



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:41 AM UTC

PDB ID : 2VE3 / pdb_00002ve3
Title : Retinoic acid bound cyanobacterial CYP120A1
Authors : Kuhnel, K.; Ke, N.; Sligar, S.G.; Schuler, M.A.; Schlichting, I.
Deposited on : 2007-10-15
Resolution : 2.10 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

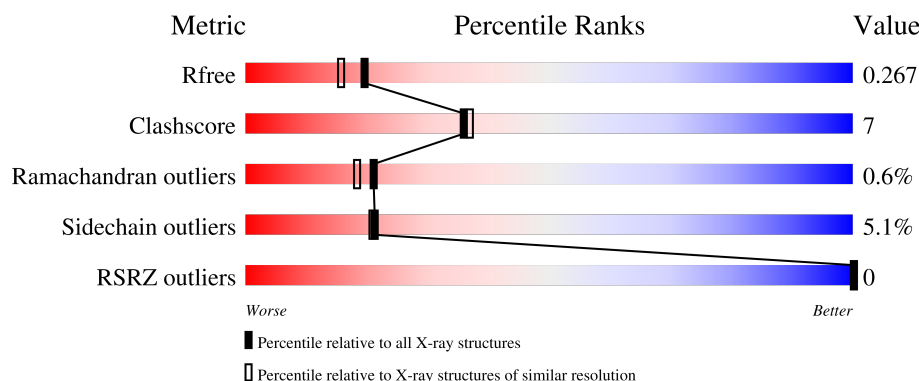
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	444	 77% 18% . .
1	B	444	 80% 15% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7324 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 PUTATIVE CYTOCHROME P450 120.

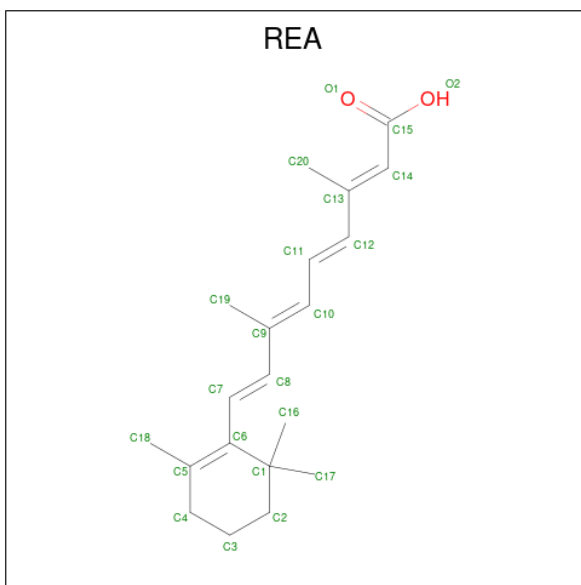
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3480	2254	601	616	9			
1	B	427	Total	C	N	O	S	0	0	0
			3411	2212	588	602	9			

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



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

- Molecule 3 is RETINOIC ACID (CCD ID: REA) (formula: $C_{20}H_{28}O_2$).



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

- Molecule 4 is water.

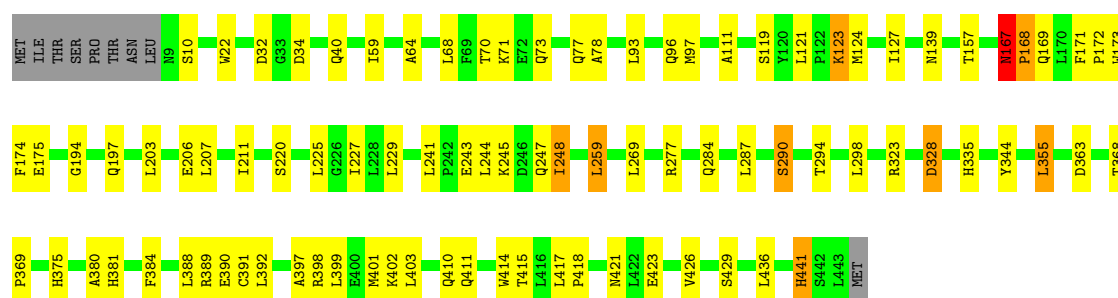
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	130	Total	O	0	0
			130	130		

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.

