:H:268:TRP:N	1:H:269:PRO:CD	2.83	0.41
2:I:401:HXC:HM21	2:I:401:HXC:HP11	1.73	0.41
1:J:303:ALA:O	1:J:304:PHE:C	2.63	0.41
1:A:174:GLU:OE1	1:A:174:GLU:C	2.63	0.41
1:E:91:ARG:NH2	2:E:401:HXC:O31	2.54	0.41
1:G:336:ARG:HG2	1:G:336:ARG:HH11	1.85	0.41
1:H:178:SER:O	1:H:180:LYS:HG3	2.19	0.41
1:H:286:HIS:HD2	3:H:663:HOH:O	2.03	0.41
1:K:221:ALA:HA	1:K:222:PRO:HD3	1.91	0.41
1:C:176:GLN:NE2	1:D:176:GLN:HG2	2.36	0.41
1:E:302:LEU:O	1:F:135:GLY:HA2	2.20	0.41
1:F:241:GLU:HB2	1:F:244:PHE:CD2	2.54	0.41
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.56	0.41
1:G:39:PRO:CB	1:G:58:THR:HG23	2.51	0.41
1:G:117:THR:O	1:H:316:ARG:HD2	2.21	0.41
1:I:80:LEU:HD22	1:I:108:TYR:CE2	2.56	0.41
1:J:196:ILE:HG12	1:J:199:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ALA:O	1:D:323:ASN:C	2.64	0.40
1:G:268:TRP:N	1:G:269:PRO:CD	2.83	0.40
1:G:135:GLY:HA2	1:H:302:LEU:O	2.20	0.40
1:G:303:ALA:O	1:G:304:PHE:C	2.65	0.40
1:K:169:LEU:HB3	1:L:169:LEU:HB3	2.02	0.40
1:E:113:GLY:HA3	1:E:130:TYR:CZ	2.57	0.40
1:H:286:HIS:CE1	3:H:636:HOH:O	2.70	0.40
1:K:302:LEU:O	1:L:135:GLY:HA2	2.21	0.40
1:L:212:ARG:HG2	3:L:568:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/364 (98%)	338 (95%)	17 (5%)	2 (1%)	22	13
1	B	359/364 (99%)	345 (96%)	13 (4%)	1 (0%)	37	29
1	C	356/364 (98%)	341 (96%)	13 (4%)	2 (1%)	22	13
1	D	358/364 (98%)	344 (96%)	13 (4%)	1 (0%)	37	29
1	E	356/364 (98%)	341 (96%)	12 (3%)	3 (1%)	16	8
1	F	356/364 (98%)	335 (94%)	17 (5%)	4 (1%)	12	4
1	G	359/364 (99%)	333 (93%)	22 (6%)	4 (1%)	12	4
1	H	358/364 (98%)	339 (95%)	16 (4%)	3 (1%)	16	8
1	I	359/364 (99%)	349 (97%)	9 (2%)	1 (0%)	37	29
1	J	358/364 (98%)	347 (97%)	9 (2%)	2 (1%)	22	13
1	K	360/364 (99%)	343 (95%)	15 (4%)	2 (1%)	22	13
1	L	359/364 (99%)	347 (97%)	12 (3%)	0	100	100
All	All	4295/4368 (98%)	4102 (96%)	168 (4%)	25 (1%)	22	13

All (25) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/277 (99%)	268 (98%)	7 (2%)	42	34
1	B	277/277 (100%)	268 (97%)	9 (3%)	34	24
1	C	277/277 (100%)	270 (98%)	7 (2%)	42	34
1	D	276/277 (100%)	268 (97%)	8 (3%)	37	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	276/277 (100%)	272 (99%)	4 (1%)	62 59
1	F	277/277 (100%)	268 (97%)	9 (3%)	34 24
1	G	277/277 (100%)	268 (97%)	9 (3%)	34 24
1	H	276/277 (100%)	267 (97%)	9 (3%)	33 23
1	I	277/277 (100%)	271 (98%)	6 (2%)	47 41
1	J	276/277 (100%)	274 (99%)	2 (1%)	81 81
1	K	277/277 (100%)	267 (96%)	10 (4%)	30 20
1	L	277/277 (100%)	274 (99%)	3 (1%)	70 68
All	All	3318/3324 (100%)	3235 (98%)	83 (2%)	42 34

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	58	THR
1	A	199	MET
1	A	258	GLU
1	A	294	SER
1	A	349	ILE
1	A	350	ASP
1	B	6	SER
1	B	41	SER
1	B	85	ARG
1	B	243[A]	GLN
1	B	243[B]	GLN
1	B	258	GLU
1	B	290	VAL
1	B	323	ASN
1	B	359	ASP
1	C	40	SER
1	C	42	VAL
1	C	54	ARG
1	C	58	THR
1	C	121	SER
1	C	265	ARG
1	C	311	PRO
1	D	6	SER
1	D	43	ASP
1	D	45	ILE

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Mol	Chain	Res	Type
1	D	85	ARG
1	D	199	MET
1	D	212	ARG
1	D	290	VAL
1	D	294	SER
1	E	42	VAL
1	E	58	THR
1	E	350	ASP
1	E	351	ILE
1	F	42	VAL
1	F	56	ILE
1	F	85	ARG
1	F	121	SER
1	F	176	GLN
1	F	294	SER
1	F	323	ASN
1	F	348	THR
1	F	350	ASP
1	G	6	SER
1	G	40	SER
1	G	42	VAL
1	G	54	ARG
1	G	121	SER
1	G	176	GLN
1	G	207	MET
1	G	293	ASN
1	G	356	THR
1	H	6	SER
1	H	177	SER
1	H	209	THR
1	H	212	ARG
1	H	248	MET
1	H	265	ARG
1	H	290	VAL
1	H	323	ASN
1	H	349	ILE
1	I	38	ARG
1	I	58	THR
1	I	76	LYS
1	I	243	GLN
1	I	321	GLU
1	I	323	ASN

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Mol	Chain	Res	Type
1	J	176	GLN
1	J	177	SER
1	K	6	SER
1	K	38	ARG
1	K	40	SER
1	K	42	VAL
1	K	58	THR
1	K	176	GLN
1	K	290	VAL
1	K	349	ILE
1	K	357	ASP
1	K	359	ASP
1	L	40	SER
1	L	199	MET
1	L	212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	G	138	HIS
1	G	176	GLN
1	G	263	ASN
1	G	282	HIS
1	G	327	GLN
1	H	122	GLN
1	H	286	HIS
1	H	323	ASN
1	I	116	GLN
1	I	138	HIS
1	I	176	GLN
1	I	323	ASN
1	I	327	GLN
1	J	122	GLN
1	J	176	GLN
1	J	286	HIS
1	K	138	HIS
1	K	263	ASN
1	K	308	HIS
1	K	327	GLN
1	L	282	HIS
1	L	286	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HXC	B	401	-	49,57,57	1.54	4 (8%)	60,83,83	1.72	5 (8%)
2	HXC	D	401	-	49,57,57	1.46	3 (6%)	60,83,83	1.42	4 (6%)
2	HXC	F	401	-	49,57,57	1.63	4 (8%)	60,83,83	1.69	10 (16%)
2	HXC	J	401	-	49,57,57	1.08	5 (10%)	60,83,83	1.87	10 (16%)
2	HXC	L	401	-	49,57,57	1.19	3 (6%)	60,83,83	1.72	7 (11%)
2	HXC	C	401	-	49,57,57	1.18	2 (4%)	60,83,83	1.97	10 (16%)
2	HXC	G	401	-	49,57,57	1.52	3 (6%)	60,83,83	1.71	10 (16%)
2	HXC	A	401	-	49,57,57	1.07	2 (4%)	60,83,83	1.93	10 (16%)
2	HXC	I	401	-	49,57,57	1.54	3 (6%)	60,83,83	1.53	5 (8%)
2	HXC	K	401	-	49,57,57	1.64	3 (6%)	60,83,83	1.74	11 (18%)
2	HXC	H	401	-	49,57,57	1.44	4 (8%)	60,83,83	1.38	5 (8%)
2	HXC	E	401	-	49,57,57	0.98	2 (4%)	60,83,83	1.56	9 (15%)

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	HXC	B	401	-	-	9/52/72/72	0/3/3/3
2	HXC	D	401	-	-	7/52/72/72	0/3/3/3
2	HXC	F	401	-	-	8/52/72/72	0/3/3/3
2	HXC	J	401	-	-	10/52/72/72	0/3/3/3
2	HXC	L	401	-	-	10/52/72/72	0/3/3/3
2	HXC	C	401	-	-	10/52/72/72	0/3/3/3
2	HXC	G	401	-	-	10/52/72/72	0/3/3/3
2	HXC	A	401	-	-	8/52/72/72	0/3/3/3
2	HXC	I	401	-	-	7/52/72/72	0/3/3/3
2	HXC	K	401	-	-	8/52/72/72	0/3/3/3
2	HXC	H	401	-	-	5/52/72/72	0/3/3/3
2	HXC	E	401	-	-	9/52/72/72	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	HXC	CM1-S	8.54	1.96	1.76
2	F	401	HXC	CM1-S	8.24	1.96	1.76
2	I	401	HXC	CM1-S	8.20	1.96	1.76
2	B	401	HXC	CM1-S	8.08	1.95	1.76
2	G	401	HXC	CM1-S	8.07	1.95	1.76
2	D	401	HXC	CM1-S	7.59	1.94	1.76
2	H	401	HXC	CM1-S	6.98	1.93	1.76
2	L	401	HXC	CM1-S	5.11	1.88	1.76
2	C	401	HXC	CM1-S	4.97	1.88	1.76
2	K	401	HXC	OM2-CM1	4.78	1.28	1.21
2	I	401	HXC	OM2-CM1	4.41	1.28	1.21
2	F	401	HXC	OM2-CM1	4.32	1.28	1.21
2	B	401	HXC	OM2-CM1	4.11	1.27	1.21
2	D	401	HXC	OM2-CM1	4.10	1.27	1.21
2	A	401	HXC	CM1-S	4.06	1.86	1.76
2	H	401	HXC	OM2-CM1	3.97	1.27	1.21
2	G	401	HXC	OM2-CM1	3.92	1.27	1.21
2	J	401	HXC	CM1-S	3.62	1.84	1.76
2	E	401	HXC	CM1-S	3.59	1.84	1.76
2	L	401	HXC	CP1-CP2	3.10	1.64	1.51
2	K	401	HXC	CM2-CM1	3.05	1.54	1.50
2	F	401	HXC	OP1-CP3	2.90	1.29	1.23
2	F	401	HXC	CM2-CM1	2.67	1.53	1.50
2	E	401	HXC	OM2-CM1	2.61	1.25	1.21
2	H	401	HXC	CM2-CM1	2.59	1.53	1.50
2	J	401	HXC	CM2-CM1	2.51	1.53	1.50
2	A	401	HXC	CM2-CM1	2.51	1.53	1.50
2	J	401	HXC	OP3-CP7	2.51	1.46	1.42
2	I	401	HXC	CM2-CM1	2.46	1.53	1.50
2	L	401	HXC	P3-O3'	2.44	1.63	1.59
2	D	401	HXC	P3-O3'	2.42	1.63	1.59
2	G	401	HXC	CM2-CM1	2.35	1.53	1.50
2	B	401	HXC	P3-O3'	2.21	1.63	1.59
2	H	401	HXC	OP1-CP3	2.17	1.27	1.23
2	B	401	HXC	C8-N7	-2.15	1.30	1.34
2	J	401	HXC	OM2-CM1	2.12	1.24	1.21
2	C	401	HXC	CM2-CM1	2.11	1.53	1.50
2	J	401	HXC	CP1-CP2	2.08	1.59	1.51

