



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 11:45 AM EST

PDB ID : 1N62
Title : Crystal Structure of the Mo,Cu-CO Dehydrogenase (CODH), n-butylisocyanide-bound state
Authors : Dobbek, H.; Gremer, L.; Kiefersauer, R.; Huber, R.; Meyer, O.
Deposited on : 2002-11-08
Resolution : 1.09 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

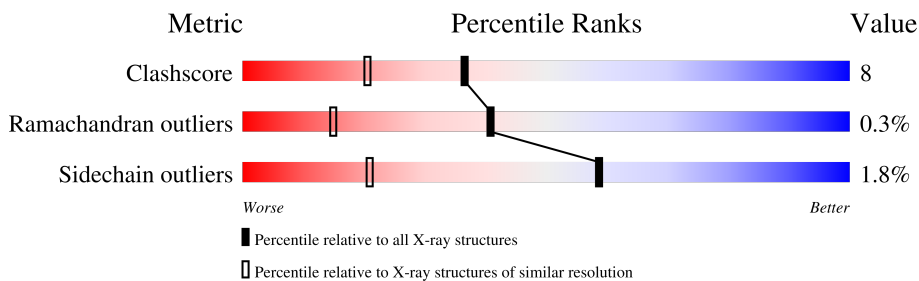
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.09 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	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)

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	166	86% 9% ...
1	D	166	85% 8% ...
2	B	809	83% 13% ...
2	E	809	84% 12% ...
3	C	288	88% 9% ..
3	F	288	84% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CUB	B	3921	X	-	-	-
6	CUB	E	4921	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22645 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 Carbon monoxide dehydrogenase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	Total	C	N	O	S	6	6	0
			1225	758	219	231	17			
1	D	159	Total	C	N	O	S	10	8	0
			1218	753	219	228	18			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	804	Total	C	N	O	S	80	15	0
			6256	3977	1067	1164	48			
2	E	796	Total	C	N	O	S	108	20	0
			6221	3959	1061	1154	47			

- Molecule 3 is a protein called Carbon monoxide dehydrogenase medium chain.

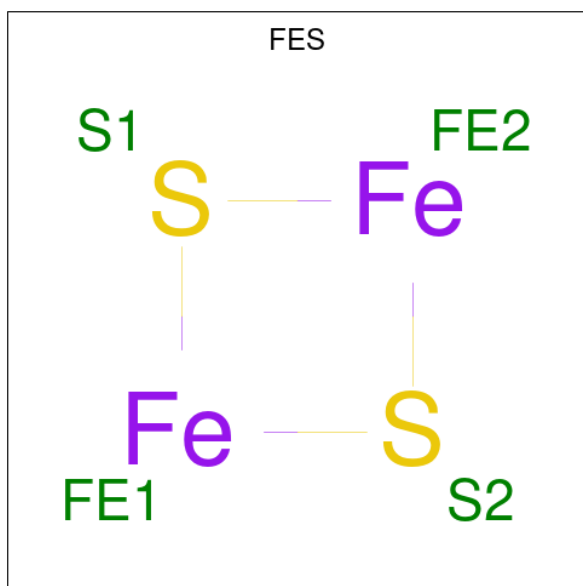
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	286	Total	C	N	O	S	33	9	0
			2144	1353	378	401	12			
3	F	286	Total	C	N	O	S	40	6	0
			2125	1341	374	398	12			

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	5	4	1	0	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



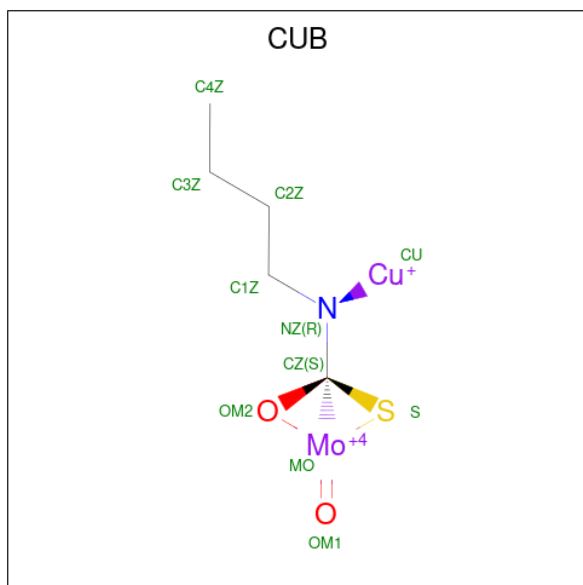
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	A	1	4	2	2	0	0
5	A	1	4	2	2	0	0
5	D	1	4	2	2	0	0

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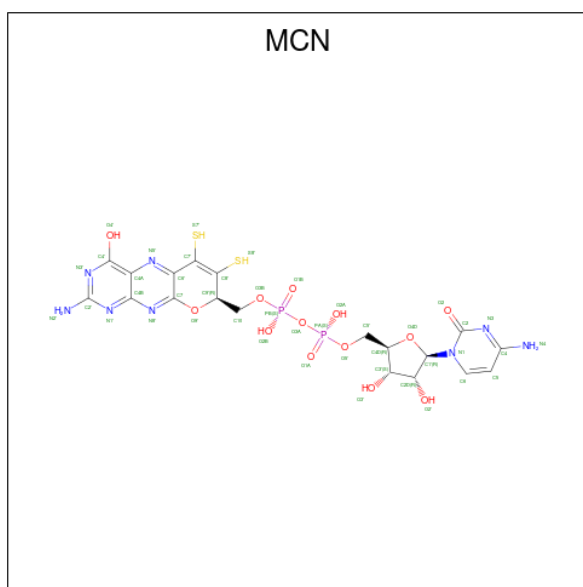
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
5	D	1	4	2	2	0	0

- Molecule 6 is CU(I)-S-MO(IV)(=O)O-NBIC CLUSTER (three-letter code: CUB) (formula: $C_5H_9CuMoNO_2S$).



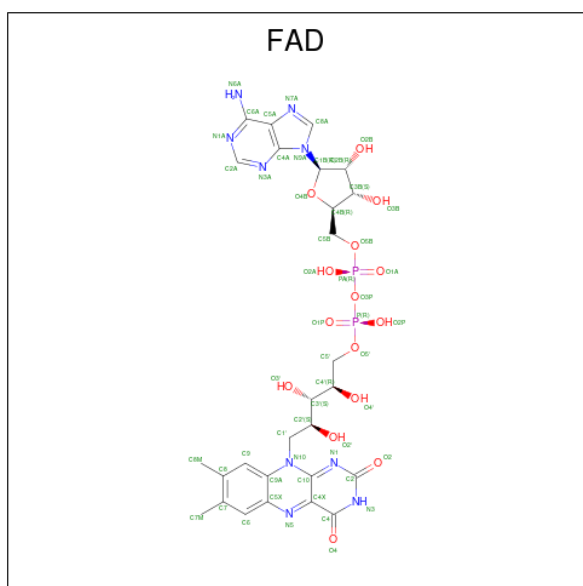
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cu	Mo	N	O	S		
6	B	1	11	5	1	1	1	2	1	0	0
6	E	1	11	5	1	1	1	2	1	0	0

- Molecule 7 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
7	B	1	44	19	8	13	2	2	0	0
7	E	1	44	19	8	13	2	2	0	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	C	1	53	27	9	15	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	F	1	53	27	9	15	2	0	0

- Molecule 9 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	217	217	217	0	0
9	B	1034	1034	1034	0	0
9	C	427	427	427	0	0
9	D	222	222	222	0	0
9	E	962	962	962	0	0
9	F	357	357	357	0	0

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.

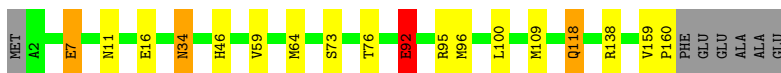
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain A:  86% 9% ...




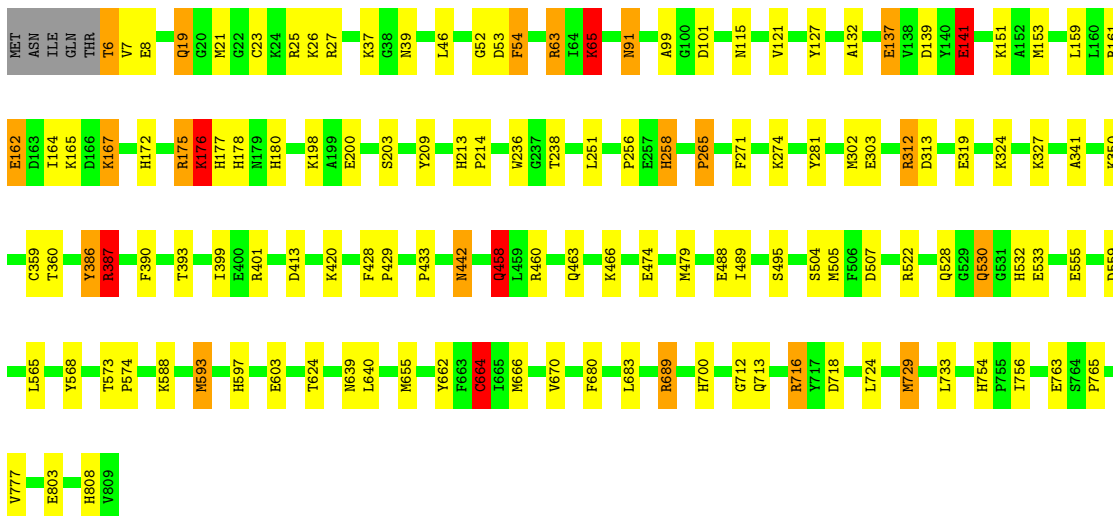
- Molecule 1: Carbon monoxide dehydrogenase small chain

Chain D:  85% 8% ...




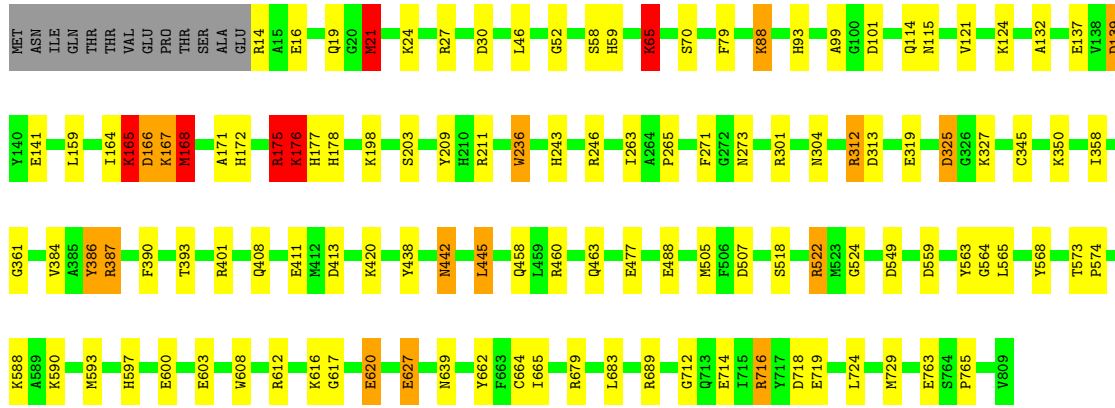
- Molecule 2: Carbon monoxide dehydrogenase large chain

Chain B:  83% 13% ...

