



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 1B86 / pdb_00001b86
Title : HUMAN DEOXYHAEMOGLOBIN-2,3-DIPHOSPHOGLYCERATE COM-
PLEX
Authors : Richard, V.; Dodson, G.G.; Mauguén, Y.
Deposited on : 1999-02-08
Resolution : 2.50 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

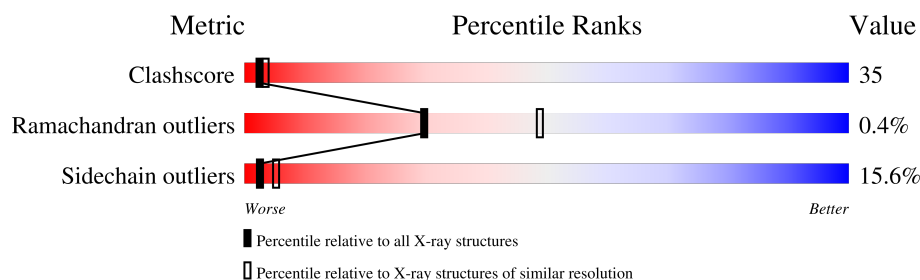
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	141	
1	C	141	
2	B	146	
2	D	146	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DG2	D	701	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4715 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.

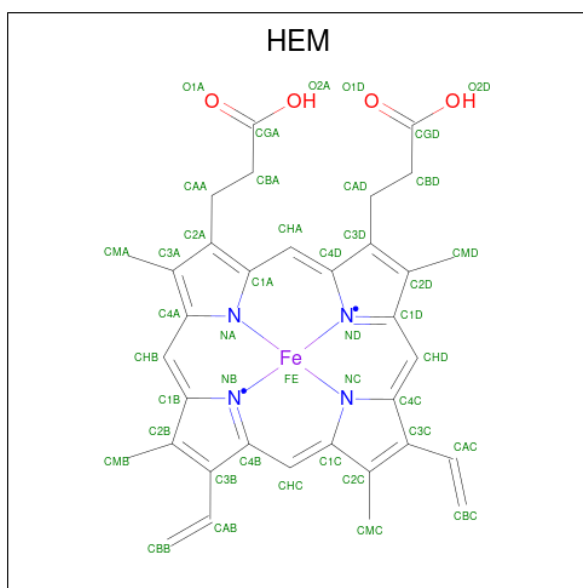
- Molecule 1 is a protein called PROTEIN (HEMOGLOBIN; ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called PROTEIN (HEMOGLOBIN; BETA CHAIN).

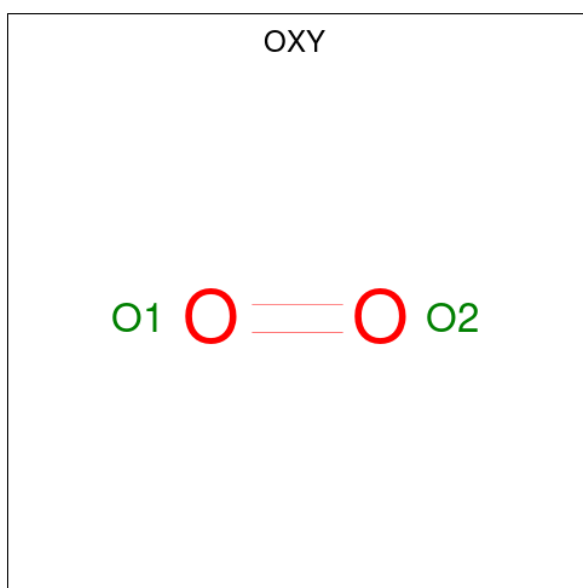
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	1	0
			1127	727	196	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



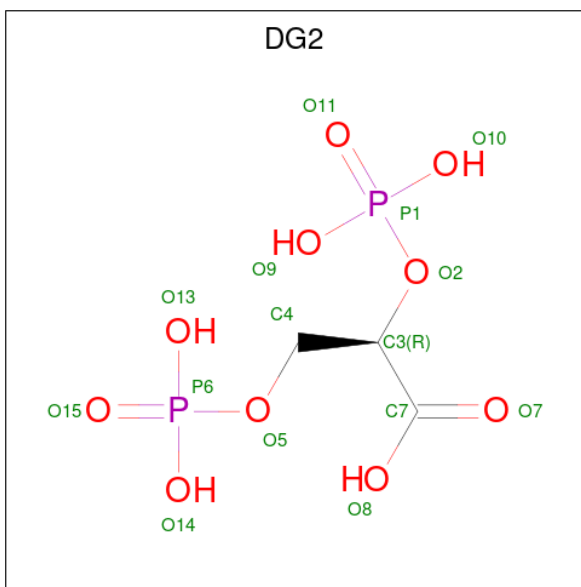
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			2	2		

- Molecule 5 is (2R)-2,3-diphosphoglyceric acid (CCD ID: DG2) (formula: C₃H₈O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	0
			15	3	10	2		

- Molecule 6 is water.

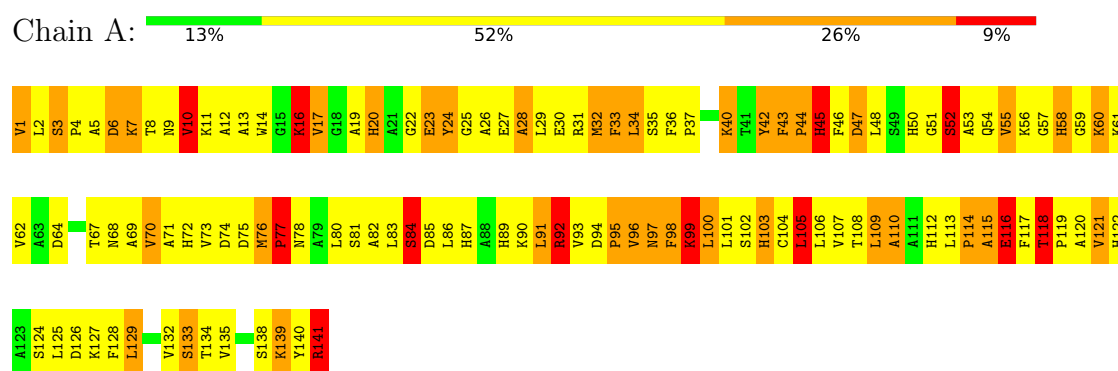
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	46	Total	O	0	0
			46	46		
6	C	16	Total	O	0	0
			16	16		
6	D	45	Total	O	0	0
			45	45		

3 Residue-property plots

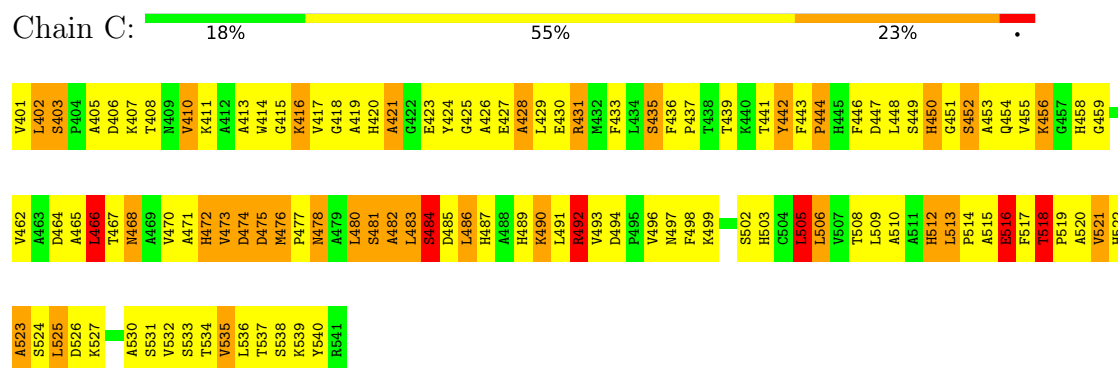
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

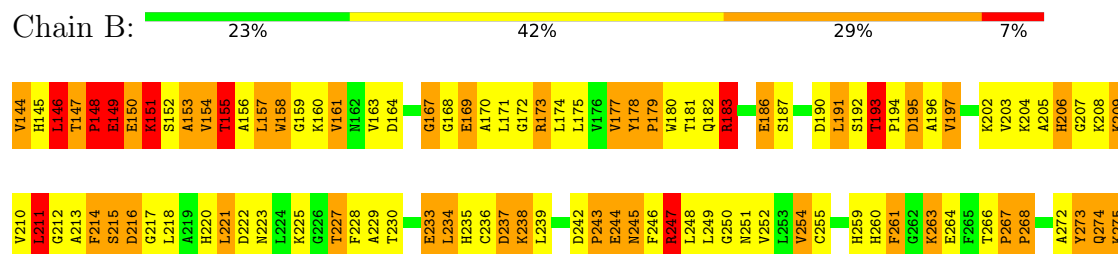
- Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

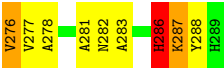


- Molecule 1: PROTEIN (HEMOGLOBIN; ALPHA CHAIN)

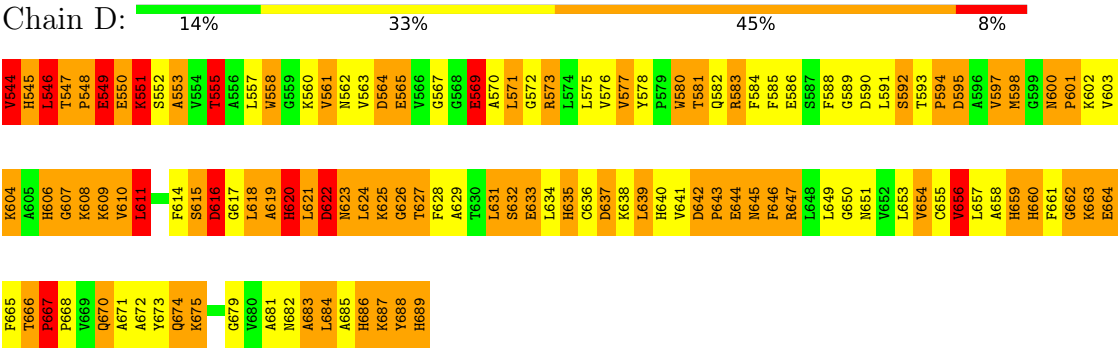


- Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)





● Molecule 2: PROTEIN (HEMOGLOBIN; BETA CHAIN)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.30 Å 98.08 Å 65.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (10.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.13	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4715	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: DG2, OXY, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.50	5/1097 (0.5%)	3.86	235/1491 (15.8%)
1	C	1.50	5/1097 (0.5%)	3.45	203/1491 (13.6%)
2	B	1.51	3/1153 (0.3%)	3.66	213/1566 (13.6%)
2	D	1.57	12/1162 (1.0%)	3.77	253/1577 (16.0%)
All	All	1.52	25/4509 (0.6%)	3.69	904/6125 (14.8%)

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	1
1	C	0	1
2	B	0	2
2	D	1	0
All	All	1	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	626	GLY	N-CA	8.47	1.56	1.45
2	D	625[A]	LYS	CA-C	7.56	1.62	1.52
2	D	625[B]	LYS	CA-C	7.56	1.62	1.52
2	B	212	GLY	N-CA	7.54	1.55	1.45
1	A	118	THR	CA-CB	6.99	1.63	1.53
2	D	650	GLY	N-CA	6.95	1.54	1.45
1	A	5	ALA	N-CA	6.58	1.54	1.46
1	C	487	HIS	CD2-NE2	6.25	1.44	1.37
1	C	436	PHE	N-CA	6.08	1.54	1.46
2	B	195	ASP	N-CA	5.96	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	TRP	N-CA	5.95	1.53	1.46
2	D	625[A]	LYS	N-CA	5.84	1.53	1.46
2	D	625[B]	LYS	N-CA	5.84	1.53	1.46
1	A	112	HIS	CA-CB	5.78	1.62	1.54
2	D	577	VAL	C-N	-5.72	1.25	1.34
1	C	527	LYS	CA-CB	-5.54	1.44	1.53
2	D	651	ASN	N-CA	5.28	1.52	1.46
2	D	685	ALA	C-N	-5.26	1.26	1.33
2	D	679	GLY	N-CA	5.25	1.52	1.45
1	A	47	ASP	C-O	5.15	1.30	1.24
2	B	235	HIS	CG-ND1	-5.09	1.32	1.38
1	C	531	SER	N-CA	5.04	1.52	1.46
2	D	586	GLU	N-CA	5.03	1.52	1.46
1	C	465	ALA	N-CA	5.03	1.52	1.46
2	D	616	ASP	N-CA	5.01	1.52	1.46

