



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 PM UTC

PDB ID : 1KQG / pdb_00001kqg
Title : FORMATE DEHYDROGENASE N FROM E. COLI
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Deposited on : 2002-01-05
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

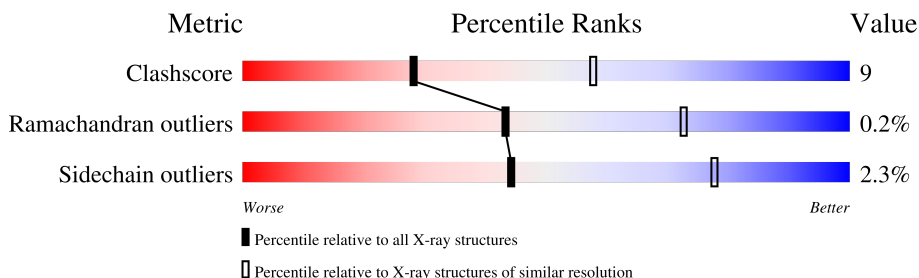
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	1015	
2	B	294	
3	C	217	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14003 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	982	Total	C	N	O	S	Se	0	0	0
			7719	4872	1352	1457	37	1			

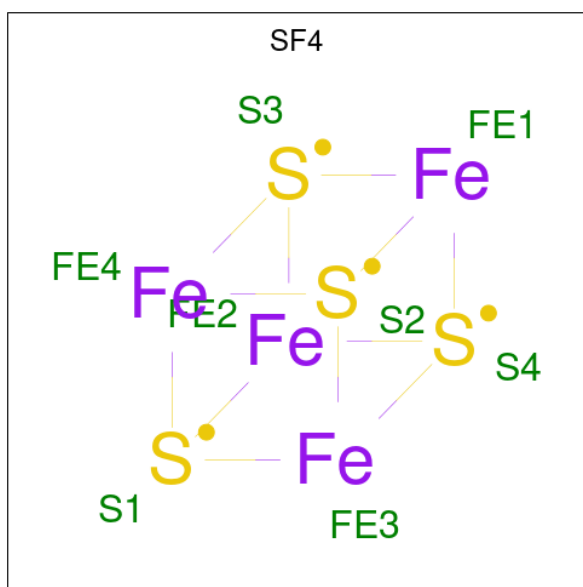
- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2207	1383	381	421	22			

- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

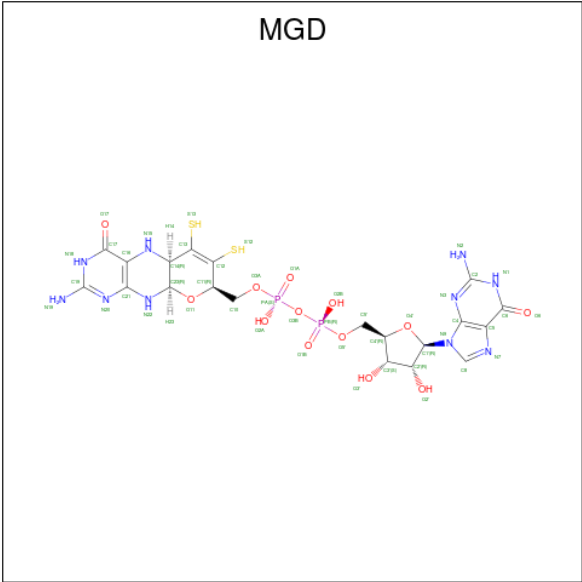
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1783	1192	301	276	14			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

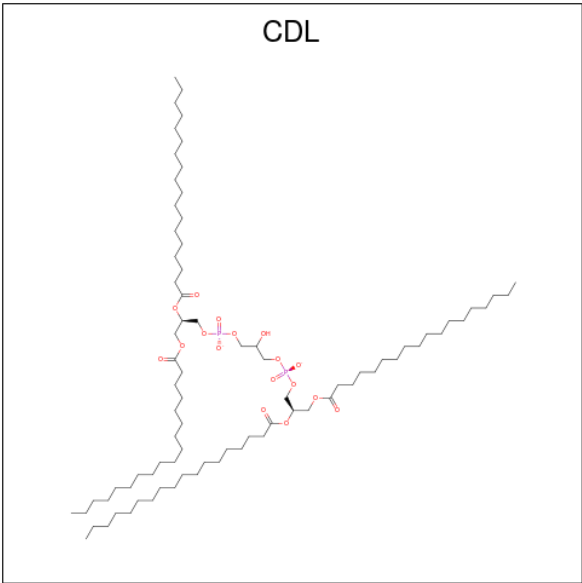


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM(VI) ION (CCD ID: 6MO) (formula: Mo).

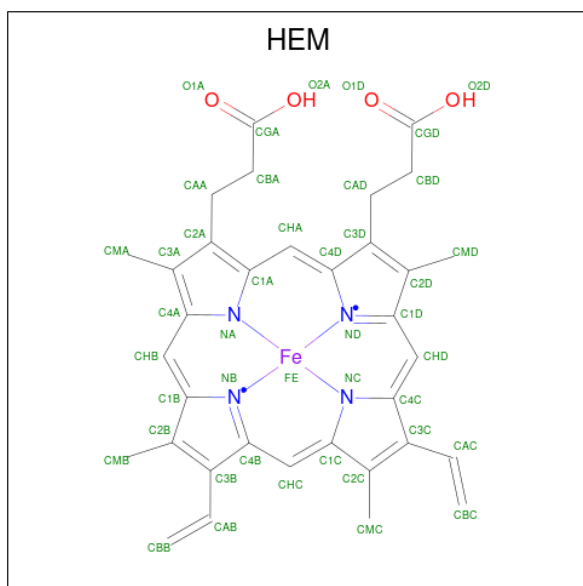
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

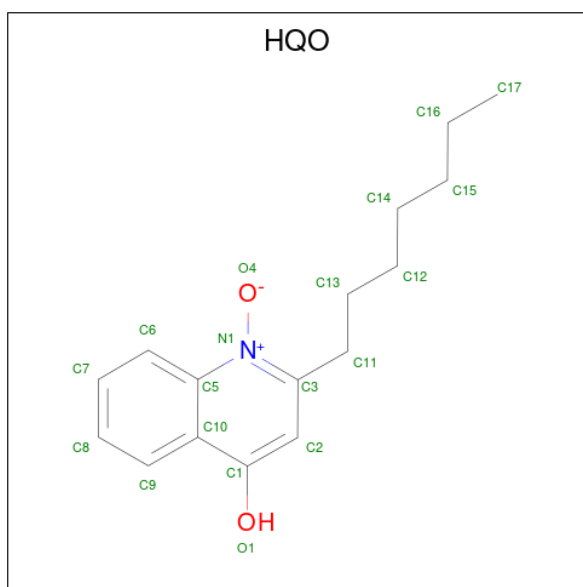
- Molecule 7 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	P	0	0
			70	51	17	2		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			19	16	1	2		

- Molecule 10 is water.

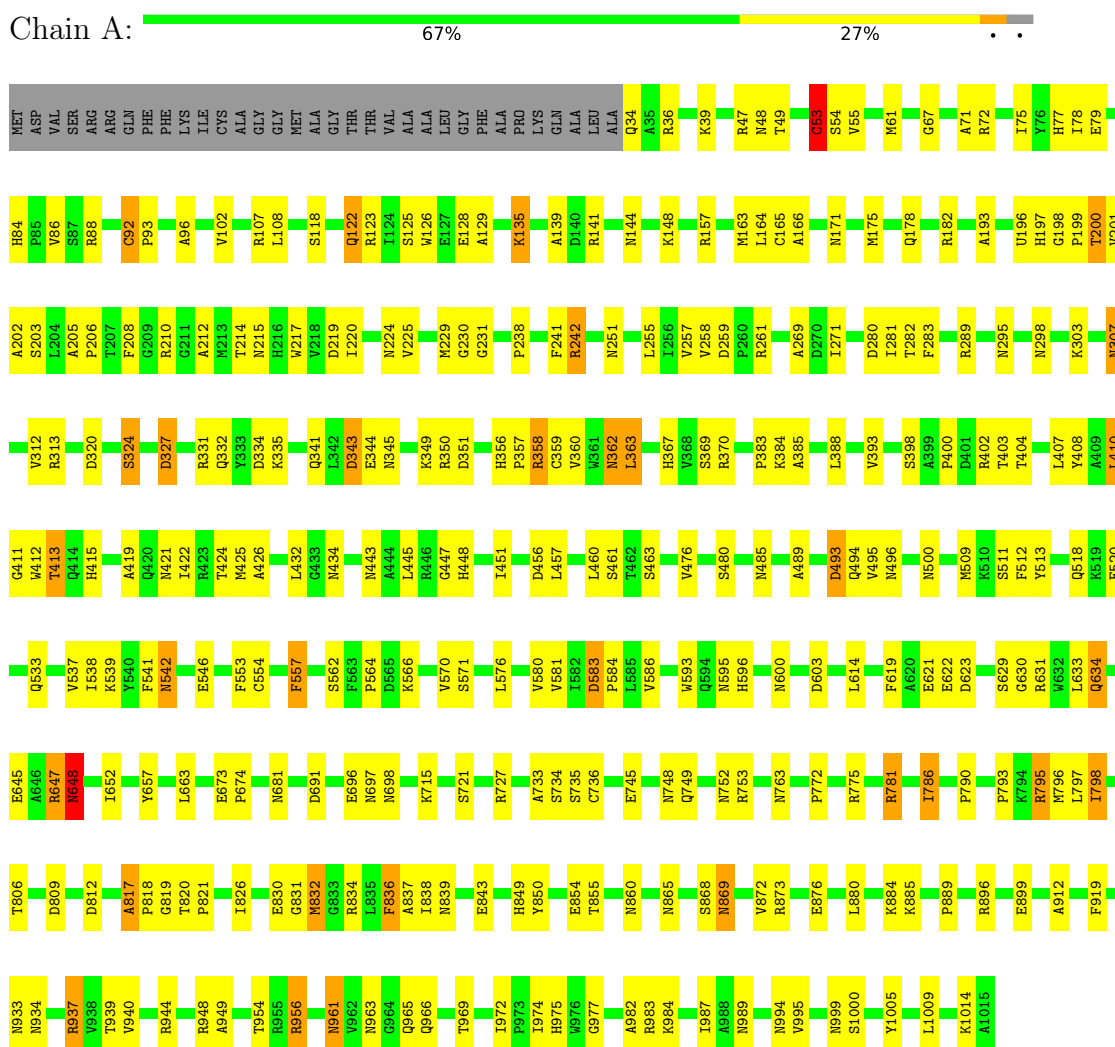
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1493	Total	O	0	0
			1493	1493		
10	B	410	Total	O	0	0
			410	410		
10	C	81	Total	O	0	0
			81	81		

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.

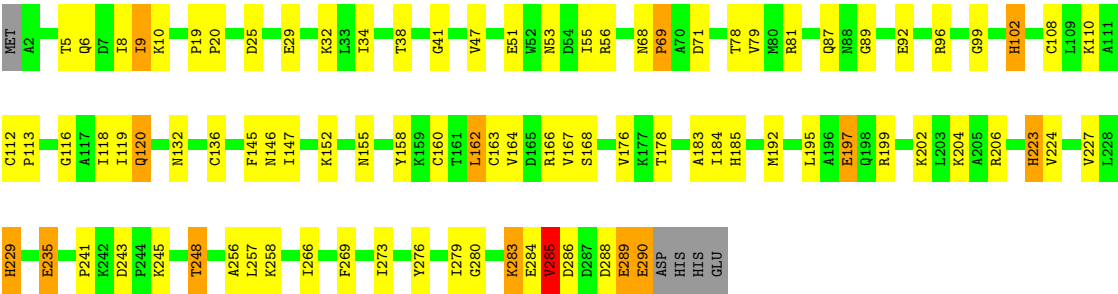
Note EDS was not executed.

• Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT



• Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT





● Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	203.00 Å 203.00 Å 203.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.8 (40.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14003	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: CDL, SF4, HEM, SEC, HQO, MGD, 6MO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	0/7910	2.09	289/10749 (2.7%)
2	B	0.91	1/2255 (0.0%)	2.03	77/3056 (2.5%)
3	C	0.80	0/1840	1.94	57/2483 (2.3%)
All	All	0.89	1/12005 (0.0%)	2.05	423/16288 (2.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	243	ASP	CA-CB	6.64	1.57	1.52

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	GLN	OE1-CD-NE2	-20.94	101.66	122.60
1	A	88	ARG	NE-CZ-NH2	-18.83	102.25	119.20
1	A	648	ASN	OD1-CG-ND2	15.46	138.06	122.60
1	A	698	ASN	OD1-CG-ND2	-14.83	107.77	122.60
2	B	6	GLN	OE1-CD-NE2	-11.71	110.89	122.60
1	A	937	ARG	NH1-CZ-NH2	11.61	134.39	119.30
1	A	937	ARG	NE-CZ-NH2	-10.70	109.57	119.20
1	A	157	ARG	NE-CZ-NH2	10.40	128.56	119.20
1	A	748	ASN	OD1-CG-ND2	10.40	133.00	122.60
3	C	86	ILE	CA-C-O	10.31	125.60	118.69
1	A	974	ILE	N-CA-C	10.00	120.81	111.91
1	A	225	VAL	CA-C-O	-9.67	109.89	120.43
1	A	178	GLN	OE1-CD-NE2	9.59	132.19	122.60
2	B	229	HIS	CA-CB-CG	9.53	123.33	113.80
1	A	583	ASP	N-CA-CB	-9.46	102.38	111.27
1	A	313	ARG	NE-CZ-NH1	-9.24	112.26	121.50
1	A	410	LEU	CA-C-O	-9.23	109.35	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH2	9.15	127.44	119.20
2	B	290	GLU	CA-C-O	-9.14	105.27	120.80
1	A	533	GLN	OE1-CD-NE2	9.11	131.71	122.60
1	A	259	ASP	CA-CB-CG	9.06	121.66	112.60
1	A	225	VAL	O-C-N	8.79	132.56	123.07
1	A	752	ASN	OD1-CG-ND2	8.72	131.32	122.60
1	A	975	HIS	N-CA-C	8.67	123.85	113.28
1	A	426	ALA	O-C-N	8.65	131.29	122.12
1	A	182	ARG	NE-CZ-NH1	-8.60	112.90	121.50
2	B	155	ASN	OD1-CG-ND2	8.53	131.13	122.60
2	B	112	CYS	O-C-N	-8.42	113.81	121.30
1	A	542	ASN	CA-C-O	8.42	129.34	120.42
2	B	276	TYR	CA-C-O	8.39	129.63	120.82
1	A	834	ARG	NH1-CZ-NH2	-8.36	108.43	119.30
2	B	81	ARG	NH1-CZ-NH2	8.31	130.10	119.30
3	C	105	ASP	CA-CB-CG	8.27	120.87	112.60
3	C	79	ASN	OD1-CG-ND2	8.24	130.84	122.60
2	B	227	VAL	N-CA-CB	8.17	121.75	111.46
1	A	873	ARG	NE-CZ-NH1	8.14	129.64	121.50
1	A	443	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	335	LYS	N-CA-CB	-8.00	99.52	110.56
1	A	88	ARG	NH1-CZ-NH2	7.99	129.69	119.30
1	A	332	GLN	CB-CG-CD	7.99	126.17	112.60
1	A	215	ASN	OD1-CG-ND2	-7.95	114.66	122.60
3	C	136	ARG	CA-C-O	-7.94	112.81	120.19
1	A	165	CYS	CA-C-O	7.91	130.10	121.16
1	A	869	ASN	OD1-CG-ND2	7.89	130.49	122.60
2	B	112	CYS	CA-C-O	7.89	127.17	119.75
1	A	956	ARG	NE-CZ-NH1	-7.86	113.64	121.50
1	A	75	ILE	O-C-N	-7.82	114.15	122.67
2	B	283	LYS	CA-C-O	-7.78	112.78	121.89
1	A	171	ASN	OD1-CG-ND2	7.76	130.36	122.60
1	A	839	ASN	OD1-CG-ND2	7.76	130.36	122.60
3	C	74	ARG	NE-CZ-NH2	-7.72	112.25	119.20
1	A	963	ASN	OD1-CG-ND2	7.71	130.31	122.60
2	B	9	ILE	O-C-N	-7.71	113.09	122.18
1	A	407	LEU	CA-C-O	-7.70	112.22	120.46
1	A	542	ASN	O-C-N	-7.63	113.45	122.15
3	C	149	ARG	NH1-CZ-NH2	7.59	129.17	119.30
1	A	157	ARG	NH1-CZ-NH2	-7.57	109.45	119.30
1	A	798	ILE	O-C-N	-7.56	114.38	123.00
1	A	1005	TYR	CA-CB-CG	7.49	127.38	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	138	TYR	N-CA-C	7.42	119.01	111.07
1	A	961	ASN	OD1-CG-ND2	7.39	129.99	122.60
1	A	648	ASN	CB-CG-ND2	-7.38	105.33	116.40
1	A	796	MET	CA-C-O	-7.38	112.28	120.69
1	A	542	ASN	OD1-CG-ND2	7.37	129.97	122.60
1	A	681	ASN	OD1-CG-ND2	7.32	129.92	122.60
1	A	937	ARG	CG-CD-NE	-7.29	95.97	112.00
1	A	614	LEU	O-C-N	7.27	130.31	121.29
2	B	276	TYR	O-C-N	-7.27	114.58	122.07
1	A	166	ALA	N-CA-C	7.25	120.70	108.23
1	A	554	CYS	CA-C-O	-7.22	111.48	120.57
1	A	974	ILE	N-CA-CB	-7.21	103.95	112.39
2	B	81	ARG	NE-CZ-NH1	-7.20	114.30	121.50
1	A	983	ARG	NH1-CZ-NH2	7.20	128.66	119.30
1	A	201	VAL	CA-C-O	-7.15	113.51	120.95
1	A	219	ASP	O-C-N	-7.14	113.11	122.39
1	A	939	THR	CA-C-O	-7.12	112.68	120.30
3	C	164	HIS	CA-C-O	7.12	128.29	120.82
1	A	410	LEU	O-C-N	7.08	130.98	122.27
1	A	734	SER	O-C-N	-7.08	114.48	123.26
1	A	786	ILE	CA-C-O	7.03	128.09	120.57
1	A	999	ASN	OD1-CG-ND2	7.00	129.60	122.60
3	C	9	ARG	NE-CZ-NH2	6.97	125.48	119.20
1	A	334	ASP	N-CA-C	-6.96	97.90	108.96
1	A	107	ARG	NE-CZ-NH2	6.95	125.45	119.20
1	A	763	ASN	CB-CG-ND2	6.94	126.81	116.40
1	A	135	LYS	O-C-N	-6.93	114.93	122.07
1	A	212	ALA	N-CA-C	6.93	120.78	110.52
1	A	621	GLU	CA-C-O	-6.93	111.78	119.95
3	C	105	ASP	CA-C-N	-6.90	114.15	123.12
3	C	105	ASP	C-N-CA	-6.90	114.15	123.12
1	A	144	ASN	N-CA-C	6.90	122.54	113.30
1	A	281	ILE	O-C-N	-6.89	114.91	121.87
1	A	520	GLU	CB-CG-CD	6.86	124.26	112.60
2	B	99	GLY	CA-C-O	-6.81	114.88	121.83
2	B	41	GLY	O-C-N	6.80	128.76	122.57
2	B	243	ASP	CA-C-O	6.79	125.71	120.48
1	A	533	GLN	CA-C-O	-6.79	114.05	121.31
1	A	280	ASP	CA-C-O	-6.78	113.31	120.63
1	A	786	ILE	O-C-N	-6.78	115.02	121.87
2	B	227	VAL	N-CA-C	-6.75	98.01	107.80
3	C	54	ARG	NE-CZ-NH2	6.74	125.27	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	934	ASN	CA-C-O	6.71	128.27	120.96
1	A	494	GLN	OE1-CD-NE2	6.68	129.28	122.60
3	C	15	ARG	NE-CZ-NH2	-6.67	113.20	119.20
2	B	289	GLU	CA-CB-CG	6.67	127.43	114.10
1	A	298	ASN	OD1-CG-ND2	-6.66	115.94	122.60
2	B	283	LYS	O-C-N	6.64	130.45	122.68
3	C	108	LYS	CA-C-O	-6.63	113.78	121.07
1	A	141	ARG	NH1-CZ-NH2	-6.62	110.69	119.30
1	A	220	ILE	O-C-N	-6.60	115.20	121.87
1	A	36	ARG	NE-CZ-NH1	-6.60	114.90	121.50
3	C	146	GLN	CA-C-O	6.57	127.38	120.42
1	A	88	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	A	972	ILE	N-CA-C	6.56	114.64	108.15
1	A	313	ARG	NH1-CZ-NH2	6.55	127.82	119.30
1	A	148	LYS	CB-CG-CD	6.55	126.37	111.30
1	A	562	SER	O-C-N	6.55	131.26	122.49
1	A	200	THR	CA-C-O	6.54	127.69	120.82
1	A	419	ALA	CA-C-O	6.54	127.48	120.55
1	A	533	GLN	CG-CD-NE2	-6.51	106.63	116.40
1	A	500	ASN	OD1-CG-ND2	6.51	129.11	122.60
2	B	102	HIS	O-C-N	-6.50	114.87	122.86
1	A	231	GLY	CA-C-O	-6.49	114.61	121.56
2	B	5	THR	OG1-CB-CG2	6.49	122.28	109.30
2	B	197	GLU	CG-CD-OE2	6.48	133.30	118.40
1	A	652	ILE	CA-C-O	-6.45	114.01	120.85
1	A	834	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	A	595	ASN	OD1-CG-ND2	6.43	129.03	122.60
1	A	873	ARG	NH1-CZ-NH2	-6.42	110.95	119.30
1	A	129	ALA	O-C-N	-6.42	115.46	122.07
1	A	369	SER	CA-C-O	-6.42	111.73	119.49
1	A	230	GLY	N-CA-C	-6.41	106.39	115.43
1	A	289	ARG	NE-CZ-NH2	6.39	124.95	119.20
3	C	177	LYS	CA-C-O	6.39	128.18	121.15
1	A	122	GLN	CG-CD-OE1	6.39	133.58	120.80
1	A	123	ARG	NH1-CZ-NH2	6.38	127.59	119.30
2	B	47	VAL	N-CA-C	6.36	116.53	110.42
2	B	167	VAL	CA-C-N	6.36	129.44	120.28
2	B	167	VAL	C-N-CA	6.36	129.44	120.28
3	C	147	VAL	CA-C-O	-6.36	114.11	120.85
1	A	541	PHE	CA-CB-CG	-6.33	107.47	113.80
2	B	285	VAL	CB-CA-C	-6.33	103.20	110.73
1	A	408	TYR	CA-C-O	-6.31	114.45	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	ASN	CA-CB-CG	-6.31	106.29	112.60
1	A	937	ARG	O-C-N	-6.29	115.85	122.96
2	B	223	HIS	CA-CB-CG	-6.29	107.51	113.80
1	A	570	VAL	CA-C-O	6.29	127.51	120.85
3	C	170	MET	N-CA-CB	6.28	119.46	110.16
1	A	865	ASN	OD1-CG-ND2	6.28	128.88	122.60
2	B	202	LYS	CA-C-O	-6.28	112.75	119.97
1	A	398	SER	N-CA-CB	6.28	120.63	110.40
1	A	463	SER	N-CA-C	6.23	119.74	110.52
1	A	781	ARG	NE-CZ-NH2	6.22	124.80	119.20
3	C	196	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	681	ASN	CA-CB-CG	-6.21	106.39	112.60
3	C	51	GLN	CA-C-O	-6.21	113.96	120.55
1	A	77	HIS	O-C-N	-6.20	116.53	123.48
1	A	581	VAL	CA-C-O	-6.20	113.90	120.48
1	A	975	HIS	N-CA-CB	-6.20	100.73	110.46
1	A	242	ARG	NE-CZ-NH1	-6.18	115.31	121.50
1	A	512	PHE	CA-C-O	6.18	127.06	120.70
1	A	39	LYS	N-CA-C	6.17	120.42	113.01
2	B	108	CYS	CA-C-O	6.16	127.28	120.82
1	A	345	ASN	OD1-CG-ND2	6.15	128.75	122.60
3	C	99	ASN	CA-CB-CG	6.15	118.75	112.60
1	A	71	ALA	O-C-N	-6.15	116.21	123.22
1	A	793	PRO	O-C-N	-6.14	114.02	122.24
1	A	118	SER	CA-C-O	-6.13	114.58	121.81
1	A	141	ARG	CD-NE-CZ	-6.12	115.83	124.40
2	B	108	CYS	O-C-N	-6.11	115.77	122.07
1	A	595	ASN	CB-CG-OD1	-6.11	108.58	120.80
2	B	53	ASN	CA-CB-CG	-6.11	106.49	112.60
2	B	199	ARG	CG-CD-NE	-6.08	98.62	112.00
1	A	350	ARG	CD-NE-CZ	-6.08	115.89	124.40
1	A	426	ALA	CA-C-O	-6.08	114.11	120.55
1	A	49	THR	CA-C-O	-6.08	113.67	120.66
1	A	576	LEU	CA-C-O	-6.08	114.35	121.16
1	A	324	SER	O-C-N	-6.08	115.34	122.81
2	B	195	LEU	N-CA-CB	6.05	119.02	110.12
1	A	343	ASP	CA-C-N	6.05	129.51	120.31
1	A	343	ASP	C-N-CA	6.05	129.51	120.31
1	A	944	ARG	CD-NE-CZ	6.04	132.85	124.40
3	C	93	VAL	CA-C-O	6.03	127.22	120.95
1	A	295	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	A	974	ILE	CB-CA-C	-6.01	105.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	132	ASN	CA-CB-CG	-6.01	106.59	112.60
1	A	698	ASN	CB-CG-OD1	6.01	132.81	120.80
1	A	178	GLN	CG-CD-OE1	-6.00	108.79	120.80
1	A	948	ARG	NH1-CZ-NH2	5.99	127.09	119.30
1	A	480	SER	O-C-N	5.98	128.23	122.07
1	A	727	ARG	NH1-CZ-NH2	5.97	127.07	119.30
1	A	940	VAL	N-CA-CB	5.97	119.38	111.25
2	B	204	LYS	CA-C-O	5.97	126.88	120.55
1	A	203	SER	CA-C-O	-5.96	112.50	119.24
2	B	146	ASN	OD1-CG-ND2	5.96	128.56	122.60
1	A	884	LYS	O-C-N	-5.96	115.13	123.11
1	A	533	GLN	O-C-N	5.95	129.35	122.99
1	A	603	ASP	CA-C-O	5.95	125.21	119.62
3	C	105	ASP	CB-CA-C	-5.95	101.32	111.31
3	C	30	LEU	CA-C-O	-5.94	114.12	120.42
1	A	489	ALA	CA-C-O	-5.94	114.51	121.16
2	B	53	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	79	GLU	CA-C-O	-5.93	114.81	121.40
3	C	187	LYS	N-CA-C	5.93	119.14	109.59
1	A	919	PHE	CA-C-O	5.91	128.13	121.51
2	B	47	VAL	O-C-N	5.90	127.69	121.91
2	B	286	ASP	N-CA-C	-5.90	106.09	113.28
1	A	261	ARG	NH1-CZ-NH2	-5.89	111.64	119.30
1	A	634	GLN	CA-C-O	-5.88	113.97	120.38
1	A	1000	SER	N-CA-CB	-5.88	101.77	110.53
2	B	120	GLN	OE1-CD-NE2	5.88	128.48	122.60
1	A	648	ASN	CB-CA-C	5.88	120.27	109.46