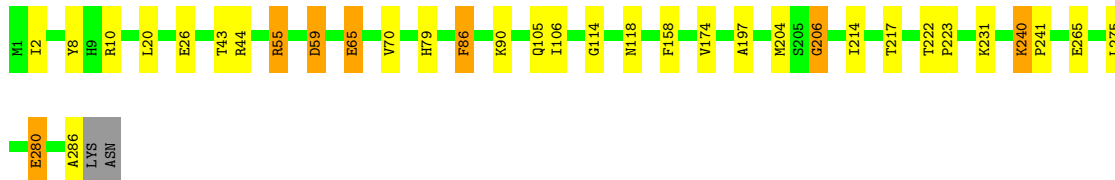
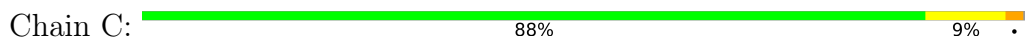


- Molecule 2: Carbon monoxide dehydrogenase large chain

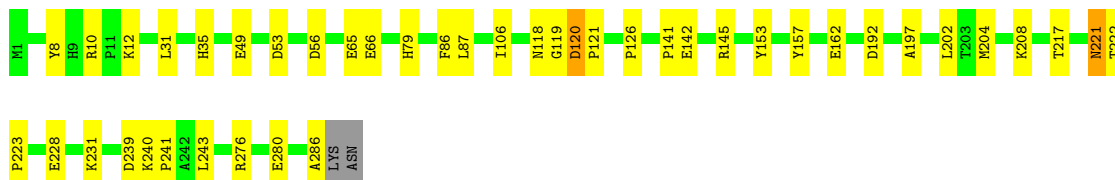
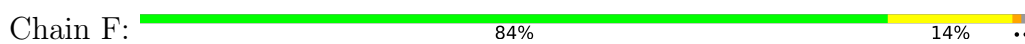
Chain E:  84% 12% ...



• Molecule 3: Carbon monoxide dehydrogenase medium chain



• Molecule 3: Carbon monoxide dehydrogenase medium chain



4 Data and refinement statistics

Xtrriage (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	117.86Å 130.02Å 156.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.80 – 1.09	Depositor
% Data completeness (in resolution range)	(Not available) (17.80-1.09)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.144 , 0.172	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22645	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: FAD, FES, PO4, CUB, MCN

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	2.66	9/1273 (0.7%)	2.65	10/1719 (0.6%)
1	D	3.27	10/1267 (0.8%)	1.83	10/1710 (0.6%)
2	B	1.15	17/6474 (0.3%)	1.44	28/8780 (0.3%)
2	E	1.35	36/6453 (0.6%)	1.01	45/8747 (0.5%)
3	C	0.94	8/2210 (0.4%)	1.05	10/3000 (0.3%)
3	F	0.83	3/2186 (0.1%)	0.83	2/2969 (0.1%)
All	All	1.53	83/19863 (0.4%)	1.37	105/26925 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	7
2	B	0	13
2	E	0	16
3	C	0	7
3	F	0	6
All	All	0	52

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92[A]	GLU	CD-OE2	75.22	2.08	1.25
1	D	92[B]	GLU	CD-OE2	75.22	2.08	1.25
1	A	95[A]	ARG	CZ-NH1	52.95	2.01	1.33
1	A	95[B]	ARG	CZ-NH1	52.95	2.01	1.33
2	E	600	GLU	CD-OE1	33.23	1.62	1.25
2	E	168	MET	CA-CB	31.19	2.22	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95[A]	ARG	CZ-NH2	-30.45	0.93	1.33
1	A	95[B]	ARG	CZ-NH2	-30.45	0.93	1.33
1	D	16	GLU	CG-CD	28.79	1.95	1.51
2	B	303	GLU	CD-OE2	-27.57	0.95	1.25
2	B	162	GLU	CD-OE1	26.87	1.55	1.25
2	E	600	GLU	CD-OE2	-24.65	0.98	1.25
2	E	137	GLU	CG-CD	-24.30	1.15	1.51
1	A	155	LYS	CE-NZ	21.69	2.03	1.49
2	B	639	ASN	CB-CG	21.23	1.99	1.51
2	E	167	LYS	CA-CB	-19.35	1.11	1.53
2	E	627	GLU	CG-CD	18.01	1.78	1.51
2	B	198	LYS	CE-NZ	-17.31	1.05	1.49
2	E	141	GLU	CB-CG	-16.92	1.20	1.52
2	B	63	ARG	CD-NE	16.76	1.75	1.46
2	E	627	GLU	CD-OE2	-16.42	1.07	1.25
3	C	158	PHE	CG-CD1	15.49	1.61	1.38
2	B	65	LYS	CG-CD	-14.33	1.03	1.52
2	E	171	ALA	CA-CB	-13.44	1.24	1.52
2	B	8	GLU	CB-CG	13.25	1.77	1.52
2	E	24	LYS	CE-NZ	11.75	1.78	1.49
2	E	617	GLY	C-N	11.60	1.60	1.34
2	E	639	ASN	CG-OD1	-11.49	0.98	1.24
2	E	65	LYS	CG-CD	11.41	1.91	1.52
2	E	639	ASN	CG-ND2	-11.26	1.04	1.32
3	C	265	GLU	CD-OE1	10.52	1.37	1.25
2	E	411	GLU	CD-OE1	10.46	1.37	1.25
2	B	141	GLU	CD-OE2	10.46	1.37	1.25
3	F	142	GLU	CB-CG	-10.28	1.32	1.52
2	E	627	GLU	CD-OE1	10.16	1.36	1.25
2	E	325	ASP	CG-OD1	-9.63	1.03	1.25
1	D	118[A]	GLN	CD-NE2	9.43	1.56	1.32
1	D	118[B]	GLN	CD-NE2	9.43	1.56	1.32
2	E	165	LYS	C-N	-9.42	1.12	1.34
2	B	141	GLU	CD-OE1	-9.08	1.15	1.25
2	E	70	SER	CB-OG	8.98	1.53	1.42
2	B	63	ARG	CZ-NH2	8.82	1.44	1.33
2	E	65	LYS	CE-NZ	8.40	1.70	1.49
2	E	141	GLU	CG-CD	-8.23	1.39	1.51
3	C	26	GLU	CB-CG	8.12	1.67	1.52
2	E	616	LYS	C-N	8.01	1.47	1.33
2	E	21[A]	MET	CB-CG	7.89	1.76	1.51
2	E	21[B]	MET	CB-CG	7.89	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	118[A]	GLN	CD-OE1	-7.74	1.06	1.24
1	D	118[B]	GLN	CD-OE1	-7.74	1.06	1.24
2	E	458	GLN	CB-CG	7.68	1.73	1.52
2	E	325	ASP	CG-OD2	7.62	1.42	1.25
1	D	7	GLU	CD-OE2	7.60	1.34	1.25
3	F	12	LYS	CG-CD	7.51	1.77	1.52
3	C	231	LYS	CG-CD	7.43	1.77	1.52
2	E	664	CYS	CB-SG	-7.12	1.70	1.82
2	E	719	GLU	CB-CG	6.99	1.65	1.52
2	B	139	ASP	CG-OD2	6.79	1.41	1.25
2	E	176	LYS	CA-CB	-6.75	1.39	1.53
2	E	639	ASN	CB-CG	6.65	1.66	1.51
3	C	240	LYS	CD-CE	-6.47	1.35	1.51
3	F	231	LYS	CG-CD	-6.20	1.31	1.52
1	A	118[A]	GLN	CD-OE1	6.20	1.37	1.24
1	A	118[B]	GLN	CD-OE1	6.20	1.37	1.24
2	E	139	ASP	CB-CG	6.20	1.64	1.51
2	B	729	MET	SD-CE	-6.16	1.43	1.77
3	C	280	GLU	CG-CD	6.13	1.61	1.51
2	B	137	GLU	CG-CD	6.02	1.60	1.51
2	B	716	ARG	NE-CZ	-5.95	1.25	1.33
2	E	21[A]	MET	CG-SD	-5.80	1.66	1.81
2	E	21[B]	MET	CG-SD	-5.80	1.66	1.81
1	A	118[A]	GLN	CD-NE2	-5.80	1.18	1.32
1	A	118[B]	GLN	CD-NE2	-5.80	1.18	1.32
3	C	158	PHE	CG-CD2	-5.80	1.30	1.38
2	B	251	LEU	CG-CD1	-5.76	1.30	1.51
2	B	151	LYS	CD-CE	5.33	1.64	1.51
2	E	19	GLN	CD-OE1	5.32	1.35	1.24
3	C	206	GLY	C-O	5.28	1.32	1.23
2	E	411	GLU	CD-OE2	-5.23	1.19	1.25
2	E	420	LYS	CD-CE	5.22	1.64	1.51
2	B	593	MET	SD-CE	-5.01	1.49	1.77
1	D	34[A]	ASN	CG-ND2	5.00	1.45	1.32
1	D	34[B]	ASN	CG-ND2	5.00	1.45	1.32