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	401	HXC	CP1-S-CM1	8.80	129.26	101.87
2	A	401	HXC	CP1-S-CM1	8.69	128.94	101.87
2	J	401	HXC	CP1-S-CM1	8.24	127.53	101.87
2	B	401	HXC	OM2-CM1-CM2	-7.06	115.66	123.99
2	E	401	HXC	CP1-S-CM1	6.78	122.97	101.87
2	B	401	HXC	OM2-CM1-S	6.70	131.31	122.61
2	I	401	HXC	OM2-CM1-S	6.38	130.90	122.61
2	G	401	HXC	OM2-CM1-CM2	-6.32	116.52	123.99
2	F	401	HXC	OM2-CM1-CM2	-6.27	116.59	123.99
2	C	401	HXC	CP4-CP3-NP1	6.20	126.85	116.42
2	D	401	HXC	OM2-CM1-CM2	-6.09	116.80	123.99
2	J	401	HXC	O22-P2-O21	6.08	142.31	112.24
2	K	401	HXC	OM2-CM1-S	5.73	130.05	122.61
2	I	401	HXC	OM2-CM1-CM2	-5.64	117.33	123.99
2	C	401	HXC	CM2-CM1-S	5.56	119.94	113.46
2	G	401	HXC	O22-P2-O21	5.45	139.19	112.24
2	C	401	HXC	CP1-S-CM1	5.44	118.82	101.87
2	C	401	HXC	O22-P2-O21	5.41	138.97	112.24
2	A	401	HXC	O22-P2-O21	5.35	138.71	112.24
2	D	401	HXC	OM2-CM1-S	5.33	129.54	122.61
2	F	401	HXC	O22-P2-O21	5.24	138.15	112.24
2	K	401	HXC	O22-P2-O21	4.98	136.87	112.24
2	F	401	HXC	OM2-CM1-S	4.88	128.96	122.61
2	H	401	HXC	OM2-CM1-S	4.64	128.64	122.61
2	K	401	HXC	OM2-CM1-CM2	-4.62	118.54	123.99
2	G	401	HXC	OM2-CM1-S	4.61	128.60	122.61
2	K	401	HXC	O32-P3-O31	4.57	125.10	107.64
2	H	401	HXC	O22-P2-O21	4.56	134.78	112.24
2	L	401	HXC	OM2-CM1-CM2	-4.39	118.80	123.99
2	H	401	HXC	OM2-CM1-CM2	-4.28	118.94	123.99
2	C	401	HXC	OM2-CM1-CM2	-4.18	119.06	123.99
2	J	401	HXC	CP9-CPA-CP7	4.00	115.75	108.82
2	J	401	HXC	CM2-CM1-S	3.94	118.04	113.46
2	E	401	HXC	O2'-C2'-C3'	3.81	121.99	111.17
2	I	401	HXC	O22-P2-O21	3.79	130.97	112.24
2	L	401	HXC	O22-P2-O21	3.72	130.61	112.24
2	C	401	HXC	OP3-CP7-CPA	-3.65	101.65	110.25
2	B	401	HXC	O22-P2-O21	3.53	129.71	112.24
2	C	401	HXC	OP1-CP3-CP4	-3.53	115.57	122.02
2	A	401	HXC	OM2-CM1-CM2	-3.51	119.84	123.99
2	G	401	HXC	O7-P2-O21	-3.48	95.48	109.07
2	A	401	HXC	O7-P2-O21	-3.31	96.15	109.07
2	G	401	HXC	O32-P3-O31	3.27	120.12	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	401	HXC	CM2-CM1-S	3.25	117.23	113.46
2	A	401	HXC	O2'-C2'-C3'	3.18	120.19	111.17
2	A	401	HXC	CP8-CPA-CPB	-3.17	103.06	108.23
2	K	401	HXC	O31-P3-O33	-3.13	98.41	110.68
2	A	401	HXC	CM2-CM1-S	3.13	117.10	113.46
2	B	401	HXC	O32-P3-O31	3.11	119.52	107.64
2	D	401	HXC	O22-P2-O21	3.10	127.59	112.24
2	F	401	HXC	OP3-CP7-CPA	-3.10	102.96	110.25
2	K	401	HXC	C5-C6-N6	3.08	125.03	120.35
2	J	401	HXC	OM2-CM1-CM2	-3.08	120.36	123.99
2	K	401	HXC	O7-P2-O21	-2.99	97.37	109.07
2	C	401	HXC	O7-P2-O21	-2.96	97.52	109.07
2	E	401	HXC	O2'-C2'-C1'	-2.95	99.95	110.85
2	G	401	HXC	O2'-C2'-C3'	-2.94	102.82	111.17
2	C	401	HXC	OP1-CP3-NP1	-2.91	117.53	123.01
2	H	401	HXC	C5-C6-N6	2.91	124.77	120.35
2	F	401	HXC	O7-CPB-CPA	-2.88	105.92	110.55
2	C	401	HXC	C5-C6-N6	2.87	124.71	120.35
2	J	401	HXC	O7-P2-O21	-2.86	97.88	109.07
2	F	401	HXC	O2'-C2'-C3'	2.81	119.14	111.17
2	G	401	HXC	C5-C6-N6	2.78	124.57	120.35
2	E	401	HXC	O22-P2-O21	2.67	125.42	112.24
2	F	401	HXC	C5-C6-N6	2.61	124.32	120.35
2	I	401	HXC	CP2-NP1-CP3	-2.56	118.08	122.84
2	L	401	HXC	O32-P3-O31	2.55	117.39	107.64
2	E	401	HXC	C5-C6-N6	2.54	124.22	120.35
2	E	401	HXC	O32-P3-O31	2.52	117.25	107.64
2	G	401	HXC	CP8-CPA-CPB	2.48	112.27	108.23
2	D	401	HXC	O3'-P3-O33	-2.45	99.92	109.39
2	G	401	HXC	O7-CPB-CPA	-2.45	106.61	110.55
2	J	401	HXC	C5-C6-N6	2.44	124.06	120.35
2	F	401	HXC	CP4-CP3-NP1	-2.43	112.32	116.42
2	H	401	HXC	C1'-N9-C4	-2.42	122.38	126.64
2	K	401	HXC	O7-CPB-CPA	-2.40	106.69	110.55
2	I	401	HXC	CP8-CPA-CP7	2.36	112.92	108.82
2	B	401	HXC	O32-P3-O33	-2.29	101.71	110.68
2	L	401	HXC	CP9-CPA-CPB	2.29	111.97	108.23
2	E	401	HXC	OM2-CM1-S	2.26	125.55	122.61
2	J	401	HXC	O32-P3-O31	2.25	116.24	107.64
2	A	401	HXC	OP3-CP7-CPA	-2.25	104.96	110.25
2	K	401	HXC	O32-P3-O33	2.22	119.37	110.68
2	A	401	HXC	O2'-C2'-C1'	-2.21	102.68	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	HXC	CP8-CPA-CP7	2.21	112.64	108.82
2	F	401	HXC	O12-P1-O11	2.17	122.95	112.24
2	J	401	HXC	CP8-CPA-CP9	-2.11	104.86	109.17
2	F	401	HXC	O3'-C3'-C2'	2.08	119.23	111.68
2	L	401	HXC	O22-P2-O7	-2.08	98.09	107.75
2	A	401	HXC	C5-C6-N6	2.06	123.49	120.35
2	G	401	HXC	O31-P3-O3'	-2.03	96.89	105.99
2	K	401	HXC	CP9-CPA-CPB	-2.03	104.92	108.23
2	K	401	HXC	O32-P3-O3'	-2.03	96.91	105.99
2	J	401	HXC	O31-P3-O3'	2.02	115.03	105.99
2	E	401	HXC	OM2-CM1-CM2	-2.00	121.62	123.99

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	HXC	C3'-O3'-P3-O31
2	A	401	HXC	CP2-CP1-S-CM1
2	A	401	HXC	CM1-CM2-CM3-CM4
2	B	401	HXC	C3'-O3'-P3-O33
2	B	401	HXC	CPB-O7-P2-O21
2	B	401	HXC	CP3-CP4-CP5-NP2
2	B	401	HXC	CM2-CM1-S-CP1
2	B	401	HXC	OM2-CM1-S-CP1
2	C	401	HXC	CP4-CP3-NP1-CP2
2	C	401	HXC	OP1-CP3-NP1-CP2
2	D	401	HXC	CM2-CM1-S-CP1
2	D	401	HXC	OM2-CM1-S-CP1
2	E	401	HXC	CPB-O7-P2-O21
2	E	401	HXC	S-CM1-CM2-CM3
2	E	401	HXC	OM2-CM1-CM2-CM3
2	F	401	HXC	CPB-O7-P2-O22
2	F	401	HXC	CP3-CP4-CP5-NP2
2	F	401	HXC	CM2-CM1-S-CP1
2	F	401	HXC	OM2-CM1-S-CP1
2	G	401	HXC	CP3-CP4-CP5-NP2
2	G	401	HXC	CM2-CM1-S-CP1
2	G	401	HXC	OM2-CM1-S-CP1
2	H	401	HXC	CM2-CM1-S-CP1
2	H	401	HXC	OM2-CM1-S-CP1
2	H	401	HXC	CM1-CM2-CM3-CM4
2	I	401	HXC	CPB-O7-P2-O21

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Mol	Chain	Res	Type	Atoms
2	I	401	HXC	CM2-CM1-S-CP1
2	I	401	HXC	OM2-CM1-S-CP1
2	J	401	HXC	CPB-O7-P2-O22
2	K	401	HXC	CP3-CP4-CP5-NP2
2	K	401	HXC	CM2-CM1-S-CP1
2	K	401	HXC	OM2-CM1-S-CP1
2	L	401	HXC	C5'-O5'-P1-O11
2	L	401	HXC	CP2-CP1-S-CM1
2	L	401	HXC	S-CM1-CM2-CM3
2	L	401	HXC	OM2-CM1-CM2-CM3
2	L	401	HXC	CM1-CM2-CM3-CM4
2	K	401	HXC	CM2-CM3-CM4-CM5
2	I	401	HXC	CM2-CM3-CM4-CM5
2	A	401	HXC	CM3-CM4-CM5-CM6
2	A	401	HXC	CP3-CP4-CP5-NP2
2	D	401	HXC	CP3-CP4-CP5-NP2
2	L	401	HXC	CM3-CM4-CM5-CM6
2	G	401	HXC	CM3-CM4-CM5-CM6
2	G	401	HXC	CM2-CM3-CM4-CM5
2	F	401	HXC	CM3-CM4-CM5-CM6
2	I	401	HXC	CM3-CM4-CM5-CM6
2	C	401	HXC	OM2-CM1-S-CP1
2	A	401	HXC	S-CM1-CM2-CM3
2	A	401	HXC	OM2-CM1-CM2-CM3
2	C	401	HXC	S-CM1-CM2-CM3
2	C	401	HXC	OM2-CM1-CM2-CM3
2	J	401	HXC	S-CM1-CM2-CM3
2	J	401	HXC	OM2-CM1-CM2-CM3
2	G	401	HXC	C3'-O3'-P3-O33
2	C	401	HXC	CM2-CM3-CM4-CM5
2	B	401	HXC	CM3-CM4-CM5-CM6
2	B	401	HXC	C5'-O5'-P1-O6
2	D	401	HXC	C5'-O5'-P1-O6
2	F	401	HXC	C3'-O3'-P3-O31
2	D	401	HXC	CM2-CM3-CM4-CM5
2	C	401	HXC	P2-O6-P1-O12
2	J	401	HXC	P2-O6-P1-O12
2	J	401	HXC	CP3-CP4-CP5-NP2
2	D	401	HXC	O4'-C4'-C5'-O5'
2	K	401	HXC	CM3-CM4-CM5-CM6
2	F	401	HXC	O4'-C4'-C5'-O5'
2	C	401	HXC	CP2-CP1-S-CM1

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Mol	Chain	Res	Type	Atoms
2	E	401	HXC	CP2-CP1-S-CM1
2	G	401	HXC	CP2-CP1-S-CM1
2	J	401	HXC	CP2-CP1-S-CM1
2	L	401	HXC	CM2-CM3-CM4-CM5
2	B	401	HXC	O4'-C4'-C5'-O5'
2	E	401	HXC	OM2-CM1-S-CP1
2	H	401	HXC	CM3-CM4-CM5-CM6
2	J	401	HXC	CM1-CM2-CM3-CM4
2	C	401	HXC	CP3-CP4-CP5-NP2
2	I	401	HXC	CP3-CP4-CP5-NP2
2	E	401	HXC	O4'-C4'-C5'-O5'
2	B	401	HXC	C3'-O3'-P3-O32
2	E	401	HXC	C3'-O3'-P3-O31
2	F	401	HXC	C3'-O3'-P3-O32
2	G	401	HXC	C3'-O3'-P3-O32
2	J	401	HXC	C3'-O3'-P3-O32
2	K	401	HXC	C5'-O5'-P1-O6
2	C	401	HXC	O4'-C4'-C5'-O5'
2	H	401	HXC	O4'-C4'-C5'-O5'
2	E	401	HXC	P2-O6-P1-O11
2	E	401	HXC	P2-O6-P1-O12
2	J	401	HXC	P2-O6-P1-O11
2	K	401	HXC	P2-O6-P1-O12
2	L	401	HXC	P2-O6-P1-O11
2	L	401	HXC	P2-O6-P1-O12
2	D	401	HXC	CM3-CM4-CM5-CM6
2	G	401	HXC	CPB-O7-P2-O22
2	A	401	HXC	O4'-C4'-C5'-O5'
2	G	401	HXC	O4'-C4'-C5'-O5'
2	I	401	HXC	O4'-C4'-C5'-O5'
2	J	401	HXC	O4'-C4'-C5'-O5'
2	K	401	HXC	O4'-C4'-C5'-O5'
2	L	401	HXC	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	HXC	3	0
2	D	401	HXC	2	0
2	F	401	HXC	2	0
2	G	401	HXC	3	0

