



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:36 AM UTC

PDB ID : 4EJG / pdb_00004ejg
Title : Human Cytochrome P450 2A13 in complex with Nicotine
Authors : DeVore, N.M.; Scott, E.E.
Deposited on : 2012-04-06
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) : 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

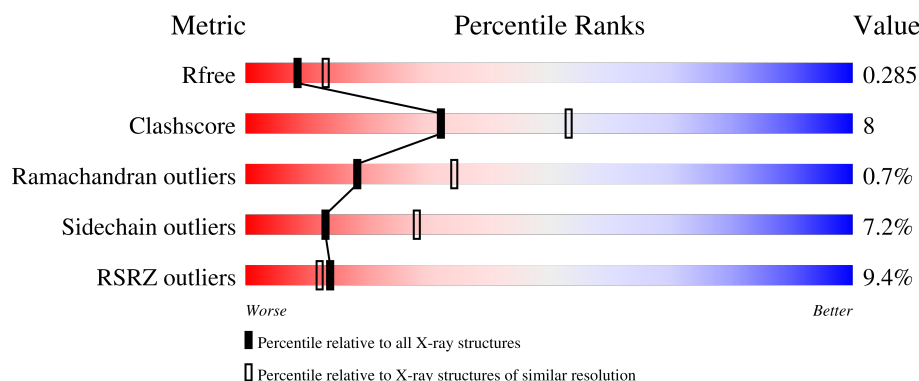
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	 76% 19% . .
1	B	476	 77% 18% . .
1	C	476	 73% 24% . .
1	D	476	 72% 23% . .
1	E	476	 5% 76% 20% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	476	
1	G	476	
1	H	476	

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	H	502	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30618 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 2A13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	1	0
			3772	2426	652	676	18			
1	B	464	Total	C	N	O	S	0	5	0
			3812	2448	663	683	18			
1	C	464	Total	C	N	O	S	0	4	0
			3798	2441	659	680	18			
1	D	465	Total	C	N	O	S	0	3	0
			3797	2441	658	680	18			
1	E	465	Total	C	N	O	S	0	3	0
			3798	2443	659	678	18			
1	F	465	Total	C	N	O	S	0	0	0
			3772	2427	652	675	18			
1	G	463	Total	C	N	O	S	0	0	0
			3735	2403	643	671	18			
1	H	458	Total	C	N	O	S	0	0	0
			3687	2365	638	666	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP Q16696
A	24	ALA	-	expression tag	UNP Q16696
A	25	LYS	-	expression tag	UNP Q16696
A	26	LYS	-	expression tag	UNP Q16696
A	27	THR	-	expression tag	UNP Q16696
A	28	SER	-	expression tag	UNP Q16696
A	29	SER	-	expression tag	UNP Q16696
A	30	LYS	-	expression tag	UNP Q16696
A	495	HIS	-	expression tag	UNP Q16696
A	496	HIS	-	expression tag	UNP Q16696
A	497	HIS	-	expression tag	UNP Q16696
A	498	HIS	-	expression tag	UNP Q16696
B	23	MET	-	expression tag	UNP Q16696

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	ALA	-	expression tag	UNP Q16696
B	25	LYS	-	expression tag	UNP Q16696
B	26	LYS	-	expression tag	UNP Q16696
B	27	THR	-	expression tag	UNP Q16696
B	28	SER	-	expression tag	UNP Q16696
B	29	SER	-	expression tag	UNP Q16696
B	30	LYS	-	expression tag	UNP Q16696
B	495	HIS	-	expression tag	UNP Q16696
B	496	HIS	-	expression tag	UNP Q16696
B	497	HIS	-	expression tag	UNP Q16696
B	498	HIS	-	expression tag	UNP Q16696
C	23	MET	-	expression tag	UNP Q16696
C	24	ALA	-	expression tag	UNP Q16696
C	25	LYS	-	expression tag	UNP Q16696
C	26	LYS	-	expression tag	UNP Q16696
C	27	THR	-	expression tag	UNP Q16696
C	28	SER	-	expression tag	UNP Q16696
C	29	SER	-	expression tag	UNP Q16696
C	30	LYS	-	expression tag	UNP Q16696
C	495	HIS	-	expression tag	UNP Q16696
C	496	HIS	-	expression tag	UNP Q16696
C	497	HIS	-	expression tag	UNP Q16696
C	498	HIS	-	expression tag	UNP Q16696
D	23	MET	-	expression tag	UNP Q16696
D	24	ALA	-	expression tag	UNP Q16696
D	25	LYS	-	expression tag	UNP Q16696
D	26	LYS	-	expression tag	UNP Q16696
D	27	THR	-	expression tag	UNP Q16696
D	28	SER	-	expression tag	UNP Q16696
D	29	SER	-	expression tag	UNP Q16696
D	30	LYS	-	expression tag	UNP Q16696
D	495	HIS	-	expression tag	UNP Q16696
D	496	HIS	-	expression tag	UNP Q16696
D	497	HIS	-	expression tag	UNP Q16696
D	498	HIS	-	expression tag	UNP Q16696
E	23	MET	-	expression tag	UNP Q16696
E	24	ALA	-	expression tag	UNP Q16696
E	25	LYS	-	expression tag	UNP Q16696
E	26	LYS	-	expression tag	UNP Q16696
E	27	THR	-	expression tag	UNP Q16696
E	28	SER	-	expression tag	UNP Q16696
E	29	SER	-	expression tag	UNP Q16696

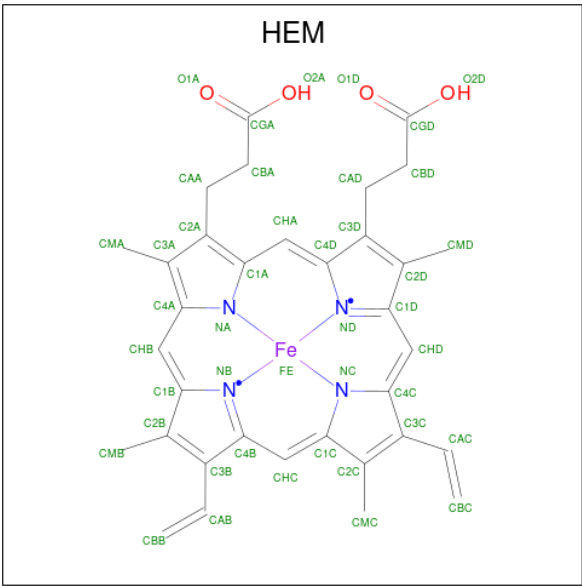
Continued on next page...

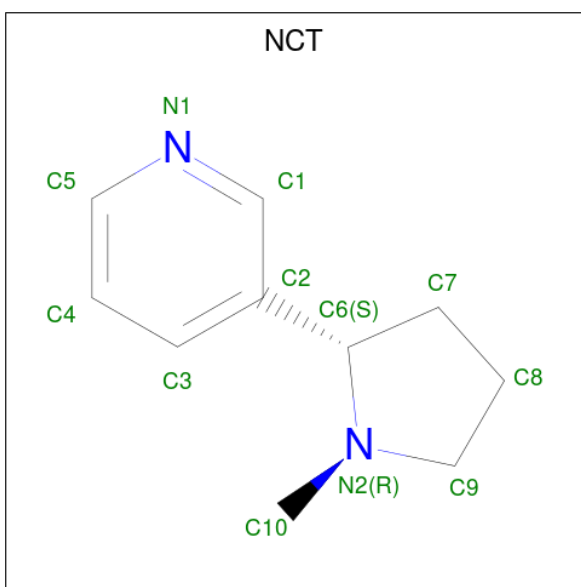
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	30	LYS	-	expression tag	UNP Q16696
E	495	HIS	-	expression tag	UNP Q16696
E	496	HIS	-	expression tag	UNP Q16696
E	497	HIS	-	expression tag	UNP Q16696
E	498	HIS	-	expression tag	UNP Q16696
F	23	MET	-	expression tag	UNP Q16696
F	24	ALA	-	expression tag	UNP Q16696
F	25	LYS	-	expression tag	UNP Q16696
F	26	LYS	-	expression tag	UNP Q16696
F	27	THR	-	expression tag	UNP Q16696
F	28	SER	-	expression tag	UNP Q16696
F	29	SER	-	expression tag	UNP Q16696
F	30	LYS	-	expression tag	UNP Q16696
F	495	HIS	-	expression tag	UNP Q16696
F	496	HIS	-	expression tag	UNP Q16696
F	497	HIS	-	expression tag	UNP Q16696
F	498	HIS	-	expression tag	UNP Q16696
G	23	MET	-	expression tag	UNP Q16696
G	24	ALA	-	expression tag	UNP Q16696
G	25	LYS	-	expression tag	UNP Q16696
G	26	LYS	-	expression tag	UNP Q16696
G	27	THR	-	expression tag	UNP Q16696
G	28	SER	-	expression tag	UNP Q16696
G	29	SER	-	expression tag	UNP Q16696
G	30	LYS	-	expression tag	UNP Q16696
G	495	HIS	-	expression tag	UNP Q16696
G	496	HIS	-	expression tag	UNP Q16696
G	497	HIS	-	expression tag	UNP Q16696
G	498	HIS	-	expression tag	UNP Q16696
H	23	MET	-	expression tag	UNP Q16696
H	24	ALA	-	expression tag	UNP Q16696
H	25	LYS	-	expression tag	UNP Q16696
H	26	LYS	-	expression tag	UNP Q16696
H	27	THR	-	expression tag	UNP Q16696
H	28	SER	-	expression tag	UNP Q16696
H	29	SER	-	expression tag	UNP Q16696
H	30	LYS	-	expression tag	UNP Q16696
H	495	HIS	-	expression tag	UNP Q16696
H	496	HIS	-	expression tag	UNP Q16696
H	497	HIS	-	expression tag	UNP Q16696
H	498	HIS	-	expression tag	UNP Q16696

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

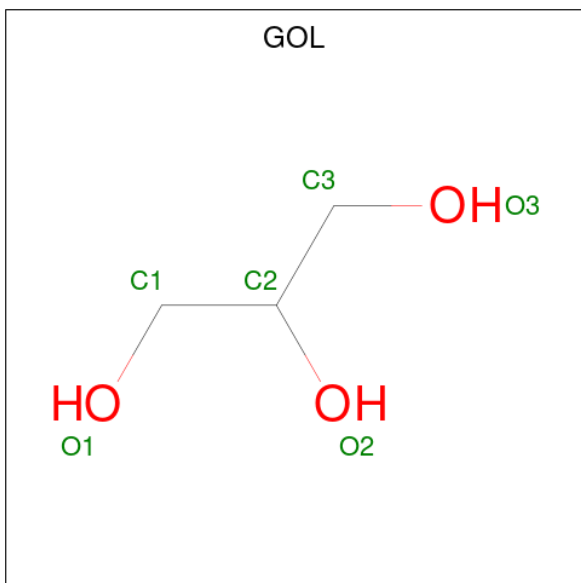
C₃₄H₃₂FeN₄O₄).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			12	10	2		
3	B	1	Total	C	N	0	0
			12	10	2		
3	C	1	Total	C	N	0	0
			12	10	2		
3	D	1	Total	C	N	0	0
			12	10	2		

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



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

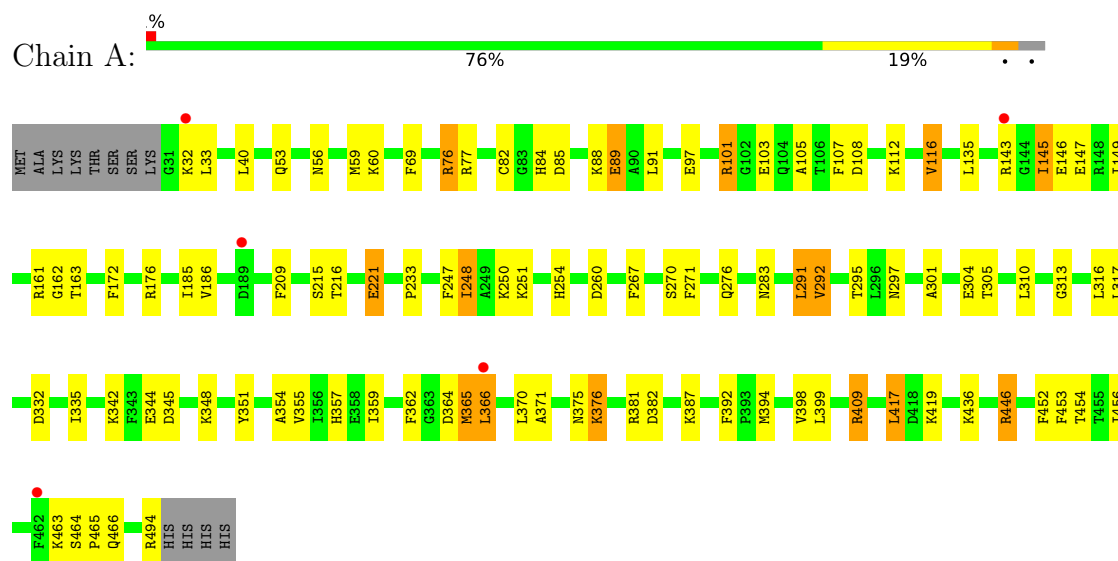
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	5	Total	O	0	0
			5	5		
5	C	6	Total	O	0	0
			6	6		
5	D	14	Total	O	0	0
			14	14		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		
5	G	9	Total	O	0	0
			9	9		
5	H	2	Total	O	0	0
			2	2		

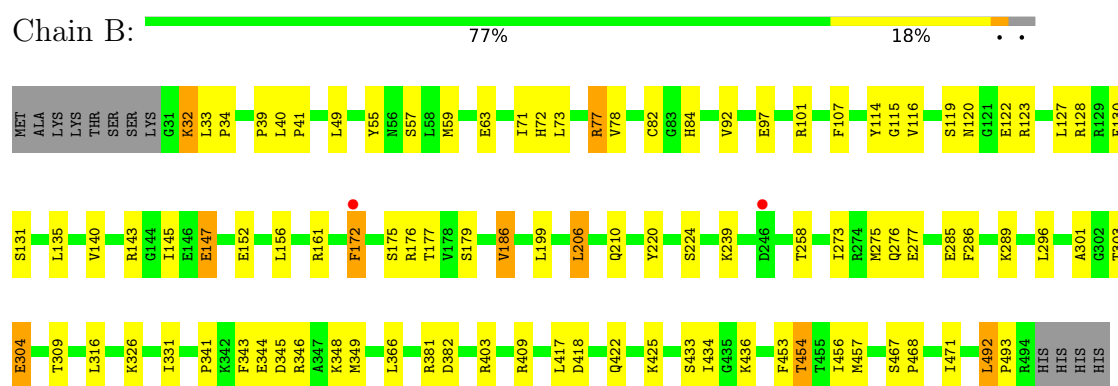
3 Residue-property plots

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 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.