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ARG	NH1-CZ-NH2	-101.31	7.96	119.40
1	A	95[A]	ARG	NE-CZ-NH2	50.85	145.73	120.30
1	A	95[B]	ARG	NE-CZ-NH2	50.85	145.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95[A]	ARG	NE-CZ-NH1	-49.76	95.42	120.30
1	A	95[B]	ARG	NE-CZ-NH1	-49.76	95.42	120.30
1	D	92[A]	GLU	OE1-CD-OE2	-45.52	68.67	123.30
1	D	92[B]	GLU	OE1-CD-OE2	-45.52	68.67	123.30
3	C	158	PHE	CB-CG-CD2	22.76	136.73	120.80
1	A	95[A]	ARG	NH1-CZ-NH2	-20.14	97.24	119.40
1	A	95[B]	ARG	NH1-CZ-NH2	-20.14	97.24	119.40
2	B	716	ARG	NE-CZ-NH1	-18.25	111.17	120.30
2	B	716	ARG	NE-CZ-NH2	17.50	129.05	120.30
3	C	206	GLY	CA-C-O	-16.08	91.66	120.60
2	E	639	ASN	CB-CG-OD1	-15.60	90.40	121.60
2	E	627	GLU	OE1-CD-OE2	15.22	141.56	123.30
2	B	139	ASP	CB-CG-OD1	15.01	131.81	118.30
2	E	165	LYS	O-C-N	-14.93	98.81	122.70
3	C	90	LYS	CD-CE-NZ	14.38	144.78	111.70
2	E	600	GLU	CG-CD-OE2	14.29	146.87	118.30
2	B	198	LYS	CD-CE-NZ	14.27	144.52	111.70
2	E	176	LYS	N-CA-CB	12.07	132.33	110.60
2	B	63	ARG	NE-CZ-NH2	11.47	126.03	120.30
3	C	158	PHE	CB-CG-CD1	-10.87	113.19	120.80
2	E	600	GLU	CG-CD-OE1	-10.63	97.03	118.30
2	E	141	GLU	CA-CB-CG	10.27	135.99	113.40
1	D	16	GLU	CG-CD-OE1	-9.96	98.38	118.30
2	E	24	LYS	CD-CE-NZ	-9.26	90.40	111.70
2	E	137	GLU	CB-CG-CD	9.26	139.19	114.20
2	B	639	ASN	CA-CB-CG	-9.19	93.19	113.40
2	E	401	ARG	NE-CZ-NH1	9.07	124.83	120.30
2	B	162	GLU	CG-CD-OE1	-9.01	100.29	118.30
2	B	139	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	D	16	GLU	CG-CD-OE2	8.62	135.54	118.30
1	D	7	GLU	OE1-CD-OE2	-8.45	113.16	123.30
2	E	167	LYS	N-CA-CB	-8.38	95.52	110.60
3	C	158	PHE	CG-CD2-CE2	8.28	129.91	120.80
2	E	600	GLU	OE1-CD-OE2	-8.20	113.46	123.30
1	D	16	GLU	CB-CG-CD	-8.13	92.24	114.20
2	B	664[A]	CYS	CA-CB-SG	8.01	128.42	114.00
2	B	664[B]	CYS	CA-CB-SG	8.01	128.42	114.00
2	E	620	GLU	CG-CD-OE1	-7.90	102.51	118.30
2	E	166	ASP	O-C-N	-7.85	110.15	122.70
2	E	639	ASN	CB-CG-ND2	7.72	135.23	116.70
2	B	175	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	D	92[A]	GLU	CG-CD-OE2	-7.63	103.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92[B]	GLU	CG-CD-OE2	-7.63	103.04	118.30
2	E	620	GLU	CG-CD-OE2	7.62	133.53	118.30
3	C	265	GLU	OE1-CD-OE2	-7.41	114.41	123.30
3	C	158	PHE	CD1-CG-CD2	-7.19	108.95	118.30
2	B	251	LEU	CB-CG-CD1	6.95	122.81	111.00
1	D	34[A]	ASN	CB-CG-ND2	-6.94	100.04	116.70
1	D	34[B]	ASN	CB-CG-ND2	-6.94	100.04	116.70
2	E	627	GLU	CG-CD-OE1	-6.91	104.48	118.30
1	A	109	MET	CG-SD-CE	-6.87	89.21	100.20
2	B	458	GLN	CG-CD-OE1	-6.74	108.12	121.60
2	E	689	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	F	142	GLU	CA-CB-CG	6.65	128.03	113.40
2	E	171	ALA	N-CA-CB	-6.62	100.83	110.10
2	B	303	GLU	OE1-CD-OE2	-6.48	115.52	123.30
2	E	139	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	84	ASP	CB-CG-OD2	6.41	124.07	118.30
2	E	21[A]	MET	CA-CB-CG	6.39	124.17	113.30
2	E	21[B]	MET	CA-CB-CG	6.39	124.17	113.30
2	E	627	GLU	CB-CG-CD	-6.32	97.14	114.20
2	B	167	LYS	N-CA-CB	6.25	121.86	110.60
2	E	386	TYR	CB-CG-CD1	6.15	124.69	121.00
2	E	171	ALA	CB-CA-C	6.12	119.28	110.10
2	E	246	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	401	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	E	401	ARG	NE-CZ-NH2	-6.09	117.26	120.30
2	E	139	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	E	65	LYS	CB-CG-CD	-5.96	96.11	111.60
2	E	325	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	B	25	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	E	559	ASP	CB-CG-OD1	5.75	123.47	118.30
2	E	101	ASP	CB-CG-OD1	5.71	123.44	118.30
2	B	176	LYS	CD-CE-NZ	-5.64	98.72	111.70
2	B	716	ARG	CD-NE-CZ	5.63	131.49	123.60
2	E	413	ASP	CB-CG-OD2	5.63	123.37	118.30
2	E	168	MET	CB-CA-C	-5.60	99.20	110.40
2	E	168	MET	N-CA-CB	-5.52	100.67	110.60
2	E	246	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	B	386	TYR	CB-CG-CD2	-5.44	117.74	121.00
2	E	301	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	E	141	GLU	CG-CD-OE2	-5.33	107.63	118.30
2	B	413	ASP	CB-CG-OD2	5.29	123.06	118.30
2	E	522	ARG	NE-CZ-NH2	-5.29	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	129	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	E	141	GLU	CG-CD-OE1	5.18	128.66	118.30
2	B	386	TYR	CB-CG-CD1	5.17	124.10	121.00
3	C	106	ILE	CG1-CB-CG2	-5.17	100.03	111.40
2	E	211	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	B	65	LYS	CB-CG-CD	5.12	124.92	111.60
2	E	679	ARG	NE-CZ-NH2	-5.11	117.75	120.30
3	C	26	GLU	CA-CB-CG	-5.10	102.18	113.40
2	B	387	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	C	90	LYS	CG-CD-CE	-5.08	96.67	111.90
2	B	101	ASP	CB-CG-OD1	5.06	122.86	118.30
2	B	281	TYR	CB-CG-CD1	5.05	124.03	121.00
3	F	239	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	236[A]	TRP	CD2-CE2-CZ2	-5.04	116.25	122.30
2	E	236[B]	TRP	CD2-CE2-CZ2	-5.04	116.25	122.30
2	B	559	ASP	CB-CG-OD1	5.03	122.83	118.30
2	E	175	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	ARG	Sidechain
1	A	95[A]	ARG	Sidechain
1	A	95[B]	ARG	Sidechain
2	B	141	GLU	Sidechain
2	B	162	GLU	Sidechain
2	B	19	GLN	Sidechain
2	B	27	ARG	Sidechain
2	B	312	ARG	Sidechain
2	B	387	ARG	Sidechain
2	B	458	GLN	Sidechain
2	B	474	GLU	Sidechain
2	B	54	PHE	Peptide
2	B	6	THR	Mainchain
2	B	689[A]	ARG	Sidechain
2	B	689[B]	ARG	Sidechain
2	B	716	ARG	Sidechain
3	C	206	GLY	Mainchain
3	C	44	ARG	Mainchain
3	C	55[A]	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	55[B]	ARG	Sidechain
3	C	59	ASP	Sidechain
3	C	65	GLU	Sidechain
3	C	86	PHE	Sidechain
1	D	138	ARG	Sidechain
1	D	34[A]	ASN	Sidechain
1	D	34[B]	ASN	Sidechain
1	D	7	GLU	Sidechain
1	D	73[B]	SER	Mainchain
1	D	92[A]	GLU	Sidechain
1	D	92[B]	GLU	Sidechain
2	E	16	GLU	Mainchain
2	E	164	ILE	Mainchain
2	E	165	LYS	Mainchain
2	E	166	ASP	Mainchain
2	E	168	MET	Mainchain
2	E	175	ARG	Sidechain,Mainchain
2	E	176	LYS	Mainchain
2	E	27	ARG	Sidechain
2	E	312	ARG	Sidechain
2	E	387	ARG	Sidechain
2	E	620	GLU	Mainchain
2	E	716[A]	ARG	Sidechain
2	E	716[B]	ARG	Sidechain
2	E	79	PHE	Sidechain
2	E	88	LYS	Mainchain
3	F	120	ASP	Sidechain
3	F	141	PRO	Mainchain
3	F	157	TYR	Sidechain
3	F	228	GLU	Sidechain
3	F	49	GLU	Sidechain
3	F	66	GLU	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1225	0	1203	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1218	0	1198	30	0
2	B	6256	0	6138	94	3
2	E	6221	0	6103	96	1
3	C	2144	0	2200	28	0
3	F	2125	0	2175	43	0
4	A	5	0	0	0	0
5	A	8	0	0	0	0
5	D	8	0	0	0	0
6	B	11	0	9	3	0
6	E	11	0	9	4	0
7	B	44	0	17	3	0
7	E	44	0	17	1	0
8	C	53	0	30	0	0
8	F	53	0	31	2	0
9	A	217	0	0	6	1
9	B	1034	0	0	18	7
9	C	427	0	0	7	0
9	D	222	0	0	5	2
9	E	962	0	0	29	2
9	F	357	0	0	13	1
All	All	22645	0	19130	302	9