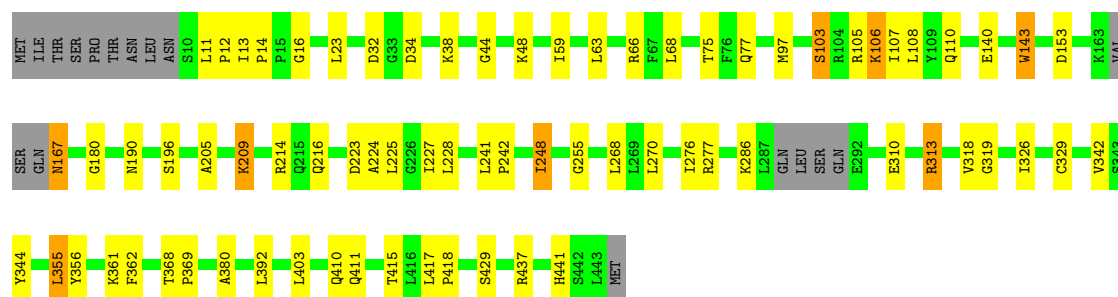
• Molecule 1: PUTATIVE CYTOCHROME P450 120

Chain A: 



• Molecule 1: PUTATIVE CYTOCHROME P450 120

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.46Å 132.97Å 67.42Å 90.00° 114.50° 90.00°	Depositor
Resolution (Å)	19.85 – 2.10 19.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.85-2.10) 80.4 (19.85-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.267 0.223 , 0.267	Depositor DCC
R_{free} test set	3238 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7324	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: REA, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/3574	0.99	9/4853 (0.2%)
1	B	0.62	0/3503	0.92	5/4755 (0.1%)
All	All	0.63	0/7077	0.96	14/9608 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASN	CA-C-N	12.66	135.66	119.84
1	A	167	ASN	C-N-CA	12.66	135.66	119.84
1	A	167	ASN	N-CA-C	7.49	121.95	108.55
1	B	167	ASN	CA-C-N	6.96	126.64	119.82
1	B	167	ASN	C-N-CA	6.96	126.64	119.82
1	B	143	TRP	N-CA-C	6.59	118.55	111.36
1	A	368	THR	CA-C-N	6.50	127.97	119.84
1	A	368	THR	C-N-CA	6.50	127.97	119.84
1	A	269	LEU	N-CA-C	5.17	116.99	111.36
1	A	363	ASP	CA-C-N	5.16	125.46	119.47
1	A	363	ASP	C-N-CA	5.16	125.46	119.47
1	A	287	LEU	CB-CA-C	-5.11	109.71	117.07
1	B	44	GLY	CA-C-N	5.00	124.66	119.56
1	B	44	GLY	C-N-CA	5.00	124.66	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	ASN	Peptide
1	A	290	SER	Peptide

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	3480	0	3486	58	0
1	B	3411	0	3404	43	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	22	0	27	0	0
3	B	22	0	27	1	0
4	A	173	0	0	2	0
4	B	130	0	0	2	0
All	All	7324	0	7004	103	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 7.

