



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:38 PM UTC

PDB ID : 1MJ3 / pdb_00001mj3
Title : Crystal Structure Analysis of rat enoyl-CoA hydratase in complex with hexadienoyl-CoA
Authors : Bell, A.F.; Feng, Y.; Hofstein, H.A.; Parikh, S.; Wu, J.; Rudolph, M.J.; Kisker, C.; Tonge, P.J.
Deposited on : 2002-08-26
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

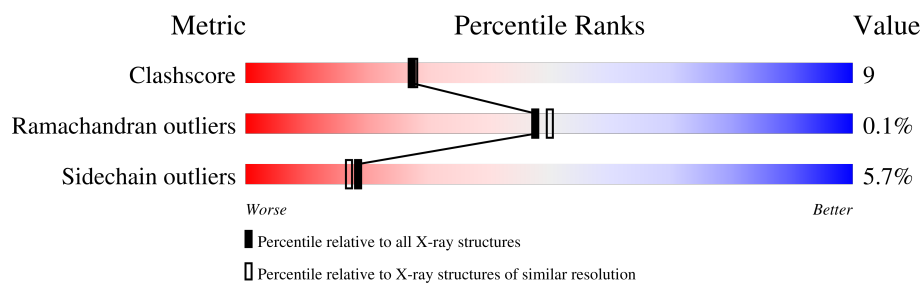
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	
1	D	260	
1	E	260	
1	F	260	

2 Entry composition [i](#)

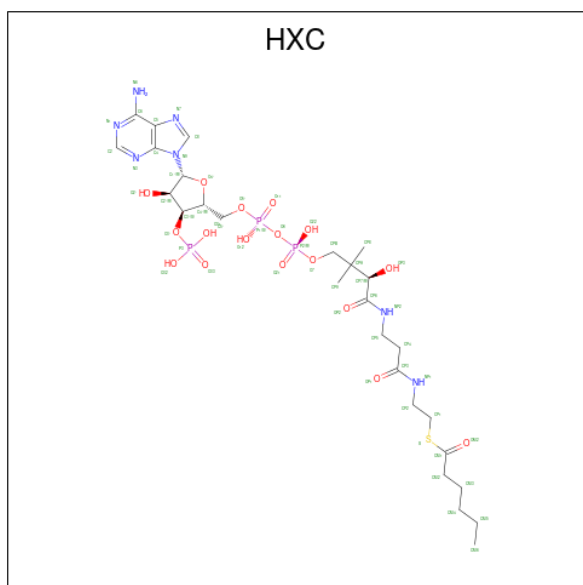
There are 3 unique types of molecules in this entry. The entry contains 12924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENOYL-COA HYDRATASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			
1	B	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			
1	C	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			
1	D	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			
1	E	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			
1	F	258	Total	C	N	O	S	0	0	0
			1955	1230	336	376	13			

- Molecule 2 is HEXANOYL-COENZYME A (CCD ID: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).



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	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total	O	0	0
			162	162		
3	B	167	Total	O	0	0
			167	167		
3	C	126	Total	O	0	0
			126	126		
3	D	145	Total	O	0	0
			145	145		
3	E	153	Total	O	0	0
			153	153		
3	F	166	Total	O	0	0
			166	166		

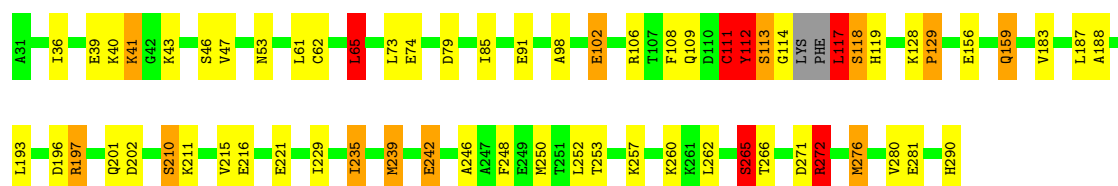
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

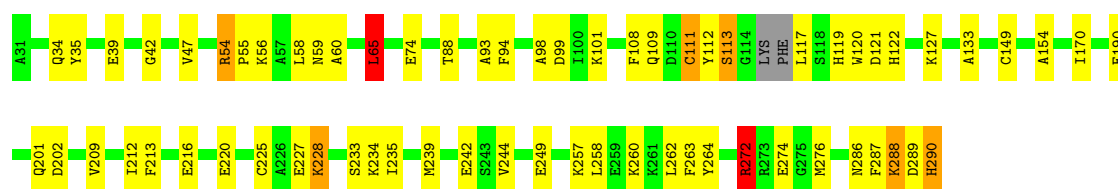
• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain A: 



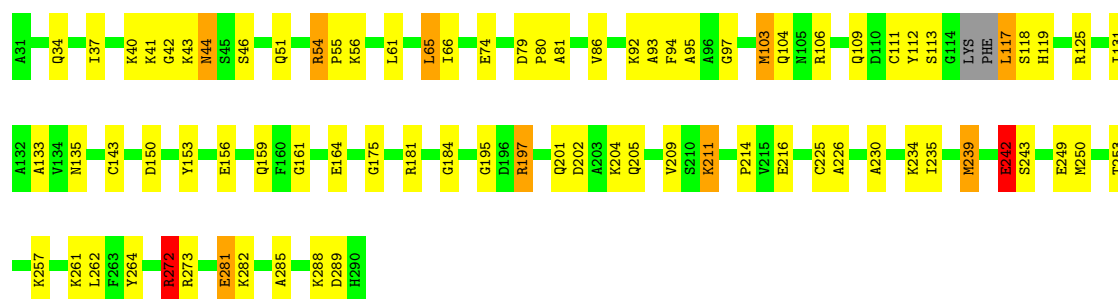
• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain B: 



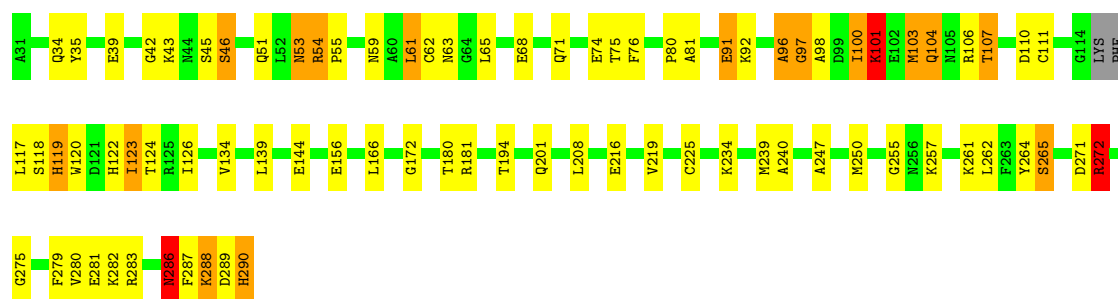
• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain C: 



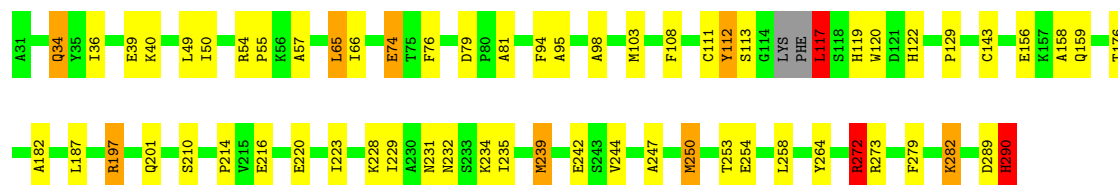
• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain D: 



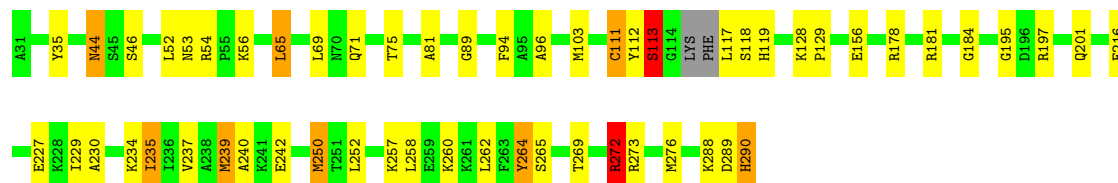
• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain E: 75% 20% ..



• Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain F: 78% 18% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.88Å 95.20Å 249.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.10	Depositor
% Data completeness (in resolution range)	90.2 (48.80-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.172 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12924	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	1.76	32/1980 (1.6%)	1.53	25/2659 (0.9%)
1	B	1.85	25/1980 (1.3%)	1.53	19/2659 (0.7%)
1	C	1.86	27/1980 (1.4%)	1.60	24/2659 (0.9%)
1	D	1.87	31/1980 (1.6%)	1.73	42/2659 (1.6%)
1	E	1.83	27/1980 (1.4%)	1.55	29/2659 (1.1%)
1	F	1.79	21/1980 (1.1%)	1.61	37/2659 (1.4%)
All	All	1.83	163/11880 (1.4%)	1.60	176/15954 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	MET	SD-CE	-14.36	1.43	1.79
1	E	272	ARG	CZ-NH1	14.07	1.52	1.32
1	B	272	ARG	CZ-NH1	14.06	1.52	1.32
1	C	239	MET	SD-CE	-12.58	1.48	1.79
1	E	239	MET	SD-CE	-12.44	1.48	1.79
1	B	119	HIS	CG-ND1	12.14	1.51	1.38
1	C	119	HIS	CG-ND1	11.94	1.51	1.38
1	D	119	HIS	CG-ND1	11.06	1.50	1.38
1	E	119	HIS	CG-ND1	10.78	1.50	1.38
1	A	276	MET	SD-CE	10.29	2.05	1.79
1	F	119	HIS	CG-ND1	9.41	1.48	1.38
1	D	272	ARG	CZ-NH1	9.36	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	MET	SD-CE	-9.24	1.56	1.79
1	C	226	ALA	CA-CB	-9.14	1.39	1.53
1	C	242	GLU	C-O	-8.96	1.13	1.24
1	D	97	GLY	CA-C	-8.95	1.42	1.51
1	F	250	MET	SD-CE	-8.62	1.57	1.79
1	A	215	VAL	CA-CB	8.58	1.64	1.54
1	D	272	ARG	NE-CZ	8.53	1.42	1.33
1	C	131	ILE	CA-CB	-8.47	1.44	1.54
1	C	164	GLU	C-O	8.42	1.34	1.24
1	E	95	ALA	CA-CB	-8.30	1.39	1.53
1	A	119	HIS	CG-ND1	8.19	1.47	1.38
1	D	250	MET	SD-CE	-8.09	1.59	1.79
1	F	272	ARG	CZ-NH1	8.04	1.44	1.32
1	A	183	VAL	CA-CB	8.00	1.63	1.54
1	E	229	ILE	CA-C	7.90	1.63	1.52
1	F	111	CYS	CA-C	-7.87	1.43	1.52
1	D	240	ALA	CA-CB	-7.65	1.41	1.53
1	C	93	ALA	CA-CB	-7.62	1.40	1.53
1	B	244	VAL	CA-CB	7.58	1.64	1.54
1	B	287	PHE	CE1-CZ	7.56	1.61	1.38
1	E	112	TYR	CA-C	-7.43	1.45	1.53
1	C	253	THR	CA-C	7.41	1.62	1.52
1	C	272	ARG	CZ-NH1	7.28	1.43	1.32
1	C	230	ALA	CA-CB	-7.24	1.40	1.53
1	C	153	TYR	CA-C	7.18	1.61	1.52
1	C	250	MET	CB-CG	-7.10	1.31	1.52
1	E	182	ALA	CA-CB	7.07	1.64	1.53
1	B	276	MET	SD-CE	7.01	1.97	1.79
1	A	272	ARG	CZ-NH1	6.87	1.42	1.32
1	A	246	ALA	CA-CB	6.74	1.64	1.53
1	B	170	ILE	N-CA	6.70	1.54	1.46
1	E	229	ILE	CA-CB	-6.66	1.45	1.54
1	D	107	THR	CA-C	6.63	1.60	1.52
1	C	81	ALA	CA-CB	6.56	1.64	1.53
1	A	239	MET	SD-CE	-6.56	1.63	1.79
1	B	112	TYR	CA-C	-6.51	1.44	1.52
1	E	81	ALA	CA-C	6.45	1.61	1.52
1	E	40	LYS	CA-C	-6.40	1.45	1.52
1	C	211	LYS	N-CA	6.37	1.54	1.45
1	D	180	THR	C-O	-6.37	1.16	1.24
1	E	103	MET	SD-CE	6.34	1.95	1.79
1	F	239	MET	SD-CE	-6.27	1.63	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	PRO	C-O	6.26	1.30	1.23
1	B	133	ALA	CA-CB	6.25	1.61	1.53
1	E	66	ILE	N-CA	-6.23	1.39	1.46
1	A	235	ILE	C-O	-6.22	1.16	1.24
1	F	184	GLY	C-O	6.17	1.30	1.23
1	A	102	GLU	C-O	-6.16	1.16	1.24
1	B	233	SER	CA-C	6.15	1.60	1.52
1	A	106	ARG	C-O	-6.14	1.16	1.23
1	C	143	CYS	CA-C	6.07	1.60	1.52
1	D	275	GLY	C-O	6.06	1.31	1.23
1	E	158	ALA	CA-CB	5.98	1.62	1.53
1	D	139	LEU	CA-C	-5.93	1.45	1.52
1	F	234	LYS	CG-CD	5.90	1.70	1.52
1	E	244	VAL	CA-CB	5.89	1.61	1.54
1	A	257	LYS	CG-CD	5.87	1.70	1.52
1	C	111	CYS	CA-C	-5.86	1.45	1.52
1	C	150	ASP	CA-C	-5.84	1.44	1.52
1	B	149	CYS	C-O	-5.82	1.15	1.23
1	C	135	ASN	CA-C	-5.79	1.46	1.52
1	D	96	ALA	C-O	-5.78	1.16	1.24
1	B	88	THR	CA-C	-5.75	1.45	1.52
1	C	161	GLY	C-O	5.74	1.29	1.23
1	F	230	ALA	CA-CB	5.73	1.62	1.53
1	F	128	LYS	C-O	-5.71	1.16	1.23
1	E	50	ILE	C-O	5.71	1.30	1.24
1	B	209	VAL	CA-CB	5.68	1.64	1.54
1	B	235	ILE	N-CA	-5.67	1.39	1.46
1	D	239	MET	CG-SD	5.67	1.95	1.80
1	F	262	LEU	C-O	-5.67	1.17	1.24
1	B	288	LYS	CE-NZ	5.66	1.66	1.49
1	F	250	MET	CB-CG	-5.66	1.35	1.52
1	F	252	LEU	CA-CB	5.65	1.62	1.53
1	A	266	THR	CA-CB	5.65	1.62	1.53
1	A	36	ILE	CA-CB	-5.63	1.45	1.54
1	D	46	SER	CA-CB	-5.62	1.43	1.53
1	D	250	MET	CB-CG	-5.62	1.35	1.52
1	A	202	ASP	C-O	-5.61	1.17	1.24
1	B	228	LYS	CA-C	-5.60	1.45	1.52
1	F	119	HIS	ND1-CE1	5.56	1.38	1.32
1	A	129	PRO	C-O	5.56	1.30	1.23
1	E	254	GLU	C-O	-5.52	1.17	1.24
1	C	86	VAL	C-O	5.51	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	123	ILE	CA-CB	-5.51	1.46	1.54
1	A	197	ARG	CD-NE	-5.49	1.38	1.46
1	A	46	SER	C-O	5.48	1.31	1.24
1	C	44	ASN	CA-C	-5.47	1.45	1.53
1	E	34	GLN	CA-C	5.46	1.59	1.52
1	E	187	LEU	CA-C	5.44	1.59	1.52
1	E	49	LEU	CA-C	-5.44	1.46	1.52
1	B	213	PHE	N-CA	-5.43	1.41	1.45
1	F	71	GLN	C-O	-5.42	1.17	1.24
1	A	271	ASP	N-CA	5.41	1.53	1.46
1	F	257	LYS	CB-CG	5.41	1.68	1.52
1	C	285	ALA	CA-C	-5.40	1.45	1.52
1	B	111	CYS	CA-C	-5.40	1.45	1.52
1	F	276	MET	CG-SD	5.39	1.94	1.80
1	B	257	LYS	CB-CG	5.39	1.68	1.52
1	D	68	GLU	C-O	5.37	1.30	1.24
1	E	254	GLU	CA-CB	5.37	1.62	1.53
1	D	181	ARG	CZ-NH1	5.36	1.40	1.32
1	D	124	THR	CA-CB	5.34	1.62	1.53
1	D	51	GLN	C-O	-5.33	1.18	1.24
1	A	193	LEU	C-O	-5.33	1.17	1.24
1	A	187	LEU	C-O	-5.32	1.17	1.24
1	D	126	ILE	CA-CB	5.31	1.60	1.54
1	C	181	ARG	N-CA	5.31	1.53	1.46
1	D	194	THR	N-CA	5.30	1.52	1.46
1	D	91	GLU	C-O	5.30	1.31	1.24
1	E	223	ILE	CA-CB	5.28	1.62	1.54
1	C	184	GLY	CA-C	5.28	1.57	1.52
1	A	272	ARG	NE-CZ	5.27	1.38	1.33
1	C	133	ALA	CA-CB	5.27	1.59	1.53
1	E	119	HIS	CD2-NE2	5.25	1.43	1.37
1	D	101	LYS	CB-CG	5.23	1.68	1.52
1	B	58	LEU	CA-C	5.22	1.59	1.52
1	B	108	PHE	CA-C	5.22	1.59	1.52
1	C	92	LYS	CA-C	5.21	1.59	1.52
1	B	170	ILE	C-O	5.21	1.30	1.24
1	F	269	THR	N-CA	5.20	1.52	1.45
1	A	73	LEU	CA-C	5.20	1.59	1.52
1	A	47	VAL	C-O	5.18	1.29	1.24
1	F	112	TYR	N-CA	-5.17	1.40	1.46
1	D	91	GLU	CA-C	5.17	1.59	1.52
1	C	202	ASP	C-O	-5.17	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLN	N-CA	5.16	1.52	1.46
1	E	39	GLU	C-O	5.16	1.30	1.23
1	E	250	MET	SD-CE	-5.15	1.66	1.79
1	D	255	GLY	CA-C	5.14	1.57	1.52
1	A	111	CYS	CB-SG	-5.13	1.64	1.81
1	D	96	ALA	CA-CB	-5.13	1.44	1.53
1	E	232	ASN	CA-C	-5.13	1.46	1.53
1	A	188	ALA	CA-CB	-5.10	1.45	1.53
1	D	239	MET	SD-CE	-5.09	1.66	1.79
1	F	75	THR	CA-C	5.08	1.59	1.52
1	B	112	TYR	N-CA	-5.07	1.40	1.46
1	B	202	ASP	CA-C	5.07	1.59	1.52
1	E	250	MET	CB-CG	-5.06	1.37	1.52
1	F	264	TYR	C-O	-5.06	1.18	1.24
1	A	111	CYS	CA-C	-5.06	1.45	1.52
1	A	250	MET	CG-SD	-5.05	1.68	1.80
1	A	85	ILE	CA-CB	-5.05	1.47	1.54
1	A	61	LEU	CA-CB	5.04	1.59	1.52
1	F	239	MET	CG-SD	5.04	1.93	1.80
1	B	119	HIS	CD2-NE2	5.04	1.43	1.37
1	D	208	LEU	CA-C	5.03	1.59	1.52
1	D	119	HIS	CD2-NE2	5.03	1.43	1.37
1	D	247	ALA	C-O	-5.03	1.17	1.24
1	D	134	VAL	CA-CB	5.02	1.59	1.53
1	A	65	LEU	CA-C	5.01	1.59	1.52