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 (302) 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:E:21[A]:MET:CG	2:E:21[A]:MET:CB	1.76	1.62
2:E:327[B]:LYS:HD3	9:E:5792:HOH:O	1.23	1.36
3:C:65:GLU:HG2	3:C:86:PHE:CZ	1.65	1.31
2:B:6:THR:CG2	9:B:4489:HOH:O	1.77	1.27
3:C:55[A]:ARG:NH2	9:C:4313:HOH:O	1.66	1.26
1:D:92[A]:GLU:CD	9:D:5018:HOH:O	1.69	1.23
2:E:593:MET:HG2	2:E:603:GLU:OE2	1.08	1.20
2:B:6:THR:HG22	9:B:4489:HOH:O	1.34	1.20
1:A:59:VAL:HG11	1:A:64[A]:MET:CE	1.74	1.18
1:A:95[A]:ARG:CZ	9:A:4137:HOH:O	1.93	1.14
1:A:59:VAL:HG11	1:A:64[A]:MET:HE1	1.28	1.14
3:F:10[B]:ARG:HH11	3:F:10[B]:ARG:CG	1.62	1.13
1:D:95[A]:ARG:NH2	1:D:96[A]:MET:CE	2.11	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:VAL:HG11	1:D:64[A]:MET:CE	1.80	1.11
1:D:95[A]:ARG:NH2	1:D:96[A]:MET:HE1	1.67	1.09
3:C:65:GLU:CG	3:C:86:PHE:CZ	2.36	1.07
2:E:159:LEU:HD21	2:E:165:LYS:HD2	1.34	1.06
2:E:593:MET:CG	2:E:603:GLU:OE2	2.05	1.05
2:E:177:HIS:N	9:E:5350:HOH:O	1.89	1.04
3:C:65:GLU:HG2	3:C:86:PHE:HZ	0.87	1.04
1:D:59:VAL:HG11	1:D:64[A]:MET:HE1	1.36	1.02
3:F:10[B]:ARG:HH11	3:F:10[B]:ARG:CB	1.70	1.02
2:E:124:LYS:HD2	9:E:5739:HOH:O	1.59	1.00
2:E:477:GLU:OE1	9:E:5591:HOH:O	1.79	0.98
1:A:96[B]:MET:HE3	9:A:4137:HOH:O	1.62	0.98
2:E:716[A]:ARG:NE	9:E:5400:HOH:O	1.77	0.98
3:F:10[B]:ARG:HH11	3:F:10[B]:ARG:HG3	1.25	0.97
3:C:280:GLU:HG3	9:C:4242:HOH:O	1.65	0.96
3:C:55[A]:ARG:NH2	9:C:4346:HOH:O	1.99	0.96
3:F:118:ASN:O	9:F:5273:HOH:O	1.82	0.95
1:D:95[A]:ARG:NH2	1:D:96[A]:MET:HE3	1.81	0.95
2:E:408:GLN:NE2	9:E:5793:HOH:O	2.00	0.94
2:E:716[A]:ARG:CZ	9:E:5171:HOH:O	2.16	0.94
2:E:21[A]:MET:CE	2:E:21[A]:MET:HB2	1.98	0.94
3:F:10[B]:ARG:HG3	3:F:10[B]:ARG:NH1	1.81	0.93
2:B:528:GLN:H	2:B:530:GLN:HE22	1.17	0.92
2:B:460:ARG:HH11	2:B:463:GLN:HE22	1.20	0.89
1:D:11:ASN:HD21	1:D:76:THR:H	1.20	0.88
1:D:95[A]:ARG:HH22	1:D:96[A]:MET:HE1	1.36	0.87
3:F:221:ASN:ND2	9:F:5116:HOH:O	2.10	0.85
1:A:59:VAL:CG1	1:A:64[A]:MET:CE	2.54	0.85
2:E:460:ARG:HH11	2:E:463:GLN:HE22	1.24	0.84
1:D:59:VAL:HG11	1:D:64[A]:MET:HE3	1.59	0.84
1:D:59:VAL:CG1	1:D:64[A]:MET:CE	2.56	0.84
3:F:286:ALA:C	9:F:5106:HOH:O	2.15	0.84
2:B:532:HIS:HE1	7:B:3920:MCN:O2B	1.60	0.84
1:D:95[A]:ARG:CZ	1:D:96[A]:MET:CE	2.56	0.83
1:D:118[A]:GLN:CD	9:D:5109:HOH:O	2.13	0.83
2:E:165:LYS:HA	9:E:5227:HOH:O	1.79	0.83
2:E:445:LEU:HD23	2:E:445:LEU:O	1.78	0.82
3:F:120:ASP:OD1	3:F:121:PRO:HD2	1.78	0.82
1:A:59:VAL:HG11	1:A:64[A]:MET:HE3	1.60	0.82
2:E:176:LYS:CA	9:E:5067:HOH:O	2.29	0.81
2:E:273:ASN:HD21	2:E:304:ASN:HD21	1.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:165:LYS:HE2	9:E:5871:HOH:O	1.82	0.80
2:E:445:LEU:HD23	2:E:445:LEU:C	2.02	0.79
2:E:21[A]:MET:CB	2:E:21[A]:MET:CE	2.60	0.79
1:D:95[A]:ARG:CZ	1:D:96[A]:MET:HE3	2.13	0.78
3:F:118:ASN:C	9:F:5273:HOH:O	2.20	0.78
2:E:168:MET:O	2:E:175:ARG:N	2.16	0.78
1:A:82:ALA:HB3	1:A:86:THR:HG22	1.65	0.77
3:F:10[B]:ARG:CB	3:F:10[B]:ARG:NH1	2.48	0.76
1:D:159:VAL:HB	1:D:160:PRO:HD3	1.69	0.75
2:B:327:LYS:HG2	2:B:420:LYS:HE3	1.67	0.75
3:F:10[B]:ARG:NH2	9:F:5100:HOH:O	2.20	0.74
2:E:590:LYS:HA	2:E:593:MET:HE2	1.69	0.74
2:E:21[A]:MET:HB2	2:E:21[A]:MET:HE2	1.68	0.74
3:F:120:ASP:CG	9:F:5191:HOH:O	2.26	0.73
2:E:159:LEU:CD2	2:E:165:LYS:HD2	2.17	0.73
1:D:92[B]:GLU:OE2	9:D:5075:HOH:O	2.04	0.73
2:E:21[A]:MET:CB	2:E:21[A]:MET:SD	2.76	0.73
2:E:327[B]:LYS:HE3	9:E:5216:HOH:O	1.89	0.72
2:B:528:GLN:H	2:B:530:GLN:NE2	1.88	0.71
1:D:59:VAL:CG1	1:D:64[A]:MET:HE3	2.18	0.71
2:E:21[A]:MET:CE	9:E:5314:HOH:O	2.38	0.71
2:B:21[B]:MET:HE3	2:B:756:ILE:HD12	1.74	0.70
2:B:37:LYS:HE2	9:B:4834:HOH:O	1.91	0.70
2:E:21[A]:MET:HE1	9:E:5314:HOH:O	1.91	0.70
2:B:46:LEU:HD11	2:B:236[B]:TRP:CZ3	2.27	0.69
3:F:119:GLY:HA3	9:F:5273:HOH:O	1.91	0.69
2:B:532:HIS:HD2	2:B:555:GLU:OE2	1.75	0.69
2:E:445:LEU:C	2:E:445:LEU:CD2	2.61	0.69
2:B:176:LYS:HD3	2:B:180:HIS:CE1	2.29	0.68
2:B:803:GLU:OE1	2:B:808:HIS:HD2	1.75	0.68
2:B:670:VAL:O	2:B:808:HIS:HE1	1.77	0.68
3:F:192:ASP:OD2	9:F:5013:HOH:O	2.13	0.67
2:B:568:TYR:HB2	6:B:3921:CUB:H21	1.75	0.67
1:A:59:VAL:CG1	1:A:64[A]:MET:HE1	2.18	0.67
2:E:46:LEU:HD11	2:E:236[B]:TRP:CZ3	2.29	0.67
6:B:3921:CUB:OM1	6:B:3921:CUB:MO	1.66	0.66
2:E:390:PHE:CZ	6:E:4921:CUB:H22	2.30	0.66
2:E:627:GLU:CG	2:E:627:GLU:OE2	2.42	0.66
3:C:43:THR:HG21	9:C:4138:HOH:O	1.94	0.66
2:E:593:MET:HG2	2:E:603:GLU:CD	2.11	0.66
2:B:458:GLN:H	2:B:458:GLN:HE21	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21[B]:MET:HE3	2:B:756:ILE:CD1	2.27	0.65
2:E:21[A]:MET:HB2	2:E:21[A]:MET:HE3	1.78	0.65
2:B:522:ARG:NH1	9:B:4933:HOH:O	2.25	0.65
1:A:59:VAL:CG1	1:A:64[A]:MET:HE3	2.24	0.65
2:E:165:LYS:O	2:E:165:LYS:HG2	1.96	0.65
3:C:65:GLU:CD	3:C:86:PHE:CE1	2.70	0.65
6:E:4921:CUB:MO	6:E:4921:CUB:OM1	1.67	0.65
2:E:159:LEU:HD21	2:E:165:LYS:CD	2.20	0.65
1:A:95[A]:ARG:CZ	9:A:4204:HOH:O	2.45	0.64
1:A:95[A]:ARG:NE	9:A:4137:HOH:O	2.19	0.64
2:E:159:LEU:HD22	2:E:165:LYS:HE3	1.80	0.64
2:B:530:GLN:H	2:B:530:GLN:HE21	1.45	0.64
1:A:68:GLN:HB3	3:C:55[B]:ARG:HH21	1.63	0.63
2:B:754:HIS:HD2	2:B:756:ILE:H	1.45	0.63
3:F:8:TYR:OH	3:F:10[A]:ARG:HD3	1.98	0.63
1:D:92[B]:GLU:HG3	9:D:5018:HOH:O	1.98	0.63
3:C:65:GLU:CG	3:C:86:PHE:CE1	2.82	0.62
1:D:59:VAL:CG1	1:D:64[A]:MET:HE1	2.20	0.62
2:B:65:LYS:CG	2:B:141:GLU:HG3	2.00	0.62
1:A:135:ASN:HD21	3:C:105:GLN:HE22	1.48	0.61
2:B:588:LYS:HD2	9:B:4227:HOH:O	2.01	0.60
1:A:135:ASN:ND2	3:C:105:GLN:HE22	1.99	0.60
2:E:568:TYR:HB2	6:E:4921:CUB:H21	1.82	0.60
2:E:175:ARG:HB2	9:E:5742:HOH:O	2.02	0.60
3:F:221:ASN:H	3:F:221:ASN:HD22	1.48	0.60
1:D:160:PRO:HG2	9:D:5096:HOH:O	2.02	0.60
3:F:10[B]:ARG:HH11	3:F:10[B]:ARG:HB2	1.64	0.60
2:E:627:GLU:CG	2:E:627:GLU:OE1	2.50	0.60
1:A:84:ASP:OD2	1:A:86:THR:HG22	2.02	0.59
2:E:21[A]:MET:CB	2:E:21[A]:MET:HE3	2.33	0.58
2:E:124:LYS:CD	9:E:5739:HOH:O	2.34	0.58
2:E:159:LEU:HD22	2:E:165:LYS:CE	2.34	0.58
2:B:21[B]:MET:HE2	9:B:4240:HOH:O	2.04	0.57
3:F:221:ASN:HD22	3:F:221:ASN:N	2.01	0.57
2:B:754:HIS:CD2	2:B:756:ILE:H	2.22	0.57
2:B:115:ASN:OD1	2:B:302[A]:MET:CE	2.53	0.56
3:C:240:LYS:HB3	3:C:241:PRO:HD3	1.86	0.56
2:B:200:GLU:HG2	2:B:324:LYS:HG3	1.88	0.55
2:E:58:SER:OG	2:E:59:HIS:HD2	1.89	0.55
2:B:327:LYS:NZ	9:B:4910:HOH:O	2.39	0.55
2:B:689[B]:ARG:NH2	9:B:4243:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ILE:HD13	3:C:275[B]:LEU:HD11	1.89	0.54
2:E:597:HIS:HD2	9:E:5402:HOH:O	1.91	0.54
3:F:119:GLY:CA	9:F:5273:HOH:O	2.53	0.54
2:E:729[A]:MET:HE3	9:E:5129:HOH:O	2.06	0.54
2:B:153:MET:HA	2:B:177:HIS:CE1	2.43	0.54
2:E:165:LYS:O	2:E:165:LYS:CG	2.56	0.54
3:F:79:HIS:HD2	9:F:5210:HOH:O	1.89	0.54
2:E:442:ASN:C	2:E:442:ASN:HD22	2.10	0.54
2:E:597:HIS:HE1	9:E:5446:HOH:O	1.90	0.54
2:B:593:MET:HE2	2:B:640:LEU:HD21	1.89	0.53
1:A:155:LYS:NZ	9:A:4054:HOH:O	1.61	0.53
3:F:119:GLY:N	9:F:5273:HOH:O	2.38	0.53
3:C:197:ALA:HB3	3:C:217:THR:HB	1.91	0.53
1:D:159:VAL:N	1:D:160:PRO:CD	2.70	0.53
3:F:120:ASP:CB	9:F:5191:HOH:O	2.57	0.53
3:F:240:LYS:HB3	3:F:241:PRO:HD3	1.91	0.53
3:C:204[A]:MET:HG3	3:C:286:ALA:CB	2.39	0.53
1:D:95[A]:ARG:CZ	1:D:96[A]:MET:HE1	2.29	0.53
2:B:700:HIS:HE1	9:B:4006:HOH:O	1.92	0.53
2:E:505:MET:HA	2:E:565:LEU:HG	1.91	0.53
2:E:390:PHE:CE1	6:E:4921:CUB:H22	2.44	0.52
2:B:666[A]:MET:SD	2:B:777:VAL:HG22	2.48	0.52
2:B:390:PHE:CZ	6:B:3921:CUB:H22	2.44	0.52
2:E:159:LEU:CD2	2:E:165:LYS:HE3	2.40	0.52
2:B:6:THR:HG21	9:B:4803:HOH:O	2.09	0.52
2:B:573:THR:HB	2:B:574:PRO:HD3	1.92	0.52
2:E:65:LYS:HG3	9:E:5426:HOH:O	2.10	0.52
2:E:714:GLU:OE1	2:E:716[A]:ARG:HD3	2.10	0.52
2:E:714:GLU:CD	2:E:716[A]:ARG:HD3	2.30	0.52
2:B:327:LYS:HE2	2:B:420:LYS:NZ	2.25	0.52
3:F:145:ARG:NH2	3:F:162:GLU:HG3	2.25	0.52
2:B:460:ARG:NH1	2:B:463:GLN:HE22	2.00	0.52
9:A:4011:HOH:O	2:B:700:HIS:HD2	1.92	0.51
2:B:442:ASN:C	2:B:442:ASN:HD22	2.13	0.51
2:B:121:VAL:HG11	2:B:132:ALA:HB3	1.92	0.51
2:B:99:ALA:O	2:B:172:HIS:HE1	1.94	0.51
3:F:10[B]:ARG:CZ	3:F:56:ASP:OD2	2.59	0.51
2:E:176:LYS:C	9:E:5067:HOH:O	2.47	0.50
2:E:325:ASP:CG	9:E:5362:HOH:O	2.49	0.50
2:B:387:ARG:HA	2:B:763:GLU:HG2	1.93	0.50
2:E:573:THR:HB	2:E:574:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:GLN:NE2	2:B:530:GLN:H	2.09	0.49
3:F:197:ALA:HB3	3:F:217:THR:HB	1.94	0.49
2:B:466:LYS:HD3	2:B:479:MET:HB2	1.94	0.49
2:B:597:HIS:HD2	9:B:4594:HOH:O	1.94	0.49
2:B:127:TYR:HA	3:C:2:ILE:HG21	1.95	0.49
3:F:10[B]:ARG:CZ	9:F:5100:HOH:O	2.55	0.49
2:B:664[B]:CYS:HB3	2:B:680:PHE:CD2	2.48	0.49
2:E:14:ARG:CZ	2:E:612:ARG:HH22	2.26	0.49
2:B:718:ASP:HB3	2:B:724:LEU:HD11	1.95	0.49
2:E:159:LEU:CD2	2:E:165:LYS:CD	2.88	0.49
2:B:729:MET:HE3	2:B:729:MET:HA	1.94	0.49
2:B:593:MET:HG2	2:B:603:GLU:OE2	2.13	0.48
2:E:114:GLN:O	2:E:115:ASN:HB2	2.13	0.48
2:B:258:HIS:HE1	2:E:549:ASP:O	1.96	0.48
2:B:803:GLU:OE1	2:B:808:HIS:CD2	2.61	0.48
3:C:70:VAL:HG23	3:C:174:VAL:HG22	1.95	0.48
3:F:118:ASN:HD22	8:F:4931:FAD:H4B	1.79	0.48
2:E:387:ARG:HA	2:E:763:GLU:HG2	1.96	0.48
2:B:238:THR:HB	2:B:274:LYS:HD3	1.96	0.48
2:B:52:GLY:HA2	2:B:121:VAL:O	2.14	0.48
2:B:664[A]:CYS:HB2	2:B:680:PHE:CD2	2.49	0.48
3:C:79:HIS:HD2	9:C:4307:HOH:O	1.97	0.47
3:C:65:GLU:HG3	3:C:86:PHE:CZ	2.43	0.47
2:E:88:LYS:HE3	2:E:93:HIS:CD2	2.49	0.47
2:B:624:THR:HB	9:B:4304:HOH:O	2.14	0.47
2:E:683:LEU:C	2:E:683:LEU:HD23	2.35	0.47
2:B:350:LYS:HE3	9:B:4455:HOH:O	2.14	0.47
2:B:258:HIS:CD2	2:E:518:SER:HB2	2.50	0.47
2:B:662:TYR:OH	2:B:765:PRO:HA	2.15	0.47
2:B:588:LYS:NZ	9:B:4783:HOH:O	2.48	0.47
3:F:8:TYR:CZ	3:F:10[A]:ARG:HD3	2.50	0.47
3:F:10[A]:ARG:HD2	3:F:53:ASP:HB3	1.97	0.47
3:F:202:LEU:HD12	3:F:202:LEU:C	2.35	0.47
2:B:161:ARG:HB3	2:B:164:ILE:HG12	1.96	0.46
3:C:20[A]:LEU:HD11	9:C:4231:HOH:O	2.16	0.46
2:E:159:LEU:CD2	2:E:165:LYS:CE	2.93	0.46
2:E:52:GLY:HA2	2:E:121:VAL:O	2.15	0.46
2:E:121:VAL:HG11	2:E:132:ALA:HB3	1.98	0.46
3:C:114:GLY:O	3:C:118:ASN:HB2	2.16	0.46
2:B:533:GLU:OE1	9:B:4954:HOH:O	2.21	0.46
2:E:165:LYS:HG3	9:E:5352:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:204[A]:MET:HG3	3:F:286:ALA:CB	2.46	0.46
2:B:19:GLN:NE2	2:B:23[A]:CYS:SG	2.89	0.45
2:B:137:GLU:HG2	9:B:4893:HOH:O	2.16	0.45
2:B:258:HIS:CD2	2:B:258:HIS:H	2.34	0.45
2:B:505:MET:HA	2:B:565:LEU:HG	1.98	0.45
2:B:6:THR:HG22	2:B:7:VAL:H	1.82	0.45
2:B:666[A]:MET:SD	2:B:777:VAL:CG2	3.04	0.45
2:E:718:ASP:HB3	2:E:724:LEU:HD11	1.99	0.45
2:B:172:HIS:HD2	9:B:4855:HOH:O	2.00	0.45
2:B:53:ASP:CG	2:B:54:PHE:H	2.20	0.45
1:A:101:GLN:HB2	1:A:139:CYS:HB3	1.99	0.45
1:D:159:VAL:CB	1:D:160:PRO:HD3	2.39	0.45
2:B:6:THR:HG22	2:B:7:VAL:N	2.31	0.45
2:E:524:GLY:HA3	2:E:564:GLY:HA3	1.99	0.45
2:B:495:SER:CB	2:B:504[A]:SER:OG	2.64	0.44
3:C:222:THR:HB	3:C:223:PRO:HD2	1.99	0.44
1:D:109[A]:MET:HE2	1:D:109[A]:MET:HB3	1.82	0.44
2:B:161:ARG:HD3	2:B:341:ALA:O	2.17	0.44
2:B:489:ILE:HD11	2:B:655[A]:MET:HG3	2.00	0.44
2:E:99:ALA:O	2:E:172:HIS:HE1	2.01	0.44
2:E:588:LYS:HE3	2:E:608:TRP:CE2	2.52	0.44
2:B:200:GLU:CD	2:B:324:LYS:HG3	2.38	0.44
2:E:358:ILE:HD11	2:E:438:TYR:CE1	2.52	0.44
2:E:729[B]:MET:HE2	2:E:729[B]:MET:HB2	1.79	0.44
2:B:175:ARG:NH2	2:B:178:HIS:O	2.51	0.44
2:B:271:PHE:HA	7:B:3920:MCN:S7'	2.58	0.43
2:E:271:PHE:HA	7:E:4920:MCN:S7'	2.58	0.43
3:F:204[A]:MET:HG3	3:F:286:ALA:HB1	2.00	0.43
2:E:175:ARG:C	9:E:5350:HOH:O	2.56	0.43
2:B:63:ARG:HG2	9:B:4877:HOH:O	2.18	0.43
3:C:275[A]:LEU:HD23	3:C:275[A]:LEU:C	2.39	0.43
1:D:46:HIS:HE1	2:E:729[B]:MET:HE2	1.83	0.43
2:B:360:THR:HG21	2:B:433:PRO:HG2	2.01	0.43
3:C:204[A]:MET:HG3	3:C:286:ALA:HB1	2.01	0.43
2:E:522:ARG:NH1	9:E:5870:HOH:O	2.47	0.43
2:E:593:MET:HE1	9:E:5675:HOH:O	2.19	0.43
3:F:222:THR:HB	3:F:223:PRO:HD2	1.99	0.43
3:F:243:LEU:HD13	3:F:243:LEU:HA	1.91	0.43
2:E:273:ASN:ND2	2:E:304:ASN:HD21	2.06	0.43
2:B:200:GLU:CG	2:B:324:LYS:HG3	2.49	0.43
1:D:11:ASN:ND2	1:D:76:THR:H	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:106:ILE:HD13	8:F:4931:FAD:C7	2.48	0.43
2:B:213:HIS:CG	2:B:214:PRO:HD2	2.54	0.42
3:F:126:PRO:HB3	3:F:153:TYR:CZ	2.54	0.42
2:B:256:PRO:HB2	2:B:258:HIS:CD2	2.54	0.42
2:B:683:LEU:C	2:B:683:LEU:HD23	2.39	0.42
2:E:345:CYS:SG	2:E:384:VAL:HG23	2.59	0.42
1:D:64[A]:MET:HE2	1:D:64[A]:MET:HB2	1.85	0.42
3:F:240:LYS:N	3:F:241:PRO:CD	2.82	0.42
2:E:361:GLY:HA2	9:E:5029:HOH:O	2.20	0.42
2:E:243:HIS:CD2	2:E:563:TYR:HA	2.55	0.42
2:B:573:THR:O	2:B:754:HIS:HE1	2.03	0.42
2:B:495:SER:HB3	2:B:504[A]:SER:OG	2.19	0.41
3:C:286:ALA:C	9:C:4279:HOH:O	2.58	0.41
3:F:65:GLU:HB2	3:F:86:PHE:HZ	1.85	0.41
2:B:21[B]:MET:CE	2:B:756:ILE:CD1	2.97	0.41
3:F:276:ARG:O	3:F:280:GLU:HG3	2.20	0.41
2:B:203:SER:O	2:B:319:GLU:HA	2.21	0.41
1:D:46:HIS:HE1	2:E:729[B]:MET:CE	2.33	0.41
2:E:203:SER:O	2:E:319:GLU:HA	2.19	0.41
2:B:713:GLN:NE2	2:B:733:LEU:HD23	2.36	0.41
2:E:65:LYS:HB2	2:E:139:ASP:HB3	2.03	0.41
3:F:65:GLU:HB2	3:F:86:PHE:CZ	2.56	0.41
2:E:159:LEU:HA	2:E:178:HIS:CD2	2.55	0.41
2:E:350:LYS:HE3	9:E:5544:HOH:O	2.21	0.41
2:E:662:TYR:OH	2:E:765:PRO:HA	2.21	0.41
1:A:82:ALA:CB	1:A:86:THR:HG22	2.43	0.41
2:B:428:PHE:HA	2:B:429:PRO:C	2.41	0.41
3:C:70:VAL:HG23	3:C:174:VAL:CG2	2.50	0.41
2:E:65:LYS:CG	9:E:5426:HOH:O	2.68	0.41
2:E:716[A]:ARG:NH1	9:E:5171:HOH:O	2.39	0.41
3:F:35:HIS:HD2	3:F:106:ILE:HG12	1.86	0.41
1:D:95[B]:ARG:HD2	2:E:30:ASP:HB2	2.02	0.41
2:B:532:HIS:CE1	7:B:3920:MCN:O2B	2.53	0.40
2:B:359:CYS:O	2:B:399:ILE:HB	2.21	0.40
2:B:593:MET:CE	2:B:640:LEU:HD21	2.50	0.40
3:C:8:TYR:OH	3:C:10[A]:ARG:HD3	2.21	0.40
2:B:39:ASN:O	2:B:265:PRO:HB2	2.21	0.40
3:F:31:LEU:HB3	3:F:53:ASP:HA	2.04	0.40

