



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:35 AM UTC

PDB ID : 2NSI / pdb_00002nsi
Title : HUMAN INDUCIBLE NITRIC OXIDE SYNTHASE, ZN-FREE, SEITU COMPLEX
Authors : Li, H.; Raman, C.S.; Glaser, C.B.; Blasko, E.; Young, T.A.; Parkinson, J.F.; Whitlow, M.; Poulos, T.L.
Deposited on : 1999-01-11
Resolution : 3.00 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

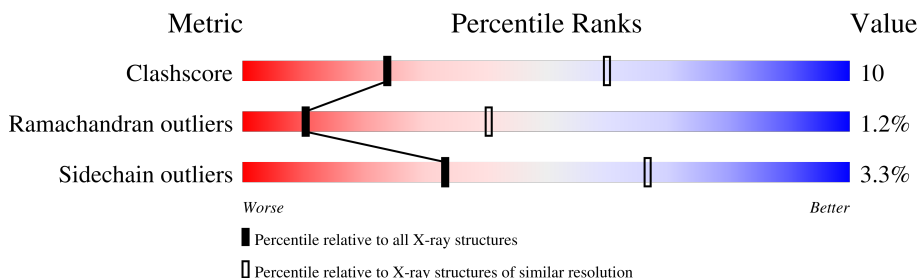
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition [i](#)

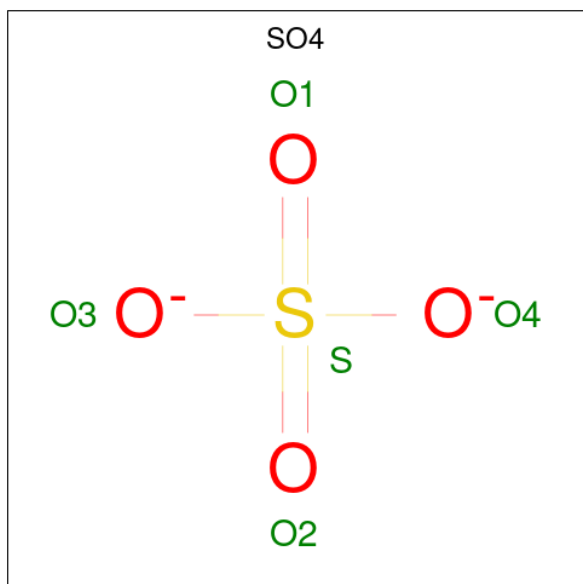
There are 5 unique types of molecules in this entry. The entry contains 13985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (NITRIC OXIDE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	B	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	C	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	D	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



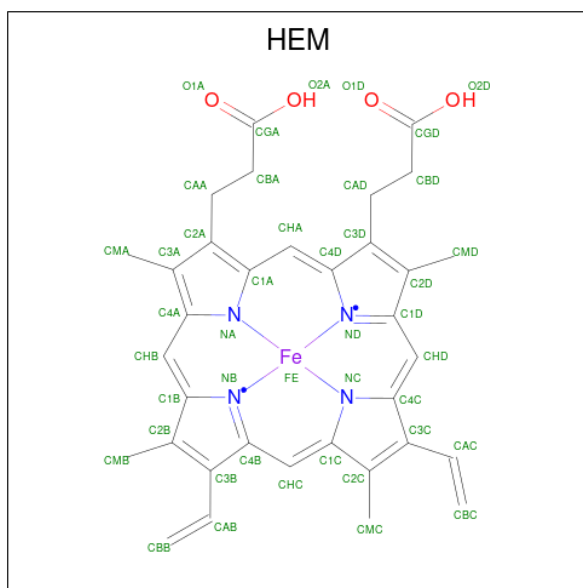
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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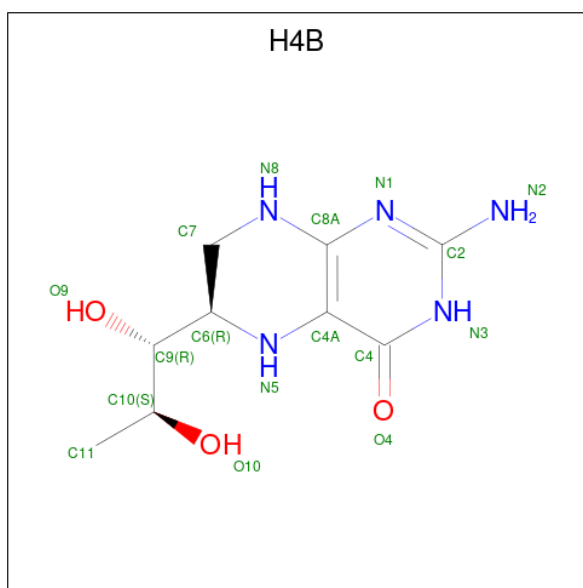
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

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



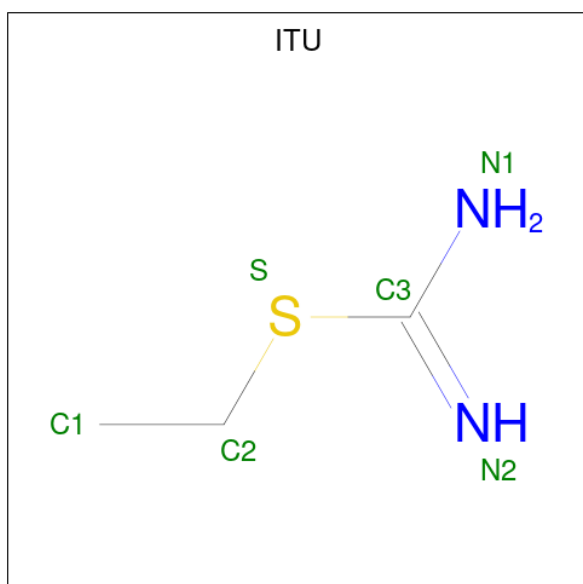
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		
4	C	1	Total	C	N	O	0	0
			17	9	5	3		
4	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is ETHYLISOTHIOUREA (CCD ID: ITU) (formula: $C_3H_8N_2S$).



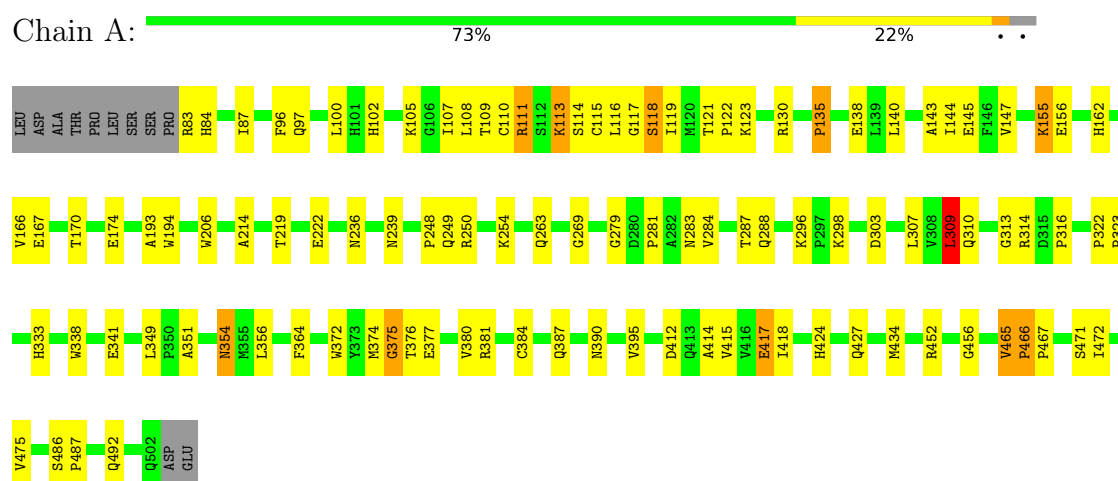
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 6	C 3	N 2	S 1	0	0
5	B	1	Total 6	C 3	N 2	S 1	0	0
5	C	1	Total 6	C 3	N 2	S 1	0	0
5	D	1	Total 6	C 3	N 2	S 1	0	0