All (904) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	286	HIS	CA-CB-CG	30.89	144.69	113.80
2	B	145	HIS	CA-CB-CG	-24.75	89.05	113.80
2	D	545	HIS	CA-CB-CG	-22.10	91.70	113.80
1	C	518	THR	N-CA-CB	-18.40	85.63	109.55
2	D	545	HIS	N-CA-CB	18.32	136.47	110.46
2	B	286	HIS	CB-CA-C	-16.90	83.78	110.81
2	B	264	GLU	CB-CG-CD	16.80	141.16	112.60
2	B	145	HIS	CB-CA-C	-16.55	84.03	111.68
1	A	64	ASP	CA-CB-CG	16.52	129.12	112.60
1	C	423	GLU	CA-CB-CG	16.33	146.77	114.10
2	B	286	HIS	N-CA-CB	16.27	134.18	109.94
1	A	7	LYS	CA-C-O	16.22	137.75	120.55
1	A	72	HIS	CA-CB-CG	-16.21	97.59	113.80
1	A	96	VAL	CA-C-O	-15.95	104.36	120.95
2	B	145	HIS	N-CA-CB	15.89	136.91	110.53
1	A	92	ARG	NE-CZ-NH2	15.43	133.09	119.20
1	A	118	THR	N-CA-CB	-15.28	88.70	109.78
1	A	114	PRO	O-C-N	15.17	143.12	122.64
2	B	235	HIS	CE1-NE2-CD2	-14.79	94.21	109.00
1	A	140	TYR	O-C-N	13.84	137.92	122.15
2	D	659	HIS	CA-C-O	13.63	135.49	120.90
2	D	617	GLY	O-C-N	13.63	137.13	122.28
1	C	485	ASP	CA-CB-CG	13.41	126.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	660	HIS	CA-C-O	-13.35	106.27	120.42
1	A	59	GLY	CA-C-O	12.91	134.34	120.66
2	D	603	VAL	CA-C-O	12.84	134.40	121.05
2	D	684	LEU	CA-C-O	12.77	134.53	120.10
2	D	565	GLU	CB-CG-CD	12.54	133.93	112.60
1	A	92	ARG	CD-NE-CZ	12.47	141.86	124.40
2	D	551	LYS	CB-CA-C	-12.37	90.25	110.79
2	D	617	GLY	CA-C-O	-12.31	106.76	120.30
2	B	177	VAL	CA-C-O	-12.26	104.74	119.58
2	B	261	PHE	CA-CB-CG	-12.18	101.62	113.80
1	A	78	ASN	OD1-CG-ND2	12.13	134.73	122.60
1	A	77	PRO	O-C-N	12.10	135.25	122.18
2	B	235	HIS	ND1-CE1-NE2	11.99	120.39	108.40
2	B	250	GLY	O-C-N	-11.98	110.69	122.19
2	B	264	GLU	CA-CB-CG	11.93	137.97	114.10
1	A	47	ASP	CA-CB-CG	-11.92	100.68	112.60
1	A	23	GLU	CA-CB-CG	11.89	137.89	114.10
2	D	582	GLN	OE1-CD-NE2	-11.86	110.74	122.60
1	C	459	GLY	O-C-N	-11.85	110.81	122.19
2	B	158	TRP	CA-C-O	11.73	133.34	120.20
2	D	666	THR	CA-C-O	-11.70	107.77	120.88
1	C	427	GLU	CB-CG-CD	11.65	132.41	112.60
1	C	459	GLY	CA-C-O	11.64	132.74	120.75
2	D	545	HIS	O-C-N	11.59	138.40	122.41
1	A	68	ASN	OD1-CG-ND2	11.56	134.16	122.60
2	D	622	ASP	CA-CB-CG	11.50	124.10	112.60
1	A	11	LYS	CD-CE-NZ	11.48	148.64	111.90
1	C	433	PHE	O-C-N	11.43	134.24	122.12
1	A	8	THR	O-C-N	11.43	135.18	122.15
1	C	497	ASN	OD1-CG-ND2	-11.40	111.20	122.60
1	A	129	LEU	O-C-N	11.40	134.20	122.12
1	A	98	PHE	CA-C-O	11.39	132.49	120.42
2	D	565	GLU	CA-CB-CG	11.38	136.85	114.10
1	A	47	ASP	CA-C-O	-11.34	107.73	120.43
1	A	24	TYR	CA-C-O	-11.22	108.53	120.42
1	C	492	ARG	NE-CZ-NH2	-11.21	109.11	119.20
2	B	228	PHE	CA-CB-CG	-11.18	102.62	113.80
1	A	122	HIS	CA-C-O	11.13	132.34	120.55
1	A	20	HIS	CA-CB-CG	-11.11	102.69	113.80
2	B	245	ASN	CA-C-O	11.10	132.32	120.55
2	B	276	VAL	N-CA-CB	-11.07	97.60	110.55
2	D	598	MET	CA-C-N	11.02	134.22	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	598	MET	C-N-CA	11.02	134.22	120.34
2	D	666	THR	O-C-N	10.96	133.80	121.53
2	D	627	THR	N-CA-C	-10.95	99.35	111.07
1	A	23	GLU	CA-C-O	10.94	132.60	120.90
2	D	580	TRP	CA-C-O	-10.93	105.75	119.31
1	A	138	SER	CA-C-O	-10.90	107.78	120.10
2	D	610	VAL	CA-CB-CG2	10.90	128.92	110.40
1	A	99	LYS	CG-CD-CE	10.89	136.35	111.30
1	A	10	VAL	CA-C-O	-10.75	108.64	120.25
2	B	223	ASN	OD1-CG-ND2	10.73	133.33	122.60
2	D	659	HIS	CA-CB-CG	-10.71	103.09	113.80
2	B	252	VAL	CA-C-O	-10.69	109.83	120.95
2	D	600	ASN	CA-C-N	10.54	130.88	119.28
2	D	600	ASN	C-N-CA	10.54	130.88	119.28
2	D	611	LEU	CA-C-O	10.49	131.67	120.55
2	D	545	HIS	CA-C-N	-10.45	107.27	122.94
2	D	545	HIS	C-N-CA	-10.45	107.27	122.94
1	A	7	LYS	O-C-N	-10.45	111.05	122.12
2	B	267	PRO	CB-CA-C	10.43	123.64	110.92
2	B	286	HIS	O-C-N	10.42	132.93	122.09
1	A	12	ALA	CA-C-O	-10.33	110.06	120.70
1	A	96	VAL	O-C-N	10.26	131.82	121.87
1	A	87	HIS	CE1-NE2-CD2	-10.24	98.75	109.00
2	B	286	HIS	N-CA-C	10.17	123.32	111.11
1	A	27	GLU	CG-CD-OE2	10.12	141.67	118.40
2	D	600	ASN	CA-CB-CG	10.07	122.67	112.60
2	D	642	ASP	O-C-N	10.06	131.34	121.28
1	A	14	TRP	CA-C-N	10.01	132.65	120.14
1	A	14	TRP	C-N-CA	10.01	132.65	120.14
1	A	36	PHE	O-C-N	9.98	130.35	121.37
2	B	193	THR	O-C-N	9.98	129.80	121.32
1	A	46	PHE	O-C-N	9.89	136.72	122.97
2	D	636	CYS	CA-C-N	9.88	135.33	120.31
2	D	636	CYS	C-N-CA	9.88	135.33	120.31
1	A	60	LYS	CA-CB-CG	9.88	133.85	114.10
1	C	450	HIS	CA-CB-CG	-9.75	104.05	113.80
2	B	282	ASN	O-C-N	9.73	133.25	122.15
2	B	154	VAL	CA-C-N	9.73	133.09	120.44
2	B	154	VAL	C-N-CA	9.73	133.09	120.44
1	C	487	HIS	CE1-NE2-CD2	-9.69	99.31	109.00
2	D	641	VAL	N-CA-CB	-9.67	100.18	110.72
2	B	268	PRO	CA-C-O	-9.66	105.14	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	VAL	CA-C-O	-9.63	110.07	120.47
2	B	274	GLN	CB-CG-CD	9.60	128.92	112.60
1	A	33	PHE	CA-CB-CG	-9.60	104.20	113.80
2	B	238	LYS	N-CA-CB	-9.55	96.55	110.40
1	C	402	LEU	O-C-N	9.51	134.16	123.04
1	A	54	GLN	N-CA-C	-9.49	101.02	111.36
1	A	102	SER	CA-C-N	9.48	133.75	120.29
1	A	102	SER	C-N-CA	9.48	133.75	120.29
1	C	521	VAL	N-CA-C	-9.47	100.68	111.00
2	B	216	ASP	CA-CB-CG	9.43	122.03	112.60
1	C	494	ASP	CA-CB-CG	-9.42	103.18	112.60
1	C	525	LEU	CA-C-O	9.38	130.49	120.55
2	B	266	THR	CA-CB-OG1	-9.38	95.53	109.60
2	D	609	LYS	CA-C-N	9.36	132.39	120.70
2	D	609	LYS	C-N-CA	9.36	132.39	120.70
1	A	72	HIS	CA-C-O	-9.29	109.22	120.65
1	C	436	PHE	O-C-N	9.29	129.73	121.37
1	A	138	SER	O-C-N	9.26	133.05	122.22
2	D	595	ASP	CA-CB-CG	9.25	121.85	112.60
1	A	117	PHE	CA-C-O	9.21	134.52	122.63
2	B	149	GLU	N-CA-C	-9.20	101.83	113.23
2	B	260	HIS	CA-CB-CG	-9.19	104.61	113.80
2	D	657	LEU	CA-C-O	9.19	130.56	120.63
1	A	109	LEU	CA-C-O	9.19	130.16	120.42
1	C	524	SER	O-C-N	-9.12	112.67	122.07
1	A	47	ASP	CA-C-N	-9.12	108.91	122.86
1	A	47	ASP	C-N-CA	-9.12	108.91	122.86
1	C	466	LEU	CA-C-O	9.12	130.39	120.82
2	D	642	ASP	CA-C-O	-9.10	110.70	119.80
2	D	638	LYS	CB-CA-C	-9.10	95.80	110.08
1	A	6	ASP	N-CA-C	-9.09	101.33	111.14
1	A	115	ALA	CA-C-O	9.09	130.18	120.55
2	D	647	ARG	O-C-N	9.04	131.86	122.09
1	A	7	LYS	N-CA-C	9.04	121.13	111.28
2	D	682	ASN	CA-C-O	-9.04	110.84	120.42
2	D	558	TRP	CA-C-N	9.03	130.14	120.03
2	D	558	TRP	C-N-CA	9.03	130.14	120.03
2	B	204	LYS	CA-C-N	9.02	136.00	120.58
2	B	204	LYS	C-N-CA	9.02	136.00	120.58
1	A	97	ASN	CB-CG-ND2	9.00	129.90	116.40
1	A	118	THR	CA-CB-CG2	8.98	125.77	110.50
2	D	672	ALA	N-CA-C	-8.96	100.94	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	ALA	CA-C-O	8.92	130.45	120.90
2	B	210	VAL	CA-CB-CG1	8.92	125.56	110.40
2	D	629	ALA	N-CA-C	8.90	122.11	111.33
2	D	656	VAL	CB-CA-C	8.90	124.17	112.24
2	D	667	PRO	O-C-N	8.90	131.97	121.46
1	A	126	ASP	CA-CB-CG	-8.86	103.74	112.60
2	D	651	ASN	CA-C-O	-8.84	111.54	120.82
2	B	235	HIS	CG-CD2-NE2	8.84	116.04	107.20
2	D	595	ASP	O-C-N	8.83	132.22	122.15
2	B	209	LYS	O-C-N	8.82	131.62	122.09
1	A	76	MET	CA-C-N	8.80	128.39	119.24
1	A	76	MET	C-N-CA	8.80	128.39	119.24
1	C	423	GLU	N-CA-C	-8.79	100.56	111.11
2	B	148	PRO	N-CA-C	-8.78	99.82	114.75
2	D	601	PRO	CB-CA-C	-8.78	98.52	112.21
2	B	282	ASN	CA-CB-CG	-8.77	103.83	112.60
1	C	431	ARG	CD-NE-CZ	-8.77	112.12	124.40
2	D	582	GLN	CG-CD-OE1	8.76	138.33	120.80
2	B	275	LYS	CA-C-O	8.76	130.02	120.82
2	D	615	SER	O-C-N	-8.75	110.95	122.59
1	A	17	VAL	N-CA-C	-8.75	101.18	110.36
1	A	125	LEU	CA-C-O	-8.75	111.15	120.42
1	A	81	SER	CA-C-O	8.74	130.07	120.63
2	B	287	LYS	CB-CA-C	-8.74	94.81	110.37
2	B	222	ASP	O-C-N	8.74	133.26	122.34
1	C	536	LEU	CB-CA-C	8.73	125.70	110.85
1	A	103	HIS	ND1-CE1-NE2	-8.72	99.68	108.40
1	A	31	ARG	CA-C-N	8.72	132.16	120.65
1	A	31	ARG	C-N-CA	8.72	132.16	120.65
2	B	195	ASP	CA-C-O	-8.72	108.65	119.38
2	B	168	GLY	CA-C-O	8.71	129.72	120.75
1	C	505	LEU	CA-C-N	8.71	138.18	121.54
1	C	505	LEU	C-N-CA	8.71	138.18	121.54
1	A	14	TRP	O-C-N	-8.70	112.90	122.12
2	B	274	GLN	CA-C-N	8.70	131.75	120.44
2	B	274	GLN	C-N-CA	8.70	131.75	120.44
2	D	615	SER	CA-CB-OG	8.70	128.49	111.10
1	A	7	LYS	N-CA-CB	-8.69	97.34	110.12
1	A	115	ALA	N-CA-C	8.66	120.72	111.28
1	C	418	GLY	CA-C-O	8.65	135.63	120.57
2	B	220	HIS	CA-CB-CG	-8.65	105.15	113.80
1	A	97	ASN	CB-CG-OD1	-8.64	103.52	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	PRO	CA-C-O	-8.64	104.88	120.60
1	A	9	ASN	CB-CG-ND2	-8.63	103.46	116.40
2	D	625[A]	LYS	N-CA-CB	8.61	122.46	109.98
2	D	625[B]	LYS	N-CA-CB	8.61	122.46	109.98
2	B	151	LYS	O-C-N	-8.60	110.91	122.43
2	D	620	HIS	CA-CB-CG	-8.59	105.21	113.80
1	C	527	LYS	CA-C-O	-8.59	110.40	120.10
2	B	245	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	A	10	VAL	O-C-N	8.57	133.56	121.82
1	C	442	TYR	CA-C-O	-8.56	109.00	119.18
1	A	47	ASP	O-C-N	8.54	132.95	123.13
1	C	450	HIS	CB-CA-C	8.54	123.56	109.89
2	D	589	GLY	CA-C-O	8.54	131.47	121.05
2	B	244	GLU	CA-C-N	8.53	131.70	120.28
2	B	244	GLU	C-N-CA	8.53	131.70	120.28
2	B	239	LEU	N-CA-CB	-8.52	97.14	110.44
1	A	122	HIS	CA-CB-CG	8.52	122.32	113.80
1	C	486	LEU	O-C-N	-8.51	113.24	122.09
1	C	534	THR	CA-C-N	8.49	134.22	120.30
1	C	534	THR	C-N-CA	8.49	134.22	120.30
1	C	468	ASN	CA-C-O	-8.48	110.22	119.97
1	A	11	LYS	CA-C-O	8.47	129.53	120.55
2	B	227	THR	CA-C-O	-8.45	112.12	121.00
1	C	431	ARG	NE-CZ-NH2	-8.44	111.60	119.20
2	D	618	LEU	CA-C-O	8.44	129.70	119.49
1	C	447	ASP	CA-C-O	-8.44	111.07	120.69
2	B	260	HIS	N-CA-CB	-8.41	97.73	110.26
2	D	553	ALA	O-C-N	8.40	133.59	122.33
2	B	282	ASN	CB-CG-ND2	-8.38	103.82	116.40
1	C	433	PHE	CA-CB-CG	-8.38	105.42	113.80
1	C	527	LYS	O-C-N	8.38	132.02	122.22
1	A	69	ALA	N-CA-C	-8.37	102.24	111.36
2	D	615	SER	CA-C-O	8.36	132.46	120.51
2	D	685	ALA	N-CA-C	8.36	122.29	112.93