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ARG	NE-CZ-NH2	-18.48	102.57	119.20
1	B	272	ARG	NE-CZ-NH2	-15.91	104.88	119.20
1	D	272	ARG	NE-CZ-NH2	-12.01	108.39	119.20
1	E	272	ARG	NE-CZ-NH1	11.61	133.11	121.50
1	D	272	ARG	NE-CZ-NH1	11.29	132.79	121.50
1	B	272	ARG	NE-CZ-NH1	11.27	132.77	121.50
1	D	98	ALA	N-CA-C	-11.11	93.39	110.17
1	D	272	ARG	CD-NE-CZ	10.58	139.21	124.40
1	D	96	ALA	CA-C-N	-9.83	107.06	121.22
1	D	96	ALA	C-N-CA	-9.83	107.06	121.22
1	E	272	ARG	CD-NE-CZ	9.59	137.82	124.40
1	C	281	GLU	N-CA-C	-9.42	101.33	112.92
1	A	272	ARG	NE-CZ-NH2	-9.34	110.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	272	ARG	CG-CD-NE	9.23	132.30	112.00
1	A	272	ARG	NE-CZ-NH1	8.81	130.31	121.50
1	F	272	ARG	NE-CZ-NH2	-8.81	111.27	119.20
1	F	94	PHE	N-CA-C	-8.76	99.94	111.24
1	F	113	SER	N-CA-C	8.68	121.89	111.82
1	D	97	GLY	N-CA-C	-8.45	98.38	110.88
1	F	89	GLY	CA-C-N	-8.24	115.10	122.43
1	F	89	GLY	C-N-CA	-8.24	115.10	122.43
1	A	197	ARG	NE-CZ-NH2	-8.22	111.80	119.20
1	D	286	ASN	CB-CA-C	-8.20	99.71	111.76
1	F	272	ARG	CD-NE-CZ	8.05	135.67	124.40
1	E	272	ARG	CG-CD-NE	8.03	129.66	112.00
1	D	281	GLU	N-CA-C	-8.00	103.97	112.93
1	D	272	ARG	CG-CD-NE	7.95	129.50	112.00
1	E	119	HIS	ND1-CG-CD2	-7.89	98.21	106.10
1	A	272	ARG	CG-CD-NE	7.83	129.22	112.00
1	E	197	ARG	NE-CZ-NH2	-7.76	112.22	119.20
1	C	272	ARG	CG-CD-NE	7.70	128.94	112.00
1	F	119	HIS	ND1-CG-CD2	-7.67	98.43	106.10
1	B	272	ARG	CD-NE-CZ	7.67	135.13	124.40
1	B	274	GLU	CA-C-N	7.51	128.48	119.99
1	B	274	GLU	C-N-CA	7.51	128.48	119.99
1	C	272	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	119	HIS	ND1-CG-CD2	-7.48	98.62	106.10
1	D	119	HIS	ND1-CG-CD2	-7.37	98.73	106.10
1	F	44	ASN	N-CA-C	-7.32	104.30	113.23
1	D	54	ARG	CB-CA-C	7.30	121.48	111.41
1	C	225	CYS	N-CA-C	-7.29	103.41	111.36
1	D	54	ARG	N-CA-C	-7.23	98.53	109.30
1	C	273	ARG	N-CA-C	-7.16	103.48	111.28
1	C	44	ASN	CB-CA-C	-7.08	100.33	111.51
1	E	253	THR	N-CA-C	7.01	119.53	111.11
1	D	61	LEU	N-CA-C	7.00	119.83	108.63
1	E	117	LEU	CA-C-N	-6.96	110.96	122.79
1	E	117	LEU	C-N-CA	-6.96	110.96	122.79
1	A	119	HIS	ND1-CG-CD2	-6.95	99.15	106.10
1	C	80	PRO	N-CA-C	-6.89	105.56	114.03
1	F	53	ASN	CA-C-N	-6.86	114.97	122.59
1	F	53	ASN	C-N-CA	-6.86	114.97	122.59
1	D	96	ALA	O-C-N	-6.86	112.24	122.39
1	F	265	SER	CA-CB-OG	-6.75	97.61	111.10
1	C	119	HIS	ND1-CG-CD2	-6.71	99.39	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	SER	N-CA-C	6.67	121.02	113.01
1	D	265	SER	CA-CB-OG	-6.66	97.78	111.10
1	B	65	LEU	N-CA-C	-6.51	104.26	111.36
1	F	54	ARG	N-CA-C	-6.49	99.62	109.30
1	C	272	ARG	CD-NE-CZ	6.49	133.48	124.40
1	D	250	MET	CG-SD-CE	-6.47	86.67	100.90
1	B	225	CYS	N-CA-C	-6.46	104.32	111.36
1	E	94	PHE	N-CA-C	-6.45	103.88	111.03
1	F	272	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	A	248	PHE	N-CA-C	6.42	120.72	113.02
1	E	112	TYR	CB-CA-C	6.41	121.58	111.39
1	F	52	LEU	CA-C-N	-6.39	113.28	122.67
1	F	52	LEU	C-N-CA	-6.39	113.28	122.67
1	C	54	ARG	CA-C-N	6.33	126.45	119.87
1	C	54	ARG	C-N-CA	6.33	126.45	119.87
1	C	250	MET	CG-SD-CE	-6.32	86.99	100.90
1	F	197	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	A	117	LEU	CA-C-N	-6.30	109.51	121.54
1	A	117	LEU	C-N-CA	-6.30	109.51	121.54
1	C	97	GLY	N-CA-C	-6.29	104.39	111.63
1	A	229	ILE	N-CA-C	-6.25	104.66	110.53
1	A	113	SER	N-CA-C	6.25	118.61	111.11
1	A	272	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	112	TYR	CA-CB-CG	-6.17	102.80	113.90
1	A	281	GLU	N-CA-C	-6.02	105.69	113.16
1	F	96	ALA	CA-C-N	-6.01	114.22	122.57
1	F	96	ALA	C-N-CA	-6.01	114.22	122.57
1	E	111	CYS	CA-C-N	-5.94	111.98	120.89
1	E	111	CYS	C-N-CA	-5.94	111.98	120.89
1	B	93	ALA	N-CA-C	5.93	119.19	108.69
1	B	113	SER	N-CA-C	-5.88	106.08	113.20
1	E	112	TYR	N-CA-CB	5.88	118.44	110.10
1	E	282	LYS	N-CA-C	5.88	119.35	111.24
1	E	108	PHE	N-CA-C	-5.87	104.88	111.28
1	F	250	MET	CB-CA-C	-5.85	97.87	110.45
1	B	39	GLU	N-CA-CB	-5.81	102.55	111.56
1	C	197	ARG	CG-CD-NE	-5.81	99.23	112.00
1	A	265	SER	CA-CB-OG	-5.79	99.52	111.10
1	D	103	MET	N-CA-C	-5.79	106.34	113.41
1	D	119	HIS	N-CA-C	-5.78	105.81	112.92
1	A	210	SER	N-CA-C	5.77	120.48	113.38
1	B	272	ARG	CG-CD-NE	5.76	124.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	TYR	N-CA-C	-5.76	102.11	111.04
1	C	118	SER	O-C-N	-5.70	115.41	122.25
1	A	265	SER	CB-CA-C	-5.69	101.00	110.68
1	B	119	HIS	N-CA-C	-5.67	106.16	112.57
1	B	47	VAL	N-CA-C	5.67	116.02	107.80
1	F	197	ARG	CG-CD-NE	-5.67	99.54	112.00
1	F	119	HIS	CG-CD2-NE2	5.65	112.85	107.20
1	E	143	CYS	N-CA-C	-5.63	105.23	111.36
1	D	166	LEU	N-CA-C	-5.61	106.28	113.01
1	C	103	MET	N-CA-C	-5.60	106.57	113.41
1	E	210	SER	CB-CA-C	5.60	118.48	109.07
1	D	54	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	C	272	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	F	112	TYR	CA-CB-CG	-5.55	103.90	113.90
1	A	108	PHE	N-CA-C	-5.55	105.14	111.07
1	F	235	ILE	N-CA-C	5.53	116.26	110.62
1	F	240	ALA	N-CA-C	-5.52	105.34	111.36
1	F	112	TYR	CA-C-N	5.52	128.70	120.31
1	F	112	TYR	C-N-CA	5.52	128.70	120.31
1	D	63	ASN	CA-C-N	5.50	125.94	119.94
1	D	63	ASN	C-N-CA	5.50	125.94	119.94
1	D	97	GLY	CA-C-O	-5.50	116.22	121.83
1	E	76	PHE	N-CA-C	5.50	117.71	111.11
1	F	54	ARG	CB-CA-C	5.48	118.97	111.41
1	D	257	LYS	N-CA-C	-5.47	105.48	111.82
1	D	98	ALA	CA-C-N	5.46	129.68	122.30
1	D	98	ALA	C-N-CA	5.46	129.68	122.30
1	D	283	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	F	118	SER	O-C-N	-5.44	115.16	122.23
1	C	175	GLY	CA-C-N	-5.41	113.61	122.54
1	C	175	GLY	C-N-CA	-5.41	113.61	122.54
1	A	117	LEU	CB-CA-C	-5.41	99.83	110.10
1	E	250	MET	CB-CA-C	-5.37	98.90	111.09
1	E	290	HIS	CA-C-O	-5.37	104.89	121.00
1	F	111	CYS	N-CA-C	-5.36	105.35	111.14
1	E	119	HIS	N-CA-C	-5.35	106.53	112.57
1	B	258	LEU	N-CA-C	-5.34	105.35	111.07
1	E	57	ALA	N-CA-C	-5.34	105.04	112.30
1	A	53	ASN	CA-C-N	-5.33	116.93	122.89
1	A	53	ASN	C-N-CA	-5.33	116.93	122.89
1	D	59	ASN	CA-C-O	-5.31	114.96	121.28
1	A	111	CYS	N-CA-C	-5.31	105.54	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	TYR	CA-CB-CG	-5.30	104.36	113.90
1	F	237	VAL	N-CA-C	-5.30	105.37	110.72
1	B	65	LEU	CB-CA-C	5.28	119.83	110.85
1	D	250	MET	CA-C-O	-5.28	115.63	121.33
1	F	56	LYS	N-CA-C	-5.27	106.36	112.89
1	D	144	GLU	N-CA-C	5.26	117.02	111.28
1	A	280	VAL	CB-CA-C	-5.26	103.59	112.16
1	B	112	TYR	CA-CB-CG	-5.26	104.43	113.90
1	D	275	GLY	CA-C-O	5.24	126.22	120.66
1	F	119	HIS	N-CA-C	-5.24	106.65	112.57
1	D	172	GLY	CA-C-N	-5.23	114.09	122.62
1	D	172	GLY	C-N-CA	-5.23	114.09	122.62
1	D	53	ASN	CA-C-N	-5.22	116.79	122.59
1	D	53	ASN	C-N-CA	-5.22	116.79	122.59
1	E	228	LYS	CB-CA-C	-5.21	102.14	110.79
1	C	249	GLU	N-CA-C	5.21	121.42	113.61
1	E	214	PRO	CB-CA-C	-5.20	104.73	111.39
1	F	178	ARG	N-CA-C	-5.19	105.69	112.23
1	B	94	PHE	N-CA-C	-5.18	105.08	111.40
1	C	195	GLY	N-CA-C	-5.17	108.18	115.32
1	F	111	CYS	CA-CB-SG	-5.16	102.53	114.40
1	E	120	TRP	CA-C-N	-5.15	114.40	122.79
1	E	120	TRP	C-N-CA	-5.15	114.40	122.79
1	A	221	GLU	N-CA-C	5.14	116.89	111.28
1	A	242	GLU	N-CA-C	-5.14	105.75	111.36
1	D	35	TYR	N-CA-C	5.13	120.40	113.72
1	D	219	VAL	N-CA-C	-5.13	105.54	110.72
1	E	176	THR	N-CA-C	-5.13	106.42	113.30
1	D	288	LYS	CA-CB-CG	-5.13	103.84	114.10
1	C	250	MET	CB-CA-C	-5.13	99.43	110.45
1	F	69	LEU	N-CA-C	-5.09	105.74	111.28
1	B	249	GLU	N-CA-C	5.04	121.17	113.61
1	A	118	SER	O-C-N	-5.01	115.93	122.59
1	D	271	ASP	CA-C-N	-5.01	113.93	120.44
1	D	271	ASP	C-N-CA	-5.01	113.93	120.44
1	F	195	GLY	N-CA-C	-5.01	108.37	115.43
1	D	75	THR	N-CA-C	-5.00	105.71	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	117	LEU	Peptide

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	1955	0	1975	47	0
1	B	1955	0	1975	42	3
1	C	1955	0	1975	33	1
1	D	1955	0	1975	48	3
1	E	1955	0	1975	41	3
1	F	1955	0	1975	35	3
2	A	55	0	40	4	0
2	B	55	0	41	6	0
2	C	55	0	41	3	0
2	E	55	0	40	2	0
2	F	55	0	39	8	0
3	A	162	0	0	16	0
3	B	167	0	0	9	0
3	C	126	0	0	8	0
3	D	145	0	0	21	0
3	E	153	0	0	3	0
3	F	166	0	0	6	0
All	All	12924	0	12051	219	7

