



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:50 PM UTC

PDB ID : 2NNH / pdb_00002nnh
Title : CYP2C8dH complexed with 2 molecules of 9-cis retinoic acid
Authors : Schoch, G.A.; Yano, J.K.; Stout, C.D.; Johnson, E.F.
Deposited on : 2006-10-24
Resolution : 2.60 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

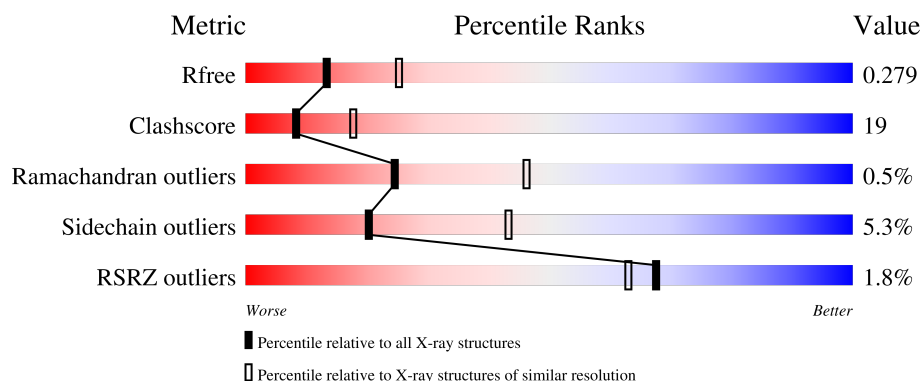
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	% 61% 33% • •
1	B	476	3% 56% 37% 5% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7694 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 2C8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3693	2362	635	674	22			
1	B	463	Total	C	N	O	S	0	0	0
			3693	2362	635	674	22			

There are 26 discrepancies between the modelled and reference sequences:

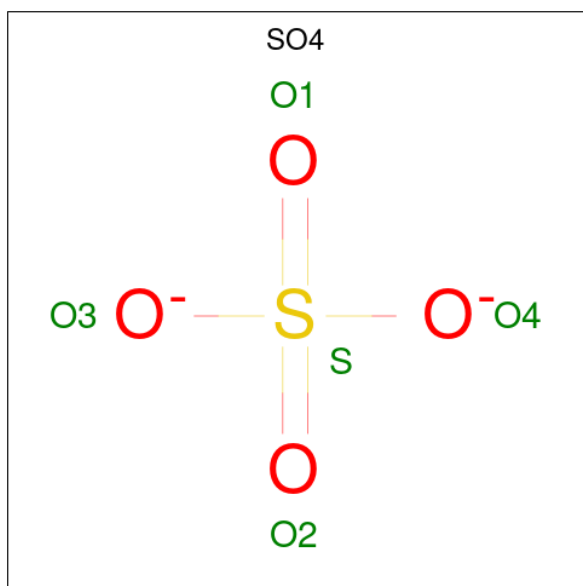
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P10632
A	20	ALA	-	expression tag	UNP P10632
A	21	LYS	-	expression tag	UNP P10632
A	22	LYS	-	expression tag	UNP P10632
A	23	THR	-	expression tag	UNP P10632
A	24	SER	-	expression tag	UNP P10632
A	25	SER	-	expression tag	UNP P10632
A	26	LYS	-	expression tag	UNP P10632
A	27	GLY	-	expression tag	UNP P10632
A	491	HIS	-	expression tag	UNP P10632
A	492	HIS	-	expression tag	UNP P10632
A	493	HIS	-	expression tag	UNP P10632
A	494	HIS	-	expression tag	UNP P10632
B	19	MET	-	expression tag	UNP P10632
B	20	ALA	-	expression tag	UNP P10632
B	21	LYS	-	expression tag	UNP P10632
B	22	LYS	-	expression tag	UNP P10632
B	23	THR	-	expression tag	UNP P10632
B	24	SER	-	expression tag	UNP P10632
B	25	SER	-	expression tag	UNP P10632
B	26	LYS	-	expression tag	UNP P10632
B	27	GLY	-	expression tag	UNP P10632
B	491	HIS	-	expression tag	UNP P10632
B	492	HIS	-	expression tag	UNP P10632
B	493	HIS	-	expression tag	UNP P10632

Continued on next page...

Continued from previous page...

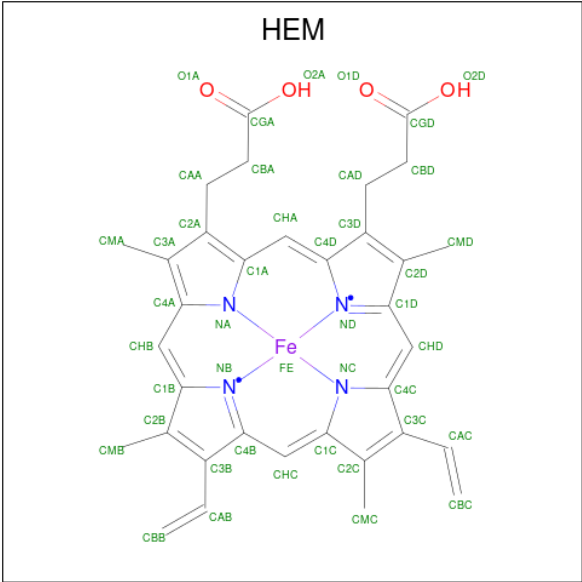
Chain	Residue	Modelled	Actual	Comment	Reference
B	494	HIS	-	expression tag	UNP P10632

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



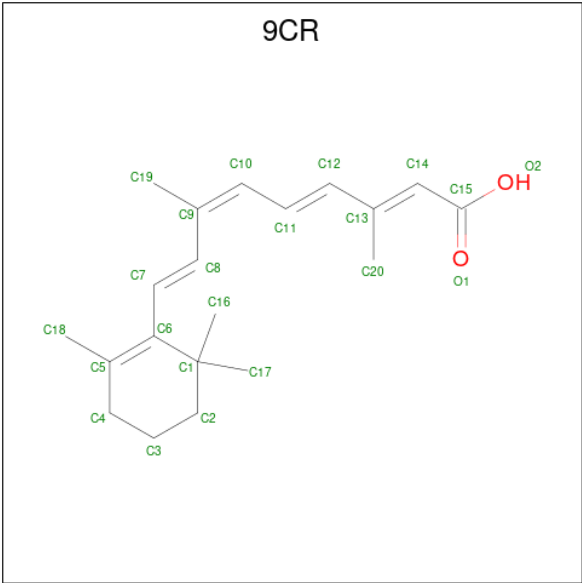
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is (9cis)-retinoic acid (CCD ID: 9CR) (formula: C₂₀H₂₈O₂).



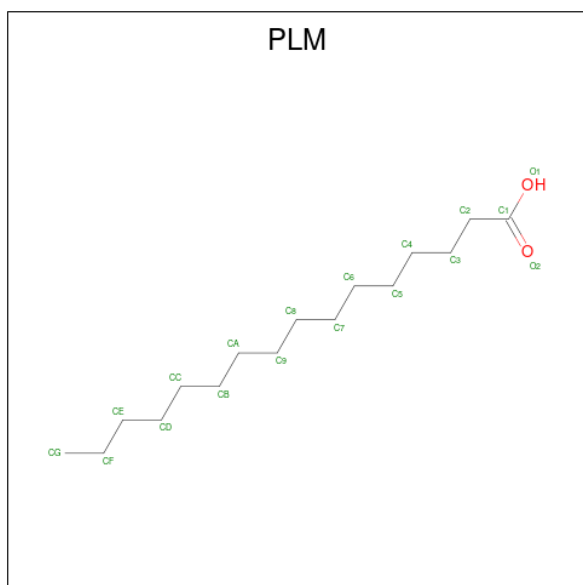
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		
4	A	1	Total	C	O	0	0
			22	20	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			22	20	2		
4	B	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			18	16	2		
5	B	1	Total	C	O	0	0
			18	16	2		

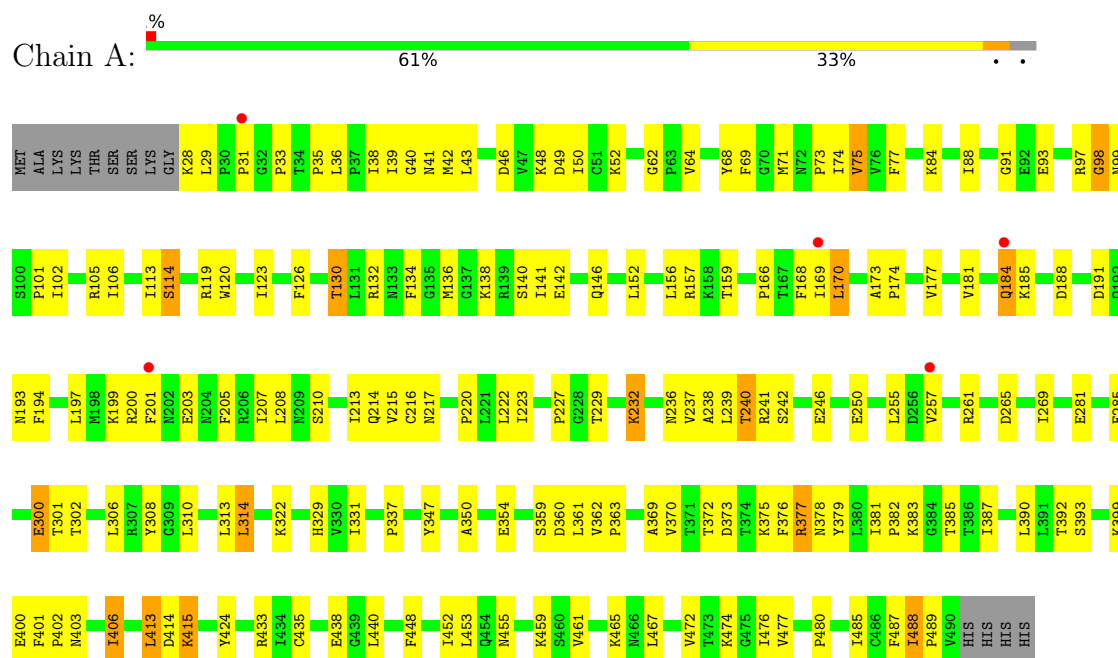
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	44	Total	O	0	0
			44	44		