All (103) 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:B:77:GLN:HG3	1:B:97:MET:HE2	1.40	1.02
1:A:77:GLN:HG3	1:A:97:MET:HE2	1.51	0.91
1:B:59:ILE:HD11	1:B:68:LEU:HD13	1.58	0.84
1:A:121:LEU:HD21	1:A:399:LEU:HD11	1.64	0.80
1:A:77:GLN:HG3	1:A:97:MET:CE	2.13	0.78
1:B:140:GLU:HG3	1:B:417:LEU:HD11	1.67	0.74
2:B:1444:HEM:HMC1	2:B:1444:HEM:HBC2	1.71	0.71
1:A:73:GLN:H	1:A:73:GLN:CD	1.97	0.71
1:A:194:GLY:HA2	1:A:197:GLN:HE21	1.57	0.69
1:A:203:LEU:O	1:A:207:LEU:HG	1.95	0.67
1:B:224:ALA:O	1:B:228:LEU:HD13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:HE2	1:B:107:ILE:HG13	1.78	0.64
1:A:68:LEU:HD22	1:A:344:TYR:HB3	1.80	0.64
1:B:77:GLN:HG3	1:B:97:MET:CE	2.25	0.64
1:B:16:GLY:O	1:B:48:LYS:NZ	2.33	0.61
1:B:59:ILE:HD11	1:B:68:LEU:CD1	2.28	0.61
1:B:318:VAL:HG13	3:B:1445:REA:H10	1.82	0.61
1:A:167:ASN:CG	1:A:167:ASN:O	2.43	0.61
1:A:121:LEU:HD22	1:A:403:LEU:HD22	1.82	0.60
1:B:205:ALA:O	1:B:209:LYS:HD2	2.01	0.60
1:A:73:GLN:HG3	1:A:388:LEU:HD11	1.83	0.60
1:B:13:ILE:HG23	1:B:14:PRO:HD2	1.83	0.60
1:A:244:LEU:O	1:A:248:ILE:HG12	2.02	0.59
1:B:225:LEU:HD13	1:B:248:ILE:HD13	1.85	0.59
1:B:415:THR:OG1	1:B:441:HIS:HE1	1.86	0.59
1:A:211:ILE:HG12	1:A:225:LEU:HD11	1.85	0.58
1:A:171:PHE:HB3	1:A:172:PRO:HD3	1.86	0.57
1:B:415:THR:OG1	1:B:441:HIS:CE1	2.58	0.57
1:B:214:ARG:HH22	1:B:223:ASP:CG	2.13	0.56
1:A:168:PRO:HD2	1:A:169:GLN:H	1.70	0.56
1:B:270:LEU:O	1:B:277:ARG:NH1	2.38	0.56
1:B:410:GLN:HG3	1:B:411:GLN:HG3	1.88	0.56
1:A:284:GLN:HE22	1:A:410:GLN:CA	2.19	0.55
1:A:381:HIS:HD2	4:A:2120:HOH:O	1.89	0.55
1:B:63:LEU:HD23	1:B:66:ARG:NH1	2.20	0.55
1:B:63:LEU:HD23	1:B:66:ARG:HH12	1.72	0.54
1:B:103:SER:HA	1:B:106:LYS:HD3	1.88	0.54
1:A:168:PRO:HD2	1:A:169:GLN:N	2.23	0.54
1:A:168:PRO:CD	1:A:169:GLN:H	2.18	0.54
1:B:68:LEU:HD11	1:B:342:VAL:HG11	1.90	0.54
1:B:310:GLU:OE1	1:B:313:ARG:HD3	2.08	0.53
1:B:68:LEU:CD2	1:B:344:TYR:HB3	2.38	0.53
1:A:384:PHE:HB3	1:A:391:CYS:HB3	1.91	0.53
1:B:106:LYS:HG2	1:B:107:ILE:N	2.24	0.52
1:A:415:THR:OG1	1:A:441:HIS:CE1	2.62	0.52
1:B:140:GLU:OE2	1:B:437:ARG:HD3	2.09	0.52
1:A:59:ILE:HD12	1:A:64:ALA:HB1	1.91	0.51
1:B:68:LEU:HD22	1:B:344:TYR:HB3	1.93	0.50
1:A:391:CYS:HB2	2:A:1444:HEM:NA	2.26	0.50
1:A:398:ARG:HA	1:A:401:MET:HE3	1.93	0.50
1:A:211:ILE:HD11	1:A:248:ILE:HD11	1.93	0.49
1:A:168:PRO:CD	1:A:169:GLN:N	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HB3	1:B:12:PRO:HD2	1.94	0.49
1:A:68:LEU:CD2	1:A:344:TYR:HB3	2.42	0.48
1:A:119:SER:O	1:A:123:LYS:NZ	2.46	0.48
2:B:1444:HEM:HBC2	2:B:1444:HEM:CMC	2.43	0.48