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 9.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:953:HXC:C2'	2:C:953:HXC:C3'	1.93	1.43
1:A:276:MET:CE	1:A:276:MET:SD	2.05	1.42
2:B:952:HXC:C2'	2:B:952:HXC:C3'	1.96	1.34
2:F:955:HXC:C2'	2:F:955:HXC:C3'	2.09	1.24
1:D:62:CYS:N	3:D:386:HOH:O	1.70	1.23
1:B:121:ASP:HB3	3:B:1107:HOH:O	1.39	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ALA:C	3:D:400:HOH:O	1.81	1.19
1:D:61:LEU:C	3:D:386:HOH:O	1.85	1.19
1:D:118:SER:HB2	3:D:370:HOH:O	1.43	1.17
1:E:117:LEU:HD11	1:F:260:LYS:CE	1.76	1.16
1:B:286:ASN:HB3	3:B:982:HOH:O	1.53	1.08
3:B:1059:HOH:O	1:C:261:LYS:HE3	1.54	1.05
1:F:117:LEU:HD13	2:F:955:HXC:HM62	1.39	1.02
1:A:109:GLN:HG2	1:F:290:HIS:HB2	1.42	1.00
1:D:100:ILE:HD13	1:E:279:PHE:CE2	1.97	1.00
1:A:114:GLY:N	3:A:1109:HOH:O	1.91	0.99
1:D:118:SER:CB	3:D:370:HOH:O	2.04	0.98
1:E:117:LEU:HD11	1:F:260:LYS:CD	1.95	0.96
1:E:117:LEU:O	1:E:117:LEU:HD13	1.63	0.96
1:B:289:ASP:O	1:B:290:HIS:HB3	1.59	0.96
1:F:117:LEU:CD1	2:F:955:HXC:HM62	1.96	0.96
1:D:96:ALA:CB	3:D:400:HOH:O	2.16	0.94
1:D:96:ALA:HB3	3:D:400:HOH:O	1.70	0.90
1:C:125:ARG:HD3	3:C:1069:HOH:O	1.71	0.89
1:E:117:LEU:HD11	1:F:260:LYS:HD2	1.55	0.87
1:D:201:GLN:HG3	3:D:330:HOH:O	1.75	0.86
2:F:955:HXC:C2'	2:F:955:HXC:O3'	2.22	0.85
1:E:234:LYS:HE2	1:E:289:ASP:OD2	1.76	0.85
1:B:127:LYS:HD2	3:B:1116:HOH:O	1.77	0.84
1:F:201:GLN:HG3	3:F:978:HOH:O	1.77	0.84
1:A:117:LEU:HD22	2:A:951:HXC:HM62	1.59	0.84
3:B:1059:HOH:O	1:C:261:LYS:HG2	1.78	0.84
1:A:113:SER:OG	3:A:1109:HOH:O	1.97	0.83
1:C:242:GLU:HG3	3:C:1046:HOH:O	1.79	0.81
1:E:117:LEU:CD1	1:F:260:LYS:HD2	2.11	0.79
1:E:117:LEU:HD11	1:F:260:LYS:HE3	1.64	0.79
1:A:201:GLN:HG3	3:A:963:HOH:O	1.80	0.79
2:C:953:HXC:HM31	3:C:994:HOH:O	1.83	0.79
1:E:117:LEU:HD11	1:F:260:LYS:NZ	1.98	0.78
1:A:112:TYR:HE2	3:A:1033:HOH:O	1.64	0.78
2:A:951:HXC:HM31	3:A:960:HOH:O	1.84	0.78
1:E:289:ASP:O	1:E:290:HIS:HB3	1.84	0.76
1:A:117:LEU:CD1	1:B:264:TYR:HE1	1.98	0.76
1:D:286:ASN:ND2	3:D:373:HOH:O	2.18	0.75
1:F:289:ASP:O	1:F:290:HIS:HB3	1.85	0.75
2:E:954:HXC:HM31	3:E:992:HOH:O	1.86	0.73
1:E:201:GLN:HG3	3:E:984:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ALA:HB2	2:B:952:HXC:HM32	1.70	0.71
1:A:117:LEU:N	3:A:1072:HOH:O	2.25	0.70
1:D:39:GLU:HG2	3:D:418:HOH:O	1.92	0.70
1:A:262:LEU:O	1:A:265:SER:HB2	1.93	0.68
1:D:100:ILE:HD13	1:E:279:PHE:CD2	2.29	0.68
1:B:201:GLN:HG3	3:B:1023:HOH:O	1.94	0.67
1:C:43:LYS:HG3	1:C:44:ASN:ND2	2.10	0.67
1:C:288:LYS:O	1:C:289:ASP:HB2	1.95	0.66
1:A:117:LEU:CD1	1:B:264:TYR:CE1	2.77	0.66
1:A:117:LEU:CD1	1:B:260:LYS:HD2	2.26	0.66
1:A:117:LEU:HD11	1:B:264:TYR:HE1	1.60	0.66
1:E:65:LEU:C	1:E:65:LEU:HD12	2.21	0.65
1:A:62:CYS:SG	3:A:1091:HOH:O	2.46	0.65
1:B:65:LEU:HD12	1:B:65:LEU:C	2.22	0.64
1:D:100:ILE:CD1	1:E:279:PHE:CE2	2.77	0.64
1:A:118:SER:CB	3:A:1107:HOH:O	2.46	0.64
1:B:289:ASP:O	1:B:290:HIS:CB	2.37	0.63
1:A:117:LEU:HD21	1:B:263:PHE:CE2	2.34	0.63
1:A:98:ALA:HB2	2:A:951:HXC:HM32	1.81	0.63
1:E:117:LEU:CD1	1:F:260:LYS:CD	2.73	0.63
2:B:952:HXC:HM31	3:B:995:HOH:O	1.97	0.62
1:D:289:ASP:O	1:D:290:HIS:HB3	1.98	0.62
1:B:109:GLN:HG2	1:E:290:HIS:HB2	1.80	0.62
1:A:111:CYS:O	1:A:112:TYR:O	2.17	0.62
1:C:204:LYS:NZ	3:C:1031:HOH:O	2.33	0.62
2:C:953:HXC:C2'	2:C:953:HXC:O3'	2.49	0.61
1:A:117:LEU:HD11	1:B:264:TYR:CE1	2.36	0.61
1:A:117:LEU:HD21	1:B:263:PHE:HE2	1.65	0.60
1:C:201:GLN:HG3	3:C:1055:HOH:O	2.01	0.60
1:A:117:LEU:HD12	1:B:264:TYR:CE1	2.35	0.60
1:B:109:GLN:HG2	1:E:290:HIS:CD2	2.36	0.60
1:F:272:ARG:HH11	1:F:272:ARG:HB3	1.67	0.60
1:D:62:CYS:CA	3:D:386:HOH:O	2.35	0.59
1:E:117:LEU:CD1	1:F:260:LYS:CE	2.69	0.59
1:E:117:LEU:HD11	1:F:260:LYS:HZ2	1.65	0.59
1:D:92:LYS:NZ	3:D:404:HOH:O	2.33	0.58
2:F:955:HXC:O3'	2:F:955:HXC:C1'	2.51	0.58
1:D:107:THR:OG1	1:D:110:ASP:CG	2.46	0.58
1:B:117:LEU:HD22	1:B:120:TRP:HE1	1.68	0.57
1:A:118:SER:HB2	3:A:1107:HOH:O	2.04	0.57
1:F:113:SER:HB2	3:F:1030:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ARG:NH2	3:F:1036:HOH:O	2.33	0.57
1:D:290:HIS:CE1	3:D:389:HOH:O	2.58	0.57
1:C:40:LYS:HE3	1:C:79:ASP:OD2	2.03	0.57
1:E:250:MET:HE1	1:E:258:LEU:HD22	1.87	0.57
1:C:43:LYS:HG3	1:C:44:ASN:HD21	1.70	0.56
1:E:74:GLU:OE1	1:E:122:HIS:HE1	1.87	0.56
1:F:235:ILE:HG12	1:F:239:MET:HE3	1.86	0.56
1:D:225:CYS:HB2	3:D:350:HOH:O	2.05	0.56
1:E:117:LEU:O	1:E:117:LEU:CD1	2.48	0.55
1:E:289:ASP:O	1:E:290:HIS:CB	2.55	0.55
1:A:40:LYS:HE3	1:A:79:ASP:OD2	2.07	0.55
1:A:117:LEU:HD12	1:B:260:LYS:HD2	1.88	0.55
1:B:228:LYS:HE2	3:B:1032:HOH:O	2.08	0.54
1:E:117:LEU:CD1	1:F:260:LYS:HE3	2.35	0.54
1:F:117:LEU:HD12	2:F:955:HXC:HM62	1.83	0.54
1:C:272:ARG:HH11	1:C:272:ARG:HB3	1.69	0.54
1:D:53:ASN:C	1:D:55:PRO:HD3	2.33	0.54
1:A:196:ASP:OD2	1:B:228:LYS:NZ	2.40	0.54
1:D:261:LYS:NZ	3:D:364:HOH:O	2.39	0.54
1:C:257:LYS:HE2	3:C:998:HOH:O	2.06	0.54
1:A:260:LYS:NZ	3:A:1061:HOH:O	2.41	0.53
2:B:952:HXC:C2'	2:B:952:HXC:O3'	2.56	0.53
1:E:235:ILE:HG12	1:E:239:MET:HE3	1.89	0.53
1:A:159:GLN:NE2	1:A:197:ARG:HD2	2.24	0.53
1:A:117:LEU:HD12	1:B:264:TYR:HE1	1.71	0.53
1:C:103:MET:O	1:C:104:GLN:C	2.50	0.52
1:A:65:LEU:C	1:A:65:LEU:HD12	2.34	0.52
1:E:98:ALA:HB2	2:E:954:HXC:HM32	1.91	0.52
1:D:264:TYR:CD1	1:F:111:CYS:HB3	2.45	0.52
1:E:65:LEU:C	1:E:65:LEU:CD1	2.82	0.52
1:F:103:MET:HE1	2:F:955:HXC:HM21	1.91	0.52
1:A:113:SER:CB	3:A:1109:HOH:O	2.56	0.52
1:A:272:ARG:NH2	3:A:1045:HOH:O	2.27	0.52
1:C:40:LYS:O	1:C:41:LYS:HG2	2.10	0.52
1:F:288:LYS:O	1:F:289:ASP:HB2	2.11	0.51
1:D:80:PRO:O	1:D:234:LYS:HE3	2.10	0.51
1:C:54:ARG:N	1:C:55:PRO:HD3	2.26	0.51
1:E:54:ARG:N	1:E:55:PRO:CD	2.73	0.51
1:B:65:LEU:C	1:B:65:LEU:CD1	2.84	0.51
1:D:103:MET:O	1:D:104:GLN:C	2.54	0.50
1:F:129:PRO:HG2	1:F:229:ILE:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:N	3:A:1107:HOH:O	2.45	0.50
1:D:96:ALA:CA	3:D:400:HOH:O	2.27	0.50
1:F:181:ARG:NE	3:F:1036:HOH:O	2.31	0.50
1:A:98:ALA:CB	2:A:951:HXC:HM32	2.42	0.49
1:C:235:ILE:HG12	1:C:239:MET:HE3	1.95	0.49
1:A:112:TYR:CE2	3:A:1033:HOH:O	2.49	0.49
1:F:250:MET:HE1	1:F:258:LEU:HD22	1.95	0.49
1:C:109:GLN:HG2	1:D:290:HIS:HB2	1.94	0.49
1:C:205:GLN:HG2	3:C:1052:HOH:O	2.12	0.49
1:A:210:SER:O	1:A:211:LYS:HG2	2.12	0.48
1:D:54:ARG:N	1:D:55:PRO:HD3	2.28	0.48
1:E:117:LEU:CD1	1:F:260:LYS:HZ2	2.26	0.48
2:F:955:HXC:HP91	2:F:955:HXC:OP2	2.12	0.48
1:D:264:TYR:CG	1:F:111:CYS:HB3	2.48	0.48
1:C:65:LEU:C	1:C:65:LEU:CD1	2.88	0.47
1:B:154:ALA:O	1:B:212:ILE:HA	2.15	0.47
1:A:91:GLU:HB2	3:A:1074:HOH:O	2.15	0.47
1:B:99:ASP:HA	2:B:952:HXC:N1	2.30	0.47
1:C:61:LEU:HB3	1:C:66:ILE:HD11	1.97	0.47
1:D:118:SER:HB3	3:D:370:HOH:O	1.91	0.47
1:C:159:GLN:NE2	1:C:197:ARG:HD2	2.30	0.46
1:C:272:ARG:HB3	1:C:272:ARG:NH1	2.30	0.46
1:A:117:LEU:HD11	1:B:263:PHE:CE2	2.51	0.46
1:B:59:ASN:O	1:B:60:ALA:C	2.57	0.46
3:D:402:HOH:O	1:E:247:ALA:HA	2.15	0.46
1:F:235:ILE:CG1	1:F:239:MET:HE3	2.45	0.46
1:B:98:ALA:CB	2:B:952:HXC:HM32	2.41	0.46
1:E:74:GLU:OE1	1:E:122:HIS:CE1	2.67	0.46
1:D:280:VAL:C	1:D:282:LYS:H	2.24	0.46
1:E:159:GLN:NE2	1:E:197:ARG:HD2	2.31	0.46
1:B:35:TYR:HD1	1:B:54:ARG:HG3	1.80	0.45
1:C:54:ARG:N	1:C:55:PRO:CD	2.80	0.45
1:A:39:GLU:OE2	1:A:41:LYS:HE3	2.16	0.45
1:C:234:LYS:HE2	1:C:289:ASP:OD2	2.17	0.45
1:D:111:CYS:HB3	1:E:264:TYR:CD1	2.52	0.45
1:F:201:GLN:HG3	3:F:1021:HOH:O	2.16	0.45
1:A:117:LEU:HD13	1:B:260:LYS:HD2	1.96	0.45
1:B:117:LEU:HD22	1:B:120:TRP:NE1	2.31	0.45
1:B:272:ARG:HH11	1:B:272:ARG:HB3	1.82	0.45
1:C:40:LYS:C	1:C:41:LYS:HG2	2.41	0.45
1:C:42:GLY:O	1:C:43:LYS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LYS:HD3	3:D:417:HOH:O	2.17	0.45
1:C:281:GLU:O	1:C:282:LYS:C	2.60	0.45
1:A:62:CYS:HB2	1:A:102:GLU:OE2	2.17	0.45
1:B:111:CYS:HB3	1:C:264:TYR:CG	2.52	0.45
1:E:117:LEU:HD12	1:F:264:TYR:OH	2.17	0.45
1:C:56:LYS:HB2	3:C:1025:HOH:O	2.16	0.44
1:D:74:GLU:OE1	1:D:122:HIS:CE1	2.71	0.44
1:F:46:SER:HA	1:F:81:ALA:O	2.18	0.44
1:D:117:LEU:HD22	1:D:120:TRP:CE2	2.52	0.44
1:E:235:ILE:O	1:E:239:MET:HG3	2.18	0.44
1:A:113:SER:C	3:A:1109:HOH:O	2.44	0.43
1:B:190:GLU:OE2	1:C:211:LYS:HE2	2.18	0.43
1:E:117:LEU:CG	1:F:260:LYS:HD2	2.49	0.43
1:D:118:SER:HB3	1:D:119:HIS:ND1	2.33	0.43
1:D:100:ILE:O	1:D:101:LYS:C	2.61	0.43
1:D:272:ARG:NH2	3:D:347:HOH:O	2.27	0.43
1:D:76:PHE:HD1	1:D:76:PHE:HA	1.76	0.43
1:E:231:ASN:HB3	3:E:1101:HOH:O	2.19	0.43
1:D:287:PHE:C	1:D:288:LYS:HG3	2.43	0.42
1:B:74:GLU:OE1	1:B:122:HIS:HE1	2.02	0.42
1:D:54:ARG:N	1:D:55:PRO:CD	2.81	0.42
1:C:37:ILE:HD13	1:C:37:ILE:HG21	1.72	0.42
1:B:56:LYS:HB2	3:B:1050:HOH:O	2.18	0.42
1:B:42:GLY:HA2	1:B:227:GLU:OE2	2.18	0.42
1:E:79:ASP:OD1	1:E:79:ASP:C	2.63	0.42
1:E:216:GLU:H	1:E:216:GLU:CD	2.28	0.42
1:A:111:CYS:O	1:A:112:TYR:C	2.54	0.42
1:A:210:SER:C	1:A:211:LYS:HG2	2.45	0.42
1:D:97:GLY:N	3:D:400:HOH:O	2.26	0.42
1:D:272:ARG:HH11	1:D:272:ARG:HB3	1.85	0.42
1:D:54:ARG:HH11	1:D:54:ARG:HD3	1.63	0.41
1:C:262:LEU:HD23	1:C:262:LEU:HA	1.90	0.41
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.67	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.93	0.41
1:C:94:PHE:O	1:C:95:ALA:HB2	2.21	0.41
1:D:46:SER:HA	1:D:81:ALA:O	2.21	0.41
1:F:181:ARG:CZ	3:F:1036:HOH:O	2.66	0.41
1:D:123:ILE:HD13	1:D:123:ILE:HG21	1.87	0.41
1:D:279:PHE:CD2	1:D:279:PHE:C	2.99	0.40
1:F:35:TYR:CB	1:F:65:LEU:HB2	2.51	0.40
1:D:117:LEU:HD22	1:D:120:TRP:NE1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:HG21	1:E:36:ILE:HD13	1.83	0.40
1:A:252:LEU:O	1:A:253:THR:C	2.63	0.40
1:D:262:LEU:O	1:D:265:SER:HB2	2.21	0.40
1:A:117:LEU:CD2	1:B:263:PHE:HE2	2.34	0.40
1:A:235:ILE:HG12	1:A:239:MET:HE3	2.03	0.40
1:B:54:ARG:N	1:B:55:PRO:HD3	2.37	0.40
1:A:128:LYS:HA	1:A:129:PRO:HD3	1.92	0.40
1:E:272:ARG:HH11	1:E:272:ARG:HB3	1.86	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:GLY:O	1:E:282:LYS:NZ[4_466]	1.45	0.75
1:B:227:GLU:OE1	1:F:288:LYS:NZ[3_756]	1.79	0.41
1:D:42:GLY:O	1:E:282:LYS:CE[4_466]	1.86	0.34
1:D:45:SER:N	1:E:282:LYS:NZ[4_466]	1.94	0.26
1:B:234:LYS:NZ	1:F:44:ASN:OD1[3_756]	2.19	0.01
1:B:288:LYS:NZ	1:F:227:GLU:OE1[3_756]	2.19	0.01
1:C:44:ASN:OD1	1:C:56:LYS:O[4_576]	2.19	0.01