2	B	148	PRO	CA-C-N	-8.35	106.96	121.66
2	B	148	PRO	C-N-CA	-8.35	106.96	121.66
2	D	601	PRO	O-C-N	8.35	132.99	122.22
2	D	635	HIS	CA-C-O	8.35	129.40	120.55
1	C	413	ALA	N-CA-CB	-8.35	97.50	109.94
1	C	427	GLU	CA-CB-CG	8.35	130.79	114.10
1	C	486	LEU	CA-C-N	8.31	132.09	120.29
1	C	486	LEU	C-N-CA	8.31	132.09	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	512	HIS	CA-C-O	-8.29	109.15	118.69
1	C	499	LYS	CA-C-O	-8.28	110.02	119.79
1	C	492	ARG	CD-NE-CZ	-8.27	112.82	124.40
1	C	454	GLN	OE1-CD-NE2	8.27	130.87	122.60
1	A	6	ASP	O-C-N	8.24	130.99	122.09
2	B	149	GLU	CB-CG-CD	8.24	126.60	112.60
2	B	209	LYS	CA-C-O	-8.21	112.25	120.70
2	B	153	ALA	N-CA-CB	-8.21	98.02	110.16
2	D	608	LYS	CA-C-O	8.20	129.37	120.10
1	A	24	TYR	CA-C-N	8.18	129.02	119.94
1	A	24	TYR	C-N-CA	8.18	129.02	119.94
1	C	420	HIS	O-C-N	8.18	132.16	122.34
1	A	26	ALA	O-C-N	-8.18	113.59	122.09
2	B	281	ALA	CA-C-O	8.17	129.64	120.90
2	D	603	VAL	N-CA-CB	-8.15	100.28	110.47
2	D	663	LYS	CB-CG-CD	8.15	130.05	111.30
2	D	550	GLU	CA-C-O	-8.12	112.47	121.00
1	A	74	ASP	CA-CB-CG	-8.12	104.48	112.60
2	B	149	GLU	CG-CD-OE1	8.12	137.07	118.40
1	A	103	HIS	CE1-NE2-CD2	8.11	117.11	109.00
2	B	216	ASP	O-C-N	-8.10	113.54	122.12
2	B	233	GLU	CA-C-O	-8.10	111.88	120.63
2	B	263	LYS	CA-CB-CG	8.09	130.28	114.10
1	C	487	HIS	ND1-CE1-NE2	8.08	116.48	108.40
2	D	646	PHE	O-C-N	8.07	132.72	122.23
1	C	441	THR	CA-CB-OG1	-8.05	97.53	109.60
2	B	147	THR	CA-CB-OG1	-8.04	97.54	109.60
1	C	471	ALA	N-CA-C	8.03	120.03	111.28
1	A	75	ASP	CA-C-O	-8.01	111.82	122.31
1	A	70	VAL	CA-CB-CG2	8.00	124.00	110.40
2	D	638	LYS	CG-CD-CE	7.98	129.65	111.30
2	B	209	LYS	N-CA-CB	7.98	121.64	110.07
1	C	453	ALA	CA-C-O	7.96	129.18	119.79
1	C	428	ALA	N-CA-C	-7.95	102.69	111.36
1	A	92	ARG	CA-C-N	7.93	132.91	121.80
1	A	92	ARG	C-N-CA	7.93	132.91	121.80
1	C	468	ASN	N-CA-C	-7.93	102.62	111.82
2	D	657	LEU	O-C-N	-7.91	113.73	122.12
2	B	212	GLY	O-C-N	7.90	131.43	122.34
1	A	82	ALA	O-C-N	7.88	130.29	122.09
1	C	497	ASN	CB-CG-OD1	7.88	136.55	120.80
1	C	462	VAL	N-CA-CB	-7.87	101.34	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	HIS	CE1-NE2-CD2	-7.86	101.14	109.00
1	C	446	PHE	CA-CB-CG	7.85	121.65	113.80
2	D	576	VAL	CA-C-O	-7.85	111.62	120.96
2	B	211	LEU	CA-C-N	-7.81	110.49	120.34
2	B	211	LEU	C-N-CA	-7.81	110.49	120.34
2	D	656	VAL	CA-C-O	-7.81	112.35	120.71
1	A	87	HIS	ND1-CE1-NE2	7.80	116.20	108.40
1	C	484	SER	O-C-N	7.79	131.03	122.15
1	A	76	MET	O-C-N	7.78	130.26	121.32
2	B	154	VAL	CA-C-O	7.78	129.50	121.41
2	D	663	LYS	CA-CB-CG	7.77	129.64	114.10
2	D	610	VAL	CA-C-N	7.75	130.67	120.28
2	D	610	VAL	C-N-CA	7.75	130.67	120.28
1	C	423	GLU	N-CA-CB	7.75	121.49	109.94
1	A	60	LYS	CG-CD-CE	7.73	129.07	111.30
1	A	30	GLU	CB-CG-CD	7.71	125.71	112.60
1	C	454	GLN	N-CA-CB	-7.68	98.84	109.98
2	D	656	VAL	N-CA-C	-7.68	102.63	111.00
1	A	55	VAL	CA-C-N	7.68	130.57	120.28
1	A	55	VAL	C-N-CA	7.68	130.57	120.28
1	A	34	LEU	N-CA-C	7.67	121.12	111.69
2	D	569	GLU	CB-CG-CD	-7.65	99.59	112.60
2	B	236	CYS	CA-C-N	7.64	130.52	120.28
2	B	236	CYS	C-N-CA	7.64	130.52	120.28
2	B	252	VAL	N-CA-CB	7.64	120.93	110.54
1	A	82	ALA	CA-C-O	-7.63	112.73	120.90
2	D	595	ASP	CA-C-O	-7.62	112.34	120.42
1	A	135	VAL	N-CA-C	-7.62	102.91	110.30
2	D	684	LEU	O-C-N	-7.60	113.32	122.22
2	B	190	ASP	CA-CB-CG	7.60	120.20	112.60
2	B	172	GLY	O-C-N	-7.58	114.91	122.18
1	C	513	LEU	O-C-N	7.58	127.56	121.20
1	C	534	THR	O-C-N	-7.58	114.09	122.12
1	C	465	ALA	CA-C-N	7.57	130.28	120.44
1	C	465	ALA	C-N-CA	7.57	130.28	120.44
2	D	586	GLU	O-C-N	7.57	132.91	122.46
1	A	59	GLY	O-C-N	-7.55	114.86	122.19
2	B	167	GLY	O-C-N	-7.55	114.86	122.19
2	B	245	ASN	CB-CG-OD1	7.54	135.88	120.80
1	A	132	VAL	CA-C-O	-7.53	113.12	120.95
2	D	545	HIS	CB-CA-C	-7.52	99.00	111.41
2	D	546	LEU	CA-C-O	-7.52	112.58	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	THR	CA-CB-CG2	7.51	123.28	110.50
2	D	620	HIS	CB-CA-C	-7.50	98.45	111.35
1	A	58	HIS	CA-C-O	7.49	128.62	119.79
1	C	472	HIS	CA-CB-CG	-7.49	106.31	113.80
1	C	531	SER	CB-CA-C	7.48	125.64	110.38
1	C	426	ALA	CA-C-O	-7.47	112.63	120.55
1	C	433	PHE	CA-C-O	-7.47	112.63	120.55
1	C	452	SER	CA-C-N	7.47	133.38	120.68
1	C	452	SER	C-N-CA	7.47	133.38	120.68
1	A	128	PHE	CA-CB-CG	-7.47	106.33	113.80
2	D	544	VAL	CA-CB-CG2	7.45	123.06	110.40
1	A	57	GLY	CA-C-O	-7.44	112.12	120.30
2	D	582	GLN	CA-C-O	-7.44	111.42	119.97
1	C	517	PHE	CA-C-O	7.43	131.92	122.64
2	B	157	LEU	O-C-N	7.42	130.04	122.03
2	B	212	GLY	N-CA-C	-7.41	102.74	113.86
1	A	90	LYS	CA-C-O	-7.41	110.42	119.61
2	B	248	LEU	O-C-N	7.39	129.68	122.07
1	C	480	LEU	CA-C-N	7.39	131.06	120.79
1	C	480	LEU	C-N-CA	7.39	131.06	120.79
2	D	611	LEU	O-C-N	-7.38	114.29	122.12
1	C	531	SER	O-C-N	-7.38	112.44	122.33
2	D	583	ARG	O-C-N	-7.34	112.78	122.33
2	D	686	HIS	N-CA-CB	-7.33	99.54	110.61
1	A	115	ALA	N-CA-CB	-7.33	99.35	110.12
2	D	597	VAL	O-C-N	7.33	129.52	121.90
2	D	583	ARG	NE-CZ-NH2	7.30	125.77	119.20
2	B	286	HIS	CA-C-O	-7.29	113.10	120.90
2	D	623	ASN	CB-CG-ND2	7.29	127.34	116.40
2	B	249	LEU	CA-C-O	-7.29	112.69	120.42
2	B	209	LYS	N-CA-C	-7.29	103.27	111.14
2	D	664	GLU	N-CA-C	7.29	121.43	112.54
1	A	125	LEU	O-C-N	7.28	130.45	122.15
2	D	675	LYS	O-C-N	7.27	132.08	122.33
2	D	689	HIS	CA-CB-CG	-7.27	106.53	113.80
1	A	98	PHE	O-C-N	-7.26	113.88	122.15
1	C	455	VAL	CA-C-O	7.25	128.49	120.95
2	D	549	GLU	O-C-N	7.24	129.53	122.07
2	B	206	HIS	O-C-N	-7.23	113.91	122.15
2	D	572	GLY	O-C-N	-7.23	115.18	122.19
1	A	24	TYR	CA-CB-CG	7.21	126.88	113.90
1	A	87	HIS	CG-CD2-NE2	7.20	114.40	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	526	ASP	CB-CG-OD1	7.19	134.95	118.40
1	A	54	GLN	O-C-N	7.19	130.34	122.15
2	D	544	VAL	N-CA-CB	7.19	123.72	111.50
2	B	233	GLU	OE1-CD-OE2	7.19	140.15	122.90
1	A	138	SER	CA-C-N	-7.18	111.25	122.67
1	A	138	SER	C-N-CA	-7.18	111.25	122.67
1	A	108	THR	CA-CB-OG1	-7.18	98.83	109.60
2	B	248	LEU	CA-C-O	-7.17	113.29	120.82
2	D	548	PRO	N-CD-CG	-7.17	92.45	103.20
2	B	283	ALA	CA-C-N	7.16	131.19	120.31
2	B	283	ALA	C-N-CA	7.16	131.19	120.31
1	C	419	ALA	CA-C-N	-7.15	111.21	122.65
1	C	419	ALA	C-N-CA	-7.15	111.21	122.65
2	B	197	VAL	N-CA-CB	-7.13	100.25	110.52
2	B	237	ASP	CA-CB-CG	7.12	119.72	112.60
2	B	251	ASN	OD1-CG-ND2	-7.11	115.49	122.60
2	D	606	HIS	N-CA-C	-7.11	102.95	111.69
2	D	583	ARG	CA-C-O	7.09	127.97	119.61
1	C	525	LEU	N-CA-CB	-7.08	99.71	110.12
2	D	645	ASN	O-C-N	7.06	131.57	122.39
1	A	32	MET	CA-CB-CG	-7.06	99.98	114.10
1	C	482	ALA	N-CA-CB	-7.06	99.47	110.06
2	D	583	ARG	CG-CD-NE	-7.06	96.47	112.00
2	B	190	ASP	CA-C-O	-7.06	112.30	120.49
2	D	640	HIS	CA-CB-CG	-7.04	106.76	113.80
1	C	471	ALA	CA-C-N	7.04	133.66	123.17
1	C	471	ALA	C-N-CA	7.04	133.66	123.17
2	D	674	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	C	512	HIS	N-CA-C	-7.02	104.20	114.39
1	A	110	ALA	N-CA-C	-7.01	103.56	111.07
1	A	9	ASN	OD1-CG-ND2	6.99	129.59	122.60
1	A	91	LEU	CA-C-O	6.99	127.83	120.42
2	B	160	LYS	CA-C-O	-6.99	110.82	119.28
2	D	627	THR	N-CA-CB	6.99	120.15	110.01
1	C	536	LEU	CA-C-O	6.99	127.83	120.42
1	C	403	SER	N-CA-C	-6.98	102.10	110.13
1	A	98	PHE	CA-CB-CG	-6.98	106.82	113.80
1	A	105	LEU	CA-C-N	6.98	129.51	120.44
1	A	105	LEU	C-N-CA	6.98	129.51	120.44
2	D	558	TRP	CA-C-O	6.96	128.15	120.63
2	D	637	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	13	ALA	CA-C-N	-6.96	110.96	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ALA	C-N-CA	-6.96	110.96	120.28
2	D	562	ASN	O-C-N	-6.96	113.84	122.68
1	A	17	VAL	O-C-N	6.94	128.88	121.94
2	D	573	ARG	CA-C-N	6.94	129.88	120.44
2	D	573	ARG	C-N-CA	6.94	129.88	120.44
1	C	452	SER	N-CA-C	-6.94	101.37	110.53
1	A	118	THR	CA-C-O	-6.93	113.12	120.88
2	B	178	TYR	N-CA-CB	6.92	119.78	110.79
2	D	623	ASN	O-C-N	6.92	131.79	122.59
1	C	450	HIS	O-C-N	6.91	131.43	122.93
1	C	476	MET	CA-CB-CG	-6.91	100.28	114.10
1	C	449	SER	CA-C-O	6.91	129.47	121.87
2	D	660	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	A	92	ARG	NE-CZ-NH1	-6.91	114.59	121.50
2	D	548	PRO	CB-CA-C	6.91	122.95	111.56
2	D	572	GLY	CA-C-O	-6.91	113.34	120.66
1	A	68	ASN	CA-C-O	6.90	127.73	120.42
2	D	561	VAL	CA-C-N	6.90	132.55	122.41
2	D	561	VAL	C-N-CA	6.90	132.55	122.41
1	A	140	TYR	CA-C-O	-6.89	113.11	120.42
2	B	156	ALA	CA-C-O	-6.89	113.12	120.42
1	A	58	HIS	ND1-CE1-NE2	6.88	115.28	108.40
2	D	625[A]	LYS	CB-CA-C	6.88	121.61	110.95
2	D	625[B]	LYS	CB-CA-C	6.88	121.61	110.95
1	C	533	SER	CA-C-O	6.88	127.71	120.42
1	A	122	HIS	ND1-CE1-NE2	6.87	115.27	108.40
1	A	114	PRO	N-CA-CB	6.87	110.47	103.25
1	A	23	GLU	CB-CA-C	-6.87	99.82	110.81
1	A	7	LYS	CA-C-N	6.87	130.04	120.29
1	A	7	LYS	C-N-CA	6.87	130.04	120.29
2	D	592	SER	CA-C-N	-6.86	110.52	122.38
2	D	592	SER	C-N-CA	-6.86	110.52	122.38
2	D	632	SER	CA-C-N	-6.85	110.42	120.28
2	D	632	SER	C-N-CA	-6.85	110.42	120.28
1	A	97	ASN	CA-CB-CG	-6.85	105.75	112.60
1	C	517	PHE	O-C-N	-6.82	113.62	122.56
2	B	177	VAL	O-C-N	6.81	131.52	122.12
2	D	670	GLN	CA-CB-CG	-6.81	100.48	114.10
1	C	437	PRO	CA-C-N	6.81	130.09	120.28
1	C	437	PRO	C-N-CA	6.81	130.09	120.28
2	B	177	VAL	CA-C-N	6.80	130.33	122.85
2	B	177	VAL	C-N-CA	6.80	130.33	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	585	PHE	CA-C-O	-6.78	113.14	121.89
2	D	671	ALA	CA-C-O	-6.78	112.44	120.10
1	C	524	SER	CA-C-O	6.78	127.94	120.82
2	D	622	ASP	CA-C-O	6.77	127.24	119.18
1	C	475	ASP	CA-CB-CG	-6.76	105.84	112.60
1	C	531	SER	N-CA-CB	-6.75	99.90	110.30
2	D	651	ASN	CB-CG-ND2	-6.75	106.28	116.40
2	B	146	LEU	CA-C-O	6.74	127.86	120.71
1	C	537	THR	CA-C-O	6.74	127.44	119.56