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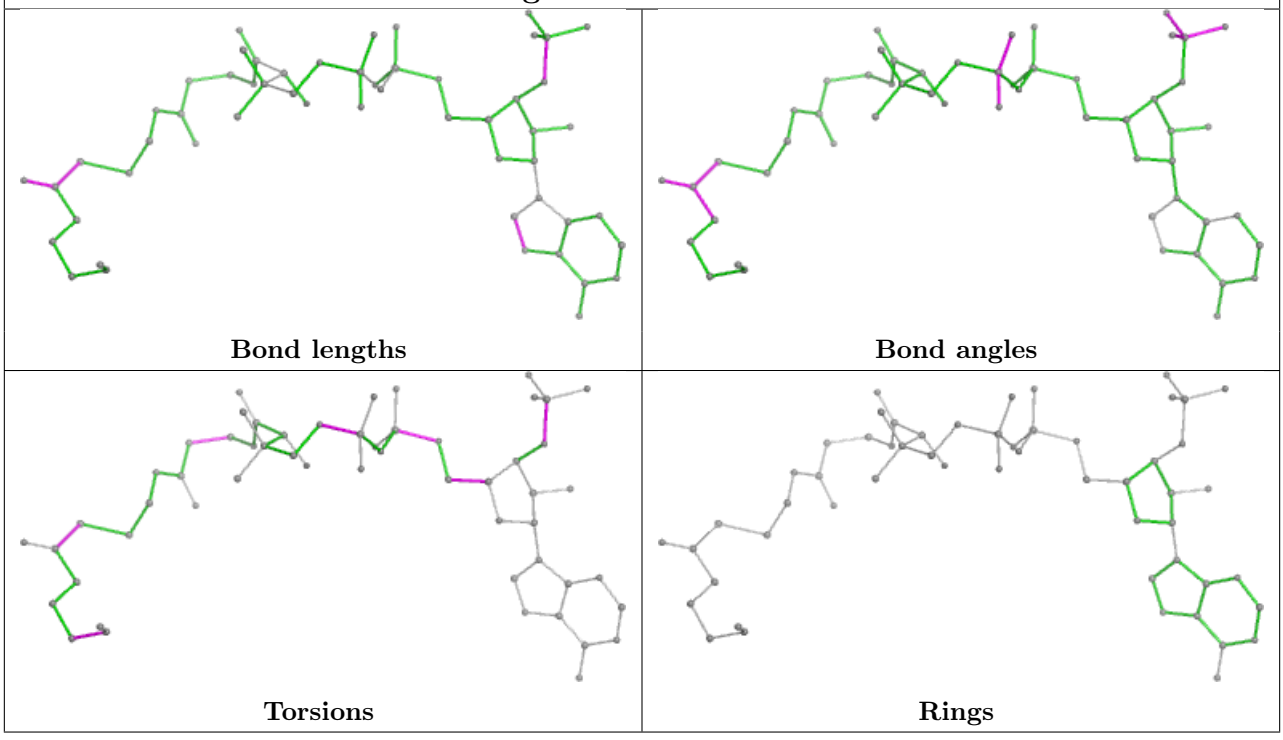
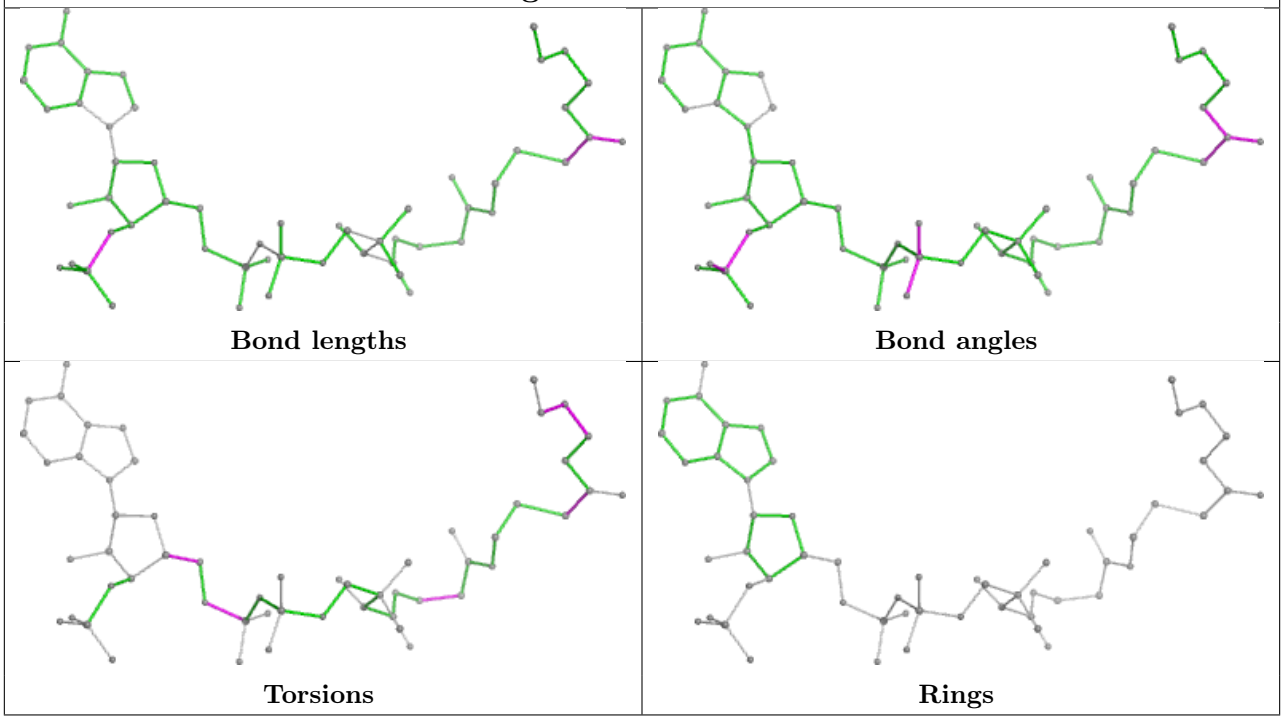
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HXC	2	0
2	I	401	HXC	1	0
2	H	401	HXC	1	0
2	E	401	HXC	1	0