2	B	89	GLY	N-CA-C	5.87	122.54	114.92
3	C	113	GLN	CG-CD-NE2	5.86	125.18	116.40
3	C	146	GLN	OE1-CD-NE2	-5.86	116.75	122.60
1	A	148	LYS	CA-C-O	-5.85	114.50	121.11
1	A	621	GLU	CB-CG-CD	5.85	122.54	112.60
2	B	204	LYS	O-C-N	-5.85	115.92	122.12
1	A	363	LEU	CA-C-O	-5.85	114.22	120.42
1	A	849	HIS	CA-C-O	-5.84	114.09	120.81
1	A	889	PRO	N-CA-C	5.84	122.15	114.27
1	A	261	ARG	O-C-N	-5.84	115.81	123.16
1	A	71	ALA	CA-C-O	5.83	126.60	120.36
3	C	66	VAL	O-C-N	-5.82	116.20	121.91
1	A	327	ASP	CA-C-O	5.82	127.33	120.70
1	A	307	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	736	CYS	N-CA-CB	5.81	120.31	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	ALA	N-CA-C	-5.81	101.36	110.36
1	A	987	ILE	O-C-N	-5.80	116.46	122.66
1	A	571	SER	CA-CB-OG	-5.80	99.51	111.10
1	A	819	GLY	O-C-N	-5.80	115.33	122.46
3	C	26	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	860	ASN	OD1-CG-ND2	5.79	128.39	122.60
2	B	145	PHE	CA-C-O	5.79	126.21	119.32
1	A	977	GLY	O-C-N	5.79	130.22	122.70
1	A	956	ARG	NH1-CZ-NH2	5.78	126.82	119.30
1	A	78	ILE	O-C-N	5.78	129.31	123.07
1	A	944	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	B	87	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	A	331	ARG	CB-CG-CD	5.75	124.53	111.30
1	A	448	HIS	CA-C-O	5.75	127.65	121.44
3	C	123	MET	CA-C-O	-5.74	114.46	120.55
2	B	34	ILE	CA-CB-CG2	5.74	120.26	110.50
3	C	143	PHE	CA-C-O	5.74	125.53	120.19
1	A	341	GLN	CA-C-O	-5.74	114.51	121.05
1	A	614	LEU	CA-C-O	-5.73	112.32	119.54
1	A	393	VAL	CA-C-O	-5.72	115.10	121.17
1	A	796	MET	O-C-N	5.72	129.73	123.04
1	A	72	ARG	O-C-N	-5.72	116.07	122.93
2	B	32	LYS	CA-C-O	-5.71	114.46	120.80
1	A	657	TYR	O-C-N	-5.71	116.19	122.07
1	A	53	CYS	N-CA-CB	-5.70	101.77	110.49
1	A	836	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	948	ARG	NE-CZ-NH2	-5.68	114.09	119.20
1	A	493	ASP	CB-CG-OD2	-5.67	105.37	118.40
3	C	37	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	210	ARG	O-C-N	5.66	129.84	123.27
3	C	194	LYS	O-C-N	5.65	128.11	122.12
1	A	806	THR	CA-C-O	-5.65	115.13	121.40
2	B	199	ARG	NE-CZ-NH1	-5.65	115.85	121.50
1	A	663	LEU	O-C-N	-5.63	116.15	122.12
2	B	71	ASP	O-C-N	5.63	129.67	123.25
2	B	116	GLY	CA-C-O	-5.62	112.78	119.02
2	B	183	ALA	N-CA-C	-5.62	105.23	111.36
3	C	91	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	A	385	ALA	CA-C-O	-5.61	114.60	120.55
3	C	149	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	55	VAL	N-CA-C	-5.60	104.91	110.62
1	A	332	GLN	OE1-CD-NE2	5.60	128.20	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	974	ILE	CA-C-O	-5.59	114.55	120.14
1	A	584	PRO	O-C-N	-5.58	114.72	122.37
1	A	995	VAL	CA-C-O	-5.58	115.44	121.19
2	B	25	ASP	CA-C-O	-5.58	113.03	119.56
1	A	554	CYS	N-CA-CB	5.58	119.90	110.69
1	A	398	SER	O-C-N	5.57	130.15	122.46
1	A	122	GLN	CG-CD-NE2	5.57	124.75	116.40
2	B	167	VAL	O-C-N	-5.56	116.47	121.87
3	C	210	LYS	CA-C-O	-5.56	114.96	121.07
1	A	850	TYR	O-C-N	-5.56	116.49	123.27
2	B	158	TYR	O-C-N	-5.55	116.45	123.17
1	A	753	ARG	NE-CZ-NH1	-5.54	115.96	121.50
2	B	19	PRO	CA-C-O	-5.54	112.53	120.56
3	C	135	TRP	N-CA-C	5.53	117.25	108.67
1	A	203	SER	O-C-N	5.52	129.76	122.36
2	B	241	PRO	N-CA-CB	5.52	108.47	103.34
1	A	280	ASP	O-C-N	5.51	127.96	122.12
1	A	681	ASN	N-CA-C	5.51	119.24	110.70
1	A	721	SER	CA-CB-OG	-5.50	100.10	111.10
1	A	619	PHE	O-C-N	-5.50	116.29	122.12
2	B	19	PRO	O-C-N	5.50	127.95	121.46
1	A	696	GLU	CA-C-O	-5.49	114.73	120.55
2	B	56	ARG	CD-NE-CZ	5.49	132.08	124.40
2	B	92	GLU	CA-C-O	-5.48	114.36	120.66
1	A	937	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	A	419	ALA	O-C-N	-5.47	116.32	122.12
1	A	557	PHE	CA-CB-CG	5.47	119.27	113.80
3	C	104	ALA	CA-C-N	5.47	130.45	122.85
3	C	104	ALA	C-N-CA	5.47	130.45	122.85
1	A	358	ARG	CA-C-N	-5.46	112.38	120.94
1	A	358	ARG	C-N-CA	-5.46	112.38	120.94
1	A	596	HIS	CA-CB-CG	-5.45	108.35	113.80
1	A	102	VAL	CA-C-N	5.45	131.33	122.67
1	A	102	VAL	C-N-CA	5.45	131.33	122.67
1	A	485	ASN	OD1-CG-ND2	5.44	128.04	122.60
1	A	554	CYS	O-C-N	5.43	131.21	122.96
1	A	388	LEU	CA-C-O	5.42	126.30	120.55
1	A	880	LEU	CA-C-O	-5.42	112.72	119.38
1	A	733	ALA	N-CA-CB	-5.42	101.51	111.37
1	A	320	ASP	O-C-N	-5.41	115.84	122.55
2	B	96	ARG	O-C-N	5.41	129.63	123.31
1	A	456	ASP	CA-CB-CG	5.39	118.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	GLN	O-C-N	5.39	127.83	122.12
2	B	38	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	210	ARG	CA-C-O	-5.38	114.81	121.06
1	A	78	ILE	CA-C-O	-5.37	114.58	120.43
1	A	831	GLY	O-C-N	-5.37	115.79	122.34
1	A	884	LYS	CA-C-O	5.36	127.74	121.46
1	A	88	ARG	CD-NE-CZ	5.36	131.91	124.40
1	A	282	THR	N-CA-C	-5.36	105.08	111.03
1	A	139	ALA	CA-C-O	-5.36	115.19	120.82
3	C	179	SER	N-CA-C	5.36	117.12	111.28
1	A	303	LYS	N-CA-C	5.35	117.11	111.28
3	C	146	GLN	N-CA-C	5.35	117.19	111.36
1	A	826	ILE	N-CA-C	5.35	119.95	113.00
3	C	216	GLY	O-C-N	5.34	129.64	122.70
1	A	67	GLY	O-C-N	-5.33	115.43	122.42
2	B	81	ARG	CD-NE-CZ	5.33	131.87	124.40
2	B	136	CYS	N-CA-C	5.33	118.01	111.82
1	A	298	ASN	O-C-N	5.33	129.13	122.63
1	A	219	ASP	CA-C-O	5.32	125.93	119.49
1	A	937	ARG	CB-CG-CD	-5.31	99.09	111.30
1	A	983	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	A	407	LEU	O-C-N	5.29	129.80	123.13
2	B	257	LEU	CA-C-O	-5.29	114.91	120.63
2	B	290	GLU	N-CA-CB	5.29	119.49	110.50
2	B	164	VAL	O-C-N	-5.29	116.53	121.87
1	A	421	ASN	CA-C-O	5.29	126.56	120.90
1	A	96	ALA	CA-C-O	-5.28	112.89	119.38
1	A	798	ILE	CA-C-O	5.28	126.87	121.28
1	A	538	ILE	CA-CB-CG2	-5.27	101.54	110.50
1	A	410	LEU	N-CA-C	5.27	117.93	111.82
1	A	600	ASN	CA-CB-CG	-5.26	107.34	112.60
1	A	413	THR	OG1-CB-CG2	5.26	119.82	109.30
1	A	1014	LYS	CA-C-O	-5.26	115.40	121.19
1	A	271	ILE	O-C-N	5.25	128.88	123.20
3	C	190	ARG	CD-NE-CZ	5.25	131.75	124.40
1	A	362	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	A	182	ARG	NH1-CZ-NH2	5.24	126.11	119.30
1	A	562	SER	CA-C-O	-5.24	113.38	119.14
3	C	119	SER	CA-C-O	5.24	126.32	120.82
1	A	868	SER	CA-CB-OG	-5.23	100.63	111.10
1	A	586	VAL	CB-CA-C	-5.23	103.53	111.33
1	A	691	ASP	O-C-N	-5.23	116.10	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	CYS	O-C-N	-5.23	115.31	121.32
1	A	404	THR	N-CA-C	-5.23	101.64	109.95
1	A	912	ALA	CA-C-O	-5.22	115.01	120.55
2	B	248	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	214	THR	N-CA-C	5.22	119.36	112.89
2	B	224	VAL	N-CA-CB	5.21	118.47	111.90
1	A	283	PHE	CA-CB-CG	5.21	119.01	113.80
3	C	65	PHE	CA-C-O	-5.21	114.89	120.42
3	C	145	MET	CA-C-O	5.21	126.26	120.63
3	C	103	VAL	CA-C-N	-5.21	114.03	122.36
3	C	103	VAL	C-N-CA	-5.21	114.03	122.36
3	C	175	TRP	N-CA-C	5.20	116.75	111.14
2	B	168	SER	CB-CA-C	-5.18	101.04	110.63
1	A	398	SER	N-CA-C	-5.18	106.47	112.89
3	C	14	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	47	ARG	NH1-CZ-NH2	5.17	126.03	119.30
1	A	899	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	72	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	A	797	LEU	N-CA-C	-5.17	105.81	112.68
1	A	564	PRO	CA-C-O	5.16	127.97	121.67
1	A	749	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	A	681	ASN	N-CA-CB	-5.16	102.34	110.49
3	C	108	LYS	O-C-N	5.16	127.60	122.08
1	A	434	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	A	933	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	107	ARG	CD-NE-CZ	5.15	131.60	124.40
1	A	107	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	621	GLU	O-C-N	5.14	128.59	122.26
1	A	727	ARG	NE-CZ-NH1	-5.14	116.36	121.50
2	B	285	VAL	N-CA-C	5.14	115.88	107.24
3	C	56	LEU	O-C-N	-5.14	115.44	122.33
1	A	208	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	367	HIS	CA-CB-CG	-5.13	108.67	113.80
1	A	969	THR	CA-C-O	5.13	126.24	120.70
3	C	179	SER	CA-C-O	-5.13	115.11	120.55
2	B	145	PHE	N-CA-CB	-5.12	102.88	110.61
2	B	286	ASP	CA-C-O	5.12	125.27	119.18
2	B	79	VAL	N-CA-CB	5.12	119.85	111.45
1	A	949	ALA	N-CA-CB	-5.12	102.98	111.57
1	A	849	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	251	ASN	N-CA-C	-5.11	105.95	113.61
2	B	256	ALA	N-CA-C	5.11	117.51	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	LEU	O-C-N	-5.10	115.42	122.46
1	A	512	PHE	O-C-N	-5.09	116.59	122.09
1	A	965	GLN	CB-CA-C	-5.09	101.30	110.36
1	A	647	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	580	VAL	CA-C-O	-5.08	115.10	120.39
1	A	697	ASN	O-C-N	-5.07	116.74	122.12
3	C	72	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	715	LYS	CA-C-O	5.07	127.44	121.36
1	A	795	ARG	NE-CZ-NH2	-5.07	114.64	119.20
2	B	147	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	A	537	VAL	CA-C-N	-5.05	114.19	120.56
1	A	537	VAL	C-N-CA	-5.05	114.19	120.56
1	A	994	ASN	O-C-N	5.05	129.03	122.71
2	B	118	ILE	CA-C-O	-5.05	115.01	120.36
1	A	581	VAL	O-C-N	5.05	128.48	123.18
1	A	255	LEU	CA-C-O	-5.04	114.96	120.36
3	C	200	TRP	CA-CB-CG	-5.04	104.02	113.60
2	B	5	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	539	LYS	O-C-N	-5.04	116.85	122.09
1	A	987	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	A	47	ARG	NE-CZ-NH2	-5.03	114.67	119.20
2	B	166	ARG	O-C-N	-5.03	115.52	122.30
1	A	809	ASP	CA-C-O	-5.02	115.89	121.51
3	C	61	GLY	N-CA-C	-5.01	106.69	112.50
1	A	745	GLU	CB-CG-CD	5.00	121.11	112.60
1	A	817	ALA	O-C-N	5.00	127.03	121.53
1	A	518	GLN	CA-C-O	-5.00	115.91	121.51
1	A	837	ALA	N-CA-C	5.00	118.27	112.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7719	0	7457	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2207	0	2140	34	0
3	C	1783	0	1836	71	0
4	A	8	0	0	0	0
4	B	32	0	0	0	0
5	A	94	0	43	5	0
6	A	1	0	0	0	0
7	B	70	0	83	4	0
8	C	86	0	60	3	0
9	C	19	0	21	1	0
10	A	1493	0	0	27	0
10	B	410	0	0	11	0
10	C	81	0	0	9	0
All	All	14003	0	11640	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:GLU:HG3	1:A:832:MET:HE2	1.40	0.98
1:A:356:HIS:HD2	1:A:358:ARG:H	1.11	0.89
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.58	0.85