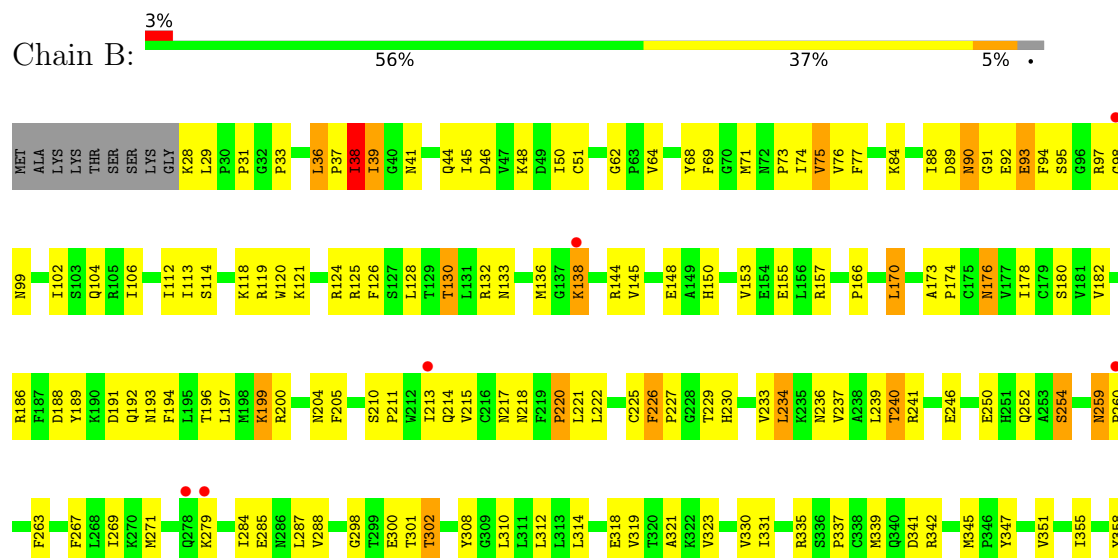
3 Residue-property plots

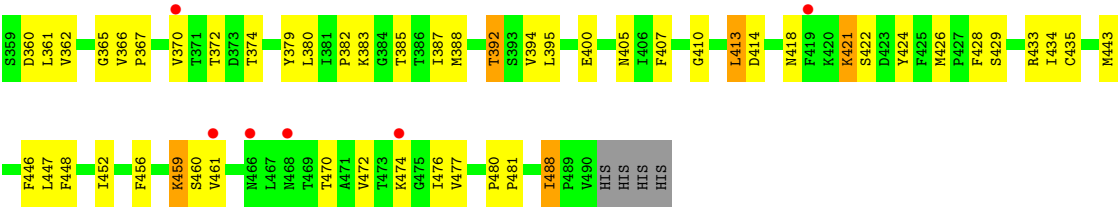
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2C8



• Molecule 1: Cytochrome P450 2C8





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.81Å 163.62Å 73.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.60) 97.2 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.290 0.233 , 0.279	Depositor DCC
R_{free} test set	2557 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7694	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.79% 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, PLM, SO4, 9CR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3778	1.01	18/5115 (0.4%)
1	B	0.48	0/3778	1.01	18/5115 (0.4%)
All	All	0.48	0/7556	1.01	36/10230 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	362	VAL	CA-C-N	8.89	128.49	119.24
1	B	362	VAL	C-N-CA	8.89	128.49	119.24
1	A	362	VAL	CA-C-N	7.75	127.03	118.97
1	A	362	VAL	C-N-CA	7.75	127.03	118.97
1	B	98	GLY	N-CA-C	7.66	125.35	113.86
1	A	138	LYS	N-CA-C	7.59	119.19	111.07
1	A	62	GLY	CA-C-N	7.24	127.58	119.32
1	A	62	GLY	C-N-CA	7.24	127.58	119.32
1	B	38	ILE	N-CA-C	7.05	118.04	112.12
1	B	62	GLY	CA-C-N	7.04	126.29	118.97
1	B	62	GLY	C-N-CA	7.04	126.29	118.97
1	A	50	ILE	N-CA-C	6.93	118.53	110.62
1	A	488	ILE	N-CA-C	6.84	113.78	107.56
1	B	259	ASN	CA-C-N	6.79	126.70	119.85
1	B	259	ASN	C-N-CA	6.79	126.70	119.85
1	A	98	GLY	N-CA-C	6.72	122.05	113.24
1	A	188	ASP	N-CA-C	-6.67	99.96	109.96
1	B	226	PHE	CA-C-N	6.66	126.16	119.24
1	B	226	PHE	C-N-CA	6.66	126.16	119.24
1	A	399	LYS	N-CA-C	-6.45	105.95	113.88
1	A	168	PHE	N-CA-C	6.31	117.85	110.97
1	B	36	LEU	CA-C-N	5.93	127.26	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	LEU	C-N-CA	5.93	127.26	119.84
1	B	365	GLY	N-CA-C	-5.76	102.21	112.58
1	B	76	VAL	N-CA-C	5.57	116.12	107.99
1	B	330	VAL	N-CA-C	5.54	116.38	111.90
1	B	188	ASP	N-CA-C	-5.50	101.50	110.20
1	A	36	LEU	CA-C-N	5.50	125.85	119.47
1	A	36	LEU	C-N-CA	5.50	125.85	119.47
1	A	329	HIS	N-CA-C	5.48	117.06	111.14
1	A	113	ILE	CB-CA-C	-5.40	105.00	112.24
1	A	91	GLY	N-CA-C	5.37	119.17	112.73
1	A	132	ARG	N-CA-C	-5.30	102.63	110.48
1	A	159	THR	N-CA-C	-5.29	106.79	113.20
1	B	488	ILE	N-CA-C	5.23	112.32	107.56
1	B	113	ILE	N-CA-C	5.21	115.42	110.42

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	3693	0	3715	135	0
1	B	3693	0	3715	160	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
4	A	44	0	54	3	0
4	B	44	0	54	2	0
5	A	18	0	31	5	0
5	B	18	0	31	4	0
6	A	44	0	0	1	0
6	B	44	0	0	4	0
All	All	7694	0	7660	293	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 19.