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

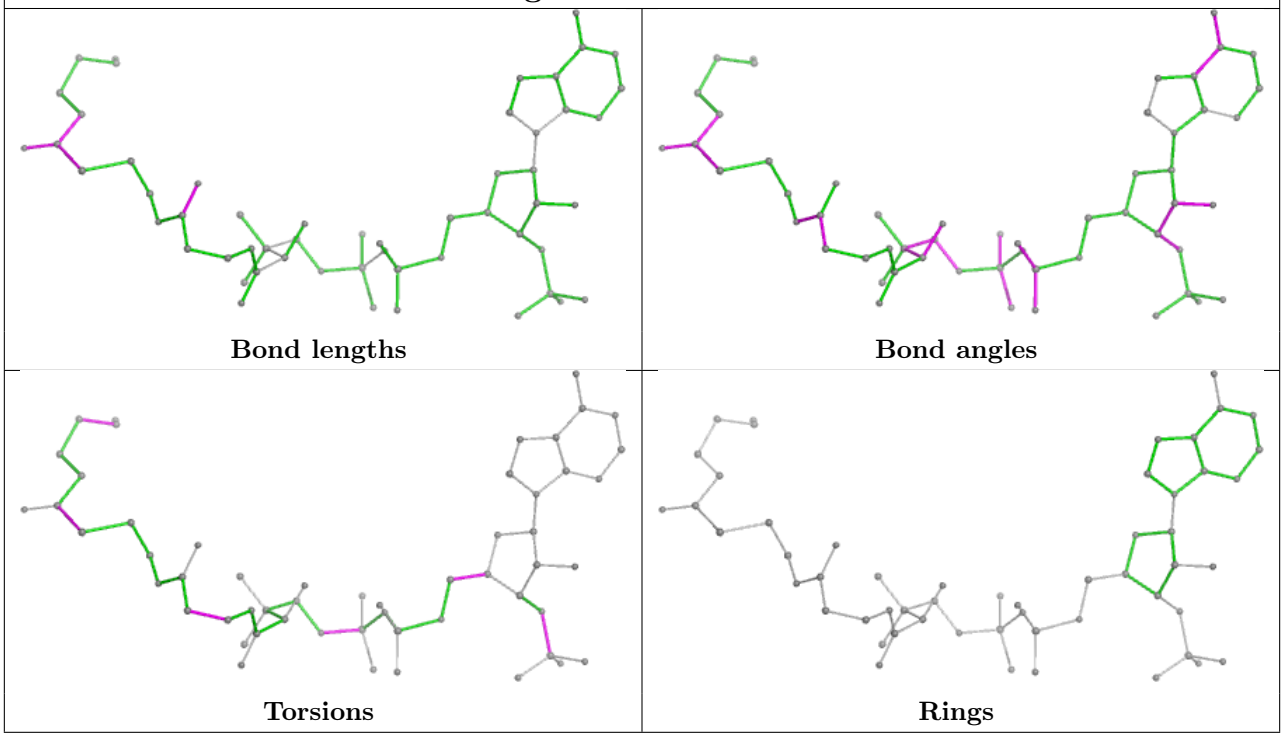
Ligand HXC B 401



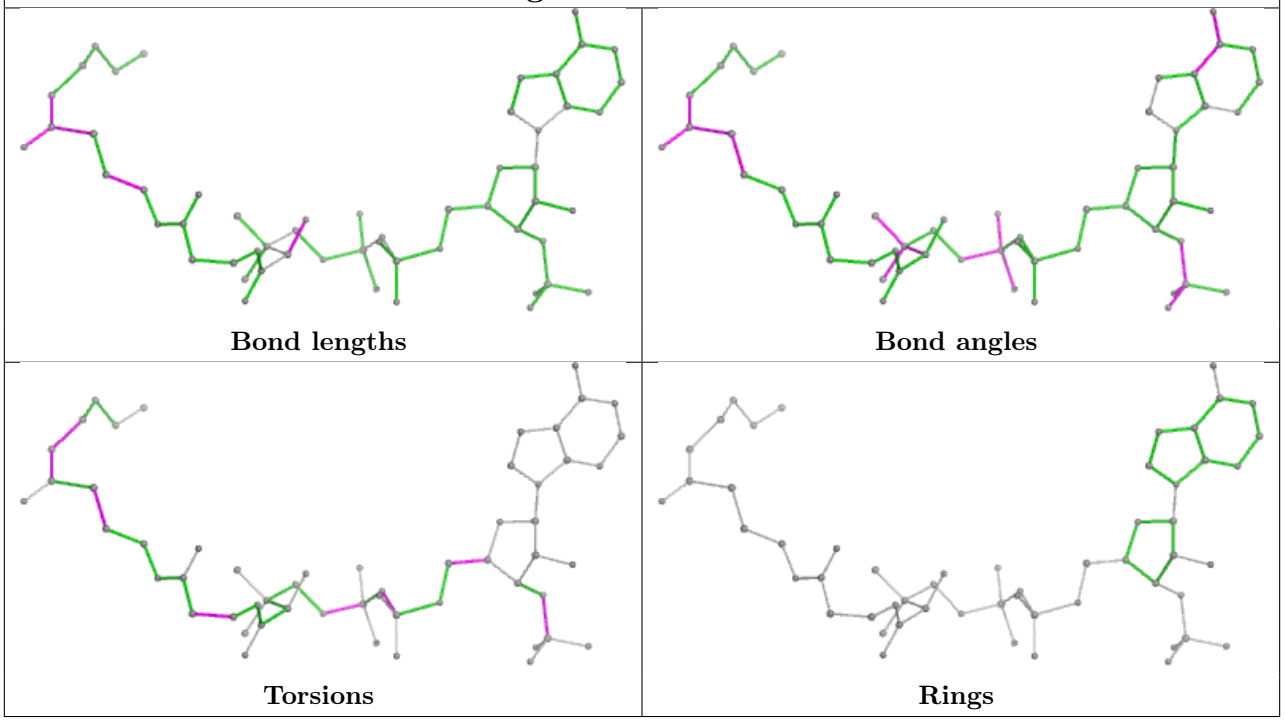
Ligand HXC D 401



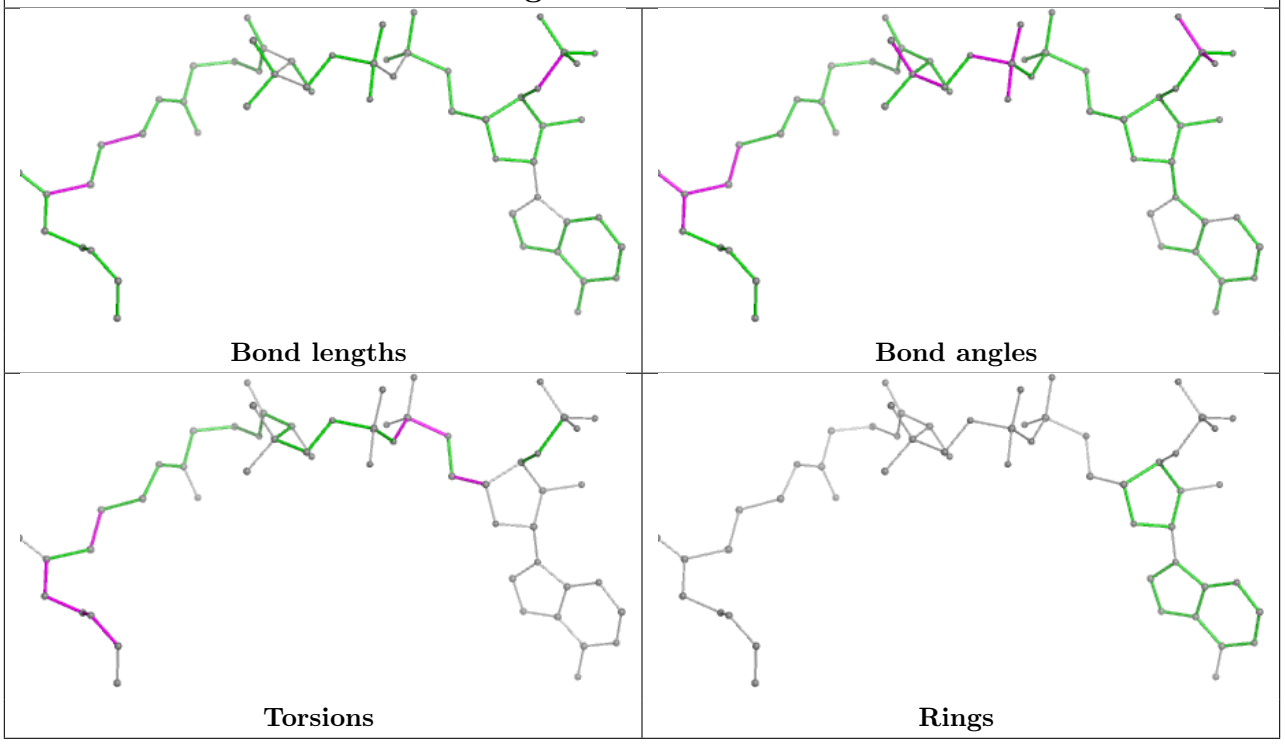
Ligand HXC F 401



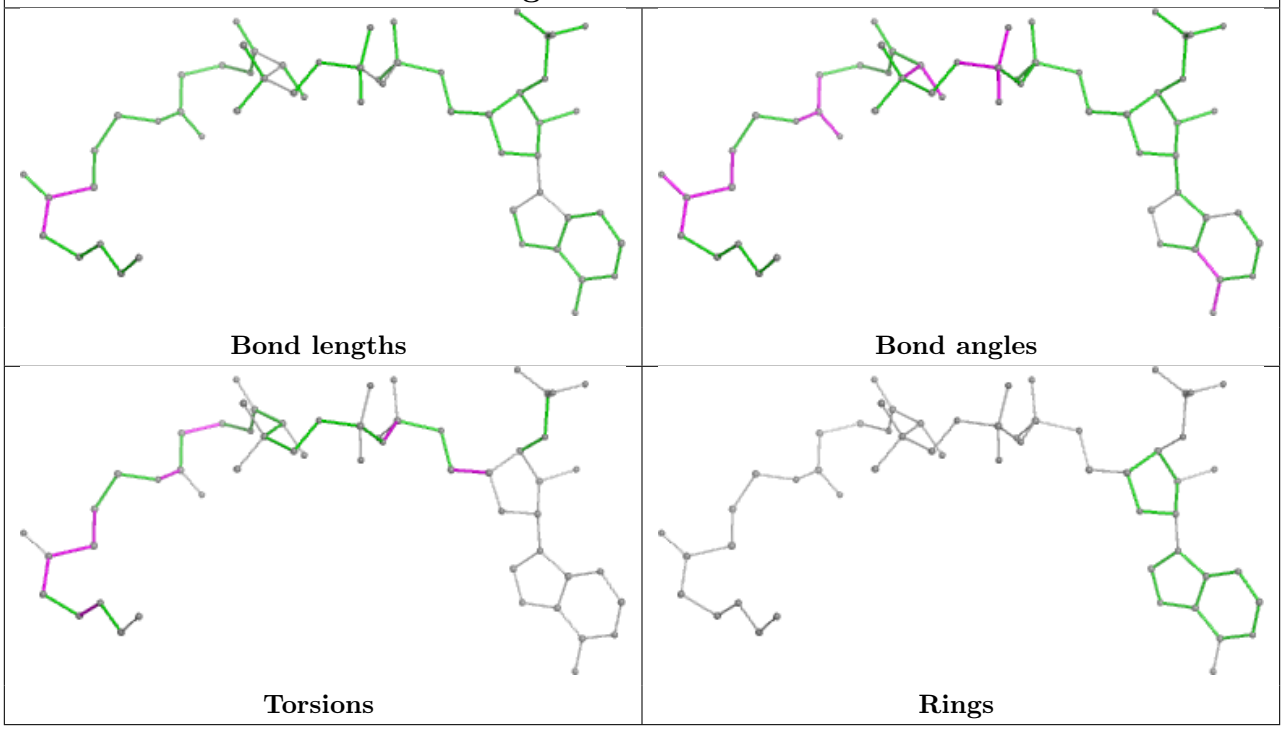
Ligand HXC J 401



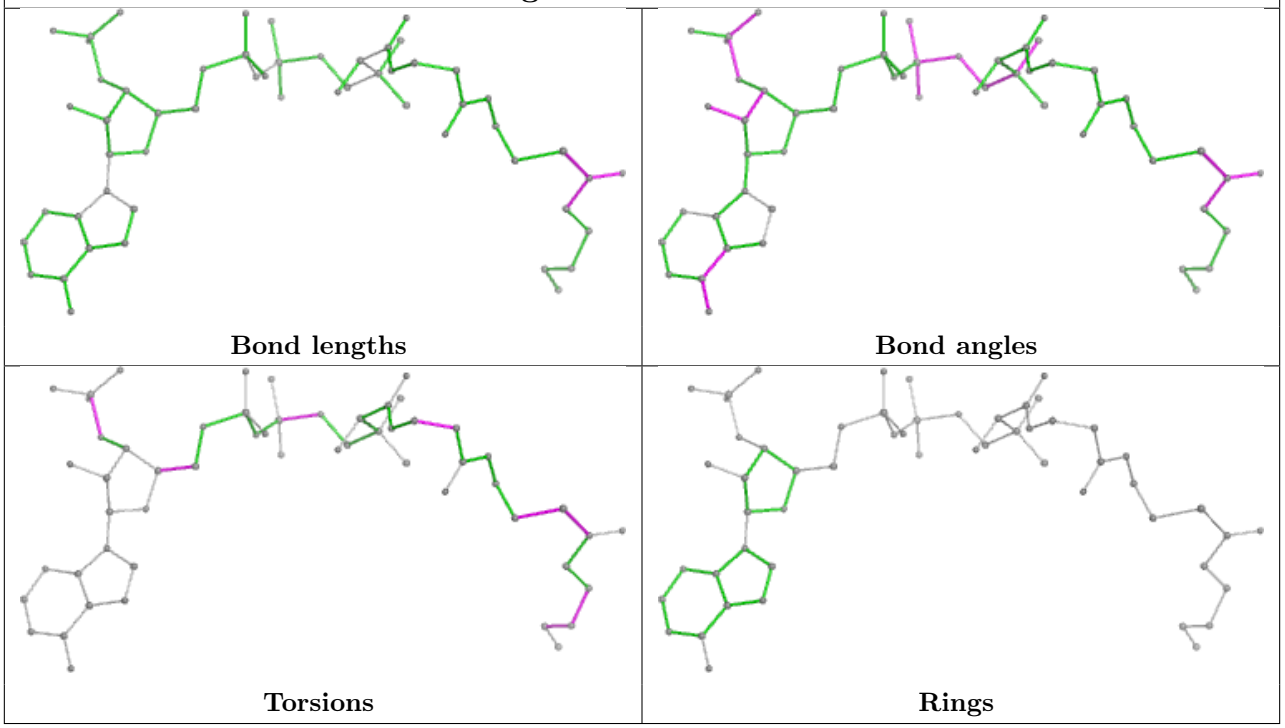
Ligand HXC L 401



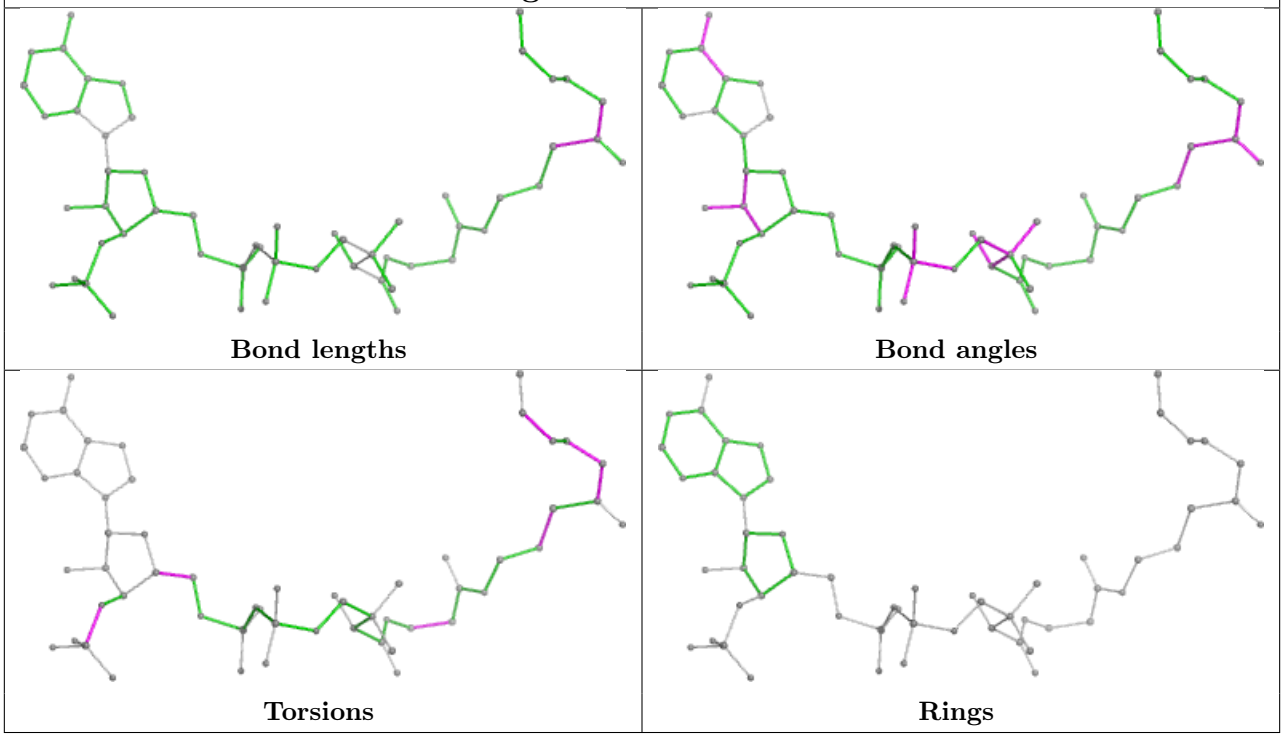
Ligand HXC C 401



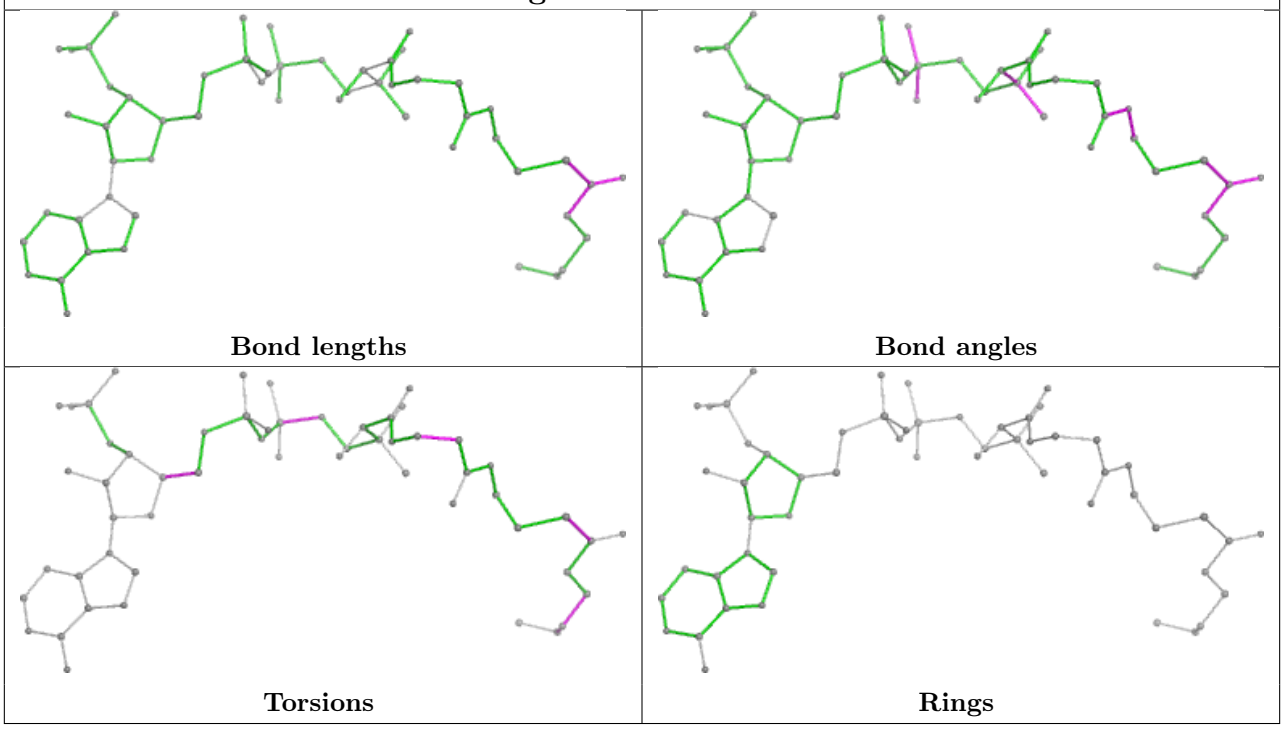
Ligand HXC G 401



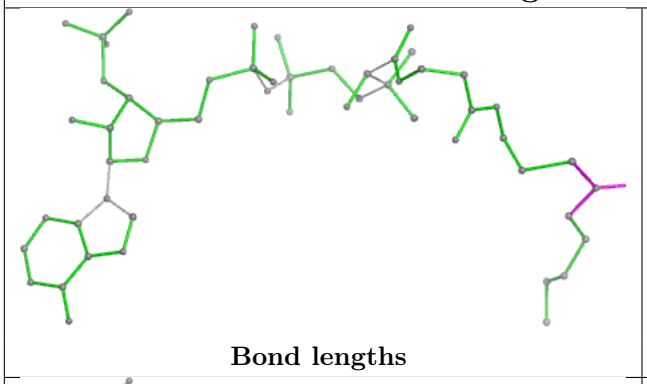
Ligand HXC A 401



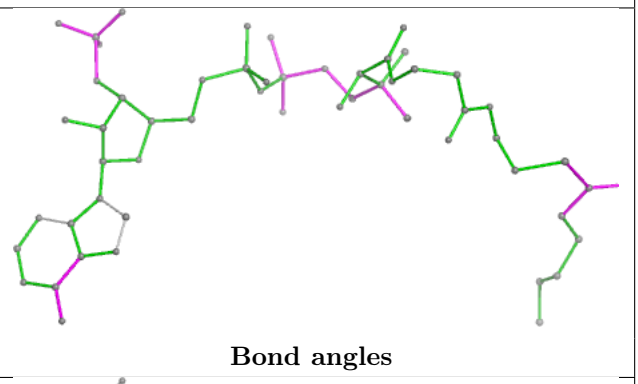
Ligand HXC I 401



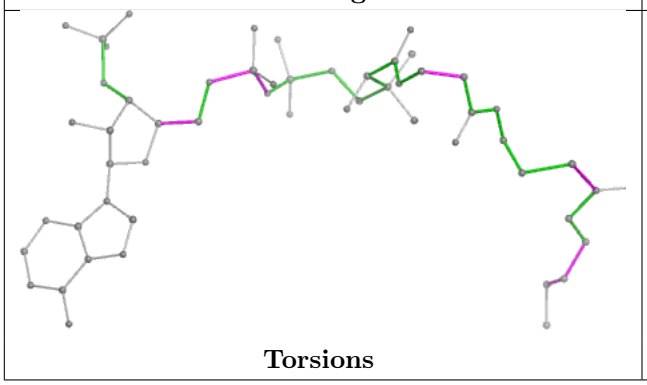
Ligand HXC K 401



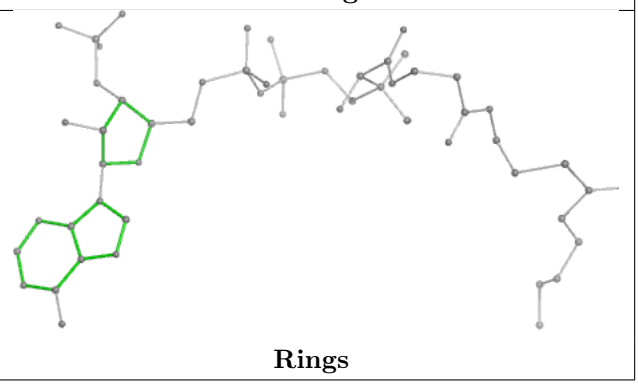
Bond lengths



Bond angles

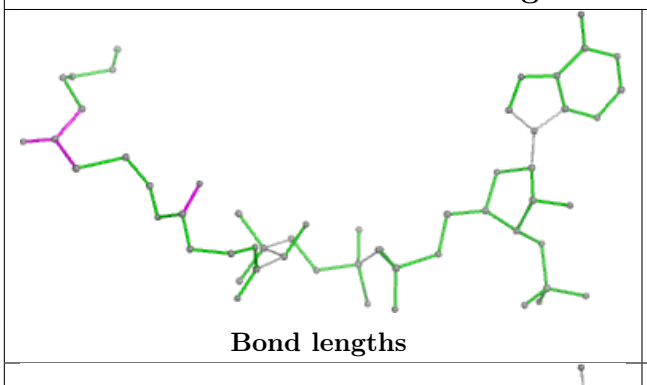


Torsions

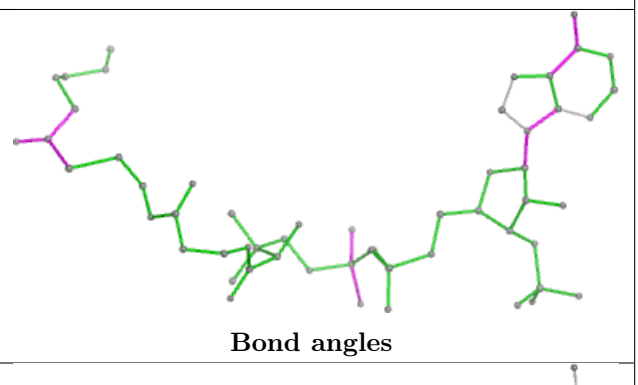


Rings

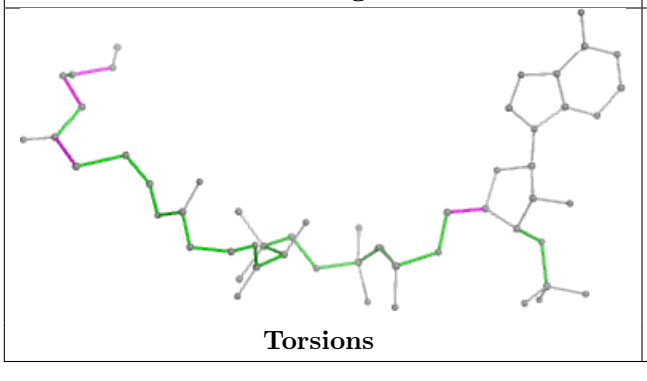
Ligand HXC H 401



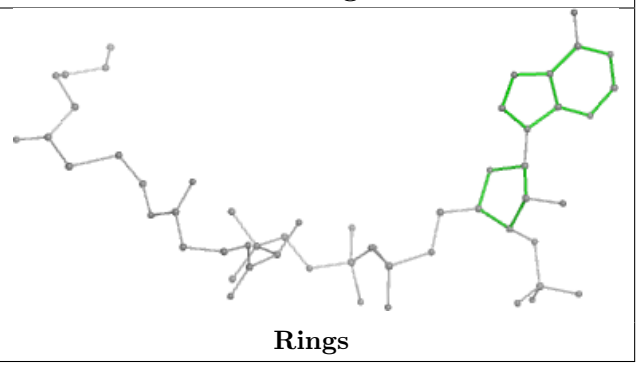
Bond lengths



Bond angles

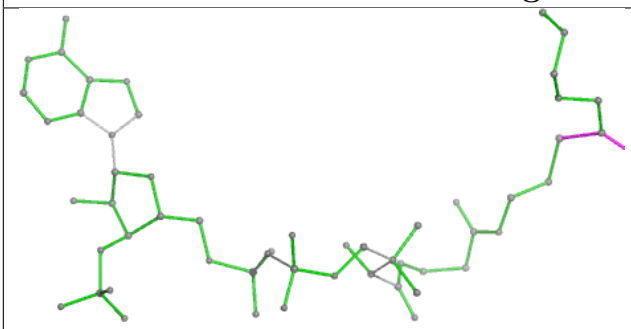


