Full wwPDB X-ray Structure Validation Report (i)

Jun 4, 2020 – 11:41 pm BST

PDB ID	:	1MJ3
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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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.
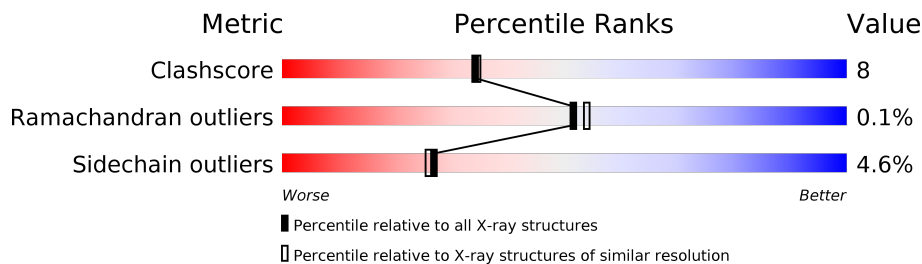
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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%

Note EDS was not executed.

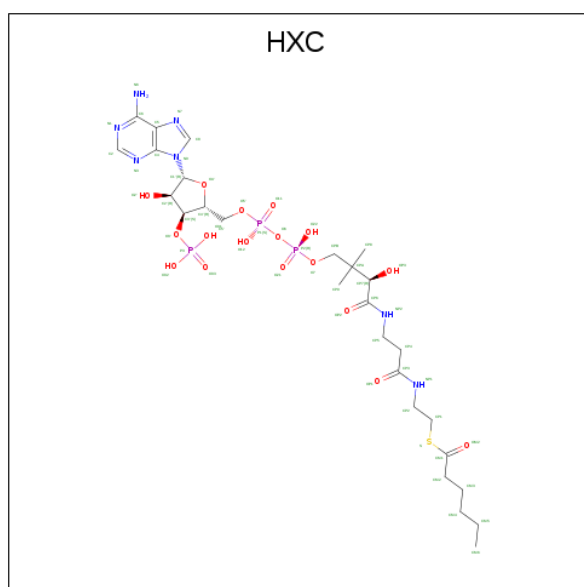| Mol	Chain	Length	Quality of chain
1	A	260	82% 13% • • •
1	B	260	79% 17% • • •
1	C	260	74% 23% • •
1	D	260	74% 20% • • •
1	E	260	85% 11% • • •
1	F	260	85% 13% • • •

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 (three-letter code: HXC) (formula: $C_{27}H_{46}N_7O_{17}P_3S$).

HXC

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

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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
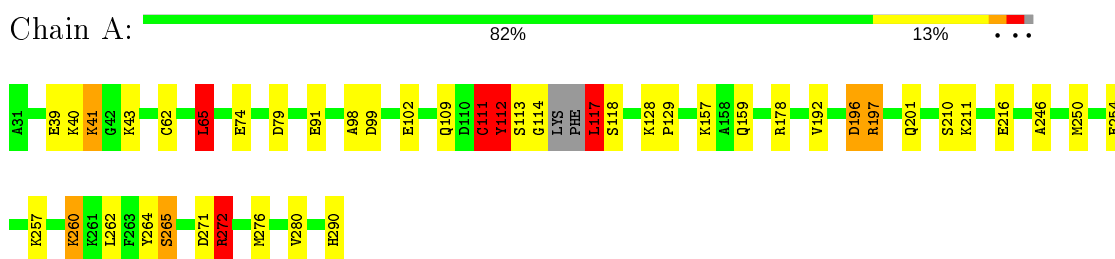
- Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

- Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

- Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

E144 D150 R181 A182 V183 G184 K185 R197 Q201 C225 K234 M239 A240 K241 E242 F248 E249 M250 K261 L262 F263 Y264 S265 D270 D271 R272 V280 E281 K282 R283 K284 A285 N286 F287 K288 D289 H290

● Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain E: ██ 85%   ██ 11% · ··

A31 I36 K41 R54 P55 L65 E74 A95 A98 R106 Y112 S113 G114 LYS PHE L117 S118 H119 H122 D150 E156 K157 A158 Q159 A182 V183 D196 R197 Q201 K211 N231 K234 I235 I236 V237 A238 M239 A247 M250

Y264 R272 R273 F279 K282 D289 H290

● Molecule 1: ENOYL-COA HYDRATASE, MITOCHONDRIAL

Chain F: ██ 85%   ██ 13% ···

A31 Y35 N44 S45 S46 V47 L65 E74 A81 C111 Y112 S113 G114 LYS PHE L117 S118 H119 P129 C149 D150 R181 R197 Q201 D202 E227 K228 I229 K234 K241 E242 M250 K257 L258 E259 K260 F263 Y264 S265 D271 R272

M276 R283 K288 D289 H290
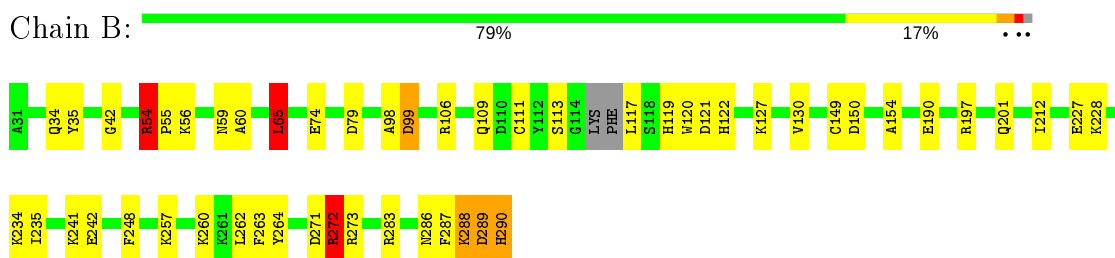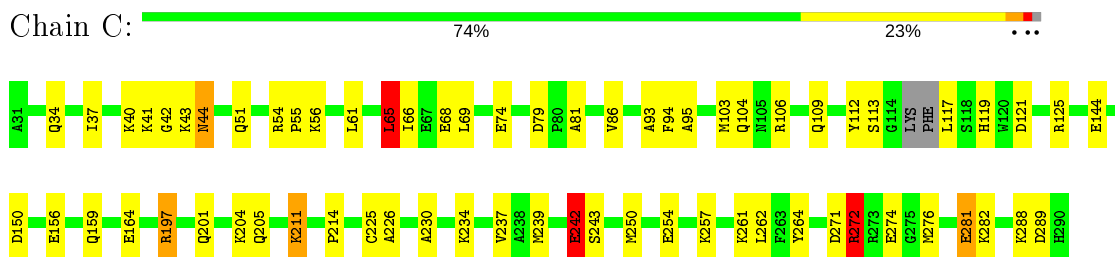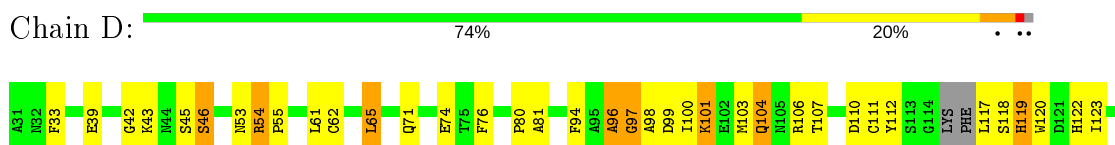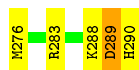
4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.44	13/1980 (0.7%)	1.36	13/2659 (0.5%)
1	B	1.52	11/1980 (0.6%)	1.46	17/2659 (0.6%)
1	C	1.49	19/1980 (1.0%)	1.34	16/2659 (0.6%)
1	D	1.54	18/1980 (0.9%)	1.55	25/2659 (0.9%)
1	E	1.47	10/1980 (0.5%)	1.55	18/2659 (0.7%)
1	F	1.43	13/1980 (0.7%)	1.35	16/2659 (0.6%)
All	All	1.48	84/11880 (0.7%)	1.44	105/15954 (0.7%)