All (293) 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:166:PRO:HB2	1:A:170:LEU:HD22	1.39	1.03
1:A:474:LYS:HE3	1:B:227:PRO:HG2	1.43	0.99
1:B:200:ARG:HH21	1:B:239:LEU:HD13	1.27	0.98
1:B:210:SER:O	1:B:213:ILE:HG13	1.65	0.94
1:B:360:ASP:OD2	1:B:392:THR:HG23	1.67	0.94
1:B:48:LYS:HE3	1:B:474:LYS:HE2	1.50	0.92
1:B:126:PHE:O	1:B:130:THR:HG23	1.70	0.92
1:A:377:ARG:HG3	1:A:378:ASN:H	1.31	0.91
1:B:331:ILE:HD13	1:B:337:PRO:HB3	1.50	0.91
1:A:200:ARG:HH21	1:A:239:LEU:HD13	1.36	0.90
1:B:421:LYS:NZ	1:B:422:SER:H	1.70	0.89
1:B:414:ASP:OD1	1:B:418:ASN:HB2	1.73	0.89
1:B:421:LYS:HZ2	1:B:422:SER:H	0.91	0.89
1:A:169:ILE:HD12	1:A:170:LEU:N	1.87	0.89
1:A:331:ILE:HD13	1:A:337:PRO:HB3	1.54	0.87
1:B:213:ILE:HD12	1:B:214:GLN:N	1.96	0.81
1:A:213:ILE:HD12	1:A:214:GLN:N	1.96	0.80
1:B:29:LEU:HD21	1:B:382:PRO:HD2	1.64	0.80
1:A:255:LEU:HD11	1:A:269:ILE:HD11	1.65	0.78
1:B:33:PRO:HB2	1:B:41:ASN:ND2	1.98	0.78
5:A:503:PLM:HD1	1:B:102:ILE:HG23	1.66	0.77
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.67	0.77
1:A:476:ILE:HG23	1:A:477:VAL:HG23	1.68	0.76
1:B:237:VAL:O	1:B:241:ARG:HD3	1.86	0.75
1:B:421:LYS:HZ2	1:B:422:SER:N	1.77	0.75
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.69	0.74
1:A:166:PRO:O	1:A:170:LEU:HB2	1.87	0.74
1:A:314:LEU:HD13	1:A:467:LEU:HD21	1.70	0.74
1:A:440:LEU:HD23	3:A:500:HEM:HBC2	1.70	0.73
1:A:84:LYS:HG3	1:A:88:ILE:HD12	1.71	0.72
1:A:210:SER:O	1:A:213:ILE:HG13	1.89	0.72
1:B:267:PHE:CG	1:B:287:LEU:HD13	2.25	0.72
1:B:170:LEU:HD21	1:B:310:LEU:HD12	1.71	0.72
1:B:200:ARG:NH2	1:B:239:LEU:HD13	2.05	0.71
1:A:64:VAL:HG21	1:A:376:PHE:HE2	1.56	0.71
1:B:166:PRO:HB2	1:B:170:LEU:HD22	1.73	0.70
1:A:203:GLU:CD	1:A:232:LYS:HZ2	2.01	0.69
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:CG	1:A:300:GLU:HG2	2.28	0.69
1:B:38:ILE:HG13	1:B:71:MET:HE1	1.74	0.69
1:A:474:LYS:CE	1:B:227:PRO:HG2	2.23	0.68
1:A:48:LYS:HE3	1:A:474:LYS:HE2	1.74	0.68
1:A:200:ARG:NH2	1:A:239:LEU:HD13	2.08	0.68
1:A:415:LYS:CD	1:A:415:LYS:H	2.05	0.68
1:A:33:PRO:HB2	1:A:41:ASN:ND2	2.09	0.68
1:A:169:ILE:CD1	1:A:170:LEU:HD13	2.24	0.67
1:B:225:CYS:C	1:B:227:PRO:HD3	2.19	0.67
1:B:28:LYS:HD2	1:B:29:LEU:H	1.60	0.67
1:A:200:ARG:HG3	1:A:200:ARG:HH11	1.58	0.67
1:B:196:THR:HB	1:B:200:ARG:HH12	1.60	0.66
1:A:415:LYS:HD3	1:A:415:LYS:N	2.11	0.66
1:A:38:ILE:HG23	1:A:39:ILE:HG23	1.78	0.65
1:A:255:LEU:HD21	1:A:269:ILE:HD13	1.79	0.65
5:A:503:PLM:HF1	1:B:106:ILE:HD11	1.79	0.65
1:B:213:ILE:HD12	1:B:214:GLN:H	1.61	0.64
1:B:308:TYR:CG	1:B:480:PRO:HB3	2.31	0.64
1:A:169:ILE:HD12	1:A:170:LEU:H	1.64	0.63
1:B:68:TYR:CE2	1:B:73:PRO:HB3	2.34	0.62
1:A:68:TYR:CE2	1:A:73:PRO:HB3	2.34	0.62
1:B:301:THR:HG22	1:B:361:LEU:HD21	1.82	0.61
1:B:97:ARG:HG2	1:B:114:SER:HA	1.82	0.61
1:B:233:VAL:O	1:B:237:VAL:HG23	2.00	0.61
1:A:134:PHE:CE1	1:A:140:SER:HB3	2.35	0.61
1:A:370:VAL:HG23	1:A:383:LYS:HA	1.83	0.60
1:B:75:VAL:HG13	1:B:387:ILE:HD13	1.82	0.60
1:A:105:ARG:HB2	5:B:503:PLM:HG1	1.84	0.60
1:A:403:ASN:O	1:A:406:ILE:HG23	2.01	0.60
1:B:45:ILE:HD12	1:B:50:ILE:CD1	2.32	0.60
1:B:196:THR:HB	1:B:200:ARG:NH1	2.17	0.60
1:B:205:PHE:CD1	1:B:300:GLU:HG2	2.37	0.60
1:B:36:LEU:HD13	1:B:44:GLN:HE21	1.65	0.59
5:A:503:PLM:HG1	1:B:234:LEU:HG	1.85	0.59
1:B:394:VAL:HG11	1:B:426:MET:HE3	1.84	0.59
1:B:226:PHE:N	1:B:227:PRO:HD3	2.17	0.59
1:A:229:THR:HG21	5:B:503:PLM:H61	1.84	0.58
1:B:267:PHE:CE2	1:B:287:LEU:HB2	2.37	0.58
1:A:216:CYS:SG	5:B:503:PLM:H91	2.44	0.58
1:B:428:PHE:O	1:B:429:SER:HB3	2.03	0.58
1:A:64:VAL:HG21	1:A:376:PHE:CE2	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG22	1:A:387:ILE:HD12	1.86	0.57
1:B:45:ILE:HD12	1:B:50:ILE:HD13	1.86	0.57
1:A:200:ARG:HG2	1:A:236:ASN:OD1	2.03	0.57
1:A:241:ARG:HG2	1:A:241:ARG:HH21	1.69	0.57
1:A:414:ASP:HB2	1:A:415:LYS:HE2	1.87	0.56
1:B:215:VAL:HG12	1:B:222:LEU:HD22	1.87	0.56
1:B:211:PRO:CG	1:B:474:LYS:HG2	2.36	0.56
1:A:134:PHE:CZ	1:A:140:SER:HB3	2.41	0.56
1:A:415:LYS:CD	1:A:415:LYS:N	2.69	0.56
1:A:166:PRO:HD3	1:A:485:ILE:HG22	1.88	0.56
1:A:257:VAL:HA	1:A:269:ILE:CD1	2.35	0.56
1:B:106:ILE:HD12	1:B:237:VAL:HG21	1.88	0.56
1:B:157:ARG:HG2	1:B:456:PHE:HZ	1.71	0.55
1:A:31:PRO:HD3	1:A:379:TYR:CE2	2.41	0.55
1:A:35:PRO:HB2	1:A:40:GLY:HA2	1.88	0.55
1:B:367:PRO:HG2	4:B:501:9CR:H25	1.89	0.55
1:A:377:ARG:HG3	1:A:378:ASN:N	2.12	0.55
1:A:415:LYS:H	1:A:415:LYS:HD3	1.68	0.55
1:B:91:GLY:O	1:B:95:SER:HB3	2.07	0.55
1:B:461:VAL:HG13	1:B:461:VAL:O	2.06	0.55
1:A:459:LYS:HD2	1:A:488:ILE:HD11	1.88	0.54
1:B:176:ASN:HD22	1:B:189:TYR:HE2	1.55	0.54
1:A:197:LEU:O	1:A:197:LEU:HD13	2.07	0.54
1:B:144:ARG:HG2	1:B:180:SER:OG	2.06	0.54
1:A:136:MET:CE	1:A:141:ILE:HG12	2.37	0.54
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.22	0.54
1:B:92:GLU:HB3	1:B:93:GLU:OE1	2.07	0.54
1:A:257:VAL:HA	1:A:269:ILE:HD11	1.90	0.54
1:B:89:ASP:O	1:B:90:ASN:CG	2.51	0.54
1:B:267:PHE:CD2	1:B:287:LEU:HB2	2.43	0.53
1:A:372:THR:HA	1:A:383:LYS:HB2	1.90	0.53
1:B:236:ASN:O	1:B:240:THR:HB	2.08	0.53
1:B:99:ASN:OD1	1:B:104:GLN:HG2	2.08	0.53
1:A:322:LYS:HD2	1:A:347:TYR:CZ	2.43	0.53
1:A:360:ASP:OD2	1:A:392:THR:HG23	2.08	0.53
1:B:374:THR:O	1:B:380:LEU:HD12	2.08	0.53
1:A:101:PRO:HG2	1:A:220:PRO:HG3	1.91	0.53
1:A:157:ARG:NH2	1:A:455:ASN:HD22	2.06	0.53
1:B:318:GLU:HG2	1:B:319:VAL:N	2.23	0.52
1:B:448:PHE:O	1:B:452:ILE:HG13	2.09	0.52
1:B:211:PRO:HG2	1:B:474:LYS:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLN:C	1:B:254:SER:H	2.16	0.52
1:B:271:MET:HE1	1:B:284:ILE:CD1	2.40	0.52
1:A:136:MET:CE	1:A:181:VAL:HG13	2.40	0.52
1:A:156:LEU:HD21	1:A:169:ILE:HD13	1.91	0.52
1:B:39:ILE:H	1:B:39:ILE:CD1	2.23	0.52
1:B:204:ASN:ND2	1:B:233:VAL:HG13	2.24	0.52
1:B:400:GLU:HG2	1:B:424:TYR:CG	2.45	0.52
1:A:472:VAL:HG23	1:A:472:VAL:O	2.10	0.51
1:B:69:PHE:HB3	1:B:218:ASN:OD1	2.10	0.51
1:B:199:LYS:O	1:B:199:LYS:HD3	2.09	0.51
1:B:341:ASP:O	1:B:345:MET:HG3	2.09	0.51
1:B:240:THR:HG22	1:B:241:ARG:HD2	1.91	0.51
1:B:460:SER:O	1:B:461:VAL:HG12	2.10	0.51
1:A:227:PRO:HG2	1:B:474:LYS:HE3	1.92	0.51
1:B:321:ALA:HB3	6:B:540:HOH:O	2.10	0.51
1:B:213:ILE:O	1:B:217:ASN:HB2	2.10	0.51
1:B:39:ILE:H	1:B:39:ILE:HD13	1.75	0.51
1:A:237:VAL:O	1:A:241:ARG:HG2	2.11	0.51
1:B:470:THR:O	1:B:481:PRO:HD3	2.10	0.51
1:B:358:TYR:HE1	1:B:405:ASN:O	1.94	0.51
1:A:49:ASP:OD2	1:A:52:LYS:HB2	2.12	0.50
1:A:136:MET:HE1	1:A:181:VAL:HG13	1.94	0.50
1:A:170:LEU:HD21	1:A:310:LEU:HD12	1.94	0.50
1:A:38:ILE:HA	1:A:71:MET:HE1	1.92	0.50
1:B:28:LYS:HD2	1:B:29:LEU:N	2.25	0.50
1:B:347:TYR:O	1:B:351:VAL:HG23	2.11	0.50
1:B:351:VAL:O	1:B:355:ILE:HG13	2.11	0.50
1:A:136:MET:HE3	1:A:141:ILE:HG12	1.94	0.50
1:B:382:PRO:HG2	1:B:385:THR:OG1	2.12	0.50
1:A:314:LEU:O	1:A:314:LEU:HD22	2.12	0.50
1:B:74:ILE:HG21	1:B:388:MET:HE3	1.94	0.49
1:B:335:ARG:HH11	1:B:335:ARG:HG2	1.76	0.49
1:A:69:PHE:CD2	1:A:74:ILE:HD12	2.48	0.49
1:A:314:LEU:HD13	1:A:467:LEU:CD2	2.40	0.49
1:B:410:GLY:HA2	1:B:413:LEU:HB2	1.94	0.49
1:B:157:ARG:HG2	1:B:456:PHE:CZ	2.47	0.49
1:B:166:PRO:O	1:B:170:LEU:HB2	2.13	0.49
1:A:213:ILE:HD12	1:A:214:GLN:H	1.75	0.49
1:B:28:LYS:O	1:B:379:TYR:HB3	2.13	0.49
1:B:260:PRO:HG3	1:B:269:ILE:CD1	2.42	0.49
1:B:31:PRO:HD2	6:B:511:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:CG1	1:B:447:LEU:HD12	2.44	0.48
1:A:308:TYR:CG	1:A:480:PRO:HB3	2.49	0.48
1:A:29:LEU:HD21	1:A:382:PRO:HD2	1.94	0.48
1:A:363:PRO:HB3	1:A:392:THR:OG1	2.13	0.48
1:A:403:ASN:HB3	1:A:406:ILE:CG2	2.44	0.48
1:B:36:LEU:HD13	1:B:44:GLN:NE2	2.28	0.48
1:B:221:LEU:HG	6:B:532:HOH:O	2.13	0.47
1:A:105:ARG:HH22	1:A:223:ILE:HD13	1.79	0.47
1:B:118:LYS:HB3	1:B:118:LYS:HE2	1.75	0.47
1:A:241:ARG:HG2	1:A:241:ARG:NH2	2.30	0.47
1:B:182:VAL:HA	1:B:263:PHE:HB3	1.96	0.47
1:A:33:PRO:HB2	1:A:41:ASN:HD22	1.78	0.47
1:A:205:PHE:CD1	1:A:300:GLU:HG2	2.50	0.47
1:A:400:GLU:HG2	1:A:424:TYR:CG	2.50	0.47
1:B:298:GLY:O	1:B:302:THR:HG23	2.15	0.47
1:A:322:LYS:HD2	1:A:347:TYR:CE1	2.50	0.46
1:A:350:ALA:HB2	1:A:413:LEU:HD13	1.97	0.46
1:B:434:ILE:O	1:B:435:CYS:C	2.59	0.46
1:B:191:ASP:O	1:B:194:PHE:HB3	2.15	0.46
1:A:306:LEU:HD11	1:A:448:PHE:CD2	2.51	0.46
1:B:75:VAL:HG13	1:B:387:ILE:CD1	2.46	0.46
1:A:102:ILE:HG12	1:A:217:ASN:OD1	2.15	0.46
1:B:69:PHE:HE1	1:B:214:GLN:OE1	1.98	0.46
1:B:246:GLU:O	1:B:250:GLU:HG3	2.16	0.46
1:B:145:VAL:HG11	1:B:447:LEU:HD12	1.98	0.46
1:A:261:ARG:HB2	1:A:265:ASP:OD2	2.16	0.46
1:B:488:ILE:HD12	1:B:488:ILE:N	2.31	0.45
1:A:39:ILE:CD1	1:A:43:LEU:HD12	2.46	0.45
1:B:45:ILE:HG13	1:B:46:ASP:N	2.31	0.45
1:B:395:LEU:HD21	1:B:426:MET:H	1.82	0.45
1:A:38:ILE:CG2	1:A:39:ILE:HG23	2.45	0.45
1:B:429:SER:CB	3:B:500:HEM:HBA1	2.47	0.45
1:A:156:LEU:HD22	1:A:487:PHE:CE1	2.51	0.45
1:A:372:THR:O	1:A:373:ASP:C	2.58	0.45
1:B:459:LYS:HB3	1:B:488:ILE:HD13	1.99	0.45
1:A:126:PHE:O	1:A:130:THR:CG2	2.65	0.45
1:A:377:ARG:CG	1:A:378:ASN:H	2.12	0.45
1:B:77:PHE:CE2	1:B:94:PHE:HE2	2.34	0.45
1:B:84:LYS:O	1:B:88:ILE:HB	2.16	0.45
1:A:414:ASP:C	1:A:414:ASP:OD2	2.60	0.45
1:B:205:PHE:CG	1:B:300:GLU:HG2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PHE:O	1:B:271:MET:HG3	2.17	0.45
1:B:421:LYS:HZ3	1:B:421:LYS:HA	1.80	0.45
1:A:257:VAL:HG23	1:A:269:ILE:HG23	1.98	0.45
1:A:246:GLU:O	1:A:250:GLU:HG3	2.17	0.45
1:A:350:ALA:CB	1:A:413:LEU:HD13	2.46	0.45
1:A:120:TRP:CZ2	1:A:433:ARG:HD2	2.52	0.45
1:B:237:VAL:HG13	1:B:241:ARG:CZ	2.47	0.44
1:A:381:ILE:N	1:A:381:ILE:HD12	2.32	0.44
1:B:121:LYS:O	1:B:125:ARG:HB2	2.17	0.44
1:B:148:GLU:CD	1:B:176:ASN:HB3	2.42	0.44
1:B:366:VAL:HG21	4:B:501:9CR:H5	1.98	0.44
1:A:308:TYR:CD1	1:A:359:SER:HB2	2.52	0.44
1:B:126:PHE:CD1	1:B:126:PHE:C	2.96	0.44
1:B:148:GLU:CD	1:B:186:ARG:HE	2.26	0.44
1:A:169:ILE:HD12	1:A:170:LEU:HD13	1.99	0.44
1:B:178:ILE:O	1:B:182:VAL:HG22	2.18	0.44
1:B:308:TYR:CD2	1:B:480:PRO:HB3	2.52	0.44
5:A:503:PLM:HG2	1:B:230:HIS:CE1	2.53	0.44
1:B:120:TRP:CZ2	1:B:433:ARG:HD2	2.53	0.44
1:B:472:VAL:O	1:B:472:VAL:HG23	2.17	0.44
1:A:98:GLY:O	1:A:99:ASN:HB3	2.17	0.44
1:A:173:ALA:O	1:A:177:VAL:HG23	2.17	0.44
1:A:191:ASP:O	1:A:194:PHE:HB3	2.18	0.44
1:B:150:HIS:O	1:B:153:VAL:HG22	2.18	0.44
1:B:372:THR:HA	1:B:383:LYS:HB2	1.98	0.44
1:B:29:LEU:CD2	1:B:382:PRO:HD2	2.40	0.43
1:B:342:ARG:HG3	1:B:446:PHE:CE2	2.53	0.43
1:B:39:ILE:HD13	1:B:39:ILE:N	2.32	0.43
1:B:459:LYS:HB3	1:B:488:ILE:CD1	2.49	0.43
1:B:48:LYS:CE	1:B:474:LYS:HG3	2.49	0.43
1:B:271:MET:HE1	1:B:284:ILE:HD11	2.00	0.43
1:A:376:PHE:CD2	1:A:377:ARG:HG2	2.52	0.43
1:B:211:PRO:O	1:B:214:GLN:HB2	2.18	0.43
1:A:301:THR:HG22	1:A:361:LEU:HD21	2.01	0.43
1:A:488:ILE:HA	1:A:489:PRO:HD2	1.87	0.43
5:A:503:PLM:H61	1:B:229:THR:HG21	2.00	0.43
1:A:126:PHE:O	1:A:130:THR:HG23	2.19	0.43
1:A:77:PHE:HE2	1:A:387:ILE:HG23	1.84	0.43
1:A:208:LEU:HD13	4:A:502:9CR:H19	2.00	0.43
1:B:193:ASN:O	1:B:197:LEU:HB2	2.19	0.43
1:A:184:GLN:HG3	1:A:185:LYS:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HD3	1:A:199:LYS:HA	1.83	0.43
1:A:215:VAL:HG12	1:A:222:LEU:HD22	2.01	0.43
1:B:93:GLU:O	1:B:370:VAL:HA	2.18	0.42
1:A:142:GLU:O	1:A:146:GLN:HG3	2.19	0.42
1:A:201:PHE:CE2	1:A:240:THR:HG21	2.54	0.42
1:A:390:LEU:O	1:A:393:SER:OG	2.28	0.42
1:B:124:ARG:O	1:B:128:LEU:HG	2.19	0.42
1:A:435:CYS:HB2	3:A:500:HEM:NA	2.33	0.42
1:B:192:GLN:C	1:B:194:PHE:N	2.75	0.42
1:B:271:MET:HE1	1:B:284:ILE:HD13	2.01	0.42
1:A:401:PHE:O	1:A:402:PRO:C	2.62	0.42
1:A:238:ALA:O	1:A:242:SER:HB2	2.19	0.42
1:B:136:MET:HE3	1:B:144:ARG:NH2	2.34	0.42
1:B:218:ASN:C	1:B:220:PRO:HD3	2.44	0.42
1:B:323:VAL:CG2	1:B:351:VAL:HG21	2.50	0.42
1:B:339:MET:HG3	1:B:443:MET:HE2	2.01	0.42
4:A:501:9CR:H10	4:A:501:9CR:H8	1.91	0.42
1:A:152:LEU:HD21	1:A:452:ILE:HD11	2.02	0.42
1:B:38:ILE:HG22	1:B:39:ILE:HG23	2.02	0.42
1:B:132:ARG:O	1:B:133:ASN:C	2.62	0.41
1:B:148:GLU:OE2	1:B:176:ASN:HB3	2.20	0.41
1:A:203:GLU:O	1:A:207:ILE:HG12	2.20	0.41
1:A:217:ASN:HD21	4:A:502:9CR:H5	1.85	0.41
1:A:369:ALA:HA	1:A:385:THR:O	2.20	0.41
1:B:284:ILE:O	1:B:288:VAL:HG23	2.21	0.41
1:A:39:ILE:O	1:A:42:MET:HB2	2.21	0.41
1:A:203:GLU:OE2	1:A:232:LYS:NZ	2.53	0.41
1:A:114:SER:HB2	6:A:515:HOH:O	2.21	0.41
1:A:119:ARG:O	1:A:123:ILE:HG12	2.19	0.41
1:A:46:ASP:OD2	1:A:48:LYS:HB2	2.20	0.41
1:B:138:LYS:CA	1:B:138:LYS:HE2	2.51	0.41
1:B:319:VAL:O	1:B:323:VAL:HG23	2.20	0.41
1:B:331:ILE:HA	1:B:335:ARG:HH12	1.86	0.41
1:A:106:ILE:HD11	5:B:503:PLM:HF2	2.03	0.41
1:A:372:THR:CA	1:A:383:LYS:HB2	2.50	0.41
1:B:48:LYS:HE3	1:B:474:LYS:CE	2.35	0.41
1:B:138:LYS:HE2	1:B:138:LYS:HA	2.03	0.41
1:B:429:SER:HB3	3:B:500:HEM:HBA1	2.02	0.41
1:A:28:LYS:O	1:A:379:TYR:HB3	2.21	0.41
1:B:31:PRO:HB2	6:B:511:HOH:O	2.20	0.41
1:B:259:ASN:HA	1:B:260:PRO:HD3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:PRO:O	1:B:383:LYS:C	2.63	0.41
1:B:424:TYR:CD1	1:B:424:TYR:N	2.89	0.41
1:B:476:ILE:HG23	1:B:477:VAL:HG23	2.02	0.41
1:A:313:LEU:HD13	1:A:453:LEU:HD11	2.04	0.41
1:A:354:GLU:HG3	1:A:354:GLU:O	2.21	0.41
1:A:119:ARG:HA	1:A:281:GLU:HG3	2.03	0.40
1:B:312:LEU:HD13	1:B:407:PHE:CE1	2.55	0.40
1:B:93:GLU:OE1	1:B:93:GLU:N	2.54	0.40
1:B:155:GLU:HG3	1:B:189:TYR:CD1	2.55	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	461/476 (97%)	425 (92%)	34 (7%)	2 (0%)	30	51
1	B	461/476 (97%)	421 (91%)	37 (8%)	3 (1%)	18	38
All	All	922/952 (97%)	846 (92%)	71 (8%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	254	SER
1	A	184	GLN
1	A	377	ARG
1	B	220	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	419/430 (97%)	399 (95%)	20 (5%)	23	47
1	B	419/430 (97%)	395 (94%)	24 (6%)	18	40
All	All	838/860 (97%)	794 (95%)	44 (5%)	20	43