1:A:224:ASN:HD22	1:A:403:THR:H	1.21	0.84
3:C:101:HIS:HD2	3:C:102:LYS:H	1.25	0.84
3:C:201:TYR:HB3	10:C:1844:HOH:O	1.77	0.83
1:A:830:GLU:CG	1:A:832:MET:HE2	2.09	0.82
3:C:213:SER:HA	10:C:1896:HOH:O	1.81	0.80
1:A:307:ASN:HB3	1:A:832:MET:HE3	1.64	0.77
3:C:15:ARG:HG2	3:C:183:MET:HE3	1.65	0.76
1:A:197:HIS:HD2	1:A:200:THR:OG1	1.70	0.75
1:A:876:GLU:HG3	10:A:1897:HOH:O	1.85	0.75
1:A:830:GLU:HG3	1:A:832:MET:CE	2.16	0.74
3:C:101:HIS:CD2	3:C:102:LYS:H	2.06	0.73
3:C:123:MET:HA	3:C:123:MET:HE2	1.71	0.73
1:A:359:CYS:HB3	10:A:1667:HOH:O	1.88	0.72
2:B:279:ILE:HD13	3:C:97:LYS:HA	1.71	0.71
3:C:101:HIS:CD2	3:C:102:LYS:HG3	2.25	0.71
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.73	0.71
3:C:112:GLY:HA3	9:C:811:HQO:H132	1.71	0.71
2:B:283:LYS:HD2	2:B:284:GLU:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:ILE:HB	3:C:87:PRO:HD3	1.76	0.68
3:C:193:ALA:HB1	3:C:201:TYR:HB2	1.76	0.67
1:A:196:SEC:SE	10:A:1476:HOH:O	2.61	0.67
3:C:84:LYS:HB3	10:C:1932:HOH:O	1.94	0.67
1:A:356:HIS:CD2	1:A:358:ARG:H	2.04	0.66
3:C:11:LYS:HG2	3:C:13:ILE:HG22	1.80	0.64
2:B:68:ASN:HA	2:B:69:PRO:C	2.23	0.63
1:A:412:TRP:CZ3	1:A:425:MET:HG3	2.34	0.63
3:C:176:VAL:HG11	10:C:1990:HOH:O	1.99	0.63
1:A:84:HIS:HE1	1:A:634:GLN:OE1	1.82	0.62
3:C:7:ILE:HG13	3:C:188:VAL:HG23	1.81	0.62
1:A:125:SER:OG	1:A:128:GLU:HG3	1.99	0.62
1:A:781:ARG:HA	1:A:798:ILE:HD11	1.82	0.62
1:A:193:ALA:HA	1:A:451:ILE:HD11	1.82	0.61
1:A:630:GLY:O	1:A:631:ARG:HB2	2.00	0.61
1:A:476:VAL:HG22	10:A:1532:HOH:O	2.01	0.59
1:A:622:GLU:OE1	1:A:648:ASN:HB2	2.02	0.59
3:C:5:LYS:HG2	3:C:6:MET:SD	2.43	0.59
3:C:198:PRO:HA	10:C:1844:HOH:O	2.03	0.59
1:A:327:ASP:OD1	1:A:327:ASP:C	2.44	0.59
1:A:820:THR:HB	1:A:821:PRO:HD2	1.85	0.59
1:A:224:ASN:HD21	1:A:795:ARG:HH22	1.51	0.58
2:B:258:LYS:HG3	10:B:970:HOH:O	2.02	0.58
3:C:4:SER:OG	3:C:190:ARG:NH2	2.34	0.58
3:C:10:THR:HG21	3:C:183:MET:HE1	1.86	0.57
3:C:202:ARG:HA	3:C:205:GLU:OE1	2.04	0.57
3:C:91:ASN:O	3:C:95:VAL:HG23	2.04	0.57
1:A:451:ILE:HD13	10:A:1476:HOH:O	2.05	0.56
1:A:896:ARG:HH22	5:A:1017:MGD:H15	1.53	0.56
1:A:199:PRO:HG2	1:A:413:THR:HB	1.88	0.56
1:A:415:HIS:HD2	10:A:1100:HOH:O	1.88	0.56
3:C:79:ASN:HA	3:C:114:LYS:HG2	1.88	0.56
3:C:86:ILE:N	3:C:87:PRO:CD	2.69	0.55
3:C:101:HIS:HD2	3:C:102:LYS:HG3	1.68	0.55
3:C:204:ILE:O	3:C:208:GLU:HB2	2.06	0.55
2:B:176:VAL:HG22	2:B:184:ILE:CG2	2.37	0.55
1:A:989:ASN:ND2	5:A:1017:MGD:H192	2.04	0.55
3:C:188:VAL:HG11	3:C:192:TRP:CZ3	2.43	0.54
1:A:961:ASN:HB3	10:A:1697:HOH:O	2.07	0.54
1:A:542:ASN:O	1:A:546:GLU:HG3	2.08	0.54
1:A:786:ILE:HG12	10:A:1720:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:ARG:O	3:C:206:LYS:HD2	2.08	0.54
1:A:411:GLY:O	1:A:415:HIS:HE1	1.90	0.54
3:C:190:ARG:O	3:C:194:LYS:HG3	2.08	0.54
1:A:307:ASN:HB3	1:A:832:MET:CE	2.35	0.54
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.38	0.53
1:A:854:GLU:HB3	1:A:1009:LEU:HD12	1.91	0.53
1:A:648:ASN:HB3	10:A:1872:HOH:O	2.09	0.52
1:A:384:LYS:HA	10:A:1708:HOH:O	2.09	0.52
3:C:190:ARG:NH1	3:C:201:TYR:OH	2.39	0.52
3:C:93:VAL:O	3:C:97:LYS:HG3	2.10	0.52
1:A:351:ASP:HB3	10:A:1667:HOH:O	2.08	0.51
3:C:127:LEU:HD21	3:C:159:GLY:N	2.25	0.51
3:C:190:ARG:O	3:C:193:ALA:HB3	2.11	0.51
1:A:135:LYS:HE2	10:A:1791:HOH:O	2.09	0.51
1:A:163:MET:HG2	1:A:553:PHE:HB2	1.92	0.51
3:C:199:ARG:O	3:C:203:GLU:HG2	2.10	0.51
1:A:832:MET:SD	10:A:1596:HOH:O	2.60	0.51
1:A:509:MET:SD	10:A:2292:HOH:O	2.60	0.50
3:C:86:ILE:N	3:C:87:PRO:HD2	2.27	0.50
3:C:105:ASP:HB2	10:C:1672:HOH:O	2.12	0.50
1:A:885:LYS:HE3	10:A:2493:HOH:O	2.11	0.50
3:C:216:GLY:O	3:C:217:ILE:C	2.55	0.50
1:A:493:ASP:CB	1:A:821:PRO:HG2	2.42	0.50
3:C:22:VAL:HG22	8:C:810:HEM:CHC	2.41	0.50
1:A:122:GLN:HG2	10:A:2081:HOH:O	2.11	0.50
1:A:200:THR:HA	1:A:422:ILE:HD13	1.93	0.50
1:A:817:ALA:HB1	1:A:818:PRO:HD2	1.92	0.49
1:A:623:ASP:HB3	10:A:1885:HOH:O	2.11	0.49
3:C:56:LEU:O	3:C:57:HIS:C	2.53	0.49
2:B:266:ILE:HG21	7:B:812:CDL:H771	1.95	0.49
2:B:266:ILE:HD13	7:B:812:CDL:H751	1.94	0.49
1:A:164:LEU:HB3	1:A:557:PHE:CD1	2.48	0.49
1:A:633:LEU:HD12	1:A:633:LEU:N	2.27	0.49
3:C:15:ARG:HA	3:C:183:MET:CE	2.42	0.49
1:A:126:TRP:CZ2	1:A:647:ARG:HG3	2.48	0.48
1:A:412:TRP:HZ3	1:A:425:MET:HG3	1.77	0.48
2:B:185:HIS:CD2	10:B:949:HOH:O	2.66	0.48
1:A:48:ASN:HB2	1:A:61:MET:HE2	1.96	0.48
1:A:53:CYS:HA	1:A:447:GLY:O	2.14	0.48
2:B:110:LYS:HE3	10:B:1125:HOH:O	2.13	0.48
2:B:176:VAL:HG22	2:B:184:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:HG13	1:A:836:PHE:HB2	1.96	0.47
1:A:34:GLN:HA	10:B:933:HOH:O	2.15	0.47
1:A:224:ASN:HD22	1:A:403:THR:N	2.01	0.47
1:A:961:ASN:OD1	1:A:966:GLN:OE1	2.31	0.47
1:A:370:ARG:HD2	10:A:2279:HOH:O	2.15	0.47
1:A:410:LEU:HA	1:A:413:THR:OG1	2.15	0.47
2:B:235:GLU:HG3	10:B:1038:HOH:O	2.15	0.47
1:A:202:ALA:O	1:A:206:PRO:HG2	2.14	0.47
3:C:208:GLU:HB3	3:C:209:ALA:H	1.48	0.47
1:A:460:LEU:O	1:A:461:SER:C	2.58	0.46
2:B:192:MET:HA	2:B:192:MET:HE2	1.95	0.46
3:C:160:ILE:O	3:C:164:HIS:HD2	1.98	0.46
1:A:199:PRO:HB2	1:A:413:THR:HG22	1.96	0.46
2:B:10:LYS:HB2	2:B:120:GLN:HB3	1.96	0.46
3:C:101:HIS:CD2	3:C:102:LYS:N	2.78	0.46
1:A:593:TRP:CD1	1:A:593:TRP:H	2.33	0.46
1:A:645:GLU:HA	10:A:1919:HOH:O	2.16	0.46
3:C:95:VAL:HG13	3:C:100:GLU:HB3	1.97	0.46
1:A:84:HIS:CD2	1:A:86:VAL:H	2.34	0.46
1:A:513:TYR:HE2	10:A:2292:HOH:O	1.99	0.46
1:A:622:GLU:CD	1:A:648:ASN:HB2	2.41	0.46
2:B:269:PHE:O	2:B:273:ILE:HD12	2.16	0.46
2:B:8:ILE:HD12	2:B:119:ILE:HD12	1.98	0.45
1:A:775:ARG:HD3	1:A:812:ASP:HA	1.98	0.45
2:B:185:HIS:HE1	10:B:891:HOH:O	1.99	0.45
1:A:224:ASN:HD21	1:A:795:ARG:NH2	2.14	0.45
3:C:170:MET:HG2	8:C:810:HEM:CAB	2.46	0.45
3:C:87:PRO:HG2	10:C:1672:HOH:O	2.16	0.45
1:A:781:ARG:O	1:A:781:ARG:HG3	2.16	0.45
2:B:285:VAL:CG2	3:C:191:ARG:HH11	2.30	0.45
3:C:123:MET:HE2	3:C:123:MET:CA	2.45	0.45
1:A:673:GLU:HB3	1:A:674:PRO:HD3	1.98	0.44
2:B:197:GLU:HG3	10:B:1199:HOH:O	2.16	0.44
1:A:343:ASP:HA	1:A:349:LYS:HE2	1.98	0.44
1:A:989:ASN:HD21	5:A:1017:MGD:H192	1.63	0.44
2:B:29:GLU:OE1	2:B:223:HIS:HE1	1.99	0.44
3:C:79:ASN:HD22	3:C:114:LYS:HA	1.81	0.44
2:B:152:LYS:HG2	10:B:917:HOH:O	2.16	0.44
3:C:214:GLU:HA	3:C:214:GLU:OE1	2.18	0.44
3:C:175:TRP:CE3	3:C:176:VAL:HG23	2.52	0.44
3:C:11:LYS:HG3	3:C:12:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:SER:OG	1:A:629:SER:HB2	2.17	0.44
1:A:495:VAL:O	1:A:496:ASN:C	2.60	0.44
1:A:108:LEU:HD12	1:A:583:ASP:O	2.17	0.43
7:B:812:CDL:H432	3:C:25:PHE:CD1	2.53	0.43
3:C:10:THR:HA	10:C:1035:HOH:O	2.18	0.43
3:C:181:LYS:HD2	3:C:185:GLU:OE1	2.18	0.43
3:C:208:GLU:O	3:C:209:ALA:C	2.60	0.43
1:A:126:TRP:CE2	1:A:647:ARG:HG3	2.54	0.43
2:B:283:LYS:HD3	3:C:177:LYS:HB2	2.00	0.43
3:C:212:GLU:HB2	10:C:1767:HOH:O	2.19	0.43
1:A:937:ARG:HH11	1:A:937:ARG:HD2	1.59	0.43
3:C:44:THR:HB	3:C:50:PRO:HG3	2.01	0.43
3:C:62:ILE:HD13	3:C:62:ILE:HA	1.74	0.43
1:A:135:LYS:HG3	10:A:1574:HOH:O	2.18	0.43
1:A:217:TRP:CH2	1:A:445:LEU:HD22	2.53	0.43
1:A:257:VAL:HG23	1:A:269:ALA:HB2	2.01	0.42
1:A:241:PHE:O	1:A:242:ARG:C	2.62	0.42
3:C:166:ILE:HD11	8:C:810:HEM:HBC2	2.01	0.42
2:B:78:THR:HG23	10:B:1204:HOH:O	2.18	0.42
1:A:229:MET:HG3	1:A:258:VAL:HB	1.99	0.42
1:A:197:HIS:CD2	1:A:200:THR:OG1	2.61	0.42
1:A:205:ALA:HB3	1:A:206:PRO:HD3	2.00	0.42
1:A:410:LEU:HD11	5:A:1018:MGD:S12	2.60	0.42
1:A:984:LYS:HE3	10:A:1726:HOH:O	2.20	0.42
1:A:566:LYS:HA	10:A:1251:HOH:O	2.19	0.42
1:A:312:VAL:HG21	1:A:363:LEU:HD12	2.01	0.42
1:A:359:CYS:SG	1:A:362:ASN:ND2	2.93	0.42
2:B:20:PRO:HD2	10:B:935:HOH:O	2.20	0.42
2:B:102:HIS:O	2:B:223:HIS:HD2	2.03	0.42
3:C:160:ILE:HD13	3:C:160:ILE:HA	1.76	0.42
3:C:205:GLU:HA	3:C:208:GLU:OE1	2.20	0.42
1:A:92:CYS:HB3	1:A:238:PRO:HG2	2.02	0.42
1:A:175:MET:HE2	1:A:457:LEU:HD22	2.02	0.42
2:B:162:LEU:O	2:B:163:CYS:C	2.62	0.42
2:B:245:LYS:HE3	2:B:245:LYS:HB3	1.78	0.42
1:A:242:ARG:O	1:A:242:ARG:HG2	2.20	0.41
2:B:68:ASN:CA	2:B:69:PRO:C	2.92	0.41
3:C:159:GLY:O	3:C:163:ILE:HG13	2.20	0.41
1:A:772:PRO:HG2	1:A:775:ARG:HD2	2.03	0.41
2:B:55:ILE:HD13	2:B:55:ILE:HG21	1.85	0.41
1:A:193:ALA:HB3	1:A:460:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:LEU:HD23	10:A:1689:HOH:O	2.21	0.41
3:C:17:CYS:SG	3:C:70:PHE:HD2	2.42	0.41
3:C:15:ARG:HA	3:C:183:MET:HE2	2.01	0.41
1:A:415:HIS:CD2	10:A:1100:HOH:O	2.70	0.41
2:B:285:VAL:HG12	2:B:288:ASP:H	1.84	0.41
3:C:170:MET:HE3	3:C:170:MET:HB2	1.97	0.41
1:A:451:ILE:HG21	10:A:1476:HOH:O	2.21	0.41
2:B:206:ARG:HH11	2:B:206:ARG:HD3	1.73	0.41
2:B:266:ILE:CG2	7:B:812:CDL:H771	2.51	0.41
1:A:896:ARG:HE	5:A:1018:MGD:H15	1.64	0.41
1:A:163:MET:HB3	1:A:163:MET:HE2	1.66	0.41
1:A:224:ASN:ND2	1:A:402:ARG:HA	2.36	0.41
2:B:9:ILE:HD11	2:B:120:GLN:CD	2.46	0.41
2:B:279:ILE:HG22	2:B:280:GLY:O	2.21	0.41
3:C:15:ARG:NH1	3:C:184:ILE:O	2.54	0.41
3:C:107:GLY:C	3:C:200:TRP:HB2	2.45	0.41
3:C:211:LYS:HA	3:C:211:LYS:HD3	1.86	0.41
1:A:400:PRO:HA	10:A:1709:HOH:O	2.21	0.40
1:A:956:ARG:HH11	1:A:956:ARG:HD2	1.55	0.40
2:B:185:HIS:HD2	10:B:907:HOH:O	2.04	0.40
1:A:356:HIS:HA	1:A:357:PRO:HD2	1.91	0.40
3:C:15:ARG:HG2	3:C:183:MET:CE	2.44	0.40
1:A:198:GLY:N	1:A:199:PRO:CD	2.85	0.40
1:A:511:SER:OG	1:A:735:SER:HB3	2.21	0.40
3:C:88:TRP:CZ2	3:C:95:VAL:HG11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	979/1015 (96%)	949 (97%)	29 (3%)	1 (0%)	48	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	287/294 (98%)	280 (98%)	7 (2%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	14	41
All	All	1480/1526 (97%)	1435 (97%)	42 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	838	ILE
3	C	198	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/837 (97%)	804 (99%)	11 (1%)	61	86
2	B	238/243 (98%)	226 (95%)	12 (5%)	22	54
3	C	188/189 (100%)	183 (97%)	5 (3%)	39	74
All	All	1241/1269 (98%)	1213 (98%)	28 (2%)	44	78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	324	SER
1	A	344	GLU
1	A	383	PRO
1	A	424	THR
1	A	648	ASN
1	A	790	PRO
1	A	832	MET
1	A	843	GLU
1	A	855	THR
1	A	954	THR