Torsions

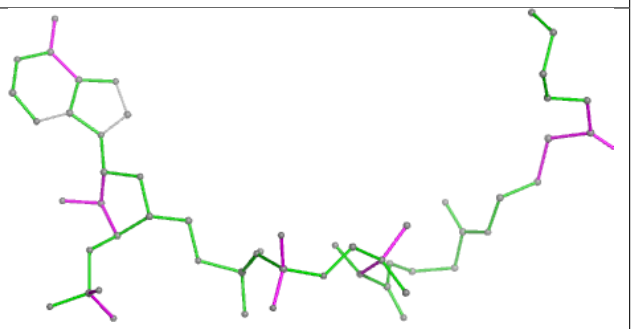


Rings

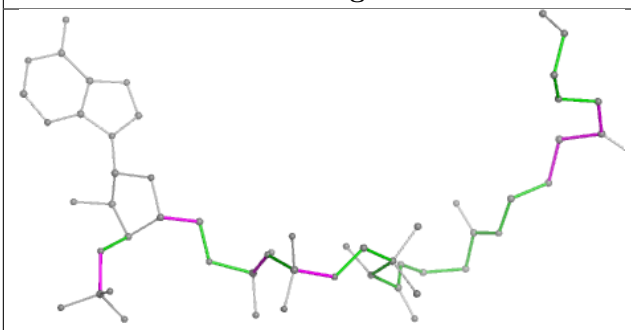
Ligand HXC E 401



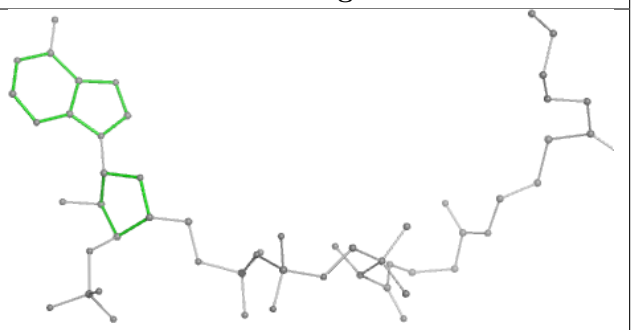
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	358/364 (98%)	0.66	50 (13%) 7 9	20, 34, 69, 100	1 (0%)
1	B	359/364 (98%)	0.62	44 (12%) 9 11	17, 34, 73, 119	2 (0%)
1	C	358/364 (98%)	0.90	87 (24%) 2 2	21, 35, 74, 100	2 (0%)
1	D	359/364 (98%)	0.56	40 (11%) 12 15	20, 34, 65, 108	1 (0%)
1	E	358/364 (98%)	0.75	53 (14%) 7 8	21, 36, 75, 99	2 (0%)
1	F	358/364 (98%)	1.03	91 (25%) 2 2	18, 37, 75, 122	2 (0%)
1	G	359/364 (98%)	1.07	92 (25%) 2 2	21, 37, 78, 117	2 (0%)
1	H	359/364 (98%)	0.70	53 (14%) 7 8	20, 36, 78, 112	1 (0%)
1	I	359/364 (98%)	0.29	18 (5%) 35 42	19, 31, 57, 98	2 (0%)
1	J	359/364 (98%)	0.51	44 (12%) 9 11	20, 31, 70, 113	1 (0%)
1	K	360/364 (98%)	0.81	74 (20%) 3 3	20, 34, 77, 109	2 (0%)
1	L	359/364 (98%)	0.39	20 (5%) 31 38	17, 33, 61, 97	2 (0%)
All	All	4305/4368 (98%)	0.69	666 (15%) 6 7	17, 34, 72, 122	20 (0%)