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 (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	272	ARG	CZ-NH1	14.93	1.52	1.33
1	B	272	ARG	CZ-NH1	14.91	1.52	1.33
1	B	287	PHE	CE1-CZ	12.61	1.61	1.37
1	A	111	CYS	CB-SG	-10.55	1.64	1.82
1	D	272	ARG	CZ-NH1	9.85	1.45	1.33
1	F	272	ARG	CZ-NH1	8.43	1.44	1.33
1	A	264	TYR	CD2-CE2	7.65	1.50	1.39
1	C	272	ARG	CZ-NH1	7.61	1.43	1.33
1	E	237	VAL	CB-CG2	7.51	1.68	1.52
1	D	272	ARG	NE-CZ	7.21	1.42	1.33
1	A	272	ARG	CZ-NH1	7.17	1.42	1.33
1	B	288	LYS	CE-NZ	6.91	1.66	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	CYS	CB-SG	6.86	1.94	1.82
1	A	254	GLU	CD-OE1	6.55	1.32	1.25
1	A	264	TYR	CD1-CE1	6.53	1.49	1.39
1	A	280	VAL	CB-CG1	6.45	1.66	1.52
1	C	226	ALA	CA-CB	-6.39	1.39	1.52
1	C	250	MET	CB-CG	-6.31	1.31	1.51
1	C	237	VAL	CB-CG1	6.24	1.66	1.52
1	D	46	SER	CA-CB	-6.21	1.43	1.52
1	E	95	ALA	CA-CB	-6.19	1.39	1.52
1	F	241	LYS	CD-CE	6.15	1.66	1.51
1	A	250	MET	SD-CE	-6.11	1.43	1.77
1	C	68	GLU	CD-OE2	6.02	1.32	1.25
1	C	254	GLU	CD-OE2	6.01	1.32	1.25
1	F	257	LYS	CB-CG	5.97	1.68	1.52
1	B	257	LYS	CB-CG	5.95	1.68	1.52
1	A	246	ALA	CA-CB	5.88	1.64	1.52
1	E	211	LYS	CD-CE	5.88	1.66	1.51
1	E	182	ALA	CA-CB	5.87	1.64	1.52
1	F	259	GLU	CD-OE2	5.87	1.32	1.25
1	D	112	TYR	CB-CG	-5.85	1.42	1.51
1	B	119	HIS	CG-ND1	5.84	1.51	1.38
1	D	101	LYS	CB-CG	5.77	1.68	1.52
1	C	119	HIS	CG-ND1	5.74	1.51	1.38
1	B	241	LYS	CE-NZ	5.72	1.63	1.49
1	C	81	ALA	CA-CB	5.72	1.64	1.52
1	D	97	GLY	CA-C	-5.72	1.42	1.51
1	F	112	TYR	CE2-CZ	5.71	1.46	1.38
1	E	273	ARG	CG-CD	5.68	1.66	1.51
1	D	183	VAL	CB-CG1	5.67	1.64	1.52
1	B	149	CYS	CB-SG	5.64	1.91	1.82
1	D	248	PHE	CE2-CZ	5.63	1.48	1.37
1	C	164	GLU	C-O	5.62	1.34	1.23
1	C	93	ALA	CA-CB	-5.59	1.40	1.52
1	C	230	ALA	CA-CB	-5.56	1.40	1.52
1	D	181	ARG	CZ-NH1	5.54	1.40	1.33
1	D	33	PHE	CE1-CZ	5.53	1.47	1.37
1	D	54	ARG	CB-CG	-5.52	1.37	1.52
1	C	197	ARG	CG-CD	5.52	1.65	1.51
1	A	192	VAL	CB-CG2	5.43	1.64	1.52
1	A	264	TYR	CG-CD2	5.42	1.46	1.39
1	C	281	GLU	CD-OE1	5.41	1.31	1.25
1	F	47	VAL	CB-CG2	5.40	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	149	CYS	CB-SG	5.32	1.91	1.82
1	C	239	MET	SD-CE	-5.31	1.48	1.77
1	B	130	VAL	CB-CG2	5.31	1.64	1.52
1	D	94	PHE	CE1-CZ	5.31	1.47	1.37
1	D	119	HIS	CG-ND1	5.30	1.50	1.38
1	D	239	MET	CG-SD	5.29	1.95	1.81
1	F	257	LYS	CE-NZ	5.28	1.62	1.49
1	F	74	GLU	CG-CD	5.27	1.59	1.51
1	E	239	MET	SD-CE	-5.25	1.48	1.77
1	D	185	LYS	CE-NZ	5.22	1.62	1.49
1	D	240	ALA	CA-CB	-5.22	1.41	1.52
1	F	234	LYS	CG-CD	5.21	1.70	1.52
1	B	248	PHE	CE1-CZ	5.20	1.47	1.37
1	D	144	GLU	CB-CG	5.19	1.62	1.52
1	A	257	LYS	CG-CD	5.18	1.70	1.52
1	D	234	LYS	CB-CG	5.17	1.66	1.52
1	E	119	HIS	CG-ND1	5.16	1.50	1.38
1	C	86	VAL	CB-CG1	5.14	1.63	1.52
1	B	288	LYS	CD-CE	5.14	1.64	1.51
1	F	111	CYS	CB-SG	-5.09	1.73	1.81
1	B	273	ARG	CG-CD	5.08	1.64	1.51
1	C	274	GLU	CG-CD	5.08	1.59	1.51
1	F	263	PHE	CD2-CE2	5.05	1.49	1.39
1	E	183	VAL	CB-CG2	5.04	1.63	1.52
1	C	242	GLU	C-O	-5.03	1.13	1.23
1	A	257	LYS	CE-NZ	5.03	1.61	1.49
1	F	276	MET	CG-SD	5.03	1.94	1.81
1	C	144	GLU	CD-OE2	5.01	1.31	1.25
1	A	250	MET	CG-SD	-5.01	1.68	1.81
1	E	158	ALA	CA-CB	5.00	1.62	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	272	ARG	NE-CZ-NH2	-35.46	102.57	120.30
1	B	272	ARG	NE-CZ-NH2	-30.85	104.88	120.30
1	E	272	ARG	NE-CZ-NH1	25.62	133.11	120.30
1	D	272	ARG	NE-CZ-NH1	24.99	132.79	120.30
1	B	272	ARG	NE-CZ-NH1	24.95	132.77	120.30
1	D	272	ARG	NE-CZ-NH2	-23.82	108.39	120.30
1	A	272	ARG	NE-CZ-NH1	20.01	130.31	120.30
1	A	272	ARG	NE-CZ-NH2	-19.00	110.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	272	ARG	NE-CZ-NH2	-18.05	111.27	120.30
1	A	197	ARG	NE-CZ-NH2	-17.00	111.80	120.30
1	E	197	ARG	NE-CZ-NH2	-16.16	112.22	120.30
1	C	272	ARG	NE-CZ-NH2	-15.71	112.44	120.30
1	F	272	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	F	197	ARG	NE-CZ-NH2	-13.56	113.52	120.30
1	C	272	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	D	272	ARG	CD-NE-CZ	11.15	139.21	123.60
1	E	272	ARG	CD-NE-CZ	10.16	137.82	123.60
1	C	271	ASP	CB-CG-OD2	10.00	127.30	118.30
1	E	197	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	F	272	ARG	CG-CD-NE	9.76	132.30	111.80