3 Residue-property plots

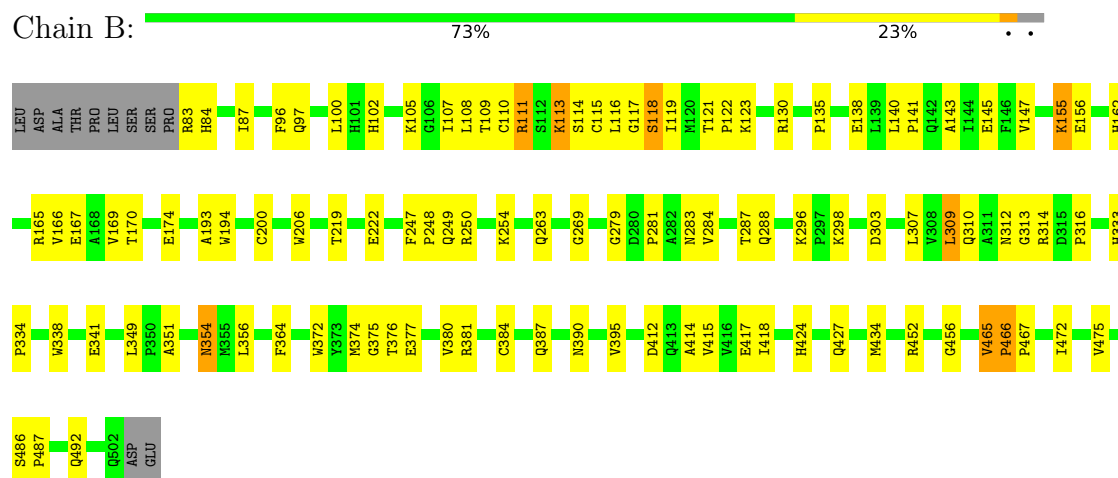
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)



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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.37Å 188.37Å 230.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	80.8 (30.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.214 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13985	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ITU, SO4, H4B, 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	0.41	0/3518	0.94	11/4774 (0.2%)
1	B	0.43	0/3518	0.94	8/4774 (0.2%)
1	C	0.43	0/3518	0.94	9/4774 (0.2%)
1	D	0.42	0/3518	0.94	9/4774 (0.2%)
All	All	0.42	0/14072	0.94	37/19096 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	PRO	CA-C-N	6.61	126.30	119.82
1	B	466	PRO	C-N-CA	6.61	126.30	119.82
1	B	465	VAL	CA-C-N	6.56	127.14	120.38
1	B	465	VAL	C-N-CA	6.56	127.14	120.38
1	D	111	ARG	N-CA-C	6.54	116.87	108.24
1	C	465	VAL	CA-C-N	6.50	127.08	120.38
1	C	465	VAL	C-N-CA	6.50	127.08	120.38
1	A	111	ARG	N-CA-C	6.43	116.73	108.24
1	B	111	ARG	N-CA-C	6.38	116.66	108.24
1	A	465	VAL	CA-C-N	6.34	126.91	120.38
1	A	465	VAL	C-N-CA	6.34	126.91	120.38
1	D	349	LEU	N-CA-C	6.25	119.93	108.69
1	C	111	ARG	N-CA-C	6.24	116.48	108.24
1	B	349	LEU	N-CA-C	6.19	119.83	108.69
1	D	465	VAL	CA-C-N	6.07	126.63	120.38
1	D	465	VAL	C-N-CA	6.07	126.63	120.38
1	A	349	LEU	N-CA-C	6.00	119.49	108.69
1	C	296	LYS	CA-C-N	5.83	125.76	119.76
1	C	296	LYS	C-N-CA	5.83	125.76	119.76
1	C	349	LEU	N-CA-C	5.78	119.09	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CA-C-N	5.59	125.52	119.76
1	A	296	LYS	C-N-CA	5.59	125.52	119.76
1	B	296	LYS	CA-C-N	5.43	125.70	119.83
1	B	296	LYS	C-N-CA	5.43	125.70	119.83
1	D	135	PRO	CA-C-N	5.39	125.47	119.32
1	D	135	PRO	C-N-CA	5.39	125.47	119.32
1	A	466	PRO	CA-C-N	5.35	125.06	119.82
1	A	466	PRO	C-N-CA	5.35	125.06	119.82
1	C	309	LEU	N-CA-C	5.34	117.94	109.24
1	C	373	TYR	N-CA-C	5.30	117.52	110.53
1	C	258	ARG	N-CA-C	5.25	117.06	108.76
1	A	135	PRO	CA-C-N	5.21	125.25	119.32
1	A	135	PRO	C-N-CA	5.21	125.25	119.32
1	D	296	LYS	CA-C-N	5.11	125.02	119.76
1	D	296	LYS	C-N-CA	5.11	125.02	119.76
1	D	258	ARG	N-CA-C	5.10	117.00	108.99
1	A	309	LEU	N-CA-C	5.04	117.46	109.24

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	3419	0	3327	75	0
1	B	3419	0	3327	74	0
1	C	3419	0	3327	67	0
1	D	3419	0	3327	75	0
2	A	15	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
3	C	43	0	30	1	0
3	D	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	15	0	0
4	B	17	0	15	0	0
4	C	17	0	15	0	0
4	D	17	0	15	0	0
5	A	6	0	7	0	0
5	B	6	0	7	0	0
5	C	6	0	7	0	0
5	D	6	0	7	0	0
All	All	13985	0	13516	278	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 10.