All (666) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	346	ALA	7.7
1	E	42	VAL	6.4
1	F	42	VAL	6.3
1	B	346	ALA	6.2
1	J	346	ALA	5.8
1	B	42	VAL	5.8
1	K	45	ILE	5.7
1	K	346	ALA	5.7
1	H	42	VAL	5.6
1	K	42	VAL	5.6
1	F	93	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	42	VAL	5.6
1	J	45	ILE	5.4
1	B	45	ILE	5.3
1	C	42	VAL	5.3
1	G	45	ILE	5.2
1	H	45	ILE	5.2
1	E	349	ILE	5.1
1	A	42	VAL	5.1
1	F	351	ILE	5.1
1	G	351	ILE	5.0
1	J	351	ILE	5.0
1	E	176	GLN	5.0
1	G	92	LEU	5.0
1	F	45	ILE	5.0
1	G	61	LEU	4.8
1	E	45	ILE	4.8
1	K	349	ILE	4.8
1	G	93	GLY	4.7
1	J	42	VAL	4.7
1	H	351	ILE	4.7
1	G	349	ILE	4.6
1	G	355	LEU	4.6
1	A	324	GLY	4.6
1	A	349	ILE	4.6
1	K	93	GLY	4.6
1	F	347	ALA	4.6
1	A	351	ILE	4.6
1	H	349	ILE	4.5
1	C	75	ALA	4.5
1	G	75	ALA	4.5
1	C	351	ILE	4.4
1	C	346	ALA	4.4
1	K	75	ALA	4.4
1	G	324	GLY	4.4
1	F	292	ALA	4.4
1	G	102	VAL	4.4
1	E	351	ILE	4.3
1	F	97	GLU	4.3
1	G	58	THR	4.3
1	G	293	ASN	4.3
1	G	59	ALA	4.3
1	L	45	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	345	PRO	4.2
1	A	45	ILE	4.2
1	G	101	LYS	4.2
1	F	41	SER	4.2
1	G	176	GLN	4.2
1	C	45	ILE	4.2
1	E	324	GLY	4.2
1	B	351	ILE	4.1
1	K	360	GLY	4.1
1	D	42	VAL	4.1
1	C	66	GLY	4.1
1	C	347	ALA	4.1
1	F	101	LYS	4.1
1	D	346	ALA	4.1
1	C	69	LEU	4.0
1	F	358	TRP	4.0
1	H	39	PRO	4.0
1	G	94	LEU	4.0
1	H	355	LEU	4.0
1	D	323	ASN	4.0
1	K	102	VAL	4.0
1	G	69	LEU	4.0
1	F	354	VAL	3.9
1	G	354	VAL	3.9
1	I	41	SER	3.9
1	G	100	ALA	3.9
1	G	292	ALA	3.9
1	K	176	GLN	3.9
1	C	61	LEU	3.9
1	G	43	ASP	3.9
1	K	72	LYS	3.9
1	B	347	ALA	3.9
1	C	93	GLY	3.9
1	F	73	LEU	3.9
1	A	346	ALA	3.8
1	G	57	VAL	3.8
1	F	180	LYS	3.8
1	E	178	SER	3.8
1	D	45	ILE	3.8
1	E	44	GLY	3.8
1	K	324	GLY	3.8
1	C	102	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	88	VAL	3.8
1	F	61	LEU	3.8
1	B	44	GLY	3.8
1	E	346	ALA	3.8
1	G	346	ALA	3.8
1	G	41	SER	3.8
1	K	73	LEU	3.8
1	G	358	TRP	3.8
1	H	346	ALA	3.8
1	G	62	LYS	3.8
1	G	10	VAL	3.7
1	G	178	SER	3.7
1	K	41	SER	3.7
1	G	73	LEU	3.7
1	I	351	ILE	3.7
1	H	358	TRP	3.7
1	K	351	ILE	3.7
1	F	207	MET	3.7
1	L	173	TRP	3.7
1	G	49	ALA	3.6
1	C	358	TRP	3.6
1	A	68	GLU	3.6
1	F	69	LEU	3.6
1	F	355	LEU	3.6
1	C	349	ILE	3.6
1	F	70	ALA	3.6
1	K	47	ARG	3.6
1	K	180	LYS	3.6
1	K	69	LEU	3.6
1	A	180	LYS	3.6
1	F	349	ILE	3.6
1	J	349	ILE	3.6
1	F	324	GLY	3.6
1	L	42	VAL	3.6
1	K	71	LEU	3.5
1	E	345	PRO	3.5
1	B	46	SER	3.5
1	F	293	ASN	3.5
1	G	72	LYS	3.5
1	F	92	LEU	3.5
1	D	349	ILE	3.5
1	G	1	MET	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	177	SER	3.5
1	C	323	ASN	3.5
1	J	347	ALA	3.5
1	J	44	GLY	3.5
1	E	40	SER	3.5
1	C	59	ALA	3.5
1	G	347	ALA	3.5
1	A	358	TRP	3.4
1	A	62	LYS	3.4
1	A	355	LEU	3.4
1	G	70	ALA	3.4
1	G	77	ALA	3.4
1	G	359	ASP	3.4
1	G	71	LEU	3.4
1	J	75	ALA	3.4
1	J	93	GLY	3.4
1	I	45	ILE	3.4
1	C	176	GLN	3.4
1	K	348	THR	3.4
1	F	79	VAL	3.4
1	K	66	GLY	3.4
1	F	94	LEU	3.4
1	H	323	ASN	3.4
1	D	358	TRP	3.3
1	D	324	GLY	3.3
1	L	323	ASN	3.3
1	C	70	ALA	3.3
1	C	74	ILE	3.3
1	F	56	ILE	3.3
1	L	324	GLY	3.3
1	F	39	PRO	3.3
1	J	350	ASP	3.3
1	K	56	ILE	3.3
1	A	47	ARG	3.3
1	J	324	GLY	3.3
1	K	44	GLY	3.3
1	F	33	VAL	3.3
1	B	257	ALA	3.3
1	K	100	ALA	3.3
1	K	347	ALA	3.3
1	L	346	ALA	3.3
1	C	43	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	73	LEU	3.3
1	F	57	VAL	3.2
1	G	353	ALA	3.2
1	K	49	ALA	3.2
1	A	69	LEU	3.2
1	A	92	LEU	3.2
1	C	173	TRP	3.2
1	B	349	ILE	3.2
1	E	58	THR	3.2
1	L	351	ILE	3.2
1	F	1	MET	3.2
1	G	97	GLU	3.2
1	J	43	ASP	3.2
1	E	39	PRO	3.2
1	F	59	ALA	3.2
1	G	34	VAL	3.2
1	K	354	VAL	3.2
1	I	47	ARG	3.2
1	C	58	THR	3.2
1	F	356	THR	3.2
1	K	181	GLY	3.2
1	L	44	GLY	3.2
1	C	36	ILE	3.2
1	E	347	ALA	3.2
1	F	75	ALA	3.2
1	F	11	VAL	3.2
1	E	355	LEU	3.2
1	I	44	GLY	3.2
1	A	348	THR	3.2
1	K	58	THR	3.2
1	G	350	ASP	3.2
1	C	107	ILE	3.2
1	G	36	ILE	3.2
1	G	56	ILE	3.2
1	J	49	ALA	3.2
1	J	353	ALA	3.2
1	C	67	LEU	3.1
1	C	94	LEU	3.1
1	K	94	LEU	3.1
1	C	76	LYS	3.1
1	G	60	ASP	3.1
1	F	173	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	36	ILE	3.1
1	G	107	ILE	3.1
1	F	49	ALA	3.1
1	I	323	ASN	3.1
1	C	355	LEU	3.1
1	F	102	VAL	3.1
1	K	11	VAL	3.1
1	G	66	GLY	3.1
1	B	350	ASP	3.1
1	C	353	ALA	3.1
1	A	93	GLY	3.1
1	H	41	SER	3.1
1	J	40	SER	3.1
1	I	349	ILE	3.1
1	K	74	ILE	3.1
1	F	87	GLY	3.1
1	A	177	SER	3.1
1	C	71	LEU	3.1
1	G	79	VAL	3.1
1	H	348	THR	3.1
1	C	68	GLU	3.0
1	F	99	CYS	3.0
1	G	99	CYS	3.0
1	E	323	ASN	3.0
1	C	49	ALA	3.0
1	C	108	TYR	3.0
1	K	43	ASP	3.0
1	K	46	SER	3.0
1	F	58	THR	3.0
1	C	99	CYS	3.0
1	F	62	LYS	3.0
1	B	345	PRO	3.0
1	J	39	PRO	3.0
1	G	322	ALA	3.0
1	A	173	TRP	3.0
1	A	58	THR	3.0
1	C	79	VAL	3.0
1	G	11	VAL	3.0
1	K	10	VAL	3.0
1	A	207	MET	3.0
1	G	91	ARG	3.0
1	F	76	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	39	PRO	3.0
1	C	171	ALA	3.0
1	H	347	ALA	3.0
1	F	47	ARG	3.0
1	F	106	LEU	3.0
1	K	67	LEU	3.0
1	C	354	VAL	3.0
1	G	64	ASP	3.0
1	E	47	ARG	2.9
1	H	47	ARG	2.9
1	F	323	ASN	2.9
1	F	71	LEU	2.9
1	G	67	LEU	2.9
1	C	10	VAL	2.9
1	G	33	VAL	2.9
1	B	43	ASP	2.9
1	K	96	PRO	2.9
1	D	347	ALA	2.9
1	E	56	ILE	2.9
1	C	62	LYS	2.9
1	F	72	LYS	2.9
1	G	76	LYS	2.9
1	H	5	LEU	2.9
1	C	350	ASP	2.9
1	C	34	VAL	2.9
1	H	34	VAL	2.9
1	G	44	GLY	2.9
1	G	345	PRO	2.9
1	C	178	SER	2.9
1	K	40	SER	2.9
1	G	180	LYS	2.9
1	H	353	ALA	2.9
1	C	56	ILE	2.9
1	F	348	THR	2.9
1	G	68	GLU	2.9
1	F	43	ASP	2.9
1	H	350	ASP	2.9
1	K	355	LEU	2.9
1	G	87	GLY	2.9
1	F	65	GLN	2.9
1	H	176	GLN	2.9
1	A	75	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	81	ILE	2.8
1	D	359	ASP	2.8
1	K	61	LEU	2.8
1	G	108	TYR	2.8
1	C	324	GLY	2.8
1	G	39	PRO	2.8
1	B	358	TRP	2.8
1	E	353	ALA	2.8
1	E	358	TRP	2.8
1	K	59	ALA	2.8
1	K	173	TRP	2.8
1	F	66	GLY	2.8
1	K	63	SER	2.8
1	G	96	PRO	2.8
1	J	352	GLU	2.8
1	B	47	ARG	2.8
1	H	173	TRP	2.8
1	D	351	ILE	2.8
1	L	349	ILE	2.8
1	J	72	LYS	2.8
1	C	11	VAL	2.8
1	A	289	ALA	2.8
1	D	59	ALA	2.8
1	D	322	ALA	2.8
1	H	49	ALA	2.8
1	J	62	LYS	2.8
1	E	66	GLY	2.8
1	G	80	LEU	2.7
1	J	73	LEU	2.7
1	C	96	PRO	2.7
1	C	47	ARG	2.7
1	H	105	ARG	2.7
1	F	34	VAL	2.7
1	C	100	ALA	2.7
1	B	1	MET	2.7
1	C	72	LYS	2.7
1	C	181	GLY	2.7
1	H	7	GLY	2.7
1	I	324	GLY	2.7
1	F	345	PRO	2.7
1	J	102	VAL	2.7
1	K	79	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	1	MET	2.7
1	A	356	THR	2.7
1	K	101	LYS	2.7
1	A	41	SER	2.7
1	G	47	ARG	2.7
1	K	107	ILE	2.7
1	A	61	LEU	2.7
1	F	67	LEU	2.7
1	D	173	TRP	2.7
1	F	326	TRP	2.7
1	E	257	ALA	2.7
1	E	179	GLY	2.7
1	C	73	LEU	2.7
1	J	355	LEU	2.7
1	K	1	MET	2.7
1	K	76	LYS	2.7
1	E	173	TRP	2.6
1	G	173	TRP	2.6
1	C	33	VAL	2.6
1	C	183	VAL	2.6
1	F	38	ARG	2.6
1	F	89	THR	2.6
1	D	7	GLY	2.6
1	A	74	ILE	2.6
1	F	96	PRO	2.6
1	G	352	GLU	2.6
1	H	1	MET	2.6
1	H	315	GLU	2.6
1	A	322	ALA	2.6
1	B	75	ALA	2.6
1	E	59	ALA	2.6
1	E	100	ALA	2.6
1	E	359	ASP	2.6
1	F	98	GLU	2.6
1	A	72	LYS	2.6
1	H	72	LYS	2.6
1	F	74	ILE	2.6
1	F	107	ILE	2.6
1	C	105	ARG	2.6
1	A	40	SER	2.6
1	H	44	GLY	2.6
1	H	59	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	10	VAL	2.6
1	K	34	VAL	2.6
1	J	359	ASP	2.6
1	A	76	LYS	2.6
1	B	76	LYS	2.6
1	H	345	PRO	2.6
1	C	80	LEU	2.6
1	C	348	THR	2.6
1	C	37	ASP	2.6
1	F	48	ASP	2.6
1	I	43	ASP	2.6
1	G	38	ARG	2.5
1	A	345	PRO	2.5
1	G	74	ILE	2.5
1	C	41	SER	2.5
1	C	106	LEU	2.5
1	E	41	SER	2.5
1	F	46	SER	2.5
1	G	106	LEU	2.5
1	L	41	SER	2.5
1	F	68	GLU	2.5
1	A	44	GLY	2.5
1	D	348	THR	2.5
1	G	348	THR	2.5
1	H	324	GLY	2.5
1	L	1	MET	2.5
1	L	43	ASP	2.5
1	F	100	ALA	2.5
1	H	2	ALA	2.5
1	L	322	ALA	2.5
1	K	358	TRP	2.5
1	G	65	GLN	2.5
1	F	40	SER	2.5
1	G	46	SER	2.5
1	K	36	ILE	2.5
1	B	355	LEU	2.5
1	J	92	LEU	2.5
1	C	101	LYS	2.5
1	B	323	ASN	2.5
1	J	323	ASN	2.5
1	K	99	CYS	2.5
1	C	39	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	97	GLU	2.5
1	D	180	LYS	2.5
1	H	180	LYS	2.5
1	B	93	GLY	2.5
1	C	7	GLY	2.5
1	G	83	GLY	2.5
1	G	105	ARG	2.5
1	J	61	LEU	2.5
1	K	80	LEU	2.5
1	B	204	ALA	2.5
1	D	2	ALA	2.5
1	E	75	ALA	2.5
1	F	353	ALA	2.5
1	G	277	GLU	2.5
1	A	102	VAL	2.5
1	C	57	VAL	2.5
1	G	7	GLY	2.4
1	B	65	GLN	2.4
1	B	322	ALA	2.4
1	D	49	ALA	2.4
1	C	40	SER	2.4
1	D	345	PRO	2.4
1	L	47	ARG	2.4
1	I	1	MET	2.4
1	C	104	ASP	2.4
1	C	359	ASP	2.4
1	E	144	ASP	2.4
1	K	350	ASP	2.4
1	B	71	LEU	2.4
1	G	323	ASN	2.4
1	J	100	ALA	2.4
1	G	63	SER	2.4
1	B	359	ASP	2.4
1	E	350	ASP	2.4
1	F	350	ASP	2.4
1	F	359	ASP	2.4
1	D	102	VAL	2.4
1	I	42	VAL	2.4
1	E	30	GLY	2.4
1	E	348	THR	2.4
1	K	323	ASN	2.4
1	K	77	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	46	SER	2.4
1	J	63	SER	2.4
1	A	354	VAL	2.4
1	B	324	GLY	2.4
1	C	30	GLY	2.4
1	F	7	GLY	2.4
1	H	354	VAL	2.4
1	A	323	ASN	2.3
1	D	47	ARG	2.3
1	J	38	ARG	2.3
1	F	80	LEU	2.3
1	J	69	LEU	2.3
1	J	71	LEU	2.3
1	D	76	LYS	2.3
1	A	59	ALA	2.3
1	E	70	ALA	2.3
1	H	322	ALA	2.3
1	B	41	SER	2.3
1	D	357	ASP	2.3
1	F	64	ASP	2.3
1	C	345	PRO	2.3
1	E	7	GLY	2.3
1	G	181	GLY	2.3
1	F	184	VAL	2.3
1	E	69	LEU	2.3
1	D	107	ILE	2.3
1	H	56	ILE	2.3
1	I	346	ALA	2.3
1	F	176	GLN	2.3
1	K	64	ASP	2.3
1	K	65	GLN	2.3
1	C	97	GLU	2.3
1	C	38	ARG	2.3
1	J	47	ARG	2.3
1	H	356	THR	2.3
1	D	73	LEU	2.3
1	E	65	GLN	2.3
1	F	60	ASP	2.3
1	G	8	LEU	2.3
1	H	69	LEU	2.3
1	J	37	ASP	2.3
1	J	176	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	60	ASP	2.3
1	K	92	LEU	2.3
1	K	178	SER	2.3
1	A	56	ILE	2.3
1	B	353	ALA	2.3
1	C	77	ALA	2.3
1	A	288	GLY	2.3
1	C	180	LYS	2.3
1	D	1	MET	2.3
1	D	290	VAL	2.3
1	F	10	VAL	2.3
1	I	176	GLN	2.3
1	H	43	ASP	2.3
1	I	350	ASP	2.3
1	F	63	SER	2.3
1	K	108	TYR	2.3
1	L	46	SER	2.3
1	C	8	LEU	2.3
1	D	355	LEU	2.3
1	G	51	LEU	2.3
1	J	94	LEU	2.3
1	C	14	ALA	2.2
1	E	338	ALA	2.2
1	F	115	GLY	2.2
1	A	1	MET	2.2
1	C	65	GLN	2.2
1	H	58	THR	2.2
1	K	57	VAL	2.2
1	A	350	ASP	2.2
1	F	144	ASP	2.2
1	H	359	ASP	2.2
1	A	91	ARG	2.2
1	E	73	LEU	2.2
1	K	322	ALA	2.2
1	J	65	GLN	2.2
1	B	68	GLU	2.2
1	K	97	GLU	2.2
1	C	91	ARG	2.2
1	J	173	TRP	2.2
1	A	66	GLY	2.2
1	H	71	LEU	2.2
1	B	49	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	72	LYS	2.2
1	G	14	ALA	2.2
1	G	98	GLU	2.2
1	G	37	ASP	2.2
1	C	177	SER	2.2
1	B	354	VAL	2.2
1	H	57	VAL	2.2
1	B	180	LYS	2.2
1	G	207	MET	2.2
1	I	173	TRP	2.2
1	C	51	LEU	2.2
1	C	322	ALA	2.2
1	D	204	ALA	2.2
1	E	61	LEU	2.2
1	H	73	LEU	2.2
1	K	353	ALA	2.2
1	L	75	ALA	2.2
1	F	352	GLU	2.2
1	H	352	GLU	2.2
1	L	315	GLU	2.2
1	A	39	PRO	2.2
1	F	108	TYR	2.2
1	C	357	ASP	2.1
1	D	43	ASP	2.1
1	G	356	THR	2.1
1	H	76	LYS	2.1
1	C	1	MET	2.1
1	D	183	VAL	2.1
1	K	183	VAL	2.1
1	H	30	GLY	2.1
1	C	257	ALA	2.1
1	D	75	ALA	2.1
1	J	67	LEU	2.1
1	B	173	TRP	2.1
1	B	105	ARG	2.1
1	K	105	ARG	2.1
1	F	37	ASP	2.1
1	K	104	ASP	2.1
1	L	350	ASP	2.1
1	B	348	THR	2.1
1	B	356	THR	2.1
1	D	178	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	40	SER	2.1
1	K	62	LYS	2.1
1	E	93	GLY	2.1
1	F	88	VAL	2.1
1	F	105	ARG	2.1
1	C	5	LEU	2.1
1	C	172	LEU	2.1
1	G	2	ALA	2.1
1	K	70	ALA	2.1
1	K	344	PRO	2.1
1	J	56	ILE	2.1
1	C	356	THR	2.1
1	H	63	SER	2.1
1	I	58	THR	2.1
1	L	6	SER	2.1
1	C	87	GLY	2.1
1	D	44	GLY	2.1
1	E	325	GLY	2.1
1	A	43	ASP	2.1
1	H	357	ASP	2.1
1	B	69	LEU	2.1
1	H	92	LEU	2.1
1	I	101	LYS	2.1
1	E	68	GLU	2.1
1	E	352	GLU	2.1
1	I	326	TRP	2.1
1	J	358	TRP	2.1
1	L	314	ILE	2.1
1	A	38	ARG	2.1
1	B	325	GLY	2.1
1	F	83	GLY	2.1
1	H	179	GLY	2.1
1	F	357	ASP	2.0
1	B	102	VAL	2.0
1	C	184	VAL	2.0
1	F	183	VAL	2.0
1	E	77	ALA	2.0
1	F	171	ALA	2.0
1	J	59	ALA	2.0
1	J	77	ALA	2.0
1	A	73	LEU	2.0
1	C	92	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	172	LEU	2.0
1	B	62	LYS	2.0
1	B	72	LYS	2.0
1	E	76	LYS	2.0
1	J	101	LYS	2.0
1	B	352	GLU	2.0
1	K	352	GLU	2.0
1	D	177	SER	2.0
1	E	314	ILE	2.0
1	G	89	THR	2.0
1	H	16	ILE	2.0
1	H	326	TRP	2.0
1	B	66	GLY	2.0
1	D	30	GLY	2.0
1	A	10	VAL	2.0
1	A	290	VAL	2.0
1	D	176	GLN	2.0
1	D	315	GLU	2.0
1	D	353	ALA	2.0
1	D	354	VAL	2.0
1	E	354	VAL	2.0
1	A	46	SER	2.0
1	A	94	LEU	2.0
1	F	5	LEU	2.0
1	J	41	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