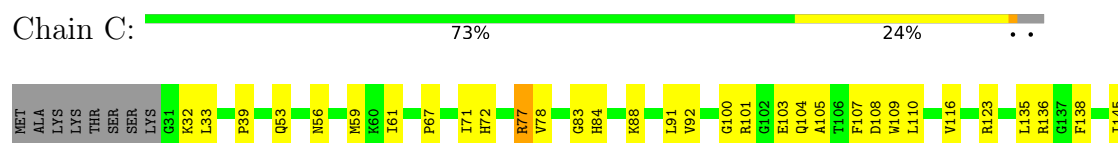
• Molecule 1: Cytochrome P450 2A13

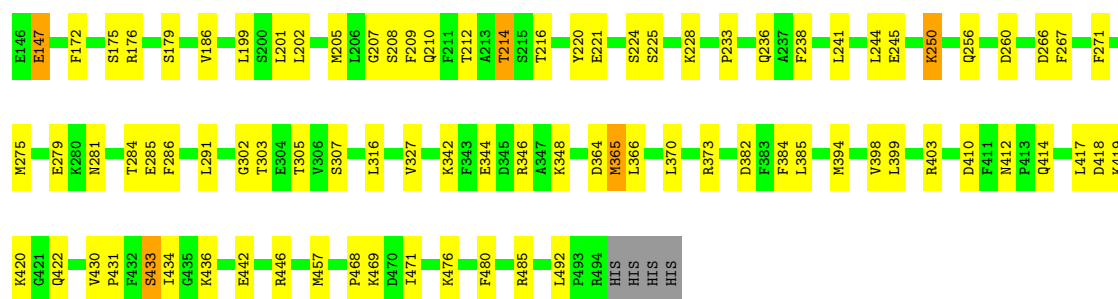


• Molecule 1: Cytochrome P450 2A13

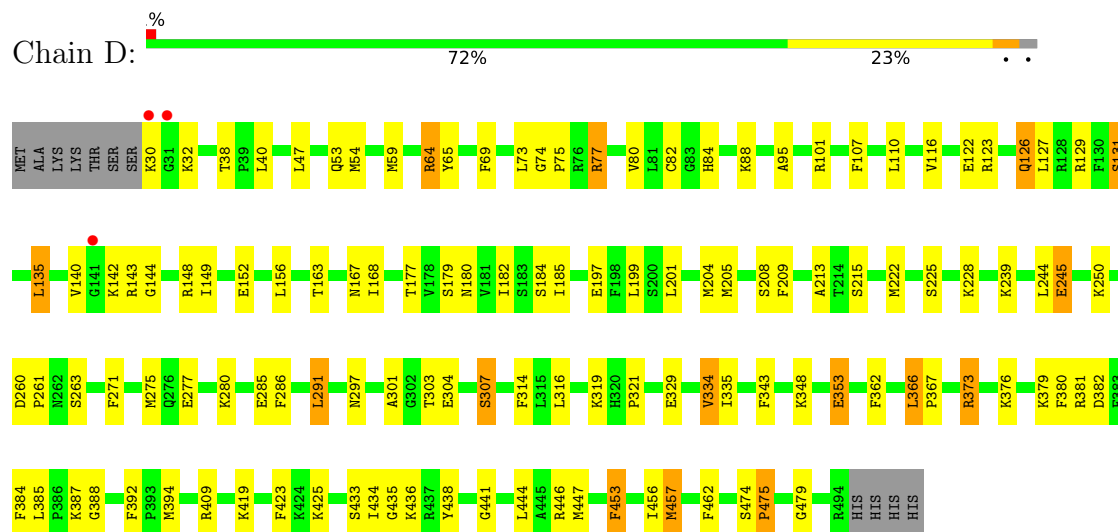


• Molecule 1: Cytochrome P450 2A13

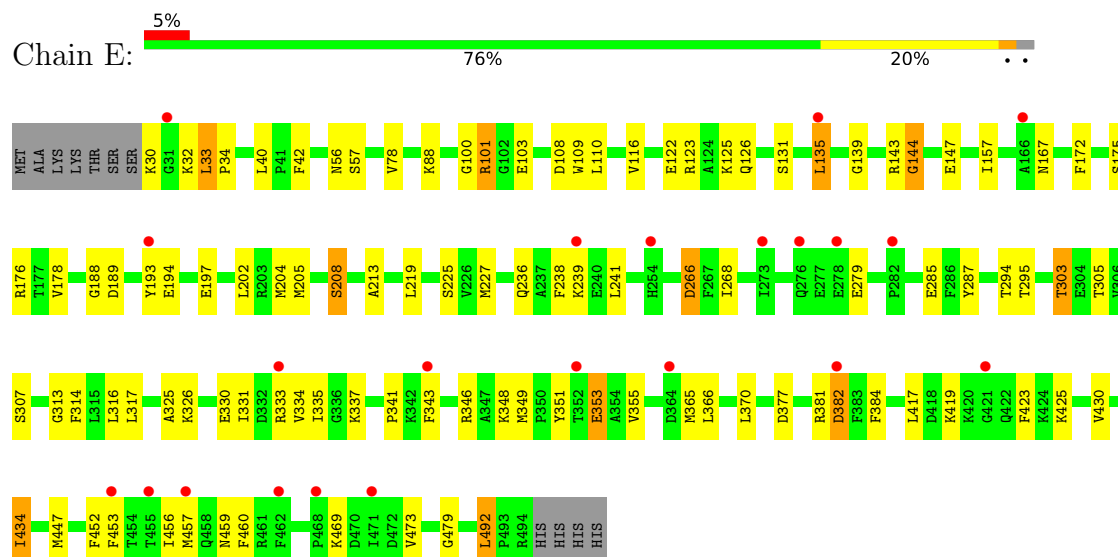




• Molecule 1: Cytochrome P450 2A13

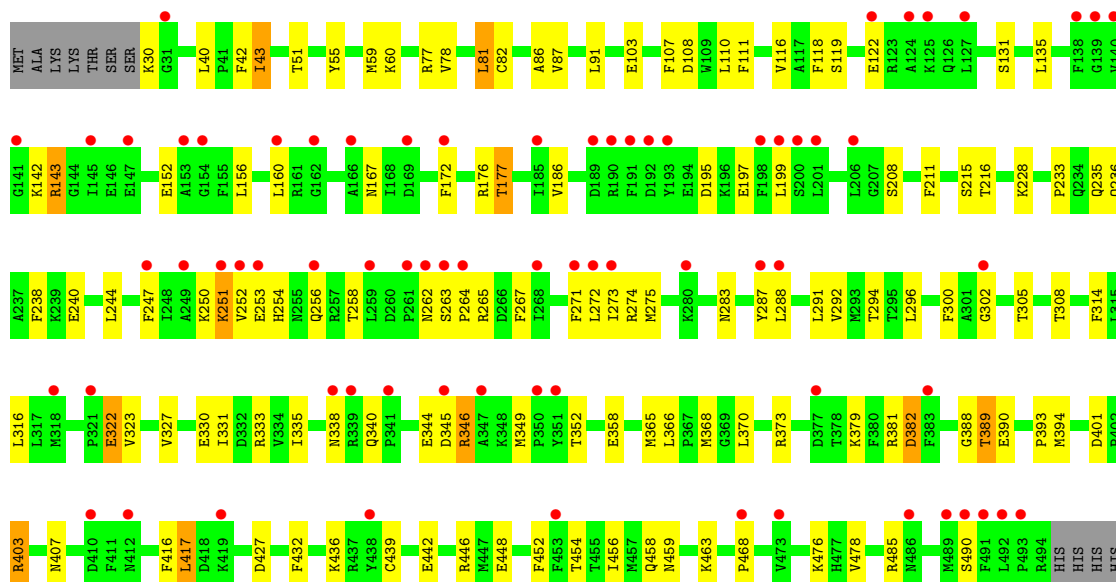


• Molecule 1: Cytochrome P450 2A13

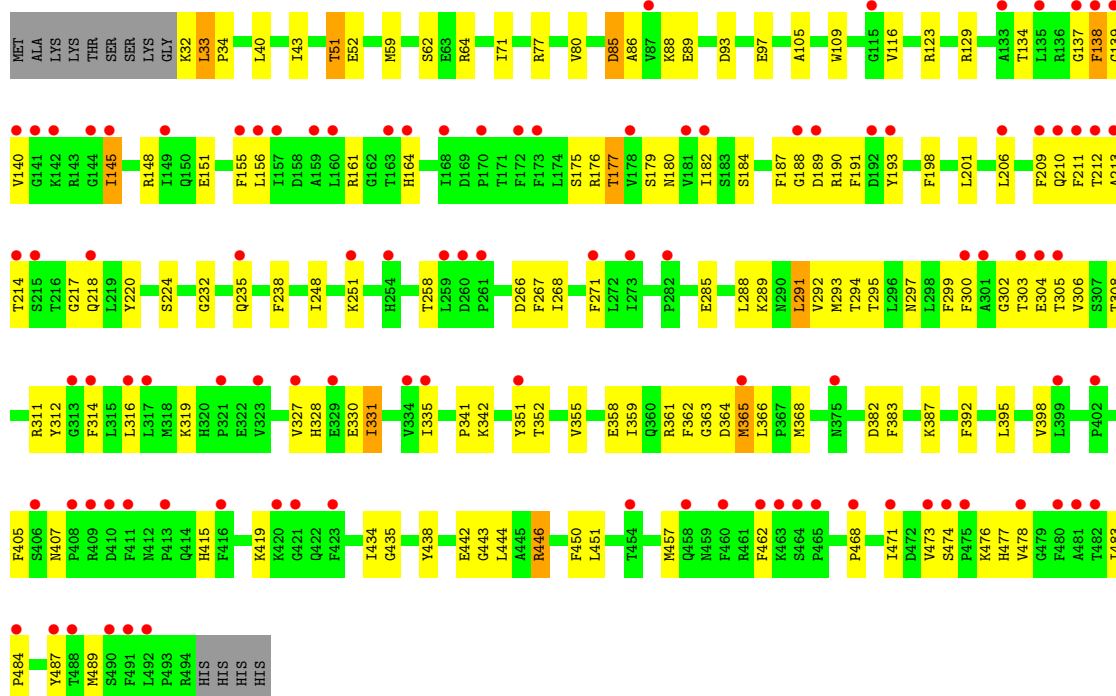


• Molecule 1: Cytochrome P450 2A13



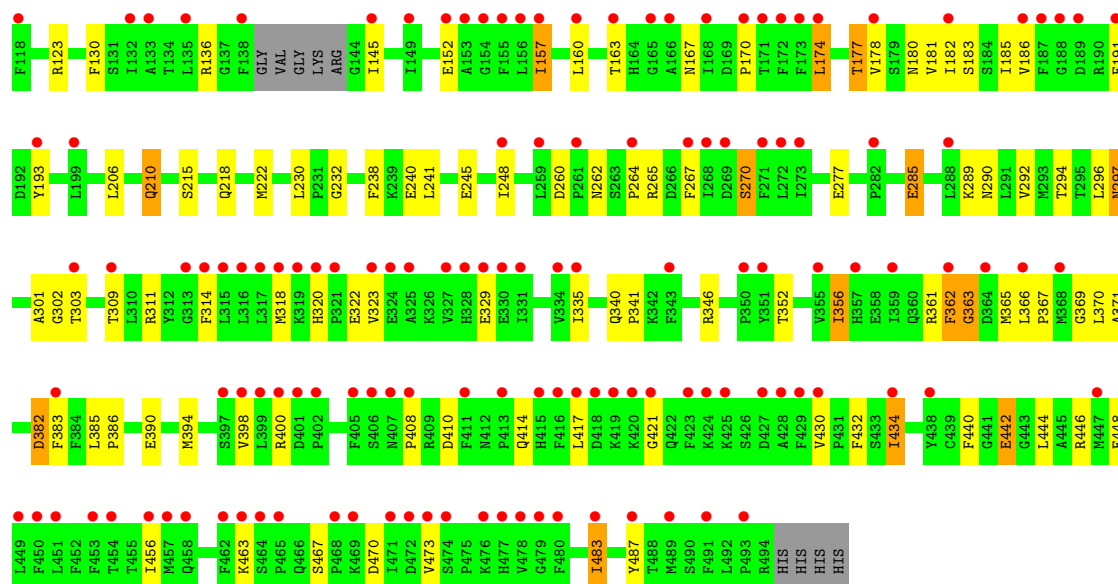


• Molecule 1: Cytochrome P450 2A13



• Molecule 1: Cytochrome P450 2A13





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.66Å 120.32Å 153.73Å 100.62° 101.82° 93.73°	Depositor
Resolution (Å)	102.58 – 2.50 102.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (102.58-2.50) 96.7 (102.58-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.52Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.224 , 0.285 0.222 , 0.285	Depositor DCC
R_{free} test set	8525 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30618	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% 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: NCT, HEM, 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	1.19	5/3869 (0.1%)	1.26	18/5210 (0.3%)
1	B	1.20	9/3909 (0.2%)	1.23	11/5262 (0.2%)
1	C	1.18	4/3898 (0.1%)	1.21	8/5248 (0.2%)
1	D	1.17	6/3897 (0.2%)	1.23	15/5246 (0.3%)
1	E	1.04	6/3898 (0.2%)	1.16	14/5246 (0.3%)
1	F	0.95	2/3869 (0.1%)	1.11	5/5209 (0.1%)
1	G	0.91	2/3832 (0.1%)	1.15	16/5166 (0.3%)
1	H	0.90	1/3780 (0.0%)	1.11	7/5094 (0.1%)
All	All	1.08	35/30952 (0.1%)	1.19	94/41681 (0.2%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	100	GLY	C-N	-9.65	1.20	1.33
1	H	483	ILE	CA-CB	6.72	1.59	1.54
1	G	214	THR	CA-CB	6.62	1.62	1.53
1	A	116	VAL	CA-CB	6.36	1.62	1.54
1	B	130	PHE	C-O	-6.34	1.16	1.24
1	E	101	ARG	C-N	-6.20	1.23	1.33
1	B	71	ILE	CA-C	6.02	1.59	1.52
1	F	42	PHE	C-O	-5.98	1.16	1.24
1	E	42	PHE	C-O	-5.93	1.16	1.24
1	D	47	LEU	N-CA	5.92	1.53	1.46
1	B	128	ARG	C-O	-5.78	1.17	1.24
1	D	475	PRO	N-CD	5.74	1.55	1.47
1	B	127	LEU	C-O	-5.64	1.17	1.24
1	D	380	PHE	C-O	-5.53	1.17	1.24
1	D	101	ARG	C-O	-5.50	1.17	1.24
1	F	43	ILE	C-O	-5.45	1.16	1.24
1	E	355	VAL	CA-CB	5.44	1.61	1.54
1	B	41	PRO	C-O	5.44	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	473	VAL	CA-CB	5.38	1.61	1.54
1	B	309	THR	CA-C	5.33	1.59	1.52
1	C	78	VAL	CA-CB	5.33	1.61	1.54
1	E	227	MET	C-O	-5.32	1.17	1.24
1	C	116	VAL	CA-CB	5.26	1.61	1.54
1	D	263	SER	CA-C	5.22	1.58	1.52
1	A	149	ILE	CA-CB	5.21	1.60	1.54
1	B	34	PRO	C-O	-5.18	1.18	1.24
1	A	101	ARG	C-N	-5.15	1.27	1.33
1	C	214	THR	CA-CB	5.09	1.61	1.53
1	G	164	HIS	CE1-NE2	5.06	1.37	1.32
1	C	433	SER	CA-C	5.05	1.59	1.52
1	D	149	ILE	CA-CB	5.05	1.60	1.54
1	A	77	ARG	CZ-NH2	-5.03	1.26	1.33
1	B	131	SER	C-O	-5.01	1.18	1.24
1	A	76	ARG	C-O	-5.00	1.17	1.24
1	B	186	VAL	CA-CB	5.00	1.60	1.54

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ARG	N-CA-C	8.79	120.94	111.36
1	A	32	LYS	N-CA-C	7.44	121.71	109.06
1	H	105	ALA	N-CA-C	7.44	120.04	111.11
1	B	120	ASN	N-CA-C	7.31	120.03	109.14
1	E	139	GLY	N-CA-C	7.04	124.50	114.64
1	G	366	LEU	CA-C-N	6.85	126.65	119.05
1	G	366	LEU	C-N-CA	6.85	126.65	119.05
1	A	270	SER	N-CA-C	-6.70	104.06	111.36
1	A	105	ALA	N-CA-C	6.63	118.51	111.28
1	A	304	GLU	N-CA-C	6.46	120.42	112.54
1	G	398	VAL	N-CA-C	-6.45	105.45	111.45
1	B	172	PHE	N-CA-C	6.37	119.21	111.82
1	G	161	ARG	N-CA-C	-6.36	106.15	114.04
1	A	247	PHE	N-CA-C	6.34	117.85	111.07
1	G	232	GLY	CA-C-N	6.34	127.76	119.84
1	G	232	GLY	C-N-CA	6.34	127.76	119.84
1	H	232	GLY	CA-C-N	6.30	127.72	119.84
1	H	232	GLY	C-N-CA	6.30	127.72	119.84
1	G	368	MET	N-CA-C	-6.26	104.95	112.59
1	D	373	ARG	O-C-N	-6.12	116.63	123.48
1	E	492	LEU	CA-C-N	6.11	126.14	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	492	LEU	C-N-CA	6.11	126.14	119.90
1	H	230	LEU	CA-C-N	-6.11	113.65	119.76
1	H	230	LEU	C-N-CA	-6.11	113.65	119.76
1	H	69	PHE	N-CA-C	6.05	118.32	108.76
1	B	304	GLU	N-CA-C	6.03	117.85	111.28
1	B	116	VAL	N-CA-C	5.99	116.63	110.82
1	D	144	GLY	N-CA-C	5.93	119.85	112.73
1	F	366	LEU	CA-C-N	5.78	125.64	119.28
1	F	366	LEU	C-N-CA	5.78	125.64	119.28
1	D	131	SER	N-CA-C	5.75	117.55	111.28
1	B	32	LYS	N-CA-C	5.73	118.90	109.85
1	A	260	ASP	CA-C-N	5.62	126.86	119.84
1	A	260	ASP	C-N-CA	5.62	126.86	119.84
1	A	292	VAL	N-CA-C	-5.62	105.05	110.72
1	B	492	LEU	CA-C-N	5.61	126.86	119.84
1	B	492	LEU	C-N-CA	5.61	126.86	119.84
1	A	221	GLU	N-CA-C	5.60	118.15	111.71
1	E	325	ALA	N-CA-C	5.60	117.07	110.97
1	A	392	PHE	CA-C-N	-5.58	112.87	119.84
1	A	392	PHE	C-N-CA	-5.58	112.87	119.84
1	G	331	ILE	CB-CA-C	-5.56	104.94	111.94
1	G	213	ALA	N-CA-C	5.54	117.00	111.07
1	C	260	ASP	CA-C-N	5.54	126.77	119.84
1	C	260	ASP	C-N-CA	5.54	126.77	119.84
1	A	362	PHE	CA-C-N	5.54	126.09	120.00
1	A	362	PHE	C-N-CA	5.54	126.09	120.00
1	D	129	ARG	N-CA-C	-5.53	105.33	111.36
1	G	407	ASN	CA-C-N	5.49	126.70	119.84
1	G	407	ASN	C-N-CA	5.49	126.70	119.84
1	H	87	VAL	N-CA-C	5.47	115.56	110.42
1	E	303	THR	N-CA-C	-5.45	106.68	113.55
1	G	40	LEU	CA-C-N	-5.43	114.13	119.99
1	G	40	LEU	C-N-CA	-5.43	114.13	119.99
1	C	207	GLY	CA-C-N	5.42	127.55	120.28
1	C	207	GLY	C-N-CA	5.42	127.55	120.28
1	E	337	LYS	N-CA-C	-5.42	105.32	113.89
1	B	345	ASP	CA-C-N	5.42	128.32	120.79
1	B	345	ASP	C-N-CA	5.42	128.32	120.79
1	A	69	PHE	N-CA-C	5.40	117.40	109.24
1	A	375	ASN	CB-CA-C	-5.38	101.69	110.85
1	G	489	MET	N-CA-C	5.37	117.24	109.07
1	D	69	PHE	N-CA-C	5.37	117.35	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	VAL	N-CA-C	5.37	116.01	108.17
1	A	295	THR	N-CA-C	-5.36	105.52	111.36
1	D	362	PHE	CA-C-N	5.36	125.93	119.98
1	D	362	PHE	C-N-CA	5.36	125.93	119.98
1	C	105	ALA	N-CA-C	5.36	117.12	111.28
1	A	398	VAL	N-CA-C	-5.35	106.48	111.45
1	F	119	SER	N-CA-C	5.35	116.12	108.74
1	B	78	VAL	N-CA-C	5.31	115.54	108.11
1	D	84	HIS	N-CA-C	5.29	117.74	111.33
1	D	453	PHE	N-CA-C	5.28	117.45	111.11
1	E	460	PHE	N-CA-C	5.26	117.39	109.23
1	G	105	ALA	N-CA-C	5.26	117.10	111.36
1	E	56	ASN	CA-C-N	5.25	127.31	120.28
1	E	56	ASN	C-N-CA	5.25	127.31	120.28
1	D	180	ASN	N-CA-C	5.20	117.86	111.82
1	D	334	VAL	N-CA-C	5.20	116.67	111.00
1	A	335	ILE	N-CA-C	5.20	116.36	111.48
1	E	266	ASP	N-CA-C	5.17	115.35	108.38
1	E	219	LEU	N-CA-C	-5.14	105.68	111.28
1	E	135	LEU	N-CA-C	5.14	116.57	111.07
1	G	86	ALA	N-CA-C	5.09	116.91	111.36
1	D	314	PHE	N-CA-C	-5.08	106.18	112.38
1	E	334	VAL	N-CA-C	5.08	116.06	111.13
1	D	307	SER	N-CA-C	5.06	116.48	111.07
1	F	454	THR	N-CA-C	5.04	116.86	111.36
1	D	47	LEU	N-CA-C	5.04	118.89	112.34
1	C	83	GLY	CA-C-N	5.03	127.27	120.38
1	C	83	GLY	C-N-CA	5.03	127.27	120.38
1	F	208	SER	N-CA-C	5.03	116.45	111.07
1	B	84	HIS	N-CA-C	5.01	119.64	111.37
1	C	398	VAL	N-CA-C	-5.00	106.80	111.45

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	3772	0	3735	56	0
1	B	3812	0	3771	48	0
1	C	3798	0	3762	58	0
1	D	3797	0	3764	63	0
1	E	3798	0	3773	45	0
1	F	3772	0	3741	77	0
1	G	3735	0	3670	82	0
1	H	3687	0	3614	57	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	0	0
2	H	43	0	30	2	0
3	A	12	0	14	3	0
3	B	12	0	14	3	0
3	C	12	0	14	3	0
3	D	12	0	14	3	0
4	H	6	0	8	1	0
5	A	9	0	0	0	0
5	B	5	0	0	1	0
5	C	6	0	0	0	0
5	D	14	0	0	1	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	9	0	0	1	0
5	H	2	0	0	0	0
All	All	30618	0	30134	488	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 8.