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	254/260 (98%)	249 (98%)	4 (2%)	1 (0%)	30	28
1	B	254/260 (98%)	247 (97%)	7 (3%)	0	100	100
1	C	254/260 (98%)	246 (97%)	8 (3%)	0	100	100
1	D	254/260 (98%)	244 (96%)	9 (4%)	1 (0%)	30	28
1	E	254/260 (98%)	249 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	254/260 (98%)	250 (98%)	4 (2%)	0	100	100
All	All	1524/1560 (98%)	1485 (97%)	37 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	TYR
1	D	104	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/205 (98%)	189 (94%)	13 (6%)	16	14
1	B	202/205 (98%)	192 (95%)	10 (5%)	22	22
1	C	202/205 (98%)	188 (93%)	14 (7%)	14	12
1	D	202/205 (98%)	190 (94%)	12 (6%)	18	16
1	E	202/205 (98%)	190 (94%)	12 (6%)	18	16
1	F	202/205 (98%)	194 (96%)	8 (4%)	28	29
All	All	1212/1230 (98%)	1143 (94%)	69 (6%)	18	17

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

Mol	Chain	Res	Type
1	A	41	LYS
1	A	43	LYS
1	A	65	LEU
1	A	74	GLU
1	A	111	CYS
1	A	112	TYR
1	A	117	LEU
1	A	156	GLU
1	A	216	GLU

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Mol	Chain	Res	Type
1	A	242	GLU
1	A	265	SER
1	A	272	ARG
1	A	290	HIS
1	B	34	GLN
1	B	54	ARG
1	B	65	LEU
1	B	101	LYS
1	B	113	SER
1	B	216	GLU
1	B	220	GLU
1	B	242	GLU
1	B	272	ARG
1	B	290	HIS
1	C	34	GLN
1	C	51	GLN
1	C	65	LEU
1	C	74	GLU
1	C	106	ARG
1	C	113	SER
1	C	117	LEU
1	C	156	GLU
1	C	209	VAL
1	C	214	PRO
1	C	216	GLU
1	C	242	GLU
1	C	243	SER
1	C	272	ARG
1	D	34	GLN
1	D	65	LEU
1	D	71	GLN
1	D	91	GLU
1	D	100	ILE
1	D	101	LYS
1	D	106	ARG
1	D	156	GLU
1	D	216	GLU
1	D	272	ARG
1	D	286	ASN
1	D	290	HIS
1	E	34	GLN
1	E	65	LEU

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Mol	Chain	Res	Type
1	E	74	GLU
1	E	112	TYR
1	E	113	SER
1	E	117	LEU
1	E	156	GLU
1	E	220	GLU
1	E	242	GLU
1	E	272	ARG
1	E	273	ARG
1	E	290	HIS
1	F	65	LEU
1	F	113	SER
1	F	156	GLU
1	F	216	GLU
1	F	242	GLU
1	F	272	ARG
1	F	273	ARG
1	F	290	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	122	HIS
1	A	286	ASN
1	B	122	HIS
1	B	159	GLN
1	B	162	GLN
1	B	224	GLN
1	C	44	ASN
1	C	122	HIS
1	C	159	GLN
1	D	53	ASN
1	D	122	HIS
1	D	159	GLN
1	E	44	ASN
1	E	53	ASN
1	E	122	HIS
1	E	159	GLN
1	E	290	HIS
1	F	34	GLN
1	F	122	HIS

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Mol	Chain	Res	Type
1	F	159	GLN
1	F	224	GLN

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 ⓘ

5 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	E	954	-	55,57,57	4.08	27 (49%)	77,83,83	3.05	31 (40%)
2	HXC	B	952	-	55,57,57	4.90	24 (43%)	77,83,83	2.71	28 (36%)
2	HXC	C	953	-	55,57,57	4.79	21 (38%)	77,83,83	2.64	27 (35%)
2	HXC	F	955	-	55,57,57	5.64	18 (32%)	77,83,83	2.90	34 (44%)
2	HXC	A	951	-	55,57,57	4.17	26 (47%)	77,83,83	3.34	35 (45%)