1	D	270	ASP	CB-CG-OD2	9.56	126.90	118.30
1	A	197	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	197	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	E	196	ASP	CB-CG-OD1	9.07	126.46	118.30
1	D	54	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	B	197	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	F	272	ARG	CD-NE-CZ	8.62	135.67	123.60
1	E	272	ARG	CG-CD-NE	8.50	129.66	111.80
1	D	250	MET	CG-SD-CE	-8.46	86.67	100.20
1	D	272	ARG	CG-CD-NE	8.43	129.50	111.80
1	A	272	ARG	CG-CD-NE	8.29	129.22	111.80
1	C	250	MET	CG-SD-CE	-8.26	86.99	100.20
1	B	271	ASP	CB-CG-OD2	8.24	125.72	118.30
1	B	272	ARG	CD-NE-CZ	8.24	135.13	123.60
1	D	197	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	C	272	ARG	CG-CD-NE	8.16	128.94	111.80
1	A	271	ASP	CB-CG-OD2	7.95	125.45	118.30
1	F	150	ASP	CB-CG-OD2	7.76	125.28	118.30
1	E	289	ASP	CB-CG-OD2	7.72	125.25	118.30
1	D	283	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	F	271	ASP	CB-CG-OD2	7.42	124.98	118.30
1	F	65	LEU	CA-CB-CG	7.32	132.12	115.30
1	A	196	ASP	CB-CG-OD1	7.28	124.85	118.30
1	D	96	ALA	C-N-CA	-7.26	107.06	122.30
1	E	290	HIS	CA-C-O	-7.24	104.89	120.10
1	D	150	ASP	CB-CG-OD2	7.18	124.77	118.30
1	D	65	LEU	CA-CB-CG	7.13	131.70	115.30
1	C	150	ASP	CB-CG-OD2	7.07	124.66	118.30
1	C	272	ARG	CD-NE-CZ	7.06	133.48	123.60
1	A	272	ARG	CD-NE-CZ	6.80	133.12	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	289	ASP	CB-CG-OD2	6.72	124.35	118.30
1	D	98	ALA	N-CA-C	-6.52	93.39	111.00
1	A	99	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	96	ALA	O-C-N	-6.45	112.24	123.20
1	B	283	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	F	111	CYS	CA-CB-SG	-6.37	102.53	114.00
1	E	150	ASP	CB-CG-OD2	6.36	124.03	118.30
1	F	250	MET	CB-CA-C	-6.26	97.87	110.40
1	B	272	ARG	CG-CD-NE	6.13	124.67	111.80
1	B	54	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	287	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	C	197	ARG	CG-CD-NE	-5.99	99.23	111.80
1	B	150	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	181	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	54	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	99	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	97	GLY	N-CA-C	-5.89	98.38	113.10
1	F	197	ARG	CG-CD-NE	-5.84	99.54	111.80
1	E	65	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	65	LEU	CB-CG-CD1	5.78	120.82	111.00
1	F	202	ASP	CB-CG-OD2	5.76	123.48	118.30
1	E	250	MET	CB-CA-C	-5.75	98.90	110.40
1	C	65	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	289	ASP	CB-CG-OD2	5.70	123.43	118.30
1	E	112	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	B	99	ASP	CB-CG-OD2	5.63	123.37	118.30
1	D	283	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	E	112	TYR	CB-CA-C	5.59	121.58	110.40
1	B	235	ILE	CG1-CB-CG2	-5.58	99.12	111.40
1	A	112	TYR	CA-CB-CG	-5.58	102.80	113.40
1	C	121	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	119	HIS	ND1-CG-CD2	-5.56	98.21	106.00
1	D	54	ARG	CB-CA-C	5.54	121.48	110.40
1	C	250	MET	CB-CA-C	-5.49	99.43	110.40
1	B	283	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	117	LEU	CB-CA-C	-5.46	99.83	110.20
1	F	119	HIS	ND1-CG-CD2	-5.41	98.43	106.00
1	D	96	ALA	CA-C-N	5.41	127.01	116.20
1	A	65	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	286	ASN	CB-CA-C	-5.35	99.71	110.40
1	F	283	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	119	HIS	ND1-CG-CD2	-5.27	98.62	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	MET	CG-SD-CE	-5.20	91.88	100.20
1	D	119	HIS	ND1-CG-CD2	-5.19	98.73	106.00
1	E	54	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	69	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	E	197	ARG	CG-CD-NE	-5.08	101.14	111.80
1	B	65	LEU	CB-CA-C	5.07	119.83	110.20
1	B	79	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	288	LYS	CD-CE-NZ	5.05	123.33	111.70
1	D	289	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	178	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	44	ASN	CB-CA-C	-5.04	100.33	110.40
1	C	211	LYS	CB-CA-C	-5.03	100.33	110.40
1	F	265	SER	CA-CB-OG	-5.03	97.61	111.20

