



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:29 AM UTC

PDB ID : 1Z10 / pdb_00001z10
Title : Crystal Structure of Human Microsomal P450 2A6 with Coumarin Bound
Authors : Yano, J.K.; Hsu, M.H.; Griffin, K.J.; Stout, C.D.; Johnson, E.F.
Deposited on : 2005-03-02
Resolution : 1.90 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

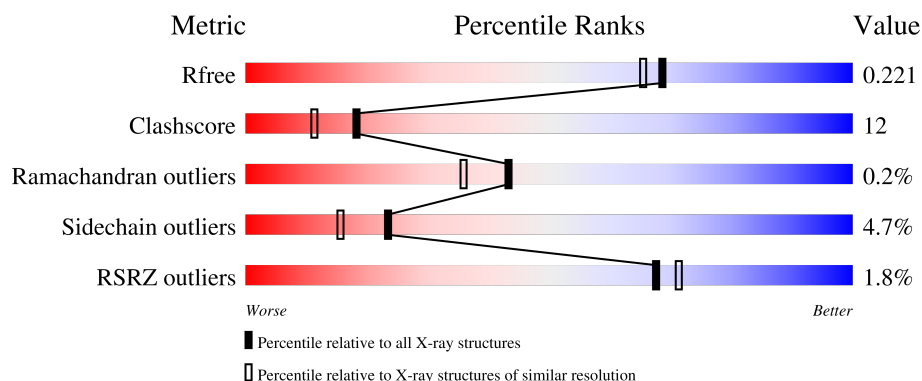
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	0% 75% 20% ..
1	B	476	3% 71% 22% ..
1	C	476	0% 73% 20% ..
1	D	476	2% 74% 20% ..

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
4	GOL	B	900	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16075 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 cytochrome P450, family 2, subfamily A, polypeptide 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3768	2420	651	679	18			
1	B	465	Total	C	N	O	S	0	0	0
			3767	2418	653	678	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

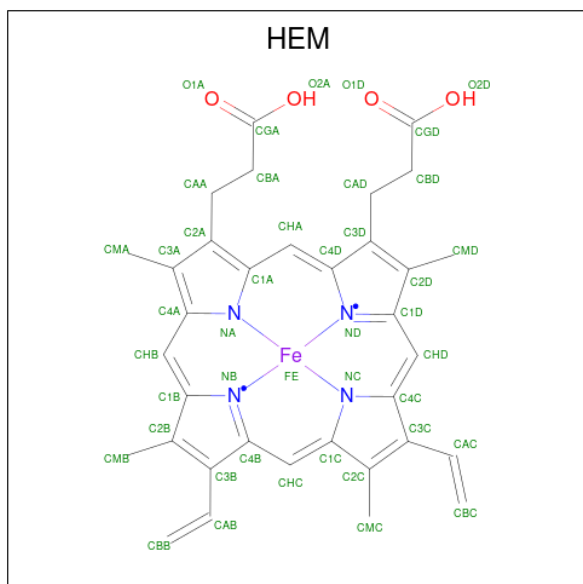
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P11509
A	24	ALA	-	SEE REMARK 999	UNP P11509
A	25	LYS	-	SEE REMARK 999	UNP P11509
A	26	LYS	-	SEE REMARK 999	UNP P11509
A	27	THR	-	SEE REMARK 999	UNP P11509
A	28	SER	-	SEE REMARK 999	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	SEE REMARK 999	UNP P11509
B	24	ALA	-	SEE REMARK 999	UNP P11509
B	25	LYS	-	SEE REMARK 999	UNP P11509
B	26	LYS	-	SEE REMARK 999	UNP P11509
B	27	THR	-	SEE REMARK 999	UNP P11509
B	28	SER	-	SEE REMARK 999	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	SEE REMARK 999	UNP P11509

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	SEE REMARK 999	UNP P11509
C	25	LYS	-	SEE REMARK 999	UNP P11509
C	26	LYS	-	SEE REMARK 999	UNP P11509
C	27	THR	-	SEE REMARK 999	UNP P11509
C	28	SER	-	SEE REMARK 999	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	SEE REMARK 999	UNP P11509
D	24	ALA	-	SEE REMARK 999	UNP P11509
D	25	LYS	-	SEE REMARK 999	UNP P11509
D	26	LYS	-	SEE REMARK 999	UNP P11509
D	27	THR	-	SEE REMARK 999	UNP P11509
D	28	SER	-	SEE REMARK 999	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



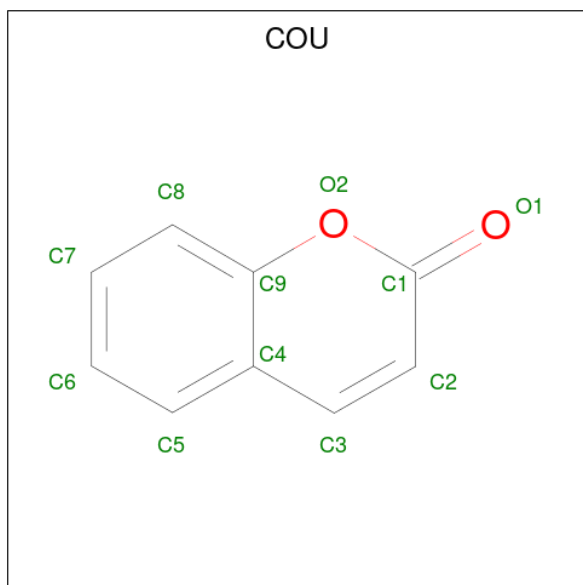
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is COUMARIN (CCD ID: COU) (formula: $C_9H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			11	9	2		
3	B	1	Total	C	O		
			11	9	2		
3	C	1	Total	C	O		
			11	9	2		
3	D	1	Total	C	O		
			11	9	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

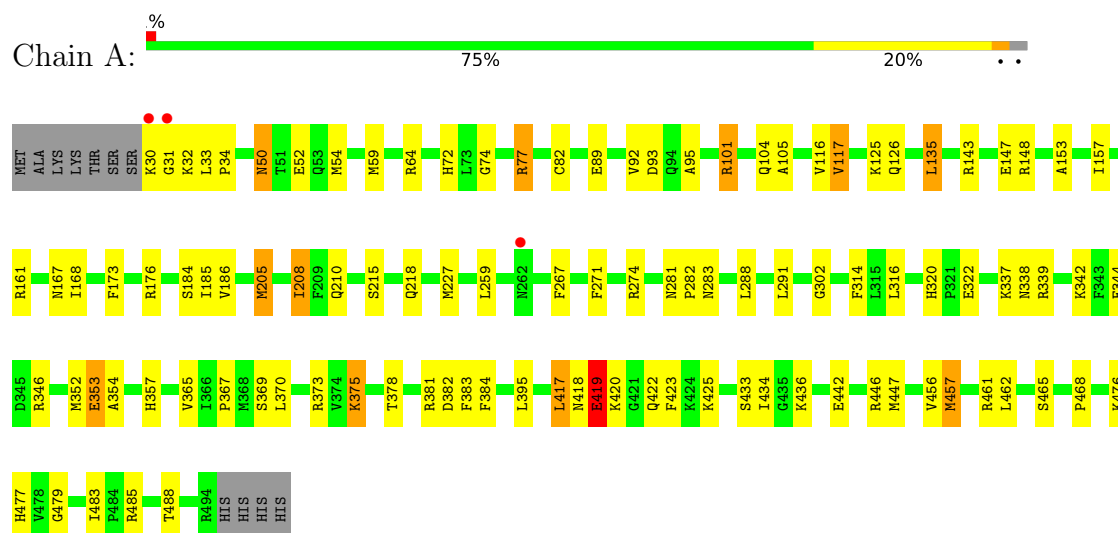
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	224	Total	O	0	0
			224	224		
5	B	140	Total	O	0	0
			140	140		
5	C	237	Total	O	0	0
			237	237		
5	D	215	Total	O	0	0
			215	215		

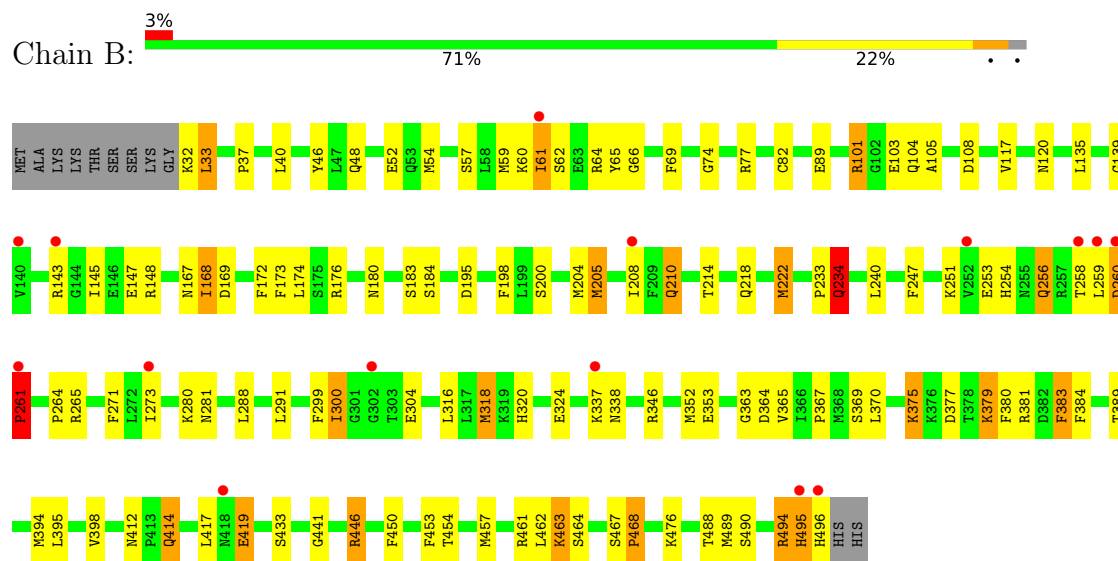
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

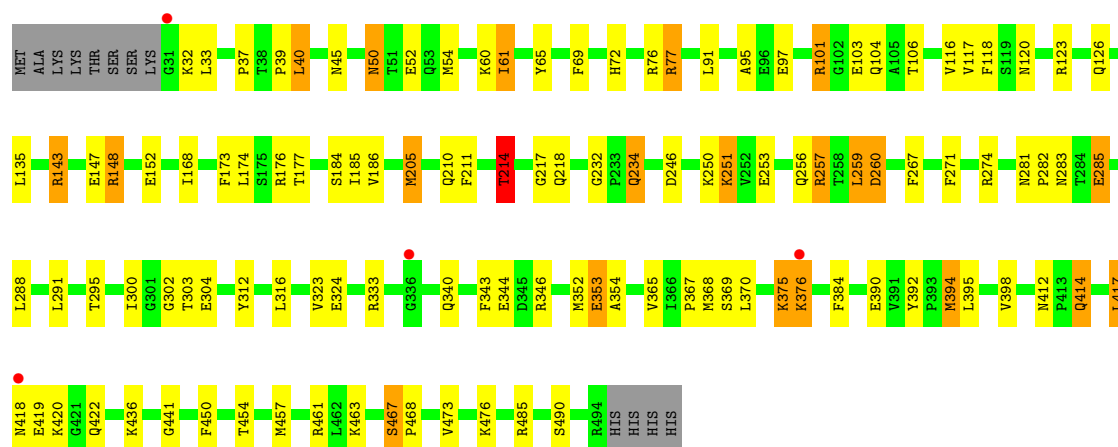


- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6

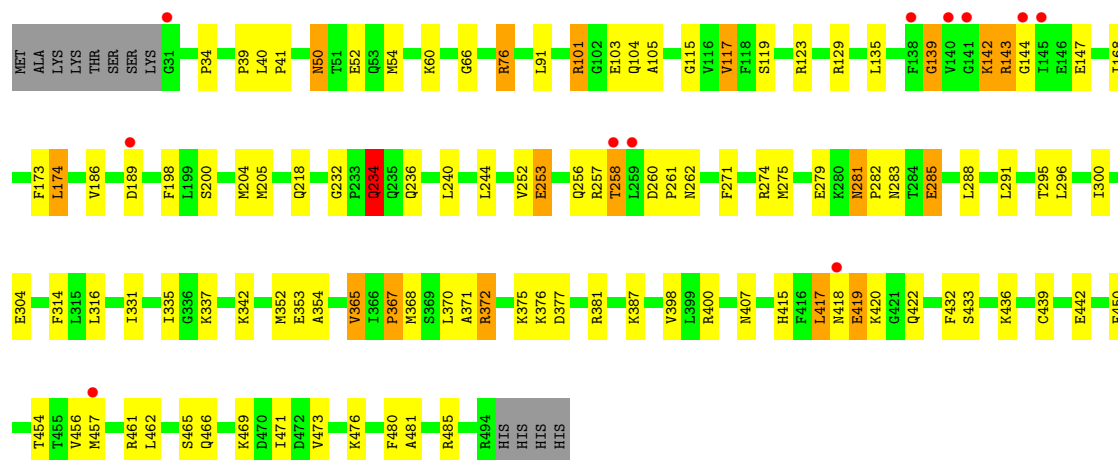
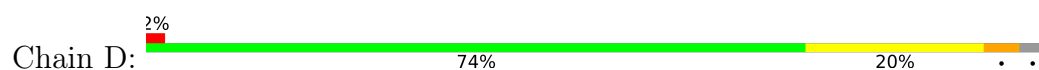


- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6





- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.61Å 157.59Å 103.54Å 90.00° 92.25° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-1.90) 92.9 (50.00-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.230 0.187 , 0.221	Depositor DCC
R_{free} test set	8756 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16075	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, COU, GOL

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	1.03	7/3859 (0.2%)	1.18	25/5197 (0.5%)
1	B	0.95	3/3860 (0.1%)	1.17	28/5200 (0.5%)
1	C	1.07	5/3842 (0.1%)	1.19	33/5175 (0.6%)
1	D	0.98	2/3842 (0.1%)	1.18	33/5175 (0.6%)
All	All	1.01	17/15403 (0.1%)	1.18	119/20747 (0.6%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	394	MET	SD-CE	-19.08	1.31	1.79
1	B	222	MET	SD-CE	-12.67	1.47	1.79
1	A	205	MET	SD-CE	-8.91	1.57	1.79
1	B	205	MET	SD-CE	-8.11	1.59	1.79
1	C	205	MET	SD-CE	-7.83	1.59	1.79
1	A	447	MET	SD-CE	7.57	1.98	1.79
1	D	368	MET	SD-CE	6.96	1.97	1.79
1	B	318	MET	SD-CE	-6.71	1.62	1.79
1	A	457	MET	SD-CE	-6.60	1.63	1.79
1	A	227	MET	SD-CE	-6.48	1.63	1.79
1	C	214	THR	CB-CG2	-6.04	1.32	1.52
1	D	34	PRO	CA-C	5.93	1.55	1.51
1	A	105	ALA	CA-CB	5.88	1.62	1.53
1	A	352	MET	SD-CE	-5.78	1.65	1.79
1	A	34	PRO	CA-C	5.21	1.54	1.51
1	C	303	THR	CA-C	5.21	1.57	1.52
1	C	368	MET	SD-CE	5.03	1.92	1.79

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	N-CA-C	-10.25	100.03	112.54
1	D	419	GLU	N-CA-C	-10.13	99.47	112.23
1	C	419	GLU	N-CA-C	-9.86	100.38	111.82
1	A	116	VAL	N-CA-C	8.81	119.62	110.72
1	A	365	VAL	N-CA-C	8.64	119.44	110.62
1	D	365	VAL	N-CA-C	8.09	119.84	110.62
1	D	335	ILE	N-CA-C	8.02	118.70	111.81
1	B	101	ARG	NE-CZ-NH2	-7.85	112.13	119.20
1	B	367	PRO	N-CA-C	7.67	124.01	113.65
1	A	101	ARG	NE-CZ-NH2	-7.48	112.47	119.20
1	B	365	VAL	N-CA-C	7.40	118.13	110.36
1	C	173	PHE	N-CA-C	-7.39	103.30	111.36
1	D	372	ARG	NE-CZ-NH2	-7.38	112.56	119.20
1	D	436	LYS	N-CA-C	7.37	121.37	112.38
1	A	367	PRO	N-CA-C	7.28	123.30	113.84
1	C	461	ARG	N-CA-C	-7.27	98.88	110.14
1	C	101	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	A	101	ARG	NE-CZ-NH1	7.09	128.59	121.50
1	C	232	GLY	CA-C-N	7.09	127.69	119.47
1	C	232	GLY	C-N-CA	7.09	127.69	119.47
1	C	367	PRO	N-CA-C	7.00	123.10	113.65
1	B	383	PHE	N-CA-C	-6.97	98.49	109.50
1	B	139	GLY	N-CA-C	6.81	123.77	114.92
1	D	104	GLN	N-CA-C	-6.79	94.34	107.44
1	D	117	VAL	N-CA-C	6.68	116.81	110.53
1	A	320	HIS	CA-C-N	6.61	126.86	119.32
1	A	320	HIS	C-N-CA	6.61	126.86	119.32
1	B	173	PHE	N-CA-C	-6.61	104.00	111.07
1	A	419	GLU	N-CA-C	6.59	118.46	111.28
1	B	304	GLU	N-CA-C	6.57	119.44	111.82
1	C	104	GLN	N-CA-C	-6.51	94.87	107.44
1	A	104	GLN	N-CA-C	-6.49	96.57	107.80
1	D	101	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	B	288	LEU	N-CA-C	6.44	118.84	111.11
1	D	285	GLU	N-CA-C	-6.32	105.61	113.38
1	A	288	LEU	N-CA-C	6.27	118.64	111.11
1	D	398	VAL	N-CA-C	-6.27	105.62	111.45
1	C	365	VAL	N-CA-C	6.25	118.86	111.05
1	D	66	GLY	CA-C-N	6.24	125.87	119.56
1	D	66	GLY	C-N-CA	6.24	125.87	119.56
1	C	260	ASP	CA-C-N	6.23	127.63	119.84
1	C	260	ASP	C-N-CA	6.23	127.63	119.84
1	C	40	LEU	CA-C-N	6.21	126.23	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	LEU	C-N-CA	6.21	126.23	119.90
1	D	370	LEU	N-CA-C	-6.19	99.15	109.24
1	C	288	LEU	N-CA-C	6.17	118.51	111.11
1	D	304	GLU	N-CA-C	6.14	118.94	111.82
1	A	338	ASN	N-CA-C	6.04	120.71	112.68
1	A	105	ALA	N-CA-C	6.00	117.83	111.28
1	D	234	GLN	CB-CA-C	-5.97	100.88	110.79
1	C	185	ILE	N-CA-C	5.95	116.12	110.53
1	C	214	THR	N-CA-CB	-5.95	100.72	110.41
1	D	372	ARG	CG-CD-NE	-5.89	99.04	112.00
1	C	91	LEU	CA-C-N	-5.85	117.24	122.97
1	C	91	LEU	C-N-CA	-5.85	117.24	122.97
1	A	173	PHE	N-CA-C	-5.85	104.83	111.14
1	C	101	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	B	104	GLN	N-CA-C	-5.82	96.21	107.44
1	B	398	VAL	N-CA-C	-5.80	105.43	111.58
1	B	461	ARG	N-CA-C	-5.80	100.73	109.95
1	B	441	GLY	N-CA-C	-5.79	105.53	115.61
1	C	285	GLU	N-CA-C	-5.79	106.26	113.38
1	A	74	GLY	N-CA-C	-5.69	100.73	112.34
1	D	173	PHE	N-CA-C	-5.69	105.08	111.28
1	C	116	VAL	N-CA-C	5.69	116.46	110.72
1	D	371	ALA	N-CA-C	5.65	118.21	110.24
1	C	441	GLY	N-CA-C	-5.65	105.78	115.61
1	B	320	HIS	CA-C-N	5.63	126.88	119.84
1	B	320	HIS	C-N-CA	5.63	126.88	119.84
1	C	398	VAL	N-CA-C	-5.62	106.23	111.45
1	A	483	ILE	CA-C-N	-5.60	114.82	120.31
1	A	483	ILE	C-N-CA	-5.60	114.82	120.31
1	C	168	ILE	N-CA-C	5.58	116.89	108.96
1	C	323	VAL	N-CA-C	-5.57	105.10	110.72
1	D	91	LEU	CA-C-N	-5.57	117.51	122.97
1	D	91	LEU	C-N-CA	-5.57	117.51	122.97
1	A	479	GLY	N-CA-C	-5.51	100.11	113.18
1	D	461	ARG	N-CA-C	-5.51	101.19	109.95
1	B	168	ILE	N-CA-C	5.51	118.04	108.90
1	D	381	ARG	CA-C-N	-5.50	114.35	122.83
1	D	381	ARG	C-N-CA	-5.50	114.35	122.83
1	C	304	GLU	N-CA-C	5.50	118.20	111.82
1	D	258	THR	N-CA-C	5.49	118.98	112.72
1	B	74	GLY	N-CA-C	-5.48	101.16	112.34
1	C	118	PHE	N-CA-C	5.47	119.59	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	LEU	N-CA-C	5.46	118.15	110.23
1	B	169	ASP	CA-C-O	5.43	122.82	119.29
1	C	370	LEU	N-CA-C	-5.41	100.42	109.24
1	D	139	GLY	N-CA-C	5.40	125.99	113.18
1	B	198	PHE	N-CA-C	-5.40	105.30	111.07
1	D	198	PHE	N-CA-C	-5.37	105.43	111.28
1	D	442	GLU	N-CA-C	5.37	117.82	111.33
1	A	161	ARG	N-CA-C	-5.35	105.62	111.82
1	B	105	ALA	N-CA-C	5.35	117.11	111.28
1	A	259	LEU	N-CA-C	5.35	118.19	110.28
1	A	378	THR	N-CA-C	5.29	118.08	109.24
1	A	117	VAL	N-CA-C	5.28	115.49	110.53
1	C	60	LYS	CA-C-N	-5.28	111.98	120.64
1	C	60	LYS	C-N-CA	-5.28	111.98	120.64
1	A	101	ARG	CD-NE-CZ	5.25	131.74	124.40
1	B	338	ASN	N-CA-C	5.24	119.37	112.92
1	D	372	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	D	76	ARG	CB-CA-C	-5.20	102.08	110.77
1	D	367	PRO	N-CA-C	5.19	120.66	113.65
1	D	274	ARG	N-CA-C	-5.19	105.63	111.28
1	C	106	THR	N-CA-C	-5.16	105.57	111.14
1	B	234	GLN	CA-CB-CG	5.16	124.41	114.10
1	B	66	GLY	CA-C-N	5.14	124.80	119.56
1	B	66	GLY	C-N-CA	5.14	124.80	119.56
1	B	33	LEU	N-CA-C	-5.08	102.83	110.24
1	A	64	ARG	N-CA-C	5.08	117.94	111.69
1	D	105	ALA	N-CA-C	5.08	116.81	111.28
1	B	300	ILE	CB-CA-C	-5.07	105.33	111.87
1	B	260	ASP	CA-C-N	5.06	126.17	119.84
1	B	260	ASP	C-N-CA	5.06	126.17	119.84
1	D	253	GLU	N-CA-C	-5.06	105.46	110.97
1	A	461	ARG	N-CA-C	-5.02	101.97	109.95
1	C	343	PHE	N-CA-C	5.01	116.74	111.28
1	A	383	PHE	N-CA-C	-5.00	101.68	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	3768	0	3757	79	0
1	B	3767	0	3745	107	0
1	C	3751	0	3734	102	0
1	D	3751	0	3734	78	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	11	0	6	0	0
3	B	11	0	6	0	0
3	C	11	0	6	0	0
3	D	11	0	6	0	0
4	B	6	0	5	3	0
5	A	224	0	0	3	0
5	B	140	0	0	2	0
5	C	237	0	0	4	0
5	D	215	0	0	5	0
All	All	16075	0	15119	367	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 12.