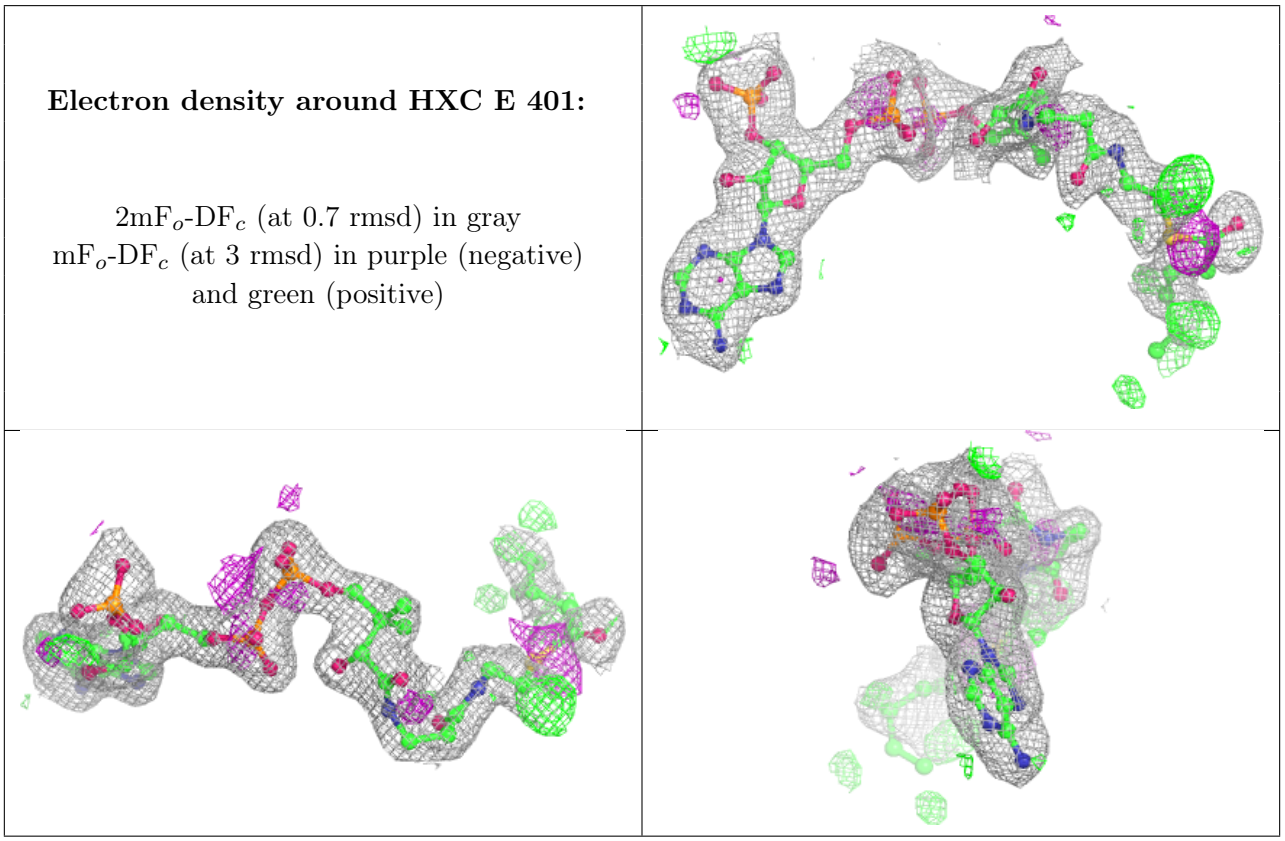
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HXC	E	401	55/55	0.89	0.15	34,47,84,109	0
2	HXC	C	401	55/55	0.90	0.14	27,42,68,83	0
2	HXC	H	401	55/55	0.90	0.15	34,48,87,91	0
2	HXC	F	401	55/55	0.91	0.15	27,47,84,86	0
2	HXC	A	401	55/55	0.91	0.14	28,43,72,90	0
2	HXC	G	401	55/55	0.92	0.14	25,45,76,78	0
2	HXC	J	401	55/55	0.92	0.14	24,39,79,87	0
2	HXC	K	401	55/55	0.92	0.13	26,40,81,86	0
2	HXC	B	401	55/55	0.94	0.12	25,40,75,83	0
2	HXC	L	401	55/55	0.94	0.12	21,30,76,81	0
2	HXC	I	401	55/55	0.96	0.10	22,31,79,84	0
2	HXC	D	401	55/55	0.96	0.10	20,32,72,76	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.

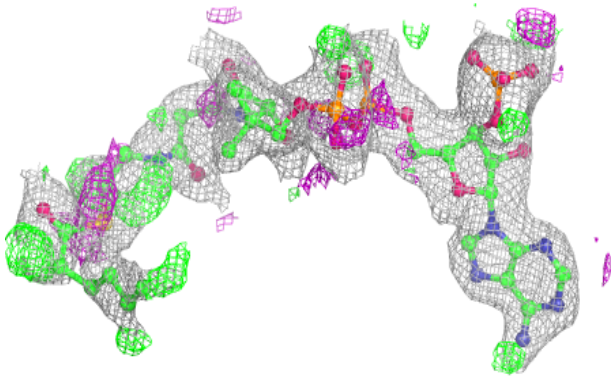
Electron density around HXC E 401:

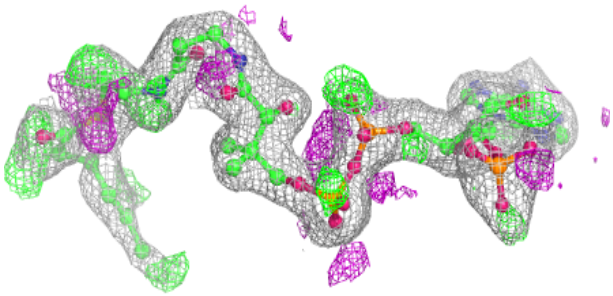
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

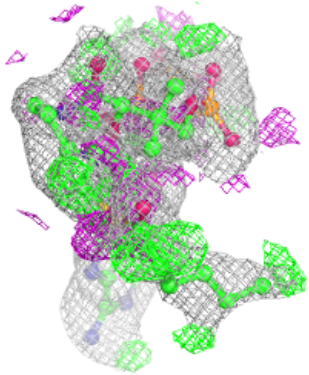


Electron density around HXC C 401:

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

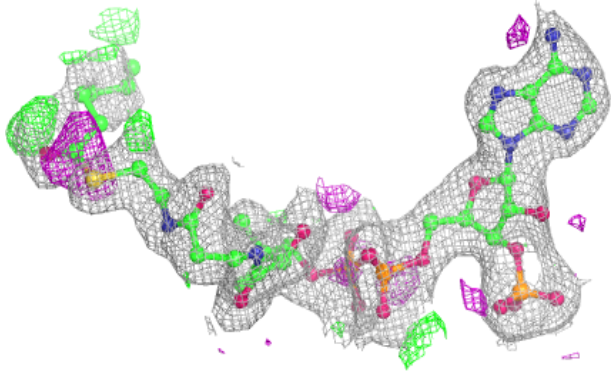


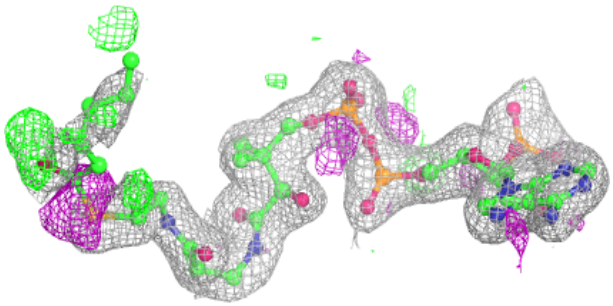


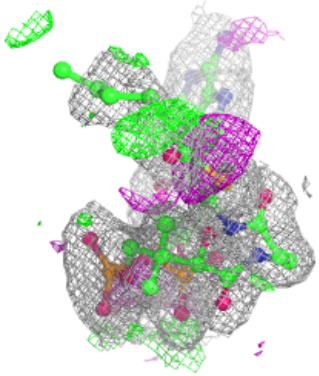


Electron density around HXC H 401:

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

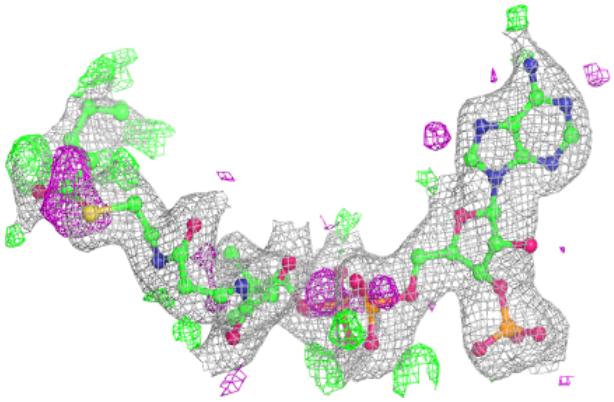


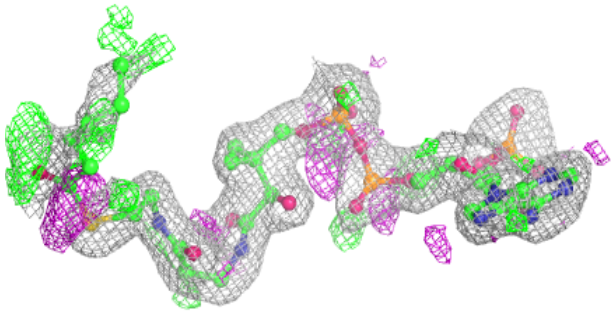


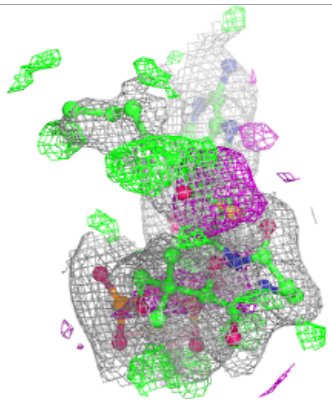


Electron density around HXC F 401:

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

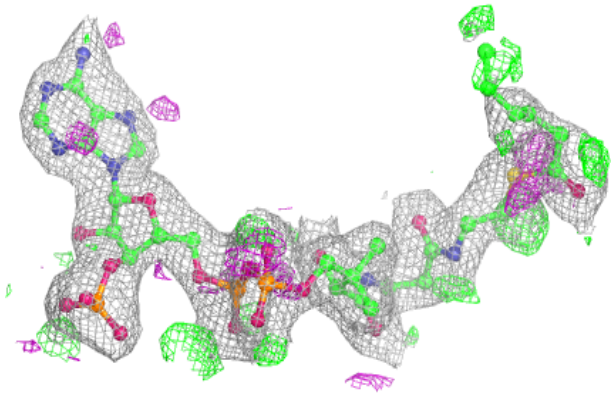


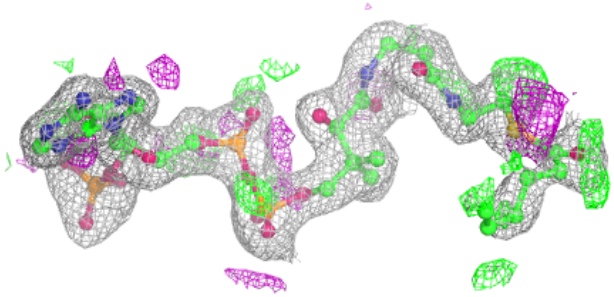


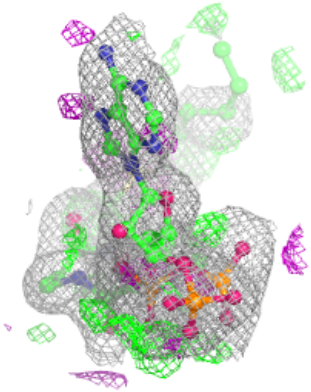


Electron density around HXC A 401:

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

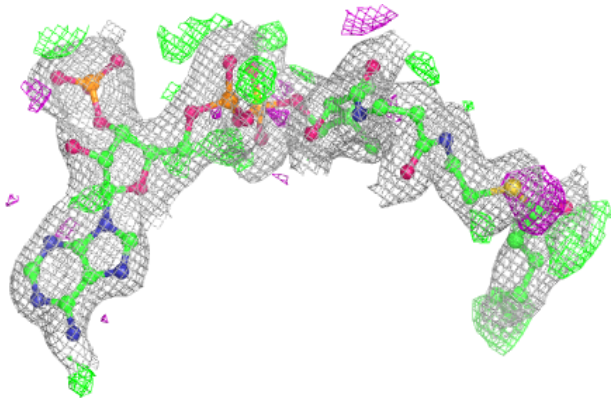


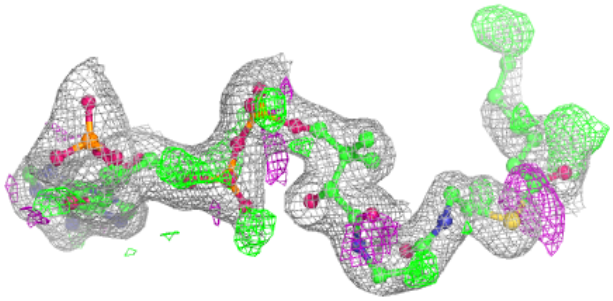


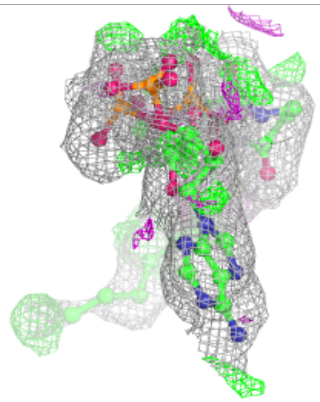


Electron density around HXC G 401:

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

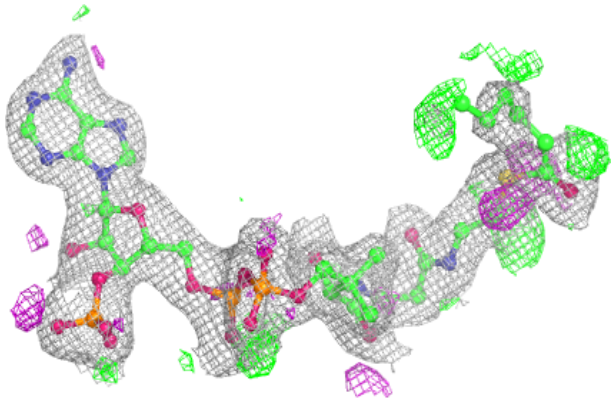


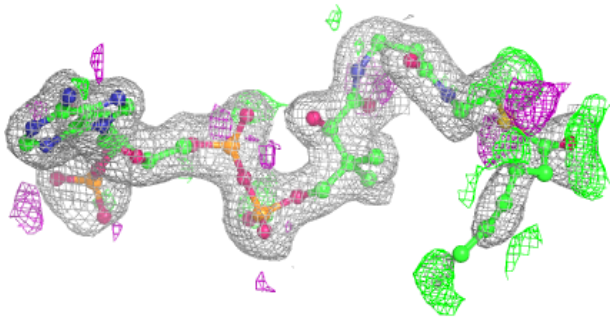


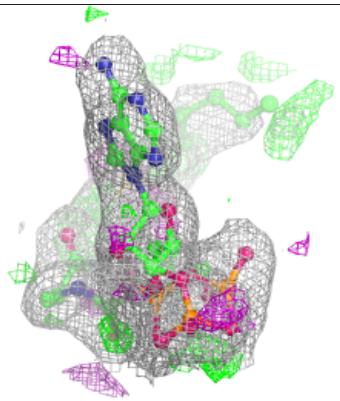


Electron density around HXC J 401:

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

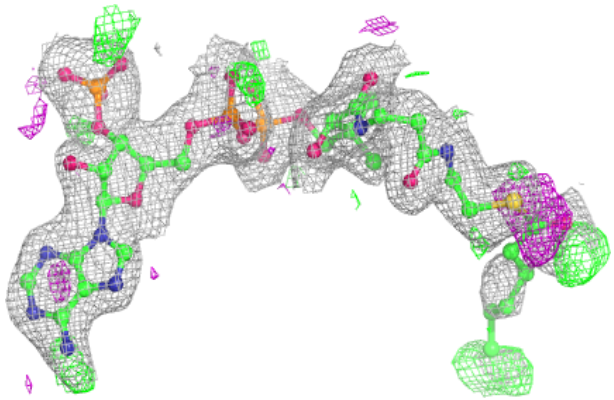


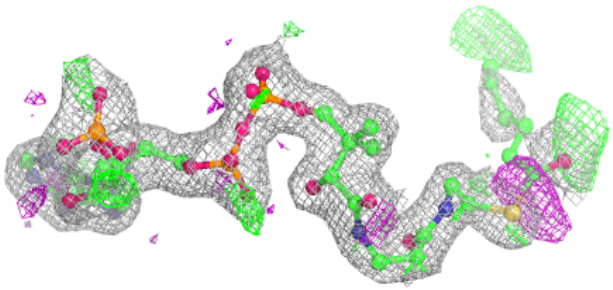


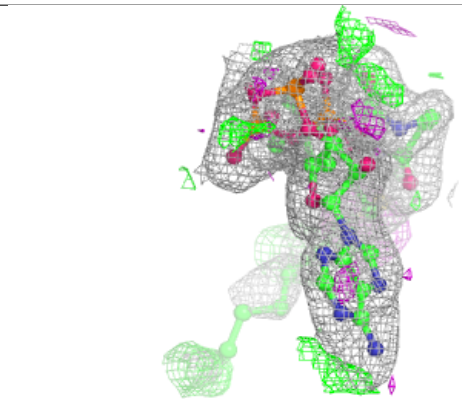


Electron density around HXC K 401:

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

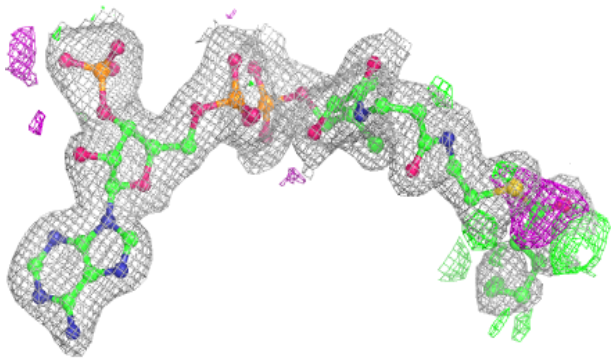


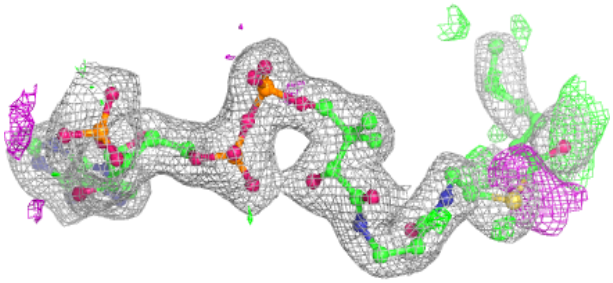


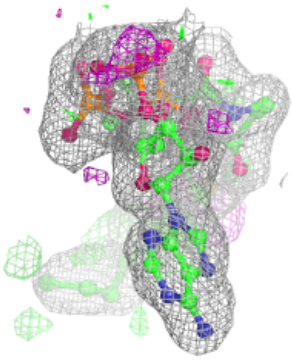


Electron density around HXC B 401:

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

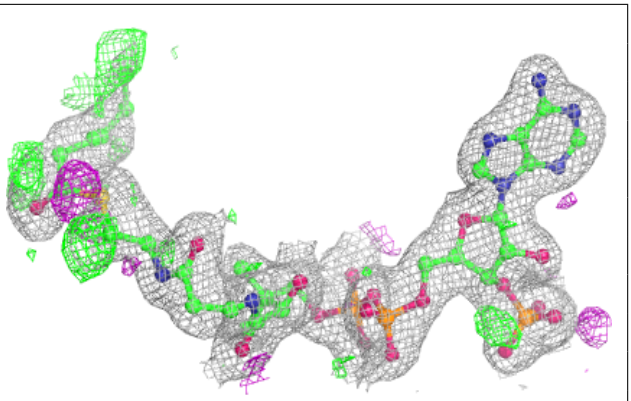


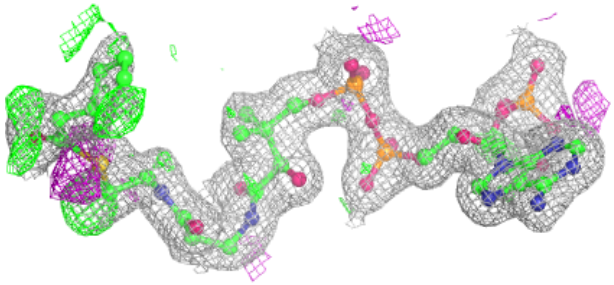


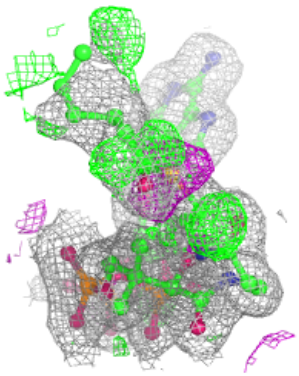


Electron density around HXC L 401:

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

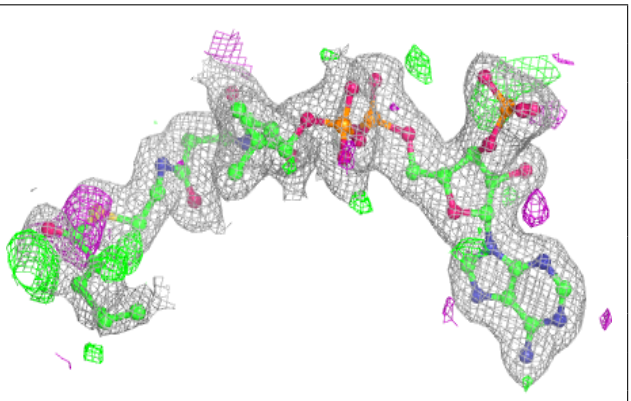


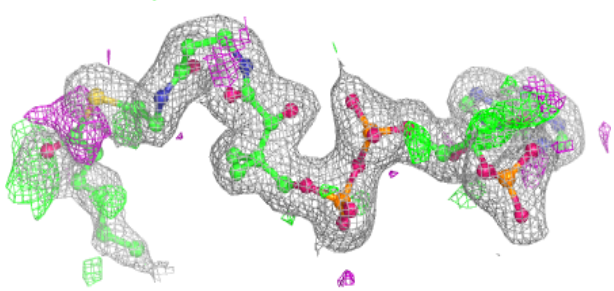


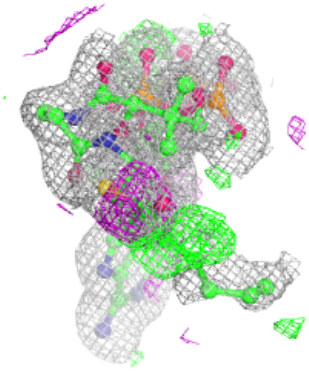


Electron density around HXC I 401:

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

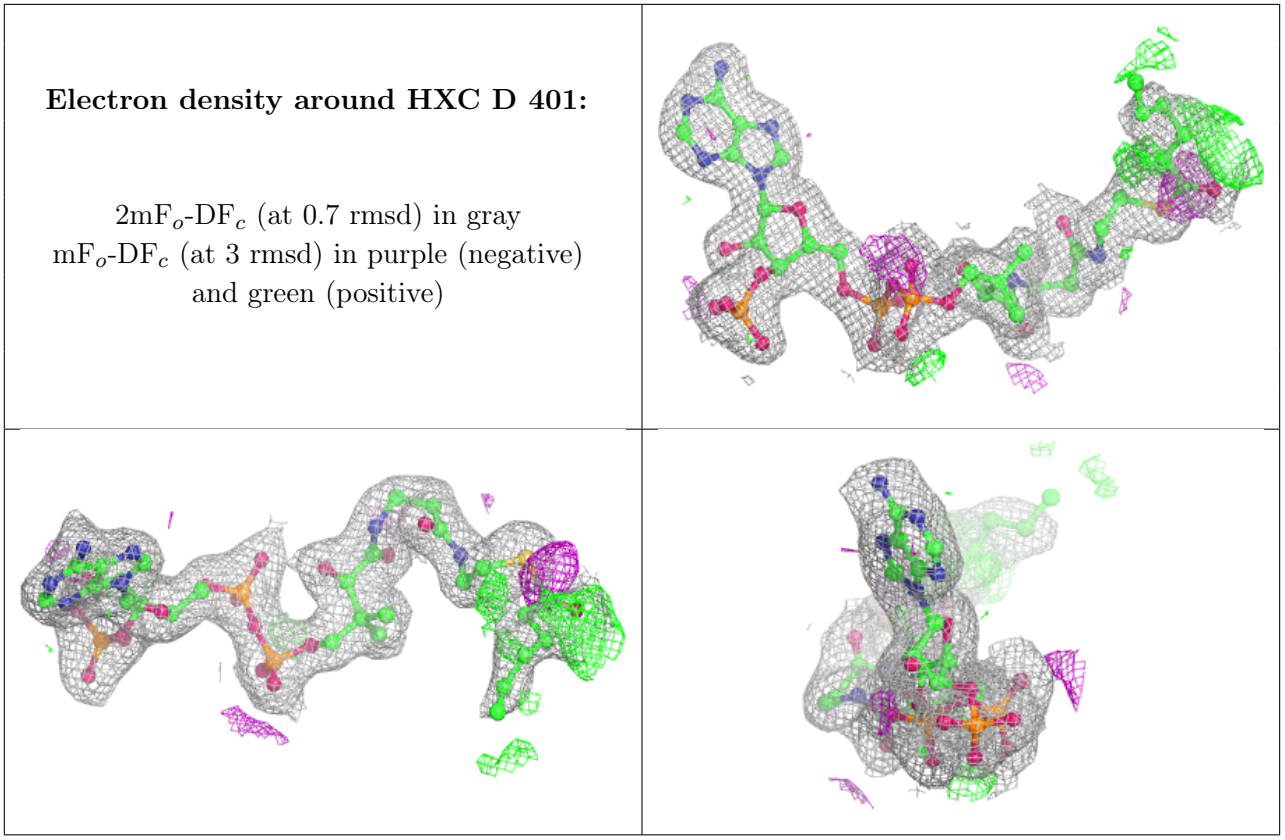






Electron density around HXC D 401:

$2mF_o$-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.