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	93	GLU
1	A	97	ARG
1	A	114	SER
1	A	130	THR
1	A	170	LEU
1	A	193	ASN
1	A	232	LYS
1	A	240	THR
1	A	285	GLU
1	A	300	GLU
1	A	302	THR
1	A	314	LEU
1	A	375	LYS
1	A	406	ILE
1	A	413	LEU
1	A	415	LYS
1	A	438	GLU
1	A	461	VAL
1	A	465	LYS
1	B	37	PRO
1	B	38	ILE
1	B	39	ILE
1	B	51	CYS
1	B	64	VAL
1	B	75	VAL
1	B	93	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	112	ILE
1	B	119	ARG
1	B	130	THR
1	B	138	LYS
1	B	170	LEU
1	B	176	ASN
1	B	199	LYS
1	B	234	LEU
1	B	240	THR
1	B	279	LYS
1	B	285	GLU
1	B	302	THR
1	B	314	LEU
1	B	392	THR
1	B	413	LEU
1	B	421	LYS
1	B	459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	193	ASN
1	A	202	ASN
1	A	214	GLN
1	A	329	HIS
1	A	344	HIS
1	A	455	ASN
1	B	72	ASN
1	B	104	GLN
1	B	146	GLN
1	B	252	GLN
1	B	324	GLN
1	B	466	ASN
1	B	468	ASN

5.3.3 RNA ⓘ

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](#)