All (367) 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)
4:B:900:GOL:C1	4:B:900:GOL:O1	1.71	1.35
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.17	1.08
1:C:418:ASN:HD22	1:C:422:GLN:HB2	1.15	1.08
1:D:189:ASP:HB2	5:D:695:HOH:O	1.55	1.06
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.12	1.04
1:D:253:GLU:HG2	1:D:257:ARG:NH2	1.74	1.02
1:C:234:GLN:H	1:C:234:GLN:HE21	1.05	1.01
1:B:318:MET:HE1	1:B:489:MET:HB2	1.38	1.00
1:D:139:GLY:HA2	1:D:142:LYS:HE3	1.42	0.99
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.26	0.98
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.45	0.97
1:B:205:MET:HE2	1:B:300:ILE:HA	1.44	0.96
1:B:101:ARG:H	1:B:120:ASN:ND2	1.65	0.94
1:B:352:MET:HE3	1:B:454:THR:HG22	1.48	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:MET:HE3	1:C:454:THR:HG22	1.49	0.92
1:A:314:PHE:HE2	1:A:457:MET:HE3	1.34	0.91
1:C:45:ASN:HD22	1:C:72:HIS:H	1.17	0.91
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.34	0.91
1:B:208:ILE:HD11	1:B:240:LEU:CB	2.01	0.91
1:B:318:MET:HE3	1:B:489:MET:HE3	1.53	0.90
1:B:205:MET:CE	1:B:300:ILE:HA	2.02	0.90
1:B:234:GLN:H	1:B:234:GLN:HE21	1.20	0.90
1:C:101:ARG:H	1:C:120:ASN:ND2	1.70	0.90
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.53	0.89
1:D:253:GLU:HG2	1:D:257:ARG:HH21	1.34	0.89
1:D:54:MET:HG3	1:D:218:GLN:HE21	1.40	0.86
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.41	0.85
1:A:54:MET:HG3	1:A:218:GLN:HE21	1.37	0.85
1:A:322:GLU:OE2	1:A:322:GLU:N	2.08	0.85
1:B:234:GLN:H	1:B:234:GLN:NE2	1.73	0.85
1:A:420:LYS:HB2	1:A:422:GLN:HE21	1.42	0.85
1:B:54:MET:HG3	1:B:218:GLN:HE21	1.42	0.84
1:B:446:ARG:HG3	1:B:446:ARG:NH1	1.93	0.84
1:C:77:ARG:HH11	1:C:77:ARG:CG	1.91	0.84
1:C:418:ASN:HB2	1:C:422:GLN:H	1.44	0.83
1:C:77:ARG:HG2	1:C:77:ARG:NH1	1.95	0.82
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.62	0.82
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.81	0.81
1:C:101:ARG:H	1:C:120:ASN:HD21	1.27	0.81
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.45	0.80
1:C:214:THR:HG22	1:C:217:GLY:H	1.46	0.80
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.47	0.79
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.83	0.78
1:D:456:VAL:HG12	1:D:457:MET:CE	2.13	0.78
1:D:234:GLN:NE2	1:D:234:GLN:H	1.80	0.78
1:C:316:LEU:CD2	1:C:473:VAL:HG11	2.14	0.77
1:C:234:GLN:H	1:C:234:GLN:NE2	1.83	0.76
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.50	0.76
1:B:318:MET:CE	1:B:489:MET:HE3	2.16	0.76
1:B:208:ILE:CD1	1:B:240:LEU:HB2	2.09	0.75
1:A:456:VAL:HG12	1:A:457:MET:HE2	1.69	0.74
1:B:204:MET:O	1:B:208:ILE:HG12	1.88	0.74
1:C:251:LYS:HZ2	1:C:251:LYS:HB3	1.53	0.74
1:D:407:ASN:H	1:D:415:HIS:HE1	1.36	0.74
1:C:214:THR:HG21	5:C:646:HOH:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:VAL:HG12	1:A:457:MET:CE	2.17	0.73
1:C:418:ASN:ND2	1:C:422:GLN:HB2	1.98	0.73
1:D:139:GLY:CA	1:D:142:LYS:HE3	2.17	0.73
1:D:234:GLN:H	1:D:234:GLN:HE21	1.35	0.73
1:B:37:PRO:HD3	1:B:61:ILE:HD13	1.70	0.73
1:A:101:ARG:CD	1:A:117:VAL:O	2.38	0.72
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.01	0.72
1:D:352:MET:HE3	1:D:454:THR:HG22	1.70	0.72
1:B:59:MET:HE1	1:B:82:CYS:SG	2.29	0.71
1:B:101:ARG:H	1:B:120:ASN:HD21	1.36	0.71
1:B:148:ARG:HD3	1:B:184:SER:HB3	1.72	0.71
1:A:32:LYS:HD2	1:A:33:LEU:H	1.55	0.71
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	1.72	0.70
1:B:346:ARG:HD2	1:B:353:GLU:OE2	1.91	0.70
1:B:446:ARG:HH11	1:B:446:ARG:CG	2.05	0.70
1:A:322:GLU:H	1:A:322:GLU:CD	2.01	0.69
1:D:253:GLU:O	1:D:256:GLN:CB	2.41	0.69
1:D:372:ARG:NH2	5:D:502:HOH:O	2.25	0.69
1:C:316:LEU:HD21	1:C:473:VAL:HG11	1.75	0.68
1:D:281:ASN:ND2	1:D:283:ASN:H	1.91	0.68
1:C:392:TYR:HB3	1:C:394:MET:CE	2.24	0.67
1:B:59:MET:HE3	1:B:394:MET:HE2	1.77	0.67
1:B:77:ARG:HH11	1:B:77:ARG:CG	2.07	0.67
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.29	0.66
1:A:420:LYS:CB	1:A:422:GLN:HE21	2.07	0.66
1:B:253:GLU:O	1:B:256:GLN:HG3	1.96	0.66
1:D:139:GLY:HA2	1:D:142:LYS:HG2	1.76	0.66
1:C:234:GLN:HE21	1:C:234:GLN:N	1.85	0.66
1:C:257:ARG:HH11	1:C:257:ARG:CG	2.05	0.65
1:B:61:ILE:HD12	1:B:65:TYR:CD2	2.32	0.65
1:D:139:GLY:O	1:D:142:LYS:HG2	1.97	0.65
1:A:101:ARG:HD3	1:A:117:VAL:O	1.94	0.65
1:D:457:MET:HE2	1:D:457:MET:HA	1.78	0.65
1:A:30:LYS:HG3	1:A:32:LYS:H	1.62	0.64
1:B:148:ARG:HD3	1:B:184:SER:CB	2.28	0.64
1:B:318:MET:HE1	1:B:489:MET:CB	2.23	0.64
1:A:420:LYS:HG3	1:A:422:GLN:NE2	2.11	0.64
1:D:50:ASN:HD22	1:D:50:ASN:C	2.05	0.64
1:B:233:PRO:HD2	1:B:234:GLN:NE2	2.13	0.64
1:C:50:ASN:C	1:C:50:ASN:HD22	2.04	0.64
1:B:200:SER:O	1:B:204:MET:HG3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:HIS:NE2	1:C:77:ARG:HD3	2.14	0.63
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.79	0.63
1:B:210:GLN:HE22	1:B:476:LYS:NZ	1.97	0.63
1:A:101:ARG:HD2	1:A:117:VAL:O	1.99	0.63
1:D:50:ASN:ND2	1:D:52:GLU:H	1.96	0.62
1:A:314:PHE:HE2	1:A:457:MET:CE	2.10	0.62
1:D:253:GLU:O	1:D:256:GLN:HB2	2.00	0.62
1:C:418:ASN:HB2	1:C:422:GLN:N	2.15	0.61
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.34	0.61
1:C:101:ARG:CD	1:C:117:VAL:O	2.49	0.61
1:C:324:GLU:HG3	1:C:457:MET:HE1	1.83	0.61
1:D:101:ARG:CD	1:D:117:VAL:O	2.49	0.61
1:C:324:GLU:HG3	1:C:457:MET:CE	2.31	0.60
1:A:346:ARG:HD2	1:A:353:GLU:OE1	2.00	0.60
1:C:281:ASN:ND2	1:C:283:ASN:H	1.99	0.60
1:D:101:ARG:HD2	1:D:117:VAL:O	2.02	0.60
1:D:456:VAL:HG12	1:D:457:MET:HE2	1.83	0.60
1:B:148:ARG:HH11	1:B:184:SER:HB3	1.66	0.59
1:D:50:ASN:HD22	1:D:52:GLU:H	1.50	0.59
1:A:337:LYS:HD2	1:A:337:LYS:N	2.17	0.59
1:D:275:MET:HE3	1:D:288:LEU:N	2.17	0.59
1:B:60:LYS:HE2	5:B:958:HOH:O	2.02	0.59
1:C:45:ASN:HD22	1:C:72:HIS:N	1.93	0.59
1:A:420:LYS:CG	1:A:422:GLN:HE21	2.16	0.59
1:B:254:HIS:O	1:B:258:THR:HG22	2.03	0.59
1:C:376:LYS:HE2	1:C:376:LYS:N	2.17	0.58
1:B:253:GLU:HA	1:B:256:GLN:HG2	1.85	0.58
1:C:101:ARG:HD2	1:C:117:VAL:O	2.04	0.58
1:C:50:ASN:ND2	1:C:52:GLU:H	2.01	0.58
1:D:281:ASN:C	1:D:281:ASN:HD22	2.10	0.58
1:A:457:MET:HE2	1:A:457:MET:N	2.18	0.58
1:B:64:ARG:NH1	5:B:1038:HOH:O	2.37	0.58
1:B:101:ARG:CD	1:B:117:VAL:O	2.51	0.58
1:D:232:GLY:HA3	1:D:234:GLN:HE22	1.69	0.58
1:B:419:GLU:CD	1:B:419:GLU:H	2.11	0.57
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.39	0.57
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.34	0.57
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.85	0.57
1:C:302:GLY:HA2	2:C:500:HEM:HMC3	1.87	0.57
1:B:208:ILE:HD13	1:B:240:LEU:HD12	1.85	0.57
1:D:142:LYS:O	1:D:144:GLY:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.20	0.57
1:C:186:VAL:CG1	1:C:295:THR:HG23	2.35	0.57
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.41	0.56
1:B:337:LYS:NZ	1:B:496:HIS:CE1	2.73	0.56
1:C:473:VAL:HG12	1:C:473:VAL:O	2.05	0.56
1:A:205:MET:O	1:A:208:ILE:HG12	2.05	0.56
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.88	0.56
1:D:376:LYS:HA	1:D:387:LYS:HB2	1.88	0.56
1:B:59:MET:HE3	1:B:394:MET:CE	2.36	0.55
1:B:101:ARG:HD3	1:B:117:VAL:O	2.06	0.55
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.88	0.55
1:C:205:MET:HE2	1:C:300:ILE:HG12	1.89	0.55
1:A:117:VAL:CG1	1:A:370[A]:LEU:HD21	2.37	0.54
1:B:210:GLN:O	1:B:214:THR:HG23	2.07	0.54
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.88	0.54
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.88	0.54
1:A:353:GLU:HG2	1:A:423:PHE:CD2	2.43	0.54
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.89	0.54
1:A:314:PHE:CE2	1:A:457:MET:HE3	2.27	0.54
1:C:281:ASN:HD22	1:C:282:PRO:N	2.06	0.54
1:A:457:MET:HE2	1:A:457:MET:CA	2.37	0.54
1:C:281:ASN:HD22	1:C:281:ASN:C	2.15	0.54
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.90	0.53
1:A:420:LYS:CG	1:A:422:GLN:NE2	2.70	0.53
1:D:76:ARG:NH2	1:D:103:GLU:HG3	2.24	0.53
1:D:281:ASN:ND2	1:D:281:ASN:C	2.64	0.53
1:D:418:ASN:HB2	1:D:422:GLN:H	1.73	0.53
1:C:250:LYS:HD2	5:C:665:HOH:O	2.08	0.53
1:B:253:GLU:HA	1:B:256:GLN:CG	2.39	0.53
1:B:337:LYS:HZ2	1:B:496:HIS:CE1	2.26	0.53
4:B:900:GOL:C1	4:B:900:GOL:HO1	2.14	0.53
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.90	0.53
1:A:342:LYS:HE3	1:A:344:GLU:OE1	2.08	0.52
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.91	0.52
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.44	0.52
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.91	0.52
1:A:457:MET:HE1	1:A:462:LEU:HD21	1.92	0.52
1:C:101:ARG:HD3	1:C:117:VAL:O	2.09	0.52
1:A:72:HIS:NE2	1:A:77:ARG:HD3	2.24	0.52
1:C:77:ARG:NH1	5:C:647:HOH:O	2.07	0.52
1:B:450:PHE:O	1:B:454:THR:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:LYS:HB3	1:C:376:LYS:CE	2.38	0.52
1:B:46:TYR:HB2	1:B:222:MET:HE1	1.91	0.52
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.75	0.52
1:D:420:LYS:HB2	1:D:422:GLN:HE21	1.74	0.52
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.90	0.52
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.69	0.51
1:D:466:GLN:HG3	1:D:471:ILE:CG1	2.40	0.51
1:B:33:LEU:HD21	1:B:77:ARG:HD2	1.91	0.51
1:C:50:ASN:HD22	1:C:52:GLU:H	1.57	0.51
1:B:463:LYS:HB3	1:B:490:SER:HB2	1.93	0.51
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.75	0.51
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.93	0.51
1:C:251:LYS:HB3	1:C:251:LYS:NZ	2.24	0.51
1:A:281:ASN:ND2	1:A:283:ASN:H	2.08	0.51
1:C:253:GLU:HA	1:C:256:GLN:HE21	1.76	0.51
1:D:407:ASN:H	1:D:415:HIS:CE1	2.23	0.50
1:C:346:ARG:HG2	1:C:353:GLU:OE1	2.11	0.50
1:D:253:GLU:O	1:D:256:GLN:HB3	2.11	0.50
1:A:339:ARG:CZ	1:A:342:LYS:HZ1	2.25	0.50
1:D:129:ARG:HD2	5:D:562:HOH:O	2.12	0.50
1:C:418:ASN:HB3	1:C:420:LYS:H	1.76	0.50
1:D:418:ASN:HB3	1:D:420:LYS:H	1.76	0.50
1:B:61:ILE:HD12	1:B:65:TYR:HD2	1.76	0.50
1:C:369:SER:HB2	1:C:395:LEU:HG	1.92	0.50
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.47	0.50
1:D:142:LYS:HG3	1:D:144:GLY:H	1.77	0.50
1:A:143:ARG:O	1:A:147:GLU:HG2	2.13	0.49
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.47	0.49
1:C:72:HIS:HE2	1:C:77:ARG:HD3	1.77	0.49
1:A:50:ASN:C	1:A:50:ASN:HD22	2.20	0.49
1:C:352:MET:CE	1:C:454:THR:HG22	2.34	0.49
1:D:466:GLN:HG3	1:D:471:ILE:HG13	1.93	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.95	0.49
1:A:281:ASN:C	1:A:281:ASN:HD22	2.20	0.49
1:D:281:ASN:HD22	1:D:282:PRO:HD2	1.77	0.49
1:A:302:GLY:HA2	2:A:500:HEM:HMC2	1.94	0.49
1:D:314:PHE:HE2	1:D:457:MET:HE3	1.78	0.49
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.95	0.49
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.95	0.48
1:B:271:PHE:HB3	1:B:291:LEU:HD13	1.94	0.48
1:C:281:ASN:HD22	1:C:282:PRO:CD	2.25	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:HD23	1:C:473:VAL:HG11	1.91	0.48
1:B:205:MET:HE1	1:B:299:PHE:O	2.13	0.48
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.94	0.48
1:C:251:LYS:NZ	1:C:251:LYS:CB	2.77	0.48
1:D:457:MET:HE2	1:D:457:MET:CA	2.43	0.48
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.44	0.48
1:D:418:ASN:HD22	1:D:422:GLN:NE2	2.11	0.48
1:A:89:GLU:O	1:A:93:ASP:HB2	2.14	0.47
1:B:101:ARG:N	1:B:120:ASN:HD21	2.07	0.47
1:B:32:LYS:HE2	1:B:379:LYS:NZ	2.29	0.47
1:C:463:LYS:HB3	1:C:490:SER:HB2	1.96	0.47
1:B:103:GLU:HB2	1:B:108:ASP:OD2	2.14	0.47
1:D:205:MET:HE2	1:D:300:ILE:HA	1.96	0.47
1:B:281:ASN:C	1:B:281:ASN:HD22	2.22	0.47
1:B:120:ASN:OD1	1:B:375:LYS:HE2	2.14	0.47
1:D:400:ARG:CZ	5:D:569:HOH:O	2.63	0.47
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.30	0.47
1:C:101:ARG:N	1:C:120:ASN:HD21	2.04	0.47
1:A:30:LYS:HG3	1:A:31:GLY:N	2.30	0.47
1:A:50:ASN:ND2	1:A:52:GLU:H	2.13	0.47
1:C:205:MET:HE2	1:C:300:ILE:CG1	2.45	0.46
1:B:494:ARG:O	1:B:495:HIS:HB2	2.14	0.46
1:B:101:ARG:HD2	1:B:117:VAL:O	2.15	0.46
1:B:369:SER:HB2	1:B:395:LEU:HG	1.97	0.46
1:A:50:ASN:C	1:A:50:ASN:ND2	2.74	0.46
1:B:210:GLN:HE22	1:B:476:LYS:HZ1	1.62	0.46
1:B:195:ASP:OD1	1:B:195:ASP:C	2.58	0.46
1:D:143:ARG:O	1:D:147:GLU:HG3	2.15	0.46
1:B:233:PRO:HD2	1:B:234:GLN:HE22	1.78	0.46
1:B:324:GLU:HG3	1:B:457:MET:CE	2.46	0.46
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.97	0.46
1:C:312:TYR:HE2	1:C:473:VAL:CG1	2.29	0.46
1:A:457:MET:HE2	1:A:457:MET:HA	1.96	0.46
1:B:205:MET:HE1	1:B:300:ILE:HA	1.92	0.46
1:B:318:MET:SD	1:B:464:SER:HB3	2.56	0.46
1:D:139:GLY:N	1:D:142:LYS:HE3	2.31	0.46
1:D:76:ARG:CZ	1:D:103:GLU:HG3	2.45	0.46
1:A:215:SER:CB	1:B:233:PRO:HG3	2.46	0.45
1:B:77:ARG:NH1	1:B:389:THR:HG23	2.24	0.45
1:B:259:LEU:O	1:B:261:PRO:HD3	2.15	0.45
1:D:101:ARG:HD3	1:D:117:VAL:O	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LYS:HE2	1:B:379:LYS:HZ2	1.81	0.45
1:B:271:PHE:CG	1:B:291:LEU:HD13	2.51	0.45
1:C:251:LYS:HA	1:C:251:LYS:HZ3	1.81	0.45
1:D:115:GLY:O	1:D:119:SER:HB3	2.15	0.45
1:C:77:ARG:CG	1:C:77:ARG:NH1	2.61	0.45
1:D:331:ILE:HD11	1:D:352:MET:CE	2.47	0.45
1:C:312:TYR:HE2	1:C:473:VAL:HG12	1.81	0.45
1:A:135:LEU:HD12	1:A:185:ILE:HG21	1.98	0.45
1:A:357:HIS:NE2	1:A:446:ARG:NH2	2.65	0.45
1:D:432:PHE:HB3	1:D:439:CYS:HB3	1.99	0.45
1:A:302:GLY:HA2	2:A:500:HEM:CMC	2.47	0.45
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.99	0.45
1:C:281:ASN:ND2	1:C:281:ASN:C	2.75	0.45
1:D:60:LYS:HE2	5:D:611:HOH:O	2.16	0.45
1:B:46:TYR:HA	1:B:222:MET:HE1	1.99	0.44
1:B:168:ILE:O	1:B:488:THR:HA	2.17	0.44
1:C:52:GLU:HG2	1:C:52:GLU:O	2.17	0.44
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.98	0.44
1:B:453:PHE:O	1:B:457:MET:HG2	2.17	0.44
1:D:236:GLN:O	1:D:240:LEU:HG	2.18	0.44
1:B:363:GLY:O	1:B:364:ASP:C	2.59	0.44
1:C:61:ILE:HD12	1:C:61:ILE:O	2.18	0.44
1:C:186:VAL:HA	1:C:267:PHE:HB3	2.00	0.44
1:A:33:LEU:HD12	1:A:384:PHE:O	2.17	0.44
1:B:264:PRO:HG3	1:B:273:ILE:CD1	2.48	0.44
1:B:370:LEU:HA	4:B:900:GOL:H12	1.99	0.44
1:D:367:PRO:HD2	1:D:480:PHE:O	2.18	0.44
1:C:61:ILE:HD12	1:C:65:TYR:HD2	1.83	0.44
1:C:418:ASN:HB3	1:C:420:LYS:N	2.33	0.43
1:C:97:GLU:HG3	5:C:705:HOH:O	2.18	0.43
1:A:125:LYS:HD2	5:A:556:HOH:O	2.18	0.43
1:A:322:GLU:N	1:A:322:GLU:CD	2.69	0.43
1:C:210:GLN:NE2	1:C:476:LYS:NZ	2.66	0.43
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.75	0.43
1:A:423:PHE:HE1	1:A:425:LYS:HG2	1.83	0.43
1:C:259:LEU:HG	1:C:260:ASP:N	2.32	0.43
1:D:450:PHE:O	1:D:454:THR:HG23	2.18	0.43
1:A:375:LYS:HD2	1:A:375:LYS:HA	1.85	0.43
1:D:314:PHE:CE2	1:D:457:MET:HE3	2.54	0.43
1:A:92:VAL:HG23	1:A:434:ILE:HD12	2.01	0.43
1:A:101:ARG:NH2	1:A:370[A]:LEU:HB3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:SER:O	1:C:468:PRO:C	2.60	0.43
1:A:89:GLU:CD	1:A:381:ARG:HH21	2.26	0.43
1:A:153:ALA:O	1:A:157:ILE:HG12	2.19	0.43
1:A:176:ARG:NE	5:A:627:HOH:O	2.32	0.43
1:B:37:PRO:HD3	1:B:61:ILE:CD1	2.45	0.43
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.71	0.43
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.48	0.43
1:A:274:ARG:HD2	1:A:274:ARG:HA	1.68	0.43
1:C:257:ARG:CG	1:C:257:ARG:NH1	2.72	0.43
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.54	0.43
1:C:33:LEU:HD12	1:C:384:PHE:O	2.19	0.43
1:C:352:MET:HE3	1:C:454:THR:CG2	2.35	0.42
1:D:260:ASP:O	1:D:262:ASN:N	2.52	0.42
1:B:54:MET:HE3	1:B:54:MET:HB3	1.94	0.42
1:B:253:GLU:C	1:B:256:GLN:HG3	2.44	0.42
1:A:418:ASN:OD1	1:A:418:ASN:C	2.61	0.42
1:A:126:GLN:HG2	5:A:594:HOH:O	2.19	0.42
1:A:354:ALA:HB2	1:A:417:LEU:HD13	2.01	0.42
1:B:143:ARG:O	1:B:147:GLU:HG3	2.19	0.42
1:D:365:VAL:O	1:D:481:ALA:HA	2.20	0.42
1:A:59:MET:HE1	1:A:82:CYS:SG	2.59	0.42
1:A:281:ASN:ND2	1:A:281:ASN:C	2.77	0.42
1:A:281:ASN:HD22	1:A:282:PRO:CD	2.32	0.42
1:B:271:PHE:CB	1:B:291:LEU:HD13	2.50	0.42
1:B:377:ASP:HB3	1:B:384:PHE:CZ	2.55	0.42
1:C:143:ARG:NE	1:C:147:GLU:HG3	2.34	0.42
1:C:152:GLU:HG3	1:C:177:THR:HG23	2.01	0.42
1:C:450:PHE:O	1:C:454:THR:HG23	2.19	0.42
1:D:168:ILE:C	1:D:168:ILE:HD12	2.45	0.42
1:B:318:MET:HE2	1:B:463:LYS:C	2.44	0.42
1:D:456:VAL:HG12	1:D:457:MET:HE3	1.96	0.42
1:A:32:LYS:HG3	1:A:33:LEU:O	2.19	0.42
1:C:39:PRO:C	1:C:40:LEU:HD12	2.45	0.42
1:B:380:PHE:O	1:B:383:PHE:HB2	2.20	0.41
1:A:442:GLU:O	1:A:446:ARG:HG3	2.21	0.41
1:B:210:GLN:NE2	1:B:476:LYS:NZ	2.67	0.41
1:C:205:MET:HE2	1:C:300:ILE:HA	2.01	0.41
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.28	0.41
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.21	0.41
1:A:381:ARG:O	1:A:382:ASP:HB2	2.21	0.41
1:C:148:ARG:HD3	1:C:184:SER:OG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:ALA:HB2	1:D:417:LEU:HD13	2.02	0.41
1:A:346:ARG:HE	1:A:346:ARG:HB3	1.55	0.41
1:C:211:PHE:O	1:C:214:THR:HB	2.21	0.41
1:D:376:LYS:O	1:D:377:ASP:C	2.64	0.41
1:A:476:LYS:HB2	1:A:485:ARG:HA	2.03	0.41
1:A:148:ARG:HD3	1:A:184:SER:OG	2.21	0.40
1:A:314:PHE:CE2	1:A:457:MET:CE	2.98	0.40
1:B:172:PHE:O	1:B:176:ARG:HG3	2.20	0.40
1:C:352:MET:HG2	1:C:454:THR:HG22	2.02	0.40
1:D:200:SER:O	1:D:204:MET:HG3	2.21	0.40
1:B:57:SER:O	1:B:61:ILE:HG23	2.21	0.40
1:B:54:MET:HG3	1:B:218:GLN:NE2	2.23	0.40
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.79	0.40
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.22	0.40
1:D:174:LEU:HD12	1:D:174:LEU:HA	1.91	0.40
1:D:342:LYS:HE3	1:D:342:LYS:HB2	1.71	0.40
1:A:95:ALA:HB1	1:A:436:LYS:HG2	2.04	0.40
1:B:180:ASN:HA	1:B:183:SER:HB2	2.02	0.40
1:B:467:SER:O	1:B:468:PRO:C	2.64	0.40
1:C:176:ARG:HE	1:C:176:ARG:HB2	1.73	0.40
1:C:246:ASP:O	1:C:250:LYS:HG3	2.21	0.40
1:A:168:ILE:O	1:A:488:THR:HA	2.22	0.40
1:A:369:SER:HB2	1:A:395:LEU:HG	2.03	0.40
1:B:247:PHE:CZ	1:B:251:LYS:HE3	2.55	0.40
1:B:258:THR:O	1:B:258:THR:OG1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/476 (98%)	453 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	463/476 (97%)	445 (96%)	16 (4%)	2 (0%)	30	22
1	C	462/476 (97%)	447 (97%)	15 (3%)	0	100	100
1	D	462/476 (97%)	447 (97%)	13 (3%)	2 (0%)	30	22
All	All	1851/1904 (97%)	1792 (97%)	55 (3%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	HIS
1	D	143	ARG
1	B	261	PRO
1	D	261	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/422 (98%)	399 (97%)	14 (3%)	32	25
1	B	413/422 (98%)	391 (95%)	22 (5%)	20	12
1	C	411/422 (97%)	390 (95%)	21 (5%)	21	13
1	D	411/422 (97%)	390 (95%)	21 (5%)	21	13
All	All	1648/1688 (98%)	1570 (95%)	78 (5%)	23	15