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Mol	Chain	Res	Type
2	B	51	GLU
2	B	69	PRO
2	B	113	PRO
2	B	160	CYS
2	B	162	LEU
2	B	178	THR
2	B	229	HIS
2	B	235	GLU
2	B	248	THR
2	B	285	VAL
2	B	289	GLU
2	B	290	GLU
3	C	101	HIS
3	C	189	SER
3	C	204	ILE
3	C	205	GLU
3	C	206	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	122	GLN
1	A	191	ASN
1	A	197	HIS
1	A	224	ASN
1	A	304	HIS
1	A	341	GLN
1	A	345	ASN
1	A	356	HIS
1	A	362	ASN
1	A	415	HIS
1	A	479	GLN
1	A	522	ASN
1	A	542	ASN
1	A	689	GLN
1	A	865	ASN
1	A	966	GLN
1	A	989	ASN
2	B	185	HIS
2	B	223	HIS
3	C	79	ASN

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Mol	Chain	Res	Type
3	C	101	HIS
3	C	164	HIS
3	C	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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
8	HEM	C	809	3	50,50,50	1.24	5 (10%)	67,82,82	0.92	2 (2%)
9	HQO	C	811	-	19,20,20	3.09	9 (47%)	20,26,26	3.02	7 (35%)
5	MGD	A	1018	6	47,52,52	2.23	8 (17%)	58,81,81	1.92	17 (29%)
4	SF4	B	805	2	0,12,12	-	-	-	-	-
8	HEM	C	810	3	50,50,50	1.35	8 (16%)	67,82,82	1.27	8 (11%)
4	SF4	A	1016	1	0,12,12	-	-	-	-	-
4	SF4	B	806	2	0,12,12	-	-	-	-	-
4	SF4	B	807	2	0,12,12	-	-	-	-	-
4	SF4	B	808	2	0,12,12	-	-	-	-	-
7	CDL	B	812	-	69,69,99	2.96	20 (28%)	75,81,111	2.68	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	A	1017	6	47,52,52	2.05	7 (14%)	58,81,81	2.40	18 (31%)