10 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	$\# Z > 2$
4	9CR	B	502	-	22,22,22	4.07	11 (50%)	30,30,30	2.23	11 (36%)
2	SO4	B	504	-	4,4,4	0.40	0	6,6,6	0.05	0
5	PLM	A	503	-	17,17,17	0.48	0	17,17,17	0.81	0
3	HEM	A	500	1	50,50,50	2.38	24 (48%)	67,82,82	1.35	10 (14%)
4	9CR	B	501	-	22,22,22	3.97	10 (45%)	30,30,30	2.31	10 (33%)
3	HEM	B	500	1	50,50,50	2.42	24 (48%)	67,82,82	1.32	11 (16%)
2	SO4	A	505	-	4,4,4	0.41	0	6,6,6	0.08	0
5	PLM	B	503	-	17,17,17	0.52	0	17,17,17	0.82	0
4	9CR	A	501	-	22,22,22	3.94	11 (50%)	30,30,30	2.27	11 (36%)
4	9CR	A	502	-	22,22,22	4.12	10 (45%)	30,30,30	2.29	12 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9CR	B	502	-	-	6/15/32/32	0/1/1/1
5	PLM	A	503	-	-	5/15/15/15	-
3	HEM	A	500	1	-	2/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	9CR	B	501	-	-	5/15/32/32	0/1/1/1
3	HEM	B	500	1	-	4/14/54/54	-
5	PLM	B	503	-	-	3/15/15/15	-
4	9CR	A	501	-	-	5/15/32/32	0/1/1/1
4	9CR	A	502	-	-	7/15/32/32	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	9CR	C1-C6	12.48	1.69	1.53
4	B	502	9CR	C1-C6	12.16	1.69	1.53
4	B	501	9CR	C1-C6	11.93	1.69	1.53
4	A	501	9CR	C1-C6	11.77	1.68	1.53
4	A	502	9CR	C5-C6	10.05	1.51	1.34
4	B	501	9CR	C5-C6	9.70	1.50	1.34
4	A	501	9CR	C5-C6	9.53	1.50	1.34
4	B	502	9CR	C5-C6	9.34	1.50	1.34
4	A	502	9CR	C16-C1	4.98	1.63	1.53
4	B	502	9CR	C16-C1	4.78	1.62	1.53
4	A	501	9CR	C16-C1	4.62	1.62	1.53
4	B	501	9CR	C16-C1	4.50	1.62	1.53
3	B	500	HEM	C4A-NA	-4.43	1.31	1.39
3	A	500	HEM	C4D-ND	-4.41	1.32	1.40
4	B	502	9CR	C20-C13	4.35	1.59	1.50
3	B	500	HEM	C1B-NB	-4.29	1.32	1.40
3	A	500	HEM	C1D-ND	-4.26	1.30	1.38
3	B	500	HEM	CMA-C3A	4.14	1.59	1.50
4	A	502	9CR	C20-C13	4.09	1.59	1.50
3	B	500	HEM	C1D-ND	-4.06	1.30	1.38
3	B	500	HEM	CBB-CAB	4.04	1.49	1.30
3	B	500	HEM	C1C-NC	-4.01	1.32	1.39
3	B	500	HEM	CAC-C3C	-3.98	1.36	1.47
3	A	500	HEM	C1B-NB	-3.94	1.33	1.40
3	B	500	HEM	FE-ND	3.91	2.06	1.94
3	A	500	HEM	FE-NB	3.86	2.06	1.94
3	A	500	HEM	C4A-NA	-3.80	1.32	1.39
3	A	500	HEM	CMA-C3A	3.79	1.58	1.50
4	B	502	9CR	C4-C5	3.78	1.58	1.51
3	A	500	HEM	CBB-CAB	3.75	1.48	1.30
3	B	500	HEM	C4D-ND	-3.71	1.33	1.40
3	A	500	HEM	C1C-NC	-3.67	1.32	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	FE-ND	3.62	2.06	1.94
4	A	501	9CR	C2-C1	3.62	1.62	1.54
4	A	501	9CR	C20-C13	3.60	1.58	1.50
4	B	501	9CR	C20-C13	3.60	1.58	1.50
4	B	502	9CR	C2-C1	3.60	1.62	1.54
4	A	502	9CR	C2-C1	3.59	1.62	1.54
3	B	500	HEM	FE-NB	3.57	2.05	1.94
3	A	500	HEM	C4B-NB	-3.55	1.31	1.38
4	B	501	9CR	C10-C9	3.48	1.43	1.35
3	B	500	HEM	C1C-C2C	-3.47	1.38	1.45
4	A	501	9CR	C4-C5	3.44	1.57	1.51
4	B	501	9CR	C14-C13	3.43	1.40	1.35
3	B	500	HEM	FE-NA	3.36	2.06	1.95
3	A	500	HEM	C1C-C2C	-3.36	1.38	1.45
3	B	500	HEM	C4B-NB	-3.36	1.32	1.38
3	A	500	HEM	FE-NC	3.32	2.06	1.95
4	B	501	9CR	C2-C1	3.30	1.61	1.54
3	A	500	HEM	FE-NA	3.29	2.06	1.95
4	B	502	9CR	C2-C3	3.28	1.60	1.52
4	A	502	9CR	C4-C5	3.26	1.57	1.51
4	B	501	9CR	C14-C15	3.24	1.56	1.47
4	A	502	9CR	C14-C13	3.22	1.39	1.35
3	A	500	HEM	CAC-C3C	-3.18	1.38	1.47
4	A	501	9CR	C2-C3	3.17	1.60	1.52
4	B	502	9CR	C14-C13	3.14	1.39	1.35
3	B	500	HEM	CMC-C2C	3.09	1.57	1.50
4	B	502	9CR	C10-C9	3.07	1.42	1.35
4	B	501	9CR	C4-C5	3.07	1.56	1.51
4	A	501	9CR	C10-C9	3.02	1.42	1.35
4	A	502	9CR	C10-C9	2.98	1.42	1.35
3	A	500	HEM	C4C-NC	-2.85	1.34	1.39
4	A	502	9CR	C14-C15	2.84	1.55	1.47
4	A	502	9CR	C2-C3	2.78	1.59	1.52
3	B	500	HEM	FE-NC	2.76	2.04	1.95
4	B	502	9CR	O2-C15	-2.72	1.23	1.30
4	A	501	9CR	C14-C15	2.72	1.54	1.47
4	A	501	9CR	C14-C13	2.68	1.39	1.35
3	A	500	HEM	CMC-C2C	2.68	1.56	1.50
4	B	501	9CR	C2-C3	2.65	1.58	1.52
4	B	502	9CR	C14-C15	2.58	1.54	1.47
3	B	500	HEM	C3B-C2B	2.58	1.42	1.37
3	B	500	HEM	C4C-NC	-2.53	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	HEM	C3C-C2C	2.47	1.42	1.37
3	A	500	HEM	CBC-CAC	2.44	1.42	1.30
3	A	500	HEM	C3B-C2B	2.42	1.42	1.37
3	A	500	HEM	C3C-C4C	-2.39	1.41	1.46
3	B	500	HEM	CBC-CAC	2.37	1.41	1.30
3	A	500	HEM	O2A-CGA	-2.37	1.23	1.30
3	B	500	HEM	C3C-C4C	-2.33	1.42	1.46
3	B	500	HEM	O2A-CGA	-2.22	1.23	1.30
3	A	500	HEM	CAD-C3D	2.22	1.57	1.51
3	A	500	HEM	C4D-C3D	-2.17	1.41	1.45
3	B	500	HEM	CBD-CGD	2.15	1.55	1.50
3	A	500	HEM	CBD-CGD	2.13	1.55	1.50
3	B	500	HEM	C4D-C3D	-2.13	1.41	1.45
3	B	500	HEM	CAD-C3D	2.13	1.56	1.51
3	B	500	HEM	C3C-C2C	2.06	1.41	1.37
4	A	501	9CR	C12-C13	-2.02	1.41	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	9CR	C7-C8-C9	4.70	133.19	126.23
4	A	502	9CR	C17-C1-C6	4.65	117.54	110.24
4	B	502	9CR	C17-C1-C6	4.54	117.36	110.24
4	A	502	9CR	C19-C9-C10	-4.52	115.50	122.82
4	B	501	9CR	C17-C1-C6	4.35	117.06	110.24
4	A	501	9CR	C19-C9-C10	-4.32	115.82	122.82
4	B	501	9CR	C19-C9-C10	-4.29	115.87	122.82
4	A	501	9CR	C7-C8-C9	4.22	132.48	126.23
4	A	502	9CR	C7-C8-C9	4.21	132.46	126.23
4	B	502	9CR	C19-C9-C10	-4.17	116.07	122.82
4	A	501	9CR	C20-C13-C12	4.13	124.40	118.09
4	A	502	9CR	C19-C9-C8	4.02	124.23	118.09
4	A	501	9CR	C17-C1-C6	4.01	116.53	110.24
4	A	501	9CR	C19-C9-C8	4.01	124.21	118.09
4	B	501	9CR	C20-C13-C12	3.95	124.12	118.09
4	B	502	9CR	C20-C13-C12	3.94	124.11	118.09
4	B	501	9CR	C19-C9-C8	3.90	124.05	118.09
4	B	502	9CR	C19-C9-C8	3.71	123.75	118.09
4	B	502	9CR	C7-C8-C9	3.68	131.69	126.23
4	A	502	9CR	C20-C13-C12	3.62	123.62	118.09
4	B	502	9CR	C8-C7-C6	3.46	136.24	127.00
4	B	501	9CR	C1-C6-C5	-3.42	117.96	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	9CR	C2-C1-C6	3.42	115.41	110.44
4	A	501	9CR	C2-C1-C6	3.40	115.38	110.44
3	A	500	HEM	CHD-C4C-NC	-3.31	120.84	124.45
4	A	502	9CR	C1-C6-C5	-3.31	118.12	122.64
4	B	502	9CR	C2-C1-C6	3.30	115.23	110.44
4	A	502	9CR	C8-C7-C6	3.12	135.33	127.00
4	A	501	9CR	C1-C6-C5	-3.06	118.46	122.64
4	A	502	9CR	C2-C1-C6	3.02	114.83	110.44
4	A	501	9CR	C8-C7-C6	2.92	134.80	127.00
4	B	502	9CR	C1-C6-C5	-2.86	118.72	122.64
4	B	501	9CR	C8-C7-C6	2.82	134.54	127.00
3	B	500	HEM	C4B-C3B-C2B	-2.74	104.76	107.28
4	B	502	9CR	C16-C1-C6	-2.72	105.98	110.24
3	B	500	HEM	C1B-NB-C4B	2.65	108.34	105.21
3	A	500	HEM	C4C-C3C-C2C	-2.64	104.53	106.81
3	A	500	HEM	CHC-C1C-NC	-2.63	121.58	124.45
3	A	500	HEM	C4B-C3B-C2B	-2.59	104.90	107.28
4	A	502	9CR	C11-C10-C9	-2.58	123.66	127.28
4	B	501	9CR	O2-C15-C14	2.56	121.01	113.40
3	B	500	HEM	CHC-C4B-NB	-2.55	121.68	124.42
4	A	502	9CR	C16-C1-C6	-2.53	106.28	110.24
3	A	500	HEM	C1C-CHC-C4B	2.51	131.36	126.02
3	B	500	HEM	C1C-CHC-C4B	2.51	131.34	126.02
3	B	500	HEM	C4C-C3C-C2C	-2.50	104.64	106.81
3	B	500	HEM	CHD-C4C-NC	-2.42	121.82	124.45
4	A	501	9CR	O2-C15-C14	2.39	120.51	113.40
4	B	501	9CR	C16-C1-C6	-2.39	106.50	110.24
3	A	500	HEM	C1B-NB-C4B	2.38	108.02	105.21
4	A	501	9CR	C11-C10-C9	-2.30	124.06	127.28
4	A	501	9CR	C16-C1-C6	-2.27	106.69	110.24
3	B	500	HEM	C3B-C2B-C1B	-2.25	104.72	106.41
3	B	500	HEM	O2A-CGA-CBA	2.24	121.07	114.00
3	A	500	HEM	C3B-C2B-C1B	-2.23	104.74	106.41
4	B	502	9CR	C11-C10-C9	-2.19	124.20	127.28
4	A	502	9CR	O2-C15-C14	2.19	119.92	113.40
3	A	500	HEM	C4A-CHB-C1B	2.15	131.30	126.25
3	A	500	HEM	C4D-ND-C1D	2.14	107.75	105.21
3	A	500	HEM	O2A-CGA-CBA	2.14	120.76	114.00
3	B	500	HEM	C3B-C4B-NB	2.13	111.00	109.47
3	B	500	HEM	C4D-ND-C1D	2.10	107.69	105.21
4	B	502	9CR	C12-C13-C14	-2.04	113.48	119.15
4	A	502	9CR	C7-C6-C5	2.02	126.20	121.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	HEM	CAD-CBD-CGD	2.00	118.97	113.67

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	HEM	C2C-C3C-CAC-CBC
3	B	500	HEM	C4C-C3C-CAC-CBC
4	A	501	9CR	C13-C14-C15-O2
4	B	501	9CR	C13-C14-C15-O1
4	B	501	9CR	C13-C14-C15-O2
4	B	502	9CR	C7-C8-C9-C19
4	A	502	9CR	C7-C8-C9-C19
4	A	502	9CR	C7-C8-C9-C10
4	B	502	9CR	C7-C8-C9-C10
4	A	501	9CR	C13-C14-C15-O1
5	A	503	PLM	C8-C9-CA-CB
5	A	503	PLM	CC-CD-CE-CF
4	A	501	9CR	C6-C7-C8-C9
5	B	503	PLM	CC-CD-CE-CF
4	A	502	9CR	C13-C14-C15-O1
4	A	502	9CR	C13-C14-C15-O2
4	B	502	9CR	C13-C14-C15-O2
4	B	502	9CR	C13-C14-C15-O1
5	A	503	PLM	C4-C5-C6-C7
4	B	501	9CR	C6-C7-C8-C9
4	A	501	9CR	C11-C10-C9-C19
4	A	502	9CR	C6-C7-C8-C9
4	A	502	9CR	C11-C10-C9-C19
4	B	501	9CR	C11-C10-C9-C19
4	B	502	9CR	C11-C10-C9-C19
3	B	500	HEM	CAA-CBA-CGA-O1A
5	A	503	PLM	O1-C1-C2-C3
4	A	501	9CR	C11-C10-C9-C8
4	A	502	9CR	C11-C10-C9-C8
4	B	501	9CR	C11-C10-C9-C8
4	B	502	9CR	C11-C10-C9-C8
3	A	500	HEM	CAA-CBA-CGA-O1A
5	A	503	PLM	O2-C1-C2-C3
3	A	500	HEM	CAA-CBA-CGA-O2A
3	B	500	HEM	CAA-CBA-CGA-O2A
5	B	503	PLM	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