All (278) 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:115:CYS:HB2	1:B:110:CYS:SG	2.11	0.91
1:A:110:CYS:SG	1:B:115:CYS:HB2	2.17	0.85
1:B:83:ARG:HB3	1:B:102:HIS:HE1	1.45	0.80
1:D:83:ARG:HB3	1:D:102:HIS:HE1	1.45	0.80
1:C:83:ARG:HB3	1:C:102:HIS:HE1	1.46	0.79
1:A:83:ARG:HB3	1:A:102:HIS:HE1	1.47	0.78
1:B:269:GLY:H	1:B:287:THR:HG21	1.51	0.76
1:C:109:THR:HG22	1:C:116:LEU:HG	1.67	0.75
1:A:269:GLY:H	1:A:287:THR:HG21	1.52	0.73
1:D:109:THR:HG22	1:D:116:LEU:HG	1.70	0.73
1:D:269:GLY:H	1:D:287:THR:HG21	1.53	0.72
1:A:109:THR:HG22	1:A:116:LEU:HG	1.70	0.72
1:C:269:GLY:H	1:C:287:THR:HG21	1.54	0.72
1:C:115:CYS:HB2	1:D:110:CYS:SG	2.31	0.69
1:B:109:THR:HG22	1:B:116:LEU:HG	1.72	0.69
1:C:110:CYS:SG	1:D:115:CYS:HB2	2.33	0.68
1:D:110:CYS:HB3	1:D:116:LEU:H	1.57	0.68
1:C:372:TRP:H	3:C:550:HEM:HAB	1.59	0.67
1:B:83:ARG:HB3	1:B:102:HIS:CE1	2.29	0.67
1:D:83:ARG:HB3	1:D:102:HIS:CE1	2.28	0.67
1:A:372:TRP:H	3:A:550:HEM:HAB	1.59	0.66
1:D:372:TRP:H	3:D:550:HEM:HAB	1.59	0.66
1:B:110:CYS:HB3	1:B:116:LEU:H	1.61	0.66
1:A:110:CYS:HB3	1:A:116:LEU:H	1.62	0.65
1:C:83:ARG:HB3	1:C:102:HIS:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HB3	1:A:102:HIS:CE1	2.31	0.65
1:B:372:TRP:H	3:B:550:HEM:HAB	1.62	0.65
1:B:155:LYS:H	1:B:155:LYS:HD3	1.63	0.62
1:B:354:ASN:HD22	1:B:354:ASN:H	1.48	0.61
1:D:155:LYS:H	1:D:155:LYS:HD3	1.66	0.61
1:A:354:ASN:H	1:A:354:ASN:HD22	1.49	0.61
1:C:354:ASN:H	1:C:354:ASN:HD22	1.47	0.61
1:C:414:ALA:O	1:C:418:ILE:HG13	2.01	0.61
1:C:110:CYS:HB3	1:C:116:LEU:H	1.65	0.60
1:D:354:ASN:HD22	1:D:354:ASN:H	1.49	0.59
1:C:110:CYS:HB2	1:C:115:CYS:HA	1.84	0.59
1:B:412:ASP:O	1:B:415:VAL:HG12	2.03	0.59
1:C:155:LYS:H	1:C:155:LYS:HD3	1.68	0.59
1:B:219:THR:HG23	1:B:222:GLU:H	1.68	0.59
1:C:219:THR:HG23	1:C:222:GLU:H	1.67	0.59
1:A:155:LYS:H	1:A:155:LYS:HD3	1.66	0.58
1:A:380:VAL:HG11	1:A:467:PRO:HB2	1.86	0.58
1:A:219:THR:HG23	1:A:222:GLU:H	1.69	0.57
1:C:380:VAL:HG11	1:C:467:PRO:HB2	1.85	0.57
1:C:354:ASN:HD22	1:C:354:ASN:N	2.03	0.57
1:C:110:CYS:HA	1:C:116:LEU:HD23	1.87	0.56
1:D:380:VAL:HG11	1:D:467:PRO:HB2	1.88	0.56
1:B:380:VAL:HG11	1:B:467:PRO:HB2	1.88	0.56
1:B:135:PRO:HB2	1:B:138:GLU:HG2	1.88	0.56
1:C:135:PRO:HB2	1:C:138:GLU:HG2	1.88	0.56
1:B:414:ALA:O	1:B:418:ILE:HG13	2.07	0.55
1:C:263:GLN:HA	1:C:351:ALA:O	2.07	0.55
1:C:412:ASP:O	1:C:415:VAL:HG12	2.07	0.55
1:A:414:ALA:O	1:A:418:ILE:HG13	2.07	0.55
1:A:412:ASP:O	1:A:415:VAL:HG12	2.06	0.54
1:B:263:GLN:HA	1:B:351:ALA:O	2.07	0.54
1:A:110:CYS:HB2	1:A:115:CYS:HA	1.89	0.54
1:C:279:GLY:O	1:C:281:PRO:HD3	2.08	0.54
1:D:219:THR:HG23	1:D:222:GLU:H	1.72	0.54
1:B:283:ASN:O	1:B:287:THR:HG23	2.08	0.54
1:B:354:ASN:HD22	1:B:354:ASN:N	2.04	0.53
1:B:110:CYS:HB2	1:B:115:CYS:HA	1.89	0.53
1:A:354:ASN:HD22	1:A:354:ASN:N	2.06	0.53
1:D:110:CYS:HB3	1:D:116:LEU:N	2.22	0.53
1:C:110:CYS:CB	1:C:116:LEU:H	2.21	0.53
1:C:283:ASN:O	1:C:287:THR:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ASN:HD22	1:D:354:ASN:N	2.07	0.52
1:A:135:PRO:HB2	1:A:138:GLU:HG2	1.91	0.52
1:A:263:GLN:HA	1:A:351:ALA:O	2.09	0.52
1:D:143:ALA:O	1:D:147:VAL:HG23	2.08	0.52
1:B:111:ARG:HG3	1:B:113:LYS:HG2	1.92	0.52
1:D:263:GLN:HA	1:D:351:ALA:O	2.10	0.52
1:D:412:ASP:O	1:D:415:VAL:HG12	2.09	0.52
1:D:110:CYS:CB	1:D:116:LEU:H	2.22	0.52
1:B:110:CYS:HA	1:B:116:LEU:HD23	1.92	0.52
1:D:110:CYS:HB2	1:D:115:CYS:HA	1.91	0.52
1:D:465:VAL:HG22	1:D:475:VAL:HG23	1.92	0.51
1:A:110:CYS:HA	1:A:116:LEU:HD23	1.92	0.51
1:C:119:ILE:HB	1:C:122:PRO:HG3	1.92	0.51
1:C:193:ALA:HB2	1:C:487:PRO:HB2	1.92	0.51
1:D:117:GLY:O	1:D:118:SER:CB	2.59	0.51
1:A:110:CYS:CB	1:A:116:LEU:H	2.23	0.51
1:A:111:ARG:HG3	1:A:113:LYS:HG2	1.93	0.51
1:C:486:SER:HA	1:C:487:PRO:C	2.36	0.51
1:A:111:ARG:C	1:B:111:ARG:HA	2.36	0.51
1:B:110:CYS:CB	1:B:116:LEU:H	2.23	0.50
1:B:281:PRO:HB2	1:B:387:GLN:O	2.11	0.50
1:A:143:ALA:O	1:A:147:VAL:HG23	2.11	0.50
1:A:283:ASN:O	1:A:287:THR:HG23	2.11	0.50
1:A:117:GLY:O	1:A:118:SER:CB	2.59	0.50
1:D:135:PRO:HB2	1:D:138:GLU:HG2	1.93	0.50
1:B:110:CYS:HB3	1:B:116:LEU:N	2.26	0.49
1:B:452:ARG:NH1	1:B:452:ARG:HG2	2.27	0.49
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.47	0.49
1:D:356:LEU:HB2	1:D:492:GLN:CD	2.37	0.49
1:B:117:GLY:O	1:B:118:SER:CB	2.60	0.49
1:A:110:CYS:HB3	1:A:116:LEU:N	2.27	0.49
1:C:117:GLY:O	1:C:118:SER:CB	2.61	0.49
1:A:193:ALA:HB2	1:A:487:PRO:HB2	1.94	0.48
1:C:143:ALA:O	1:C:147:VAL:HG23	2.12	0.48
1:D:193:ALA:HB2	1:D:487:PRO:HB2	1.95	0.48
1:A:111:ARG:HA	1:B:111:ARG:C	2.37	0.48
1:A:119:ILE:HB	1:A:122:PRO:HG3	1.96	0.48
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.48	0.48
1:C:105:LYS:HG3	1:C:107:ILE:HG12	1.96	0.48
1:D:162:HIS:O	1:D:166:VAL:HG23	2.14	0.48
1:D:110:CYS:HA	1:D:116:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:GLU:O	1:C:381:ARG:HB2	2.14	0.48
1:D:111:ARG:HG3	1:D:113:LYS:HG2	1.95	0.48
1:C:111:ARG:HG3	1:C:113:LYS:HG2	1.94	0.47
1:A:466:PRO:HA	1:A:467:PRO:HD3	1.78	0.47
1:B:298:LYS:HB2	1:B:303:ASP:OD2	2.14	0.47
1:D:140:LEU:O	1:D:144:ILE:HG12	2.14	0.47
1:A:471:SER:HB2	1:B:467:PRO:HB3	1.95	0.47
1:B:486:SER:HA	1:B:487:PRO:C	2.39	0.47
1:C:452:ARG:NH1	1:C:452:ARG:HG2	2.30	0.47
1:A:105:LYS:HG3	1:A:107:ILE:HG12	1.96	0.47
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.50	0.47
1:C:356:LEU:HB2	1:C:492:GLN:CD	2.39	0.47
1:D:283:ASN:O	1:D:287:THR:HG23	2.15	0.47
1:D:298:LYS:HB2	1:D:303:ASP:OD2	2.14	0.47
1:A:281:PRO:HB2	1:A:387:GLN:O	2.14	0.47
1:D:105:LYS:HG3	1:D:107:ILE:HG12	1.95	0.47
1:A:162:HIS:O	1:A:166:VAL:HG23	2.15	0.46
1:A:452:ARG:NH1	1:A:452:ARG:HG2	2.30	0.46
1:A:486:SER:HA	1:A:487:PRO:C	2.40	0.46
1:B:84:HIS:HB3	1:B:97:GLN:NE2	2.31	0.46
1:B:87:ILE:HG13	1:B:96:PHE:HB2	1.98	0.46
1:B:193:ALA:HB2	1:B:487:PRO:HB2	1.97	0.46
1:D:219:THR:HG22	1:D:222:GLU:HG3	1.97	0.46
1:A:356:LEU:HB2	1:A:492:GLN:CD	2.41	0.46
1:D:414:ALA:O	1:D:418:ILE:HG13	2.15	0.46
1:B:380:VAL:O	1:B:384:CYS:HB2	2.16	0.46
1:B:424:HIS:HA	1:B:427:GLN:HE21	1.80	0.46
1:D:130:ARG:HG2	1:D:250:ARG:HD3	1.98	0.46
1:A:219:THR:HG22	1:A:222:GLU:HG3	1.97	0.46
1:A:281:PRO:O	1:A:284:VAL:HG23	2.15	0.46
1:B:143:ALA:O	1:B:147:VAL:HG23	2.15	0.46
1:C:110:CYS:HB3	1:C:116:LEU:N	2.30	0.46