All (488) 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:59:MET:HE1	1:A:82:CYS:SG	1.81	1.18
1:C:32:LYS:HD2	1:C:33:LEU:H	1.19	1.07
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.23	1.03
1:B:32:LYS:HD2	1:B:33:LEU:H	1.25	0.96
1:C:32:LYS:HD2	1:C:33:LEU:N	1.81	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:MET:HG2	1:F:394:MET:HE1	1.52	0.91
1:H:352:THR:O	1:H:356:ILE:HD13	1.72	0.90
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.37	0.89
1:G:476:LYS:HG3	1:G:477:HIS:H	1.39	0.87
1:G:457:MET:HE2	1:G:462:PHE:HE2	1.39	0.85
1:F:403:ARG:HG3	1:F:403:ARG:HH11	1.40	0.85
1:G:190:ARG:HH22	1:G:193:TYR:HE1	1.23	0.84
1:F:186:VAL:HA	1:F:267:PHE:HB3	1.58	0.84
1:A:53[B]:GLN:HG3	1:A:56:ASN:HB2	1.62	0.82
1:F:172:PHE:O	1:F:176:ARG:HG3	1.80	0.81
1:A:376:LYS:HA	1:A:387:LYS:HG3	1.62	0.81
1:H:215:SER:HB3	4:H:502:GOL:H2	1.61	0.81
1:A:216:THR:HG21	1:A:233:PRO:HG2	1.61	0.80
1:G:305:THR:HG22	1:G:365:MET:HG3	1.63	0.79
1:D:54:MET:HE1	1:D:222:MET:HE2	1.64	0.78
1:E:205:MET:HE1	1:E:303:THR:HG21	1.64	0.78
1:A:271:PHE:HB3	1:A:291:LEU:HD22	1.66	0.77
1:F:305:THR:HA	1:F:365:MET:CE	2.14	0.77
1:F:253:GLU:HA	1:F:256:GLN:OE1	1.85	0.77
1:G:190:ARG:NH2	1:G:193:TYR:HE1	1.83	0.76
1:F:308:THR:HB	1:F:365:MET:HE1	1.67	0.76
1:D:381:ARG:O	1:D:382:ASP:HB2	1.86	0.76
1:E:33:LEU:HD12	1:E:34:PRO:HD2	1.67	0.75
1:E:303:THR:O	1:E:307:SER:HB2	1.87	0.75
1:F:305:THR:HA	1:F:365:MET:HE2	1.67	0.74
1:G:442:GLU:OE2	1:G:446:ARG:NH1	2.20	0.74
1:B:32:LYS:HD2	1:B:33:LEU:N	2.02	0.74
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.70	0.74
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.52	0.73
1:F:442:GLU:O	1:F:446:ARG:HG3	1.89	0.73
1:G:311:ARG:HH11	1:G:484:PRO:HD2	1.54	0.72
1:G:140:VAL:HG21	1:G:444:LEU:HB2	1.70	0.72
1:H:170:PRO:O	1:H:174:LEU:HB2	1.88	0.72
1:C:92:VAL:HG23	1:C:434:ILE:HD12	1.70	0.71
1:B:273:ILE:O	1:B:277:GLU:HG3	1.91	0.71
1:E:101:ARG:NH1	1:E:370:LEU:HB3	2.05	0.70
1:F:216:THR:HG21	1:F:233:PRO:HG2	1.73	0.70
1:C:364:ASP:OD1	1:C:399:LEU:HD12	1.92	0.69
1:A:59:MET:CE	1:A:82:CYS:SG	2.73	0.69
1:H:51:THR:HG23	1:H:218:GLN:HG3	1.73	0.69
1:F:186:VAL:HA	1:F:267:PHE:CB	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53[B]:GLN:HG3	1:C:56:ASN:HB2	1.75	0.68
1:C:303:THR:O	1:C:307:SER:HB2	1.94	0.67
1:B:172:PHE:O	1:B:176[B]:ARG:HG3	1.94	0.67
1:G:182:ILE:HD11	1:G:302:GLY:C	2.19	0.67
1:H:59:MET:C	1:H:61:ILE:H	2.01	0.67
1:A:101:ARG:NH1	1:A:370:LEU:HB3	2.09	0.67
1:H:365:MET:O	1:H:367:PRO:HD3	1.94	0.67
1:C:216:THR:HG21	1:C:233:PRO:HG2	1.77	0.66
1:H:366:LEU:HB3	1:H:369:GLY:HA2	1.77	0.66
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.01	0.66
1:B:179:SER:HB2	1:B:303:THR:HG23	1.76	0.66
1:G:209:PHE:HE2	1:G:300:PHE:HD1	1.41	0.65
1:G:156:LEU:HB2	1:G:177:THR:HG21	1.79	0.65
1:E:101:ARG:HH12	1:E:370:LEU:HB3	1.60	0.65
1:H:123:ARG:HA	1:H:285:GLU:HG2	1.80	0.64
1:E:331:ILE:HG23	1:E:335:ILE:HD12	1.78	0.64
1:G:88:LYS:HE2	5:G:603:HOH:O	1.96	0.64
1:B:92:VAL:HG23	1:B:434:ILE:HD12	1.80	0.64
1:G:209:PHE:CE2	1:G:300:PHE:HD1	2.15	0.63
1:F:40:LEU:HD22	1:F:43:ILE:HD11	1.79	0.63
1:H:180:ASN:OD1	1:H:191:PHE:HB2	1.98	0.63
1:H:248:ILE:HG22	1:H:292:VAL:HG13	1.80	0.63
1:A:59:MET:HE3	1:A:394:MET:HE3	1.81	0.62
1:B:206:LEU:O	1:B:210[B]:GLN:HG3	1.99	0.62
1:H:356:ILE:N	1:H:356:ILE:CD1	2.62	0.62
1:F:403:ARG:HH11	1:F:403:ARG:CG	2.09	0.62
1:G:351:TYR:O	1:G:355:VAL:HG23	2.00	0.61
1:C:107:PHE:CE1	3:C:501:NCT:HC4	2.35	0.61
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.81	0.61
1:G:116:VAL:CG1	1:G:294:THR:HG23	2.31	0.61
1:G:311:ARG:NH1	1:G:484:PRO:HD2	2.15	0.61
1:D:280:LYS:HE3	5:D:612:HOH:O	2.00	0.61
1:G:327:VAL:HG21	1:G:355:VAL:HG21	1.83	0.61
1:A:143:ARG:O	1:A:147:GLU:HG2	2.00	0.61
1:H:240:GLU:OE1	1:H:240:GLU:HA	2.01	0.61
1:D:209:PHE:CD2	1:D:304:GLU:HG3	2.36	0.61
1:D:271:PHE:CD1	1:D:291:LEU:HB2	2.36	0.61
1:D:64:ARG:HG2	1:D:65:TYR:CE2	2.36	0.60
1:A:381:ARG:O	1:A:382:ASP:HB2	2.01	0.60
1:B:101:ARG:NH1	2:B:500:HEM:O2A	2.31	0.60
1:D:376:LYS:HA	1:D:387:LYS:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PRO:HG3	1:B:72:HIS:CE1	2.37	0.60
1:H:180:ASN:HA	1:H:183:SER:HB2	1.83	0.60
1:D:142:LYS:HG2	1:D:143:ARG:N	2.17	0.59
1:F:403:ARG:HG3	1:F:403:ARG:O	2.01	0.59
1:G:64:ARG:O	1:G:64:ARG:HG3	2.02	0.59
1:B:206:LEU:HD12	1:B:304:GLU:OE2	2.02	0.59
1:G:355:VAL:O	1:G:359:ILE:HG12	2.02	0.59
1:A:351:TYR:O	1:A:355:VAL:HG23	2.02	0.59
1:G:176:ARG:O	1:G:180:ASN:ND2	2.33	0.59
3:C:501:NCT:HC3	3:C:501:NCT:H102	1.84	0.59
1:G:175:SER:O	1:G:179:SER:HB2	2.02	0.59
1:B:143:ARG:O	1:B:147:GLU:HG2	2.03	0.59
5:B:605:HOH:O	1:C:403:ARG:HD2	2.01	0.59
1:F:432:PHE:HB3	1:F:439:CYS:HB3	1.84	0.59
1:G:235:GLN:OE1	1:G:238:PHE:HD2	1.85	0.59
1:C:59:MET:CE	1:C:394:MET:HE2	2.32	0.59
1:A:452:PHE:O	1:A:456:ILE:HD12	2.03	0.58
1:B:122:GLU:OE1	1:B:122:GLU:HA	2.01	0.58
1:C:202:LEU:HD23	1:C:205:MET:HE3	1.85	0.58
1:C:305:THR:HG22	1:C:365:MET:HE2	1.84	0.58
1:E:172:PHE:O	1:E:176:ARG:HG3	2.04	0.58
1:A:59:MET:HE3	1:A:394:MET:CE	2.34	0.58
1:A:107:PHE:CZ	3:A:501:NCT:HC4	2.38	0.58
1:G:116:VAL:HG12	1:G:294:THR:HG23	1.85	0.58
1:B:107:PHE:CE1	3:B:501:NCT:HC4	2.38	0.58
1:A:271:PHE:HB3	1:A:291:LEU:CD2	2.33	0.58
1:D:59:MET:HE3	1:D:394:MET:HE3	1.86	0.57
1:F:368:MET:HG2	1:F:394:MET:CE	2.28	0.57
1:C:172:PHE:O	1:C:176:ARG:HG3	2.03	0.57
1:F:152:GLU:HG3	1:F:177:THR:HG22	1.86	0.57
1:G:457:MET:HE2	1:G:462:PHE:CE2	2.30	0.57
1:G:312:TYR:O	1:G:316:LEU:HD12	2.05	0.57
1:A:271:PHE:CG	1:A:291:LEU:HD22	2.39	0.57
1:G:34:PRO:HD3	1:G:383:PHE:HB3	1.87	0.57
1:D:179:SER:HB2	1:D:303:THR:HG23	1.86	0.57
1:C:100:GLY:HA3	1:C:373:ARG:O	2.05	0.56
1:D:201:LEU:HA	1:D:204:MET:HE3	1.87	0.56
1:E:335:ILE:HD13	1:E:341:PRO:HB3	1.87	0.56
1:A:271:PHE:CB	1:A:291:LEU:HD22	2.34	0.56
1:E:123:ARG:HA	1:E:285:GLU:HG3	1.86	0.56
1:H:109:TRP:CH2	1:H:238:PHE:HB3	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:LEU:O	1:H:448:GLU:HG3	2.06	0.56
1:A:313:GLY:O	1:A:317:LEU:HG	2.05	0.56
1:G:335:ILE:HD13	1:G:341:PRO:HB3	1.88	0.56
1:D:301:ALA:HB2	3:D:501:NCT:HC6	1.88	0.55
1:E:313:GLY:O	1:E:317:LEU:HG	2.06	0.55
1:B:49:LEU:HD23	1:B:57:SER:HB3	1.88	0.55
1:B:453:PHE:O	1:B:457:MET:HG3	2.07	0.55
1:C:209:PHE:HZ	1:C:365:MET:CE	2.19	0.55
1:F:302:GLY:HA2	2:F:500:HEM:HMC2	1.88	0.55
1:G:473:VAL:HG23	1:G:474:SER:H	1.71	0.55
1:G:139:GLY:HA2	1:G:145:ILE:HB	1.88	0.55
1:G:211:PHE:CZ	1:G:217:GLY:HA2	2.41	0.55
1:A:366:LEU:HD12	2:A:500:HEM:HMA3	1.89	0.55
1:D:213:ALA:HA	1:D:479:GLY:HA3	1.88	0.55
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.89	0.55
1:A:464:SER:HB2	1:A:465:PRO:HD2	1.89	0.54
1:E:331:ILE:HG12	1:E:349:MET:HE1	1.88	0.54
1:A:355:VAL:O	1:A:359:ILE:HG13	2.08	0.54
1:G:442:GLU:CD	1:G:446:ARG:HH11	2.15	0.54
1:C:175:SER:O	1:C:179:SER:HB2	2.08	0.54
1:A:305:THR:HA	1:A:365:MET:HE2	1.89	0.54
1:E:381:ARG:O	1:E:382:ASP:OD2	2.25	0.54
1:H:311:ARG:HH12	1:H:483:ILE:HG23	1.72	0.54
1:C:103:GLU:HB2	1:C:108:ASP:OD2	2.08	0.54
1:D:182:ILE:HA	1:D:185:ILE:HD12	1.89	0.54
1:D:95:ALA:HB1	1:D:436:LYS:HG2	1.89	0.53
1:E:430:VAL:HG11	1:E:434:ILE:HD13	1.90	0.53
1:A:89:GLU:OE1	1:A:381:ARG:NE	2.38	0.53
1:D:435:GLY:O	1:D:438:TYR:HD1	1.91	0.53
1:E:305:THR:HA	1:E:365:MET:CE	2.39	0.53
1:F:358:GLU:HA	1:F:358:GLU:OE1	2.08	0.53
1:G:294:THR:O	1:G:297:ASN:HB2	2.09	0.53
1:B:32:LYS:CD	1:B:33:LEU:H	2.12	0.53
1:F:448:GLU:O	1:F:452:PHE:HD2	1.91	0.53
1:F:59:MET:HA	1:F:59:MET:HE2	1.91	0.53
1:A:354:ALA:HB2	1:A:417:LEU:HD13	1.91	0.52
1:F:458:GLN:HG3	1:F:459:ASN:N	2.23	0.52
1:F:296:LEU:O	1:F:300:PHE:HB2	2.09	0.52
1:F:302:GLY:HA2	2:F:500:HEM:CMC	2.39	0.52
1:H:110:LEU:HD22	1:H:241:LEU:HB3	1.91	0.52
1:C:302:GLY:HA2	2:C:500:HEM:HMC3	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:ARG:HD3	1:G:184:SER:OG	2.10	0.52
1:A:357:HIS:NE2	1:A:446:ARG:NH2	2.57	0.52
1:C:430:VAL:N	1:C:431:PRO:CD	2.73	0.52
1:E:33:LEU:HD12	1:E:34:PRO:CD	2.36	0.52
1:C:39:PRO:HG3	1:C:72:HIS:CE1	2.45	0.52
1:E:326:LYS:HB2	1:E:351:TYR:CE1	2.44	0.52
1:H:59:MET:C	1:H:61:ILE:N	2.65	0.52
1:A:409:ARG:HH11	1:A:409:ARG:HB3	1.75	0.52
1:B:172:PHE:O	1:B:176[A]:ARG:HB2	2.10	0.52
1:C:109:TRP:CH2	1:C:238:PHE:HB3	2.45	0.52
1:C:342:LYS:HG3	1:C:344:GLU:HG2	1.92	0.52
1:F:416:PHE:O	1:F:417:LEU:HD13	2.09	0.52
1:A:172:PHE:O	1:A:176:ARG:HG3	2.10	0.52
1:H:101:ARG:HD3	1:H:371:ALA:O	2.10	0.52
1:A:145:ILE:HD11	1:A:185:ILE:HD11	1.91	0.51
1:A:381:ARG:O	1:A:382:ASP:CB	2.58	0.51
1:C:136:ARG:NH1	1:D:277:GLU:OE2	2.41	0.51
1:A:271:PHE:CD1	1:A:291:LEU:HD22	2.46	0.51
1:F:247:PHE:CZ	1:F:251:LYS:HG2	2.45	0.51
1:G:51:THR:HG23	1:G:218:GLN:HB2	1.92	0.51
1:E:452:PHE:O	1:E:456:ILE:HG13	2.10	0.51
1:H:206:LEU:O	1:H:210:GLN:HB2	2.10	0.51
1:C:271:PHE:CE1	1:C:291:LEU:HB2	2.45	0.51
1:G:363:GLY:O	1:G:365:MET:HE2	2.11	0.51
1:C:250:LYS:HB2	1:C:250:LYS:NZ	2.25	0.51
1:E:305:THR:HA	1:E:365:MET:HE2	1.92	0.51
1:G:123:ARG:HA	1:G:285:GLU:HG3	1.93	0.51
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.76	0.51
1:E:109:TRP:CH2	1:E:238:PHE:HB3	2.46	0.51
1:F:211:PHE:HE1	1:F:233:PRO:HB2	1.76	0.51
1:F:107:PHE:O	1:F:111:PHE:HD2	1.94	0.51
1:E:188:GLY:N	1:E:266:ASP:HB3	2.26	0.51
1:C:61:ILE:HD13	1:C:71:ILE:HD13	1.92	0.50
1:D:122:GLU:O	1:D:126:GLN:HB2	2.11	0.50
1:E:305:THR:HB	2:E:500:HEM:CAB	2.42	0.50
1:F:40:LEU:CD2	1:F:43:ILE:HD11	2.41	0.50
1:H:78:VAL:HG22	1:H:390:GLU:HB2	1.92	0.50
1:G:405:PHE:HD1	1:G:415:HIS:HB3	1.77	0.50
1:H:302:GLY:HA2	2:H:501:HEM:CMC	2.41	0.50
1:D:140:VAL:HG13	1:D:444:LEU:HD13	1.92	0.50
1:D:453:PHE:O	1:D:457:MET:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:356:ILE:N	1:H:356:ILE:HD12	2.27	0.50
1:F:59:MET:HE1	1:F:82:CYS:SG	2.52	0.50
1:B:156:LEU:CD2	1:B:456:ILE:HD11	2.42	0.50
1:G:138:PHE:N	1:G:138:PHE:CD2	2.79	0.50
1:F:271:PHE:CD1	1:F:291:LEU:HB2	2.47	0.50
1:D:205:MET:HE1	1:D:303:THR:HG21	1.94	0.50
1:E:343:PHE:CD2	1:E:447:MET:HE2	2.47	0.50
1:C:209:PHE:HZ	1:C:365:MET:HE3	1.75	0.49
1:F:118:PHE:HE1	1:F:370:LEU:HD11	1.77	0.49
1:G:365:MET:HE2	1:G:365:MET:HA	1.94	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.94	0.49
1:E:202:LEU:HA	1:E:205:MET:HE2	1.94	0.49
1:G:89:GLU:O	1:G:93:ASP:HB2	2.12	0.49
1:B:114:TYR:CD1	1:B:289:LYS:HE3	2.47	0.49
1:A:161:ARG:C	1:A:163:THR:H	2.20	0.49
1:H:88:LYS:HG2	1:H:434:ILE:HD13	1.93	0.49
1:H:152:GLU:HG3	1:H:177:THR:HG22	1.95	0.49
1:H:414:GLN:OE1	1:H:417:LEU:HD12	2.13	0.49
1:E:131:SER:O	1:E:135:LEU:HB2	2.11	0.49
1:D:384:PHE:C	1:D:385:LEU:HD12	2.37	0.49
1:F:55:TYR:CE1	1:F:59:MET:HG3	2.48	0.49
1:A:76:ARG:NH1	1:A:221:GLU:O	2.45	0.49
1:C:412:ASN:HD21	1:C:414:GLN:HB2	1.78	0.49
1:D:441:GLY:HA2	2:D:500:HEM:HBC2	1.95	0.49
1:G:140:VAL:CG2	1:G:444:LEU:HB2	2.40	0.49
1:G:188:GLY:H	1:G:266:ASP:HB3	1.77	0.49
1:H:440:PHE:HD1	1:H:440:PHE:O	1.96	0.49
1:A:209:PHE:HZ	1:A:365:MET:HE3	1.78	0.48
1:B:115:GLY:O	1:B:119:SER:HB3	2.13	0.48
1:H:309:THR:HA	1:H:365:MET:HE3	1.95	0.48
1:A:146:GLU:OE2	1:A:342:LYS:HB2	2.14	0.48
1:B:63:GLU:O	1:C:67:PRO:HG3	2.13	0.48
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.95	0.48
1:C:77:ARG:HH11	1:C:77:ARG:CG	2.21	0.48
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.95	0.48
1:H:440:PHE:O	1:H:440:PHE:CD1	2.67	0.48
1:C:84:HIS:NE2	1:C:88:LYS:HD3	2.28	0.48
1:D:225:SER:HA	1:D:228:LYS:HE2	1.96	0.48
1:F:327:VAL:O	1:F:331:ILE:HG13	2.13	0.48
1:F:381:ARG:O	1:F:382:ASP:HB2	2.14	0.48
1:B:275:MET:HG2	1:B:286:PHE:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:HA	1:C:267:PHE:HB3	1.95	0.47
1:D:107:PHE:CZ	3:D:501:NCT:HC4	2.48	0.47
1:G:187:PHE:HZ	1:G:248:ILE:HD13	1.79	0.47
1:G:271:PHE:CD1	1:G:291:LEU:HB2	2.48	0.47
1:G:316:LEU:HD21	1:G:362:PHE:CD2	2.49	0.47
1:H:73:LEU:HB3	1:H:222:MET:HG2	1.95	0.47
1:A:85:ASP:O	1:A:89:GLU:HB2	2.15	0.47
1:C:275:MET:HG2	1:C:286:PHE:O	2.15	0.47
1:G:189:ASP:OD1	1:G:190:ARG:N	2.45	0.47
1:A:107:PHE:CE2	3:A:501:NCT:HC4	2.50	0.47
1:B:156:LEU:HD21	1:B:456:ILE:HD11	1.95	0.47
1:G:33:LEU:HD21	1:G:77:ARG:HD2	1.96	0.47
1:A:84:HIS:CE1	1:A:88:LYS:HD3	2.50	0.47
1:F:314:PHE:HZ	1:F:456:ILE:HD13	1.78	0.47
1:A:310:LEU:HD23	1:A:453:PHE:CE1	2.49	0.47
1:E:343:PHE:CE1	1:E:346:ARG:HD3	2.49	0.47
1:A:53[B]:GLN:HG3	1:A:56:ASN:CB	2.40	0.47
1:E:377:ASP:HB3	1:E:384:PHE:CE1	2.49	0.47
1:F:143:ARG:C	1:F:143:ARG:HD2	2.40	0.47
1:F:235:GLN:OE1	1:F:238:PHE:HD2	1.97	0.47
1:F:322:GLU:CD	1:F:322:GLU:H	2.23	0.47
1:G:182:ILE:HD11	1:G:302:GLY:O	2.15	0.47
1:H:186:VAL:HA	1:H:267:PHE:HB2	1.96	0.47
1:D:334:VAL:HG12	1:D:335:ILE:HG13	1.97	0.47
1:G:193:TYR:HD1	1:G:193:TYR:N	2.13	0.47
1:G:288:LEU:O	1:G:292:VAL:HG23	2.14	0.47
1:D:53[B]:GLN:C	1:D:53[B]:GLN:OE1	2.57	0.47
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.97	0.47
1:B:59:MET:HE2	1:B:59:MET:HA	1.97	0.46
1:D:131:SER:O	1:D:135:LEU:HB2	2.15	0.46
1:F:211:PHE:CE1	1:F:233:PRO:HB2	2.50	0.46
1:G:268:ILE:HG23	1:G:291:LEU:HD11	1.96	0.46
1:H:88:LYS:HE3	1:H:434:ILE:HG21	1.96	0.46
1:A:464:SER:C	1:A:466:GLN:H	2.24	0.46
1:F:152:GLU:HG3	1:F:177:THR:CG2	2.45	0.46
1:G:193:TYR:N	1:G:193:TYR:CD1	2.83	0.46
1:B:301:ALA:HB2	3:B:501:NCT:HC6	1.98	0.46
1:H:262:ASN:O	1:H:264:PRO:HD3	2.15	0.46
1:B:72:HIS:NE2	1:B:77:ARG:HD3	2.31	0.46
1:D:343:PHE:CE1	1:D:447:MET:HA	2.51	0.46
1:G:358:GLU:OE2	1:G:361:ARG:NH2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HD11	1:D:245:GLU:HB2	1.98	0.46
1:E:204:MET:O	1:E:208:SER:HB2	2.16	0.46
1:G:450:PHE:HD2	1:G:451:LEU:HD23	1.79	0.46
1:E:285:GLU:HA	1:E:287:TYR:CE2	2.51	0.46
1:F:51:THR:OG1	1:F:215:SER:HB2	2.15	0.46
1:A:59:MET:HA	1:A:59:MET:HE2	1.98	0.46
1:D:474:SER:HB2	1:D:475:PRO:HD2	1.98	0.46
1:F:448:GLU:O	1:F:452:PHE:CD2	2.68	0.46
1:A:248:ILE:HG22	1:A:292:VAL:HG13	1.97	0.46
1:G:191:PHE:CD1	1:G:198:PHE:HB2	2.51	0.45
1:B:140:VAL:HA	1:B:145:ILE:HG21	1.98	0.45
1:B:344:GLU:C	1:B:346:ARG:H	2.23	0.45
1:H:301:ALA:O	2:H:501:HEM:C1C	2.70	0.45
1:D:156:LEU:CD2	1:D:456:ILE:HD11	2.46	0.45
1:H:77:ARG:NH2	1:H:386:PRO:HG2	2.30	0.45
1:C:104:GLN:NE2	1:C:221:GLU:OE2	2.49	0.45
1:D:54:MET:HE1	1:D:222:MET:CE	2.42	0.45
1:D:319:LYS:O	1:D:319:LYS:HG3	2.16	0.45
2:E:500:HEM:HMB2	2:E:500:HEM:HBB2	1.99	0.45
1:G:266:ASP:HB2	1:G:267:PHE:H	1.62	0.45
1:G:327:VAL:CG2	1:G:355:VAL:HG21	2.47	0.45
1:H:265:ARG:HB3	1:H:265:ARG:CZ	2.46	0.45
1:D:275:MET:HG2	1:D:286:PHE:O	2.16	0.45
1:F:156:LEU:O	1:F:160:LEU:N	2.49	0.45
1:H:260:ASP:OD1	1:H:262:ASN:HB2	2.16	0.45
1:B:97[A]:GLU:CD	1:B:97[A]:GLU:H	2.25	0.45
1:C:201:LEU:HD22	1:C:244:LEU:HD23	1.99	0.45
1:D:123:ARG:O	1:D:127:LEU:HG	2.17	0.45
1:F:373:ARG:NH1	1:F:388:GLY:O	2.48	0.45
1:G:182:ILE:HD13	1:G:299:PHE:HA	1.99	0.45
1:H:432:PHE:CG	1:H:442:GLU:HG3	2.52	0.45
1:A:301:ALA:HB2	3:A:501:NCT:HC6	1.98	0.45
1:C:110:LEU:HD22	1:C:241:LEU:HB3	1.99	0.45
1:C:220:TYR:O	1:C:224:SER:HB3	2.17	0.45
1:C:365:MET:HG3	1:C:366:LEU:HD13	1.99	0.45
1:F:82:CYS:O	1:F:86:ALA:HB3	2.17	0.45
1:G:450:PHE:CD2	1:G:451:LEU:HD23	2.52	0.45
1:H:290:ASN:O	1:H:294:THR:OG1	2.30	0.44
1:G:193:TYR:HD1	1:G:193:TYR:H	1.64	0.44
1:A:342:LYS:O	1:A:345:ASP:HB2	2.17	0.44
1:F:403:ARG:CG	1:F:403:ARG:O	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:VAL:HG22	1:G:392:PHE:HB2	1.99	0.44
1:G:206:LEU:O	1:G:210:GLN:HB2	2.18	0.44
1:A:101:ARG:HD3	1:A:371:ALA:O	2.18	0.44
1:B:418:ASP:OD2	1:B:422:GLN:HB2	2.17	0.44
1:C:101:ARG:NH1	2:C:500:HEM:O2A	2.45	0.44
1:E:314:PHE:HE1	1:E:453:PHE:CE1	2.36	0.44
1:E:423:PHE:CE2	1:E:425:LYS:HG2	2.52	0.44
1:F:240:GLU:O	1:F:244:LEU:HG	2.18	0.44
1:F:258:THR:O	1:F:265:ARG:NH2	2.50	0.44
1:G:220:TYR:CE1	1:G:224:SER:HB3	2.52	0.44
1:G:330:GLU:OE2	1:G:352:THR:N	2.51	0.44
1:H:178:VAL:CG1	1:H:303:THR:HA	2.48	0.44
1:H:398:VAL:C	1:H:400:ARG:H	2.26	0.44
1:C:101:ARG:O	1:C:373:ARG:HG2	2.17	0.44
1:F:403:ARG:CG	1:F:403:ARG:NH1	2.73	0.44
1:A:332:ASP:OD2	1:A:494:ARG:NH2	2.46	0.44
1:H:340:GLN:HA	1:H:341:PRO:HD3	1.78	0.44
1:D:107:PHE:CE2	3:D:501:NCT:HC4	2.53	0.44
1:D:205:MET:HG3	1:D:244:LEU:HD11	2.00	0.44
1:D:156:LEU:HD23	1:D:456:ILE:HD11	2.00	0.44
1:H:181:VAL:O	1:H:185:ILE:HG13	2.18	0.44
1:C:327:VAL:HG11	1:C:457:MET:CE	2.48	0.44
1:F:78:VAL:HG22	1:F:390:GLU:HB2	2.00	0.44
1:F:288:LEU:O	1:F:292:VAL:HG23	2.18	0.44
1:F:401:ASP:C	1:F:403:ARG:H	2.25	0.44
1:A:103:GLU:HB2	1:A:108:ASP:OD2	2.18	0.43
1:D:148:ARG:HD3	1:D:184:SER:OG	2.17	0.43
1:E:157:ILE:HD12	1:E:459:ASN:HB2	2.00	0.43
1:G:476:LYS:HG3	1:G:477:HIS:N	2.18	0.43
1:A:419:LYS:HD2	1:A:419:LYS:HA	1.88	0.43
1:B:381:ARG:O	1:B:382:ASP:CB	2.66	0.43
1:G:235:GLN:OE1	1:G:238:PHE:CD2	2.68	0.43
3:C:501:NCT:C10	3:C:501:NCT:C3	2.96	0.43
1:G:442:GLU:O	1:G:443:GLY:C	2.61	0.43
1:H:136:ARG:HE	1:H:136:ARG:HA	1.83	0.43
1:D:457:MET:HE3	1:D:462:PHE:CZ	2.54	0.43
1:A:101:ARG:NH1	1:A:370:LEU:HD23	2.34	0.43
1:C:138:PHE:CZ	1:C:266:ASP:HA	2.54	0.43
1:C:418:ASP:OD2	1:C:422[A]:GLN:HB2	2.19	0.43
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.15	0.43
1:C:250:LYS:HB2	1:C:250:LYS:HZ2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ASN:HB3	1:C:284:THR:HB	2.00	0.43
1:D:205:MET:CG	1:D:244:LEU:HD11	2.48	0.43
1:E:116:VAL:CG1	1:E:294:THR:HG23	2.49	0.43
1:G:442:GLU:CD	1:G:446:ARG:NH1	2.74	0.43
1:F:77:ARG:NH1	1:F:389:THR:OG1	2.52	0.43
1:G:85:ASP:O	1:G:89:GLU:HB2	2.19	0.43
1:H:130:PHE:HZ	1:H:270:SER:HB3	1.84	0.43
1:A:101:ARG:HH12	1:A:370:LEU:HB3	1.79	0.43
1:D:453:PHE:O	1:D:457:MET:CG	2.67	0.43
1:E:423:PHE:HE2	1:E:425:LYS:HG2	1.83	0.43
1:H:32:LYS:O	1:H:383:PHE:HA	2.19	0.43
1:D:80:VAL:HG22	1:D:392:PHE:HB2	2.00	0.42
1:A:116:VAL:HG12	1:A:297:ASN:HD22	1.85	0.42
1:G:59:MET:HA	1:G:62:SER:HB3	2.00	0.42
1:G:435:GLY:O	1:G:438:TYR:HD2	2.02	0.42
1:B:343:PHE:O	1:B:346:ARG:HB2	2.18	0.42
1:D:260:ASP:HA	1:D:261:PRO:HD3	1.84	0.42
1:G:209:PHE:CE1	1:G:304:GLU:HG2	2.54	0.42
1:E:103:GLU:HB2	1:E:108:ASP:OD2	2.19	0.42
1:F:305:THR:CA	1:F:365:MET:HE2	2.42	0.42
1:G:109:TRP:CH2	1:G:238:PHE:HB3	2.53	0.42
1:H:297:ASN:HD22	1:H:297:ASN:HA	1.63	0.42
1:D:423:PHE:HE1	1:D:425:LYS:HG3	1.85	0.42
1:E:353:GLU:OE1	1:E:353:GLU:HA	2.19	0.42
1:A:101:ARG:NH2	2:A:500:HEM:O2D	2.53	0.42
1:A:251:LYS:O	1:A:254:HIS:HB3	2.19	0.42
1:B:107:PHE:CZ	3:B:501:NCT:HC4	2.55	0.42
1:C:250:LYS:NZ	1:C:250:LYS:CB	2.82	0.42
1:D:197:GLU:OE2	1:D:250:LYS:NZ	2.53	0.42
1:H:320:HIS:HB3	1:H:323:VAL:HG22	2.01	0.42
1:F:103:GLU:HB2	1:F:108:ASP:OD2	2.19	0.42
1:F:195:ASP:OD2	1:F:197:GLU:HB3	2.19	0.42
1:F:272:LEU:HA	1:F:275:MET:HB3	2.01	0.42
1:G:314:PHE:HB2	1:G:487:TYR:OH	2.19	0.42
1:B:220:TYR:CZ	1:B:224:SER:HB2	2.54	0.42
1:E:330:GLU:HG3	1:E:333[A]:ARG:NH2	2.34	0.42
1:F:81:LEU:HB2	1:F:87:VAL:HG22	2.02	0.42
1:F:463:LYS:HB3	1:F:490:SER:HB2	2.02	0.42
1:G:304:GLU:O	1:G:308:THR:OG1	2.29	0.42
1:B:331:ILE:HG12	1:B:349:MET:HE1	2.02	0.42
1:C:210[B]:GLN:O	1:C:214:THR:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:ILE:HD12	1:G:295:THR:HG22	2.02	0.42
1:H:53:GLN:OE1	1:H:56:ASN:ND2	2.53	0.42
1:H:314:PHE:HB2	1:H:487:TYR:OH	2.20	0.42
1:C:442:GLU:OE2	1:C:446:ARG:NH1	2.53	0.42
1:D:366:LEU:HA	1:D:367:PRO:HD3	1.88	0.42
1:F:308:THR:CB	1:F:365:MET:HE1	2.45	0.42
1:F:271:PHE:CG	1:F:291:LEU:HD13	2.55	0.41
1:F:331:ILE:HG23	1:F:335:ILE:HD12	2.02	0.41
1:G:328:HIS:HA	1:G:331:ILE:HD12	2.02	0.41
1:H:157:ILE:HD11	1:H:456:ILE:HA	2.02	0.41
1:A:364:ASP:OD1	1:A:399:LEU:HD12	2.20	0.41
1:B:152:GLU:HG3	1:B:177:THR:HG23	2.03	0.41
1:C:384:PHE:C	1:C:385:LEU:HD12	2.45	0.41
1:A:291:LEU:C	1:A:291:LEU:CD1	2.93	0.41
1:D:353:GLU:HG2	1:D:423:PHE:CD2	2.56	0.41
1:E:143:ARG:O	1:E:144:GLY:C	2.64	0.41
1:B:32:LYS:CD	1:B:33:LEU:N	2.78	0.41
1:B:468:PRO:HA	1:B:471:ILE:HD12	2.01	0.41
1:F:271:PHE:CB	1:F:291:LEU:HD13	2.51	0.41
1:G:190:ARG:NH2	1:G:193:TYR:CE1	2.67	0.41
1:D:433:SER:HB3	2:D:500:HEM:HBA1	2.03	0.41
1:E:116:VAL:HG12	1:E:294:THR:HG23	2.02	0.41
1:F:116:VAL:HG12	1:F:294:THR:HG23	2.02	0.41
1:F:271:PHE:CE1	1:F:291:LEU:HB2	2.56	0.41
1:F:323:VAL:O	1:F:327:VAL:HG23	2.20	0.41
1:B:436:LYS:HA	1:B:436:LYS:HD3	1.84	0.41
1:D:163:THR:HG21	1:D:168:ILE:HD13	2.02	0.41
1:E:101:ARG:NH1	1:E:370:LEU:CB	2.81	0.41
1:F:314:PHE:CZ	1:F:456:ILE:HD13	2.54	0.41
1:H:382:ASP:OD2	1:H:382:ASP:N	2.51	0.41
1:C:147:GLU:OE2	1:D:143:ARG:NH1	2.52	0.41
1:E:101:ARG:NH1	1:E:370:LEU:CG	2.84	0.41
1:E:110:LEU:HD13	1:E:241:LEU:HB3	2.01	0.41
1:F:263:SER:HA	1:F:264:PRO:HD3	1.76	0.41
1:H:81:LEU:O	1:H:394:MET:HG2	2.21	0.41
1:B:341:PRO:HB3	1:B:454:THR:HG21	2.03	0.41
1:C:225:SER:HA	1:C:228:LYS:HE3	2.02	0.41
1:D:74:GLY:HA3	1:D:75:PRO:HD2	1.89	0.41
1:D:116:VAL:HG12	1:D:297:ASN:HD22	1.86	0.41
1:D:303:THR:O	1:D:307:SER:HB3	2.21	0.41
1:D:373:ARG:NH1	1:D:388:GLY:O	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:LYS:HB2	1:F:485:ARG:HA	2.02	0.41
1:G:138:PHE:N	1:G:138:PHE:HD2	2.18	0.41
1:G:289:LYS:O	1:G:293:MET:HG2	2.21	0.41
1:H:109:TRP:CZ2	1:H:238:PHE:HB3	2.56	0.41
1:D:54:MET:HE3	1:D:73:LEU:HD21	2.02	0.41
1:D:319:LYS:C	1:D:321:PRO:HD3	2.46	0.41
1:F:452:PHE:O	1:F:456:ILE:HD12	2.21	0.41
2:F:500:HEM:HBD2	2:F:500:HEM:HHA	2.01	0.41
1:B:492:LEU:HA	1:B:493:PRO:HD3	1.95	0.40
1:E:213:ALA:HA	1:E:479:GLY:HA3	2.02	0.40
1:G:395:LEU:HD23	1:G:395:LEU:HA	1.91	0.40
1:H:69:PHE:CE1	1:H:80:VAL:HB	2.56	0.40
1:B:467:SER:O	1:B:468:PRO:C	2.64	0.40
1:C:199:LEU:HD12	1:C:199:LEU:HA	1.92	0.40
1:C:468:PRO:HA	1:C:471:ILE:HD12	2.03	0.40
1:E:178:VAL:HG12	1:E:303:THR:HA	2.04	0.40
1:F:330:GLU:OE1	1:F:349:MET:HB3	2.21	0.40
1:H:68:VAL:HA	1:H:80:VAL:O	2.21	0.40
1:B:175:SER:O	1:B:179:SER:CB	2.69	0.40
1:D:64:ARG:HG2	1:D:65:TYR:CD2	2.56	0.40
1:F:344:GLU:C	1:F:346:ARG:H	2.29	0.40
1:B:55:TYR:CE1	1:B:59:MET:HG3	2.56	0.40
1:C:370:LEU:HD12	1:C:370:LEU:HA	1.86	0.40
1:E:122:GLU:O	1:E:126:GLN:HB2	2.22	0.40
1:F:116:VAL:CG1	1:F:294:THR:HG23	2.51	0.40
1:C:212:THR:HB	1:C:480:PHE:HB3	2.04	0.40
2:D:500:HEM:HBB2	2:D:500:HEM:HMB1	2.02	0.40
1:E:268:ILE:HD11	1:E:295:THR:HG21	2.04	0.40
1:F:142:LYS:H	1:F:142:LYS:HG2	1.69	0.40
1:F:458:GLN:CG	1:F:459:ASN:N	2.85	0.40
1:G:473:VAL:HG23	1:G:474:SER:N	2.36	0.40
1:H:362:PHE:O	1:H:363:GLY:C	2.64	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	463/476 (97%)	441 (95%)	21 (4%)	1 (0%)	43	63
1	B	467/476 (98%)	433 (93%)	33 (7%)	1 (0%)	43	63
1	C	466/476 (98%)	438 (94%)	26 (6%)	2 (0%)	30	49
1	D	466/476 (98%)	445 (96%)	21 (4%)	0	100	100
1	E	466/476 (98%)	448 (96%)	16 (3%)	2 (0%)	30	49
1	F	463/476 (97%)	413 (89%)	44 (10%)	6 (1%)	9	18
1	G	461/476 (97%)	404 (88%)	52 (11%)	5 (1%)	11	22
1	H	454/476 (95%)	396 (87%)	49 (11%)	9 (2%)	6	10
All	All	3706/3808 (97%)	3418 (92%)	262 (7%)	26 (1%)	18	34