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 (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	1955	0	1975	43	0
1	B	1955	0	1975	42	3
1	C	1955	0	1975	32	1
1	D	1955	0	1975	44	3
1	E	1955	0	1975	37	3
1	F	1955	0	1975	31	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	7	0
3	A	162	0	0	16	0
3	B	167	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	126	0	0	8	0
3	D	145	0	0	20	0
3	E	153	0	0	3	0
3	F	166	0	0	6	0
All	All	12924	0	12051	202	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 8.

All (202) 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:C3'	2:C:953:HXC:C2'	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
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:D:96:ALA:C	3:D:400:HOH:O	1.81	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:D:61:LEU:C	3:D:386:HOH:O	1.85	1.03
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:HD13	1:E:117:LEU:O	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:O3'	2:F:955:HXC:C2'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:96:ALA:CA	3:D:400:HOH:O	2.27	0.73
1:E:201:GLN:HG3	3:E:984:HOH:O	1.89	0.72
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:A:62:CYS:SG	3:A:1091:HOH:O	2.46	0.65
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:D:289:ASP:O	1:D:290:HIS:HB3	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:LYS:NZ	3:C:1031:HOH:O	2.33	0.62
2:C:953:HXC:O3'	2:C:953:HXC:C2'	2.49	0.61
1:A:117:LEU:HD11	1:B:264:TYR:CE1	2.36	0.61
1:E:65:LEU:C	1:E:65:LEU:HD12	2.21	0.61
1:E:117:LEU:HD11	1:F:260:LYS:HZ2	1.64	0.60
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:B:65:LEU:C	1:B:65:LEU:HD12	2.22	0.59
2:F:955:HXC:O3'	2:F:955:HXC:C1'	2.51	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
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: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:D:225:CYS:HB2	3:D:350:HOH:O	2.05	0.56
1:E:117:LEU:CD1	1:E:117:LEU:O	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: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
2:B:952:HXC:C2'	2:B:952:HXC:O3'	2.56	0.53
1:D:107:THR:OG1	1:D:110:ASP:CG	2.46	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:A:260:LYS:NZ	3:A:1061:HOH:O	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:129:PRO:HG2	1:F:229:ILE:HG21	1.93	0.50
1:E:117:LEU:CD1	1:F:260:LYS:HZ2	2.25	0.50
1:D:53:ASN:C	1:D:55:PRO:HD3	2.33	0.50
1:A:118:SER:N	3:A:1107:HOH:O	2.45	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:A:112:TYR:CE2	3:A:1033:HOH:O	2.49	0.49
1:C:205:GLN:HG2	3:C:1052:HOH:O	2.12	0.49
1:C:109:GLN:HG2	1:D:290:HIS:HB2	1.94	0.49
1:C:103:MET:O	1:C:104:GLN:C	2.50	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:A:65:LEU:C	1:A:65:LEU:HD12	2.34	0.48
2:F:955:HXC:OP2	2:F:955:HXC:HP91	2.12	0.48
1:D:264:TYR:CG	1:F:111:CYS:HB3	2.48	0.48
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:E:65:LEU:C	1:E:65:LEU:CD1	2.82	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:NH1	1:C:272:ARG:HB3	2.30	0.46
1:A:117:LEU:HD11	1:B:263:PHE:CE2	2.51	0.46
1:B:65:LEU:C	1:B:65:LEU:CD1	2.84	0.46
3:D:402:HOH:O	1:E:247:ALA:HA	2.15	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:E:159:GLN:NE2	1:E:197:ARG:HD2	2.31	0.46
1:D:103:MET:O	1:D:104:GLN:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:43:LYS:HD3	3:D:417:HOH:O	2.17	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: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: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:B:74:GLU:OE1	1:B:122:HIS:HE1	2.02	0.42
1:C:65:LEU:CD1	1:C:65:LEU:C	2.88	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:D:97:GLY:N	3:D:400:HOH:O	2.26	0.42
1:D:272:ARG:HB3	1:D:272:ARG:HH11	1.85	0.42
1:D:54:ARG:HH11	1:D:54:ARG:HD3	1.63	0.41
1:B:59:ASN:O	1:B:60:ALA:C	2.57	0.41
1:C:262:LEU:HA	1:C:262:LEU:HD23	1.90	0.41
1:D:280:VAL:C	1:D:282:LYS:H	2.24	0.41
1:B:117:LEU:HA	1:B:117:LEU:HD23	1.67	0.41
1:D:46:SER:HA	1:D:81:ALA:O	2.21	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:F:181:ARG:CZ	3:F:1036:HOH:O	2.66	0.41
1:D:123:ILE:HG21	1:D:123:ILE:HD13	1.87	0.41
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
1:E:36:ILE:HG21	1:E:36:ILE:HD13	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:C	1:C:41:LYS:HG2	2.41	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:B:54:ARG:N	1:B:55:PRO:HD3	2.37	0.40
1:C:42:GLY:O	1:C:43:LYS:C	2.59	0.40
1:A:113:SER:C	3:A:1109:HOH:O	2.44	0.40
1:A:128:LYS:HA	1:A:129:PRO:HD3	1.92	0.40
1:C:281:GLU:O	1:C:282:LYS:C	2.60	0.40
1:E:272:ARG:HB3	1:E:272:ARG:HH11	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:C:44:ASN:OD1	1:C:56:LYS:O[4_576]	2.19	0.01
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

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	254/260 (98%)	249 (98%)	4 (2%)	1 (0%)	34	32
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%)	34	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	254/260 (98%)	249 (98%)	5 (2%)	0	100	100
1	F	254/260 (98%)	250 (98%)	4 (2%)	0	100	100
All	All	1524/1560 (98%)	1485 (97%)	37 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

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

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	202/205 (98%)	189 (94%)	13 (6%)	17	14
1	B	202/205 (98%)	194 (96%)	8 (4%)	31	32
1	C	202/205 (98%)	190 (94%)	12 (6%)	19	17
1	D	202/205 (98%)	193 (96%)	9 (4%)	27	27
1	E	202/205 (98%)	192 (95%)	10 (5%)	24	23
1	F	202/205 (98%)	198 (98%)	4 (2%)	55	60
All	All	1212/1230 (98%)	1156 (95%)	56 (5%)	27	26

All (56) 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	157	LYS

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Mol	Chain	Res	Type
1	A	216	GLU
1	A	260	LYS
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	106	ARG
1	B	113	SER
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	112	TYR
1	C	113	SER
1	C	156	GLU
1	C	214	PRO
1	C	242	GLU
1	C	243	SER
1	C	272	ARG
1	D	65	LEU
1	D	71	GLN
1	D	101	LYS
1	D	106	ARG
1	D	242	GLU
1	D	272	ARG
1	D	284	LYS
1	D	286	ASN
1	D	290	HIS
1	E	41	LYS
1	E	65	LEU
1	E	74	GLU
1	E	106	ARG
1	E	112	TYR
1	E	113	SER
1	E	156	GLU
1	E	272	ARG