1:D:424:HIS:HA	1:D:427:GLN:HE21	1.81	0.46
1:A:84:HIS:HB3	1:A:97:GLN:NE2	2.31	0.46
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.50	0.46
1:A:465:VAL:HG22	1:A:475:VAL:HG23	1.98	0.46
1:C:413:GLN:HG3	1:D:416:VAL:HG11	1.98	0.46
1:D:115:CYS:C	1:D:117:GLY:H	2.25	0.46
1:C:336:TYR:N	1:C:336:TYR:CD1	2.84	0.45
1:A:140:LEU:O	1:A:144:ILE:HG12	2.16	0.45
1:B:130:ARG:HG2	1:B:250:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ILE:HG13	1:C:368:PRO:O	2.16	0.45
1:B:338:TRP:O	1:B:341:GLU:HB2	2.16	0.45
1:D:119:ILE:HB	1:D:122:PRO:HG3	1.97	0.45
1:B:281:PRO:O	1:B:284:VAL:HG23	2.17	0.45
1:A:322:PRO:HA	1:A:323:PRO:HD2	1.80	0.45
1:A:377:GLU:O	1:A:381:ARG:HB2	2.16	0.45
1:D:84:HIS:HB3	1:D:97:GLN:NE2	2.32	0.45
1:D:309:LEU:O	1:D:316:PRO:HA	2.16	0.45
1:C:115:CYS:C	1:C:117:GLY:H	2.25	0.45
1:A:115:CYS:C	1:A:117:GLY:H	2.25	0.45
1:B:249:GLN:HB3	1:B:364:PHE:CE2	2.52	0.45
1:D:279:GLY:O	1:D:281:PRO:HD3	2.16	0.45
1:A:380:VAL:O	1:A:384:CYS:HB2	2.17	0.44
1:B:100:LEU:CB	1:B:456:GLY:HA3	2.47	0.44
1:B:119:ILE:HB	1:B:122:PRO:HG3	1.98	0.44
1:C:471:SER:HB2	1:D:467:PRO:HB3	2.00	0.44
1:D:380:VAL:O	1:D:384:CYS:HB2	2.18	0.44
1:A:87:ILE:HG13	1:A:96:PHE:HB2	1.98	0.44
1:C:130:ARG:HG2	1:C:250:ARG:HD3	1.99	0.44
1:B:107:ILE:HG13	1:B:107:ILE:O	2.17	0.44
1:B:107:ILE:C	1:B:108:LEU:HD12	2.43	0.44
1:A:130:ARG:HG2	1:A:250:ARG:HD3	1.99	0.44
1:C:84:HIS:HB3	1:C:97:GLN:NE2	2.32	0.44
1:D:87:ILE:HG13	1:D:96:PHE:HB2	1.98	0.44
1:D:423:LEU:O	1:D:427:GLN:HG3	2.18	0.44
1:A:108:LEU:HD13	1:B:113:LYS:HA	2.00	0.44
1:B:472:ILE:O	1:B:472:ILE:HG22	2.18	0.44
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.98	0.44
1:B:115:CYS:C	1:B:117:GLY:H	2.25	0.44
1:B:140:LEU:HB3	1:B:141:PRO:HD3	2.00	0.44
1:B:310:GLN:HG3	1:B:314:ARG:O	2.18	0.44
1:B:465:VAL:HG22	1:B:475:VAL:HG23	2.00	0.44
1:D:254:LYS:O	1:D:313:GLY:HA3	2.18	0.44
1:D:377:GLU:O	1:D:381:ARG:HB2	2.18	0.44
1:A:279:GLY:O	1:A:281:PRO:HD3	2.17	0.43
1:A:333:HIS:NE2	1:A:417:GLU:HG3	2.33	0.43
1:D:281:PRO:O	1:D:284:VAL:HG23	2.18	0.43
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.34	0.43
1:A:310:GLN:HG3	1:A:314:ARG:O	2.18	0.43
1:B:219:THR:HG22	1:B:222:GLU:HG3	2.00	0.43
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PRO:HB2	1:C:387:GLN:O	2.18	0.43
1:D:249:GLN:HB3	1:D:364:PHE:CE2	2.52	0.43
1:A:298:LYS:HB2	1:A:303:ASP:OD2	2.18	0.43
1:C:322:PRO:HA	1:C:323:PRO:HD2	1.83	0.43
1:D:247:PHE:HB3	1:D:248:PRO:HD2	2.01	0.43
1:D:338:TRP:O	1:D:341:GLU:HB2	2.18	0.43
1:D:486:SER:HA	1:D:487:PRO:C	2.44	0.43
1:A:111:ARG:HA	1:B:111:ARG:HA	2.00	0.43
1:B:170:THR:O	1:B:174:GLU:HG2	2.18	0.43
1:C:219:THR:HG22	1:C:222:GLU:HG3	2.00	0.43
1:B:105:LYS:HG3	1:B:107:ILE:HG12	1.99	0.43
1:B:162:HIS:O	1:B:166:VAL:HG23	2.18	0.43
1:B:279:GLY:O	1:B:281:PRO:HD3	2.18	0.43
1:C:281:PRO:O	1:C:284:VAL:HG23	2.19	0.43
1:A:100:LEU:HB3	1:A:456:GLY:HA3	2.00	0.43
1:C:107:ILE:O	1:C:107:ILE:HG13	2.19	0.43
1:D:307:LEU:HG	1:D:309:LEU:HD11	2.01	0.43
1:A:338:TRP:O	1:A:341:GLU:HB2	2.19	0.43
1:D:107:ILE:C	1:D:108:LEU:HD12	2.44	0.43
1:A:236:ASN:ND2	2:A:930:SO4:O2	2.51	0.42
1:A:333:HIS:HE2	1:A:417:GLU:HG3	1.83	0.42
1:C:333:HIS:NE2	1:C:417:GLU:HG3	2.34	0.42
1:D:135:PRO:HA	1:D:136:PRO:HD3	1.92	0.42
1:C:310:GLN:HG3	1:C:314:ARG:O	2.19	0.42
1:A:100:LEU:CB	1:A:456:GLY:HA3	2.49	0.42
1:D:100:LEU:CB	1:D:456:GLY:HA3	2.49	0.42
1:B:309:LEU:O	1:B:316:PRO:HA	2.19	0.42
1:B:333:HIS:CG	1:B:334:PRO:HD2	2.54	0.42
1:D:465:VAL:HA	1:D:466:PRO:HD3	1.88	0.42
1:A:249:GLN:HB3	1:A:364:PHE:CE2	2.55	0.42
1:B:155:LYS:H	1:B:155:LYS:CD	2.25	0.42
1:B:356:LEU:HB2	1:B:492:GLN:CD	2.44	0.42
1:D:281:PRO:HB2	1:D:387:GLN:O	2.20	0.42
1:D:459:ALA:HB3	1:D:480:MET:HB2	2.01	0.42
1:B:254:LYS:O	1:B:313:GLY:HA3	2.19	0.42
1:B:333:HIS:NE2	1:B:417:GLU:HG3	2.35	0.42
1:C:162:HIS:O	1:C:166:VAL:HG23	2.20	0.42
1:C:309:LEU:O	1:C:316:PRO:HA	2.20	0.42
1:C:333:HIS:HE2	1:C:417:GLU:HG3	1.84	0.42
1:A:214:ALA:O	1:A:248:PRO:HD3	2.20	0.42
1:A:424:HIS:HA	1:A:427:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:HG13	1:C:96:PHE:HB2	2.00	0.42
1:D:333:HIS:NE2	1:D:417:GLU:HG3	2.35	0.42
1:A:465:VAL:HA	1:A:466:PRO:HD3	1.87	0.42
1:C:165:ARG:O	1:C:169:VAL:HG23	2.19	0.42
1:C:423:LEU:O	1:C:427:GLN:HG3	2.20	0.42
1:A:107:ILE:HG13	1:A:107:ILE:O	2.20	0.42
1:A:107:ILE:C	1:A:108:LEU:HD12	2.44	0.42
1:A:254:LYS:O	1:A:313:GLY:HA3	2.20	0.42
1:C:236:ASN:HB3	1:C:239:ASN:O	2.20	0.42
1:D:171:LYS:O	1:D:175:THR:HG23	2.20	0.42
1:D:310:GLN:HG3	1:D:314:ARG:O	2.19	0.42
1:C:416:VAL:HG11	1:D:413:GLN:HG3	2.00	0.41
1:C:472:ILE:HG22	1:C:472:ILE:O	2.20	0.41
1:D:472:ILE:O	1:D:472:ILE:HG22	2.19	0.41
1:A:374:MET:HE3	1:A:376:THR:OG1	2.19	0.41
1:D:100:LEU:HB3	1:D:456:GLY:HA3	2.01	0.41
1:A:472:ILE:HG22	1:A:472:ILE:O	2.19	0.41
1:B:374:MET:HE3	1:B:376:THR:OG1	2.20	0.41
1:B:377:GLU:O	1:B:381:ARG:HB2	2.21	0.41
1:D:155:LYS:H	1:D:155:LYS:CD	2.29	0.41
1:B:200:CYS:HB2	3:B:550:HEM:ND	2.36	0.41
1:A:236:ASN:HB3	1:A:239:ASN:O	2.20	0.41
1:B:247:PHE:HB3	1:B:248:PRO:HD2	2.02	0.41
1:A:374:MET:O	1:A:375:GLY:C	2.64	0.41
1:B:466:PRO:HA	1:B:467:PRO:HD3	1.76	0.41
1:A:170:THR:O	1:A:174:GLU:HG2	2.20	0.41
1:A:374:MET:HA	1:A:434:MET:O	2.21	0.41
1:A:471:SER:CB	1:B:467:PRO:HB3	2.51	0.41
1:C:100:LEU:HB3	1:C:456:GLY:HA3	2.03	0.41
1:C:107:ILE:C	1:C:108:LEU:HD12	2.46	0.41
1:C:109:THR:O	1:C:116:LEU:HG	2.21	0.41
1:C:338:TRP:O	1:C:341:GLU:HB2	2.21	0.41
1:C:424:HIS:HA	1:C:427:GLN:HE21	1.86	0.41
1:C:465:VAL:HG22	1:C:475:VAL:HG23	2.02	0.41
1:C:466:PRO:HA	1:C:467:PRO:HD3	1.79	0.41
1:D:214:ALA:O	1:D:248:PRO:HD3	2.20	0.41
1:B:374:MET:HA	1:B:434:MET:O	2.20	0.41
1:D:296:LYS:HA	1:D:297:PRO:HD2	1.91	0.41
1:D:333:HIS:HE2	1:D:417:GLU:HG3	1.86	0.40
1:A:309:LEU:O	1:A:316:PRO:HA	2.20	0.40
1:B:165:ARG:O	1:B:169:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ILE:HG13	1:D:368:PRO:O	2.21	0.40
1:C:298:LYS:HB2	1:C:303:ASP:OD2	2.21	0.40
1:C:336:TYR:CE2	1:C:417:GLU:HG2	2.56	0.40
1:D:433:ILE:HG13	1:D:434:MET:N	2.36	0.40
1:D:466:PRO:HA	1:D:467:PRO:HD3	1.77	0.40
1:C:122:PRO:HD2	1:C:125:LEU:HD12	2.03	0.40
1:D:107:ILE:O	1:D:107:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