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	77	ARG
1	A	135	LEU
1	A	167	ASN
1	A	208	ILE
1	A	210	GLN
1	A	316	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	353	GLU
1	A	373	ARG
1	A	375	LYS
1	A	417	LEU
1	A	419	GLU
1	A	465	SER
1	A	468	PRO
1	B	40	LEU
1	B	48	GLN
1	B	52	GLU
1	B	61	ILE
1	B	135	LEU
1	B	167	ASN
1	B	174	LEU
1	B	210	GLN
1	B	234	GLN
1	B	256	GLN
1	B	260	ASP
1	B	261	PRO
1	B	280	LYS
1	B	316	LEU
1	B	375	LYS
1	B	379	LYS
1	B	414	GLN
1	B	417	LEU
1	B	419	GLU
1	B	446	ARG
1	B	463	LYS
1	B	468	PRO
1	C	50	ASN
1	C	61	ILE
1	C	77	ARG
1	C	126	GLN
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	214	THR
1	C	234	GLN
1	C	251	LYS
1	C	257	ARG
1	C	274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	340	GLN
1	C	344	GLU
1	C	353	GLU
1	C	375	LYS
1	C	376	LYS
1	C	414	GLN
1	C	417	LEU
1	C	467	SER
1	D	39	PRO
1	D	40	LEU
1	D	41	PRO
1	D	50	ASN
1	D	135	LEU
1	D	142	LYS
1	D	174	LEU
1	D	234	GLN
1	D	252	VAL
1	D	258	THR
1	D	279	GLU
1	D	281	ASN
1	D	316	LEU
1	D	337	LYS
1	D	353	GLU
1	D	375	LYS
1	D	417	LEU
1	D	419	GLU
1	D	465	SER
1	D	469	LYS
1	D	473	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	53	GLN
1	A	56	ASN
1	A	167	ASN
1	A	210	GLN
1	A	218	GLN
1	A	229	HIS
1	A	235	GLN
1	A	276	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	281	ASN
1	A	283	ASN
1	A	407	ASN
1	A	414	GLN
1	A	422	GLN
1	B	48	GLN
1	B	50	ASN
1	B	56	ASN
1	B	94	GLN
1	B	210	GLN
1	B	218	GLN
1	B	234	GLN
1	B	236	GLN
1	B	256	GLN
1	B	281	ASN
1	B	328	HIS
1	B	340	GLN
1	B	477	HIS
1	C	45	ASN
1	C	50	ASN
1	C	53	GLN
1	C	56	ASN
1	C	126	GLN
1	C	167	ASN
1	C	210	GLN
1	C	218	GLN
1	C	234	GLN
1	C	236	GLN
1	C	239	GLN
1	C	256	GLN
1	C	281	ASN
1	C	297	ASN
1	C	320	HIS
1	C	328	HIS
1	C	418	ASN
1	C	422	GLN
1	C	466	GLN
1	D	50	ASN
1	D	53	GLN
1	D	56	ASN
1	D	72	HIS
1	D	210	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	218	GLN
1	D	234	GLN
1	D	239	GLN
1	D	256	GLN
1	D	262	ASN
1	D	276	GLN
1	D	281	ASN
1	D	283	ASN
1	D	297	ASN
1	D	415	HIS
1	D	418	ASN
1	D	422	GLN