1	C	521	VAL	O-C-N	6.74	130.73	121.84
2	B	148	PRO	O-C-N	6.72	131.90	122.55
1	A	42	TYR	CA-C-O	-6.72	111.49	119.15
2	B	170	ALA	O-C-N	-6.72	113.50	122.23
2	D	581	THR	CA-CB-OG1	-6.69	99.57	109.60
1	A	91	LEU	O-C-N	-6.68	114.53	122.15
2	B	248	LEU	CD1-CG-CD2	-6.67	96.12	110.80
2	B	251	ASN	CA-C-N	6.67	129.60	120.46
2	B	251	ASN	C-N-CA	6.67	129.60	120.46
2	D	660	HIS	O-C-N	6.67	129.75	122.15
1	A	94	ASP	O-C-N	6.66	127.23	121.30
1	A	22	GLY	O-C-N	6.66	131.35	122.70
2	D	663	LYS	CG-CD-CE	6.66	126.61	111.30
2	D	610	VAL	N-CA-CB	-6.65	103.37	110.62
2	D	682	ASN	OD1-CG-ND2	-6.65	115.95	122.60
2	B	191	LEU	CA-C-O	6.64	126.42	119.51
1	C	513	LEU	CA-C-O	-6.64	114.52	121.29
2	B	197	VAL	CA-CB-CG2	6.64	121.68	110.40
1	C	467	THR	CA-CB-OG1	6.64	119.56	109.60
1	C	520	ALA	CA-C-O	-6.62	111.10	119.31
2	B	168	GLY	O-C-N	-6.61	115.84	122.19
2	B	173	ARG	CA-C-N	6.59	129.01	120.44
2	B	173	ARG	C-N-CA	6.59	129.01	120.44
1	A	6	ASP	CA-C-O	-6.59	113.91	120.70
2	B	242	ASP	O-C-N	6.58	127.04	121.31
2	B	179	PRO	CA-C-N	6.56	129.73	120.28
2	B	179	PRO	C-N-CA	6.56	129.73	120.28
1	C	431	ARG	NE-CZ-NH1	6.55	128.05	121.50
2	D	585	PHE	CA-C-N	-6.55	109.67	121.14
2	D	585	PHE	C-N-CA	-6.55	109.67	121.14
2	D	597	VAL	CA-C-O	-6.54	113.79	121.05
2	D	607	GLY	O-C-N	-6.54	114.20	122.70
2	D	547	THR	N-CA-C	-6.54	100.79	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ASN	CA-CB-CG	-6.54	106.06	112.60
2	B	227	THR	OG1-CB-CG2	-6.53	96.23	109.30
2	D	646	PHE	N-CA-CB	6.52	119.92	110.20
1	C	523	ALA	CA-C-O	-6.51	113.65	120.55
1	C	427	GLU	N-CA-CB	-6.49	99.82	110.40
2	D	673	TYR	O-C-N	6.48	129.54	122.15
1	A	27	GLU	O-C-N	-6.47	115.26	122.12
2	B	230	THR	N-CA-C	-6.46	104.09	112.23
1	C	489	HIS	O-C-N	6.45	130.29	122.48
2	D	651	ASN	CB-CG-OD1	6.44	133.68	120.80
2	B	282	ASN	CB-CG-OD1	6.44	133.68	120.80
2	D	638	LYS	CA-C-O	-6.44	111.38	120.07
2	B	222	ASP	CA-CB-CG	-6.42	106.18	112.60
2	D	597	VAL	CA-C-N	6.42	128.89	120.28
2	D	597	VAL	C-N-CA	6.42	128.89	120.28
2	D	633	GLU	CA-C-O	-6.42	112.84	120.10
1	A	8	THR	CA-C-N	-6.42	111.67	120.28
1	A	8	THR	C-N-CA	-6.42	111.67	120.28
2	D	549	GLU	N-CA-CB	6.41	119.31	110.01
2	D	561	VAL	N-CA-CB	6.40	117.69	110.72
2	B	282	ASN	N-CA-C	6.39	118.33	111.36
2	B	156	ALA	O-C-N	6.39	129.44	122.15
2	B	238	LYS	CA-CB-CG	-6.39	101.32	114.10
1	A	20	HIS	O-C-N	6.39	130.79	122.42
2	B	264	GLU	CG-CD-OE2	6.38	133.09	118.40
1	C	452	SER	CA-C-O	-6.38	114.46	121.87
1	A	52	SER	N-CA-C	-6.38	101.67	110.35
2	D	674	GLN	N-CA-CB	6.38	120.04	110.22
1	C	510	ALA	O-C-N	6.36	128.86	122.12
1	C	456	LYS	N-CA-CB	6.36	119.23	110.01
2	D	547	THR	CA-CB-CG2	6.35	121.30	110.50
1	C	462	VAL	CG1-CB-CG2	6.35	124.77	110.80
2	D	628	PHE	CA-CB-CG	-6.35	107.45	113.80
1	C	462	VAL	CA-CB-CG2	-6.35	99.61	110.40
1	C	536	LEU	N-CA-CB	-6.33	100.79	110.16
2	B	242	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	518	THR	CA-CB-OG1	6.32	119.08	109.60
2	D	548	PRO	O-C-N	6.32	131.17	122.64
1	C	498	PHE	CA-CB-CG	-6.32	107.48	113.80
2	D	643	PRO	CA-C-O	6.31	128.21	119.18
1	A	96	VAL	CB-CA-C	6.31	120.66	112.14
2	D	655	CYS	CA-CB-SG	6.31	128.91	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CB-CA-C	6.31	120.86	110.90
1	A	58	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
2	D	550	GLU	N-CA-C	-6.30	104.11	110.97
2	D	647	ARG	N-CA-C	-6.30	104.34	111.14
1	A	11	LYS	CB-CG-CD	6.29	125.77	111.30
1	C	471	ALA	O-C-N	-6.29	115.46	122.12
1	A	2	LEU	O-C-N	6.28	130.38	123.22
1	C	537	THR	CA-CB-OG1	-6.26	100.21	109.60
2	D	670	GLN	O-C-N	-6.26	115.58	122.09
2	D	567	GLY	O-C-N	-6.25	115.46	122.28
1	A	133	SER	CA-C-N	6.25	129.16	120.29
1	A	133	SER	C-N-CA	6.25	129.16	120.29
1	C	415	GLY	O-C-N	-6.23	115.96	122.13
1	C	506	LEU	O-C-N	6.23	130.88	122.59
1	C	467	THR	CA-C-N	6.21	129.76	120.31
1	C	467	THR	C-N-CA	6.21	129.76	120.31
1	C	492	ARG	CB-CG-CD	-6.21	97.01	111.30
1	A	133	SER	CA-CB-OG	-6.21	98.68	111.10
2	D	616	ASP	N-CA-C	6.20	118.84	111.71
1	A	68	ASN	O-C-N	-6.19	115.09	122.15
1	A	99	LYS	O-C-N	-6.19	114.66	122.27
1	A	72	HIS	O-C-N	6.19	130.49	122.20
2	B	192	SER	CA-C-N	-6.19	115.05	123.96
2	B	192	SER	C-N-CA	-6.19	115.05	123.96
2	B	282	ASN	CA-C-O	-6.18	113.87	120.42
1	C	420	HIS	CA-CB-CG	-6.18	107.62	113.80
2	B	186	GLU	CA-C-O	6.17	127.07	120.10
2	B	252	VAL	O-C-N	6.17	127.85	121.87
2	D	639	LEU	O-C-N	6.17	130.91	122.46
1	A	56	LYS	O-C-N	-6.16	115.59	122.12
2	B	149	GLU	O-C-N	6.15	130.88	122.46
1	C	433	PHE	N-CA-CB	6.15	119.16	110.12
2	B	251	ASN	CA-C-O	-6.14	114.37	120.82
1	C	508	THR	OG1-CB-CG2	6.12	121.55	109.30
1	C	444	PRO	CA-C-O	6.12	127.93	119.18
2	D	570	ALA	N-CA-CB	6.12	118.89	110.01
1	A	54	GLN	CA-C-N	6.12	128.27	120.56
1	A	54	GLN	C-N-CA	6.12	128.27	120.56
1	C	416	LYS	N-CA-C	6.12	120.21	112.87
1	C	458	HIS	CA-CB-CG	-6.12	107.69	113.80
1	A	86	LEU	N-CA-CB	-6.11	100.84	109.94
1	C	532	VAL	N-CA-CB	-6.10	102.24	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	TYR	O-C-N	6.10	129.10	122.15
2	D	544	VAL	CA-C-N	-6.10	111.59	122.32
2	D	544	VAL	C-N-CA	-6.10	111.59	122.32
2	B	196	ALA	CA-C-O	-6.10	112.96	119.97
2	B	247	ARG	CD-NE-CZ	-6.10	115.86	124.40
1	A	135	VAL	CA-C-N	6.08	130.34	120.60
1	A	135	VAL	C-N-CA	6.08	130.34	120.60
1	A	76	MET	CA-C-O	-6.08	111.83	120.16
2	B	242	ASP	CA-C-O	-6.08	113.55	119.51
2	B	235	HIS	CA-C-N	-6.08	113.27	121.71
2	B	235	HIS	C-N-CA	-6.08	113.27	121.71
2	B	215	SER	CA-CB-OG	-6.07	98.95	111.10
1	C	454	GLN	CG-CD-NE2	-6.07	107.30	116.40
2	D	572	GLY	CA-C-N	6.06	129.01	120.28
2	D	572	GLY	C-N-CA	6.06	129.01	120.28
1	A	43	PHE	CA-C-O	6.06	128.46	120.16
2	B	186	GLU	CA-CB-CG	6.04	126.17	114.10
1	C	462	VAL	CA-C-O	-6.04	114.77	121.17
1	C	456	LYS	CA-CB-CG	6.04	126.17	114.10
1	A	78	ASN	CB-CG-ND2	-6.04	107.35	116.40
2	B	210	VAL	CB-CA-C	6.03	119.60	111.88
2	D	679	GLY	CA-C-N	-6.03	112.84	120.56
2	D	679	GLY	C-N-CA	-6.03	112.84	120.56
1	A	19	ALA	N-CA-CB	-6.02	101.23	110.44
2	B	251	ASN	CB-CG-OD1	6.01	132.82	120.80
2	D	644	GLU	OE1-CD-OE2	6.01	137.31	122.90
1	C	447	ASP	N-CA-C	-6.00	100.21	109.76
2	B	222	ASP	CA-C-O	-6.00	112.33	119.35
2	D	601	PRO	N-CD-CG	-6.00	94.20	103.20
2	B	169	GLU	N-CA-CB	-6.00	101.26	110.20
1	C	425	GLY	N-CA-C	-5.99	105.55	112.50
1	A	84	SER	CA-C-O	-5.98	114.08	120.42
1	C	489	HIS	CB-CA-C	-5.98	99.03	109.07
1	C	403	SER	CA-CB-OG	-5.97	99.15	111.10
1	C	414	TRP	CB-CA-C	5.97	120.25	110.88
2	B	145	HIS	CA-C-O	5.96	128.07	121.39
2	D	569	GLU	OE1-CD-OE2	5.96	137.22	122.90
2	D	575	LEU	O-C-N	-5.96	115.80	122.12
1	A	14	TRP	CA-C-O	5.96	126.86	120.55
1	C	471	ALA	CA-C-O	5.96	126.86	120.55
1	C	482	ALA	CA-C-O	5.95	127.05	120.63
1	C	526	ASP	OD1-CG-OD2	-5.94	108.65	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	589	GLY	N-CA-C	5.93	117.55	111.56
1	C	494	ASP	CA-C-O	-5.93	114.18	119.75
1	C	420	HIS	CA-C-O	-5.92	112.63	119.56
2	D	623	ASN	CA-C-N	-5.92	111.05	122.06
2	D	623	ASN	C-N-CA	-5.92	111.05	122.06
2	B	178	TYR	CA-C-O	5.91	127.78	121.28
1	C	448	LEU	CD1-CG-CD2	5.90	123.78	110.80
2	B	191	LEU	N-CA-C	-5.89	103.64	112.54
2	D	654	VAL	N-CA-CB	-5.89	103.10	110.47
1	C	402	LEU	CA-C-O	-5.88	113.98	120.69
1	C	435	SER	CA-C-N	-5.88	115.92	123.16
1	C	435	SER	C-N-CA	-5.88	115.92	123.16
1	C	455	VAL	O-C-N	-5.88	116.17	121.87
1	A	68	ASN	CA-CB-CG	-5.88	106.72	112.60
2	D	641	VAL	CA-C-N	5.87	128.54	120.67
2	D	641	VAL	C-N-CA	5.87	128.54	120.67
1	A	68	ASN	N-CA-CB	-5.87	101.47	110.16
2	B	246	PHE	CA-CB-CG	5.87	119.67	113.80
1	C	442	TYR	CA-CB-CG	-5.86	103.36	113.90
1	C	446	PHE	CA-C-N	-5.86	113.13	121.50
1	C	446	PHE	C-N-CA	-5.86	113.13	121.50
2	D	658	ALA	N-CA-CB	-5.85	101.52	110.01
2	D	685	ALA	N-CA-CB	-5.85	102.49	110.56
2	D	569	GLU	CA-CB-CG	5.84	125.78	114.10
1	C	499	LYS	CB-CA-C	-5.84	98.47	110.38
2	D	637	ASP	CA-C-O	-5.84	113.26	119.97
1	A	96	VAL	N-CA-C	-5.83	104.67	110.62
1	A	12	ALA	N-CA-C	5.83	117.44	111.14
2	B	242	ASP	CA-C-N	5.83	125.50	119.56
2	B	242	ASP	C-N-CA	5.83	125.50	119.56
1	C	490	LYS	CA-C-O	5.82	126.83	119.61
1	A	75	ASP	CA-C-N	-5.82	107.60	121.80
1	A	75	ASP	C-N-CA	-5.82	107.60	121.80
1	C	491	LEU	O-C-N	5.82	128.37	122.09
2	B	276	VAL	CB-CA-C	5.82	119.41	111.97
2	B	155	THR	OG1-CB-CG2	5.81	120.91	109.30
2	D	591	LEU	O-C-N	5.80	130.21	122.26
1	A	105	LEU	O-C-N	-5.80	115.83	122.09
2	B	149	GLU	N-CA-CB	5.79	119.48	110.44
1	C	464	ASP	CA-C-N	-5.79	111.50	120.31
1	C	464	ASP	C-N-CA	-5.79	111.50	120.31
1	A	86	LEU	N-CA-C	5.79	118.06	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	MET	O-C-N	5.79	126.05	120.55
2	B	276	VAL	CA-C-N	-5.78	111.04	120.64
2	B	276	VAL	C-N-CA	-5.78	111.04	120.64
2	D	551	LYS	O-C-N	5.78	128.25	122.12
2	D	600	ASN	CA-C-O	5.78	125.21	119.49
2	D	603	VAL	O-C-N	-5.78	116.23	121.89
2	D	688	TYR	N-CA-C	-5.78	102.35	110.50
2	D	658	ALA	CA-C-O	5.77	126.88	120.82
2	D	663	LYS	CA-C-N	5.77	130.36	120.72
2	D	663	LYS	C-N-CA	5.77	130.36	120.72
1	C	408	THR	O-C-N	5.77	128.32	122.09
2	B	287	LYS	CA-C-O	-5.76	112.46	119.43
2	B	173	ARG	CG-CD-NE	-5.75	99.35	112.00
1	C	430	GLU	OE1-CD-OE2	5.74	136.68	122.90
1	A	16	LYS	CB-CG-CD	-5.73	98.12	111.30
2	B	170	ALA	N-CA-CB	-5.73	101.67	110.20
1	C	478	ASN	CA-C-N	-5.72	111.61	120.31
1	C	478	ASN	C-N-CA	-5.72	111.61	120.31
1	A	118	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	67	THR	O-C-N	-5.72	116.06	122.12
2	D	681	ALA	N-CA-C	-5.72	104.41	111.33
2	D	545	HIS	CA-C-O	-5.71	114.98	121.66
2	D	619	ALA	CA-C-O	-5.70	111.82	119.11
2	D	581	THR	CA-C-O	5.70	126.46	119.05
2	D	562	ASN	N-CA-C	-5.70	97.97	107.99
1	A	70	VAL	CA-C-N	5.69	130.22	120.72
1	A	70	VAL	C-N-CA	5.69	130.22	120.72