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Mol	Chain	Res	Type
1	E	273	ARG
1	E	290	HIS
1	F	65	LEU
1	F	113	SER
1	F	242	GLU
1	F	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	B	122	HIS
1	B	159	GLN
1	B	162	GLN
1	B	290	HIS
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	290	HIS
1	F	122	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	F	955	-	49,57,57	5.82	18 (36%)	60,83,83	3.04	27 (45%)
2	HXC	C	953	-	49,57,57	4.87	17 (34%)	60,83,83	2.61	19 (31%)
2	HXC	E	954	-	49,57,57	4.10	22 (44%)	60,83,83	2.95	23 (38%)
2	HXC	A	951	-	49,57,57	4.29	22 (44%)	60,83,83	3.04	27 (45%)
2	HXC	B	952	-	49,57,57	5.00	18 (36%)	60,83,83	2.87	25 (41%)

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	F	955	-	-	6/52/72/72	0/3/3/3
2	HXC	C	953	-	-	3/52/72/72	0/3/3/3
2	HXC	E	954	-	-	1/52/72/72	0/3/3/3
2	HXC	A	951	-	-	2/52/72/72	0/3/3/3
2	HXC	B	952	-	-	3/52/72/72	0/3/3/3

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	955	HXC	C2'-C3'	25.37	2.09	1.52
2	F	955	HXC	CM2-CM1	-23.32	1.27	1.50
2	B	952	HXC	C2'-C3'	19.56	1.96	1.52
2	A	951	HXC	CM2-CM1	-18.82	1.31	1.50
2	C	953	HXC	C2'-C3'	18.34	1.93	1.52
2	E	954	HXC	CM2-CM1	-18.17	1.32	1.50
2	C	953	HXC	CM2-CM1	-16.93	1.33	1.50
2	B	952	HXC	CM2-CM1	-15.22	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	953	HXC	OM2-CM1	14.26	1.44	1.21
2	B	952	HXC	OM2-CM1	13.72	1.43	1.21
2	F	955	HXC	OM2-CM1	11.03	1.39	1.21
2	B	952	HXC	OP1-CP3	9.64	1.42	1.23
2	B	952	HXC	O2'-C2'	-8.69	1.22	1.43
2	A	951	HXC	OM2-CM1	8.55	1.34	1.21
2	E	954	HXC	OM2-CM1	8.44	1.34	1.21
2	A	951	HXC	C2'-C3'	8.39	1.71	1.52
2	A	951	HXC	O2'-C2'	-8.37	1.23	1.43
2	E	954	HXC	OP1-CP3	8.33	1.40	1.23
2	F	955	HXC	OP1-CP3	8.26	1.40	1.23
2	E	954	HXC	C2'-C3'	8.05	1.70	1.52
2	C	953	HXC	OP1-CP3	8.02	1.39	1.23
2	A	951	HXC	C4-N3	7.77	1.46	1.35
2	E	954	HXC	CP3-NP1	7.50	1.50	1.33
2	C	953	HXC	O2'-C2'	-7.44	1.25	1.43
2	A	951	HXC	OP1-CP3	7.41	1.38	1.23
2	F	955	HXC	CP3-NP1	6.87	1.49	1.33
2	F	955	HXC	CM3-CM2	-6.82	1.27	1.52
2	E	954	HXC	O2'-C2'	-6.60	1.27	1.43
2	F	955	HXC	O2'-C2'	-6.54	1.27	1.43
2	B	952	HXC	CP3-NP1	6.36	1.47	1.33
2	B	952	HXC	C4-N3	6.30	1.44	1.35
2	C	953	HXC	C4-N3	5.91	1.43	1.35
2	C	953	HXC	CP3-NP1	5.76	1.46	1.33
2	E	954	HXC	C4-N3	5.75	1.43	1.35
2	B	952	HXC	CP2-NP1	-5.73	1.33	1.46
2	A	951	HXC	CP3-NP1	5.70	1.46	1.33
2	A	951	HXC	CM3-CM2	-5.61	1.31	1.52
2	E	954	HXC	CM3-CM2	-5.33	1.32	1.52
2	B	952	HXC	CM3-CM2	-5.21	1.33	1.52
2	F	955	HXC	C4-N3	5.05	1.42	1.35
2	F	955	HXC	CP2-NP1	-4.94	1.34	1.46
2	C	953	HXC	CP2-NP1	-4.48	1.35	1.46
2	C	953	HXC	CM3-CM2	-4.25	1.36	1.52
2	B	952	HXC	O4'-C1'	4.08	1.46	1.41
2	E	954	HXC	C2-N3	3.81	1.38	1.32
2	E	954	HXC	CP1-S	-3.79	1.66	1.81
2	A	951	HXC	O4'-C1'	3.74	1.46	1.41
2	C	953	HXC	CP1-S	-3.73	1.66	1.81
2	F	955	HXC	CP1-CP2	-3.66	1.35	1.51
2	F	955	HXC	CP1-S	-3.65	1.66	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	951	HXC	C2-N3	3.64	1.38	1.32
2	C	953	HXC	CP1-CP2	-3.62	1.36	1.51
2	B	952	HXC	CP1-CP2	-3.55	1.36	1.51
2	A	951	HXC	P3-O31	-3.30	1.42	1.54
2	F	955	HXC	CM4-CM3	-3.28	1.33	1.51
2	B	952	HXC	CP1-S	-3.23	1.68	1.81
2	A	951	HXC	CP4-CP3	3.21	1.57	1.51
2	A	951	HXC	CM4-CM3	-3.17	1.33	1.51
2	A	951	HXC	CP1-S	-3.16	1.68	1.81
2	E	954	HXC	CM4-CM3	-3.11	1.34	1.51
2	C	953	HXC	C2-N3	3.11	1.37	1.32
2	B	952	HXC	CM4-CM3	-3.10	1.34	1.51
2	C	953	HXC	CM4-CM3	-3.05	1.34	1.51
2	C	953	HXC	C5-C4	3.03	1.48	1.40
2	C	953	HXC	O4'-C1'	2.99	1.45	1.41
2	E	954	HXC	CP2-NP1	-2.93	1.39	1.46
2	A	951	HXC	C6-C5	2.93	1.54	1.43
2	A	951	HXC	P3-O3'	2.92	1.64	1.59
2	B	952	HXC	P3-O3'	2.90	1.64	1.59
2	E	954	HXC	OP3-CP7	2.84	1.47	1.42
2	A	951	HXC	CP5-NP2	2.80	1.52	1.46
2	A	951	HXC	CP2-NP1	-2.76	1.39	1.46
2	F	955	HXC	O4'-C1'	2.75	1.44	1.41
2	F	955	HXC	CM5-CM4	-2.68	1.32	1.51
2	A	951	HXC	P1-O12	-2.63	1.43	1.55
2	E	954	HXC	CP5-NP2	2.62	1.52	1.46
2	B	952	HXC	OP3-CP7	2.56	1.47	1.42
2	E	954	HXC	C6-C5	2.56	1.52	1.43
2	C	953	HXC	C8-N7	2.55	1.39	1.34
2	E	954	HXC	CP1-CP2	-2.55	1.40	1.51
2	A	951	HXC	CP1-CP2	-2.54	1.40	1.51
2	A	951	HXC	CM5-CM4	-2.51	1.33	1.51
2	B	952	HXC	C2-N1	2.43	1.38	1.33
2	B	952	HXC	CM5-CM4	-2.41	1.34	1.51
2	E	954	HXC	C5-N7	-2.38	1.31	1.39
2	F	955	HXC	C5-C4	2.36	1.47	1.40
2	A	951	HXC	C5-N7	-2.35	1.31	1.39
2	E	954	HXC	CM5-CM4	-2.35	1.35	1.51
2	C	953	HXC	CM5-CM4	-2.32	1.35	1.51
2	B	952	HXC	C5-C4	2.25	1.46	1.40
2	E	954	HXC	CP9-CPA	2.24	1.58	1.53
2	E	954	HXC	C8-N7	2.12	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	954	HXC	P3-O3'	2.09	1.63	1.59
2	E	954	HXC	CM6-CM5	-2.06	1.32	1.49
2	F	955	HXC	P3-O3'	2.04	1.63	1.59
2	F	955	HXC	C2'-C1'	2.03	1.56	1.53
2	F	955	HXC	C8-N7	2.01	1.38	1.34