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](#)

9 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	HEM	A	500	1	50,50,50	2.30	21 (42%)	67,82,82	1.21	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	500	1	50,50,50	2.43	23 (46%)	67,82,82	1.39	13 (19%)
3	COU	B	501	-	12,12,12	1.45	3 (25%)	16,16,16	0.73	0
4	GOL	B	900	-	5,5,5	5.01	3 (60%)	5,5,5	6.32	3 (60%)
3	COU	D	501	-	12,12,12	1.56	2 (16%)	16,16,16	0.73	0
2	HEM	B	500	1	50,50,50	2.46	25 (50%)	67,82,82	1.29	12 (17%)
2	HEM	D	500	1	50,50,50	2.41	23 (46%)	67,82,82	1.22	9 (13%)
3	COU	A	501	-	12,12,12	1.21	2 (16%)	16,16,16	0.69	0
3	COU	C	501	-	12,12,12	0.98	1 (8%)	16,16,16	0.71	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	2/14/54/54	-
2	HEM	C	500	1	-	3/14/54/54	-
3	COU	B	501	-	-	-	0/2/2/2
4	GOL	B	900	-	-	2/4/4/4	-
3	COU	D	501	-	-	-	0/2/2/2
2	HEM	B	500	1	-	4/14/54/54	-
2	HEM	D	500	1	-	3/14/54/54	-
3	COU	A	501	-	-	-	0/2/2/2
3	COU	C	501	-	-	-	0/2/2/2