1	C	435	SER	O-C-N	5.69	130.44	122.36
1	C	405	ALA	CB-CA-C	-5.69	101.18	110.85
2	D	638	LYS	CA-CB-CG	5.68	125.46	114.10
1	A	116	GLU	CG-CD-OE1	-5.68	105.34	118.40
2	B	173	ARG	NE-CZ-NH1	5.68	127.18	121.50
2	D	631	LEU	N-CA-CB	-5.68	101.48	110.22
2	B	220	HIS	CA-C-O	-5.67	114.58	121.89
2	B	149	GLU	CB-CA-C	5.67	121.05	109.55
2	D	647	ARG	CA-C-N	-5.66	112.89	120.54
2	D	647	ARG	C-N-CA	-5.66	112.89	120.54
2	B	203	VAL	N-CA-C	-5.66	105.21	110.53
2	B	277	VAL	CA-C-O	-5.66	112.84	119.85
2	B	187	SER	N-CA-CB	-5.65	101.27	110.42
1	A	19	ALA	N-CA-C	5.64	120.16	113.16
2	D	639	LEU	CA-C-O	-5.64	112.67	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	597	VAL	CB-CA-C	-5.64	104.64	112.02
2	D	635	HIS	O-C-N	-5.64	116.14	122.12
1	C	518	THR	CB-CA-C	5.63	122.21	110.50
2	D	682	ASN	N-CA-CB	5.62	118.49	110.16
2	B	243	PRO	CA-C-N	-5.62	111.60	120.60
2	B	243	PRO	C-N-CA	-5.62	111.60	120.60
2	D	549	GLU	CA-CB-CG	-5.62	102.85	114.10
1	C	464	ASP	N-CA-CB	5.62	118.88	110.22
1	C	522	HIS	CA-CB-CG	5.61	119.41	113.80
2	D	571	LEU	CA-C-N	-5.61	113.83	120.00
2	D	571	LEU	C-N-CA	-5.61	113.83	120.00
1	A	132	VAL	N-CA-CB	-5.60	102.92	110.54
2	D	550	GLU	CB-CG-CD	5.60	122.12	112.60
1	A	27	GLU	CG-CD-OE1	-5.60	105.53	118.40
2	D	624	LEU	N-CA-CB	-5.59	101.69	110.46
2	D	565	GLU	O-C-N	-5.59	116.20	122.12
2	B	160	LYS	CB-CG-CD	-5.58	98.46	111.30
2	B	255	CYS	CA-CB-SG	5.58	127.23	114.40
1	A	99	LYS	N-CA-C	-5.58	105.35	111.82
2	B	233	GLU	CB-CA-C	-5.57	101.22	110.68
2	B	146	LEU	CA-CB-CG	5.56	135.76	116.30
1	A	44	PRO	CA-C-O	5.56	126.25	118.86
1	C	429	LEU	CA-C-N	5.56	128.76	120.31
1	C	429	LEU	C-N-CA	5.56	128.76	120.31
1	C	481	SER	CA-CB-OG	-5.56	99.98	111.10
1	A	139	LYS	O-C-N	5.54	129.07	122.26
2	B	250	GLY	CA-C-N	5.54	127.64	120.44
2	B	250	GLY	C-N-CA	5.54	127.64	120.44
2	D	578	TYR	CA-CB-CG	-5.54	103.93	113.90
2	D	590	ASP	CB-CG-OD1	-5.54	105.66	118.40
2	D	614	PHE	CB-CA-C	5.54	119.54	110.95
1	A	80	LEU	CA-C-O	-5.54	113.06	119.59
1	C	421	ALA	CB-CA-C	5.53	120.09	110.68
1	C	505	LEU	N-CA-C	-5.53	105.26	112.23
2	D	665	PHE	CB-CA-C	5.53	120.91	111.68
1	A	11	LYS	O-C-N	-5.51	116.27	122.12
1	A	114	PRO	CA-C-N	5.51	127.67	120.28
1	A	114	PRO	C-N-CA	5.51	127.67	120.28
2	B	278	ALA	N-CA-C	-5.51	105.28	112.23
2	D	580	TRP	O-C-N	5.51	130.06	122.46
2	D	597	VAL	N-CA-CB	5.50	117.62	110.57
2	D	616	ASP	O-C-N	-5.50	115.78	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	8	THR	N-CA-C	-5.49	105.37	111.36
1	C	537	THR	N-CA-C	5.49	119.68	112.92
1	C	439	THR	CA-CB-OG1	-5.49	101.37	109.60
2	B	230	THR	CA-CB-OG1	-5.49	101.37	109.60
1	C	492	ARG	CA-CB-CG	-5.49	103.13	114.10
1	A	71	ALA	CA-C-O	5.47	126.11	119.38
1	A	96	VAL	CA-CB-CG2	5.47	119.71	110.40
2	B	277	VAL	O-C-N	5.47	129.22	122.05
1	A	45	HIS	CA-CB-CG	-5.47	108.33	113.80
2	B	210	VAL	CA-CB-CG2	-5.47	101.11	110.40
2	D	569	GLU	CA-C-N	5.47	127.55	120.44
2	D	569	GLU	C-N-CA	5.47	127.55	120.44
2	D	598	MET	CA-C-O	5.46	126.34	120.55
1	A	119	PRO	CA-C-N	5.45	127.90	120.54
1	A	119	PRO	C-N-CA	5.45	127.90	120.54
2	D	546	LEU	CA-C-N	5.45	129.75	121.03
2	D	546	LEU	C-N-CA	5.45	129.75	121.03
2	B	254	VAL	O-C-N	-5.45	116.58	121.87
2	D	670	GLN	CG-CD-NE2	-5.44	108.23	116.40
2	B	155	THR	CA-CB-OG1	-5.44	101.44	109.60
2	B	287	LYS	O-C-N	5.43	129.40	122.39
1	C	537	THR	N-CA-CB	-5.43	102.62	110.56
1	A	77	PRO	N-CD-CG	-5.43	95.05	103.20
2	B	233	GLU	CG-CD-OE2	-5.43	105.91	118.40
2	D	606	HIS	CA-C-O	-5.42	114.22	120.24
1	C	446	PHE	CA-C-O	-5.42	115.04	121.16
1	C	502	SER	CA-C-N	5.41	127.79	120.38
1	C	502	SER	C-N-CA	5.41	127.79	120.38
2	B	247	ARG	CA-C-O	-5.41	113.75	119.97
2	B	237	ASP	CB-CA-C	5.40	119.76	110.79
2	D	576	VAL	CA-CB-CG1	5.40	119.58	110.40
1	A	27	GLU	CA-C-N	5.40	127.52	120.28
1	A	27	GLU	C-N-CA	5.40	127.52	120.28
2	D	682	ASN	O-C-N	5.40	128.30	122.15
1	C	433	PHE	CB-CA-C	-5.39	101.84	110.79
1	A	134	THR	CA-C-O	-5.39	114.71	120.42
1	A	100	LEU	O-C-N	5.39	129.23	122.23
2	D	552	SER	N-CA-C	-5.39	105.97	112.54
1	C	478	ASN	CA-CB-CG	-5.39	107.21	112.60
1	A	8	THR	CA-C-O	-5.38	114.71	120.42
2	D	591	LEU	CB-CA-C	-5.38	102.02	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NH1-CZ-NH2	-5.38	112.31	119.30
2	D	664	GLU	N-CA-CB	-5.38	101.47	110.39
1	A	25	GLY	N-CA-C	-5.37	106.27	112.50
1	A	97	ASN	N-CA-C	5.37	119.45	113.01
1	C	464	ASP	CA-C-O	-5.37	114.04	120.10
1	C	516	GLU	CG-CD-OE1	-5.36	106.07	118.40
2	D	569	GLU	CG-CD-OE2	-5.36	106.07	118.40
2	D	679	GLY	N-CA-C	-5.36	105.82	113.86
2	B	234	LEU	N-CA-CB	5.36	117.96	109.82
2	D	616	ASP	CB-CA-C	5.34	120.52	110.63
1	C	492	ARG	NH1-CZ-NH2	5.34	126.24	119.30
2	D	632	SER	O-C-N	5.34	127.80	122.03
1	A	85	ASP	CA-C-O	5.34	126.94	121.07
2	B	193	THR	CA-CB-OG1	5.34	117.61	109.60
1	A	104	CYS	CA-C-N	5.33	127.69	120.44
1	A	104	CYS	C-N-CA	5.33	127.69	120.44
2	B	150	GLU	CA-C-N	-5.32	111.84	120.72
2	B	150	GLU	C-N-CA	-5.32	111.84	120.72
1	C	414	TRP	CD2-CE2-CZ2	5.32	127.72	122.40
1	C	523	ALA	O-C-N	5.32	127.75	122.12
1	C	414	TRP	CH2-CZ2-CE2	-5.31	110.59	117.50
2	D	688	TYR	CA-C-O	-5.31	115.77	121.56
1	C	426	ALA	N-CA-CB	5.29	117.90	110.12
1	A	3	SER	CA-CB-OG	-5.29	100.52	111.10
1	C	420	HIS	CB-CA-C	-5.29	101.63	110.56
2	D	647	ARG	CA-C-O	-5.28	115.26	120.70
2	B	243	PRO	CA-C-O	5.28	126.72	119.18
1	A	4	PRO	CA-C-N	-5.27	111.92	121.14
1	A	4	PRO	C-N-CA	-5.27	111.92	121.14
2	D	635	HIS	CA-CB-CG	-5.27	108.53	113.80
1	C	465	ALA	CB-CA-C	5.26	120.77	110.67
1	C	414	TRP	CB-CG-CD2	5.26	134.17	126.80
1	A	77	PRO	CA-CB-CG	-5.26	94.51	104.50
1	C	423	GLU	CB-CA-C	-5.26	102.40	110.81
2	B	177	VAL	CA-CB-CG1	5.25	119.33	110.40
1	C	518	THR	CA-C-N	5.25	125.31	119.32
1	C	518	THR	C-N-CA	5.25	125.31	119.32
1	C	462	VAL	O-C-N	5.25	127.05	121.91
2	B	149	GLU	OE1-CD-OE2	-5.25	110.31	122.90
2	B	170	ALA	CA-C-N	5.24	127.57	120.44
2	B	170	ALA	C-N-CA	5.24	127.57	120.44
2	B	213	ALA	CA-C-N	5.24	127.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	ALA	C-N-CA	5.24	127.26	120.44
2	D	606	HIS	N-CA-CB	5.24	118.01	110.20
1	C	521	VAL	N-CA-CB	5.24	119.31	110.56
2	B	222	ASP	CB-CG-OD1	5.24	130.44	118.40
2	D	660	HIS	N-CA-C	5.24	117.07	111.36
1	A	122	HIS	O-C-N	-5.23	116.58	122.12
2	D	616	ASP	N-CA-CB	-5.22	102.18	110.22
1	A	61	LYS	CG-CD-CE	5.22	123.30	111.30
1	C	474	ASP	CA-C-O	-5.22	113.20	119.15
1	A	1	VAL	CA-CB-CG2	-5.21	101.54	110.40
2	B	205	ALA	CA-C-O	-5.21	114.46	120.24
2	B	288	TYR	CB-CG-CD2	-5.20	113.00	120.80
1	A	40	LYS	CG-CD-CE	-5.20	99.34	111.30
2	B	287	LYS	CA-CB-CG	-5.19	103.71	114.10
1	C	524	SER	CA-C-N	5.19	127.24	120.28
1	C	524	SER	C-N-CA	5.19	127.24	120.28
2	B	146	LEU	N-CA-CB	-5.19	102.34	110.69
2	D	640	HIS	CB-CA-C	-5.18	104.53	111.89
2	B	167	GLY	N-CA-C	-5.18	106.14	112.77
2	B	193	THR	CB-CA-C	-5.18	101.74	109.56
1	A	7	LYS	CB-CG-CD	-5.18	99.39	111.30
2	D	629	ALA	CA-C-N	5.18	129.43	120.58
2	D	629	ALA	C-N-CA	5.18	129.43	120.58
2	D	654	VAL	O-C-N	-5.18	116.82	121.89
2	D	549	GLU	CB-CG-CD	-5.17	103.81	112.60
2	D	614	PHE	N-CA-C	-5.17	105.29	111.03
1	A	108	THR	O-C-N	-5.17	116.71	122.09
1	A	89	HIS	N-CA-C	5.17	120.59	113.97
1	A	99	LYS	CA-C-O	-5.16	114.04	119.97
2	B	247	ARG	N-CA-C	-5.16	105.84	111.82
2	D	660	HIS	ND1-CE1-NE2	5.16	113.56	108.40
2	B	228	PHE	N-CA-C	5.15	119.20	113.02
2	D	604	LYS	CB-CA-C	-5.15	102.79	110.88
2	D	550	GLU	CG-CD-OE1	-5.14	106.58	118.40
1	A	54	GLN	CG-CD-NE2	-5.13	108.70	116.40
2	D	570	ALA	CA-C-N	5.12	129.38	120.68
2	D	570	ALA	C-N-CA	5.12	129.38	120.68
2	D	594	PRO	N-CA-C	-5.12	105.49	113.78
2	D	564	ASP	CB-CG-OD1	5.12	130.17	118.40
2	D	683	ALA	N-CA-C	-5.12	105.79	112.23
1	C	530	ALA	CA-C-N	-5.11	111.99	120.68
1	C	530	ALA	C-N-CA	-5.11	111.99	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	THR	O-C-N	5.11	127.35	122.03
2	B	238	LYS	N-CA-C	5.11	119.99	113.55
2	B	227	THR	N-CA-CB	5.11	117.37	109.91
1	C	413	ALA	CA-C-N	5.11	127.08	120.44
1	C	413	ALA	C-N-CA	5.11	127.08	120.44
1	A	124	SER	CA-C-O	5.10	126.17	120.82
1	C	442	TYR	O-C-N	5.09	129.63	122.41
2	D	547	THR	CA-CB-OG1	-5.08	101.98	109.60
2	B	273	TYR	CB-CA-C	5.08	119.22	110.79
1	C	538	SER	CA-CB-OG	5.07	121.23	111.10
1	C	414	TRP	CA-CB-CG	-5.06	103.98	113.60
1	A	28	ALA	O-C-N	5.06	127.48	122.12
1	A	44	PRO	CA-C-N	-5.05	114.56	122.65
1	A	44	PRO	C-N-CA	-5.05	114.56	122.65
2	D	687	LYS	CA-C-O	-5.05	113.63	119.59
1	C	490	LYS	CB-CA-C	5.05	119.65	111.26
1	A	53	ALA	N-CA-CB	-5.05	102.53	110.46
2	B	153	ALA	CA-C-O	5.04	125.77	120.42
2	B	195	ASP	O-C-N	5.04	129.19	122.43
2	B	216	ASP	OD1-CG-OD2	-5.04	110.80	122.90
1	A	139	LYS	N-CA-CB	-5.04	102.86	110.92
2	B	287	LYS	CA-C-N	-5.04	113.03	121.39
2	B	287	LYS	C-N-CA	-5.04	113.03	121.39
1	C	474	ASP	CA-C-N	5.03	131.70	122.54
1	C	474	ASP	C-N-CA	5.03	131.70	122.54
2	D	548	PRO	N-CA-C	-5.03	102.10	112.47
1	A	68	ASN	CB-CG-OD1	-5.03	110.74	120.80
1	A	75	ASP	N-CA-C	-5.03	99.73	109.24
2	B	252	VAL	N-CA-C	-5.03	105.49	110.62
1	A	125	LEU	N-CA-C	-5.02	105.88	111.36
2	D	546	LEU	O-C-N	5.02	129.76	123.23
2	B	236	CYS	CA-C-O	5.02	126.23	120.71
2	D	555	THR	N-CA-CB	-5.02	102.75	110.12
1	A	141	ARG	CD-NE-CZ	-5.01	117.38	124.40
2	B	169	GLU	OE1-CD-OE2	5.01	134.94	122.90
1	C	535	VAL	CA-CB-CG1	5.01	118.92	110.40
1	A	107	VAL	O-C-N	-5.01	117.00	121.91
1	A	124	SER	CA-C-N	5.01	127.40	120.29
1	A	124	SER	C-N-CA	5.01	127.40	120.29
1	A	93	VAL	CA-CB-CG2	5.00	118.90	110.40
1	A	50	HIS	N-CA-CB	5.00	116.89	109.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	545	HIS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
2	B	183	ARG	Sidechain
2	B	247	ARG	Sidechain
1	C	492	ARG	Sidechain