All (9) 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)
2:B:7:VAL:CB	9:B:4950:HOH:O[4_477]	1.17	1.03
2:B:7:VAL:CG1	9:B:4950:HOH:O[4_477]	1.51	0.69
2:B:7:VAL:CG2	9:B:4950:HOH:O[4_477]	1.64	0.56
9:B:4928:HOH:O	9:D:5093:HOH:O[4_477]	1.69	0.51
9:E:5511:HOH:O	9:E:5739:HOH:O[2_685]	1.88	0.32
9:B:4600:HOH:O	9:E:5851:HOH:O[4_577]	2.07	0.13
2:E:21[A]:MET:CE	9:A:4107:HOH:O[4_577]	2.13	0.07
9:B:4845:HOH:O	9:D:5003:HOH:O[4_477]	2.16	0.04
9:B:4554:HOH:O	9:F:5250:HOH:O[1_545]	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	165/166 (99%)	162 (98%)	3 (2%)	0	100	100
1	D	165/166 (99%)	162 (98%)	3 (2%)	0	100	100
2	B	817/809 (101%)	785 (96%)	28 (3%)	4 (0%)	29	6
2	E	813/809 (100%)	788 (97%)	22 (3%)	3 (0%)	34	10
3	C	293/288 (102%)	287 (98%)	6 (2%)	0	100	100
3	F	290/288 (101%)	285 (98%)	5 (2%)	0	100	100
All	All	2543/2526 (101%)	2469 (97%)	67 (3%)	7 (0%)	41	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	265	PRO
2	B	312	ARG
2	B	712	GLY
2	E	312	ARG
2	E	712	GLY
2	E	265	PRO
2	B	91	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/131 (103%)	134 (99%)	1 (1%)	84	57
1	D	134/131 (102%)	133 (99%)	1 (1%)	84	57
2	B	663/653 (102%)	645 (97%)	18 (3%)	44	9
2	E	661/653 (101%)	647 (98%)	14 (2%)	53	14
3	C	219/212 (103%)	218 (100%)	1 (0%)	88	66
3	F	216/212 (102%)	213 (99%)	3 (1%)	67	30
All	All	2028/1992 (102%)	1990 (98%)	38 (2%)	59	18