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	GOL	C3-C2	-8.07	1.21	1.51
4	B	900	GOL	O1-C1	6.88	1.71	1.42
2	C	500	HEM	C1C-NC	-5.92	1.28	1.39
2	B	500	HEM	C4D-ND	-4.96	1.31	1.40
2	B	500	HEM	C4A-NA	-4.93	1.30	1.39
2	D	500	HEM	C4A-NA	-4.91	1.30	1.39
2	A	500	HEM	CMA-C3A	4.89	1.60	1.50
2	C	500	HEM	CMA-C3A	4.53	1.60	1.50
2	D	500	HEM	C1C-C2C	-4.27	1.36	1.45
2	C	500	HEM	FE-NA	4.19	2.09	1.95
2	A	500	HEM	C1C-C2C	-4.14	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1D-ND	-4.13	1.30	1.38
2	B	500	HEM	FE-ND	4.04	2.07	1.94
2	D	500	HEM	C1B-NB	-4.03	1.33	1.40
2	C	500	HEM	FE-NC	4.02	2.08	1.95
2	A	500	HEM	FE-ND	3.97	2.07	1.94
2	D	500	HEM	CMD-C2D	3.88	1.58	1.50
2	D	500	HEM	FE-ND	3.83	2.06	1.94
2	B	500	HEM	C3B-C2B	3.82	1.44	1.37
2	A	500	HEM	C4D-ND	-3.81	1.33	1.40
2	B	500	HEM	CBB-CAB	3.81	1.48	1.30
2	B	500	HEM	CMB-C2B	3.80	1.58	1.50
2	D	500	HEM	FE-NB	3.78	2.06	1.94
2	D	500	HEM	CMA-C3A	3.76	1.58	1.50
2	A	500	HEM	C1D-ND	-3.76	1.31	1.38
2	C	500	HEM	C1D-ND	-3.72	1.31	1.38
2	D	500	HEM	C4D-ND	-3.68	1.33	1.40
2	D	500	HEM	FE-NA	3.68	2.07	1.95
2	B	500	HEM	FE-NA	3.66	2.07	1.95
2	C	500	HEM	CAC-C3C	-3.58	1.37	1.47
2	C	500	HEM	C4D-ND	-3.58	1.34	1.40
2	B	500	HEM	C1C-C2C	-3.57	1.38	1.45
2	A	500	HEM	CAC-C3C	-3.56	1.37	1.47
2	C	500	HEM	C3B-C2B	3.56	1.44	1.37
2	D	500	HEM	C1D-ND	-3.54	1.31	1.38
2	D	500	HEM	CAC-C3C	-3.53	1.38	1.47
2	C	500	HEM	C4A-NA	-3.51	1.33	1.39
2	A	500	HEM	C4D-C3D	-3.50	1.39	1.45
2	C	500	HEM	CBB-CAB	3.48	1.47	1.30
2	D	500	HEM	CBB-CAB	3.47	1.47	1.30
2	C	500	HEM	FE-NB	3.45	2.05	1.94
2	A	500	HEM	CBD-CGD	3.41	1.58	1.50
2	A	500	HEM	FE-NB	3.41	2.05	1.94
2	A	500	HEM	CBB-CAB	3.39	1.46	1.30
2	A	500	HEM	CMD-C2D	3.35	1.57	1.50
2	B	500	HEM	C4D-C3D	-3.28	1.39	1.45
2	C	500	HEM	C4C-NC	-3.27	1.33	1.39
2	C	500	HEM	FE-ND	3.21	2.04	1.94
2	D	500	HEM	C1C-NC	-3.21	1.33	1.39
2	A	500	HEM	C3C-C4C	-3.19	1.40	1.46
2	B	500	HEM	C4C-NC	-3.19	1.33	1.39
2	D	500	HEM	O2A-CGA	-3.19	1.20	1.30
2	B	500	HEM	CAC-C3C	-3.15	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	GOL	O3-C3	3.09	1.55	1.42
2	D	500	HEM	FE-NC	3.08	2.05	1.95
2	C	500	HEM	C4D-C3D	-3.08	1.39	1.45
2	D	500	HEM	C3C-C4C	-3.07	1.40	1.46
2	A	500	HEM	C4A-NA	-3.07	1.33	1.39
2	B	500	HEM	C1B-NB	-3.05	1.35	1.40
2	A	500	HEM	C1A-C2A	-3.01	1.38	1.44
2	B	500	HEM	CMA-C3A	3.01	1.56	1.50
2	D	500	HEM	C4D-C3D	-2.99	1.40	1.45
2	A	500	HEM	C1C-NC	-2.96	1.34	1.39
2	C	500	HEM	C4B-NB	-2.93	1.33	1.38
2	B	500	HEM	C1C-NC	-2.92	1.34	1.39
2	B	500	HEM	C1D-C2D	-2.90	1.38	1.44
2	B	500	HEM	FE-NC	2.89	2.04	1.95
2	D	500	HEM	C4C-NC	-2.88	1.34	1.39
3	D	501	COU	O2-C9	2.85	1.42	1.38
2	B	500	HEM	O2A-CGA	-2.85	1.21	1.30
2	C	500	HEM	C1C-C2C	-2.75	1.39	1.45
2	B	500	HEM	C3C-C4C	-2.68	1.41	1.46
2	B	500	HEM	FE-NB	2.66	2.03	1.94
2	A	500	HEM	FE-NC	2.66	2.03	1.95
2	B	500	HEM	CMD-C2D	2.57	1.56	1.50
3	D	501	COU	C7-C6	2.55	1.43	1.38
2	B	500	HEM	C4B-NB	-2.54	1.33	1.38
2	C	500	HEM	CMD-C2D	2.46	1.55	1.50
3	A	501	COU	C7-C6	2.45	1.43	1.38
3	B	501	COU	C7-C6	2.45	1.43	1.38
2	A	500	HEM	FE-NA	2.44	2.03	1.95
2	A	500	HEM	CBD-CAD	2.43	1.60	1.51
2	C	500	HEM	CBC-CAC	2.36	1.41	1.30
2	C	500	HEM	C1D-C2D	-2.32	1.39	1.44
2	B	500	HEM	CMC-C2C	2.32	1.55	1.50
2	A	500	HEM	C1B-NB	-2.32	1.36	1.40
2	D	500	HEM	C3B-C2B	2.30	1.41	1.37
2	D	500	HEM	CMC-C2C	2.30	1.55	1.50
2	A	500	HEM	C1D-C2D	-2.30	1.39	1.44
2	D	500	HEM	C1A-C2A	-2.29	1.40	1.44
2	C	500	HEM	CMC-C2C	2.28	1.55	1.50
2	A	500	HEM	CMC-C2C	2.25	1.55	1.50
3	B	501	COU	C7-C8	2.23	1.42	1.38
2	B	500	HEM	C1A-C2A	-2.23	1.40	1.44
2	C	500	HEM	C3C-C4C	-2.20	1.42	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CBC-CAC	2.13	1.40	1.30
2	D	500	HEM	C1D-C2D	-2.11	1.40	1.44
2	C	500	HEM	CBD-CGD	2.11	1.55	1.50
3	A	501	COU	O2-C9	2.10	1.41	1.38
2	D	500	HEM	C3C-C2C	2.09	1.41	1.37
2	C	500	HEM	C1B-NB	-2.07	1.36	1.40
3	B	501	COU	O2-C9	2.06	1.41	1.38
3	C	501	COU	C7-C6	2.02	1.42	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	900	GOL	O3-C3-C2	11.82	163.59	110.38
4	B	900	GOL	O2-C2-C3	6.21	134.89	109.18
4	B	900	GOL	O1-C1-C2	4.31	129.80	110.38
2	C	500	HEM	CHD-C4C-NC	-4.30	119.77	124.45
2	B	500	HEM	C3B-C2B-C1B	-3.42	103.84	106.41
2	C	500	HEM	O2A-CGA-CBA	3.31	124.45	114.00
2	C	500	HEM	C4C-C3C-C2C	-3.30	103.95	106.81
2	A	500	HEM	O2A-CGA-CBA	3.23	124.22	114.00
2	A	500	HEM	C3B-C4B-NB	3.09	111.69	109.47
2	A	500	HEM	CHB-C1B-NB	-2.87	120.82	124.37
2	B	500	HEM	CHD-C4C-NC	-2.83	121.37	124.45
2	D	500	HEM	O2A-CGA-CBA	2.75	122.69	114.00
2	D	500	HEM	C4B-C3B-C2B	-2.75	104.75	107.28
2	B	500	HEM	C4A-CHB-C1B	2.50	132.12	126.25
2	D	500	HEM	C4A-CHB-C1B	2.49	132.09	126.25
2	B	500	HEM	O2A-CGA-CBA	2.46	121.78	114.00
2	D	500	HEM	C4C-CHD-C1D	2.43	131.19	126.02
2	C	500	HEM	C3B-C2B-C1B	-2.43	104.59	106.41
2	C	500	HEM	C1C-CHC-C4B	2.38	131.07	126.02
2	D	500	HEM	CHB-C1B-NB	-2.36	121.45	124.37
2	B	500	HEM	C3B-C4B-NB	2.33	111.14	109.47
2	B	500	HEM	C4B-C3B-C2B	-2.33	105.14	107.28
2	C	500	HEM	CHB-C1B-NB	-2.33	121.48	124.37
2	B	500	HEM	C4D-ND-C1D	2.27	107.90	105.21
2	D	500	HEM	CHD-C4C-NC	-2.23	122.02	124.45
2	B	500	HEM	C2B-C1B-NB	2.23	112.40	109.84
2	C	500	HEM	C3B-C4B-NB	2.22	111.07	109.47
2	C	500	HEM	C1B-NB-C4B	2.22	107.84	105.21
2	C	500	HEM	C4D-ND-C1D	2.21	107.83	105.21
2	A	500	HEM	CHD-C4C-NC	-2.21	122.05	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C4A-CHB-C1B	2.17	131.34	126.25
2	A	500	HEM	CMD-C2D-C1D	2.16	128.41	125.03
2	B	500	HEM	C4C-CHD-C1D	2.15	130.58	126.02
2	A	500	HEM	C4C-CHD-C1D	2.15	130.58	126.02
2	A	500	HEM	O2D-CGD-CBD	2.13	120.73	114.00
2	D	500	HEM	C3B-C4B-NB	2.13	111.00	109.47
2	B	500	HEM	CHB-C1B-NB	-2.11	121.76	124.37
2	D	500	HEM	C4C-C3C-C2C	-2.09	105.00	106.81
2	B	500	HEM	CHC-C1C-NC	-2.08	122.19	124.45
3	C	501	COU	C8-C9-C4	2.07	121.74	118.18
2	B	500	HEM	C4C-C3C-C2C	-2.06	105.03	106.81
2	A	500	HEM	O2D-CGD-O1D	-2.05	118.05	123.33
2	C	500	HEM	O2D-CGD-CBD	2.03	120.42	114.00
2	D	500	HEM	C4D-ND-C1D	2.02	107.61	105.21
2	C	500	HEM	C4C-CHD-C1D	2.02	130.31	126.02
2	A	500	HEM	C4A-CHB-C1B	2.01	130.96	126.25
2	A	500	HEM	O1A-CGA-CBA	-2.00	116.73	123.09
2	C	500	HEM	C4B-C3B-C2B	-2.00	105.44	107.28

There are no chirality outliers.

All (14) torsion outliers are listed below:

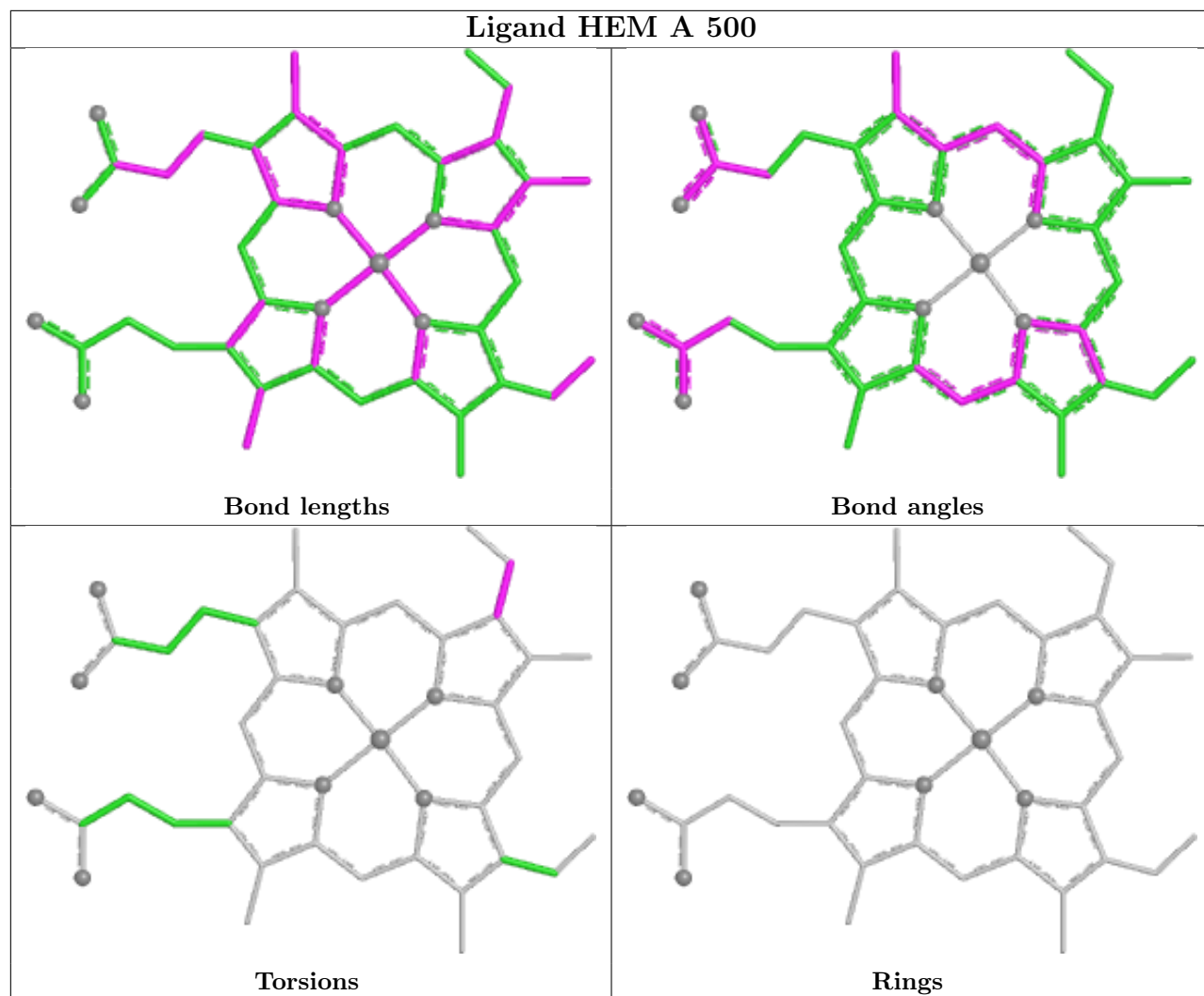
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
4	B	900	GOL	C1-C2-C3-O3
4	B	900	GOL	O1-C1-C2-O2
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O2D