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	1069	0	1073	61	1
1	C	1069	0	1070	55	0
2	B	1123	0	1115	94	0
2	D	1127	0	1124	109	0
3	A	43	0	30	2	0
3	B	43	0	30	6	0
3	C	43	0	30	0	0
3	D	43	0	30	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	D	15	0	3	2	0
6	A	29	0	0	1	1
6	B	46	0	0	9	1
6	C	16	0	0	0	0
6	D	45	0	0	9	1
All	All	4715	0	4505	316	2

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 35.

All (316) 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:D:686:HIS:NE2	6:D:102:HOH:O	1.57	1.28
2:D:571:LEU:HD22	6:D:128:HOH:O	1.12	1.24
2:B:153:ALA:HA	6:B:49:HOH:O	1.38	1.17
2:D:649:LEU:HD23	3:D:691:HEM:HBB2	1.25	1.14
1:A:118:THR:HG22	1:A:121:VAL:H	1.09	1.13
2:D:547:THR:HG22	2:D:549:GLU:N	1.64	1.12
2:B:217:GLY:HA3	6:B:44:HOH:O	1.46	1.11
2:D:686:HIS:CD2	6:D:102:HOH:O	1.85	1.09
2:B:147:THR:HG22	2:B:149:GLU:H	1.11	1.09
2:D:571:LEU:HB2	6:D:128:HOH:O	1.45	1.08
2:B:147:THR:HG23	2:B:148:PRO:HD2	1.25	1.07
2:D:549:GLU:OE1	2:D:549:GLU:HA	1.53	1.07
3:B:291:HEM:HHC	3:B:291:HEM:HBB2	1.39	1.01
2:D:547:THR:HG22	2:D:549:GLU:H	0.90	1.01
2:D:667:PRO:HB2	2:D:668:PRO:HD3	1.42	0.99
2:B:147:THR:C	2:B:151:LYS:HE3	1.87	0.98
2:B:147:THR:CG2	2:B:148:PRO:HD2	1.94	0.98
1:C:513:LEU:HB3	1:C:516:GLU:HG3	1.46	0.97
2:D:548:PRO:HA	2:D:551:LYS:HG3	1.47	0.96
2:D:544:VAL:HA	6:D:104:HOH:O	1.66	0.95
2:B:147:THR:HG22	2:B:149:GLU:N	1.81	0.94
2:B:153:ALA:CA	6:B:49:HOH:O	2.05	0.90
1:C:513:LEU:HB3	1:C:516:GLU:CG	2.03	0.89
2:B:164:ASP:HA	2:B:208:LYS:HG2	1.54	0.88
2:D:649:LEU:HD23	3:D:691:HEM:CBB	2.04	0.86
1:A:103:HIS:HE1	2:B:274:GLN:OE1	1.56	0.86
2:B:147:THR:CG2	2:B:149:GLU:H	1.89	0.86
2:B:148:PRO:CA	2:B:151:LYS:HE3	2.06	0.86
1:A:6:ASP:O	1:A:10:VAL:HG13	1.79	0.83
1:C:496:VAL:O	1:C:496:VAL:HG22	1.77	0.82
2:D:547:THR:CG2	2:D:549:GLU:H	1.85	0.82
1:A:42:TYR:C	1:A:44:PRO:HD3	2.05	0.81
2:B:148:PRO:N	2:B:151:LYS:HE3	1.95	0.81
2:B:147:THR:O	2:B:151:LYS:HE3	1.81	0.80
1:A:118:THR:HG22	1:A:121:VAL:N	1.94	0.79
1:C:484:SER:HB2	1:C:539:LYS:HD2	1.66	0.78
2:D:616:ASP:O	2:D:620:HIS:CD2	2.37	0.78
2:B:148:PRO:HB3	2:B:151:LYS:HZ1	1.48	0.78
5:D:701:DG2:C7	5:D:701:DG2:O11	2.31	0.78
2:D:632:SER:HB3	2:D:687:LYS:HG3	1.65	0.77
1:C:417:VAL:CG1	1:C:421:ALA:HB2	2.13	0.77
1:A:43:PHE:N	1:A:44:PRO:HD3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:GLY:HA2	2:B:211:LEU:HD23	1.65	0.77
2:D:547:THR:O	2:D:551:LYS:HG2	1.85	0.76
1:A:76:MET:N	1:A:77:PRO:CD	2.49	0.76
2:D:607:GLY:HA2	6:D:128:HOH:O	1.84	0.76
2:D:600:ASN:OD1	2:D:602:LYS:HB2	1.86	0.76
1:C:417:VAL:HG12	1:C:421:ALA:HB2	1.68	0.75
1:A:45:HIS:ND1	1:A:45:HIS:N	2.29	0.74
2:B:146:LEU:HD23	2:B:151:LYS:CA	2.18	0.73
1:A:17:VAL:HG13	1:A:24:TYR:CD2	2.23	0.73
1:A:76:MET:N	1:A:77:PRO:HD3	2.03	0.73
2:B:180:TRP:O	2:B:183:ARG:HG2	1.88	0.73
1:A:114:PRO:O	2:B:259:HIS:NE2	2.20	0.73
2:D:547:THR:HB	2:D:550:GLU:HG3	1.70	0.71
2:D:649:LEU:CD2	3:D:691:HEM:HBB2	2.15	0.71
1:C:401:VAL:HG13	1:C:401:VAL:O	1.90	0.70
2:B:286:HIS:ND1	2:B:287:LYS:HE2	2.05	0.70
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.27	0.69
2:B:193:THR:HG22	2:B:194:PRO:HD2	1.74	0.69
1:A:47:ASP:OD1	1:A:47:ASP:C	2.33	0.69
2:B:148:PRO:HA	2:B:151:LYS:CE	2.22	0.69
1:A:20:HIS:O	1:A:23:GLU:HB2	1.93	0.68
1:C:496:VAL:O	1:C:496:VAL:CG2	2.40	0.68
2:D:545:HIS:O	2:D:675:LYS:HE2	1.93	0.68
2:D:618:LEU:HA	2:D:621:LEU:HD13	1.75	0.68
2:B:148:PRO:HB3	2:B:151:LYS:NZ	2.09	0.67
2:D:639:LEU:HD13	3:D:691:HEM:C3D	2.30	0.67
2:B:287:LYS:HE3	6:B:42:HOH:O	1.94	0.67
2:D:667:PRO:CB	2:D:668:PRO:HD3	2.17	0.67
2:B:148:PRO:CA	2:B:151:LYS:CE	2.73	0.66
2:B:147:THR:HG23	2:B:148:PRO:CD	2.16	0.66
2:D:620:HIS:CD2	2:D:620:HIS:N	2.63	0.66
2:B:181:THR:HG22	2:B:245:ASN:HD21	1.60	0.66
1:A:32:MET:SD	1:A:101:LEU:HB2	2.36	0.65
2:B:229:ALA:O	2:B:233:GLU:HG3	1.95	0.65
2:D:667:PRO:N	2:D:668:PRO:CD	2.59	0.65
1:C:431:ARG:HD3	2:D:670:GLN:OE1	1.96	0.65
2:D:546:LEU:HD23	2:D:550:GLU:CB	2.27	0.65
2:B:148:PRO:HA	2:B:151:LYS:HE3	1.79	0.64
2:D:621:LEU:HD12	2:D:624:LEU:HD11	1.77	0.64
2:B:148:PRO:CD	2:B:149:GLU:H	2.11	0.64
2:B:148:PRO:CB	2:B:151:LYS:NZ	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:PHE:N	1:C:444:PRO:CD	2.62	0.63
2:B:217:GLY:HA2	2:B:227:THR:HG21	1.80	0.63
2:B:148:PRO:HA	2:B:151:LYS:HZ2	1.64	0.62
2:D:581:THR:HG22	2:D:645:ASN:ND2	2.14	0.62
2:D:661:PHE:HB3	2:D:664:GLU:HB3	1.80	0.62
2:B:147:THR:CG2	2:B:148:PRO:CD	2.75	0.62
1:A:58:HIS:O	1:A:62:VAL:HG23	1.99	0.62
2:B:153:ALA:C	6:B:49:HOH:O	2.37	0.62
1:A:28:ALA:HB1	1:A:105:LEU:HD13	1.80	0.62
1:C:505:LEU:O	1:C:509:LEU:HG	2.00	0.62
3:B:291:HEM:NC	6:B:126:HOH:O	2.31	0.62
2:B:146:LEU:HD23	2:B:151:LYS:HA	1.82	0.61
2:D:581:THR:HG22	2:D:645:ASN:HD22	1.65	0.61
2:D:624:LEU:O	2:D:683:ALA:HB1	2.00	0.61
1:C:503:HIS:HE1	2:D:674:GLN:OE1	1.84	0.61
2:B:148:PRO:HA	2:B:151:LYS:HG2	1.83	0.60
1:A:99:LYS:HD2	1:A:99:LYS:N	2.17	0.60
2:B:146:LEU:HD23	2:B:151:LYS:HB3	1.83	0.60
2:B:148:PRO:HA	2:B:151:LYS:NZ	2.17	0.59
2:B:148:PRO:CD	2:B:149:GLU:N	2.62	0.59
1:C:450:HIS:ND1	1:C:451:GLY:N	2.51	0.59
1:C:476:MET:HB2	1:C:477:PRO:HD3	1.84	0.59
2:B:234:LEU:CD2	3:B:291:HEM:HBA2	2.32	0.59
1:A:43:PHE:N	1:A:44:PRO:CD	2.66	0.59
1:A:103:HIS:CE1	2:B:274:GLN:OE1	2.47	0.59
1:A:113:LEU:HB3	1:A:116:GLU:HG2	1.84	0.58
1:A:44:PRO:HD2	1:A:45:HIS:ND1	2.17	0.58
3:D:691:HEM:HBB2	3:D:691:HEM:HHC	1.85	0.58
2:D:583:ARG:HD3	2:D:584:PHE:CZ	2.38	0.58
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.69	0.57
2:B:254:VAL:HG11	2:B:274:GLN:OE1	2.05	0.57
2:D:558:TRP:HH2	2:D:611:LEU:HD11	1.70	0.57
2:D:667:PRO:N	2:D:668:PRO:HD2	2.20	0.56
2:D:588:PHE:HA	2:D:602:LYS:HE3	1.86	0.56
1:C:480:LEU:HD12	1:C:535:VAL:HG11	1.86	0.56
2:D:546:LEU:HD23	2:D:550:GLU:HB2	1.88	0.56
1:A:43:PHE:HA	1:A:45:HIS:HE1	1.71	0.56
2:B:157:LEU:C	2:B:159:GLY:N	2.62	0.56
2:D:600:ASN:OD1	2:D:602:LYS:CB	2.54	0.56
1:A:3:SER:O	1:A:7:LYS:HG3	2.06	0.56
1:A:16:LYS:O	1:A:17:VAL:C	2.49	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:SER:O	1:C:456:LYS:HG3	2.06	0.56
2:D:547:THR:CG2	2:D:548:PRO:CD	2.85	0.55
2:D:667:PRO:HB2	2:D:668:PRO:CD	2.27	0.55
2:B:148:PRO:CA	2:B:151:LYS:NZ	2.70	0.54
2:B:150:GLU:OE1	2:B:275:LYS:NZ	2.40	0.54
1:C:476:MET:O	1:C:477:PRO:C	2.47	0.54
1:A:37:PRO:O	1:A:40:LYS:HG3	2.07	0.54
2:B:233:GLU:O	2:B:237:ASP:HB2	2.07	0.54
1:A:52:SER:OG	1:A:55:VAL:HG23	2.07	0.54
2:D:639:LEU:CD1	3:D:691:HEM:C3D	2.91	0.54
2:B:157:LEU:C	2:B:159:GLY:H	2.16	0.54
2:B:147:THR:O	2:B:151:LYS:CE	2.55	0.53
2:B:183:ARG:HB3	1:C:492:ARG:HD3	1.90	0.53
2:B:146:LEU:HD23	2:B:151:LYS:CB	2.37	0.53
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.38	0.53
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.43	0.53
2:D:667:PRO:CB	2:D:668:PRO:CD	2.86	0.53
2:D:558:TRP:HA	2:D:561:VAL:HG23	1.91	0.53
2:D:616:ASP:O	2:D:620:HIS:HD2	1.86	0.53
1:C:481:SER:OG	1:C:482:ALA:N	2.40	0.52
2:D:546:LEU:HD23	2:D:550:GLU:HB3	1.91	0.52
2:D:633:GLU:O	2:D:637:ASP:HB2	2.09	0.52
2:B:148:PRO:HD2	2:B:149:GLU:H	1.75	0.52
1:C:512:HIS:O	1:C:513:LEU:HD23	2.10	0.52
2:D:684:LEU:HD12	3:D:691:HEM:HAB	1.92	0.52
3:B:291:HEM:HBB2	3:B:291:HEM:CHC	2.20	0.51
2:B:193:THR:CG2	2:B:194:PRO:HD2	2.40	0.51
1:A:115:ALA:HB3	1:A:116:GLU:OE2	2.11	0.51
1:C:401:VAL:O	1:C:401:VAL:CG1	2.58	0.51
2:B:211:LEU:O	2:B:215:SER:HB2	2.11	0.51
1:A:35:SER:C	1:A:37:PRO:HD3	2.35	0.51
2:D:594:PRO:O	2:D:598:MET:HG2	2.10	0.51
2:D:592:SER:O	2:D:593:THR:HG23	2.11	0.51
1:C:403:SER:O	1:C:406:ASP:HB2	2.12	0.50
1:C:435:SER:HB3	2:D:674:GLN:HG3	1.93	0.50
2:D:620:HIS:C	2:D:622:ASP:H	2.19	0.50
1:A:98:PHE:HB3	1:A:133:SER:HB3	1.92	0.50
2:B:161:VAL:HG12	2:B:261:PHE:CZ	2.47	0.50
2:B:244:GLU:O	2:B:244:GLU:HG3	2.12	0.50
1:C:468:ASN:O	1:C:472:HIS:HD2	1.95	0.50
2:D:571:LEU:CD2	6:D:128:HOH:O	1.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LYS:O	2:B:155:THR:HB	2.11	0.50
2:D:624:LEU:O	2:D:683:ALA:CB	2.60	0.50
2:D:548:PRO:CA	2:D:551:LYS:HG3	2.33	0.49
1:A:113:LEU:HB3	1:A:116:GLU:CG	2.43	0.49
1:C:466:LEU:O	1:C:470:VAL:HG23	2.13	0.49
2:B:182:GLN:O	2:B:183:ARG:C	2.53	0.49
2:B:193:THR:HG22	2:B:194:PRO:CD	2.42	0.49
2:B:181:THR:HG22	2:B:245:ASN:ND2	2.27	0.49
1:C:514:PRO:O	1:C:515:ALA:C	2.54	0.49
1:A:118:THR:CG2	1:A:120:ALA:HB3	2.43	0.49
3:D:691:HEM:CBB	3:D:691:HEM:HHC	2.43	0.49
2:B:146:LEU:CD2	2:B:151:LYS:HB3	2.43	0.49
2:D:549:GLU:OE1	2:D:549:GLU:CA	2.41	0.49
1:A:40:LYS:NZ	2:D:689:HIS:O	2.38	0.49
2:D:616:ASP:O	2:D:619:ALA:HB3	2.13	0.49
2:D:620:HIS:HB2	2:D:627:THR:OG1	2.13	0.49
2:D:623:ASN:ND2	2:D:626:GLY:H	2.11	0.49
2:D:550:GLU:O	2:D:553:ALA:HB3	2.13	0.48
1:C:428:ALA:HB2	1:C:505:LEU:HD13	1.95	0.48
1:C:476:MET:N	1:C:477:PRO:HD2	2.28	0.48
2:D:684:LEU:CD1	3:D:691:HEM:HAB	2.43	0.48
2:B:144:VAL:HG23	2:B:146:LEU:HD13	1.95	0.48
1:C:410:VAL:HG23	1:C:470:VAL:HG13	1.96	0.48
2:D:609:LYS:HD3	3:D:691:HEM:CAA	2.43	0.48
1:A:17:VAL:HG13	1:A:24:TYR:HD2	1.78	0.48
2:B:193:THR:CB	2:B:194:PRO:CD	2.91	0.48
2:D:661:PHE:O	2:D:664:GLU:HB2	2.14	0.48
1:A:28:ALA:CB	1:A:105:LEU:CD1	2.92	0.48
1:A:58:HIS:HE1	3:A:143:HEM:CHA	2.25	0.48
2:D:661:PHE:O	2:D:662:GLY:C	2.56	0.48
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.95	0.48
1:A:97:ASN:ND2	6:A:148:HOH:O	2.31	0.48
2:D:593:THR:O	2:D:597:VAL:HG23	2.14	0.48
2:D:666:THR:HB	2:D:668:PRO:HD2	1.96	0.48
2:B:153:ALA:O	2:B:154:VAL:C	2.56	0.48
1:C:442:TYR:C	1:C:444:PRO:HD2	2.39	0.48
2:D:547:THR:CB	2:D:550:GLU:HG3	2.40	0.48
1:A:16:LYS:HZ2	1:A:16:LYS:HB3	1.78	0.47
2:B:218:LEU:O	2:B:221:LEU:HD22	2.14	0.47
2:B:272:ALA:O	2:B:276:VAL:HG23	2.13	0.47
2:D:684:LEU:HD23	2:D:684:LEU:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:LYS:NZ	1:C:474:ASP:OD1	2.30	0.47
2:D:544:VAL:HG13	2:D:546:LEU:HD12	1.97	0.47
1:A:17:VAL:HG13	1:A:24:TYR:CE2	2.49	0.47
2:B:147:THR:HG22	2:B:150:GLU:H	1.79	0.47
2:D:639:LEU:HD13	3:D:691:HEM:C2D	2.49	0.47
1:C:480:LEU:HD12	1:C:535:VAL:CG1	2.43	0.47
1:C:513:LEU:O	1:C:516:GLU:HG2	2.14	0.47
2:D:642:ASP:OD1	2:D:643:PRO:HD2	2.13	0.47
2:B:163:VAL:HG13	2:B:211:LEU:HB3	1.96	0.47
1:A:44:PRO:HD2	1:A:45:HIS:CE1	2.50	0.46
1:A:34:LEU:HD12	2:B:267:PRO:C	2.40	0.46
1:C:486:LEU:HD11	1:C:490:LYS:HD3	1.97	0.46
2:D:547:THR:O	2:D:551:LYS:CG	2.60	0.46
2:B:167:GLY:HA3	2:B:207:GLY:O	2.16	0.46
1:C:483:LEU:HD12	1:C:483:LEU:HA	1.65	0.46
2:D:571:LEU:HD21	2:D:606:HIS:HD2	1.80	0.46
1:A:113:LEU:N	1:A:114:PRO:CD	2.79	0.46
1:A:70:VAL:O	1:A:73:VAL:HB	2.15	0.46
1:A:51:GLY:O	1:A:52:SER:C	2.55	0.46
2:D:632:SER:CB	2:D:687:LYS:HG3	2.42	0.46
2:D:551:LYS:O	2:D:555:THR:HB	2.16	0.46
2:D:644:GLU:OE1	2:D:647:ARG:NH1	2.49	0.45
1:A:109:LEU:O	1:A:110:ALA:C	2.54	0.45
2:B:173:ARG:O	2:B:177:VAL:HG23	2.16	0.45
2:D:611:LEU:HD22	2:D:611:LEU:HA	1.65	0.45
1:C:442:TYR:C	1:C:444:PRO:CD	2.89	0.45
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.80	0.45
1:C:518:THR:HG22	1:C:521:VAL:HG23	1.99	0.45
2:B:217:GLY:CA	6:B:44:HOH:O	2.28	0.45
1:C:475:ASP:OD2	1:C:478:ASN:HB2	2.17	0.45
1:C:417:VAL:HG11	1:C:421:ALA:HB2	1.94	0.45
1:A:91:LEU:O	1:A:92:ARG:C	2.60	0.44
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.70	0.44
2:B:178:TYR:N	2:B:179:PRO:CD	2.80	0.44
2:D:653:LEU:O	2:D:654:VAL:C	2.61	0.44
2:B:267:PRO:N	2:B:268:PRO:CD	2.81	0.44
1:C:513:LEU:HB3	1:C:516:GLU:HG2	1.92	0.44
2:B:191:LEU:HB3	2:B:197:VAL:HG22	2.00	0.44
2:D:558:TRP:CE3	2:D:561:VAL:HG21	2.53	0.44
1:A:92:ARG:NH1	2:D:583:ARG:HB2	2.33	0.44
1:C:493:VAL:O	1:C:540:TYR:HE2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:ALA:HA	2:D:577:VAL:HG13	1.98	0.44
2:D:573:ARG:O	2:D:577:VAL:HG23	2.17	0.44
1:C:417:VAL:CG1	1:C:421:ALA:CB	2.91	0.44
2:D:546:LEU:CD2	2:D:550:GLU:HB3	2.47	0.44
3:A:143:HEM:HBC2	3:A:143:HEM:HMC1	2.00	0.44
2:B:148:PRO:CB	2:B:151:LYS:HZ2	2.29	0.44
2:B:225:LYS:HD3	2:B:286:HIS:CD2	2.53	0.44
2:B:148:PRO:CG	2:B:149:GLU:N	2.82	0.43
2:D:620:HIS:C	2:D:622:ASP:N	2.75	0.43
2:D:548:PRO:HA	2:D:551:LYS:NZ	2.33	0.43
2:D:573:ARG:HD2	2:D:656:VAL:CG2	2.49	0.43
2:B:164:ASP:CA	2:B:208:LYS:HG2	2.37	0.43
1:C:476:MET:N	1:C:477:PRO:CD	2.82	0.43
2:D:656:VAL:O	2:D:659:HIS:HB3	2.18	0.43
2:B:272:ALA:O	2:B:275:LYS:HB2	2.18	0.43
2:D:571:LEU:CB	6:D:128:HOH:O	2.20	0.43
2:D:684:LEU:CD1	3:D:691:HEM:CAB	2.96	0.43
1:A:33:PHE:HD1	1:A:33:PHE:HA	1.58	0.43
1:C:466:LEU:HD12	1:C:466:LEU:HA	1.34	0.43
2:D:547:THR:HG23	2:D:548:PRO:CD	2.49	0.43
2:D:548:PRO:CB	2:D:551:LYS:HZ2	2.31	0.43
2:B:158:TRP:HE3	2:B:273:TYR:OH	2.02	0.43
1:A:95:PRO:O	1:A:96:VAL:C	2.62	0.43
2:B:148:PRO:CA	2:B:151:LYS:HZ2	2.28	0.42
2:B:206:HIS:NE2	6:B:126:HOH:O	2.36	0.42
1:C:407:LYS:O	1:C:411:LYS:HG3	2.19	0.42
1:C:406:ASP:O	1:C:410:VAL:HG13	2.19	0.42
1:C:424:TYR:N	1:C:424:TYR:CD1	2.86	0.42
2:B:146:LEU:HD21	2:B:154:VAL:HG21	2.02	0.42
2:D:631:LEU:HD23	2:D:631:LEU:HA	1.91	0.42
1:A:47:ASP:OD1	1:A:48:LEU:N	2.53	0.42
2:B:146:LEU:HD23	2:B:151:LYS:N	2.34	0.42
2:D:558:TRP:CH2	2:D:611:LEU:HD11	2.51	0.42
2:D:569:GLU:HG2	2:D:656:VAL:HG22	2.01	0.42
2:D:661:PHE:O	2:D:664:GLU:CB	2.67	0.42
2:B:193:THR:CB	2:B:194:PRO:HD2	2.50	0.42
2:B:147:THR:O	2:B:151:LYS:CD	2.67	0.41
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.85	0.41
1:C:470:VAL:O	1:C:473:VAL:HB	2.20	0.41
1:C:516:GLU:HG2	1:C:516:GLU:H	1.31	0.41
2:B:161:VAL:HG12	2:B:261:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:O	1:A:114:PRO:C	2.63	0.41
1:C:476:MET:HB2	1:C:477:PRO:CD	2.50	0.41
2:D:600:ASN:HA	2:D:601:PRO:HD2	1.52	0.41
2:D:653:LEU:O	2:D:656:VAL:N	2.52	0.41
2:B:177:VAL:C	2:B:179:PRO:HD3	2.45	0.41
1:A:141:ARG:HD3	2:D:580:TRP:HZ3	1.86	0.41
2:B:209:LYS:HE3	3:B:291:HEM:HAA2	2.01	0.41
2:B:214:PHE:CD1	2:B:214:PHE:C	2.99	0.41
1:C:505:LEU:HD13	1:C:505:LEU:HA	1.83	0.41
2:D:545:HIS:O	2:D:675:LYS:CE	2.66	0.41
2:D:548:PRO:CA	2:D:551:LYS:HZ2	2.34	0.41
2:D:601:PRO:HG2	2:D:602:LYS:H	1.86	0.41
2:D:635:HIS:HB3	2:D:688:TYR:OH	2.20	0.41
2:B:211:LEU:HA	2:B:214:PHE:HB3	2.03	0.41
2:B:243:PRO:HB2	2:B:247:ARG:HH22	1.86	0.41
2:D:644:GLU:O	2:D:644:GLU:HG3	2.21	0.41
1:A:1:VAL:O	1:A:127:LYS:NZ	2.48	0.41
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.83	0.41
2:B:171:LEU:O	2:B:174:LEU:HB3	2.21	0.41
2:D:588:PHE:O	2:D:602:LYS:HG3	2.21	0.40
3:B:291:HEM:HAA1	6:B:65:HOH:O	2.21	0.40
1:C:525:LEU:HA	1:C:525:LEU:HD23	1.89	0.40
2:D:548:PRO:HA	2:D:551:LYS:HZ2	1.86	0.40
5:D:701:DG2:H41	6:D:106:HOH:O	2.21	0.40
1:A:20:HIS:CD2	1:A:20:HIS:N	2.88	0.40
1:C:512:HIS:C	1:C:513:LEU:HD23	2.47	0.40
2:D:547:THR:HG22	2:D:549:GLU:CA	2.44	0.40
2:D:643:PRO:HA	2:D:646:PHE:CD2	2.56	0.40