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
2	B	65	LYS
2	B	91	ASN
2	B	159	LEU
2	B	165	LYS
2	B	167	LYS
2	B	176	LYS
2	B	209	TYR
2	B	258	HIS
2	B	313	ASP
2	B	386	TYR
2	B	393	THR
2	B	442	ASN
2	B	458	GLN
2	B	488	GLU
2	B	507	ASP
2	B	530	GLN
2	B	664[A]	CYS
2	B	664[B]	CYS
3	C	59	ASP
1	D	100	LEU
2	E	21[A]	MET

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Mol	Chain	Res	Type
2	E	21[B]	MET
2	E	65	LYS
2	E	167	LYS
2	E	168	MET
2	E	198	LYS
2	E	209	TYR
2	E	313	ASP
2	E	386	TYR
2	E	393	THR
2	E	442	ASN
2	E	445	LEU
2	E	488	GLU
2	E	507	ASP
3	F	87	LEU
3	F	208	LYS
3	F	221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	135	ASN
2	B	19	GLN
2	B	91	ASN
2	B	172	HIS
2	B	258	HIS
2	B	273	ASN
2	B	304	ASN
2	B	442	ASN
2	B	458	GLN
2	B	463	GLN
2	B	530	GLN
2	B	532	HIS
2	B	592	GLN
2	B	698	GLN
2	B	700	HIS
2	B	754	HIS
2	B	808	HIS
3	C	79	HIS
3	C	118	ASN
1	D	11	ASN
2	E	59	HIS

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Mol	Chain	Res	Type
2	E	91	ASN
2	E	115	ASN
2	E	172	HIS
2	E	273	ASN
2	E	442	ASN
2	E	463	GLN
2	E	597	HIS
2	E	698	GLN
2	E	720	GLN
2	E	804	GLN
3	F	78	GLN
3	F	79	HIS
3	F	118	ASN
3	F	221	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
6	CUB	E	4921	2,7	3,12,12	2.09	1 (33%)	2,20,20	1.61	1 (50%)
8	FAD	C	3932	-	53,58,58	1.31	3 (5%)	68,89,89	1.39	9 (13%)
5	FES	D	4908	1	0,4,4	-	-	-	-	-
8	FAD	F	4931	-	53,58,58	1.20	2 (3%)	68,89,89	1.20	7 (10%)
6	CUB	B	3921	2,7	3,12,12	2.17	2 (66%)	2,20,20	1.38	0
7	MCN	B	3920	6	41,48,48	1.99	8 (19%)	49,74,74	1.67	7 (14%)
5	FES	A	3908	1	0,4,4	-	-	-	-	-
5	FES	D	4907	1	0,4,4	-	-	-	-	-
5	FES	A	3907	1	0,4,4	-	-	-	-	-
7	MCN	E	4920	6	41,48,48	2.53	9 (21%)	49,74,74	1.94	9 (18%)
4	PO4	A	4001	-	4,4,4	1.18	0	6,6,6	0.98	0

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
6	CUB	E	4921	2,7	1/1/3/3	1/2/25/25	0/2/2/2
8	FAD	F	4931	-	-	2/30/50/50	0/6/6/6
5	FES	D	4908	1	-	-	0/1/1/1
6	CUB	B	3921	2,7	1/1/3/3	1/2/25/25	0/2/2/2
7	MCN	B	3920	6	-	0/22/54/54	0/5/5/5
5	FES	D	4907	1	-	-	0/1/1/1
5	FES	A	3908	1	-	-	0/1/1/1
8	FAD	C	3932	-	-	2/30/50/50	0/6/6/6
5	FES	A	3907	1	-	-	0/1/1/1
7	MCN	E	4920	6	-	0/22/54/54	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4920	MCN	O9'-C7	9.61	1.47	1.35
7	E	4920	MCN	C6'-C7	9.09	1.57	1.43
7	B	3920	MCN	C6'-C7	8.03	1.55	1.43
7	B	3920	MCN	O9'-C7	4.74	1.41	1.35
7	B	3920	MCN	C7-N8'	4.71	1.42	1.30
7	E	4920	MCN	C10-C9'	-3.80	1.46	1.52
7	E	4920	MCN	C7-N8'	3.61	1.39	1.30
8	C	3932	FAD	C4X-N5	3.60	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4920	MCN	C2-N1	-3.40	1.32	1.40
8	F	4931	FAD	C4X-N5	3.09	1.36	1.30
8	F	4931	FAD	O4B-C4B	-3.02	1.38	1.45
8	C	3932	FAD	O4B-C4B	-2.86	1.38	1.45
7	B	3920	MCN	C6'-N5'	2.85	1.36	1.32
6	B	3921	CUB	C1Z-C2Z	-2.81	1.40	1.51
7	E	4920	MCN	C1'-N1	-2.67	1.39	1.47
6	E	4921	CUB	C4Z-C3Z	2.50	1.70	1.49
8	C	3932	FAD	C2A-N3A	2.44	1.36	1.32
7	E	4920	MCN	C4B-N8'	-2.33	1.32	1.36
7	E	4920	MCN	C5'-C4D	-2.28	1.44	1.51
7	B	3920	MCN	C4A-C4B	-2.27	1.36	1.40
7	B	3920	MCN	C2-N1	-2.23	1.35	1.40
7	B	3920	MCN	C6-C5	-2.14	1.30	1.35
7	B	3920	MCN	O4D-C1'	-2.14	1.36	1.42
7	E	4920	MCN	PB-O2B	-2.12	1.45	1.55
6	B	3921	CUB	C3Z-C2Z	-2.11	1.36	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	4920	MCN	O9'-C7-N8'	-6.59	107.13	115.30
7	B	3920	MCN	O9'-C7-N8'	-6.32	107.45	115.30
7	E	4920	MCN	N1'-C2'-N3'	-5.50	119.89	127.22
7	B	3920	MCN	N1'-C2'-N3'	-5.30	120.15	127.22
7	E	4920	MCN	N4-C4-N3	4.49	125.85	117.97
8	C	3932	FAD	O3B-C3B-C4B	4.47	123.98	111.05
7	E	4920	MCN	C5-C4-N4	-4.27	113.85	120.57
8	C	3932	FAD	N3A-C2A-N1A	-4.01	122.41	128.68
8	C	3932	FAD	C4X-C10-N10	3.49	121.58	116.48
8	C	3932	FAD	C3B-C2B-C1B	-3.38	95.89	100.98
7	B	3920	MCN	C2'-N3'-C4'	3.35	124.89	116.43
8	F	4931	FAD	C2B-C3B-C4B	-3.19	96.43	102.64
8	F	4931	FAD	O4B-C4B-C3B	3.17	111.39	105.11
7	E	4920	MCN	C7-N8'-C4B	3.16	119.30	116.61
7	E	4920	MCN	C2'-N1'-C4B	3.15	118.95	115.36
8	C	3932	FAD	C5A-C6A-N6A	2.96	124.85	120.35
7	B	3920	MCN	C5-C4-N4	-2.96	115.91	120.57
8	F	4931	FAD	C9A-C5X-N5	-2.82	119.37	122.43
7	B	3920	MCN	N4-C4-N3	2.75	122.80	117.97
7	E	4920	MCN	C2'-N3'-C4'	2.67	123.15	116.43
8	C	3932	FAD	C10-C4X-N5	-2.66	119.22	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	3932	FAD	C5B-C4B-C3B	2.46	124.39	115.18
7	B	3920	MCN	O4'-C4'-C4A	2.36	124.09	119.67
8	F	4931	FAD	C4X-C10-N10	2.36	119.93	116.48
7	E	4920	MCN	N2'-C2'-N1'	2.29	121.52	117.79
6	E	4921	CUB	C1Z-C2Z-C3Z	2.27	121.15	111.78
7	E	4920	MCN	O2-C2-N3	-2.21	118.74	122.33
8	F	4931	FAD	C5X-C9A-N10	2.16	120.19	117.95
8	F	4931	FAD	C4-N3-C2	-2.13	121.70	125.64
8	C	3932	FAD	O4B-C4B-C5B	2.12	116.36	109.37
7	B	3920	MCN	N2'-C2'-N1'	2.11	121.22	117.79
8	F	4931	FAD	O4'-C4'-C5'	-2.08	105.23	109.92
8	C	3932	FAD	O5B-C5B-C4B	-2.02	102.03	108.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	3921	CUB	CZ
6	E	4921	CUB	CZ