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	418/431 (97%)	392 (94%)	21 (5%)	5 (1%)	10	40
1	B	418/431 (97%)	387 (93%)	26 (6%)	5 (1%)	10	40
1	C	418/431 (97%)	389 (93%)	24 (6%)	5 (1%)	10	40
1	D	418/431 (97%)	390 (93%)	23 (6%)	5 (1%)	10	40
All	All	1672/1724 (97%)	1558 (93%)	94 (6%)	20 (1%)	10	40

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	B	118	SER
1	C	118	SER
1	D	118	SER
1	A	114	SER
1	A	390	ASN
1	B	114	SER
1	B	390	ASN

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Mol	Chain	Res	Type
1	C	114	SER
1	D	114	SER
1	D	390	ASN
1	A	113	LYS
1	B	113	LYS
1	C	113	LYS
1	C	390	ASN
1	D	113	LYS
1	C	375	GLY
1	A	375	GLY
1	D	375	GLY
1	B	375	GLY

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	366/376 (97%)	354 (97%)	12 (3%)	33	67
1	B	366/376 (97%)	354 (97%)	12 (3%)	33	67
1	C	366/376 (97%)	354 (97%)	12 (3%)	33	67
1	D	366/376 (97%)	354 (97%)	12 (3%)	33	67
All	All	1464/1504 (97%)	1416 (97%)	48 (3%)	33	67

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	123	LYS
1	A	145	GLU
1	A	155	LYS
1	A	156	GLU
1	A	167	GLU
1	A	288	GLN
1	A	307	LEU
1	A	309	LEU

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Mol	Chain	Res	Type
1	A	354	ASN
1	A	395	VAL
1	A	417	GLU
1	B	121	THR
1	B	123	LYS
1	B	145	GLU
1	B	155	LYS
1	B	156	GLU
1	B	167	GLU
1	B	288	GLN
1	B	307	LEU
1	B	309	LEU
1	B	312	ASN
1	B	354	ASN
1	B	395	VAL
1	C	121	THR
1	C	123	LYS
1	C	145	GLU
1	C	155	LYS
1	C	156	GLU
1	C	167	GLU
1	C	288	GLN
1	C	307	LEU
1	C	309	LEU
1	C	354	ASN
1	C	395	VAL
1	C	417	GLU
1	D	121	THR
1	D	123	LYS
1	D	145	GLU
1	D	155	LYS
1	D	156	GLU
1	D	167	GLU
1	D	288	GLN
1	D	307	LEU
1	D	309	LEU
1	D	354	ASN
1	D	395	VAL
1	D	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	102	HIS
1	A	142	GLN
1	A	192	GLN
1	A	205	GLN
1	A	283	ASN
1	A	354	ASN
1	A	390	ASN
1	A	424	HIS
1	A	427	GLN
1	A	429	GLN
1	A	482	ASN
1	B	97	GLN
1	B	102	HIS
1	B	142	GLN
1	B	192	GLN
1	B	205	GLN
1	B	208	ASN
1	B	283	ASN
1	B	310	GLN
1	B	354	ASN
1	B	390	ASN
1	B	424	HIS
1	B	427	GLN
1	B	429	GLN
1	B	502	GLN
1	C	97	GLN
1	C	102	HIS
1	C	142	GLN
1	C	192	GLN
1	C	205	GLN
1	C	208	ASN
1	C	210	GLN
1	C	249	GLN
1	C	283	ASN
1	C	354	ASN
1	C	390	ASN
1	C	424	HIS
1	C	427	GLN
1	C	429	GLN
1	C	482	ASN
1	C	502	GLN
1	D	97	GLN