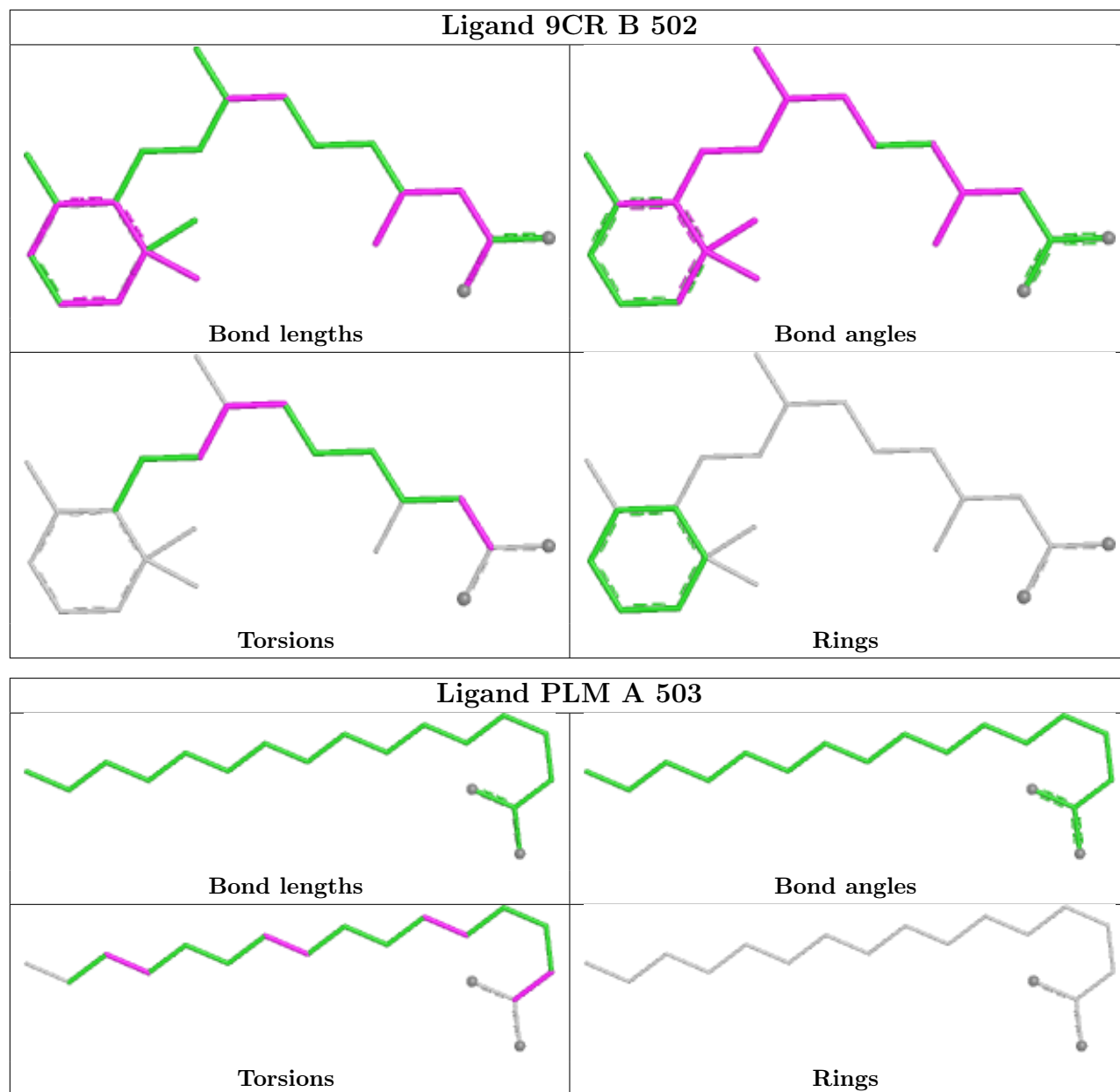
Mol	Chain	Res	Type	Atoms
5	B	503	PLM	O1-C1-C2-C3

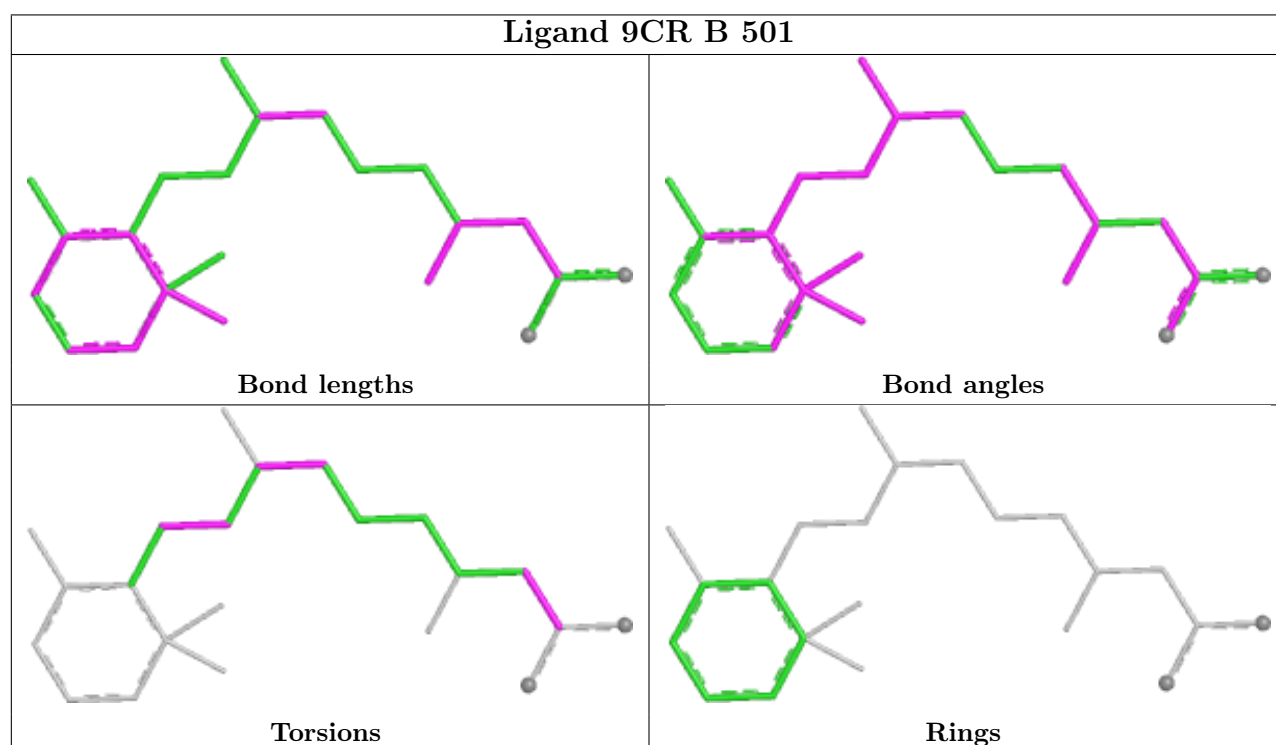
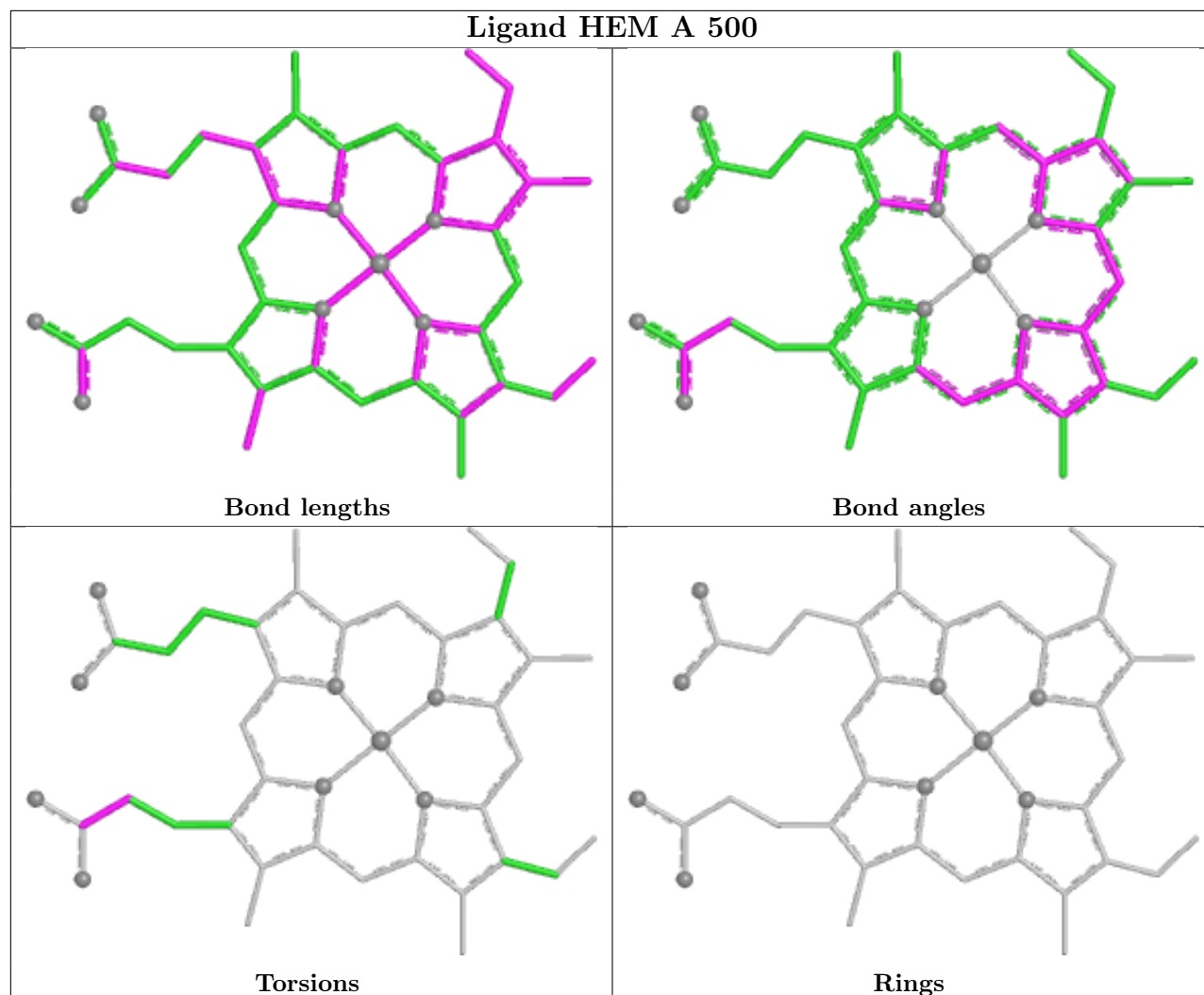
There are no ring outliers.