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	955	HXC	O3'-C3'-C2'	-10.08	75.15	111.68
2	C	953	HXC	OP1-CP3-CP4	-9.17	105.25	122.02
2	F	955	HXC	OP1-CP3-CP4	-8.79	105.93	122.02
2	A	951	HXC	O4'-C1'-C2'	8.63	119.53	106.93
2	B	952	HXC	CP5-CP4-CP3	-8.51	98.18	112.36
2	F	955	HXC	OP1-CP3-NP1	-8.25	107.44	123.01
2	E	954	HXC	CP5-CP4-CP3	-7.74	99.47	112.36
2	B	952	HXC	OP1-CP3-CP4	-7.36	108.55	122.02
2	B	952	HXC	CM3-CM2-CM1	7.30	128.51	112.33
2	A	951	HXC	CP5-CP4-CP3	-7.25	100.29	112.36
2	C	953	HXC	OP1-CP3-NP1	-7.21	109.41	123.01
2	E	954	HXC	O3'-C3'-C2'	-7.17	85.71	111.68
2	E	954	HXC	C4-C5-N7	-6.99	102.11	109.40
2	E	954	HXC	CP1-CP2-NP1	6.93	126.98	112.42
2	E	954	HXC	O2'-C2'-C3'	6.71	130.23	111.17
2	B	952	HXC	OP1-CP3-NP1	-6.28	111.16	123.01
2	E	954	HXC	OM2-CM1-S	-6.21	114.54	122.61
2	A	951	HXC	CM2-CM1-S	5.83	120.25	113.46
2	A	951	HXC	CP1-CP2-NP1	5.69	124.36	112.42
2	A	951	HXC	C3'-C2'-C1'	-5.66	87.35	99.89
2	C	953	HXC	CP5-CP4-CP3	-5.55	103.11	112.36
2	A	951	HXC	O2'-C2'-C3'	5.55	126.92	111.17
2	B	952	HXC	CP1-CP2-NP1	5.42	123.80	112.42
2	A	951	HXC	CP8-CPA-CP7	5.15	117.75	108.82
2	A	951	HXC	C2'-C3'-C4'	5.08	112.23	103.22
2	C	953	HXC	O3'-C3'-C2'	-4.94	93.78	111.68
2	A	951	HXC	OM2-CM1-S	-4.92	116.22	122.61
2	F	955	HXC	P2-O6-P1	-4.82	116.28	132.83
2	A	951	HXC	O32-P3-O31	4.82	126.04	107.64
2	E	954	HXC	OP1-CP3-NP1	-4.79	113.97	123.01
2	F	955	HXC	C3'-C2'-C1'	-4.76	89.34	99.89
2	A	951	HXC	OP1-CP3-NP1	-4.75	114.06	123.01
2	F	955	HXC	O4'-C1'-C2'	4.73	113.84	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	955	HXC	O2'-C2'-C3'	4.62	124.28	111.17
2	C	953	HXC	C4-C5-N7	-4.55	104.66	109.40
2	B	952	HXC	O3'-C3'-C2'	-4.54	95.23	111.68
2	E	954	HXC	CP9-CPA-CP7	4.53	116.67	108.82
2	E	954	HXC	CM2-CM1-S	4.46	118.65	113.46
2	E	954	HXC	OP1-CP3-CP4	-4.45	113.87	122.02
2	F	955	HXC	C4-C5-N7	-4.31	104.90	109.40
2	B	952	HXC	P2-O6-P1	-4.19	118.44	132.83
2	B	952	HXC	CP2-NP1-CP3	-4.19	115.05	122.84
2	B	952	HXC	OM2-CM1-CM2	4.17	128.91	123.99
2	A	951	HXC	OP1-CP3-CP4	-4.16	114.41	122.02
2	C	953	HXC	CP8-CPA-CP9	4.07	117.45	109.17
2	A	951	HXC	C4-C5-N7	-4.01	105.22	109.40
2	B	952	HXC	CP5-NP2-CP6	3.95	129.62	122.59
2	F	955	HXC	C1'-N9-C4	3.84	133.39	126.64
2	C	953	HXC	CP1-CP2-NP1	3.82	120.45	112.42
2	A	951	HXC	O22-P2-O21	3.78	130.95	112.24
2	B	952	HXC	CP9-CPA-CP7	3.73	115.28	108.82
2	C	953	HXC	CP8-CPA-CP7	-3.72	102.37	108.82
2	C	953	HXC	CM2-CM1-S	3.68	117.74	113.46
2	B	952	HXC	C4-C5-N7	-3.68	105.57	109.40
2	F	955	HXC	CP5-CP4-CP3	-3.67	106.25	112.36
2	C	953	HXC	N3-C2-N1	-3.66	122.95	128.68
2	E	954	HXC	CM3-CM2-CM1	3.62	120.36	112.33
2	F	955	HXC	CM2-CM1-S	-3.57	109.30	113.46
2	C	953	HXC	CP5-NP2-CP6	3.57	128.95	122.59
2	F	955	HXC	N3-C2-N1	-3.48	123.25	128.68