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Mol	Chain	Res	Type
1	D	102	HIS
1	D	142	GLN
1	D	192	GLN
1	D	205	GLN
1	D	283	ASN
1	D	354	ASN
1	D	390	ASN
1	D	424	HIS
1	D	427	GLN
1	D	429	GLN
1	D	482	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	922	-	4,4,4	0.72	0	6,6,6	0.34	0
4	H4B	A	600	-	17,18,18	1.34	2 (11%)	14,26,26	1.94	4 (28%)
2	SO4	B	911	-	4,4,4	0.80	0	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	923	-	4,4,4	0.76	0	6,6,6	0.36	0
3	HEM	B	550	1	50,50,50	1.21	3 (6%)	67,82,82	1.25	4 (5%)
2	SO4	B	921	-	4,4,4	0.74	0	6,6,6	0.44	0
2	SO4	A	920	-	4,4,4	0.76	0	6,6,6	0.38	0
4	H4B	D	603	-	17,18,18	1.30	2 (11%)	14,26,26	1.97	4 (28%)
2	SO4	A	930	-	4,4,4	0.71	0	6,6,6	0.33	0
2	SO4	D	913	-	4,4,4	0.80	0	6,6,6	0.36	0
4	H4B	C	602	-	17,18,18	1.31	2 (11%)	14,26,26	1.96	4 (28%)
5	ITU	B	801	-	4,5,5	1.11	0	3,5,5	2.77	1 (33%)
3	HEM	D	550	1	50,50,50	1.16	4 (8%)	67,82,82	1.03	2 (2%)
5	ITU	D	803	-	4,5,5	1.02	0	3,5,5	2.97	1 (33%)
2	SO4	C	912	-	4,4,4	0.76	0	6,6,6	0.41	0
3	HEM	C	550	1	50,50,50	1.24	4 (8%)	67,82,82	1.30	8 (11%)
4	H4B	B	601	-	17,18,18	1.34	2 (11%)	14,26,26	2.04	4 (28%)
3	HEM	A	550	1	50,50,50	1.10	3 (6%)	67,82,82	1.15	3 (4%)
5	ITU	A	800	-	4,5,5	0.81	0	3,5,5	3.37	1 (33%)
5	ITU	C	802	-	4,5,5	0.76	0	3,5,5	3.11	1 (33%)
2	SO4	A	910	-	4,4,4	0.85	0	6,6,6	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H4B	A	600	-	-	0/8/17/17	0/2/2/2
3	HEM	B	550	1	-	2/14/54/54	-
4	H4B	D	603	-	-	0/8/17/17	0/2/2/2
5	ITU	B	801	-	-	3/3/3/3	-
5	ITU	C	802	-	-	3/3/3/3	-
3	HEM	C	550	1	-	2/14/54/54	-
4	H4B	B	601	-	-	0/8/17/17	0/2/2/2
4	H4B	C	602	-	-	0/8/17/17	0/2/2/2
3	HEM	A	550	1	-	2/14/54/54	-
5	ITU	A	800	-	-	3/3/3/3	-
3	HEM	D	550	1	-	2/14/54/54	-
5	ITU	D	803	-	-	3/3/3/3	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	H4B	C4A-N5	3.56	1.46	1.37
4	A	600	H4B	C4A-N5	3.52	1.46	1.37
4	C	602	H4B	C4A-N5	3.45	1.46	1.37
4	B	601	H4B	C4A-N5	3.35	1.45	1.37
4	B	601	H4B	C6-N5	3.30	1.53	1.47
3	D	550	HEM	CAB-C3B	-3.27	1.38	1.47
3	B	550	HEM	CAB-C3B	-3.19	1.38	1.47
4	A	600	H4B	C6-N5	3.16	1.53	1.47
3	C	550	HEM	CAB-C3B	-3.13	1.39	1.47
4	C	602	H4B	C6-N5	3.02	1.52	1.47
3	A	550	HEM	CAB-C3B	-2.93	1.39	1.47
3	A	550	HEM	CAC-C3C	-2.90	1.39	1.47
3	B	550	HEM	CAC-C3C	-2.89	1.39	1.47
4	D	603	H4B	C6-N5	2.85	1.52	1.47
3	C	550	HEM	C2A-C3A	-2.53	1.32	1.38
3	C	550	HEM	CAC-C3C	-2.53	1.40	1.47
3	C	550	HEM	C4D-ND	-2.53	1.35	1.40
3	D	550	HEM	CAC-C3C	-2.47	1.40	1.47
3	D	550	HEM	FE-NB	2.20	2.01	1.94
3	B	550	HEM	C2A-C3A	-2.14	1.33	1.38
3	D	550	HEM	C2A-C3A	-2.12	1.33	1.38
3	A	550	HEM	C2A-C3A	-2.09	1.33	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	ITU	C2-S-C3	5.83	109.21	103.15
5	C	802	ITU	C2-S-C3	5.37	108.74	103.15
5	D	803	ITU	C2-S-C3	5.13	108.48	103.15
4	C	602	H4B	C2-N1-C8A	5.07	122.31	113.36
4	D	603	H4B	C2-N1-C8A	4.91	122.02	113.36
4	A	600	H4B	C2-N1-C8A	4.90	122.01	113.36
4	B	601	H4B	C2-N1-C8A	4.89	121.99	113.36
5	B	801	ITU	C2-S-C3	4.79	108.13	103.15
3	B	550	HEM	C3B-C4B-NB	4.09	112.41	109.47
4	B	601	H4B	O10-C10-C9	-3.72	103.61	109.77
3	C	550	HEM	C3B-C4B-NB	3.38	111.90	109.47
3	A	550	HEM	C3B-C4B-NB	3.20	111.77	109.47
4	D	603	H4B	O10-C10-C9	-3.17	104.53	109.77
4	A	600	H4B	O10-C10-C9	-3.09	104.66	109.77
4	D	603	H4B	N3-C2-N1	-2.82	118.16	123.32
4	C	602	H4B	O10-C10-C9	-2.76	105.19	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	H4B	O9-C9-C6	2.76	115.89	109.28
4	C	602	H4B	N3-C2-N1	-2.75	118.29	123.32
4	A	600	H4B	N3-C2-N1	-2.65	118.47	123.32
4	B	601	H4B	N3-C2-N1	-2.63	118.51	123.32
4	C	602	H4B	O9-C9-C6	2.61	115.53	109.28
4	D	603	H4B	O9-C9-C6	2.60	115.51	109.28
3	D	550	HEM	C3B-C4B-NB	2.58	111.32	109.47
3	C	550	HEM	CBD-CAD-C3D	-2.57	105.42	112.53
4	A	600	H4B	O9-C9-C6	2.52	115.32	109.28
3	D	550	HEM	CBD-CAD-C3D	-2.44	105.80	112.53
3	A	550	HEM	CBD-CAD-C3D	-2.41	105.87	112.53
3	C	550	HEM	C2D-C1D-ND	2.36	112.63	109.90
3	C	550	HEM	C2B-C1B-NB	2.29	112.47	109.84
3	C	550	HEM	C4C-C3C-C2C	-2.27	104.84	106.81
3	C	550	HEM	CHD-C4C-C3C	-2.20	121.50	125.21
3	B	550	HEM	CBD-CAD-C3D	-2.19	106.47	112.53
3	C	550	HEM	CAD-C3D-C4D	2.19	128.51	124.70
3	B	550	HEM	CAA-C2A-C1A	2.13	129.11	124.94
3	B	550	HEM	CMD-C2D-C1D	2.08	128.29	125.03
3	A	550	HEM	C2D-C1D-ND	2.01	112.23	109.90
3	C	550	HEM	CAD-C3D-C2D	-2.00	124.12	127.87

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	550	HEM	C2B-C3B-CAB-CBB
3	B	550	HEM	C2B-C3B-CAB-CBB
3	C	550	HEM	C2B-C3B-CAB-CBB
3	D	550	HEM	C2B-C3B-CAB-CBB
3	B	550	HEM	C4B-C3B-CAB-CBB
5	A	800	ITU	N1-C3-S-C2
5	B	801	ITU	N1-C3-S-C2
5	C	802	ITU	N1-C3-S-C2
5	D	803	ITU	N1-C3-S-C2
3	A	550	HEM	C4B-C3B-CAB-CBB
3	C	550	HEM	C4B-C3B-CAB-CBB
3	D	550	HEM	C4B-C3B-CAB-CBB
5	A	800	ITU	N2-C3-S-C2
5	B	801	ITU	N2-C3-S-C2
5	C	802	ITU	N2-C3-S-C2
5	D	803	ITU	N2-C3-S-C2