All (2) 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)
6:A:170:HOH:O	6:D:132:HOH:O[4_554]	0.01	2.19
1:A:23:GLU:OE1	6:B:28:HOH:O[3_445]	1.65	0.55

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	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	C	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
2	B	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
2	D	145/146 (99%)	133 (92%)	10 (7%)	2 (1%)	9	17
All	All	567/574 (99%)	528 (93%)	37 (6%)	2 (0%)	30	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	662	GLY
2	D	564	ASP

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	113/113 (100%)	99 (88%)	14 (12%)	4	9
1	C	113/113 (100%)	102 (90%)	11 (10%)	8	17
2	B	118/118 (100%)	97 (82%)	21 (18%)	2	3
2	D	119/118 (101%)	92 (77%)	27 (23%)	1	1
All	All	463/462 (100%)	390 (84%)	73 (16%)	2	5

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	16	LYS
1	A	45	HIS
1	A	52	SER
1	A	60	LYS
1	A	77	PRO
1	A	83	LEU
1	A	84	SER
1	A	92	ARG
1	A	95	PRO
1	A	99	LYS
1	A	105	LEU
1	A	116	GLU
1	A	118	THR
2	B	144	VAL
2	B	146	LEU
2	B	148	PRO
2	B	149	GLU
2	B	151	LYS
2	B	152	SER
2	B	155	THR
2	B	161	VAL
2	B	169	GLU
2	B	175	LEU
2	B	183	ARG
2	B	186	GLU
2	B	193	THR
2	B	195	ASP
2	B	202	LYS
2	B	211	LEU
2	B	216	ASP
2	B	221	LEU
2	B	238	LYS
2	B	263	LYS
2	B	286	HIS
1	C	410	VAL
1	C	416	LYS
1	C	466	LEU
1	C	473	VAL
1	C	483	LEU
1	C	484	SER
1	C	505	LEU
1	C	506	LEU

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Mol	Chain	Res	Type
1	C	516	GLU
1	C	518	THR
1	C	519	PRO
2	D	544	VAL
2	D	546	LEU
2	D	549	GLU
2	D	551	LYS
2	D	555	THR
2	D	557	LEU
2	D	560	LYS
2	D	563	VAL
2	D	565	GLU
2	D	569	GLU
2	D	595	ASP
2	D	604	LYS
2	D	608	LYS
2	D	610	VAL
2	D	611	LEU
2	D	615	SER
2	D	616	ASP
2	D	620	HIS
2	D	621	LEU
2	D	622	ASP
2	D	625[A]	LYS
2	D	625[B]	LYS
2	D	634	LEU
2	D	656	VAL
2	D	660	HIS
2	D	663	LYS
2	D	667	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	78	ASN
1	A	103	HIS
2	B	223	ASN
2	B	240	HIS
2	B	245	ASN
1	C	420	HIS
1	C	468	ASN

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Mol	Chain	Res	Type
1	C	472	HIS
1	C	478	ASN
1	C	503	HIS
2	D	620	HIS
2	D	623	ASN
2	D	640	HIS
2	D	645	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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
3	HEM	A	143	1,4	50,50,50	1.44	7 (14%)	67,82,82	2.22	24 (35%)
3	HEM	D	691	2,6	50,50,50	1.41	7 (14%)	67,82,82	2.07	21 (31%)
3	HEM	C	543	1,4	50,50,50	1.28	6 (12%)	67,82,82	2.07	18 (26%)
5	DG2	D	701	-	13,14,14	2.04	3 (23%)	18,21,21	6.26	8 (44%)
4	OXY	A	144	3	1,1,1	0.31	0	-		
4	OXY	C	544	3	1,1,1	0.44	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	291	2,6	50,50,50	1.48	9 (18%)	67,82,82	1.37	8 (11%)

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
3	HEM	A	143	1,4	-	2/14/54/54	-
3	HEM	D	691	2,6	-	4/14/54/54	-
3	HEM	C	543	1,4	-	6/14/54/54	-
5	DG2	D	701	-	1/1/4/4	7/15/15/15	-
3	HEM	B	291	2,6	-	5/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	DG2	O5-C4	-4.83	1.26	1.44
3	B	291	HEM	C2A-C3A	-4.47	1.27	1.38
3	A	143	HEM	FE-NC	3.34	2.06	1.95
5	D	701	DG2	P6-O15	-3.20	1.40	1.50
5	D	701	DG2	P1-O11	-3.15	1.40	1.50
3	D	691	HEM	CAB-C3B	3.02	1.55	1.47
3	B	291	HEM	CAB-C3B	2.79	1.54	1.47
3	D	691	HEM	FE-NB	2.78	2.03	1.94
3	C	543	HEM	CAB-C3B	2.76	1.54	1.47
3	D	691	HEM	C2A-C3A	-2.76	1.31	1.38
3	B	291	HEM	FE-NB	2.76	2.03	1.94
3	A	143	HEM	CAC-C3C	2.73	1.54	1.47
3	B	291	HEM	CAC-C3C	2.59	1.54	1.47
3	A	143	HEM	CMB-C2B	2.54	1.56	1.50
3	B	291	HEM	CMB-C2B	2.51	1.55	1.50
3	A	143	HEM	CHC-C1C	2.49	1.43	1.38
3	C	543	HEM	CMD-C2D	2.48	1.55	1.50
3	C	543	HEM	FE-ND	2.47	2.02	1.94
3	B	291	HEM	FE-NA	2.46	2.03	1.95
3	C	543	HEM	CMB-C2B	2.40	1.55	1.50
3	D	691	HEM	FE-NA	2.36	2.02	1.95
3	A	143	HEM	FE-NB	2.35	2.02	1.94
3	D	691	HEM	CMA-C3A	2.32	1.55	1.50
3	C	543	HEM	C3B-C2B	-2.23	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	143	HEM	C2A-C3A	-2.17	1.33	1.38
3	A	143	HEM	CMC-C2C	2.15	1.55	1.50
3	D	691	HEM	CMC-C2C	2.12	1.55	1.50
3	D	691	HEM	C3D-C2D	-2.08	1.32	1.36
3	C	543	HEM	FE-NA	2.07	2.02	1.95
3	B	291	HEM	O2A-CGA	-2.07	1.24	1.30
3	B	291	HEM	C3C-C2C	-2.06	1.33	1.37
3	B	291	HEM	FE-NC	2.04	2.01	1.95

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	DG2	O5-C4-C3	22.54	164.22	108.58
5	D	701	DG2	O13-P6-O5	7.76	126.89	106.67
5	D	701	DG2	P1-O2-C3	-7.30	106.30	123.04
3	D	691	HEM	O1D-CGD-CBD	-7.03	100.79	123.09
5	D	701	DG2	O14-P6-O5	-6.57	89.54	106.67
3	C	543	HEM	CHD-C4C-NC	6.19	131.19	124.45
3	D	691	HEM	O2D-CGD-O1D	6.12	139.07	123.33
3	A	143	HEM	CAD-CBD-CGD	5.92	129.36	113.67
3	A	143	HEM	CHB-C1B-NB	5.30	130.92	124.37
3	C	543	HEM	O1D-CGD-CBD	-5.08	106.98	123.09
3	C	543	HEM	O2D-CGD-O1D	4.97	136.12	123.33
3	C	543	HEM	CHC-C1C-NC	4.93	129.82	124.45
3	A	143	HEM	CHA-C4D-ND	-4.60	118.67	124.37
3	A	143	HEM	CMA-C3A-C4A	4.28	131.94	125.42
3	B	291	HEM	O2A-CGA-O1A	4.13	133.96	123.33
3	C	543	HEM	CMB-C2B-C1B	-4.07	118.67	125.03
3	C	543	HEM	C4C-CHD-C1D	-4.07	117.37	126.02
3	A	143	HEM	CHA-C4D-C3D	4.01	132.62	125.23
3	A	143	HEM	CMB-C2B-C1B	-3.93	118.90	125.03
3	D	691	HEM	CHD-C1D-ND	3.71	128.42	124.42
3	C	543	HEM	C1C-CHC-C4B	-3.68	118.21	126.02
3	D	691	HEM	CHD-C4C-NC	3.60	128.37	124.45
3	D	691	HEM	CHB-C4A-NA	3.55	130.31	123.86
3	C	543	HEM	CMA-C3A-C4A	-3.52	120.05	125.42
3	D	691	HEM	C3D-C4D-ND	-3.50	106.33	110.17
3	A	143	HEM	O2A-CGA-O1A	3.46	132.23	123.33
3	A	143	HEM	CBB-CAB-C3B	3.39	144.46	127.53
3	A	143	HEM	CHD-C4C-NC	3.39	128.14	124.45
3	A	143	HEM	C1A-CHA-C4D	3.32	134.06	126.25
3	A	143	HEM	O2D-CGD-O1D	3.28	131.78	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	543	HEM	CMA-C3A-C2A	3.23	132.47	125.62
3	B	291	HEM	CAA-C2A-C1A	-3.19	118.71	124.94
3	B	291	HEM	CHD-C1D-ND	3.16	127.82	124.42
3	A	143	HEM	C4A-CHB-C1B	-3.15	118.85	126.25
5	D	701	DG2	O8-C7-C3	3.12	120.83	112.71
3	D	691	HEM	C4A-CHB-C1B	-3.11	118.94	126.25
3	A	143	HEM	C3B-C2B-C1B	3.11	108.74	106.41
3	D	691	HEM	CHA-C4D-ND	3.04	128.12	124.37
3	A	143	HEM	CHD-C4C-C3C	-3.02	120.12	125.21
5	D	701	DG2	O8-C7-O7	-3.01	117.25	124.08
3	B	291	HEM	CBA-CAA-C2A	-2.94	104.40	112.53
3	C	543	HEM	CHD-C4C-C3C	-2.92	120.28	125.21
3	C	543	HEM	C3B-C2B-C1B	2.89	108.58	106.41
3	D	691	HEM	CMA-C3A-C2A	2.87	131.72	125.62
3	D	691	HEM	CMA-C3A-C4A	-2.87	121.05	125.42
3	A	143	HEM	C4C-CHD-C1D	-2.86	119.94	126.02
3	C	543	HEM	O1A-CGA-CBA	-2.84	114.08	123.09
3	C	543	HEM	CHB-C1B-NB	2.79	127.82	124.37
3	D	691	HEM	CHB-C1B-NB	2.77	127.80	124.37
3	A	143	HEM	C4D-C3D-C2D	2.73	110.87	106.89
3	C	543	HEM	CHA-C1A-NA	-2.70	118.96	123.86
3	D	691	HEM	CHC-C1C-NC	2.70	127.39	124.45
3	A	143	HEM	C1D-C2D-C3D	-2.66	104.18	106.98
3	B	291	HEM	CMD-C2D-C1D	-2.66	120.88	125.03
3	D	691	HEM	C4C-CHD-C1D	-2.57	120.55	126.02
3	D	691	HEM	C1A-CHA-C4D	-2.52	120.32	126.25
3	A	143	HEM	CHD-C1D-C2D	-2.46	121.15	125.03
3	A	143	HEM	O1A-CGA-CBA	-2.46	115.30	123.09
5	D	701	DG2	O10-P1-O9	-2.46	98.60	107.80
3	C	543	HEM	CHC-C1C-C2C	-2.45	120.39	125.49
3	D	691	HEM	C4D-C3D-C2D	2.43	110.43	106.89
3	A	143	HEM	O1D-CGD-CBD	-2.43	115.39	123.09
5	D	701	DG2	O10-P1-O2	2.41	115.22	105.85
3	D	691	HEM	CAD-CBD-CGD	-2.40	107.30	113.67
3	D	691	HEM	CAD-C3D-C2D	-2.40	123.38	127.87
3	D	691	HEM	CHB-C4A-C3A	-2.39	120.49	127.43
3	A	143	HEM	CMD-C2D-C1D	2.32	128.66	125.03
3	A	143	HEM	CHB-C1B-C2B	-2.32	120.36	126.95
3	D	691	HEM	CBD-CAD-C3D	-2.31	106.14	112.53
3	D	691	HEM	O2A-CGA-O1A	2.25	129.13	123.33
3	B	291	HEM	CHA-C1A-NA	2.21	127.87	123.86
3	C	543	HEM	CHD-C1D-ND	2.21	126.80	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	143	HEM	C2D-C1D-ND	2.21	112.45	109.90
3	A	143	HEM	CHA-C1A-C2A	2.13	129.96	125.30
3	C	543	HEM	CHC-C4B-NB	2.13	126.71	124.42
3	B	291	HEM	CAA-C2A-C3A	2.10	131.77	127.07
3	C	543	HEM	O2A-CGA-CBA	2.05	120.46	114.00
3	B	291	HEM	C1A-CHA-C4D	-2.02	121.50	126.25
3	D	691	HEM	C2A-C1A-NA	-2.02	107.92	110.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	701	DG2	C3

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	701	DG2	C7-C3-C4-O5
5	D	701	DG2	C7-C3-O2-P1
5	D	701	DG2	O2-C3-C7-O7
5	D	701	DG2	C3-C4-O5-P6
5	D	701	DG2	C4-O5-P6-O15
5	D	701	DG2	C4-O5-P6-O14
5	D	701	DG2	O2-C3-C7-O8
3	B	291	HEM	C2C-C3C-CAC-CBC
3	B	291	HEM	C4B-C3B-CAB-CBB
3	B	291	HEM	C4C-C3C-CAC-CBC
3	C	543	HEM	C4D-C3D-CAD-CBD
3	D	691	HEM	CAD-CBD-CGD-O1D
3	A	143	HEM	CAA-CBA-CGA-O1A
3	A	143	HEM	CAA-CBA-CGA-O2A
3	D	691	HEM	CAD-CBD-CGD-O2D
3	C	543	HEM	CAD-CBD-CGD-O1D
3	C	543	HEM	CAD-CBD-CGD-O2D
3	C	543	HEM	CAA-CBA-CGA-O2A
3	D	691	HEM	CAA-CBA-CGA-O2A
3	C	543	HEM	C2D-C3D-CAD-CBD
3	C	543	HEM	CAA-CBA-CGA-O1A
3	B	291	HEM	CAD-CBD-CGD-O1D
3	B	291	HEM	CAD-CBD-CGD-O2D
3	D	691	HEM	CAA-CBA-CGA-O1A