2	B	952	HXC	C2-N1-C6	3.35	124.48	118.75
2	A	951	HXC	CP2-NP1-CP3	-3.30	116.71	122.84
2	F	955	HXC	C2-N1-C6	3.29	124.38	118.75
2	E	954	HXC	CP8-CPA-CP7	3.27	114.49	108.82
2	E	954	HXC	P2-O6-P1	-3.26	121.64	132.83
2	F	955	HXC	CP1-S-CM1	-3.26	91.73	101.87
2	E	954	HXC	O4'-C1'-C2'	3.25	111.67	106.93
2	C	953	HXC	O2'-C2'-C3'	3.18	120.19	111.17
2	F	955	HXC	O7-CPB-CPA	-3.08	105.59	110.55
2	F	955	HXC	O32-P3-O33	3.06	122.67	110.68
2	C	953	HXC	O7-CPB-CPA	-3.06	105.63	110.55
2	E	954	HXC	OP2-CP6-NP2	-3.03	116.48	122.99
2	C	953	HXC	O2'-C2'-C1'	2.97	121.80	110.85
2	E	954	HXC	N3-C2-N1	-2.96	124.05	128.68
2	A	951	HXC	CP9-CPA-CP7	-2.95	103.70	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	952	HXC	O32-P3-O33	2.95	122.22	110.68
2	A	951	HXC	O3'-P3-O33	-2.94	98.06	109.39
2	C	953	HXC	CM3-CM2-CM1	2.93	118.83	112.33
2	B	952	HXC	O5'-C5'-C4'	-2.89	99.05	108.99
2	E	954	HXC	O2'-C2'-C1'	2.88	121.50	110.85
2	A	951	HXC	CM3-CM2-CM1	2.87	118.70	112.33
2	F	955	HXC	N6-C6-N1	2.85	124.49	118.57
2	B	952	HXC	N6-C6-N1	2.85	124.48	118.57
2	B	952	HXC	OM2-CM1-S	-2.81	118.97	122.61
2	A	951	HXC	CP4-CP3-NP1	2.77	121.09	116.42
2	A	951	HXC	O2'-C2'-C1'	2.69	120.78	110.85
2	A	951	HXC	O7-CPB-CPA	-2.68	106.23	110.55
2	A	951	HXC	O3'-C3'-C2'	-2.68	101.96	111.68
2	F	955	HXC	O4'-C4'-C3'	2.68	110.61	104.87
2	E	954	HXC	CP4-CP3-NP1	2.65	120.88	116.42
2	A	951	HXC	C5-C6-N6	2.61	124.32	120.35
2	B	952	HXC	N3-C2-N1	-2.61	124.61	128.68
2	F	955	HXC	O2'-C2'-C1'	2.60	120.45	110.85
2	E	954	HXC	O32-P3-O33	2.57	120.73	110.68
2	F	955	HXC	CP9-CPA-CP7	2.52	113.20	108.82
2	B	952	HXC	O4'-C4'-C3'	2.52	110.26	104.87
2	B	952	HXC	O3'-C3'-C4'	-2.45	101.23	110.08
2	C	953	HXC	OM2-CM1-CM2	-2.44	121.11	123.99
2	B	952	HXC	C1'-N9-C4	2.43	130.91	126.64
2	E	954	HXC	O4'-C4'-C3'	2.43	110.07	104.87
2	E	954	HXC	OM2-CM1-CM2	2.38	126.80	123.99
2	C	953	HXC	O32-P3-O33	2.38	119.99	110.68
2	C	953	HXC	C3'-C2'-C1'	-2.38	94.62	99.89
2	F	955	HXC	CP2-NP1-CP3	-2.36	118.46	122.84
2	A	951	HXC	P2-O6-P1	-2.35	124.76	132.83
2	E	954	HXC	O31-P3-O3'	-2.35	95.47	105.99
2	C	953	HXC	CP9-CPA-CP7	-2.33	104.78	108.82
2	F	955	HXC	O22-P2-O21	2.33	123.76	112.24
2	B	952	HXC	C2'-C3'-C4'	-2.29	99.16	103.22
2	F	955	HXC	OM2-CM1-S	2.24	125.52	122.61
2	A	951	HXC	CP8-CPA-CPB	-2.23	104.59	108.23
2	A	951	HXC	O32-P3-O33	-2.22	102.00	110.68
2	B	952	HXC	CM4-CM3-CM2	2.21	121.13	113.19
2	B	952	HXC	C5-C6-N1	-2.12	115.54	120.35
2	F	955	HXC	O7-P2-O21	-2.11	100.81	109.07
2	B	952	HXC	O32-P3-O3'	-2.11	96.56	105.99
2	F	955	HXC	CP7-CP6-NP2	2.08	120.72	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	955	HXC	OP2-CP6-CP7	-2.08	114.72	121.06
2	F	955	HXC	C5-C6-N1	-2.08	115.64	120.35
2	E	954	HXC	CP2-NP1-CP3	-2.07	119.00	122.84
2	A	951	HXC	O5'-P1-O11	2.02	116.96	109.07