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	262	ASN
1	F	338	ASN
1	H	95	ALA
1	H	408	PRO
1	F	345	ASP
1	G	364	ASP
1	H	277	GLU
1	H	421	GLY
1	F	382	ASP
1	H	60	LYS
1	B	433	SER
1	C	433	SER
1	G	387	LYS
1	G	468	PRO
1	H	362	PHE
1	C	365	MET
1	E	193	TYR
1	H	85	ASP
1	H	193	TYR
1	F	393	PRO
1	F	468	PRO
1	G	137	GLY
1	G	471	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	GLY
1	E	144	GLY
1	H	363	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	409/419 (98%)	382 (93%)	27 (7%)	15	32
1	B	413/419 (99%)	391 (95%)	22 (5%)	20	42
1	C	412/419 (98%)	390 (95%)	22 (5%)	20	42
1	D	412/419 (98%)	385 (93%)	27 (7%)	15	32
1	E	412/419 (98%)	382 (93%)	30 (7%)	13	27
1	F	409/419 (98%)	373 (91%)	36 (9%)	9	20
1	G	402/419 (96%)	371 (92%)	31 (8%)	12	25
1	H	396/419 (94%)	355 (90%)	41 (10%)	7	14
All	All	3265/3352 (97%)	3029 (93%)	236 (7%)	13	28