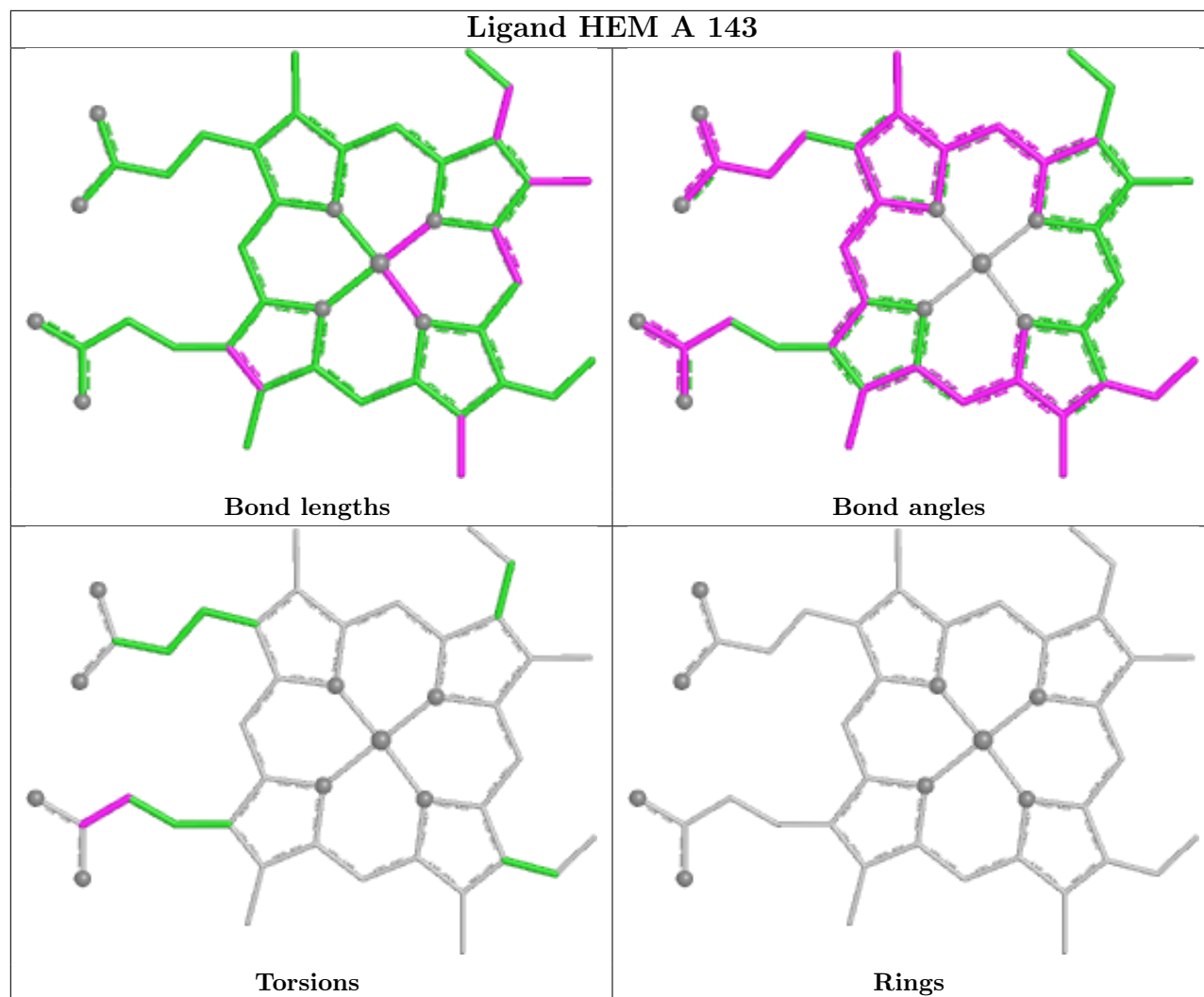
There are no ring outliers.

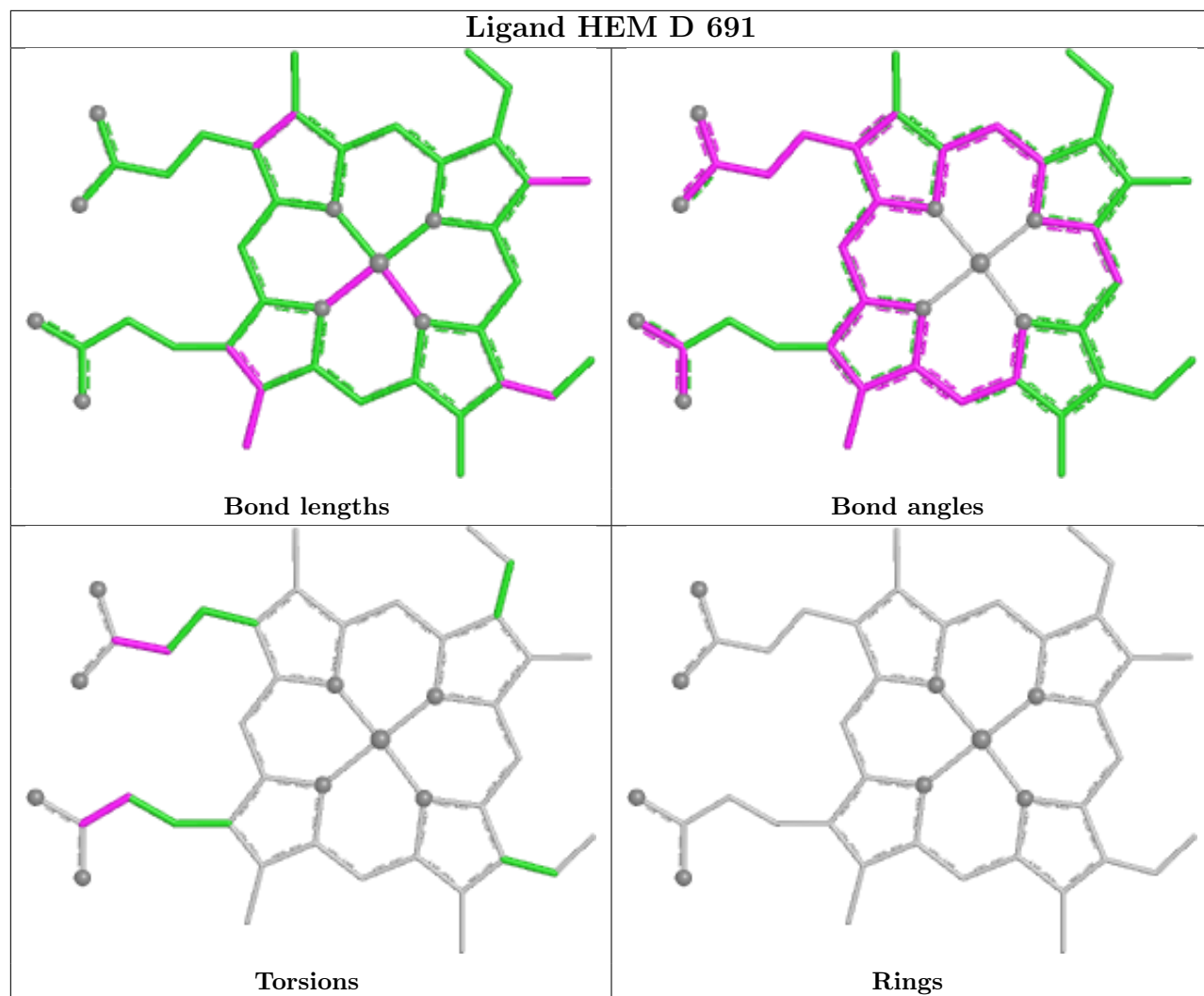
4 monomers are involved in 22 short contacts:

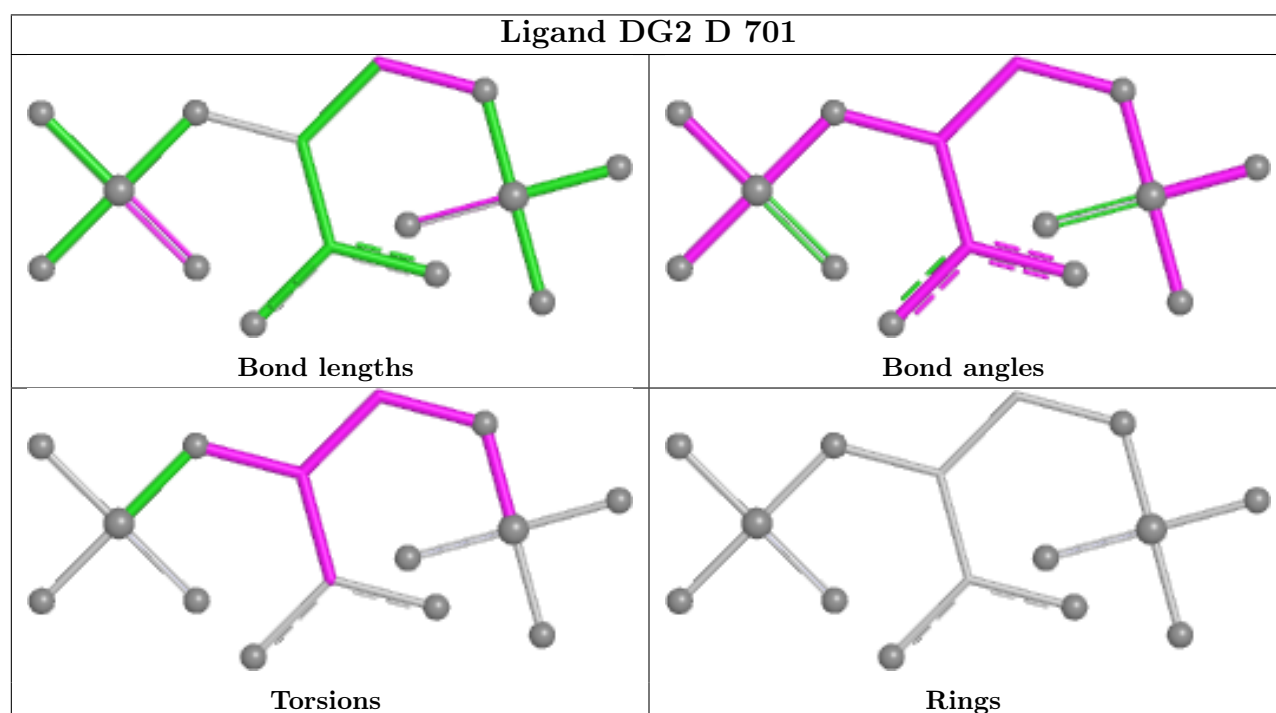
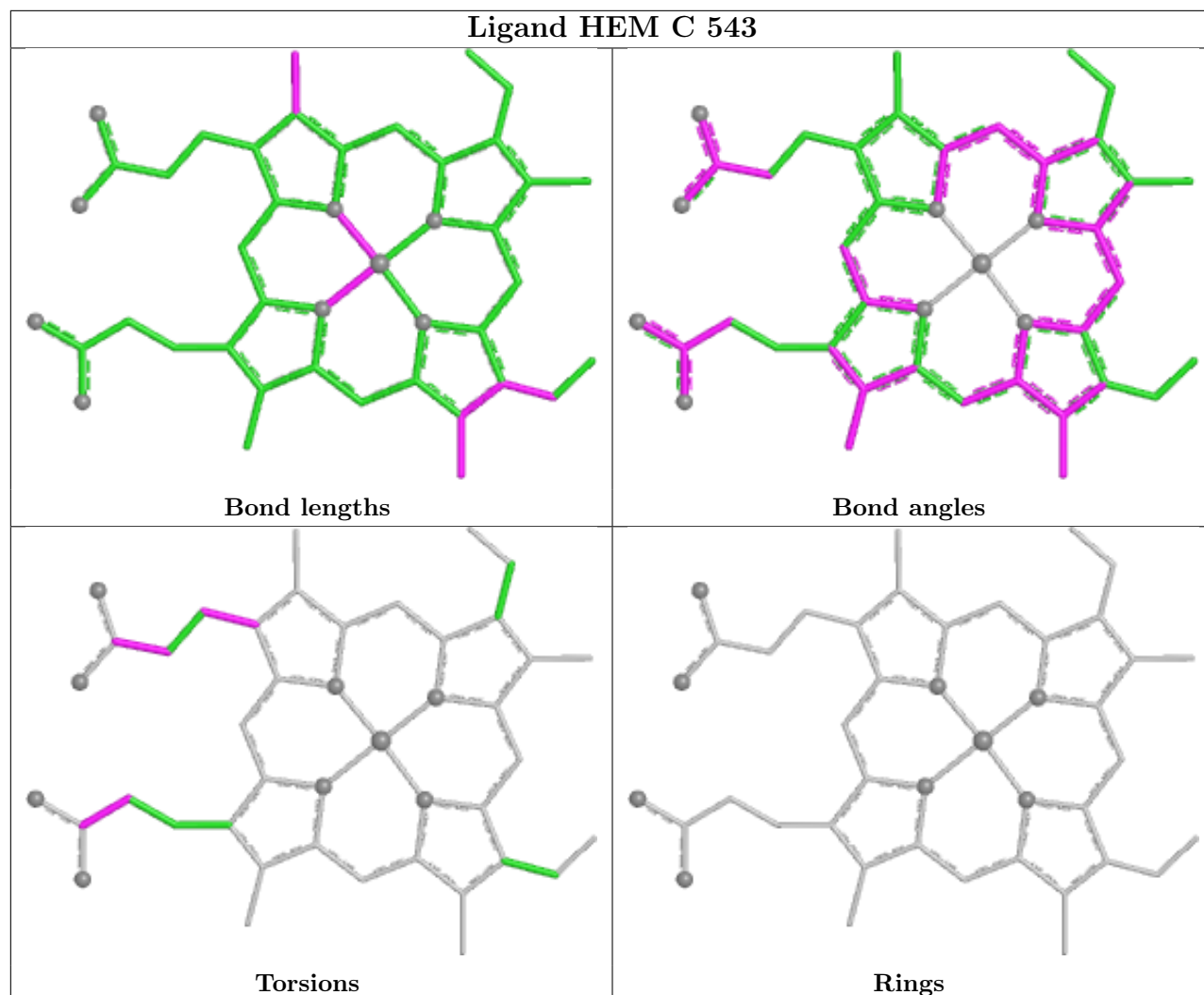
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	143	HEM	2	0
3	D	691	HEM	12	0
5	D	701	DG2	2	0
3	B	291	HEM	6	0

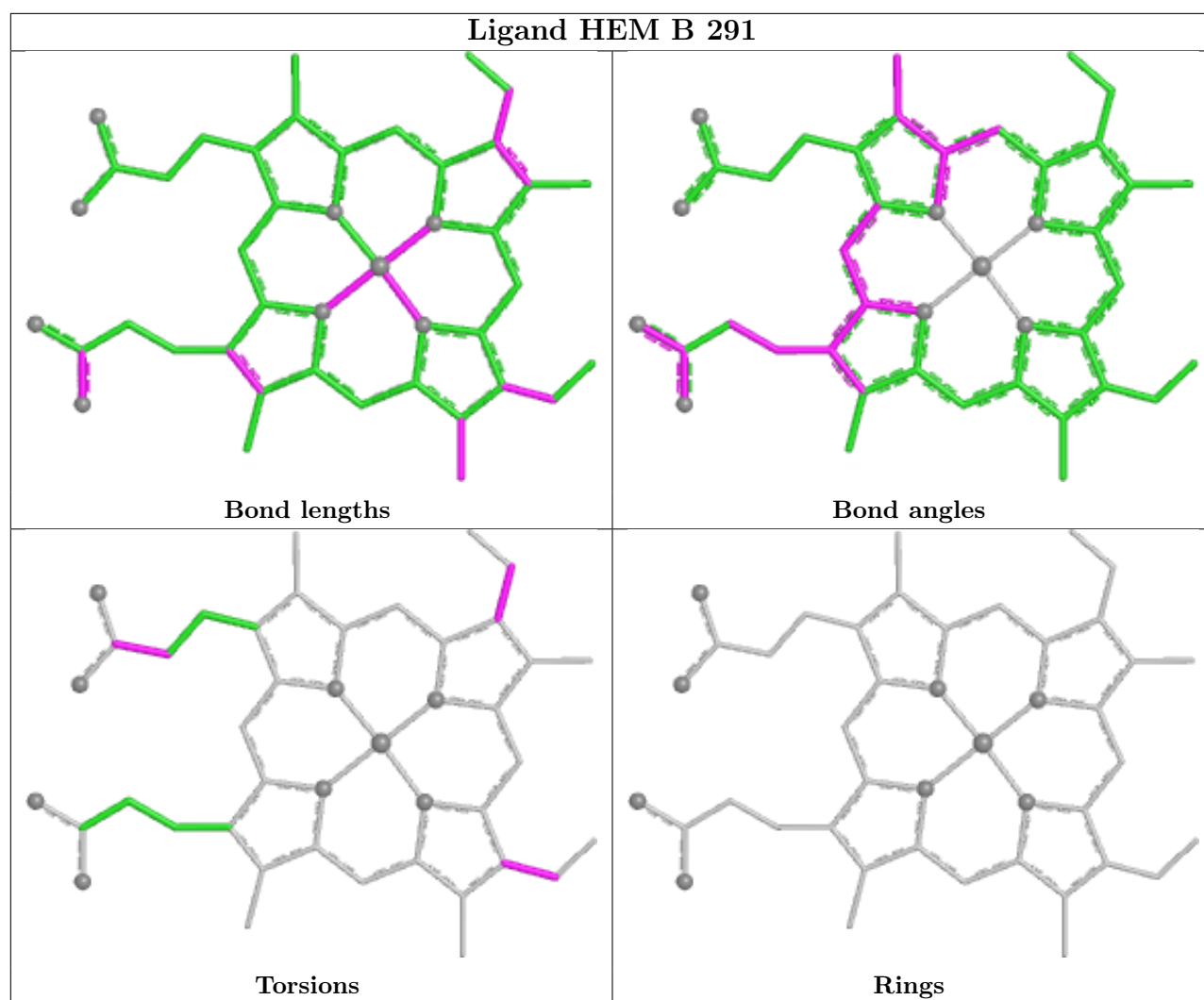
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HEM A 143









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.