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
8	HEM	C	809	3	-	6/14/54/54	-
9	HQO	C	811	-	-	2/7/7/7	0/2/2/2
5	MGD	A	1018	6	-	7/22/66/66	0/6/6/6
8	HEM	C	810	3	-	3/14/54/54	-
4	SF4	B	805	2	-	-	0/6/5/5
4	SF4	A	1016	1	-	-	0/6/5/5
4	SF4	B	806	2	-	-	0/6/5/5
4	SF4	B	807	2	-	-	0/6/5/5
4	SF4	B	808	2	-	-	0/6/5/5
7	CDL	B	812	-	-	40/80/80/110	-
5	MGD	A	1017	6	-	8/22/66/66	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	812	CDL	OB8-CB6	-15.57	1.10	1.45
5	A	1018	MGD	O3A-C10	-10.54	1.04	1.44
5	A	1017	MGD	O3A-C10	-10.11	1.06	1.44
7	B	812	CDL	OA6-CA5	8.42	1.58	1.34
9	C	811	HQO	C11-C3	7.80	1.71	1.50
7	B	812	CDL	OB6-CB5	7.18	1.54	1.34
9	C	811	HQO	O1-C1	5.93	1.53	1.36
5	A	1018	MGD	PB-O3B	5.88	1.65	1.59
7	B	812	CDL	PA1-OA3	5.65	1.70	1.50
7	B	812	CDL	C51-CB5	5.28	1.66	1.50
9	C	811	HQO	O4-N1	-4.77	1.32	1.38
5	A	1017	MGD	PB-O3B	4.18	1.64	1.59
7	B	812	CDL	OA8-CA7	3.83	1.44	1.33
5	A	1018	MGD	C23-C14	-3.68	1.50	1.53
5	A	1017	MGD	C21-N22	3.59	1.39	1.35
9	C	811	HQO	C8-C9	3.52	1.44	1.36
5	A	1018	MGD	O5'-C5'	-3.34	1.32	1.44
7	B	812	CDL	PB2-OB3	3.31	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	811	HQO	C2-C3	3.25	1.44	1.38
7	B	812	CDL	C79-C78	3.24	1.73	1.50
7	B	812	CDL	OB8-CB7	-3.21	1.24	1.33
5	A	1018	MGD	C14-N15	-3.20	1.42	1.46
8	C	810	HEM	CAB-C3B	3.13	1.55	1.47
9	C	811	HQO	C7-C6	3.06	1.43	1.36
5	A	1017	MGD	C5'-C4'	-3.03	1.42	1.51
8	C	810	HEM	FE-NC	3.02	2.05	1.95
7	B	812	CDL	OB6-CB4	-2.99	1.39	1.46
7	B	812	CDL	C39-C38	-2.94	1.37	1.51
7	B	812	CDL	PB2-OB4	2.91	1.68	1.55
7	B	812	CDL	C11-CA5	2.86	1.59	1.50
9	C	811	HQO	C3-N1	2.86	1.42	1.36
7	B	812	CDL	C42-C41	-2.85	1.37	1.51
8	C	809	HEM	CAC-C3C	2.84	1.55	1.47
8	C	810	HEM	CAC-C3C	2.79	1.54	1.47
5	A	1017	MGD	O5'-C5'	-2.72	1.34	1.44
7	B	812	CDL	C19-C18	-2.72	1.34	1.51
8	C	810	HEM	CMC-C2C	2.72	1.56	1.50
8	C	809	HEM	CAB-C3B	2.67	1.54	1.47
9	C	811	HQO	C2-C1	2.62	1.43	1.37
9	C	811	HQO	C8-C7	2.59	1.43	1.38
7	B	812	CDL	CA3-CA4	-2.58	1.42	1.50
7	B	812	CDL	C12-C11	2.52	1.61	1.52
7	B	812	CDL	PA1-OA5	2.40	1.68	1.59
7	B	812	CDL	C52-C51	2.40	1.61	1.52
5	A	1018	MGD	O11-C11	-2.39	1.39	1.43
7	B	812	CDL	CB3-CB4	2.35	1.58	1.50
5	A	1017	MGD	C14-N15	-2.29	1.43	1.46
8	C	809	HEM	CMC-C2C	2.24	1.55	1.50
8	C	810	HEM	FE-NB	2.23	2.01	1.94
8	C	809	HEM	CMA-C3A	2.22	1.55	1.50
8	C	810	HEM	CAD-C3D	2.20	1.57	1.51
5	A	1018	MGD	PB-O1B	-2.17	1.43	1.50
5	A	1018	MGD	C5'-C4'	-2.17	1.45	1.51
8	C	810	HEM	O1A-CGA	2.09	1.28	1.22
5	A	1017	MGD	C16-C21	2.05	1.42	1.38
8	C	809	HEM	FE-NA	2.02	2.01	1.95
8	C	810	HEM	CMD-C2D	2.00	1.54	1.50

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	812	CDL	OB6-CB5-C51	13.28	140.21	111.48
9	C	811	HQO	C11-C3-C2	9.25	139.33	121.06
5	A	1017	MGD	O11-C23-C14	8.49	114.63	108.96
7	B	812	CDL	C52-C51-CB5	-7.17	87.41	113.69
7	B	812	CDL	CA6-CA4-CA3	-6.99	95.49	111.78
7	B	812	CDL	CB6-OB8-CB7	-6.86	92.04	117.12
7	B	812	CDL	OB7-CB5-C51	-6.08	100.01	123.78
9	C	811	HQO	C13-C11-C3	-6.06	97.03	113.91
5	A	1017	MGD	C19-N20-C21	5.73	123.48	113.36
5	A	1017	MGD	C23-C14-N15	5.55	113.32	107.87
5	A	1017	MGD	O4'-C1'-N9	-5.50	95.90	108.36
5	A	1018	MGD	C19-N20-C21	5.23	122.58	113.36
7	B	812	CDL	OA6-CA5-OA7	-4.91	112.22	123.70
5	A	1018	MGD	O4'-C1'-C2'	-4.70	96.55	106.62
8	C	810	HEM	O2A-CGA-O1A	4.14	133.98	123.33
9	C	811	HQO	O1-C1-C10	4.08	123.41	116.42
5	A	1017	MGD	O5'-C5'-C4'	3.86	122.14	108.99
5	A	1017	MGD	N2-C2-N3	3.80	127.08	119.67
7	B	812	CDL	OB8-CB7-OB9	3.78	133.09	123.63
7	B	812	CDL	OB6-CB5-OB7	-3.77	114.89	123.70
5	A	1017	MGD	O17-C17-N18	-3.72	113.12	120.11
5	A	1018	MGD	O4'-C1'-N9	-3.61	100.19	108.36
5	A	1018	MGD	O17-C17-C16	-3.57	118.65	127.26
7	B	812	CDL	CB6-CB4-CB3	-3.49	103.66	111.78
5	A	1018	MGD	C4'-O4'-C1'	-3.45	101.86	109.47
9	C	811	HQO	C2-C3-N1	3.41	122.69	118.94
5	A	1018	MGD	O11-C23-C14	-3.36	106.72	108.96
5	A	1017	MGD	O3B-PB-O1B	-3.34	100.67	110.70
7	B	812	CDL	CA4-OA6-CA5	-3.23	110.07	117.80
5	A	1018	MGD	N18-C19-N20	-3.14	117.58	123.32
7	B	812	CDL	CA6-OA8-CA7	-3.00	106.16	117.12
8	C	809	HEM	O2D-CGD-O1D	2.91	130.83	123.33
8	C	810	HEM	O1D-CGD-CBD	-2.91	113.85	123.09
5	A	1017	MGD	O4'-C1'-C2'	-2.87	100.47	106.62
8	C	809	HEM	O1D-CGD-CBD	-2.85	114.05	123.09
5	A	1018	MGD	O2A-PA-O3B	-2.84	99.59	107.27
7	B	812	CDL	O1-C1-CA2	-2.83	99.92	109.70
7	B	812	CDL	CB4-OB6-CB5	-2.83	111.03	117.80
7	B	812	CDL	OA6-CA5-C11	2.82	117.59	111.48
5	A	1018	MGD	C19-N18-C17	-2.82	119.99	125.11
8	C	810	HEM	O1A-CGA-CBA	-2.79	114.26	123.09
8	C	810	HEM	CMA-C3A-C2A	2.73	131.41	125.62
7	B	812	CDL	OA4-PA1-OA3	-2.69	99.94	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1018	MGD	O5'-C5'-C4'	2.69	118.14	108.99
9	C	811	HQO	C1-C2-C3	2.60	120.41	118.45
5	A	1017	MGD	O6-C6-N1	2.56	124.92	120.11
9	C	811	HQO	C12-C13-C11	-2.51	103.25	113.74
5	A	1018	MGD	C16-C17-N18	2.51	119.01	112.13
8	C	810	HEM	CMA-C3A-C4A	-2.47	121.65	125.42
9	C	811	HQO	C1-C10-C5	2.46	121.15	117.87
5	A	1017	MGD	N18-C19-N20	-2.44	118.86	123.32
8	C	810	HEM	CBC-CAC-C3C	-2.40	115.55	127.53
5	A	1018	MGD	O11-C23-N22	-2.39	106.44	108.61
5	A	1017	MGD	O3A-C10-C11	2.33	114.34	108.58
5	A	1018	MGD	N2-C2-N3	2.30	124.16	119.67
5	A	1018	MGD	O4'-C4'-C5'	2.28	116.63	109.33
5	A	1017	MGD	C5'-C4'-C3'	-2.25	107.12	115.21
5	A	1017	MGD	N2-C2-N1	-2.22	112.07	116.76
5	A	1017	MGD	O2B-PB-O3B	-2.20	101.31	107.27
5	A	1018	MGD	C23-C14-N15	2.19	110.02	107.87
7	B	812	CDL	OB9-CB7-C71	-2.18	115.26	123.78
5	A	1018	MGD	C17-C16-N15	2.16	122.16	116.27
5	A	1017	MGD	O4'-C4'-C5'	2.16	116.25	109.33
5	A	1017	MGD	PA-O3A-C10	-2.13	109.15	121.35
5	A	1017	MGD	O11-C23-N22	2.12	110.53	108.61
7	B	812	CDL	OB2-PB2-OB3	-2.09	100.64	108.94
5	A	1018	MGD	N19-C19-N18	2.08	121.14	116.76
8	C	810	HEM	CAD-C3D-C2D	2.02	131.65	127.87
8	C	810	HEM	CHD-C1D-ND	2.01	126.59	124.42