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	40	LEU
1	A	60	LYS
1	A	89	GLU
1	A	91	LEU
1	A	97	GLU
1	A	112	LYS
1	A	135	LEU
1	A	145	ILE
1	A	215	SER
1	A	248	ILE
1	A	250	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	276	GLN
1	A	283	ASN
1	A	291	LEU
1	A	316	LEU
1	A	344	GLU
1	A	348	LYS
1	A	365	MET
1	A	366	LEU
1	A	376	LYS
1	A	409	ARG
1	A	417	LEU
1	A	436	LYS
1	A	446	ARG
1	A	454	THR
1	A	463	LYS
1	B	40	LEU
1	B	73	LEU
1	B	77	ARG
1	B	82	CYS
1	B	135	LEU
1	B	147	GLU
1	B	186	VAL
1	B	199	LEU
1	B	206	LEU
1	B	239	LYS
1	B	258	THR
1	B	276	GLN
1	B	296	LEU
1	B	316	LEU
1	B	326	LYS
1	B	348	LYS
1	B	366	LEU
1	B	403	ARG
1	B	409	ARG
1	B	417	LEU
1	B	425	LYS
1	B	454	THR
1	C	77	ARG
1	C	91	LEU
1	C	135	LEU
1	C	145	ILE
1	C	147	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	208	SER
1	C	236	GLN
1	C	245	GLU
1	C	250	LYS
1	C	256	GLN
1	C	279	GLU
1	C	316	LEU
1	C	346	ARG
1	C	348	LYS
1	C	382	ASP
1	C	410	ASP
1	C	417	LEU
1	C	419	LYS
1	C	420	LYS
1	C	436	LYS
1	C	469	LYS
1	C	492	LEU
1	D	30	LYS
1	D	32	LYS
1	D	38	THR
1	D	40	LEU
1	D	77	ARG
1	D	82	CYS
1	D	88	LYS
1	D	126	GLN
1	D	135	LEU
1	D	167	ASN
1	D	199	LEU
1	D	208	SER
1	D	215	SER
1	D	239	LYS
1	D	245	GLU
1	D	291	LEU
1	D	316	LEU
1	D	329	GLU
1	D	348	LYS
1	D	353	GLU
1	D	366	LEU
1	D	379	LYS
1	D	409	ARG
1	D	419	LYS
1	D	434	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	446	ARG
1	D	457	MET
1	E	30	LYS
1	E	32	LYS
1	E	33	LEU
1	E	40	LEU
1	E	57	SER
1	E	88	LYS
1	E	125	LYS
1	E	147	GLU
1	E	167	ASN
1	E	175	SER
1	E	189	ASP
1	E	194	GLU
1	E	197	GLU
1	E	208	SER
1	E	225	SER
1	E	236	GLN
1	E	239[A]	LYS
1	E	239[B]	LYS
1	E	279	GLU
1	E	316	LEU
1	E	348	LYS
1	E	353	GLU
1	E	366	LEU
1	E	382	ASP
1	E	417	LEU
1	E	419	LYS
1	E	434	ILE
1	E	457	MET
1	E	469	LYS
1	E	492	LEU
1	F	30	LYS
1	F	60	LYS
1	F	81	LEU
1	F	91	LEU
1	F	110	LEU
1	F	122	GLU
1	F	131	SER
1	F	135	LEU
1	F	143	ARG
1	F	167	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	177	THR
1	F	199	LEU
1	F	228	LYS
1	F	236	GLN
1	F	250	LYS
1	F	251	LYS
1	F	252	VAL
1	F	254	HIS
1	F	273	ILE
1	F	274	ARG
1	F	283	ASN
1	F	287	TYR
1	F	316	LEU
1	F	322	GLU
1	F	333	ARG
1	F	340	GLN
1	F	346	ARG
1	F	352	THR
1	F	379	LYS
1	F	389	THR
1	F	403	ARG
1	F	407	ASN
1	F	417	LEU
1	F	427	ASP
1	F	436	LYS
1	F	478	VAL
1	G	32	LYS
1	G	33	LEU
1	G	43	ILE
1	G	51	THR
1	G	52	GLU
1	G	71	ILE
1	G	85	ASP
1	G	97	GLU
1	G	129	ARG
1	G	134	THR
1	G	138	PHE
1	G	145	ILE
1	G	151	GLU
1	G	155	PHE
1	G	177	THR
1	G	201	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	212	THR
1	G	251	LYS
1	G	258	THR
1	G	291	LEU
1	G	303	THR
1	G	306	VAL
1	G	319	LYS
1	G	342	LYS
1	G	365	MET
1	G	382	ASP
1	G	419	LYS
1	G	434	ILE
1	G	446	ARG
1	G	478	VAL
1	G	483	ILE
1	H	33	LEU
1	H	50	ASN
1	H	51	THR
1	H	57	SER
1	H	62	SER
1	H	85	ASP
1	H	91	LEU
1	H	145	ILE
1	H	157	ILE
1	H	160	LEU
1	H	163	THR
1	H	167	ASN
1	H	174	LEU
1	H	177	THR
1	H	182	ILE
1	H	210	GLN
1	H	245	GLU
1	H	270	SER
1	H	285	GLU
1	H	289	LYS
1	H	296	LEU
1	H	297	ASN
1	H	318	MET
1	H	322	GLU
1	H	329	GLU
1	H	335	ILE
1	H	346	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	356	ILE
1	H	361	ARG
1	H	370	LEU
1	H	382	ASP
1	H	385	LEU
1	H	410	ASP
1	H	430	VAL
1	H	434	ILE
1	H	442	GLU
1	H	446	ARG
1	H	463	LYS
1	H	467	SER
1	H	470	ASP
1	H	473	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	164	HIS
1	A	167	ASN
1	A	276	GLN
1	A	297	ASN
1	A	407	ASN
1	A	414	GLN
1	A	477	HIS
1	B	297	ASN
1	B	360	GLN
1	C	56	ASN
1	C	104	GLN
1	C	164	HIS
1	C	242	GLN
1	C	262	ASN
1	C	297	ASN
1	C	412	ASN
1	C	477	HIS
1	C	486	ASN
1	D	72	HIS
1	D	235	GLN
1	D	297	ASN
1	D	375	ASN
1	D	477	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	50	ASN
1	E	72	HIS
1	E	297	ASN
1	E	459	ASN
1	F	164	HIS
1	F	167	ASN
1	F	210	GLN
1	F	229	HIS
1	F	477	HIS
1	F	486	ASN
1	G	72	HIS
1	G	126	GLN
1	G	297	ASN
1	G	320	HIS
1	G	340	GLN
1	G	412	ASN
1	G	486	ASN
1	H	50	ASN
1	H	56	ASN
1	H	72	HIS
1	H	94	GLN
1	H	218	GLN
1	H	256	GLN
1	H	320	HIS
1	H	338	ASN
1	H	412	ASN
1	H	477	HIS

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

13 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	NCT	C	501	-	13,13,13	1.14	1 (7%)	17,17,17	2.41	5 (29%)
2	HEM	B	500	1	50,50,50	2.08	11 (22%)	67,82,82	1.43	4 (5%)
2	HEM	G	500	1	50,50,50	2.12	12 (24%)	67,82,82	1.48	10 (14%)
3	NCT	D	501	-	13,13,13	0.76	1 (7%)	17,17,17	1.93	6 (35%)
4	GOL	H	502	-	5,5,5	1.01	0	5,5,5	2.19	3 (60%)
2	HEM	E	500	1	50,50,50	2.08	11 (22%)	67,82,82	1.53	13 (19%)
2	HEM	F	500	1	50,50,50	2.17	10 (20%)	67,82,82	1.45	5 (7%)
2	HEM	A	500	1	50,50,50	2.07	12 (24%)	67,82,82	1.53	10 (14%)
3	NCT	A	501	-	13,13,13	0.82	0	17,17,17	2.23	7 (41%)
2	HEM	D	500	1	50,50,50	1.90	11 (22%)	67,82,82	1.15	7 (10%)
3	NCT	B	501	-	13,13,13	1.23	1 (7%)	17,17,17	2.33	6 (35%)
2	HEM	H	501	1	50,50,50	2.08	8 (16%)	67,82,82	1.42	8 (11%)
2	HEM	C	500	1	50,50,50	2.36	12 (24%)	67,82,82	1.73	15 (22%)

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	NCT	C	501	-	-	0/4/14/14	0/2/2/2
2	HEM	B	500	1	-	4/14/54/54	-
2	HEM	G	500	1	-	4/14/54/54	-
3	NCT	D	501	-	-	0/4/14/14	0/2/2/2
4	GOL	H	502	-	-	4/4/4/4	-
2	HEM	E	500	1	-	4/14/54/54	-
2	HEM	F	500	1	-	9/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	4/14/54/54	-
3	NCT	A	501	-	-	0/4/14/14	0/2/2/2
2	HEM	D	500	1	-	5/14/54/54	-
3	NCT	B	501	-	-	0/4/14/14	0/2/2/2
2	HEM	H	501	1	-	3/14/54/54	-
2	HEM	C	500	1	-	6/14/54/54	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	HEM	C3D-C2D	8.59	1.55	1.36
2	F	500	HEM	C3D-C2D	8.23	1.54	1.36
2	C	500	HEM	C3D-C2D	7.90	1.53	1.36
2	E	500	HEM	C3D-C2D	7.72	1.53	1.36
2	H	501	HEM	C3D-C2D	7.42	1.52	1.36
2	B	500	HEM	FE-ND	7.31	2.17	1.94
2	F	500	HEM	FE-ND	7.27	2.17	1.94
2	C	500	HEM	FE-NB	7.04	2.16	1.94
2	A	500	HEM	C3D-C2D	6.99	1.51	1.36
2	H	501	HEM	FE-ND	6.90	2.16	1.94
2	C	500	HEM	FE-ND	6.78	2.15	1.94
2	B	500	HEM	C3D-C2D	6.76	1.51	1.36
2	G	500	HEM	FE-ND	6.41	2.14	1.94
2	D	500	HEM	C3D-C2D	6.33	1.50	1.36
2	A	500	HEM	FE-ND	6.13	2.13	1.94
2	H	501	HEM	FE-NC	5.66	2.13	1.95
2	C	500	HEM	FE-NC	5.29	2.12	1.95
2	E	500	HEM	FE-ND	5.10	2.10	1.94
2	F	500	HEM	FE-NC	5.02	2.11	1.95
2	D	500	HEM	FE-NC	4.35	2.09	1.95
2	B	500	HEM	FE-NC	4.28	2.09	1.95
2	E	500	HEM	FE-NC	4.09	2.08	1.95
2	E	500	HEM	FE-NA	4.02	2.08	1.95
2	E	500	HEM	FE-NB	3.89	2.06	1.94
2	A	500	HEM	FE-NB	3.89	2.06	1.94
2	F	500	HEM	FE-NB	3.88	2.06	1.94
2	B	500	HEM	CMB-C2B	3.67	1.58	1.50
2	F	500	HEM	CAC-C3C	3.57	1.56	1.47
2	H	501	HEM	CAC-C3C	3.56	1.56	1.47
2	G	500	HEM	FE-NC	3.50	2.06	1.95
2	G	500	HEM	CAB-C3B	3.49	1.56	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	CMB-C2B	3.45	1.57	1.50
2	E	500	HEM	CAB-C3B	3.45	1.56	1.47
2	D	500	HEM	CAB-C3B	3.39	1.56	1.47
2	A	500	HEM	CMA-C3A	3.38	1.57	1.50
2	E	500	HEM	CAC-C3C	3.38	1.56	1.47
2	G	500	HEM	FE-NA	3.36	2.06	1.95
2	A	500	HEM	CAB-C3B	3.34	1.56	1.47
3	C	501	NCT	C2-C6	-3.31	1.46	1.51
2	C	500	HEM	CAB-C3B	3.29	1.56	1.47
2	B	500	HEM	CAB-C3B	3.28	1.56	1.47
2	D	500	HEM	CAC-C3C	3.28	1.56	1.47
2	A	500	HEM	CAC-C3C	3.16	1.55	1.47
2	F	500	HEM	CAB-C3B	3.12	1.55	1.47
2	H	501	HEM	CAB-C3B	3.10	1.55	1.47
2	B	500	HEM	CAC-C3C	3.08	1.55	1.47
2	A	500	HEM	CMB-C2B	3.07	1.57	1.50
2	H	501	HEM	CMB-C2B	3.04	1.57	1.50
2	C	500	HEM	CMC-C2C	2.98	1.56	1.50
2	C	500	HEM	CAC-C3C	2.97	1.55	1.47
2	E	500	HEM	CMA-C3A	2.93	1.56	1.50
3	B	501	NCT	C1-C2	2.92	1.43	1.39
2	E	500	HEM	CMB-C2B	2.88	1.56	1.50
2	C	500	HEM	C1B-NB	-2.84	1.35	1.40
2	D	500	HEM	CMC-C2C	2.84	1.56	1.50
2	D	500	HEM	FE-NA	2.83	2.04	1.95
2	D	500	HEM	C2A-C3A	-2.77	1.31	1.38
2	B	500	HEM	CMC-C2C	2.75	1.56	1.50
2	B	500	HEM	FE-NB	2.74	2.03	1.94
2	G	500	HEM	FE-NB	2.74	2.03	1.94
2	D	500	HEM	FE-ND	2.64	2.03	1.94
2	D	500	HEM	C3C-C4C	-2.62	1.41	1.46
2	A	500	HEM	C1B-NB	-2.61	1.35	1.40
2	F	500	HEM	CMB-C2B	2.58	1.56	1.50
2	G	500	HEM	CMD-C2D	2.56	1.56	1.50
2	A	500	HEM	FE-NA	2.52	2.03	1.95
2	H	501	HEM	FE-NB	2.50	2.02	1.94
2	A	500	HEM	CAA-C2A	2.48	1.57	1.51
2	B	500	HEM	C1B-NB	-2.41	1.36	1.40
2	G	500	HEM	CAC-C3C	2.33	1.53	1.47
2	E	500	HEM	CMD-C2D	2.30	1.55	1.50
2	C	500	HEM	C2A-C3A	-2.28	1.32	1.38
2	F	500	HEM	CMC-C2C	2.28	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	CMB-C2B	2.27	1.55	1.50
2	B	500	HEM	C2A-C3A	-2.27	1.33	1.38
2	H	501	HEM	CMA-C3A	2.26	1.55	1.50
2	B	500	HEM	CAA-C2A	2.25	1.57	1.51
2	C	500	HEM	C3C-C2C	-2.25	1.32	1.37
2	D	500	HEM	CMA-C3A	2.23	1.55	1.50
2	G	500	HEM	CMA-C3A	2.21	1.55	1.50
2	G	500	HEM	CMC-C2C	2.19	1.55	1.50
2	A	500	HEM	C2A-C3A	-2.18	1.33	1.38
2	F	500	HEM	CMA-C3A	2.18	1.55	1.50
2	F	500	HEM	CMD-C2D	2.12	1.55	1.50
2	G	500	HEM	C3C-C2C	-2.11	1.32	1.37
3	D	501	NCT	C2-C6	-2.11	1.48	1.51
2	C	500	HEM	C4B-NB	-2.09	1.34	1.38
2	A	500	HEM	O2A-CGA	-2.04	1.24	1.30
2	G	500	HEM	CAD-C3D	2.02	1.56	1.51
2	E	500	HEM	O2A-CGA	-2.01	1.24	1.30

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C4D-ND-C1D	7.08	113.60	105.21
2	G	500	HEM	C4D-ND-C1D	6.35	112.72	105.21
2	B	500	HEM	C4D-ND-C1D	6.27	112.63	105.21
2	F	500	HEM	C4D-ND-C1D	6.11	112.44	105.21
3	C	501	NCT	C10-N2-C6	5.96	130.53	112.78
2	A	500	HEM	C4D-ND-C1D	5.93	112.23	105.21
3	B	501	NCT	C10-N2-C6	5.81	130.09	112.78
2	E	500	HEM	C4D-ND-C1D	5.65	111.89	105.21
3	A	501	NCT	C10-N2-C6	5.23	128.37	112.78
3	D	501	NCT	C10-N2-C6	4.54	126.29	112.78
2	B	500	HEM	CMD-C2D-C1D	4.31	131.76	125.03
2	C	500	HEM	C1B-NB-C4B	4.30	110.30	105.21
2	A	500	HEM	CMD-C2D-C1D	4.24	131.66	125.03
2	H	501	HEM	C4D-ND-C1D	4.02	109.97	105.21
2	F	500	HEM	CAD-C3D-C4D	4.01	131.69	124.70
3	C	501	NCT	C3-C2-C1	3.98	120.99	116.89
3	B	501	NCT	C2-C6-N2	3.80	122.18	112.17
3	A	501	NCT	C4-C3-C2	-3.66	116.26	120.65
2	H	501	HEM	C3B-C4B-NB	-3.44	107.00	109.47
2	B	500	HEM	CAD-C3D-C4D	3.38	130.58	124.70
2	G	500	HEM	CAA-CBA-CGA	-3.33	104.83	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NCT	C10-N2-C9	3.31	122.63	112.68
3	C	501	NCT	C4-C3-C2	-3.30	116.70	120.65
2	E	500	HEM	CMD-C2D-C1D	3.18	130.00	125.03
4	H	502	GOL	O2-C2-C3	-3.18	96.02	109.18
3	C	501	NCT	C10-N2-C9	3.16	122.19	112.68
2	H	501	HEM	CHC-C1C-NC	3.14	127.87	124.45
2	D	500	HEM	C4D-ND-C1D	3.10	108.88	105.21
3	D	501	NCT	C9-N2-C6	3.06	113.33	104.28
2	E	500	HEM	CHC-C1C-NC	3.00	127.72	124.45
2	E	500	HEM	CAA-CBA-CGA	-2.92	105.92	113.67
2	H	501	HEM	C3C-C2C-C1C	2.90	109.79	107.05
2	D	500	HEM	CAD-C3D-C4D	2.88	129.71	124.70
3	B	501	NCT	C4-C3-C2	-2.81	117.29	120.65
2	A	500	HEM	C1B-NB-C4B	2.75	108.46	105.21
2	H	501	HEM	CAA-CBA-CGA	-2.72	106.45	113.67
2	H	501	HEM	CHA-C4D-ND	2.69	127.70	124.37
2	A	500	HEM	O2D-CGD-O1D	-2.67	116.45	123.33
2	C	500	HEM	C1C-CHC-C4B	2.66	131.67	126.02
2	E	500	HEM	CHA-C4D-ND	2.65	127.65	124.37
2	C	500	HEM	C2B-C1B-NB	-2.61	106.83	109.84
2	E	500	HEM	C2A-C1A-NA	-2.60	107.27	110.15
2	F	500	HEM	C2A-C1A-NA	-2.58	107.29	110.15
2	E	500	HEM	C4C-NC-C1C	2.57	110.02	105.82
3	B	501	NCT	C10-N2-C9	2.57	120.42	112.68
2	C	500	HEM	C4A-C3A-C2A	2.56	109.75	106.82
3	D	501	NCT	C10-N2-C9	2.55	120.36	112.68
2	B	500	HEM	C2D-C1D-ND	-2.54	106.96	109.90
2	C	500	HEM	O1D-CGD-CBD	-2.51	115.12	123.09
2	D	500	HEM	CAA-CBA-CGA	-2.50	107.03	113.67
2	A	500	HEM	O2D-CGD-CBD	2.47	121.80	114.00
2	C	500	HEM	O2A-CGA-CBA	2.46	121.78	114.00
4	H	502	GOL	O3-C3-C2	-2.46	99.32	110.38
4	H	502	GOL	C3-C2-C1	-2.44	102.83	111.80
2	D	500	HEM	CMD-C2D-C1D	2.44	128.85	125.03
2	E	500	HEM	O2D-CGD-CBD	2.44	121.71	114.00
2	H	501	HEM	CHD-C4C-NC	2.44	127.11	124.45
2	C	500	HEM	C4C-CHD-C1D	2.39	131.10	126.02
2	D	500	HEM	CBC-CAC-C3C	-2.39	115.59	127.53
2	C	500	HEM	C4C-C3C-C2C	2.37	108.87	106.81
2	E	500	HEM	C4C-C3C-C2C	2.37	108.86	106.81
2	D	500	HEM	C4C-NC-C1C	2.35	109.65	105.82
2	A	500	HEM	CAD-C3D-C4D	2.35	128.79	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	NCT	C4-C3-C2	-2.34	117.85	120.65
2	G	500	HEM	C3B-C2B-C1B	2.31	108.15	106.41
2	D	500	HEM	CHD-C1D-ND	2.30	126.90	124.42
3	A	501	NCT	C3-C4-C5	2.29	122.24	118.92
2	H	501	HEM	C4B-C3B-C2B	2.29	109.39	107.28
2	C	500	HEM	CMC-C2C-C1C	2.27	128.73	124.73
2	G	500	HEM	O2D-CGD-CBD	2.24	121.08	114.00
2	G	500	HEM	CBC-CAC-C3C	-2.23	116.38	127.53
3	B	501	NCT	C1-C2-C6	-2.22	116.92	121.56
2	C	500	HEM	C3B-C2B-C1B	2.21	108.07	106.41
3	C	501	NCT	C1-C2-C6	-2.20	116.97	121.56
2	E	500	HEM	CBD-CAD-C3D	-2.20	106.46	112.53
2	F	500	HEM	C4C-CHD-C1D	2.20	130.69	126.02
2	A	500	HEM	CHD-C1D-C2D	2.19	128.49	125.03
2	C	500	HEM	C3A-C4A-NA	-2.18	106.65	110.14
3	A	501	NCT	C2-C6-N2	2.17	117.89	112.17
3	D	501	NCT	C3-C2-C1	2.16	119.12	116.89
3	B	501	NCT	C8-C9-N2	-2.16	97.42	103.56
2	G	500	HEM	CHA-C4D-ND	2.15	127.03	124.37
2	G	500	HEM	C1A-CHA-C4D	2.14	131.28	126.25
3	A	501	NCT	C3-C2-C1	2.13	119.09	116.89
2	A	500	HEM	CAD-CBD-CGD	-2.13	108.02	113.67
2	G	500	HEM	C1D-C2D-C3D	-2.12	104.75	106.98
2	F	500	HEM	C2D-C1D-ND	-2.12	107.46	109.90
2	G	500	HEM	C2A-C1A-NA	-2.10	107.82	110.15
2	E	500	HEM	C1D-C2D-C3D	-2.10	104.77	106.98
2	C	500	HEM	C3D-C4D-ND	-2.10	107.87	110.17
3	A	501	NCT	C8-C9-N2	-2.09	97.62	103.56
2	C	500	HEM	CBD-CAD-C3D	-2.08	106.77	112.53
2	A	500	HEM	CHA-C4D-ND	2.07	126.93	124.37
2	A	500	HEM	CMA-C3A-C4A	2.07	128.57	125.42
2	C	500	HEM	CHB-C4A-NA	2.07	127.61	123.86
2	E	500	HEM	CHD-C4C-C3C	2.06	128.69	125.21
2	E	500	HEM	C3B-C4B-NB	-2.06	107.99	109.47
3	D	501	NCT	C5-N1-C1	2.04	120.43	116.85
2	G	500	HEM	C4C-C3C-C2C	2.00	108.55	106.81