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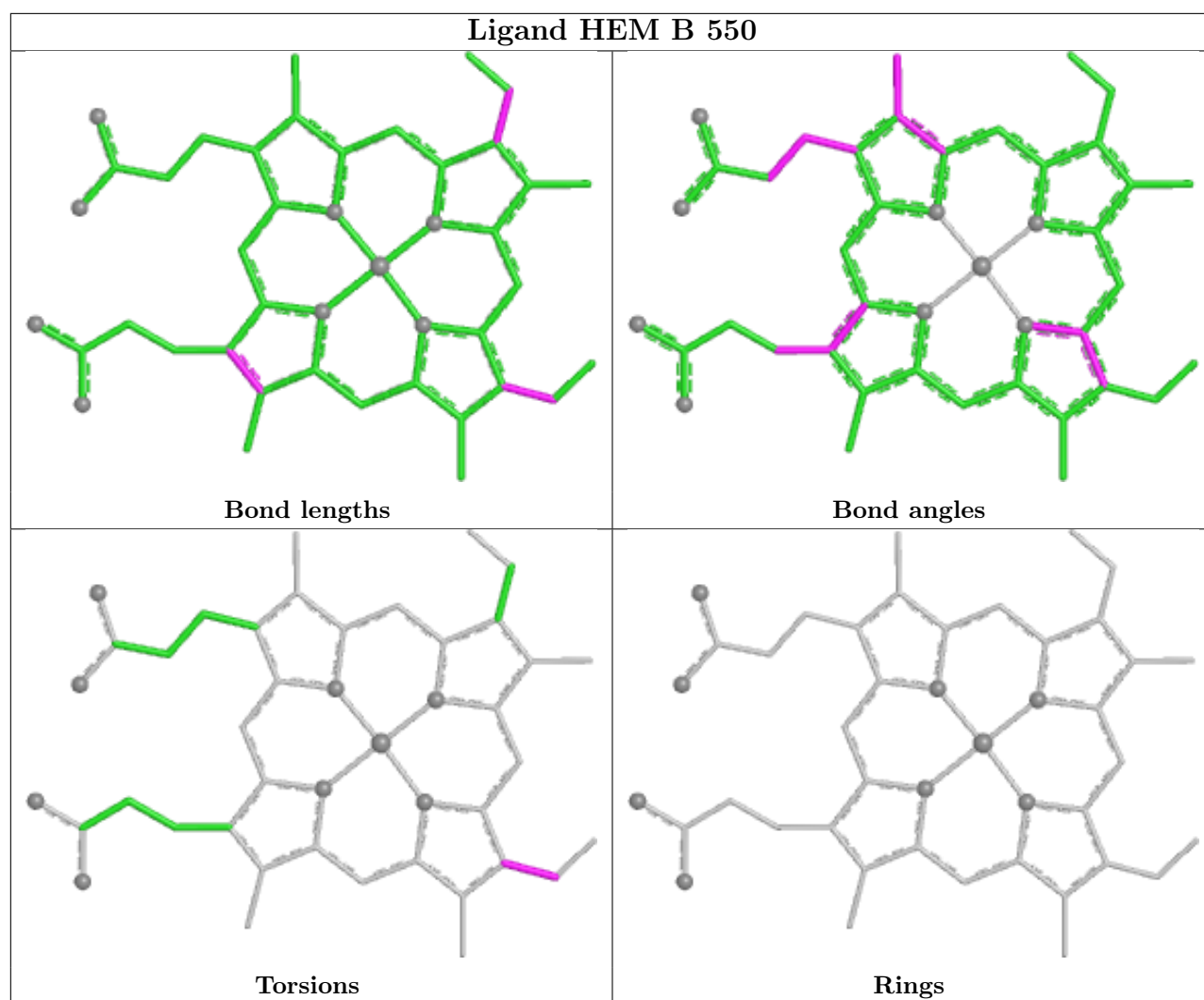
Mol	Chain	Res	Type	Atoms
5	C	802	ITU	C1-C2-S-C3
5	A	800	ITU	C1-C2-S-C3
5	B	801	ITU	C1-C2-S-C3
5	D	803	ITU	C1-C2-S-C3

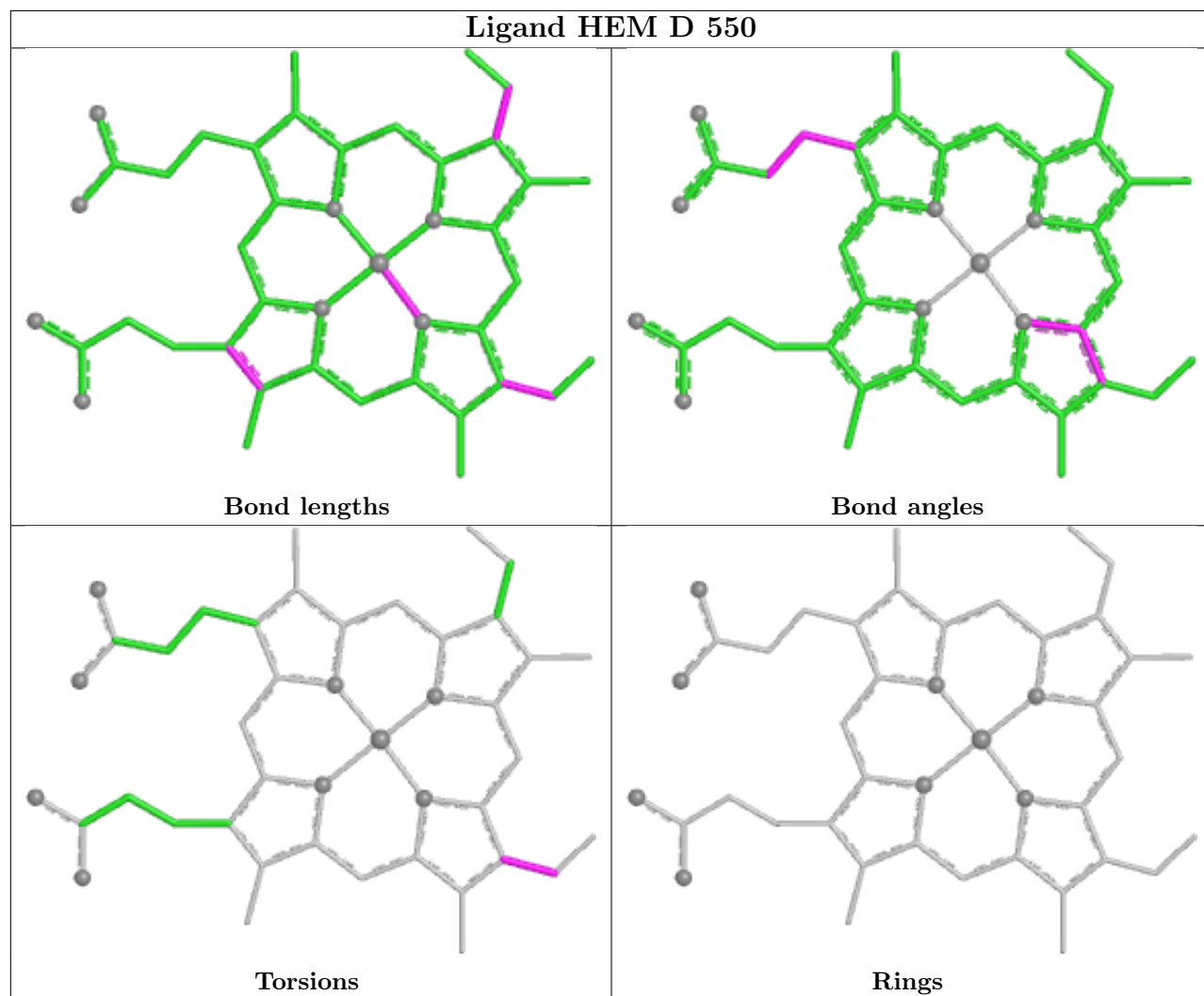
There are no ring outliers.