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	4921	CUB	NZ-C1Z-C2Z-C3Z
6	B	3921	CUB	NZ-C1Z-C2Z-C3Z
8	C	3932	FAD	PA-O3P-P-O1P
8	C	3932	FAD	PA-O3P-P-O2P
8	F	4931	FAD	PA-O3P-P-O1P
8	F	4931	FAD	PA-O3P-P-O2P

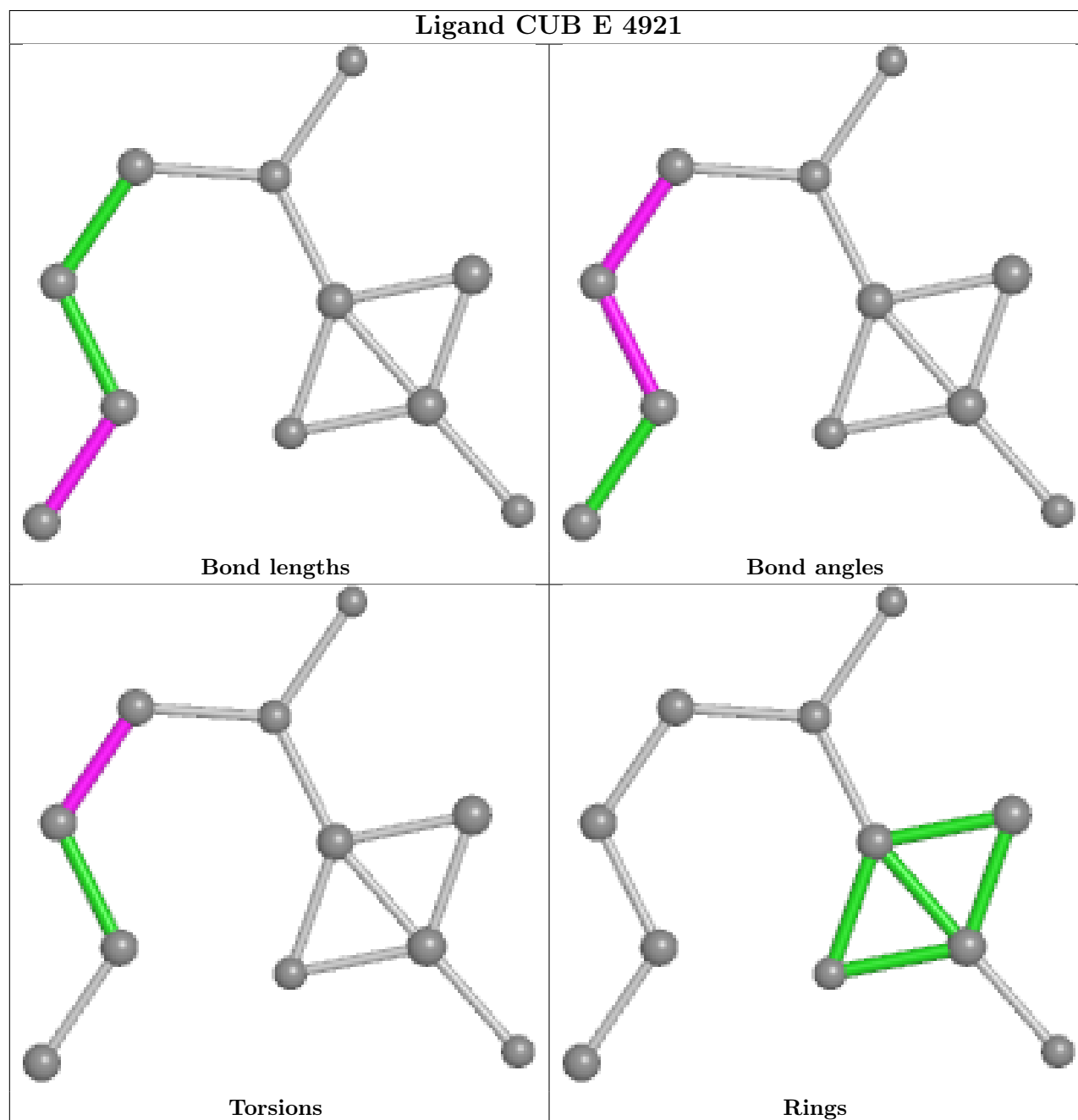
There are no ring outliers.

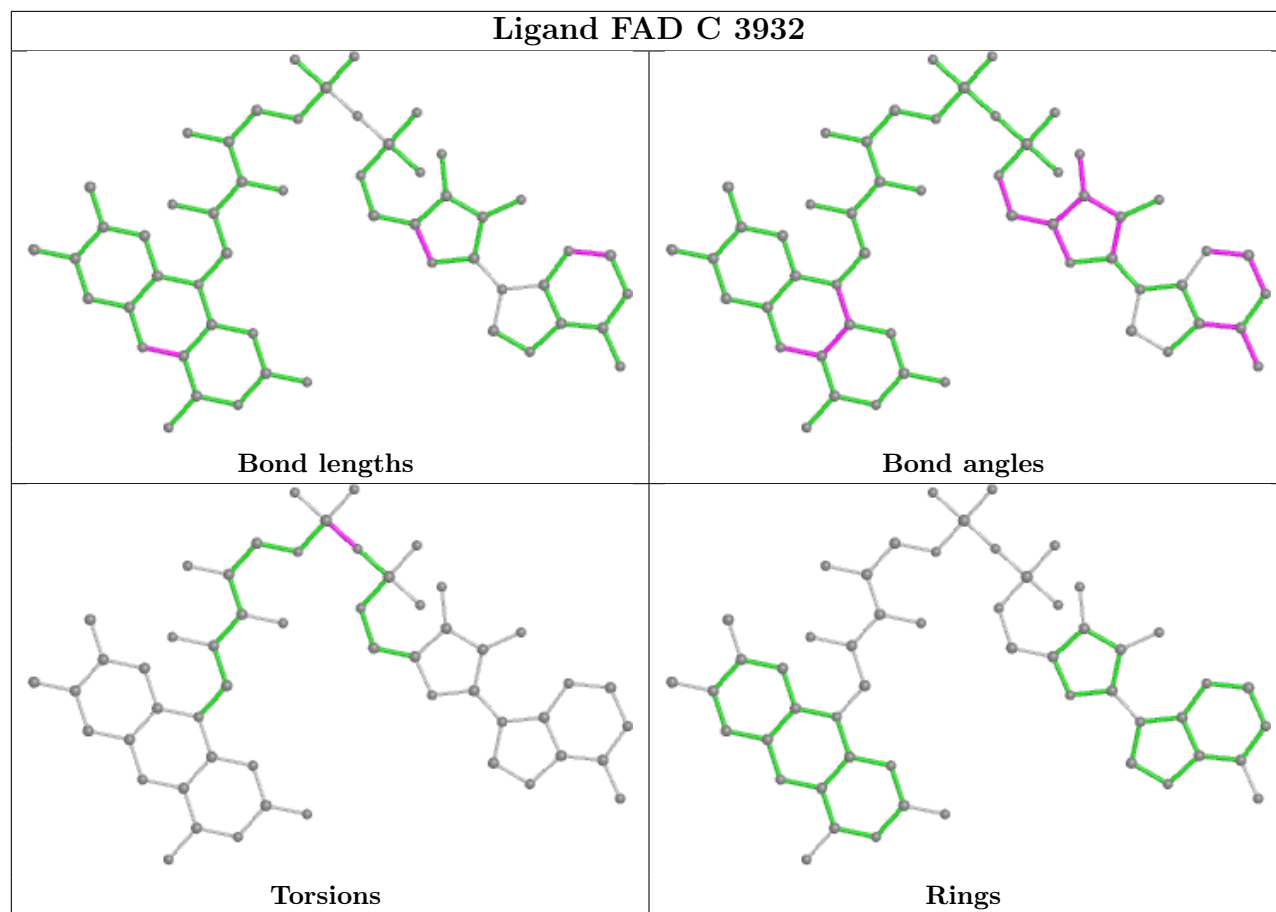
5 monomers are involved in 13 short contacts:

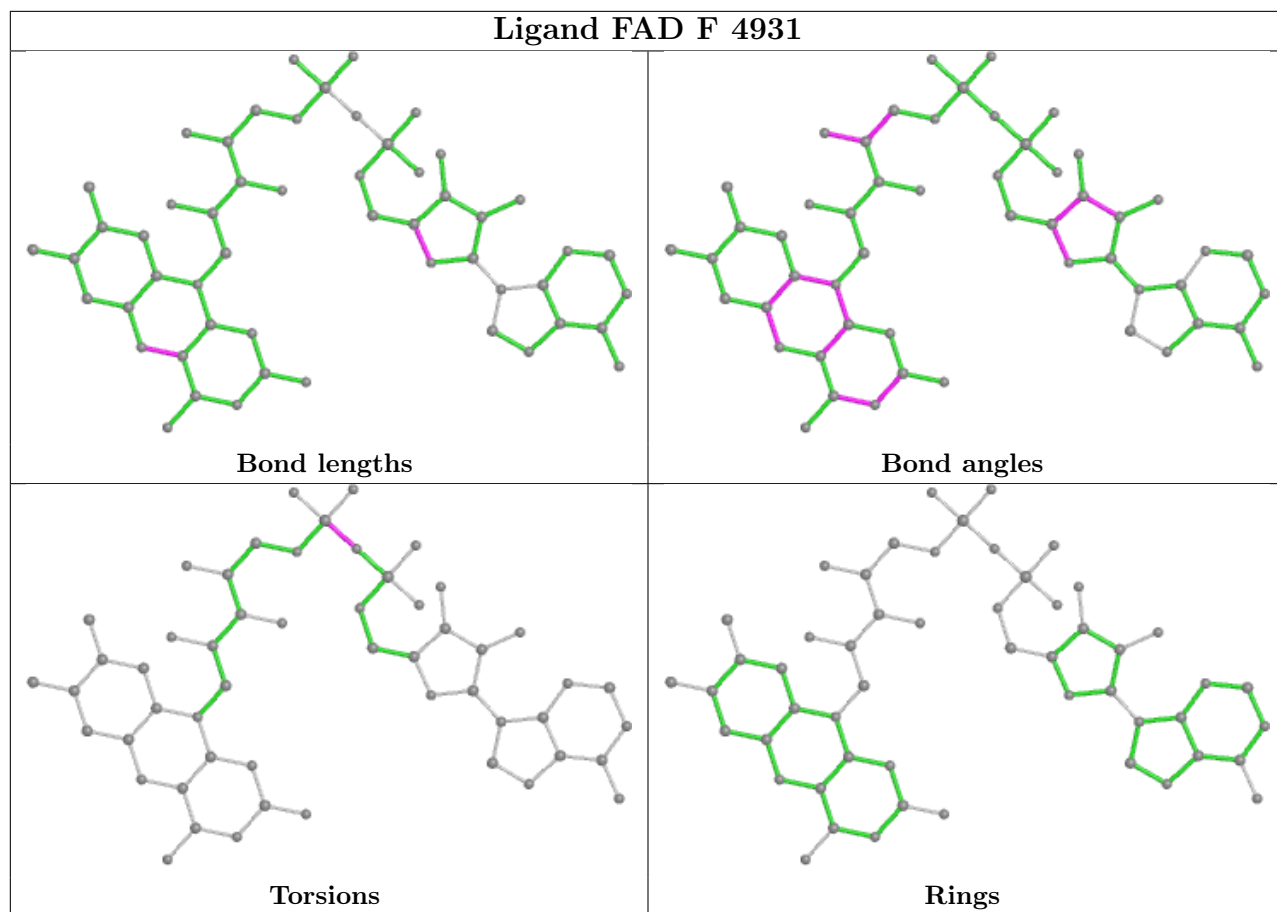
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	4921	CUB	4	0
8	F	4931	FAD	2	0
6	B	3921	CUB	3	0
7	B	3920	MCN	3	0
7	E	4920	MCN	1	0

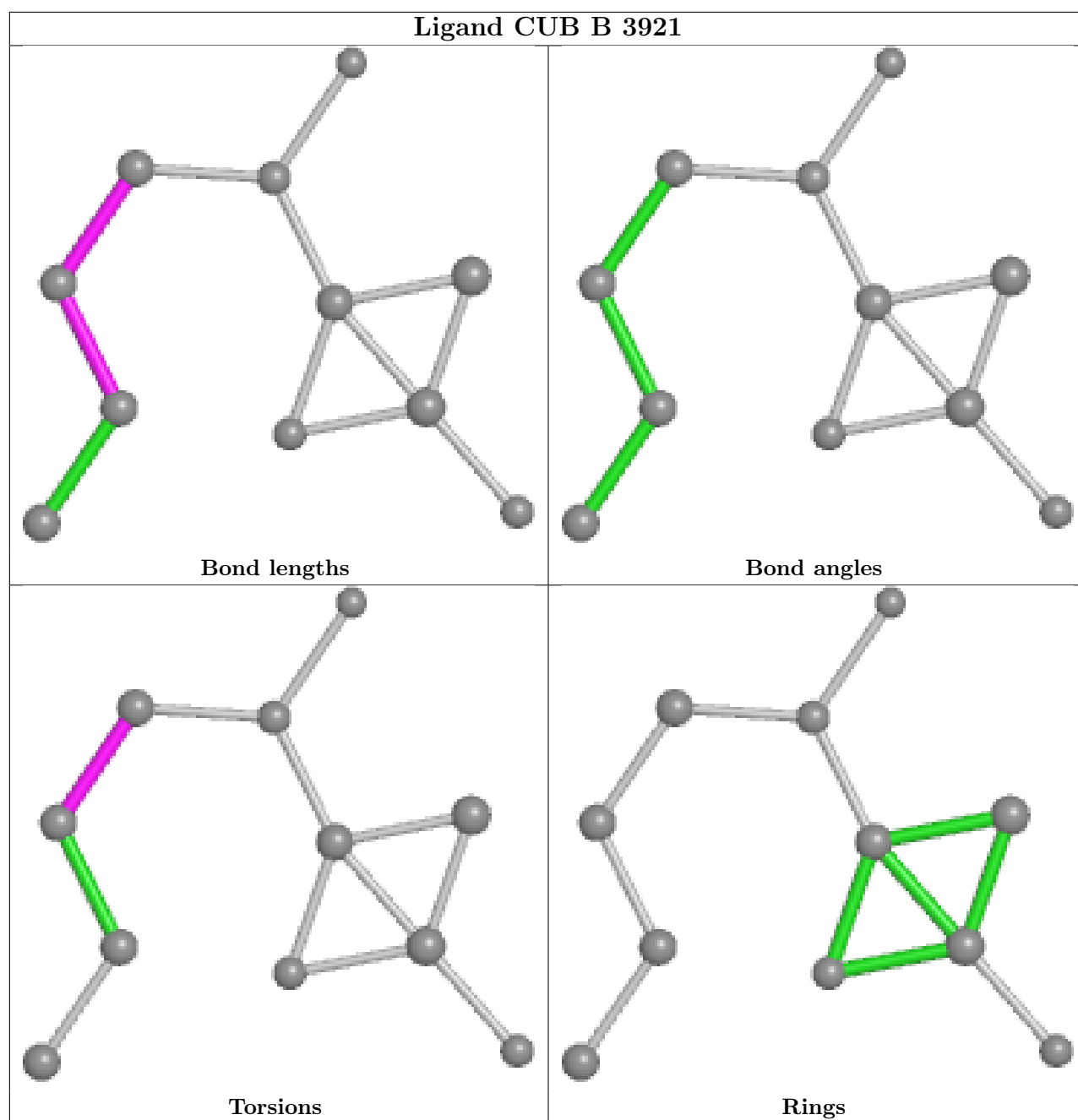
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

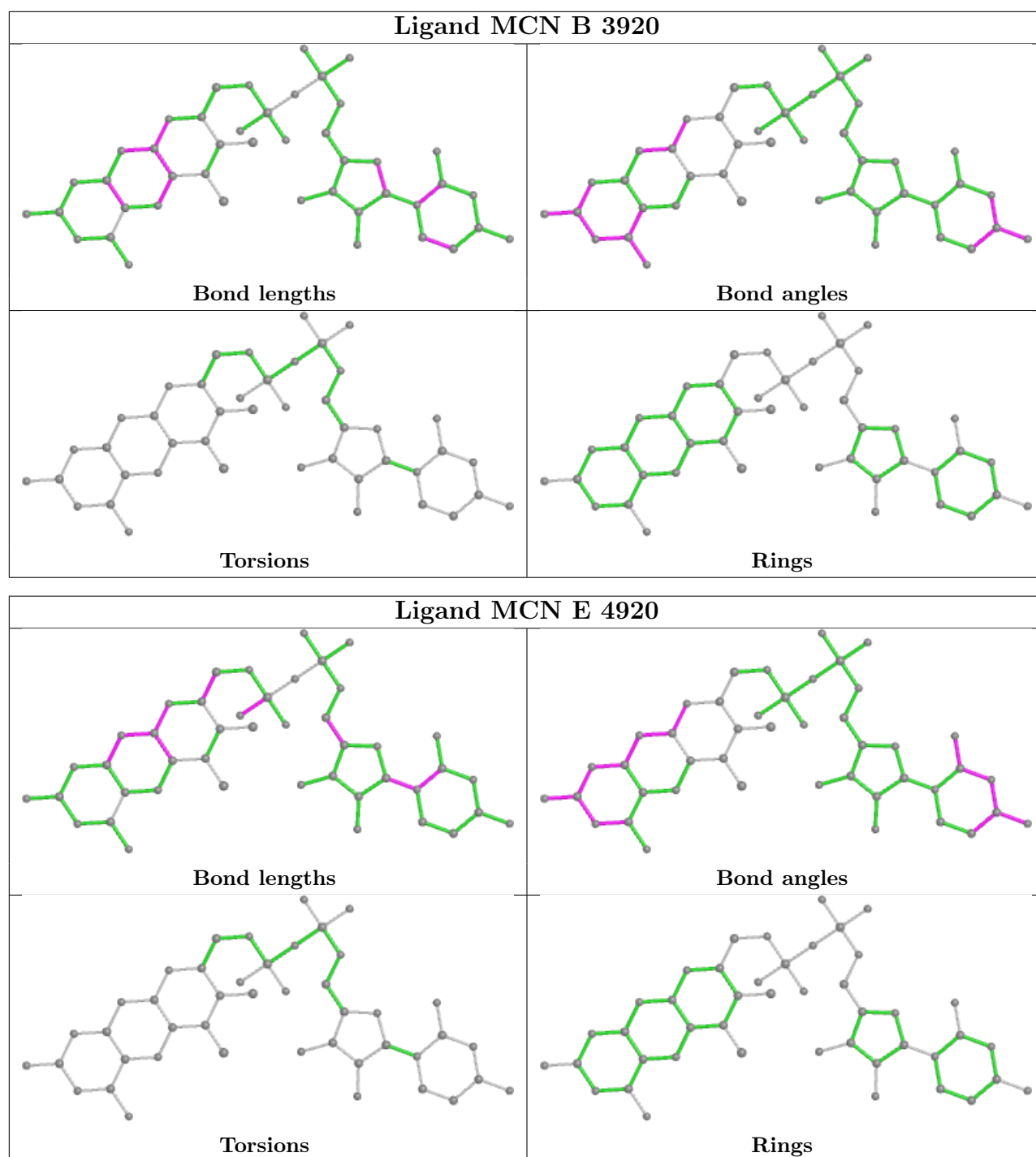
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	617:GLY	C	618:LEU	N	1.60
1	E	165:LYS	C	166:ASP	N	1.12

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.