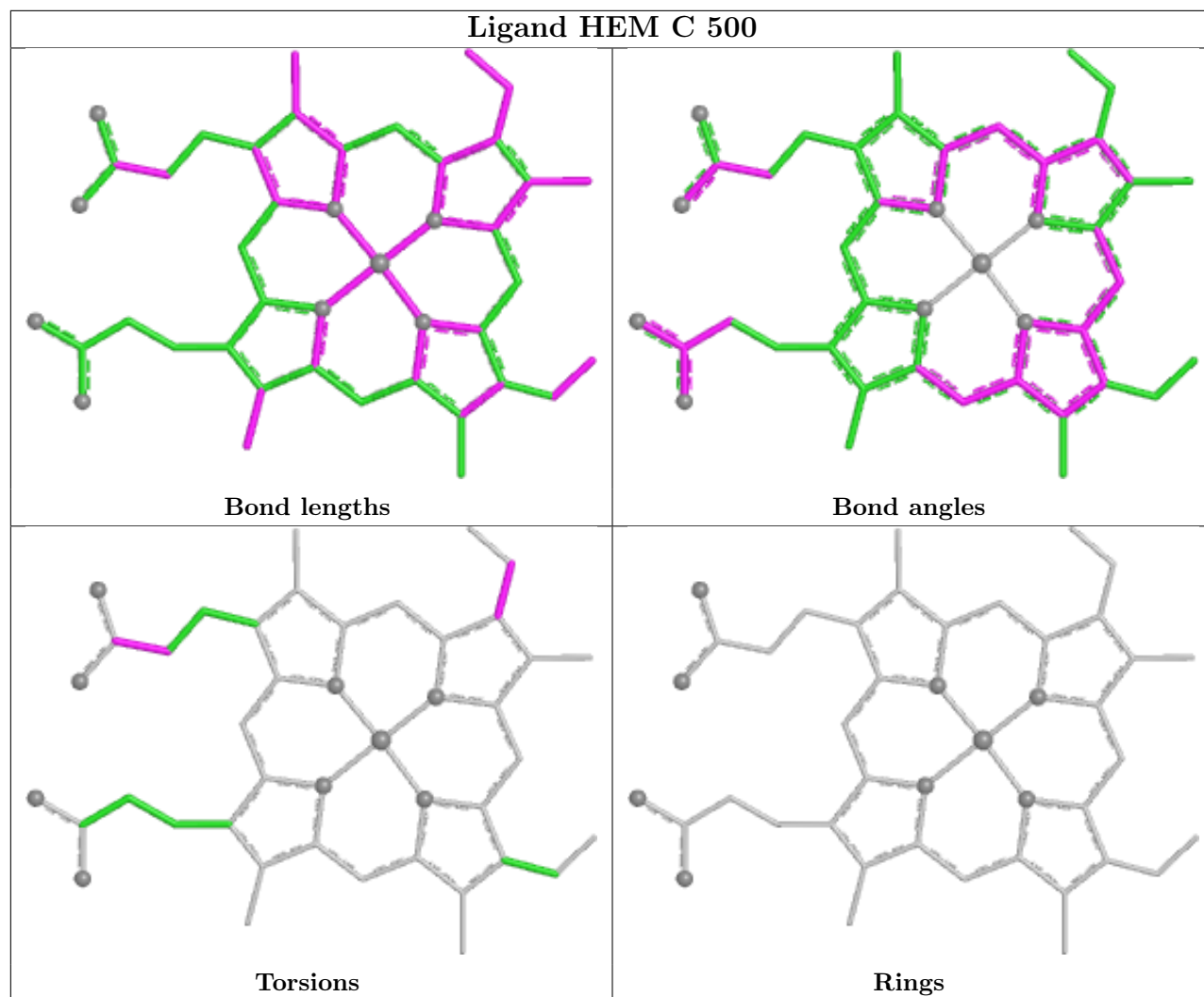
There are no ring outliers.

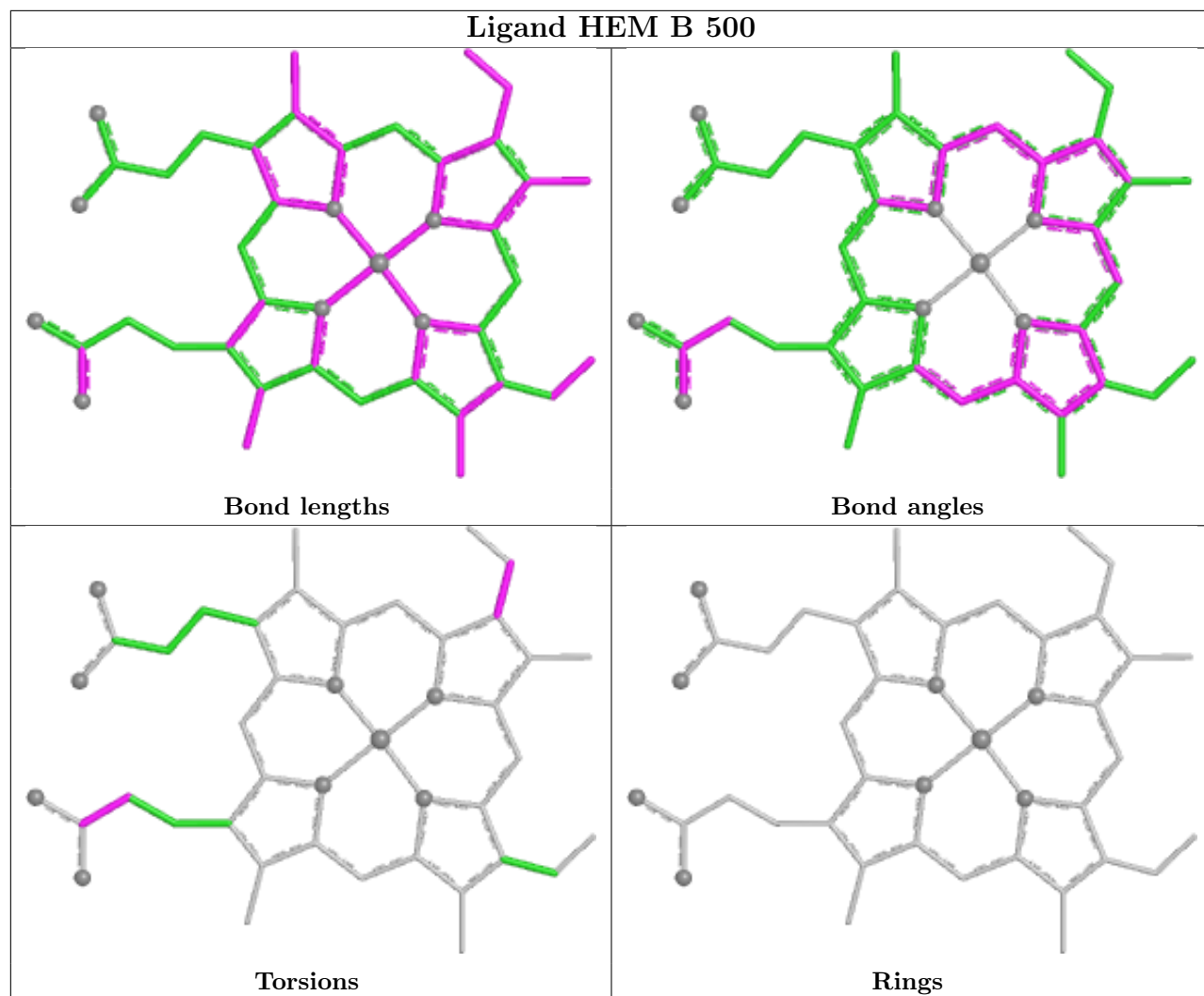
5 monomers are involved in 12 short contacts:

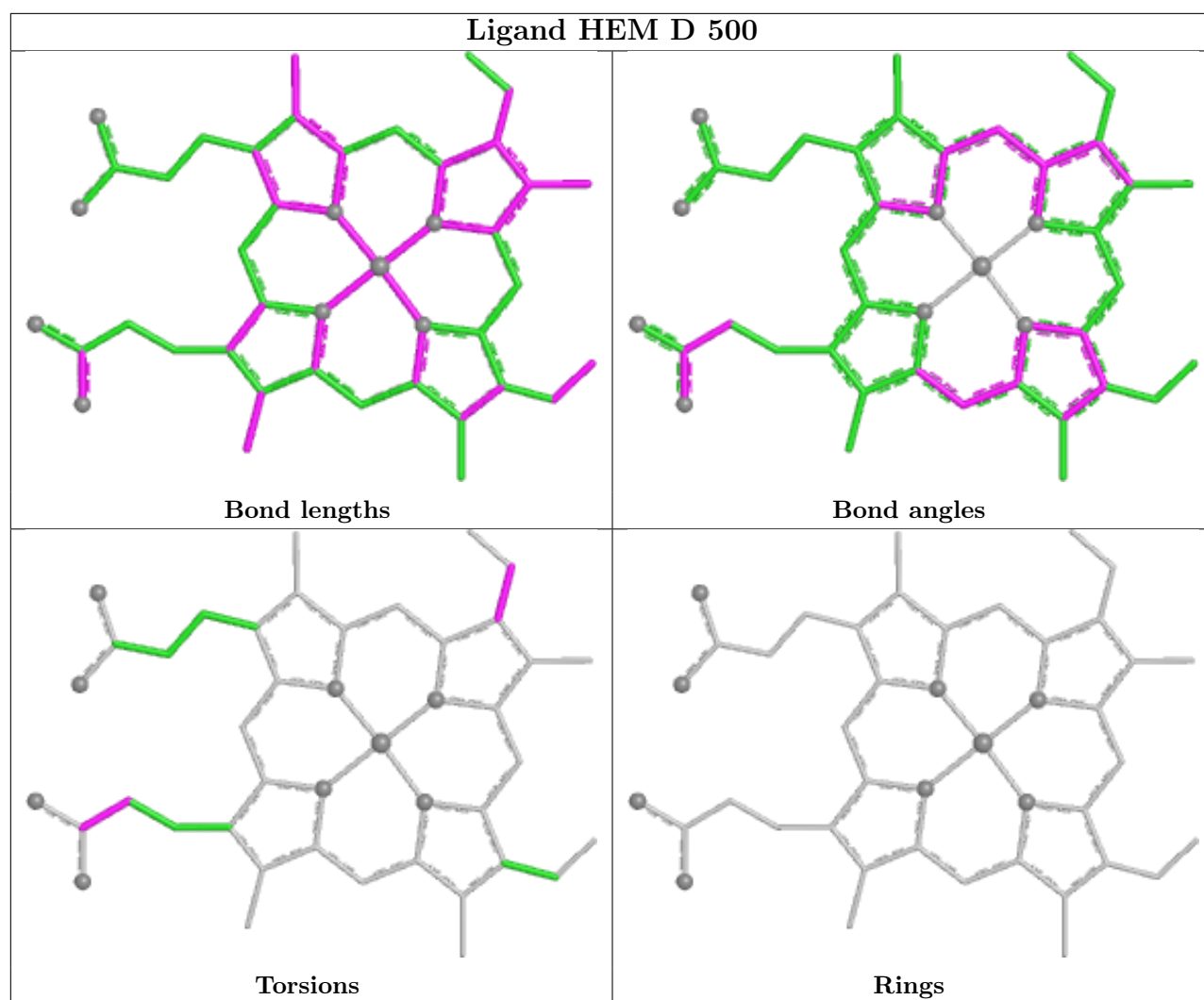
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
2	C	500	HEM	2	0
4	B	900	GOL	3	0
2	B	500	HEM	1	0
2	D	500	HEM	2	0