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

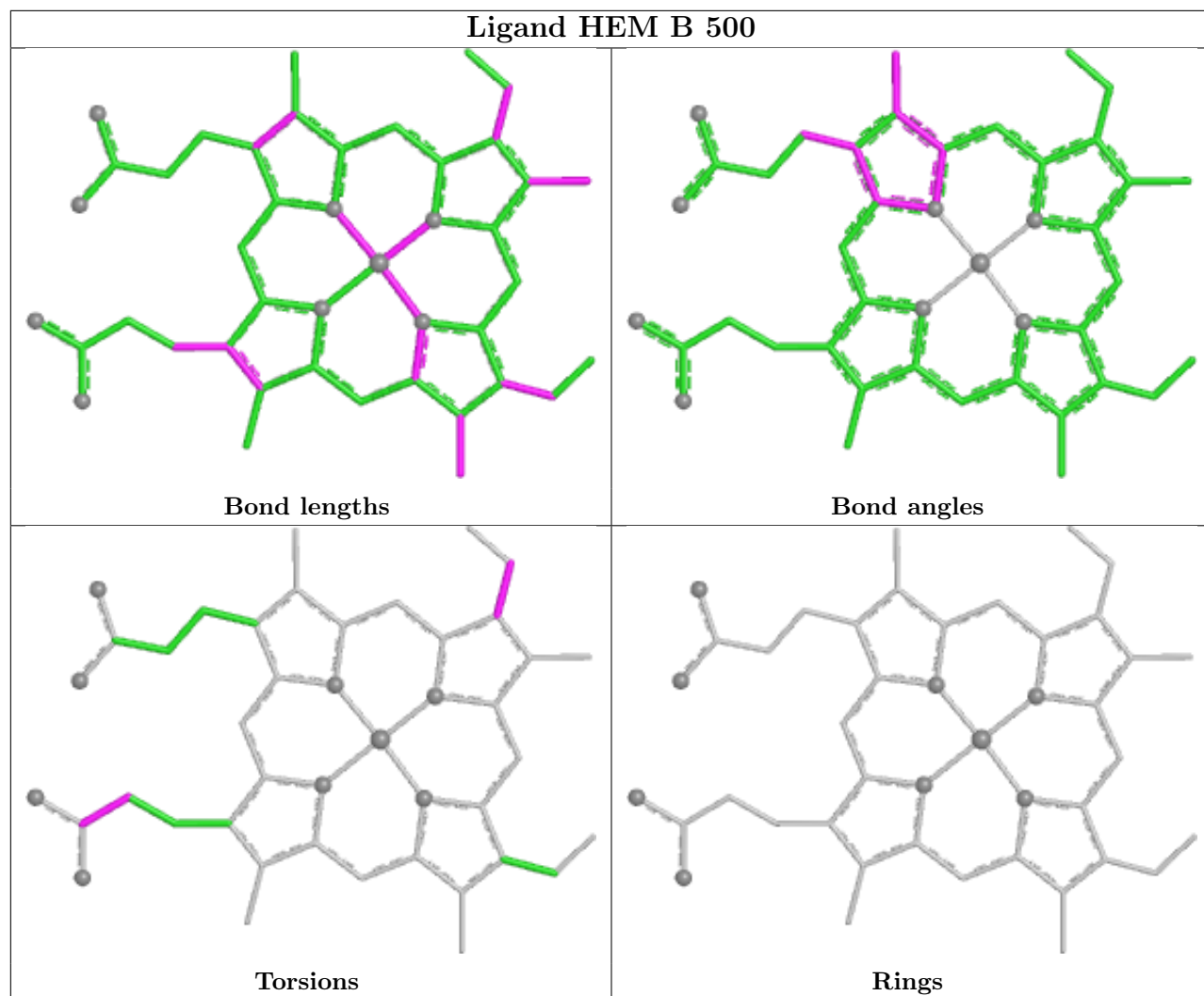
Mol	Chain	Res	Type	Atoms
2	D	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	E	500	HEM	C2C-C3C-CAC-CBC
2	F	500	HEM	C2C-C3C-CAC-CBC
2	F	500	HEM	C4C-C3C-CAC-CBC
2	G	500	HEM	C2C-C3C-CAC-CBC
4	H	502	GOL	O1-C1-C2-C3
4	H	502	GOL	C1-C2-C3-O3
2	F	500	HEM	C2D-C3D-CAD-CBD
2	F	500	HEM	C4D-C3D-CAD-CBD
2	F	500	HEM	C3D-CAD-CBD-CGD
2	H	501	HEM	C3D-CAD-CBD-CGD
4	H	502	GOL	O1-C1-C2-O2
2	A	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	H	501	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	G	500	HEM	C4C-C3C-CAC-CBC
4	H	502	GOL	O2-C2-C3-O3
2	A	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	E	500	HEM	C4C-C3C-CAC-CBC
2	H	501	HEM	C4C-C3C-CAC-CBC
2	D	500	HEM	CAA-CBA-CGA-O1A
2	F	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	E	500	HEM	CAA-CBA-CGA-O1A
2	G	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	E	500	HEM	CAA-CBA-CGA-O2A
2	F	500	HEM	CAD-CBD-CGD-O1D
2	F	500	HEM	CAA-CBA-CGA-O2A
2	G	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	F	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAD-CBD-CGD-O1D
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O2D

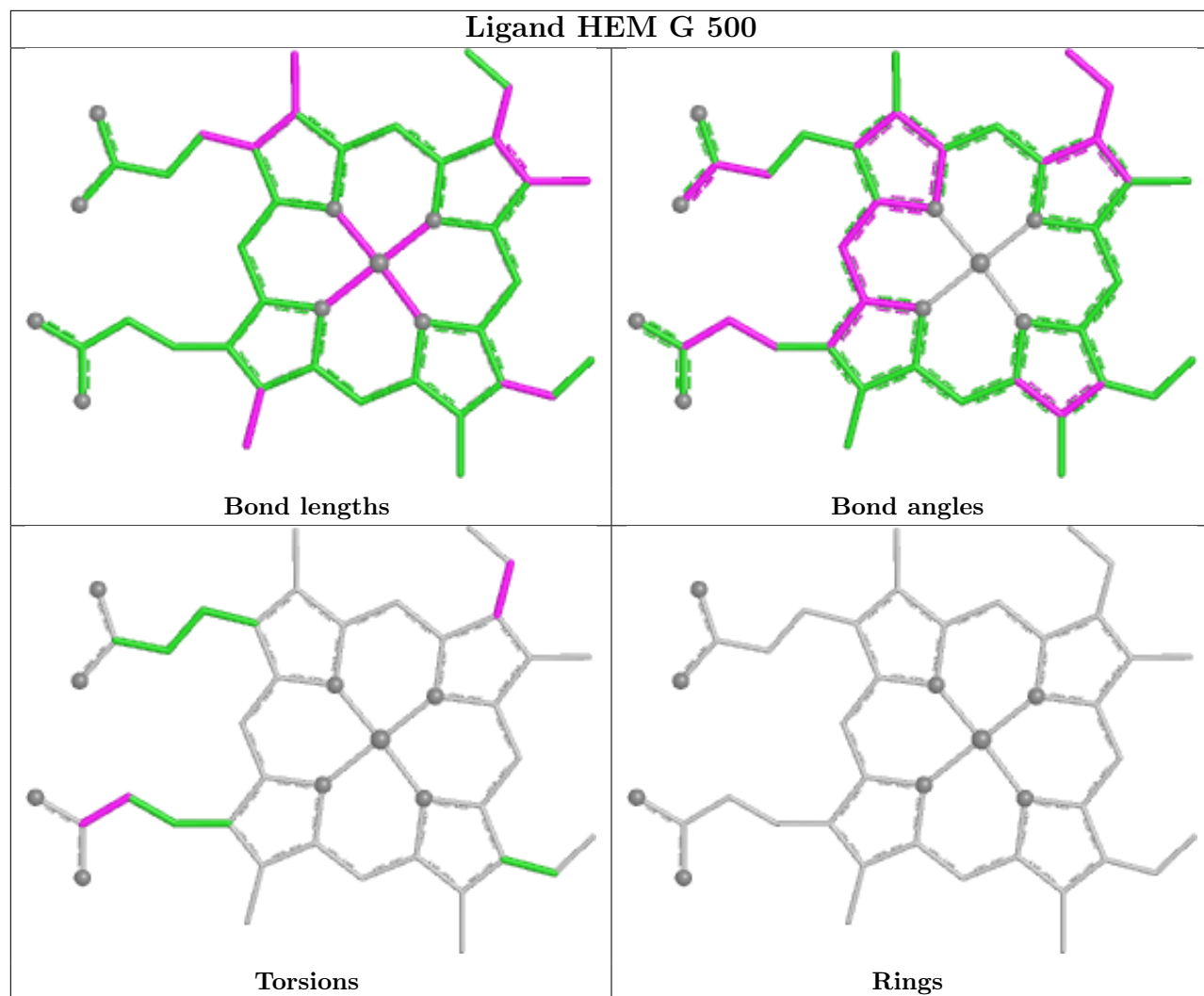
There are no ring outliers.

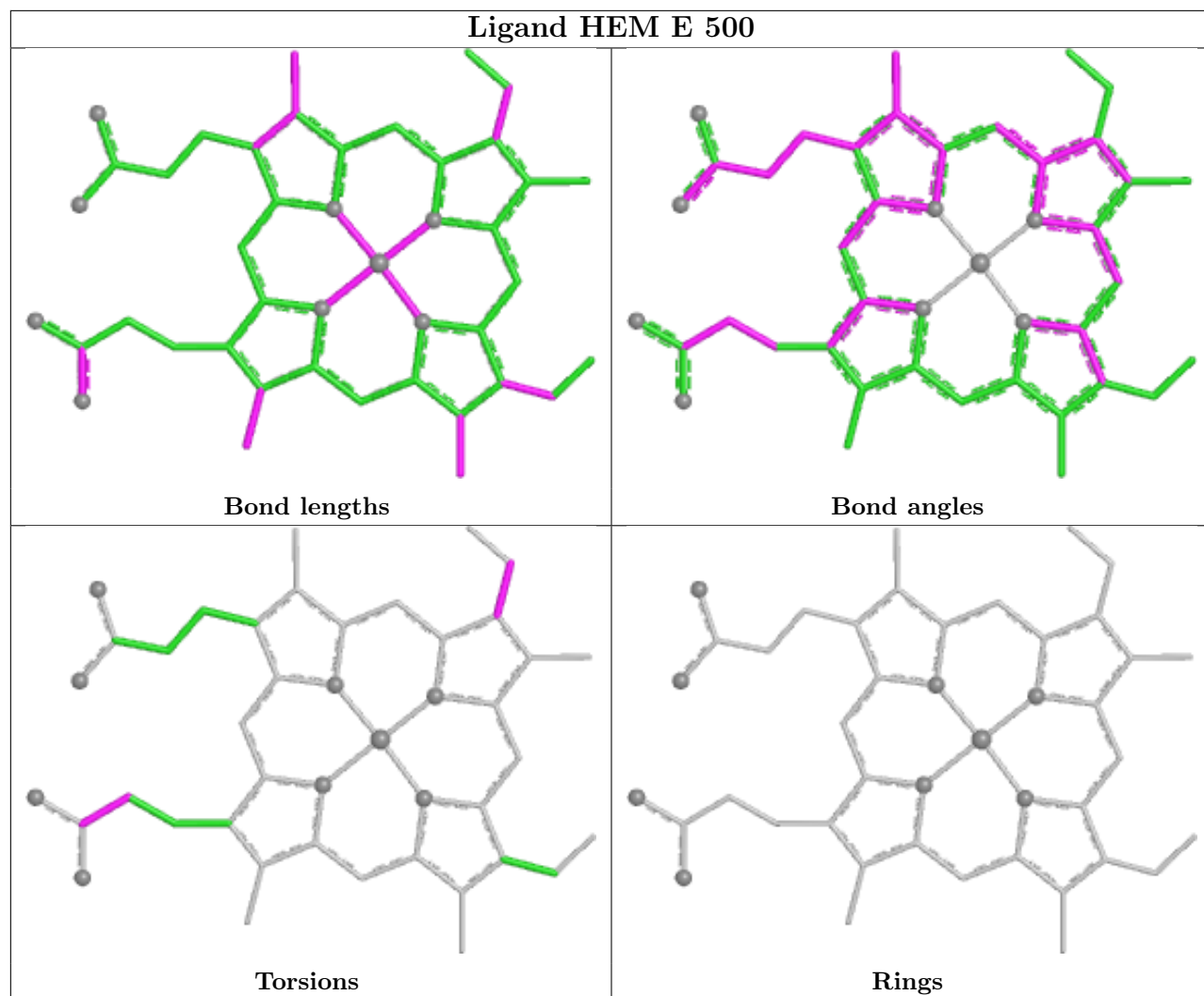
12 monomers are involved in 28 short contacts:

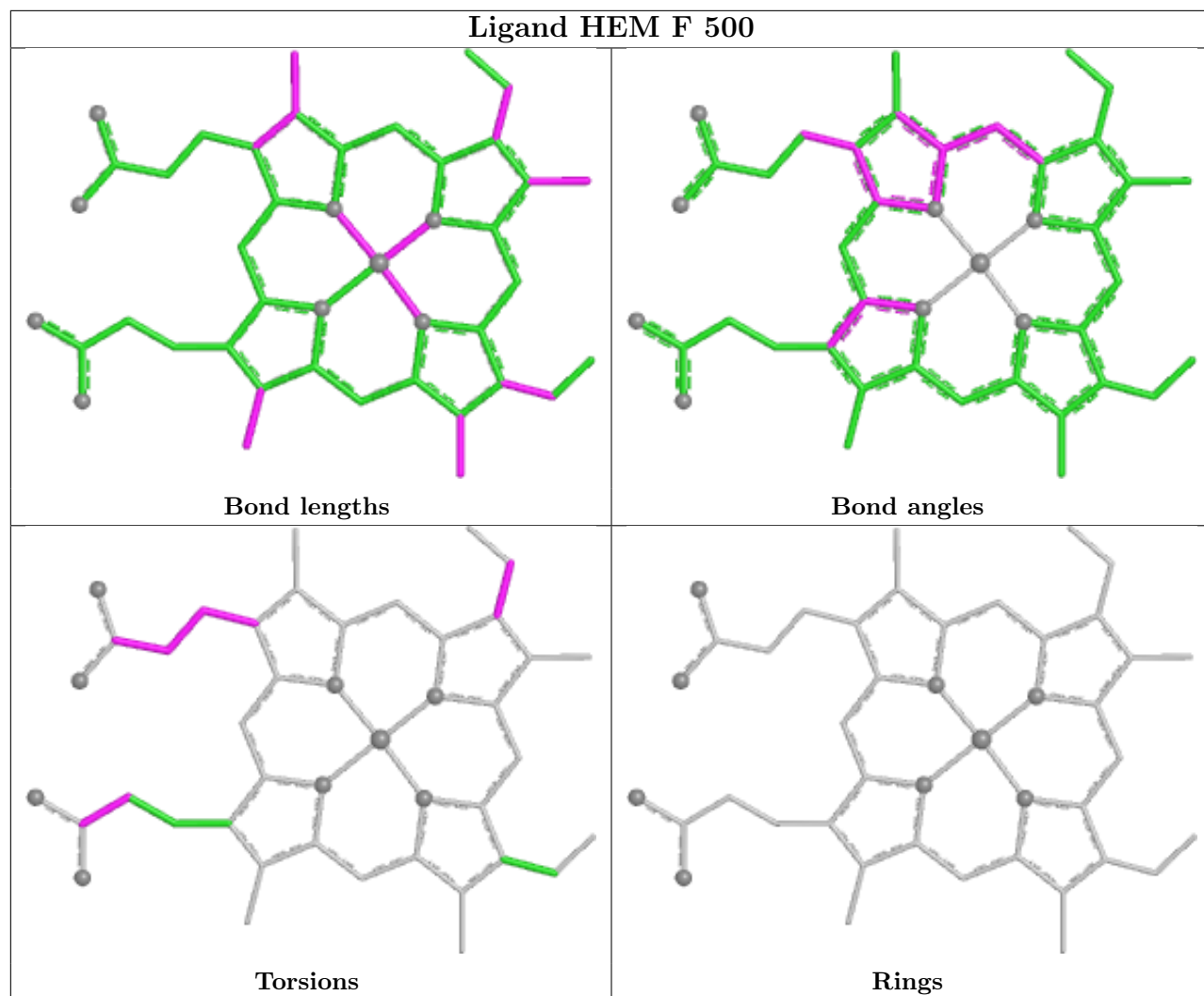
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	NCT	3	0
2	B	500	HEM	1	0
3	D	501	NCT	3	0
4	H	502	GOL	1	0
2	E	500	HEM	2	0
2	F	500	HEM	3	0
2	A	500	HEM	2	0
3	A	501	NCT	3	0
2	D	500	HEM	3	0
3	B	501	NCT	3	0
2	H	501	HEM	2	0
2	C	500	HEM	2	0

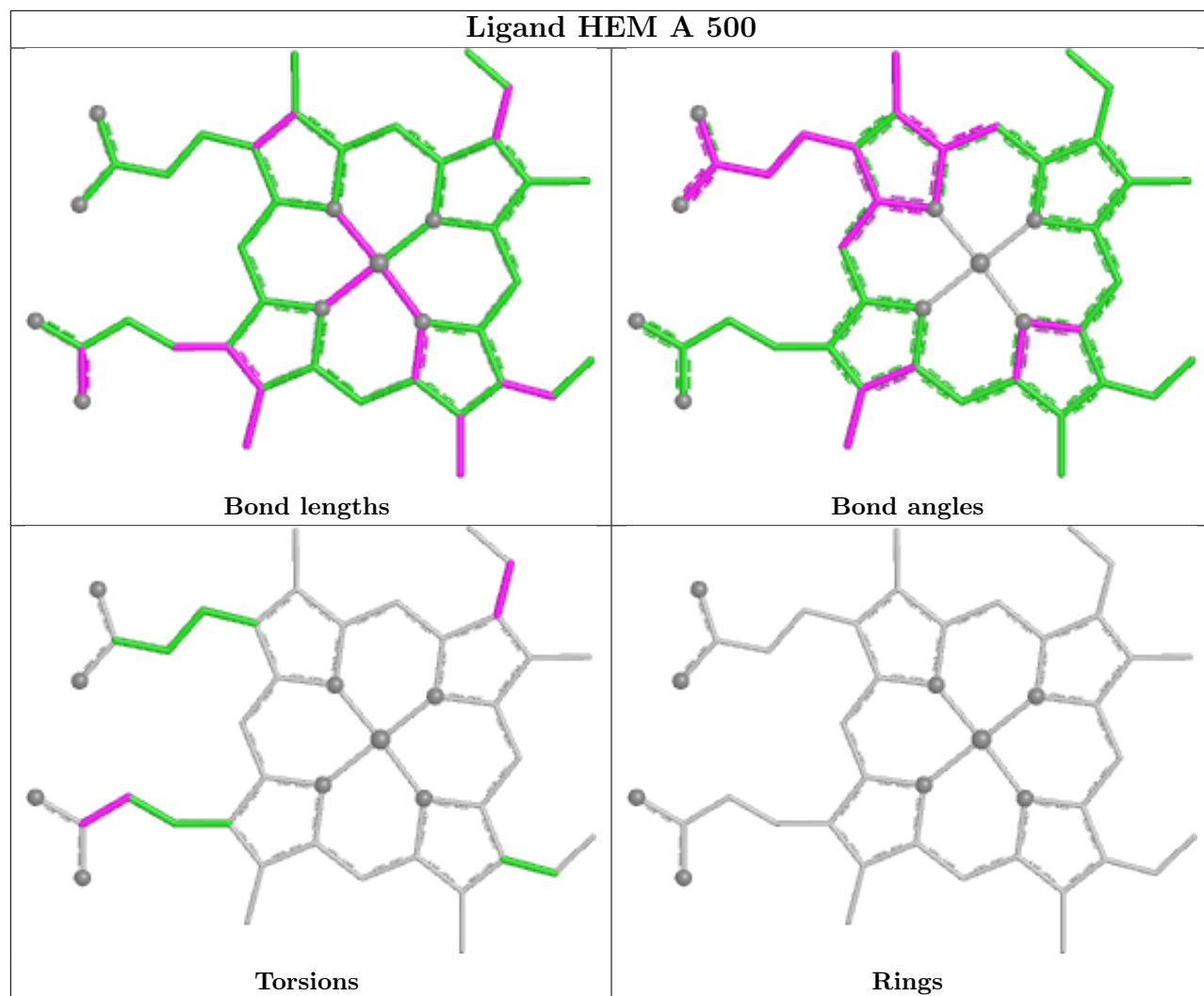
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