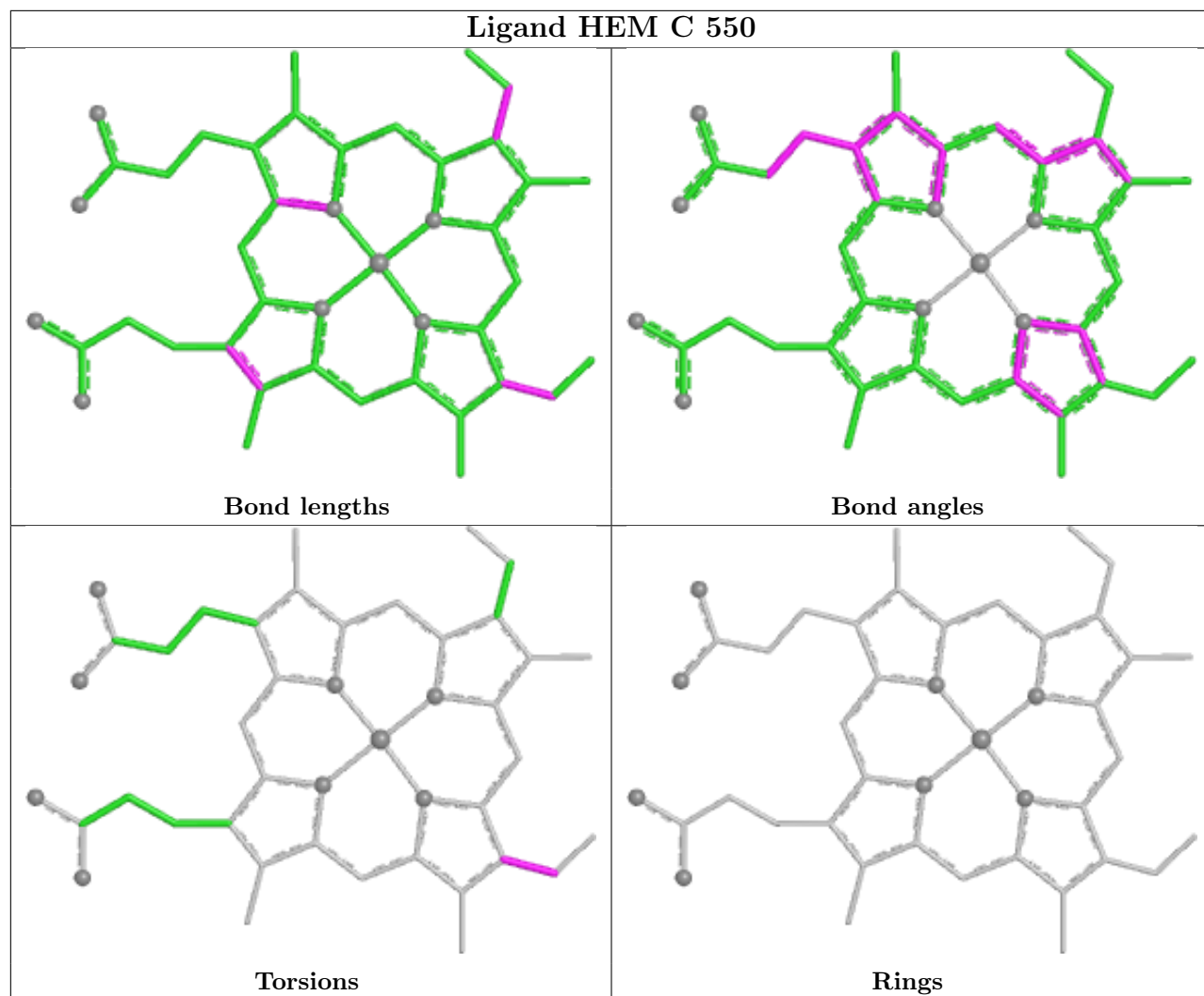
5 monomers are involved in 6 short contacts:

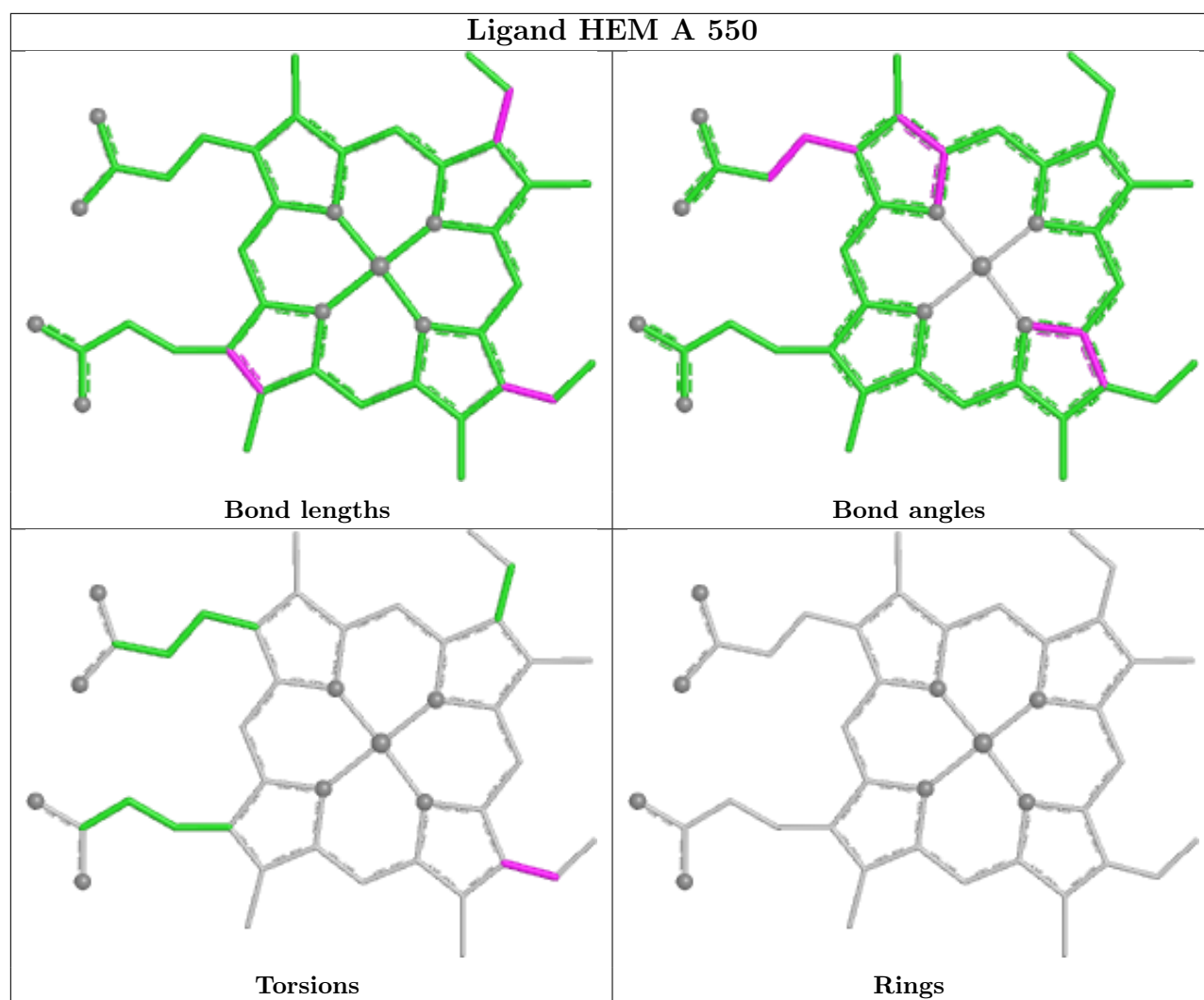
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	550	HEM	2	0
2	A	930	SO4	1	0
3	D	550	HEM	1	0
3	C	550	HEM	1	0
3	A	550	HEM	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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.