1:B:368:THR:HG23	1:B:369:PRO:HD2	1.96	0.47
1:B:225:LEU:HD13	1:B:248:ILE:CD1	2.44	0.47
1:B:313:ARG:HD2	1:B:356:TYR:CD1	2.49	0.47
1:A:167:ASN:O	1:A:167:ASN:OD1	2.33	0.47
1:A:124:MET:HE1	1:A:399:LEU:HD23	1.97	0.46
1:A:415:THR:HG1	1:A:441:HIS:CE1	2.33	0.46
1:A:32:ASP:C	1:A:34:ASP:H	2.23	0.46
1:A:111:ALA:HA	1:A:227:ILE:CD1	2.46	0.46
1:A:410:GLN:HG3	1:A:411:GLN:HG3	1.97	0.45
1:A:421:ASN:OD1	1:A:423:GLU:HB2	2.16	0.45
1:B:190:ASN:ND2	4:B:2051:HOH:O	2.48	0.45
1:A:96:GLN:O	1:A:389:ARG:NH2	2.44	0.45
1:A:78:ALA:HA	1:A:323:ARG:HD3	1.98	0.44
1:A:173:TRP:HZ3	1:A:206:GLU:HG3	1.81	0.44
1:A:243:GLU:O	1:A:247:GLN:HG2	2.17	0.44
1:B:319:GLY:HA2	4:B:2099:HOH:O	2.16	0.44
1:A:123:LYS:HE2	1:A:123:LYS:HB2	1.52	0.44
1:B:34:ASP:HB3	1:B:38:LYS:HD2	2.00	0.44
1:A:241:LEU:O	1:A:245:LYS:HG3	2.17	0.44
1:A:277:ARG:HD2	1:A:414:TRP:CZ3	2.53	0.44
1:B:108:LEU:HD23	1:B:228:LEU:HD11	1.98	0.44
1:A:127:ILE:HD11	1:A:157:THR:HG21	2.00	0.43
1:A:417:LEU:HA	1:A:418:PRO:HD3	1.87	0.43
1:B:214:ARG:NH2	1:B:223:ASP:OD2	2.51	0.43
1:A:171:PHE:O	1:A:175:GLU:HG2	2.19	0.43
1:B:110:GLN:HB2	1:B:227:ILE:HG21	2.01	0.43
1:B:180:GLY:HA3	1:B:196:SER:OG	2.19	0.42
1:B:255:GLY:HA2	2:B:1444:HEM:HMC3	2.01	0.42
1:B:276:ILE:HD12	1:B:362:PHE:CE2	2.54	0.42
1:B:355:LEU:HB3	1:B:356:TYR:CD2	2.54	0.42
1:A:121:LEU:HA	1:A:121:LEU:HD23	1.78	0.42
1:A:355:LEU:HG	1:A:380:ALA:HB1	2.00	0.42
1:B:241:LEU:HB3	1:B:242:PRO:HD3	2.01	0.42
1:A:225:LEU:HD13	1:A:248:ILE:HD13	2.00	0.42
1:A:390:GLU:O	1:A:391:CYS:C	2.63	0.41
1:B:355:LEU:HG	1:B:380:ALA:HB1	2.01	0.41
1:A:111:ALA:HA	1:A:227:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HD11	1:A:397:ALA:HA	2.01	0.41
1:A:167:ASN:OD1	1:A:167:ASN:C	2.64	0.41
1:B:417:LEU:HA	1:B:418:PRO:HD3	1.93	0.41
1:A:328:ASP:CG	1:A:335:HIS:HE2	2.28	0.41
1:A:93:LEU:CD2	1:A:392:LEU:HD13	2.51	0.40
1:A:298:LEU:HB3	1:A:402:LYS:HD2	2.03	0.40
1:A:70:THR:O	1:A:71:LYS:C	2.64	0.40
1:A:284:GLN:HE22	1:A:410:GLN:HA	1.86	0.40
1:A:426:VAL:HG11	4:A:2124:HOH:O	2.21	0.40
1:A:70:THR:HG22	1:A:71:LYS:HG3	2.04	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	433/444 (98%)	415 (96%)	13 (3%)	5 (1%)	10	7
1	B	421/444 (95%)	407 (97%)	14 (3%)	0	100	100
All	All	854/888 (96%)	822 (96%)	27 (3%)	5 (1%)	21	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PRO
1	A	22	TRP
1	A	139	ASN
1	A	290	SER
1	A	168	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	374/390 (96%)	358 (96%)	16 (4%)	26	27
1	B	364/390 (93%)	342 (94%)	22 (6%)	17	15
All	All	738/780 (95%)	700 (95%)	38 (5%)	21	21