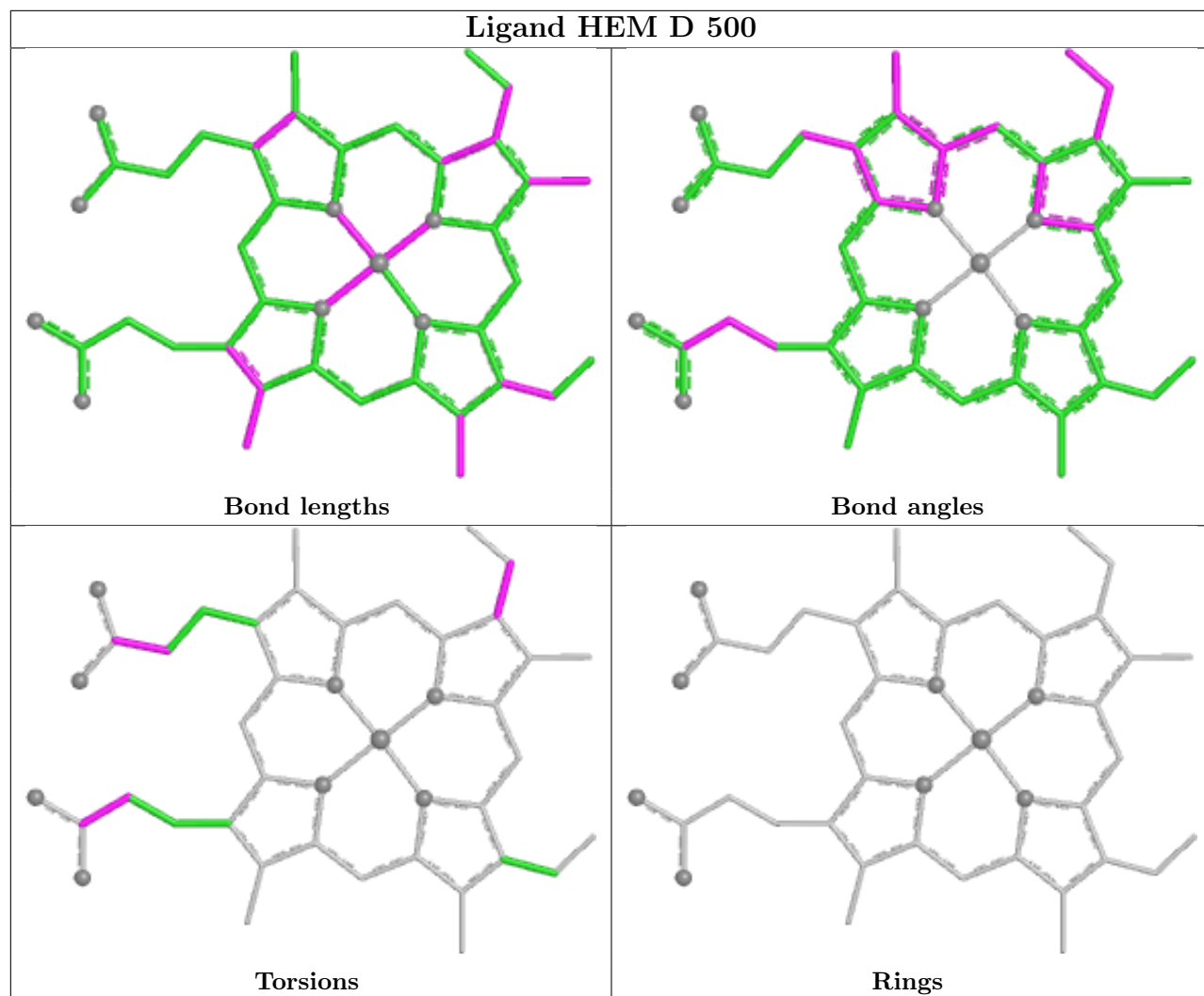


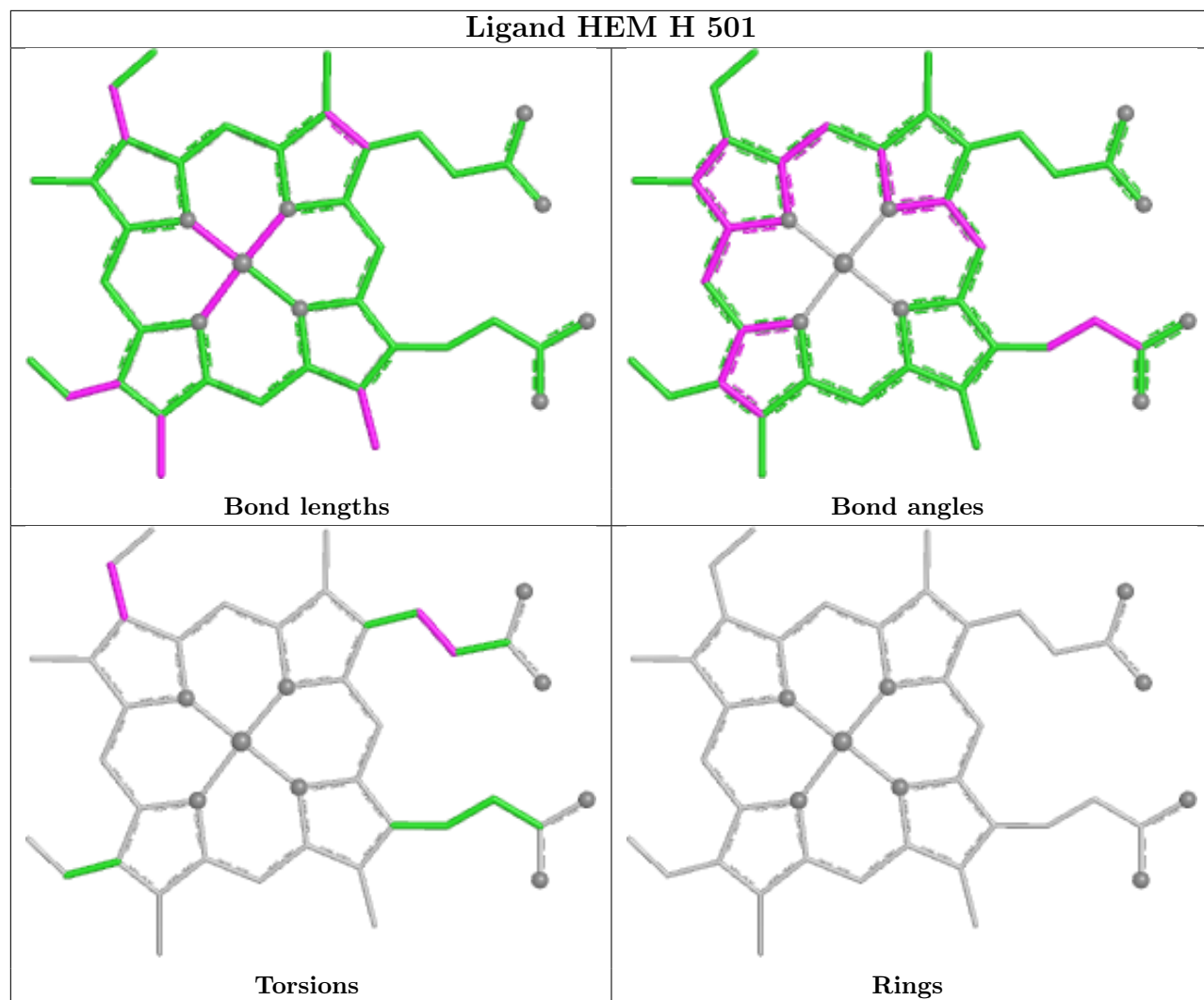


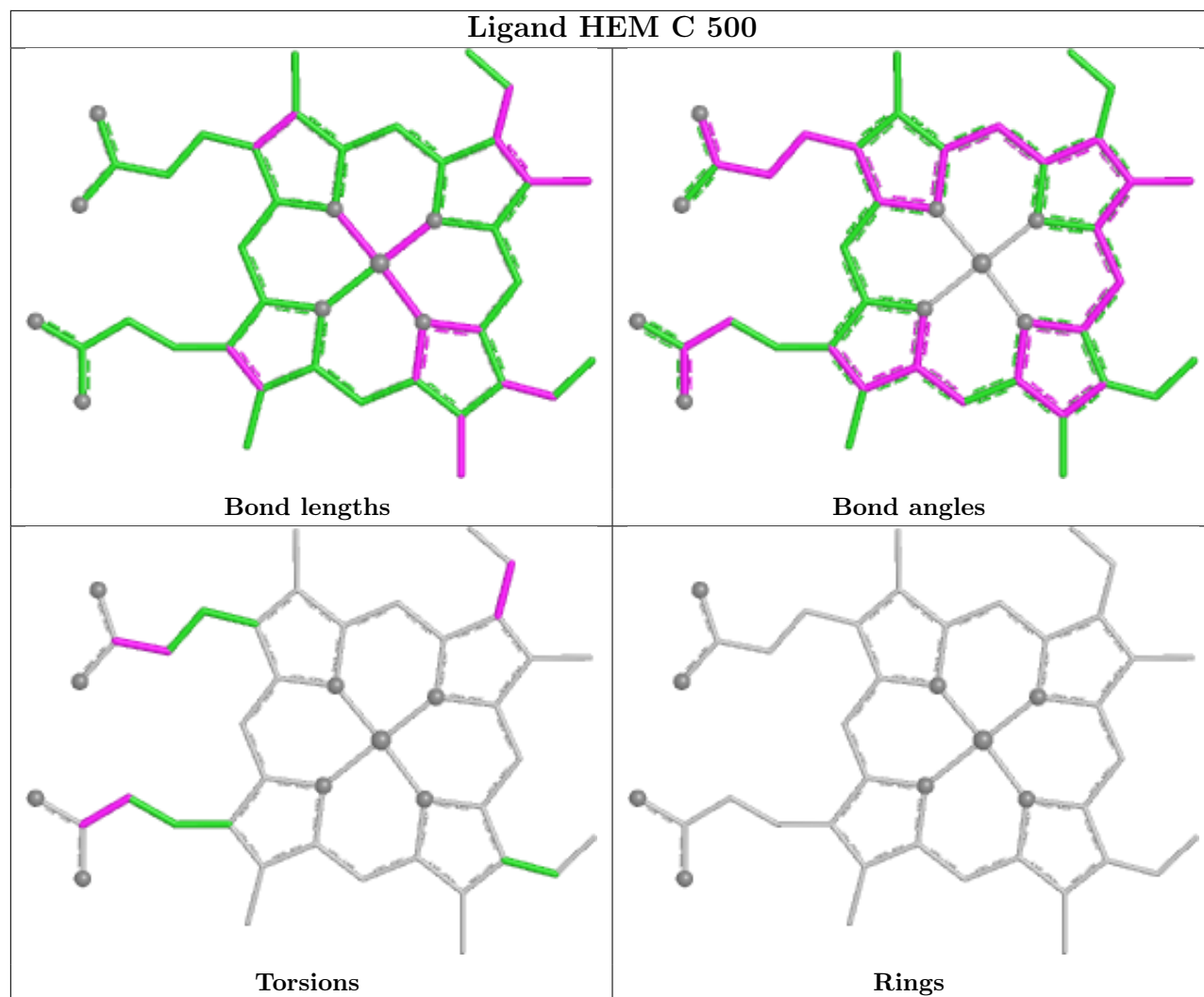












5.7 Other polymers [i](#)

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	464/476 (97%)	0.07	5 (1%) 78 75	14, 33, 53, 58	1 (0%)
1	B	464/476 (97%)	0.02	2 (0%) 88 86	13, 33, 52, 61	5 (1%)
1	C	464/476 (97%)	-0.03	0 100 100	12, 33, 49, 58	4 (0%)
1	D	465/476 (97%)	0.10	3 (0%) 85 83	13, 34, 52, 59	3 (0%)
1	E	465/476 (97%)	0.46	22 (4%) 36 32	17, 48, 66, 74	3 (0%)
1	F	465/476 (97%)	1.05	72 (15%) 5 4	23, 61, 83, 90	0
1	G	463/476 (97%)	1.33	101 (21%) 2 2	29, 65, 85, 95	0
1	H	458/476 (96%)	1.60	143 (31%) 1 1	23, 75, 94, 99	0
All	All	3708/3808 (97%)	0.57	348 (9%) 14 12	12, 45, 85, 99	16 (0%)

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	133	ALA	8.1
1	G	471	ILE	6.1
1	H	471	ILE	5.6
1	H	454	THR	5.5
1	G	155	PHE	5.4
1	H	145	ILE	5.3
1	H	462	PHE	5.1
1	H	480	PHE	5.0
1	G	137	GLY	4.7
1	H	417	LEU	4.5
1	G	408	PRO	4.5
1	H	267	PHE	4.5
1	H	468	PRO	4.4
1	H	408	PRO	4.4
1	H	478	VAL	4.3
1	F	140	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	173	PHE	4.1
1	H	138	PHE	4.1
1	G	420	LYS	4.1
1	H	423	PHE	4.1
1	H	173	PHE	4.1
1	G	413	PRO	4.0
1	G	168	ILE	4.0
1	G	488	THR	4.0
1	G	157	ILE	3.9
1	H	282	PRO	3.9
1	F	492	LEU	3.9
1	H	402	PRO	3.9
1	H	416	PHE	3.8
1	F	252	VAL	3.8
1	H	473	VAL	3.8
1	H	413	PRO	3.8
1	H	323	VAL	3.8
1	H	327	VAL	3.8
1	G	411	PHE	3.8
1	H	334	VAL	3.7
1	H	168	ILE	3.7
1	G	491	PHE	3.7
1	G	492	LEU	3.7
1	H	259	LEU	3.7
1	H	316	LEU	3.7
1	G	468	PRO	3.7
1	H	272	LEU	3.7
1	F	261	PRO	3.7
1	F	271	PHE	3.6
1	F	256	GLN	3.6
1	H	489	MET	3.5
1	G	214	THR	3.5
1	G	156	LEU	3.5
1	G	475	PRO	3.5
1	H	405	PHE	3.5
1	E	333[A]	ARG	3.5
1	G	163	THR	3.5
1	H	273	ILE	3.5
1	G	423	PHE	3.5
1	G	159	ALA	3.4
1	G	480	PHE	3.4
1	G	323	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	351	TYR	3.4
1	H	317	LEU	3.4
1	G	115	GLY	3.4
1	F	263	SER	3.4
1	H	464	SER	3.3
1	H	476	LYS	3.3
1	H	331	ILE	3.3
1	H	429	PHE	3.3
1	H	453	PHE	3.3
1	F	189	ASP	3.3
1	F	264	PRO	3.3
1	G	473	VAL	3.3
1	F	172	PHE	3.3
1	H	355	VAL	3.3
1	H	343	PHE	3.2
1	H	156	LEU	3.2
1	E	421	GLY	3.2
1	F	166	ALA	3.2
1	G	209	PHE	3.2
1	F	468	PRO	3.2
1	H	157	ILE	3.1
1	H	174	LEU	3.1
1	G	478	VAL	3.1
1	G	212	THR	3.1
1	H	188	GLY	3.1
1	H	430	VAL	3.1
1	H	335	ILE	3.1
1	G	213	ALA	3.1
1	H	415	HIS	3.1
1	F	351	TYR	3.0
1	F	412	ASN	3.0
1	H	154	GLY	3.0
1	G	482	THR	3.0
1	F	493	PRO	3.0
1	H	411	PHE	3.0
1	G	421	GLY	3.0
1	H	398	VAL	3.0
1	H	456	ILE	3.0
1	H	320	HIS	3.0
1	F	288	LEU	3.0
1	F	31	GLY	3.0
1	F	141	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	140	VAL	3.0
1	H	359	ILE	3.0
1	G	218	GLN	3.0
1	H	86	ALA	2.9
1	H	199	LEU	2.9
1	F	191	PHE	2.9
1	F	453	PHE	2.9
1	G	215	SER	2.9
1	F	318	MET	2.9
1	G	484	PRO	2.9
1	G	351	TYR	2.9
1	H	153	ALA	2.9
1	F	199	LEU	2.9
1	G	487	TYR	2.9
1	G	327	VAL	2.9
1	F	138	PHE	2.9
1	G	462	PHE	2.9
1	H	191	PHE	2.9
1	G	474	SER	2.8
1	H	248	ILE	2.8
1	H	493	PRO	2.8
1	F	491	PHE	2.8
1	G	460	PHE	2.8
1	H	264	PRO	2.8
1	F	124	ALA	2.8
1	H	271	PHE	2.8
1	G	490	SER	2.8
1	F	321	PRO	2.8
1	G	454	THR	2.8
1	G	181	VAL	2.8
1	G	321	PRO	2.8
1	G	303	THR	2.8
1	H	135	LEU	2.8
1	H	366	LEU	2.8
1	F	251	LYS	2.8
1	G	314	PHE	2.8
1	F	262	ASN	2.7
1	A	143	ARG	2.7
1	H	193	TYR	2.7
1	H	487	TYR	2.7
1	F	339	ARG	2.7
1	G	170	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	193	TYR	2.7
1	G	305	THR	2.7
1	H	132	ILE	2.7
1	H	477	HIS	2.7
1	E	364	ASP	2.6
1	H	189	ASP	2.6
1	E	453	PHE	2.6
1	G	138	PHE	2.6
1	G	172	PHE	2.6
1	G	273	ILE	2.6
1	G	416	PHE	2.6
1	G	465	PRO	2.6
1	G	160	LEU	2.6
1	H	160	LEU	2.6
1	H	397	SER	2.6
1	F	139	GLY	2.6
1	H	421	GLY	2.6
1	H	463	LYS	2.6
1	F	489	MET	2.6
1	G	317	LEU	2.6
1	F	147	GLU	2.6
1	G	133	ALA	2.6
1	H	325	ALA	2.6
1	A	32	LYS	2.6
1	H	424	LYS	2.6
1	H	268	ILE	2.6
1	H	315	LEU	2.6
1	F	473	VAL	2.6
1	F	490	SER	2.6
1	F	438	TYR	2.6
1	E	468	PRO	2.6
1	G	192	ASP	2.6
1	H	172	PHE	2.6
1	H	458	GLN	2.6
1	F	154	GLY	2.5
1	H	324	GLU	2.5
1	G	210	GLN	2.5
1	G	145	ILE	2.5
1	G	142	LYS	2.5
1	G	463	LYS	2.5
1	H	92	VAL	2.5
1	H	38	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	54	MET	2.5
1	H	261	PRO	2.5
1	H	83	GLY	2.5
1	H	149	ILE	2.5
1	H	419	LYS	2.5
1	H	328	HIS	2.5
1	G	409	ARG	2.5
1	E	31	GLY	2.5
1	G	329	GLU	2.5
1	H	479	GLY	2.5
1	A	189	ASP	2.5
1	H	472	ASP	2.5
1	F	259	LEU	2.5
1	E	462	PHE	2.5
1	H	428	ALA	2.5
1	H	406	SER	2.5
1	G	251	LYS	2.4
1	G	335	ILE	2.4
1	H	55	TYR	2.4
1	H	187	PHE	2.4
1	H	383	PHE	2.4
1	H	400	ARG	2.4
1	G	301	ALA	2.4
1	G	406	SER	2.4
1	H	165	GLY	2.4
1	F	185	ILE	2.4
1	H	483	ILE	2.4
1	F	127	LEU	2.4
1	F	272	LEU	2.4
1	H	450	PHE	2.4
1	F	338	ASN	2.4
1	H	51	THR	2.4
1	H	425	LYS	2.4
1	H	469	LYS	2.4
1	F	145	ILE	2.4
1	G	189	ASP	2.4
1	G	410	ASP	2.4
1	H	427	ASP	2.4
1	H	438	TYR	2.4
1	H	491	PHE	2.4
1	F	153	ALA	2.4
1	H	329	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	458	GLN	2.4
1	H	288	LEU	2.4
1	B	172	PHE	2.4
1	E	193	TYR	2.4
1	G	271	PHE	2.4
1	G	178	VAL	2.4
1	F	347	ALA	2.4
1	G	481	ALA	2.4
1	E	352	THR	2.3
1	G	313	GLY	2.3
1	F	345	ASP	2.3
1	H	82	CYS	2.3
1	H	118	PHE	2.3
1	G	261	PRO	2.3
1	G	464	SER	2.3
1	D	31	GLY	2.3
1	A	366	LEU	2.3
1	B	246	ASP	2.3
1	F	125	LYS	2.3
1	H	155	PHE	2.3
1	H	362	PHE	2.3
1	G	193	TYR	2.3
1	F	341	PRO	2.3
1	F	377	ASP	2.3
1	F	247	PHE	2.3
1	H	314	PHE	2.3
1	H	163	THR	2.3
1	D	141	GLY	2.3
1	H	313	GLY	2.3
1	G	135	LEU	2.3
1	H	368	MET	2.3
1	H	420	LYS	2.3
1	H	152	GLU	2.3
1	G	282	PRO	2.3
1	H	170	PRO	2.3
1	H	321	PRO	2.3
1	E	273	ILE	2.2
1	G	399	LEU	2.2
1	E	343	PHE	2.2
1	F	198	PHE	2.2
1	H	98	PHE	2.2
1	G	402	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	186	VAL	2.2
1	H	407	ASN	2.2
1	F	280	LYS	2.2
1	G	139	GLY	2.2
1	G	188	GLY	2.2
1	H	401	ASP	2.2
1	E	278	GLU	2.2
1	F	160	LEU	2.2
1	F	201	LEU	2.2
1	E	239[A]	LYS	2.2
1	E	254	HIS	2.2
1	E	276	GLN	2.2
1	H	357	HIS	2.2
1	H	447	MET	2.2
1	F	287	TYR	2.2
1	G	206	LEU	2.2
1	G	316	LEU	2.2
1	H	474	SER	2.2
1	F	192	ASP	2.2
1	F	253	GLU	2.2
1	F	410	ASP	2.2
1	H	465	PRO	2.2
1	E	166	ALA	2.1
1	H	318	MET	2.1
1	H	457	MET	2.1
1	F	206	LEU	2.1
1	H	171	THR	2.1
1	H	303	THR	2.1
1	H	182	ILE	2.1
1	A	462	PHE	2.1
1	F	383	PHE	2.1
1	G	144	GLY	2.1
1	H	449	LEU	2.1
1	F	273	ILE	2.1
1	F	122	GLU	2.1
1	H	364	ASP	2.1
1	F	419	LYS	2.1
1	E	282	PRO	2.1
1	F	350	PRO	2.1
1	E	457	MET	2.1
1	G	365	MET	2.1
1	F	486	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	375	ASN	2.1
1	G	259	LEU	2.1
1	H	451	LEU	2.1
1	E	455	THR	2.1
1	F	268	ILE	2.1
1	H	434	ILE	2.1
1	H	319	LYS	2.1
1	H	418	ASP	2.1
1	G	164	HIS	2.1
1	G	235	GLN	2.1
1	G	87	VAL	2.1
1	G	300	PHE	2.1
1	G	334	VAL	2.1
1	H	166	ALA	2.1
1	H	399	LEU	2.1
1	G	304	GLU	2.1
1	G	149	ILE	2.1
1	G	182	ILE	2.1
1	G	260	ASP	2.1
1	H	269	ASP	2.1
1	F	200	SER	2.1
1	H	350	PRO	2.1
1	G	254	HIS	2.1
1	G	211	PHE	2.0
1	F	249	ALA	2.0
1	E	135	LEU	2.0
1	G	141	GLY	2.0
1	H	330	GLU	2.0
1	D	30	LYS	2.0
1	E	471	ILE	2.0
1	E	382	ASP	2.0
1	F	169	ASP	2.0
1	F	190	ARG	2.0
1	H	178	VAL	2.0
1	H	52	GLU	2.0
1	F	162	GLY	2.0
1	F	302	GLY	2.0
1	H	309	THR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