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	E	954	-	-	1/56/72/72	0/3/3/3
2	HXC	B	952	-	-	3/56/72/72	0/3/3/3
2	HXC	C	953	-	-	4/56/72/72	0/3/3/3
2	HXC	F	955	-	-	5/56/72/72	0/3/3/3
2	HXC	A	951	-	-	3/56/72/72	0/3/3/3

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	955	HXC	C2'-C3'	25.85	2.09	1.53
2	F	955	HXC	CM2-CM1	-23.98	1.27	1.50
2	B	952	HXC	C2'-C3'	19.93	1.96	1.53
2	A	951	HXC	CM2-CM1	-19.36	1.31	1.50
2	E	954	HXC	CM2-CM1	-18.70	1.32	1.50
2	C	953	HXC	C2'-C3'	18.69	1.93	1.53
2	C	953	HXC	CM2-CM1	-17.42	1.33	1.50
2	B	952	HXC	CM2-CM1	-15.67	1.35	1.50
2	C	953	HXC	OM2-CM1	14.88	1.44	1.21
2	B	952	HXC	OM2-CM1	14.31	1.43	1.21
2	F	955	HXC	OM2-CM1	11.50	1.39	1.21
2	B	952	HXC	OP1-CP3	9.89	1.42	1.23
2	A	951	HXC	OM2-CM1	8.91	1.34	1.21
2	E	954	HXC	OM2-CM1	8.80	1.34	1.21
2	E	954	HXC	OP1-CP3	8.55	1.40	1.23
2	A	951	HXC	C2'-C3'	8.54	1.71	1.53
2	F	955	HXC	OP1-CP3	8.48	1.40	1.23
2	B	952	HXC	O2'-C2'	-8.26	1.22	1.43
2	C	953	HXC	OP1-CP3	8.22	1.39	1.23
2	E	954	HXC	C2'-C3'	8.19	1.70	1.53
2	A	951	HXC	O2'-C2'	-7.96	1.23	1.43
2	A	951	HXC	OP1-CP3	7.60	1.38	1.23
2	E	954	HXC	CP3-NP1	7.19	1.50	1.33
2	C	953	HXC	O2'-C2'	-7.06	1.25	1.43
2	F	955	HXC	CM3-CM2	-6.85	1.27	1.52
2	F	955	HXC	CP3-NP1	6.58	1.49	1.33
2	A	951	HXC	C4-N3	6.39	1.46	1.34
2	E	954	HXC	O2'-C2'	-6.26	1.27	1.43
2	F	955	HXC	O2'-C2'	-6.22	1.27	1.43
2	B	952	HXC	CP3-NP1	6.10	1.47	1.33
2	B	952	HXC	CP2-NP1	-5.83	1.33	1.46
2	A	951	HXC	CM3-CM2	-5.64	1.31	1.52
2	C	953	HXC	CP3-NP1	5.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	953	HXC	C5-C4	5.52	1.48	1.39
2	A	951	HXC	CP3-NP1	5.46	1.46	1.33
2	E	954	HXC	CM3-CM2	-5.36	1.32	1.52
2	B	952	HXC	C4-N3	5.31	1.44	1.34
2	B	952	HXC	CM3-CM2	-5.24	1.33	1.52
2	B	952	HXC	P1-O6	5.06	1.65	1.59
2	F	955	HXC	CP2-NP1	-5.03	1.34	1.46
2	C	953	HXC	C4-N3	5.02	1.43	1.34
2	E	954	HXC	C4-N3	4.90	1.43	1.34
2	E	954	HXC	P1-O6	4.82	1.64	1.59
2	A	951	HXC	C5-C6	4.74	1.54	1.41
2	C	953	HXC	CP2-NP1	-4.56	1.35	1.46
2	F	955	HXC	C5-C4	4.54	1.47	1.39
2	F	955	HXC	C4-N3	4.38	1.42	1.34
2	E	954	HXC	C5-N7	-4.37	1.31	1.39
2	B	952	HXC	C5-C4	4.37	1.46	1.39
2	A	951	HXC	P1-O6	4.33	1.64	1.59
2	A	951	HXC	C5-N7	-4.32	1.31	1.39
2	C	953	HXC	CM3-CM2	-4.27	1.36	1.52
2	E	954	HXC	C5-C6	4.24	1.52	1.41
2	C	953	HXC	C8-N7	3.94	1.39	1.31
2	C	953	HXC	P1-O6	3.89	1.63	1.59
2	F	955	HXC	CP1-CP2	-3.75	1.35	1.51
2	F	955	HXC	CM4-CM3	-3.74	1.33	1.51
2	E	954	HXC	CP1-S	-3.71	1.66	1.81
2	C	953	HXC	CP1-CP2	-3.71	1.36	1.51
2	C	953	HXC	CP1-S	-3.66	1.66	1.81
2	B	952	HXC	CP1-CP2	-3.63	1.36	1.51
2	A	951	HXC	CM4-CM3	-3.62	1.33	1.51
2	F	955	HXC	CP1-S	-3.57	1.66	1.81
2	E	954	HXC	CM4-CM3	-3.55	1.34	1.51
2	B	952	HXC	CM4-CM3	-3.54	1.34	1.51
2	E	954	HXC	C8-N7	3.54	1.38	1.31
2	C	953	HXC	CM4-CM3	-3.48	1.34	1.51
2	F	955	HXC	C8-N7	3.43	1.38	1.31
2	A	951	HXC	P3-O31	-3.41	1.42	1.54
2	C	953	HXC	C5-C6	3.35	1.50	1.41
2	B	952	HXC	C5-N7	-3.27	1.33	1.39
2	B	952	HXC	C8-N7	3.23	1.37	1.31
2	B	952	HXC	CP1-S	-3.16	1.68	1.81
2	A	951	HXC	CP1-S	-3.10	1.68	1.81
2	F	955	HXC	CM5-CM4	-3.08	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	951	HXC	CP4-CP3	3.05	1.57	1.51
2	A	951	HXC	P3-O3'	3.02	1.64	1.59
2	B	952	HXC	P3-O3'	3.00	1.64	1.59
2	E	954	HXC	CP2-NP1	-2.99	1.39	1.46
2	E	954	HXC	OP3-CP7	2.94	1.47	1.42
2	E	954	HXC	C4-N9	-2.93	1.31	1.37
2	A	951	HXC	CM5-CM4	-2.89	1.33	1.51
2	C	953	HXC	C8-N9	2.87	1.42	1.37
2	A	951	HXC	C4-N9	-2.84	1.31	1.37
2	A	951	HXC	CP5-NP2	2.84	1.52	1.46
2	A	951	HXC	CP2-NP1	-2.81	1.39	1.46
2	B	952	HXC	CM5-CM4	-2.76	1.34	1.51
2	E	954	HXC	CM5-CM4	-2.69	1.35	1.51
2	B	952	HXC	C4-N9	-2.68	1.32	1.37
2	C	953	HXC	CM5-CM4	-2.67	1.35	1.51
2	A	951	HXC	P1-O12	-2.67	1.43	1.55
2	E	954	HXC	CP5-NP2	2.66	1.52	1.46
2	B	952	HXC	OP3-CP7	2.66	1.47	1.42
2	E	954	HXC	CP1-CP2	-2.61	1.40	1.51
2	A	951	HXC	CP1-CP2	-2.60	1.40	1.51
2	B	952	HXC	C2-N1	2.53	1.38	1.33
2	F	955	HXC	C5-C6	2.53	1.48	1.41
2	E	954	HXC	CM6-CM5	-2.44	1.32	1.50
2	E	954	HXC	C2-N3	2.42	1.38	1.33
2	E	954	HXC	CP9-CPA	2.40	1.58	1.53
2	E	954	HXC	P2-O6	-2.36	1.57	1.59
2	E	954	HXC	C5-C4	2.33	1.43	1.39
2	A	951	HXC	C2-N3	2.26	1.38	1.33
2	F	955	HXC	CM6-CM5	-2.26	1.34	1.50
2	C	953	HXC	C4-N9	-2.22	1.33	1.37
2	B	952	HXC	CM6-CM5	-2.18	1.34	1.50
2	A	951	HXC	C8-N9	-2.18	1.33	1.37
2	C	953	HXC	C1'-N9	2.16	1.52	1.46
2	E	954	HXC	C8-N9	-2.16	1.33	1.37
2	B	952	HXC	C5-C6	2.15	1.47	1.41
2	C	953	HXC	CM6-CM5	-2.15	1.35	1.50
2	E	954	HXC	P3-O3'	2.13	1.63	1.59
2	A	951	HXC	CM6-CM5	-2.13	1.35	1.50
2	F	955	HXC	P3-O3'	2.08	1.63	1.59
2	B	952	HXC	O4'-C1'	2.07	1.46	1.42
2	A	951	HXC	OP2-CP6	2.01	1.27	1.23