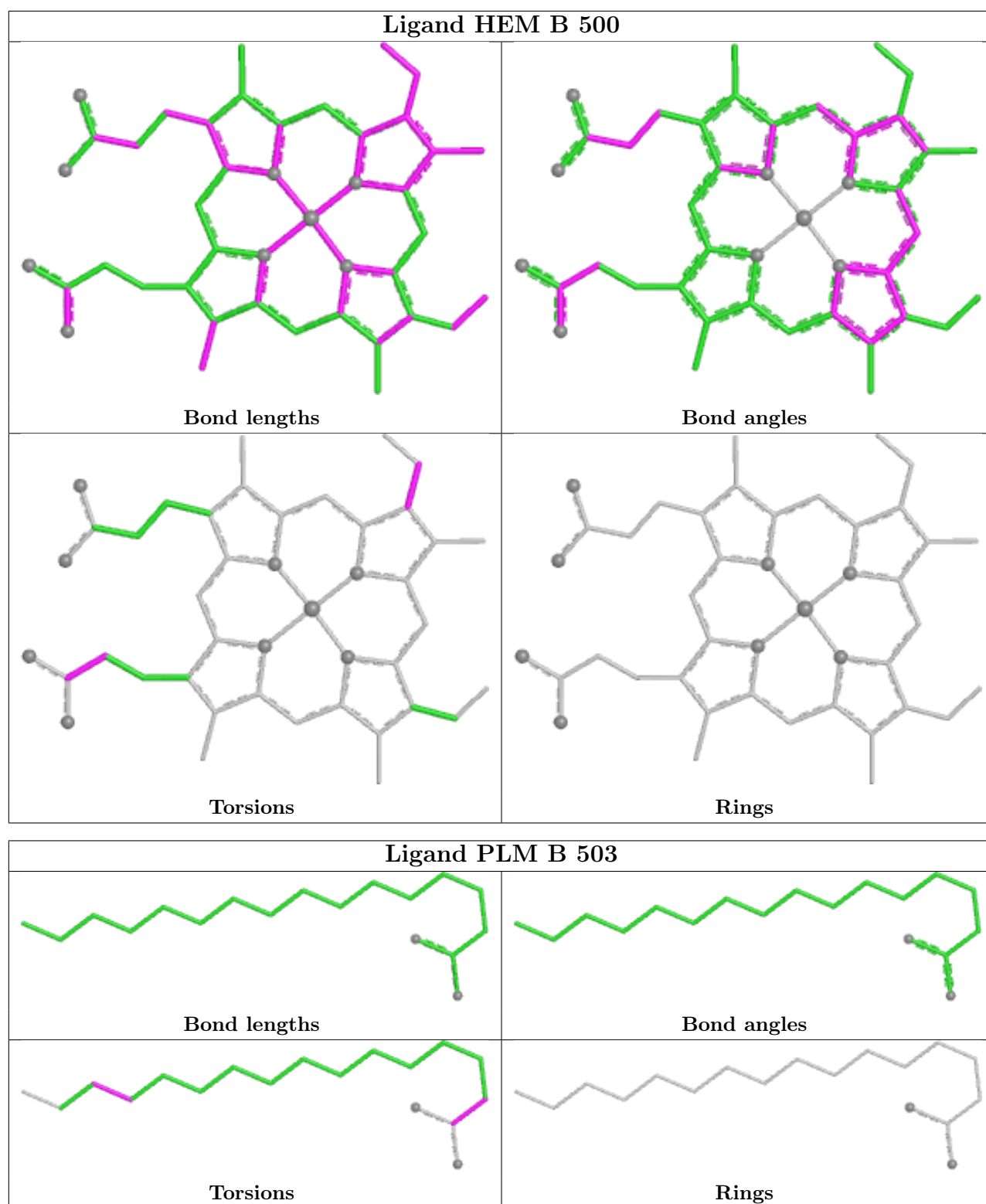
7 monomers are involved in 18 short contacts:

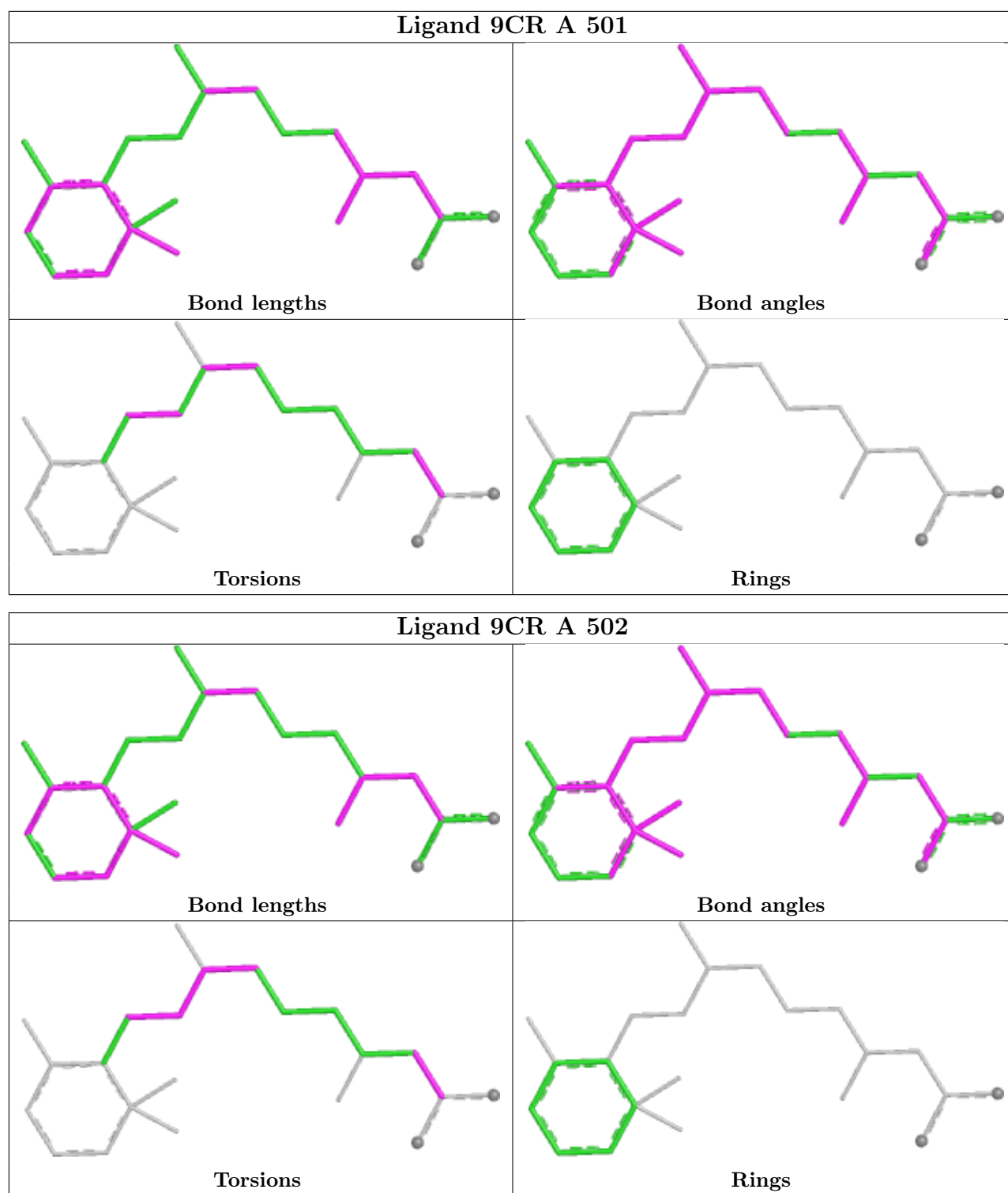
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	PLM	5	0
3	A	500	HEM	2	0
4	B	501	9CR	2	0
3	B	500	HEM	2	0
5	B	503	PLM	4	0
4	A	501	9CR	1	0
4	A	502	9CR	2	0

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	463/476 (97%)	0.29	5 (1%) 78 74	29, 47, 66, 86	0
1	B	463/476 (97%)	0.42	12 (2%) 57 51	30, 50, 73, 87	0
All	All	926/952 (97%)	0.35	17 (1%) 67 63	29, 49, 69, 87	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	VAL	3.2
1	B	461	VAL	2.5
1	B	260	PRO	2.4
1	B	278	GLN	2.3
1	B	466	ASN	2.2
1	A	184	GLN	2.2
1	B	138	LYS	2.2
1	B	213	ILE	2.2
1	A	201	PHE	2.1
1	A	257	VAL	2.1
1	B	419	PHE	2.1
1	B	279	LYS	2.1
1	A	169	ILE	2.1
1	B	98	GLY	2.0
1	B	474	LYS	2.0
1	A	31	PRO	2.0
1	B	468	ASN	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](#)

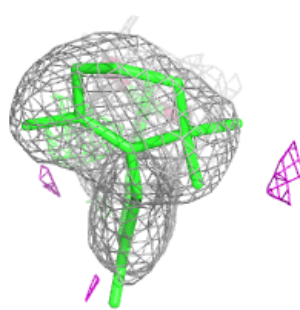
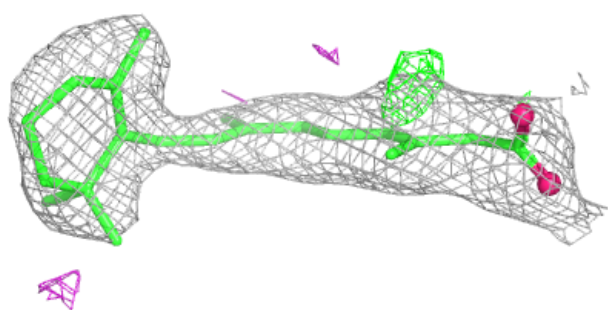
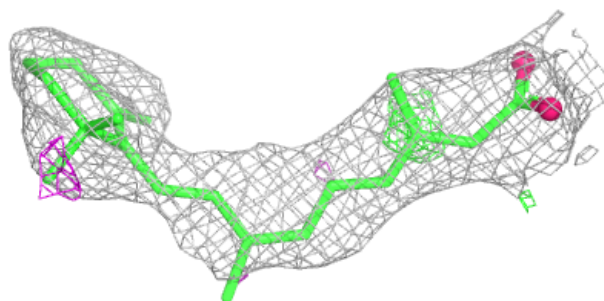
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	504	5/5	0.81	0.19	87,87,88,88	0
4	9CR	A	501	22/22	0.88	0.17	47,53,67,69	0
5	PLM	A	503	18/18	0.88	0.17	49,53,59,60	0
4	9CR	B	501	22/22	0.89	0.18	50,55,67,68	0
2	SO4	A	505	5/5	0.90	0.14	63,64,64,65	0
4	9CR	A	502	22/22	0.90	0.14	49,55,56,58	0
5	PLM	B	503	18/18	0.90	0.16	55,57,59,63	0
4	9CR	B	502	22/22	0.91	0.13	45,50,53,54	0
3	HEM	A	500	43/43	0.97	0.08	25,33,41,43	0
3	HEM	B	500	43/43	0.97	0.09	27,33,44,48	0

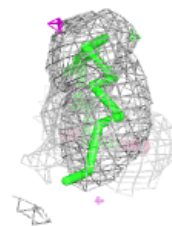
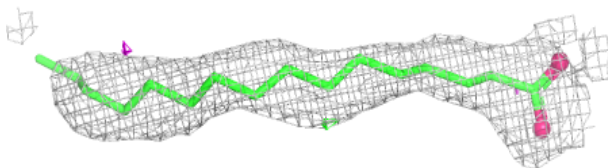
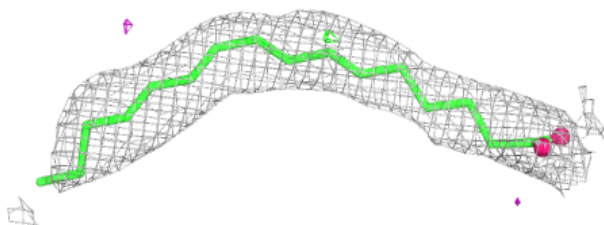
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9CR A 501:

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

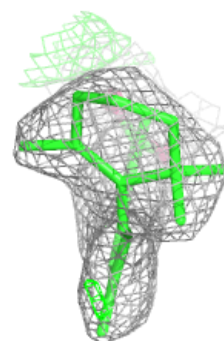
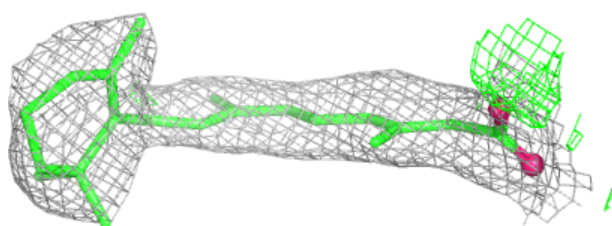
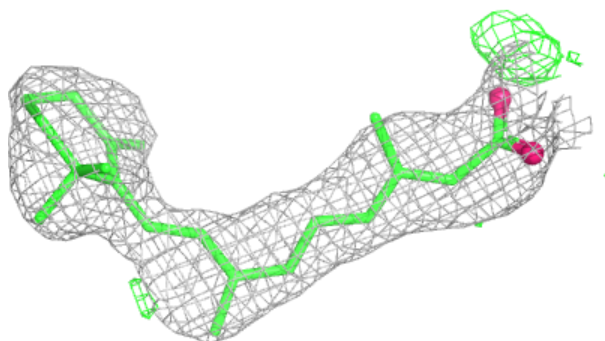
**Electron density around PLM A 503:**

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

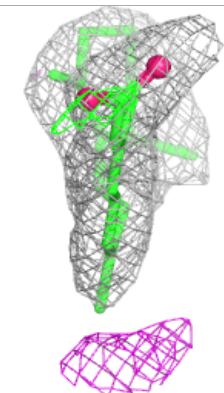
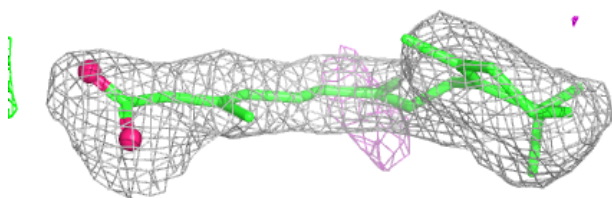
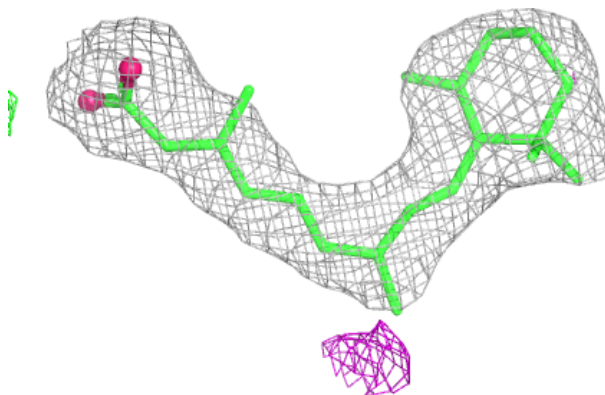


Electron density around 9CR B 501:

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

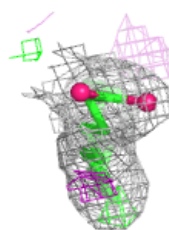
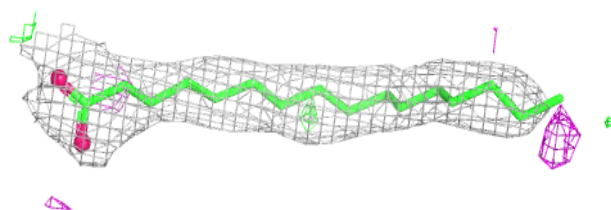
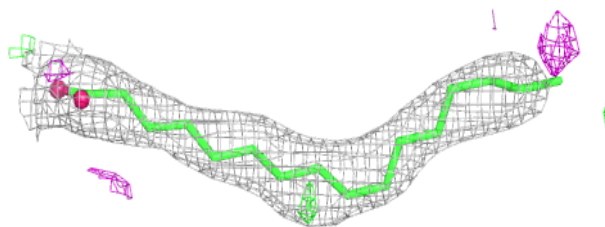
**Electron density around 9CR A 502:**

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

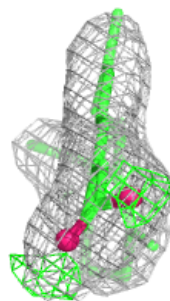
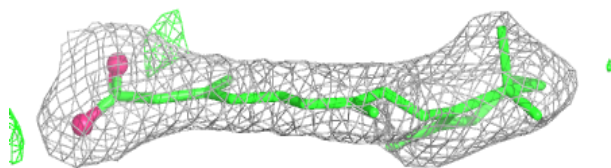
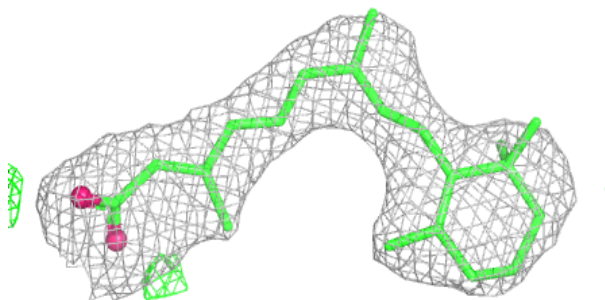


Electron density around PLM B 503:

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

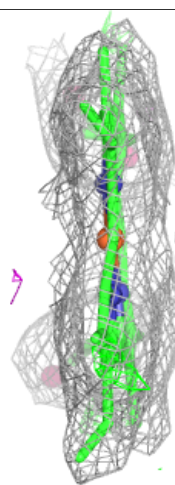
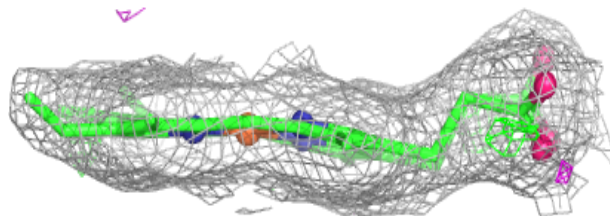
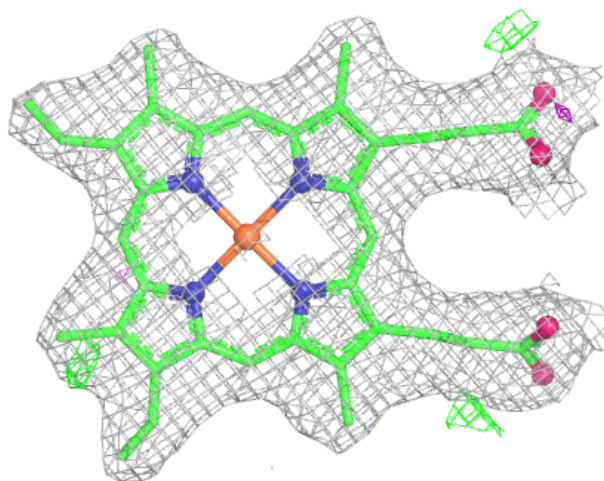
**Electron density around 9CR B 502:**

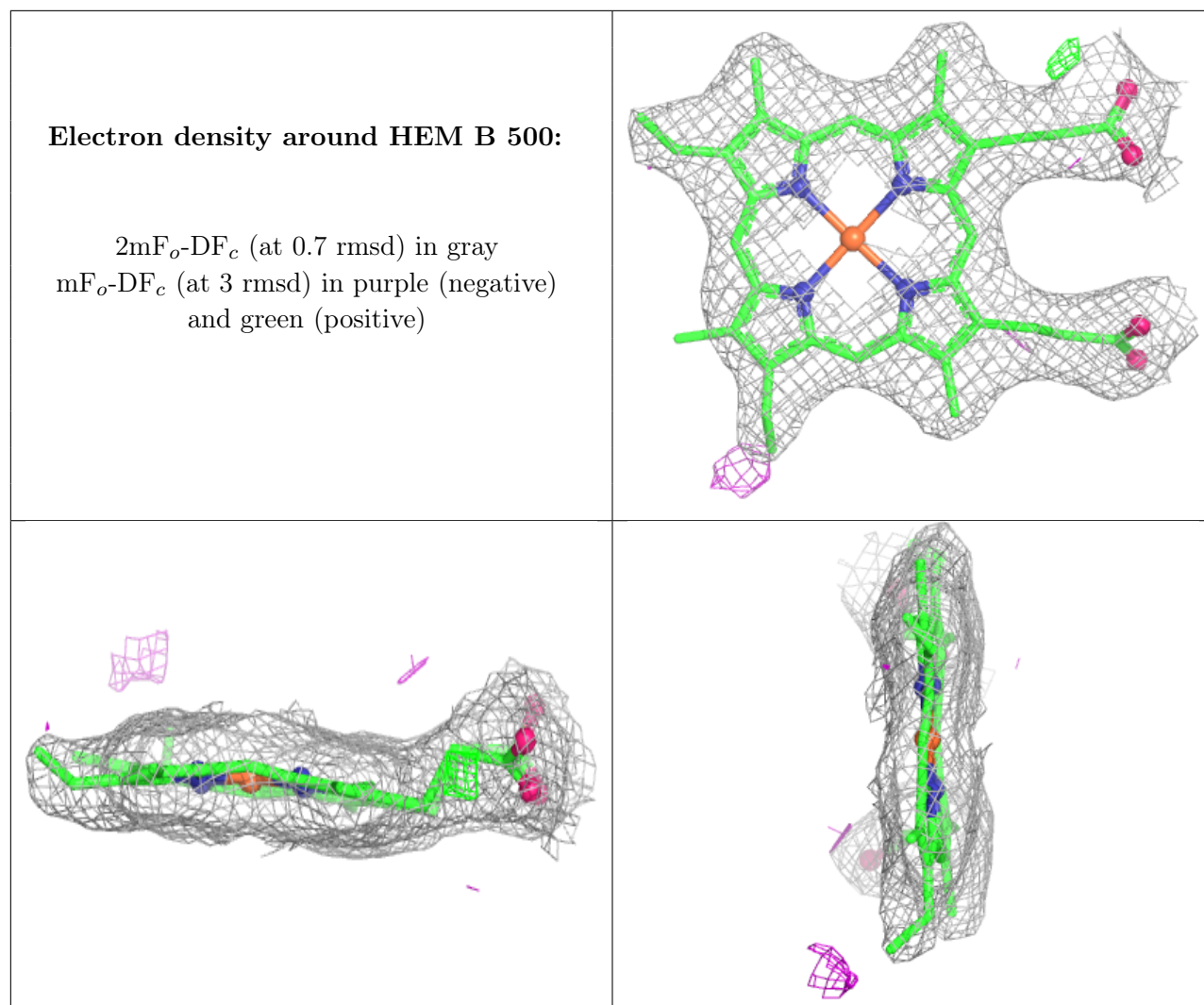
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.