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1017	MGD	PA-O3B-PB-O5'
5	A	1017	MGD	C5'-O5'-PB-O1B
5	A	1017	MGD	C5'-O5'-PB-O3B
5	A	1017	MGD	C10-O3A-PA-O3B
5	A	1017	MGD	C10-O3A-PA-O1A
5	A	1018	MGD	C10-O3A-PA-O1A
7	B	812	CDL	CA3-OA5-PA1-OA2
7	B	812	CDL	CA3-OA5-PA1-OA3
7	B	812	CDL	CA3-OA5-PA1-OA4
7	B	812	CDL	CB2-OB2-PB2-OB3
7	B	812	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
7	B	812	CDL	CB3-OB5-PB2-OB2
7	B	812	CDL	CB3-OB5-PB2-OB3
7	B	812	CDL	CB3-OB5-PB2-OB4
8	C	809	HEM	C2C-C3C-CAC-CBC
7	B	812	CDL	C11-CA5-OA6-CA4
7	B	812	CDL	CB2-C1-CA2-OA2
7	B	812	CDL	O1-C1-CA2-OA2
7	B	812	CDL	CA7-C31-C32-C33
9	C	811	HQO	C3-C11-C13-C12
7	B	812	CDL	OB7-CB5-OB6-CB4
7	B	812	CDL	O1-C1-CB2-OB2
7	B	812	CDL	C36-C37-C38-C39
7	B	812	CDL	C37-C38-C39-C40
7	B	812	CDL	OB9-CB7-OB8-CB6
8	C	809	HEM	C4C-C3C-CAC-CBC
8	C	810	HEM	C3D-CAD-CBD-CGD
7	B	812	CDL	CA2-C1-CB2-OB2
7	B	812	CDL	CB3-CB4-CB6-OB8
7	B	812	CDL	C40-C41-C42-C43
7	B	812	CDL	C71-C72-C73-C74
9	C	811	HQO	C13-C12-C14-C15
7	B	812	CDL	C1-CA2-OA2-PA1
7	B	812	CDL	CB5-C51-C52-C53
7	B	812	CDL	C73-C74-C75-C76
7	B	812	CDL	OB5-CB3-CB4-OB6
7	B	812	CDL	CA5-C11-C12-C13
7	B	812	CDL	C71-CB7-OB8-CB6
5	A	1018	MGD	PA-O3B-PB-O5'
7	B	812	CDL	C17-C18-C19-C20
7	B	812	CDL	C41-C42-C43-C44
8	C	809	HEM	C2B-C3B-CAB-CBB
7	B	812	CDL	OA5-CA3-CA4-OA6
8	C	809	HEM	C4B-C3B-CAB-CBB
7	B	812	CDL	OB6-CB4-CB6-OB8
7	B	812	CDL	OA5-CA3-CA4-CA6
5	A	1017	MGD	C10-O3A-PA-O2A
5	A	1018	MGD	C5'-O5'-PB-O1B
5	A	1018	MGD	C10-O3A-PA-O3B
7	B	812	CDL	C39-C40-C41-C42
7	B	812	CDL	C52-C53-C54-C55
5	A	1017	MGD	O3A-C10-C11-O11
5	A	1018	MGD	O3A-C10-C11-O11

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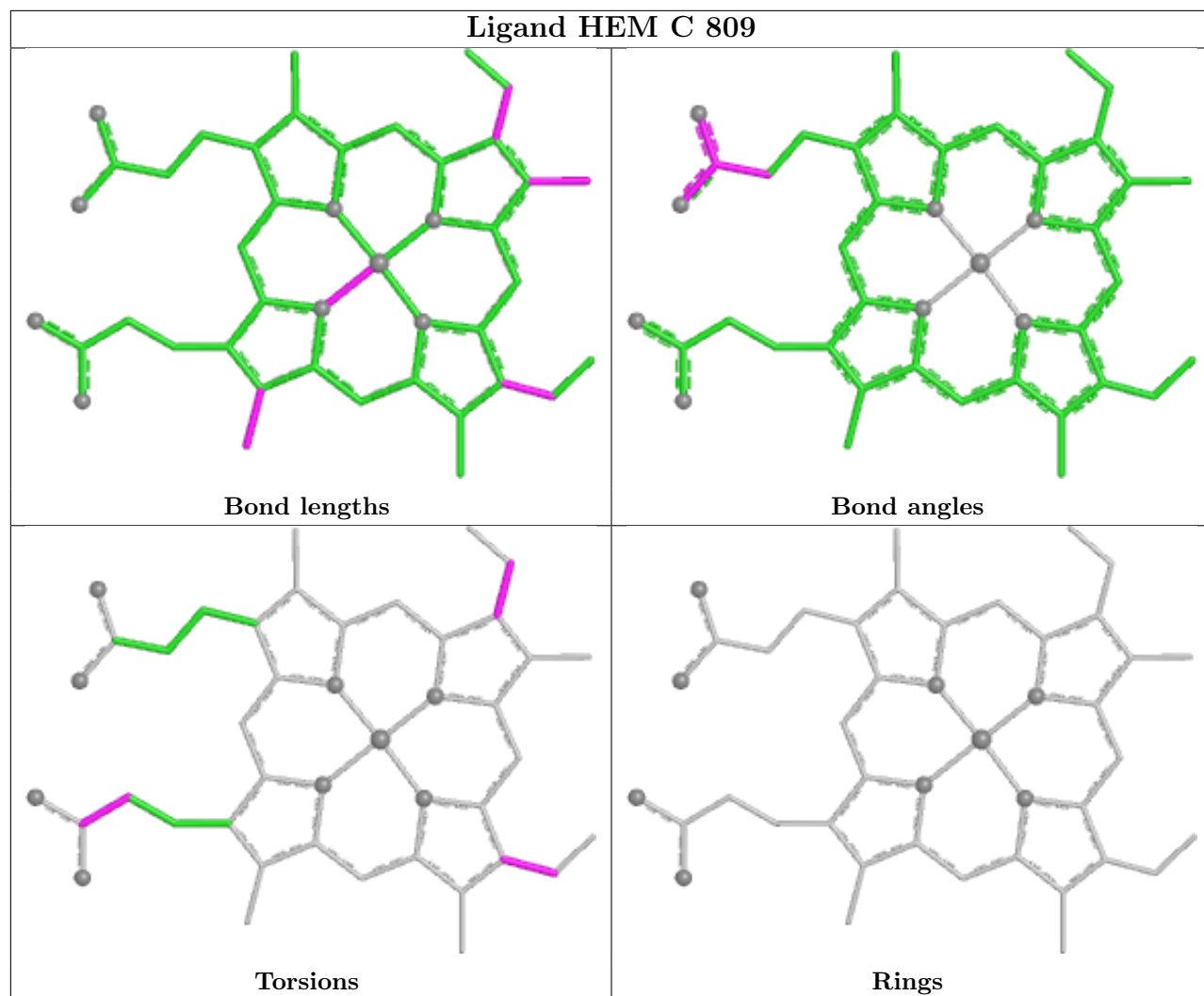
Mol	Chain	Res	Type	Atoms
7	B	812	CDL	C15-C16-C17-C18
7	B	812	CDL	OA7-CA5-OA6-CA4
7	B	812	CDL	C32-C31-CA7-OA8
8	C	809	HEM	CAA-CBA-CGA-O2A
7	B	812	CDL	OB5-CB3-CB4-CB6
5	A	1018	MGD	C2'-C1'-N9-C4
5	A	1017	MGD	C2'-C1'-N9-C8
7	B	812	CDL	C52-C51-CB5-OB6
8	C	810	HEM	CAA-CBA-CGA-O1A
8	C	809	HEM	CAA-CBA-CGA-O1A
7	B	812	CDL	C12-C11-CA5-OA7
8	C	810	HEM	CAA-CBA-CGA-O2A
5	A	1018	MGD	PB-O3B-PA-O2A

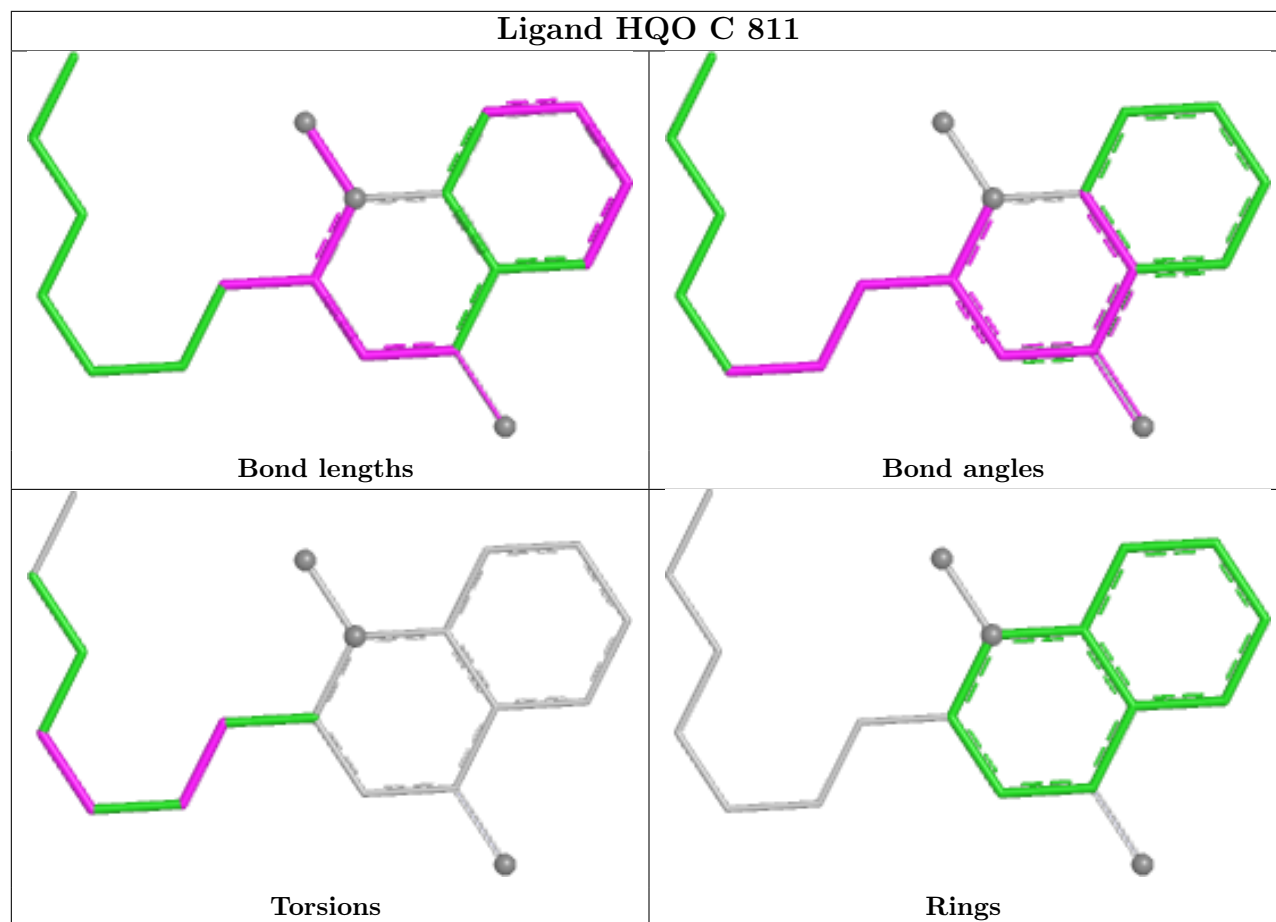
There are no ring outliers.

5 monomers are involved in 13 short contacts:

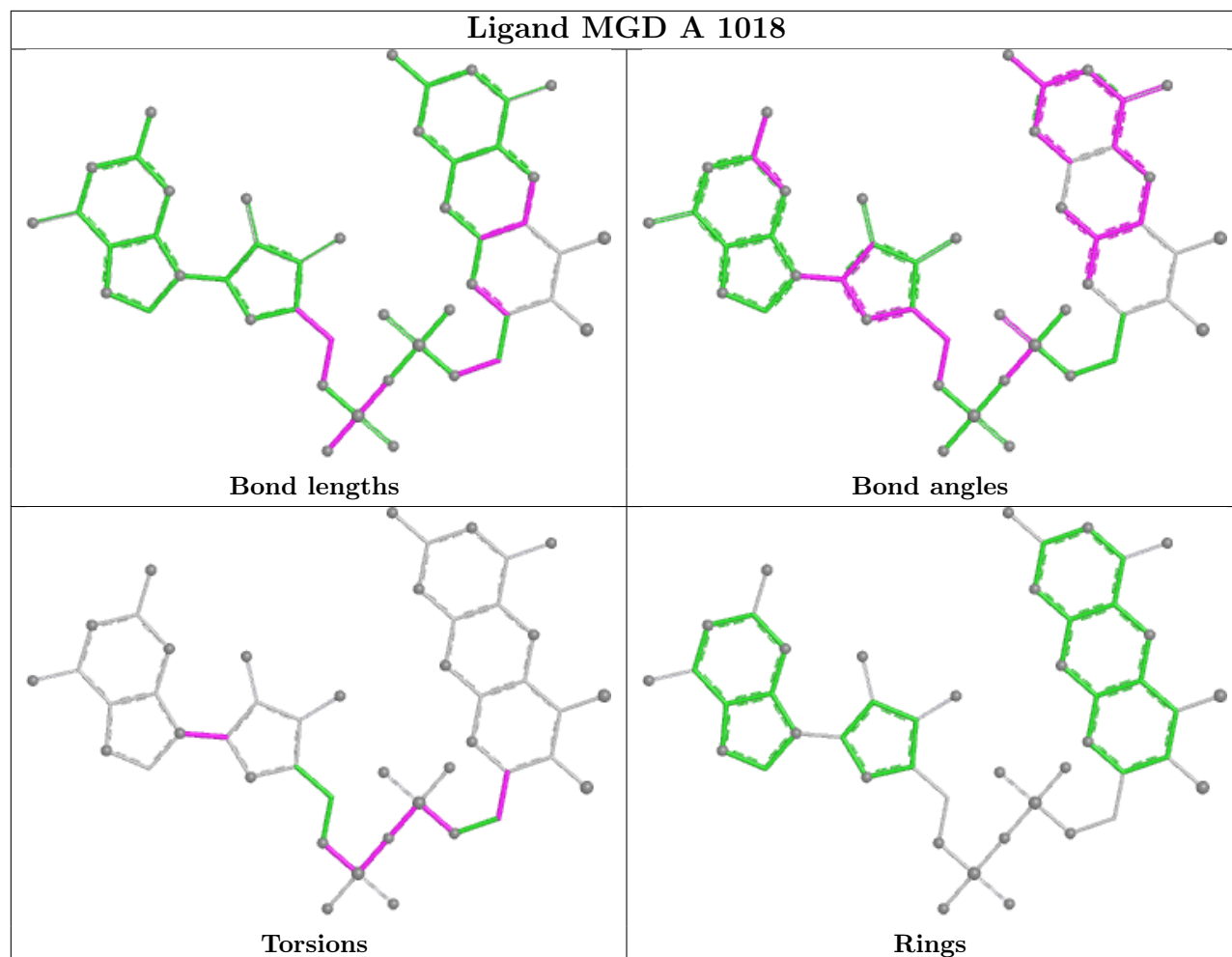
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	811	HQO	1	0
5	A	1018	MGD	2	0
8	C	810	HEM	3	0
7	B	812	CDL	4	0
5	A	1017	MGD	3	0