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	40	GLN
1	A	123	LYS
1	A	167	ASN
1	A	174	PHE
1	A	220	SER
1	A	229	LEU
1	A	248	ILE
1	A	259	LEU
1	A	294	THR
1	A	328	ASP
1	A	355	LEU
1	A	375	HIS
1	A	429	SER
1	A	436	LEU
1	A	441	HIS
1	B	23	LEU
1	B	32	ASP
1	B	75	THR
1	B	103	SER
1	B	105	ARG
1	B	106	LYS
1	B	143	TRP
1	B	153	ASP
1	B	167	ASN
1	B	209	LYS
1	B	216	GLN

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Mol	Chain	Res	Type
1	B	248	ILE
1	B	268	LEU
1	B	286	LYS
1	B	313	ARG
1	B	326	ILE
1	B	329	CYS
1	B	355	LEU
1	B	361	LYS
1	B	392	LEU
1	B	403	LEU
1	B	429	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	42	GLN
1	A	179	GLN
1	A	197	GLN
1	A	215	GLN
1	A	236	ASN
1	A	284	GLN
1	A	285	ASN
1	A	291	GLN
1	A	345	GLN
1	A	348	GLN
1	A	381	HIS
1	B	42	GLN
1	B	77	GLN
1	B	91	ASN
1	B	190	ASN
1	B	236	ASN
1	B	306	GLN
1	B	332	GLN
1	B	376	ASN
1	B	441	HIS

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](#)

4 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	REA	B	1445	-	22,22,22	2.33	5 (22%)	30,30,30	1.93	9 (30%)
2	HEM	B	1444	1	50,50,50	2.01	10 (20%)	67,82,82	1.36	6 (8%)
2	HEM	A	1444	1	50,50,50	2.05	10 (20%)	67,82,82	1.25	7 (10%)
3	REA	A	1445	-	22,22,22	2.13	6 (27%)	30,30,30	2.03	10 (33%)