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	951	HXC	C5-C4-N3	-11.40	111.02	126.72
2	F	955	HXC	O3'-C3'-C2'	-10.18	75.15	111.68
2	C	953	HXC	OP1-CP3-CP4	-9.26	105.25	122.02
2	F	955	HXC	OP1-CP3-CP4	-8.88	105.93	122.02
2	B	952	HXC	CP5-CP4-CP3	-8.53	98.18	112.39
2	F	955	HXC	OP1-CP3-NP1	-7.94	107.44	123.03
2	E	954	HXC	CP5-CP4-CP3	-7.76	99.47	112.39
2	E	954	HXC	C5-C4-N3	-7.45	116.46	126.72
2	B	952	HXC	OP1-CP3-CP4	-7.43	108.55	122.02
2	E	954	HXC	C4-C5-N7	-7.41	102.11	110.58
2	B	952	HXC	CM3-CM2-CM1	7.36	128.51	112.27
2	A	951	HXC	CP5-CP4-CP3	-7.27	100.29	112.39
2	E	954	HXC	O3'-C3'-C2'	-7.24	85.71	111.68
2	E	954	HXC	CP1-CP2-NP1	6.98	126.98	112.41
2	C	953	HXC	OP1-CP3-NP1	-6.94	109.41	123.03
2	E	954	HXC	O2'-C2'-C3'	6.81	130.23	111.19
2	F	955	HXC	C5-C4-N3	-6.62	117.61	126.72
2	C	953	HXC	C5-C4-N3	-6.53	117.72	126.72
2	E	954	HXC	OM2-CM1-S	-6.40	114.54	122.68
2	B	952	HXC	OP1-CP3-NP1	-6.05	111.16	123.03
2	A	951	HXC	C5-C4-N9	6.04	112.39	105.81
2	A	951	HXC	O4'-C1'-C2'	6.04	119.53	106.62
2	A	951	HXC	O22-P2-O6	-6.04	90.96	107.27
2	A	951	HXC	CM2-CM1-S	5.75	120.25	113.40
2	A	951	HXC	CP1-CP2-NP1	5.72	124.36	112.41
2	A	951	HXC	C3'-C2'-C1'	-5.70	87.35	99.89
2	A	951	HXC	O2'-C2'-C3'	5.62	126.92	111.19
2	C	953	HXC	CP5-CP4-CP3	-5.57	103.11	112.39
2	E	954	HXC	C5-C4-N9	5.54	111.85	105.81
2	A	951	HXC	N3-C4-N9	5.54	136.59	127.17
2	B	952	HXC	CP1-CP2-NP1	5.45	123.80	112.41
2	C	953	HXC	C5-C4-N9	5.34	111.63	105.81
2	A	951	HXC	C6-C5-C4	5.28	124.39	117.18
2	A	951	HXC	CP8-CPA-CP7	5.27	117.75	108.77
2	E	954	HXC	C5-N7-C8	5.21	111.64	103.45
2	C	953	HXC	C4-C5-N7	-5.18	104.66	110.58
2	A	951	HXC	C2'-C3'-C4'	5.14	112.23	103.24
2	A	951	HXC	OM2-CM1-S	-5.08	116.22	122.68
2	A	951	HXC	C4-N9-C8	-5.03	100.46	105.74
2	C	953	HXC	O3'-C3'-C2'	-4.99	93.78	111.68
2	F	955	HXC	C4-C5-N7	-4.97	104.90	110.58
2	A	951	HXC	O32-P3-O31	4.87	126.04	107.80
2	B	952	HXC	C5-C4-N3	-4.80	120.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	955	HXC	C3'-C2'-C1'	-4.79	89.34	99.89
2	A	951	HXC	C4-C5-N7	-4.69	105.22	110.58
2	F	955	HXC	O2'-C2'-C3'	4.68	124.28	111.19
2	E	954	HXC	CP9-CPA-CP7	4.64	116.67	108.77
2	E	954	HXC	OP1-CP3-NP1	-4.62	113.97	123.03
2	B	952	HXC	O3'-C3'-C2'	-4.59	95.23	111.68
2	A	951	HXC	OP1-CP3-NP1	-4.57	114.06	123.03
2	E	954	HXC	OP1-CP3-CP4	-4.50	113.87	122.02
2	E	954	HXC	CM2-CM1-S	4.41	118.65	113.40
2	E	954	HXC	N9-C8-N7	-4.40	107.69	113.94
2	B	952	HXC	C4-C5-N7	-4.39	105.57	110.58
2	B	952	HXC	OM2-CM1-CM2	4.27	128.91	123.98
2	A	951	HXC	OP1-CP3-CP4	-4.20	114.41	122.02
2	B	952	HXC	CP2-NP1-CP3	-4.17	115.05	122.82
2	C	953	HXC	CP8-CPA-CP9	4.14	117.45	109.20
2	B	952	HXC	C5-C4-N9	4.10	110.28	105.81
2	F	955	HXC	C5-C4-N9	4.07	110.25	105.81
2	A	951	HXC	C2-N3-C4	4.02	121.64	111.83
2	A	951	HXC	O22-P2-O21	3.98	130.95	112.44
2	B	952	HXC	CP5-NP2-CP6	3.94	129.62	122.55
2	C	953	HXC	CP1-CP2-NP1	3.85	120.45	112.41
2	B	952	HXC	CP9-CPA-CP7	3.82	115.28	108.77
2	C	953	HXC	CP8-CPA-CP7	-3.75	102.37	108.77
2	E	954	HXC	C6-C5-N7	3.75	139.32	132.09
2	E	954	HXC	C2-N3-C4	3.75	120.98	111.83
2	C	953	HXC	N1-C2-N3	-3.72	122.95	128.58
2	F	955	HXC	CP5-CP4-CP3	-3.69	106.25	112.39
2	E	954	HXC	CM3-CM2-CM1	3.67	120.36	112.27
2	C	953	HXC	CM2-CM1-S	3.64	117.74	113.40
2	C	953	HXC	CP5-NP2-CP6	3.56	128.95	122.55
2	E	954	HXC	O22-P2-O6	-3.54	97.69	107.27
2	F	955	HXC	N1-C2-N3	-3.53	123.25	128.58
2	B	952	HXC	C2-N1-C6	3.50	124.48	118.73
2	F	955	HXC	CM2-CM1-S	-3.44	109.30	113.40
2	F	955	HXC	C2-N1-C6	3.44	124.38	118.73
2	F	955	HXC	CP1-S-CM1	-3.42	91.73	101.84
2	C	953	HXC	O2'-C2'-C1'	3.40	121.80	110.10
2	F	955	HXC	O4'-C1'-C2'	3.38	113.84	106.62
2	E	954	HXC	CP8-CPA-CP7	3.35	114.49	108.77
2	C	953	HXC	C4'-O4'-C1'	3.34	116.84	109.47
2	E	954	HXC	O2'-C2'-C1'	3.31	121.50	110.10
2	A	951	HXC	CP2-NP1-CP3	-3.28	116.71	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	953	HXC	O2'-C2'-C3'	3.22	120.19	111.19
2	C	953	HXC	C6-C5-N7	3.21	138.28	132.09
2	A	951	HXC	O3'-P3-O33	-3.16	98.06	109.33
2	A	951	HXC	O2'-C2'-C1'	3.10	120.78	110.10
2	F	955	HXC	O7-CPB-CPA	-3.08	105.59	110.55
2	F	955	HXC	O4'-C1'-N9	-3.08	102.18	108.09
2	E	954	HXC	OP2-CP6-NP2	-3.07	116.48	122.98
2	F	955	HXC	C2-N3-C4	3.06	119.31	111.83
2	C	953	HXC	O7-CPB-CPA	-3.06	105.63	110.55
2	F	955	HXC	O32-P3-O33	3.04	122.67	110.83
2	F	955	HXC	O2'-C2'-C1'	3.01	120.45	110.10
2	A	951	HXC	P3-O3'-C3'	-3.00	115.42	123.43
2	E	954	HXC	N1-C2-N3	-3.00	124.05	128.58
2	A	951	HXC	CP9-CPA-CP7	-2.97	103.70	108.77
2	C	953	HXC	CM3-CM2-CM1	2.97	118.83	112.27
2	B	952	HXC	O32-P3-O33	2.92	122.22	110.83
2	B	952	HXC	OM2-CM1-S	-2.92	118.97	122.68
2	B	952	HXC	O5'-C5'-C4'	-2.92	99.05	108.99
2	A	951	HXC	CM3-CM2-CM1	2.91	118.70	112.27
2	B	952	HXC	C4'-O4'-C1'	2.89	115.85	109.47
2	F	955	HXC	C4-N9-C1'	2.89	133.39	126.63
2	A	951	HXC	O6-P2-O21	-2.87	102.08	110.70
2	F	955	HXC	N3-C4-N9	2.86	132.03	127.17
2	F	955	HXC	C1'-N9-C8	-2.76	120.96	127.09
2	F	955	HXC	C5-N7-C8	2.75	107.77	103.45
2	F	955	HXC	N6-C6-N1	2.75	124.49	118.38
2	B	952	HXC	N6-C6-N1	2.74	124.48	118.38
2	C	953	HXC	C2-N3-C4	2.72	118.47	111.83
2	A	951	HXC	O3'-C3'-C2'	-2.71	101.96	111.68
2	F	955	HXC	O4'-C4'-C3'	2.70	110.61	104.92
2	A	951	HXC	O7-CPB-CPA	-2.68	106.23	110.55
2	E	954	HXC	O31-P3-O3'	-2.66	95.47	105.85
2	F	955	HXC	C4'-O4'-C1'	2.65	115.33	109.47
2	E	954	HXC	N3-C4-N9	2.64	131.66	127.17
2	B	952	HXC	N1-C2-N3	-2.63	124.61	128.58
2	A	951	HXC	CP4-CP3-NP1	2.61	121.09	116.34
2	F	955	HXC	CP9-CPA-CP7	2.60	113.20	108.77
2	A	951	HXC	O4'-C1'-N9	2.56	113.00	108.09
2	E	954	HXC	O32-P3-O33	2.54	120.73	110.83
2	B	952	HXC	O4'-C4'-C3'	2.53	110.26	104.92
2	B	952	HXC	O4'-C1'-N9	2.51	112.92	108.09
2	B	952	HXC	O3'-C3'-C4'	-2.50	101.23	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	955	HXC	C2'-C1'-N9	-2.49	107.11	113.30
2	C	953	HXC	OM2-CM1-CM2	-2.49	121.11	123.98
2	E	954	HXC	CP4-CP3-NP1	2.49	120.88	116.34
2	B	952	HXC	O22-P2-O6	2.49	114.00	107.27
2	C	953	HXC	C5-N7-C8	2.48	107.35	103.45
2	E	954	HXC	OM2-CM1-CM2	2.44	126.80	123.98
2	E	954	HXC	O4'-C4'-C3'	2.44	110.07	104.92
2	F	955	HXC	O22-P2-O21	2.43	123.76	112.44
2	C	953	HXC	C3'-C2'-C1'	-2.39	94.62	99.89
2	B	952	HXC	O32-P3-O3'	-2.38	96.56	105.85
2	E	954	HXC	O4'-C1'-C2'	2.36	111.67	106.62
2	C	953	HXC	O32-P3-O33	2.35	119.99	110.83
2	F	955	HXC	CP2-NP1-CP3	-2.35	118.46	122.82
2	C	953	HXC	CP9-CPA-CP7	-2.34	104.78	108.77
2	B	952	HXC	C2'-C3'-C4'	-2.33	99.16	103.24
2	B	952	HXC	C5-N7-C8	2.32	107.10	103.45
2	A	951	HXC	O32-P3-O33	-2.27	102.00	110.83
2	F	955	HXC	CP7-CP6-NP2	2.23	120.72	116.48
2	F	955	HXC	OM2-CM1-S	2.23	125.52	122.68
2	F	955	HXC	OP2-CP6-CP7	-2.21	114.72	120.89
2	A	951	HXC	CP8-CPA-CPB	-2.20	104.59	108.22
2	B	952	HXC	CM4-CM3-CM2	2.18	121.13	113.13
2	E	954	HXC	O3'-P3-O33	-2.10	101.86	109.33
2	E	954	HXC	CP2-NP1-CP3	-2.05	119.00	122.82
2	F	955	HXC	O7-P2-O21	-2.05	100.81	108.94
2	C	953	HXC	N3-C4-N9	2.05	130.65	127.17
2	A	951	HXC	O5'-P1-O11	2.02	116.96	108.94
2	C	953	HXC	CP1-S-CM1	-2.00	95.91	101.84

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	953	HXC	CP8-CPA-CPB-O7
2	F	955	HXC	CPB-O7-P2-O22
2	F	955	HXC	CP7-CPA-CPB-O7
2	F	955	HXC	CP9-CPA-CPB-O7
2	F	955	HXC	CP8-CPA-CPB-O7
2	B	952	HXC	OP1-CP3-NP1-CP2
2	C	953	HXC	OP1-CP3-NP1-CP2
2	F	955	HXC	OP1-CP3-NP1-CP2
2	A	951	HXC	OP1-CP3-NP1-CP2

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Mol	Chain	Res	Type	Atoms
2	E	954	HXC	OP1-CP3-NP1-CP2
2	B	952	HXC	CP9-CPA-CPB-O7
2	C	953	HXC	C3'-O3'-P3-O33
2	C	953	HXC	C3'-O3'-P3-O32
2	B	952	HXC	CP8-CPA-CPB-O7
2	A	951	HXC	C3'-O3'-P3-O33
2	A	951	HXC	CP2-CP1-S-CM1