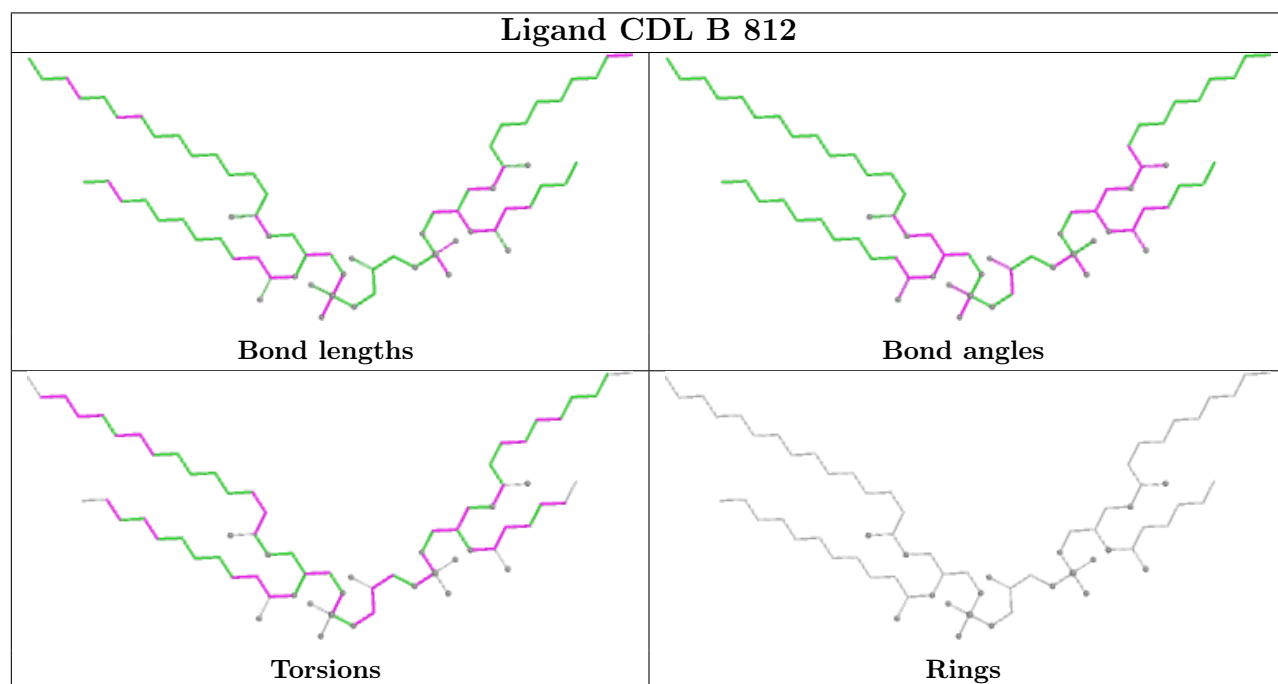
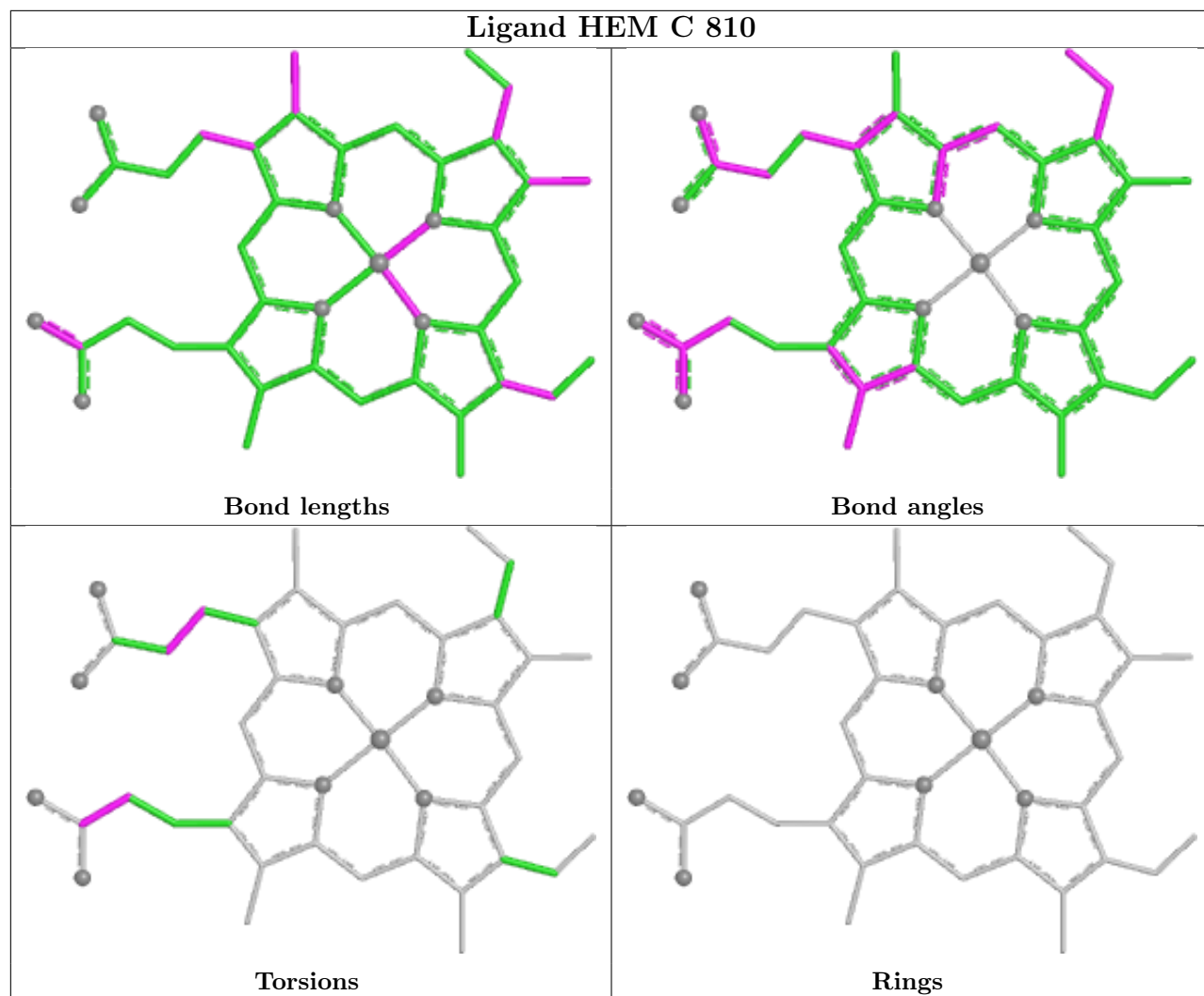
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

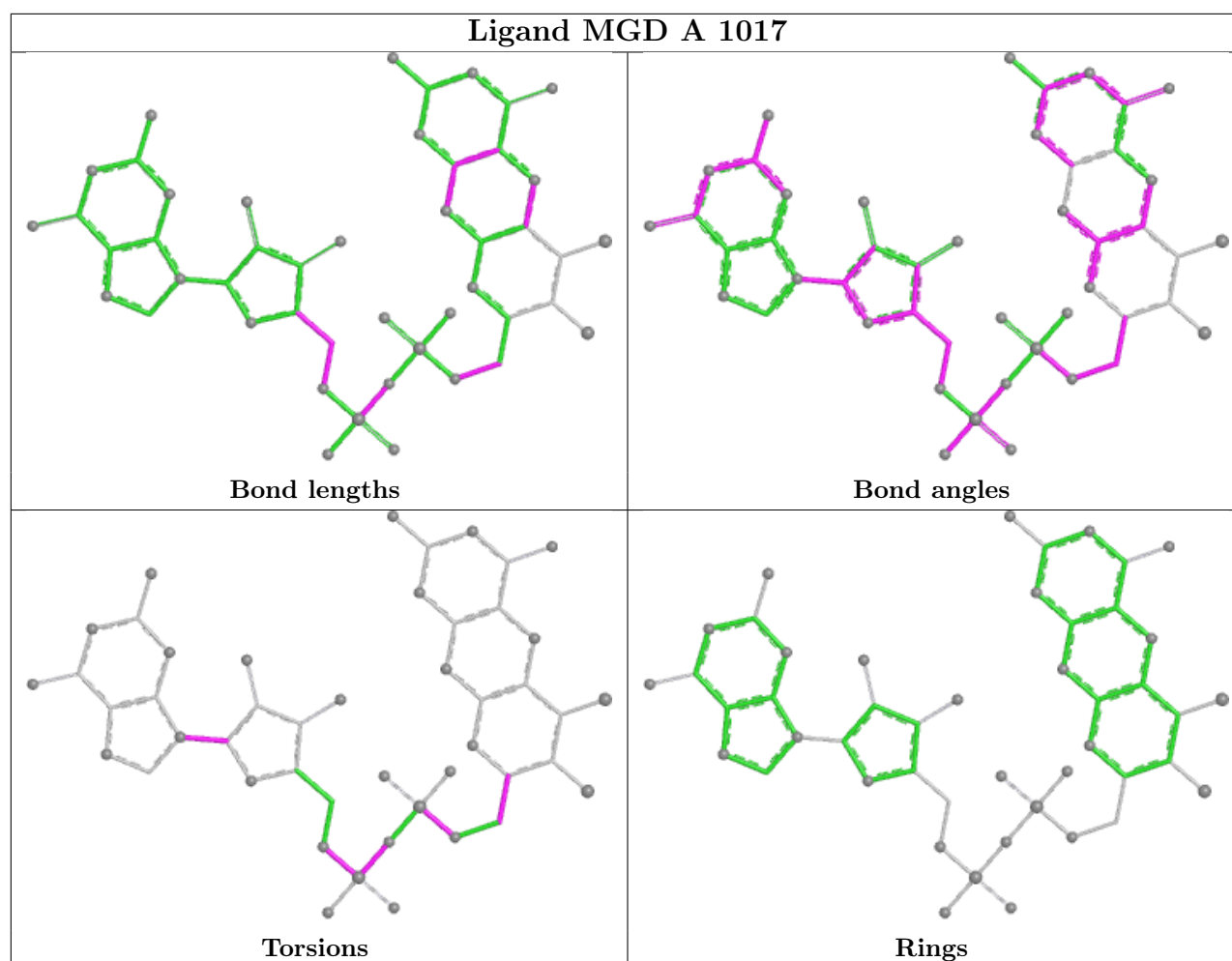




Ligand MGD A 1018







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.