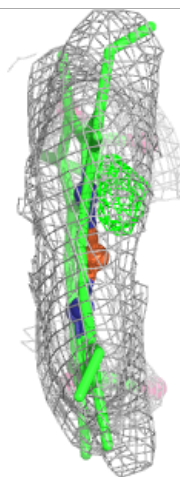
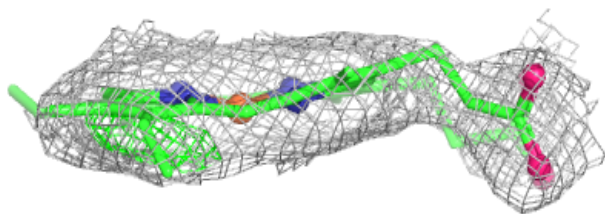
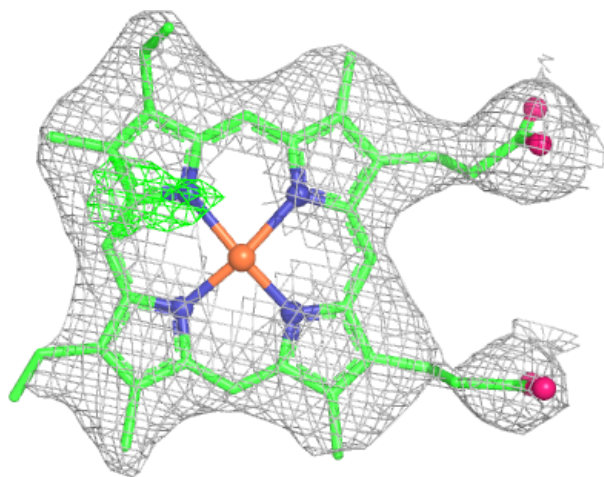
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NCT	C	501	12/12	0.90	0.21	61,62,67,68	0
4	GOL	H	502	6/6	0.90	0.19	28,32,35,37	0
3	NCT	A	501	12/12	0.91	0.15	50,52,53,54	0
3	NCT	D	501	12/12	0.91	0.20	80,81,82,82	0
3	NCT	B	501	12/12	0.91	0.12	40,43,44,47	0
2	HEM	H	501	43/43	0.93	0.15	58,61,67,68	0
2	HEM	D	500	43/43	0.96	0.09	16,26,28,28	0
2	HEM	F	500	43/43	0.96	0.09	44,48,50,51	0
2	HEM	E	500	43/43	0.97	0.07	26,33,35,35	0
2	HEM	A	500	43/43	0.97	0.08	16,23,27,31	0
2	HEM	G	500	43/43	0.97	0.08	32,38,43,49	0
2	HEM	B	500	43/43	0.98	0.06	13,23,25,28	0
2	HEM	C	500	43/43	0.98	0.07	15,23,27,29	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.

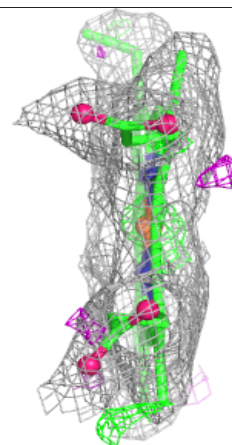
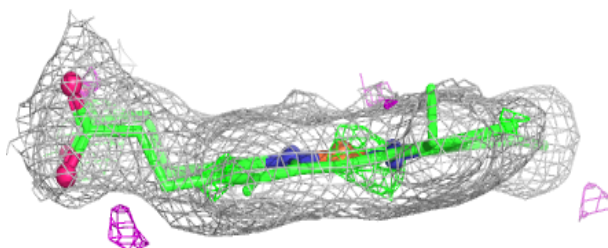
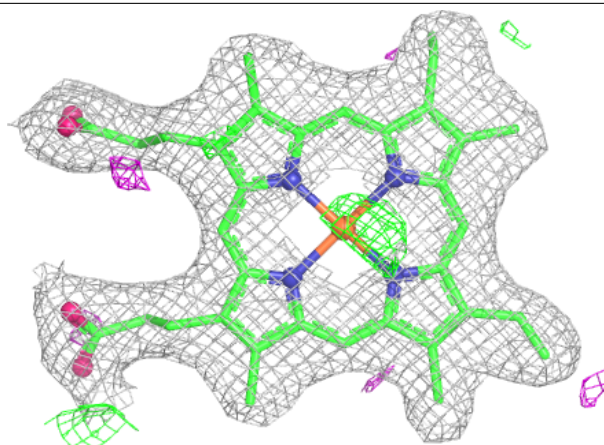
Electron density around HEM H 501:

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



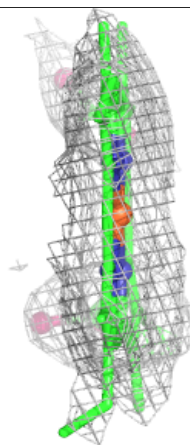
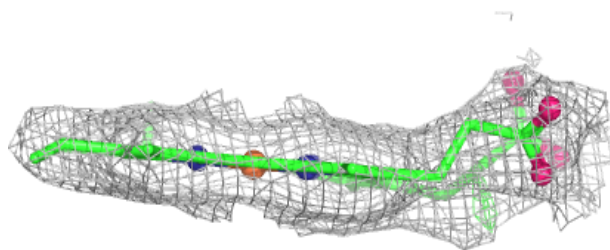
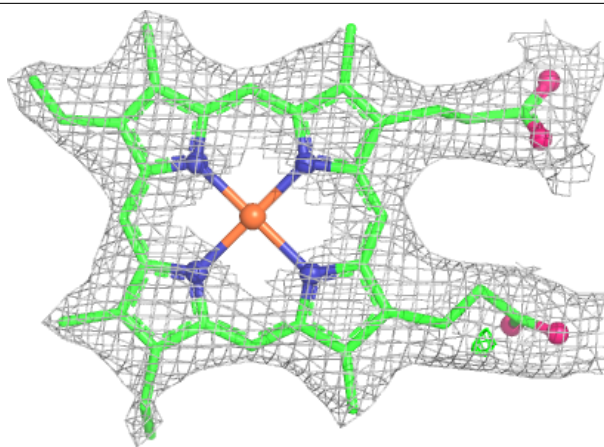
Electron density around HEM D 500:

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



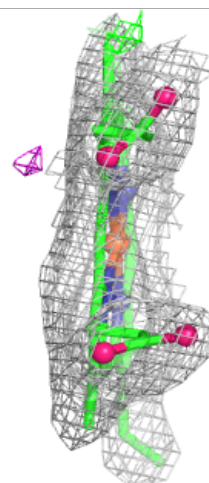
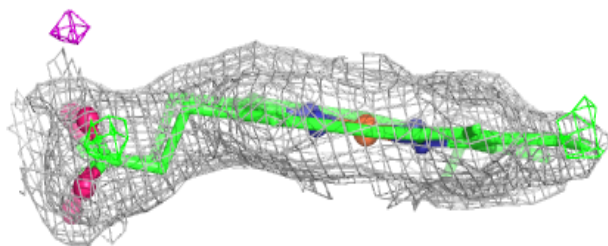
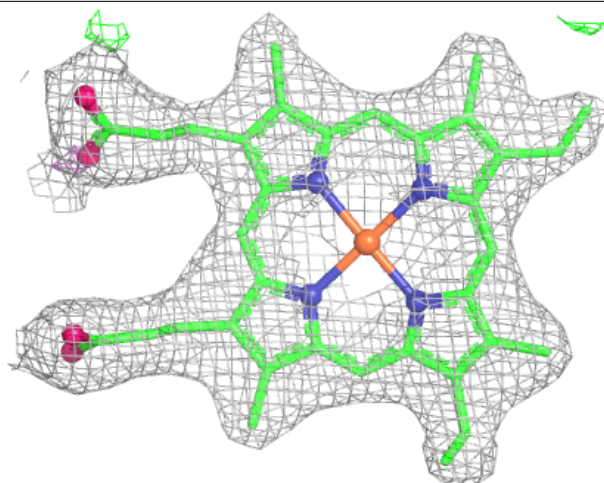
Electron density around HEM F 500:

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



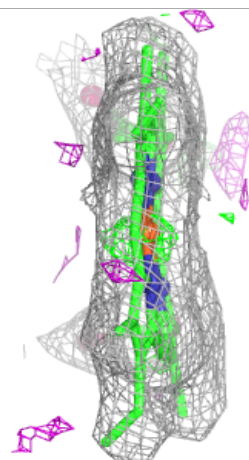
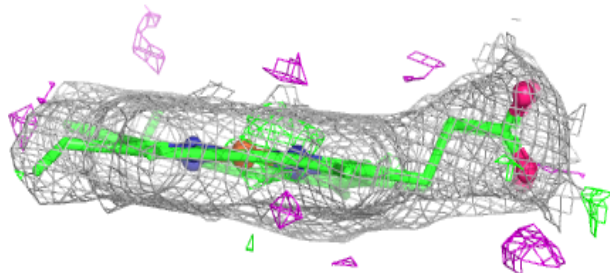
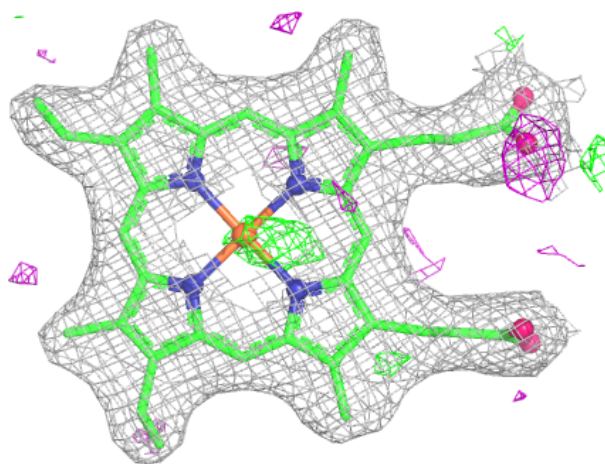
Electron density around HEM E 500:

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



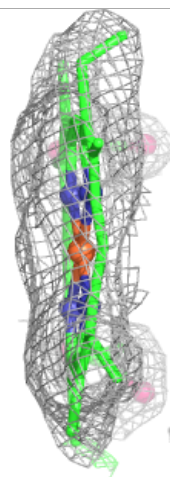
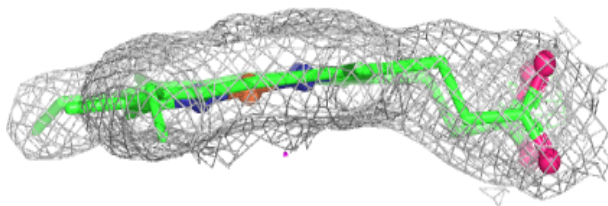
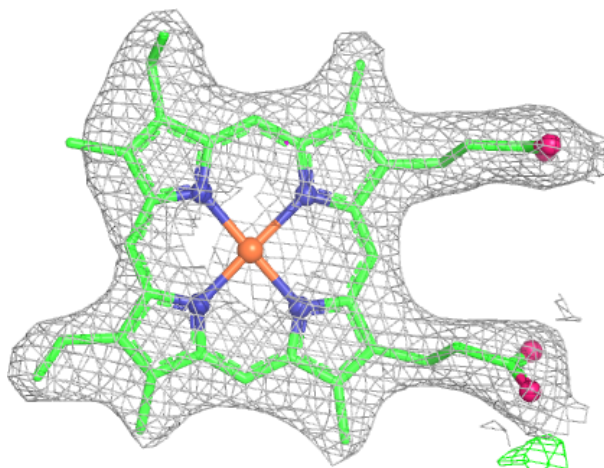
Electron density around HEM A 500:

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



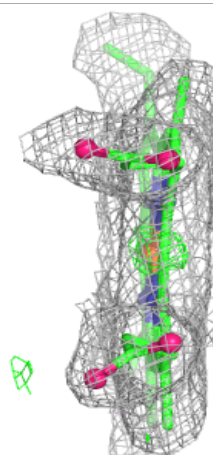
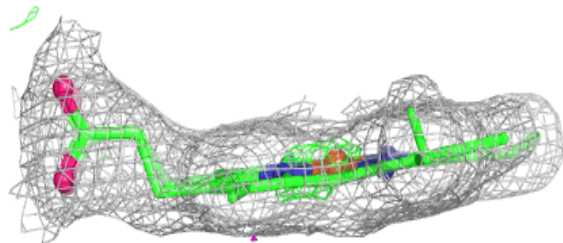
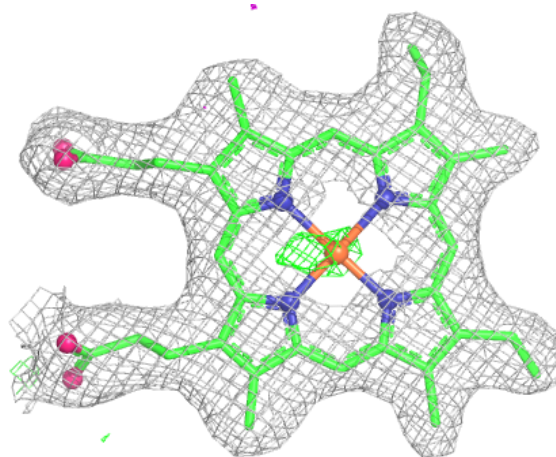
Electron density around HEM G 500:

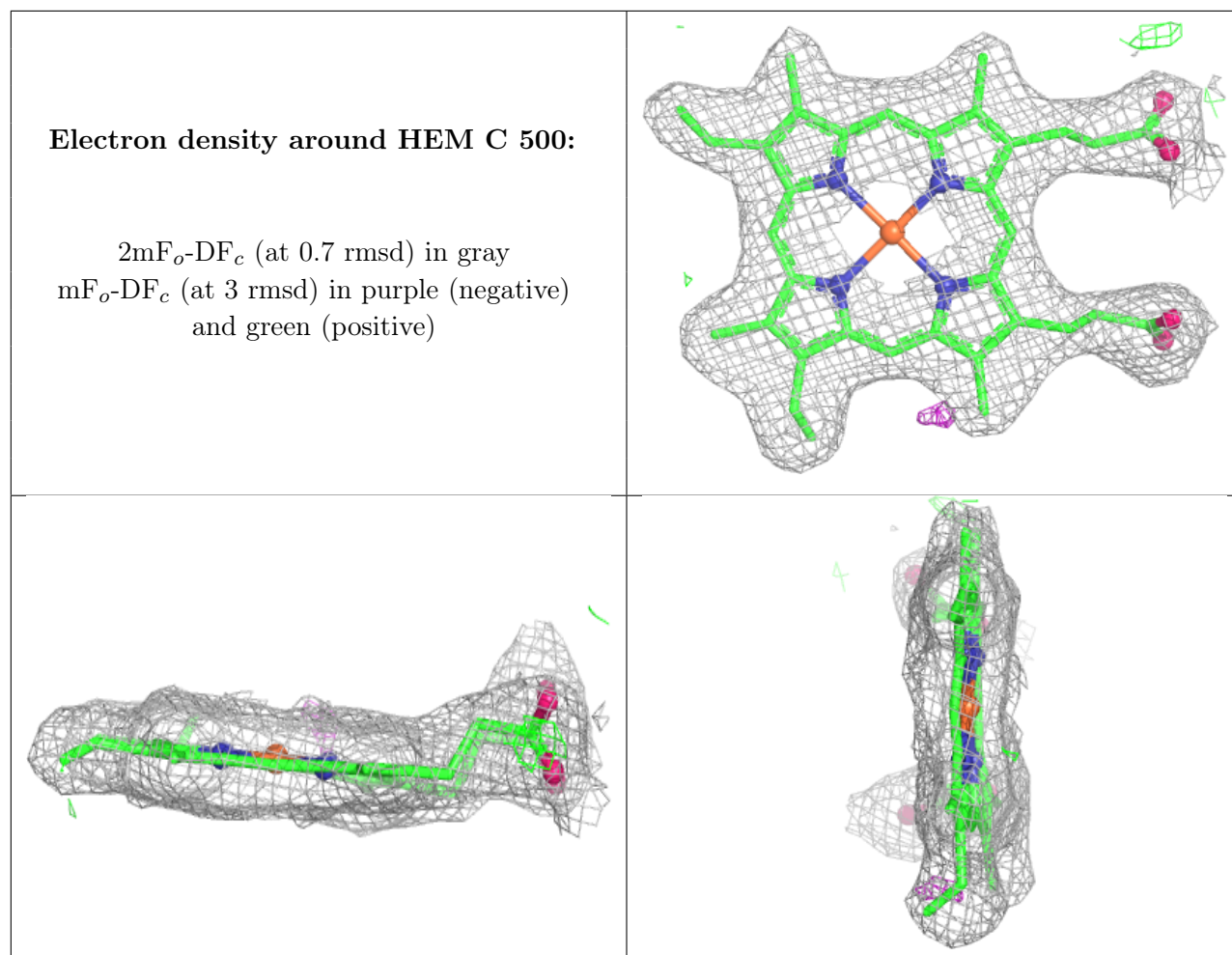
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.