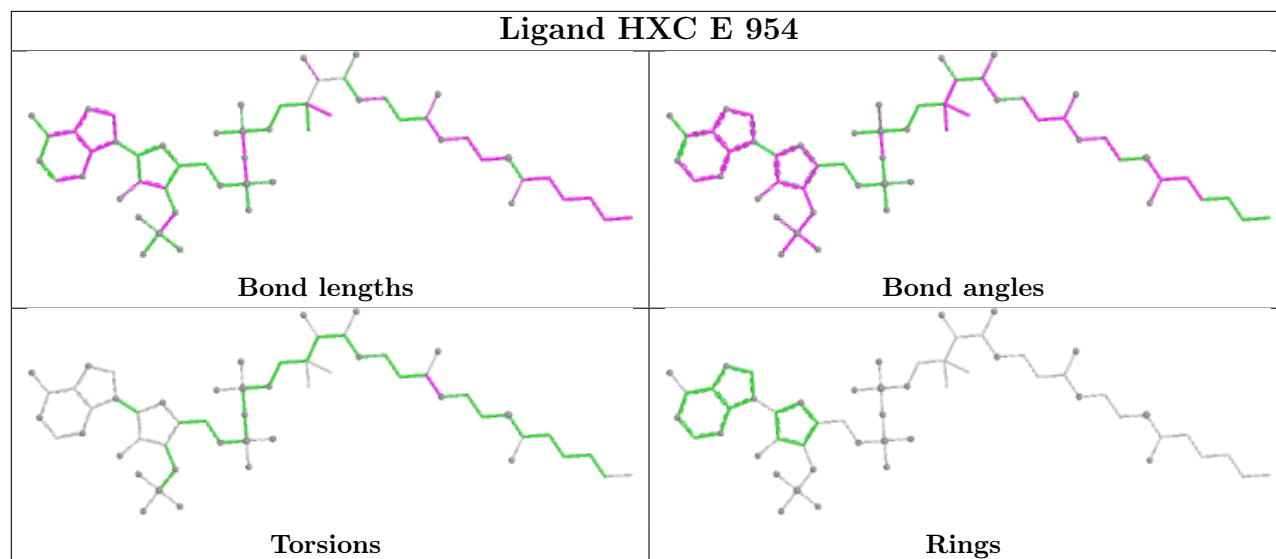
There are no ring outliers.

5 monomers are involved in 23 short contacts:

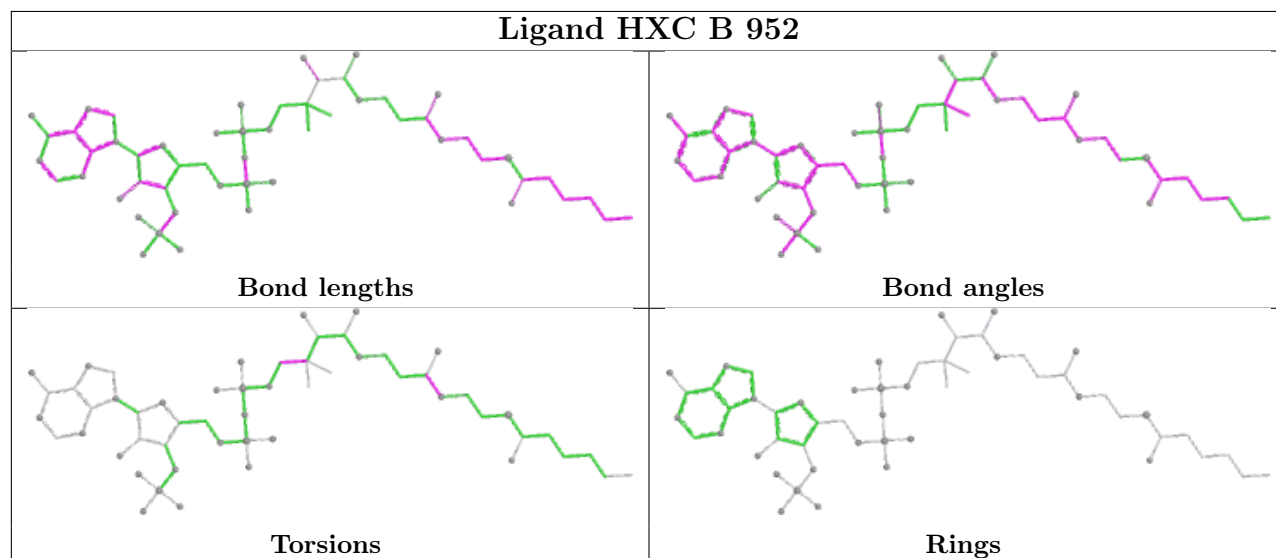
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	954	HXC	2	0
2	B	952	HXC	6	0
2	C	953	HXC	3	0
2	F	955	HXC	8	0
2	A	951	HXC	4	0

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.

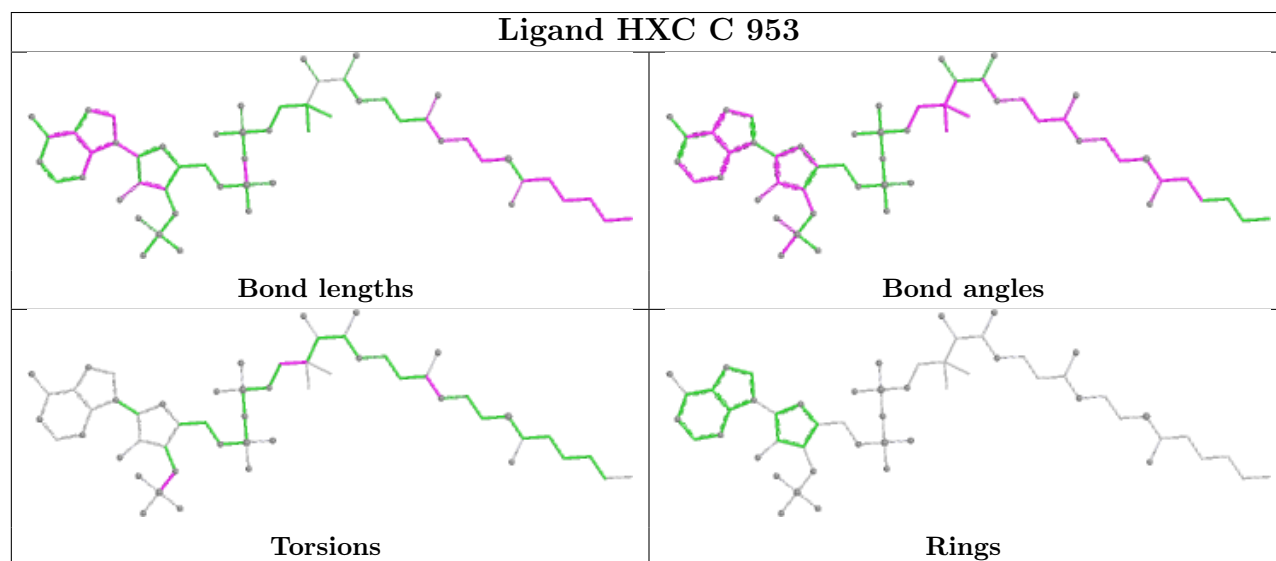
Ligand HXC E 954

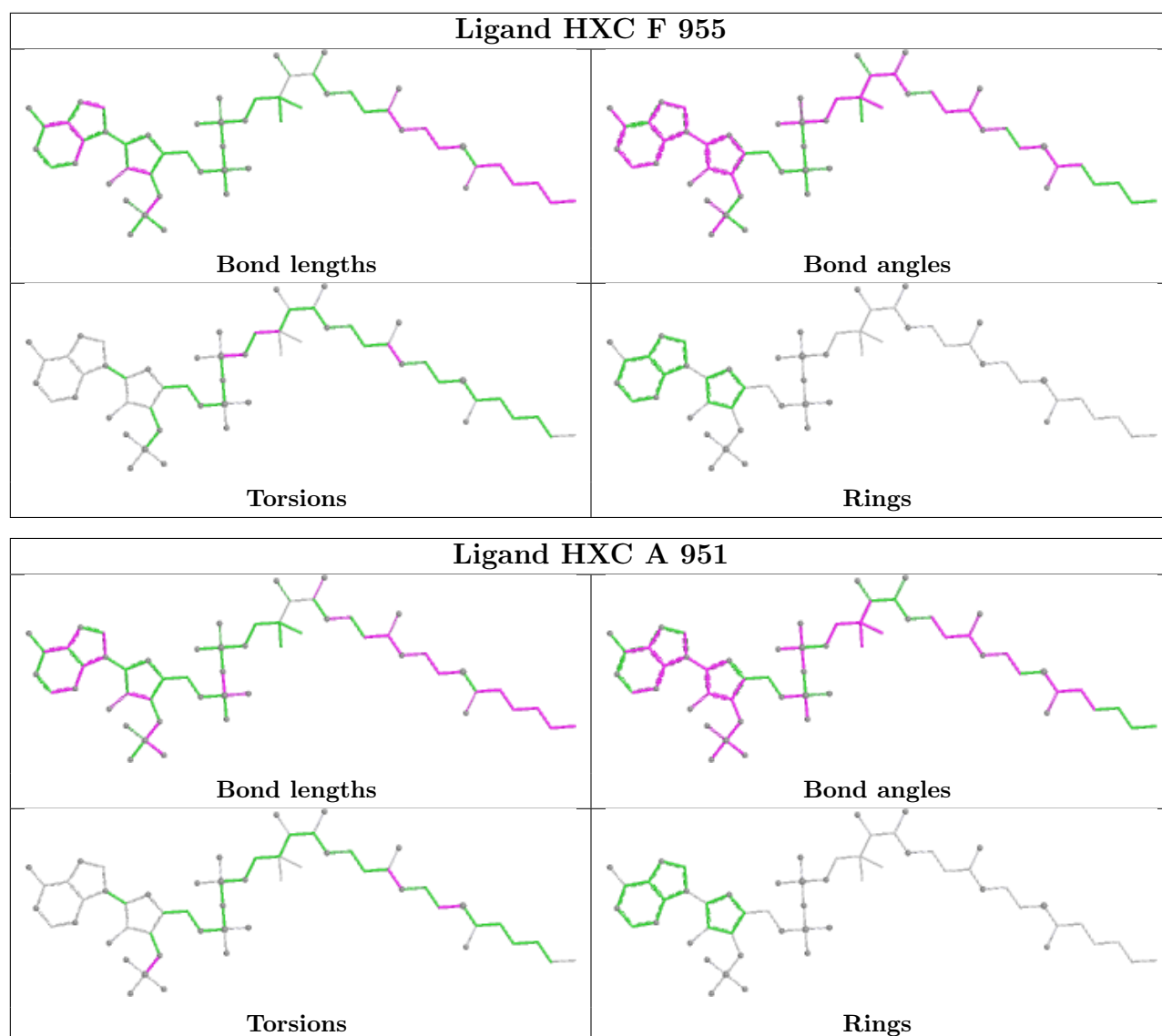


Ligand HXC B 952



Ligand HXC C 953





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.