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C	953	HXC	OP1-CP3-NP1-CP2
2	B	952	HXC	OP1-CP3-NP1-CP2
2	F	955	HXC	OP1-CP3-NP1-CP2
2	A	951	HXC	OP1-CP3-NP1-CP2
2	E	954	HXC	OP1-CP3-NP1-CP2
2	C	953	HXC	CP8-CPA-CPB-O7
2	B	952	HXC	C5'-O5'-P1-O6
2	B	952	HXC	CP9-CPA-CPB-O7
2	C	953	HXC	C3'-O3'-P3-O31
2	F	955	HXC	CPB-O7-P2-O6
2	A	951	HXC	C5'-O5'-P1-O11

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	955	HXC	7	0
2	C	953	HXC	3	0
2	E	954	HXC	2	0
2	A	951	HXC	4	0
2	B	952	HXC	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 F 955

Bond lengths

Bond angles

Torsions

Rings

Ligand HXC C 953

Bond lengths

Bond angles

Torsions

Rings

Ligand HXC E 954

Bond lengths

Bond angles

Torsions

Rings

Ligand HXC A 951

Bond lengths

Bond angles

Torsions

Rings

Ligand HXC B 952

Bond lengths

Bond angles

Torsions

Rings
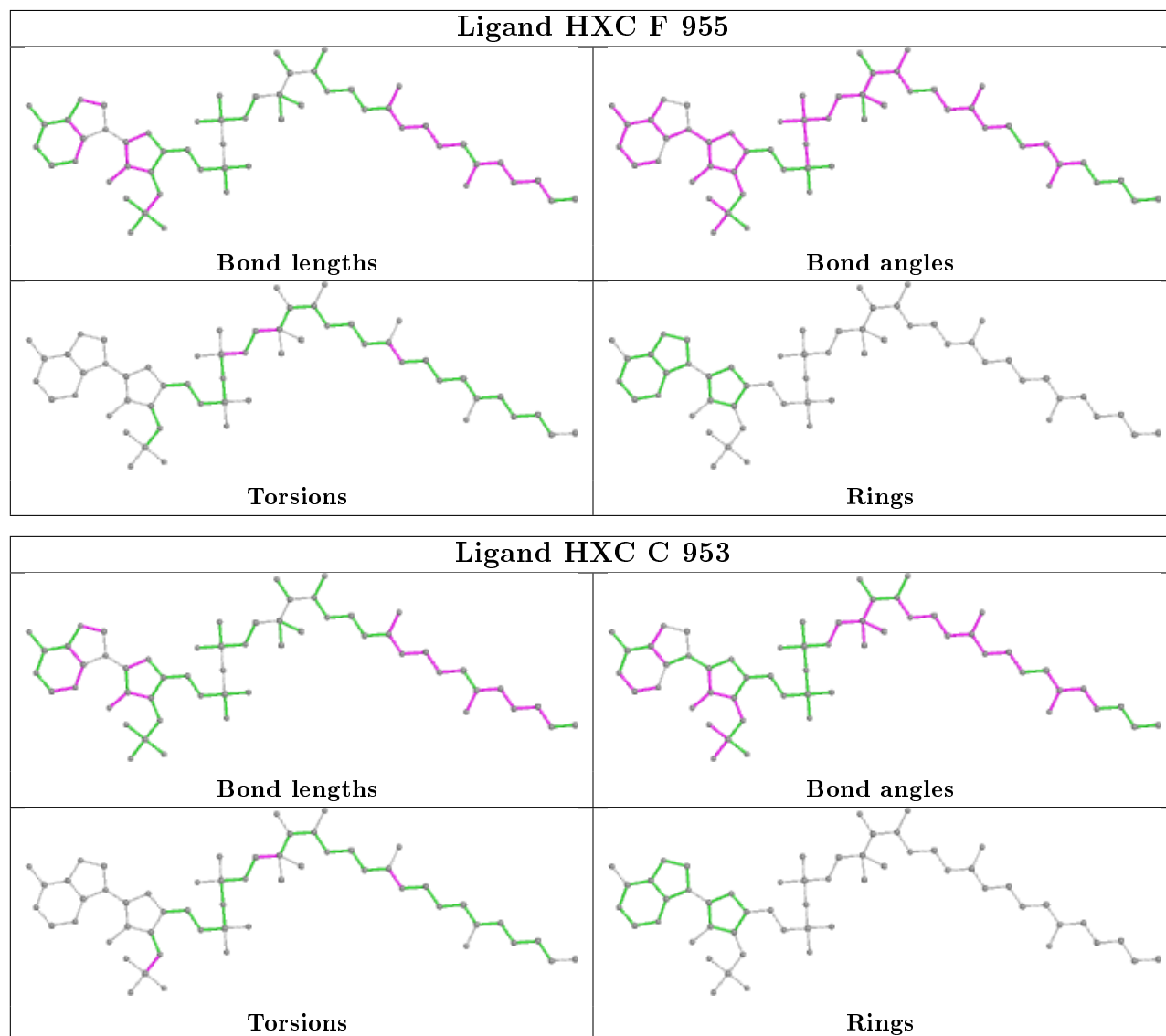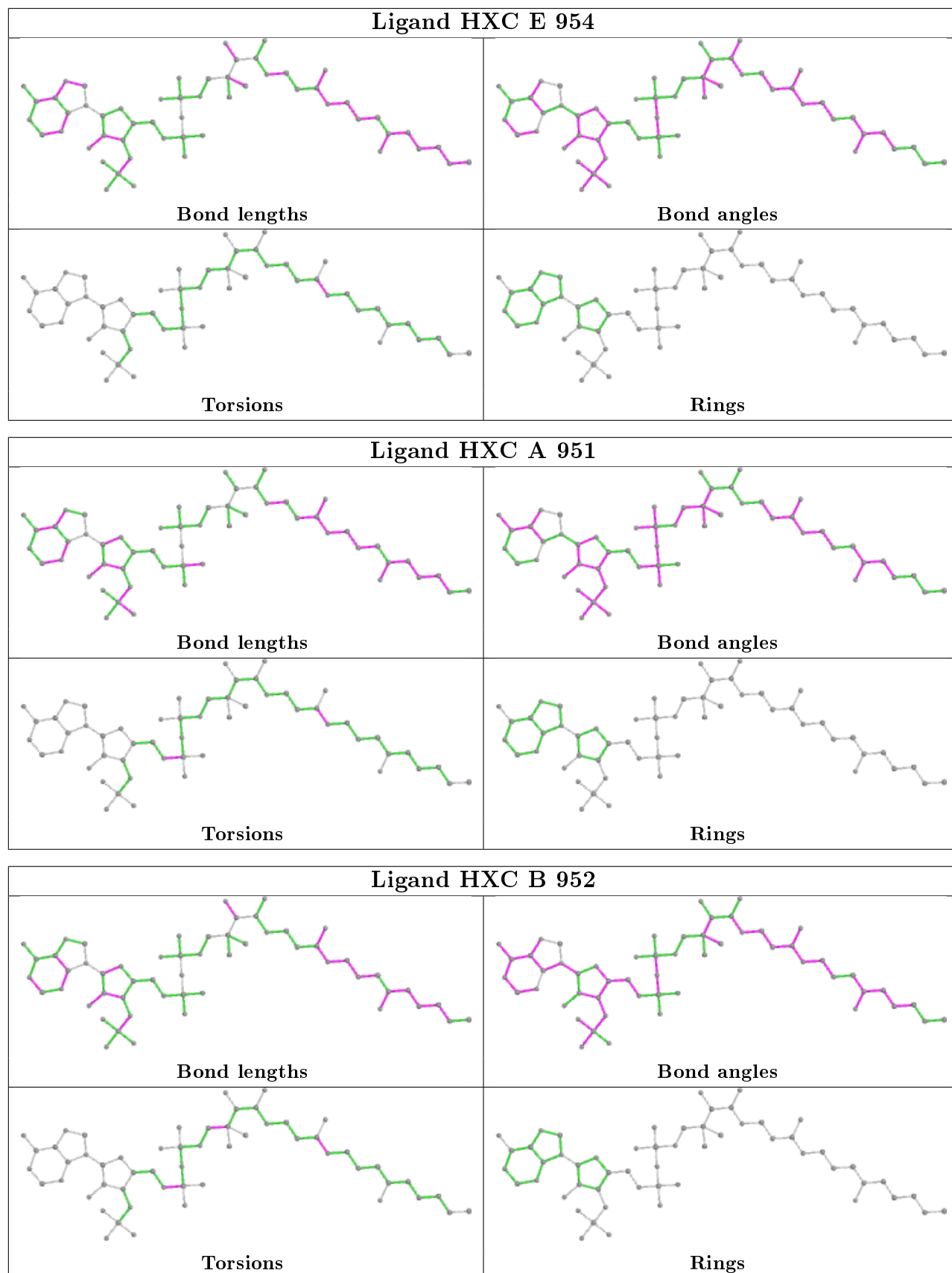
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.