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/476 (97%)	0.11	3 (0%) 85 87	15, 38, 57, 80	1 (0%)
1	B	465/476 (97%)	0.44	15 (3%) 50 54	30, 44, 63, 92	0
1	C	464/476 (97%)	0.06	4 (0%) 81 83	26, 38, 56, 71	0
1	D	464/476 (97%)	0.20	11 (2%) 59 63	26, 39, 66, 79	0
All	All	1858/1904 (97%)	0.20	33 (1%) 67 71	15, 40, 61, 92	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	HIS	4.1
1	D	140	VAL	3.8
1	A	31	GLY	3.4
1	B	61	ILE	2.9
1	B	258	THR	2.9
1	D	144	GLY	2.9
1	D	138	PHE	2.8
1	C	31	GLY	2.7
1	B	261	PRO	2.7
1	C	376	LYS	2.6
1	D	141	GLY	2.5
1	B	252	VAL	2.5
1	D	418	ASN	2.5
1	B	143	ARG	2.5
1	D	258	THR	2.5
1	B	208	ILE	2.4
1	B	140	VAL	2.4
1	B	273	ILE	2.3
1	B	302	GLY	2.3
1	C	336	GLY	2.3
1	C	418	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	259	LEU	2.2
1	B	259	LEU	2.2
1	D	145	ILE	2.1
1	B	495	HIS	2.1
1	A	30	LYS	2.1
1	D	31	GLY	2.1
1	B	418	ASN	2.1
1	D	457	MET	2.0
1	A	262	ASN	2.0
1	B	260	ASP	2.0
1	D	189	ASP	2.0
1	B	337	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

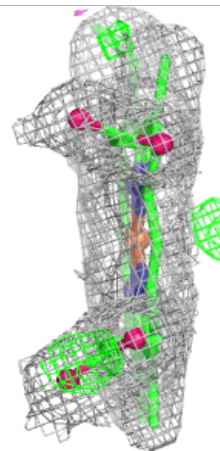
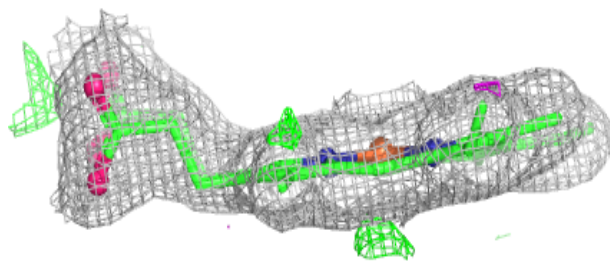
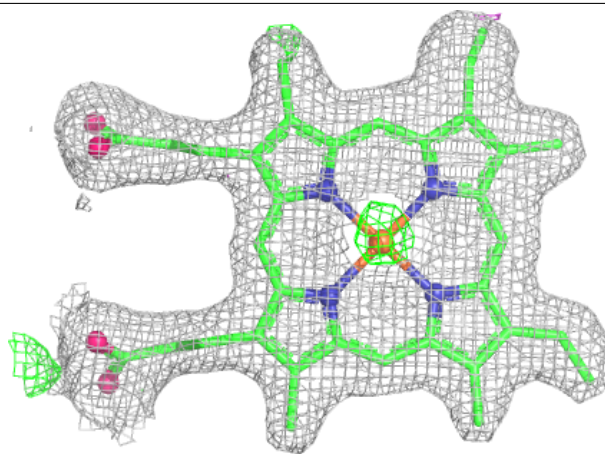
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	900	6/6	0.83	0.13	37,43,43,46	0
3	COU	D	501	11/11	0.85	0.14	50,56,57,57	0
3	COU	A	501	11/11	0.89	0.14	56,59,60,60	0
3	COU	B	501	11/11	0.91	0.12	63,64,64,65	0
3	COU	C	501	11/11	0.92	0.13	59,61,62,62	0
2	HEM	D	500	43/43	0.98	0.05	27,31,34,40	0
2	HEM	A	500	43/43	0.98	0.05	24,28,34,37	0
2	HEM	B	500	43/43	0.98	0.05	28,33,39,42	0
2	HEM	C	500	43/43	0.99	0.05	26,32,34,36	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

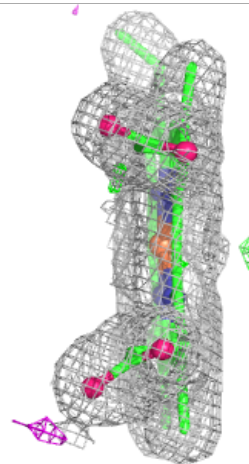
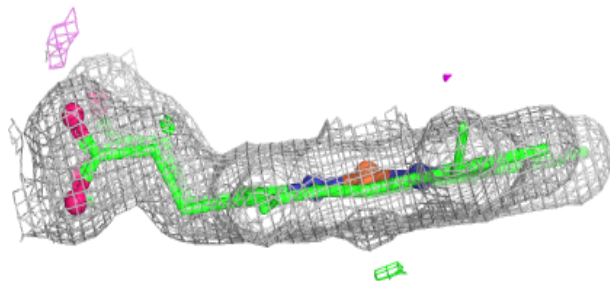
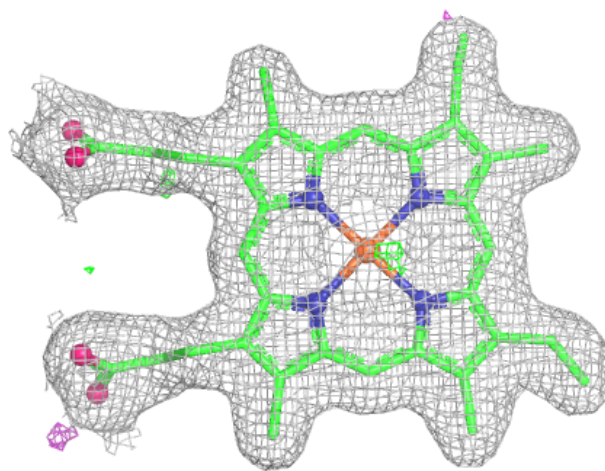
Electron density around HEM D 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



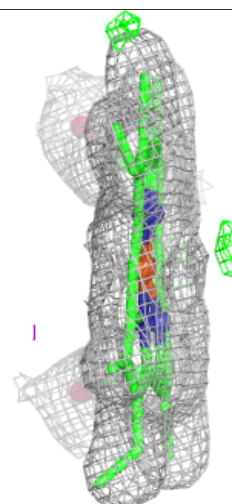
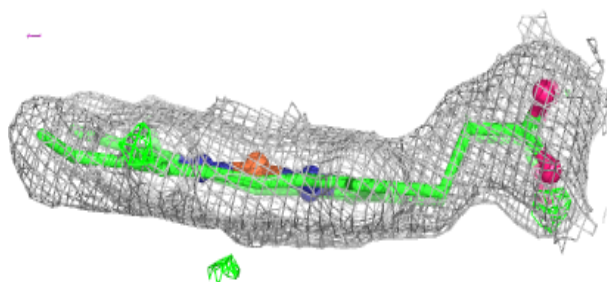
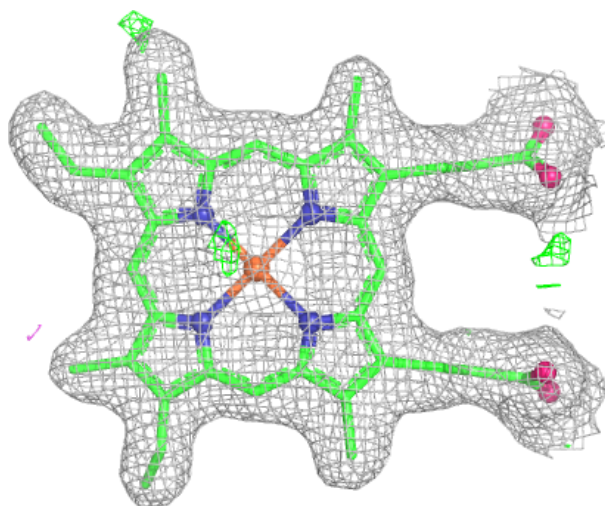
Electron density around HEM A 500:

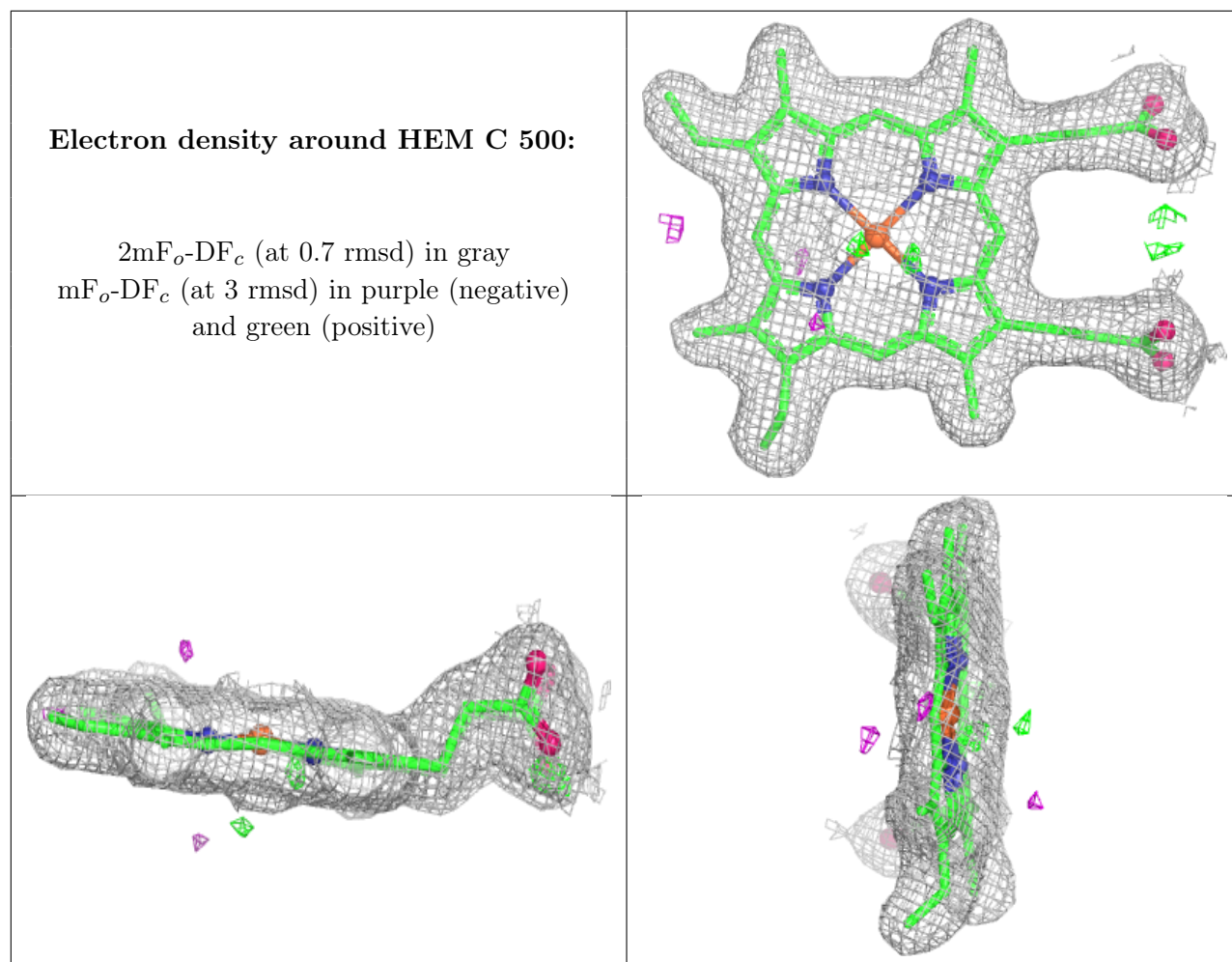
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.