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	REA	B	1445	-	-	8/15/32/32	0/1/1/1
2	HEM	B	1444	1	-	4/14/54/54	-
2	HEM	A	1444	1	-	4/14/54/54	-
3	REA	A	1445	-	-	5/15/32/32	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1444	HEM	C3D-C2D	7.86	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1444	HEM	C3D-C2D	7.57	1.53	1.36
2	B	1444	HEM	FE-NB	6.24	2.14	1.94
2	A	1444	HEM	FE-ND	5.36	2.11	1.94
2	A	1444	HEM	FE-NA	5.30	2.12	1.95
2	B	1444	HEM	FE-NA	5.12	2.12	1.95
3	B	1445	REA	C5-C6	4.81	1.42	1.34
3	B	1445	REA	C14-C13	4.74	1.42	1.35
3	B	1445	REA	C8-C7	4.72	1.47	1.33
3	B	1445	REA	C11-C12	4.70	1.46	1.34
3	A	1445	REA	C11-C12	4.60	1.46	1.34
3	A	1445	REA	C8-C7	4.59	1.46	1.33
3	B	1445	REA	C10-C9	4.55	1.46	1.35
2	B	1444	HEM	FE-ND	4.36	2.08	1.94
3	A	1445	REA	C14-C13	4.28	1.41	1.35
3	A	1445	REA	C10-C9	4.07	1.45	1.35
2	A	1444	HEM	FE-NC	3.94	2.08	1.95
3	A	1445	REA	C5-C6	3.54	1.40	1.34
2	A	1444	HEM	CAB-C3B	3.52	1.56	1.47
2	B	1444	HEM	CAB-C3B	3.30	1.56	1.47
2	A	1444	HEM	FE-NB	3.27	2.05	1.94
2	A	1444	HEM	CAC-C3C	3.26	1.56	1.47
2	B	1444	HEM	CAC-C3C	2.73	1.54	1.47
2	A	1444	HEM	CMC-C2C	2.45	1.55	1.50
2	A	1444	HEM	CMD-C2D	2.32	1.55	1.50
3	A	1445	REA	O2-C15	-2.32	1.24	1.30
2	B	1444	HEM	CMD-C2D	2.14	1.55	1.50
2	B	1444	HEM	C2A-C3A	-2.13	1.33	1.38
2	B	1444	HEM	CMA-C3A	2.06	1.55	1.50
2	B	1444	HEM	CMB-C2B	2.05	1.55	1.50
2	A	1444	HEM	CMB-C2B	2.03	1.54	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1445	REA	C7-C8-C9	-5.35	118.32	126.23
2	B	1444	HEM	C4D-ND-C1D	5.22	111.39	105.21
2	A	1444	HEM	C4D-ND-C1D	5.00	111.13	105.21
3	B	1445	REA	C15-C14-C13	-4.99	120.97	128.40
3	B	1445	REA	C7-C8-C9	-4.51	119.56	126.23
3	A	1445	REA	C10-C11-C12	-3.88	111.95	123.20
3	A	1445	REA	C18-C5-C6	-3.48	120.68	124.48
3	A	1445	REA	C19-C9-C8	3.37	123.24	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1445	REA	C11-C10-C9	-2.93	123.17	127.28
2	A	1444	HEM	C3B-C2B-C1B	2.90	108.58	106.41
3	B	1445	REA	C8-C7-C6	-2.87	119.32	127.00
2	B	1444	HEM	CBD-CAD-C3D	-2.82	104.73	112.53
3	B	1445	REA	C18-C5-C6	-2.74	121.49	124.48
2	B	1444	HEM	C3B-C2B-C1B	2.74	108.47	106.41
3	A	1445	REA	C8-C7-C6	-2.72	119.73	127.00
2	B	1444	HEM	CAA-CBA-CGA	-2.67	106.58	113.67
3	B	1445	REA	C3-C4-C5	-2.65	109.32	114.06
2	B	1444	HEM	C2A-C1A-NA	-2.44	107.45	110.15
3	A	1445	REA	C15-C14-C13	-2.39	124.84	128.40
2	A	1444	HEM	CAA-CBA-CGA	-2.39	107.32	113.67
3	A	1445	REA	C20-C13-C12	2.39	121.74	118.09
3	B	1445	REA	O2-C15-C14	2.24	120.06	113.40
2	A	1444	HEM	CHD-C1D-ND	2.15	126.73	124.42
3	A	1445	REA	O2-C15-C14	2.14	119.77	113.40
3	A	1445	REA	C8-C9-C10	-2.14	115.65	119.01
3	B	1445	REA	C11-C12-C13	-2.12	120.55	126.36
2	A	1444	HEM	O2D-CGD-CBD	2.11	120.68	114.00
3	A	1445	REA	C11-C10-C9	-2.09	124.35	127.28
2	A	1444	HEM	C2A-C1A-NA	-2.09	107.84	110.15
2	B	1444	HEM	O1A-CGA-CBA	-2.06	116.56	123.09
2	A	1444	HEM	C1B-NB-C4B	2.05	107.64	105.21
3	B	1445	REA	C19-C9-C8	2.00	121.14	118.09

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1444	HEM	C2C-C3C-CAC-CBC
3	A	1445	REA	C11-C10-C9-C8
3	A	1445	REA	C11-C10-C9-C19
3	A	1445	REA	C10-C11-C12-C13
3	A	1445	REA	C12-C13-C14-C15
3	A	1445	REA	C20-C13-C14-C15
3	B	1445	REA	C11-C10-C9-C8
3	B	1445	REA	C11-C10-C9-C19
3	B	1445	REA	C10-C11-C12-C13
3	B	1445	REA	C12-C13-C14-C15
3	B	1445	REA	C20-C13-C14-C15
3	B	1445	REA	C13-C14-C15-O1
3	B	1445	REA	C13-C14-C15-O2

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Mol	Chain	Res	Type	Atoms
2	A	1444	HEM	C4C-C3C-CAC-CBC
2	B	1444	HEM	C2B-C3B-CAB-CBB
2	B	1444	HEM	C4B-C3B-CAB-CBB
2	B	1444	HEM	CAA-CBA-CGA-O2A
3	B	1445	REA	C9-C10-C11-C12
2	A	1444	HEM	CAA-CBA-CGA-O2A
2	B	1444	HEM	CAA-CBA-CGA-O1A
2	A	1444	HEM	CAA-CBA-CGA-O1A

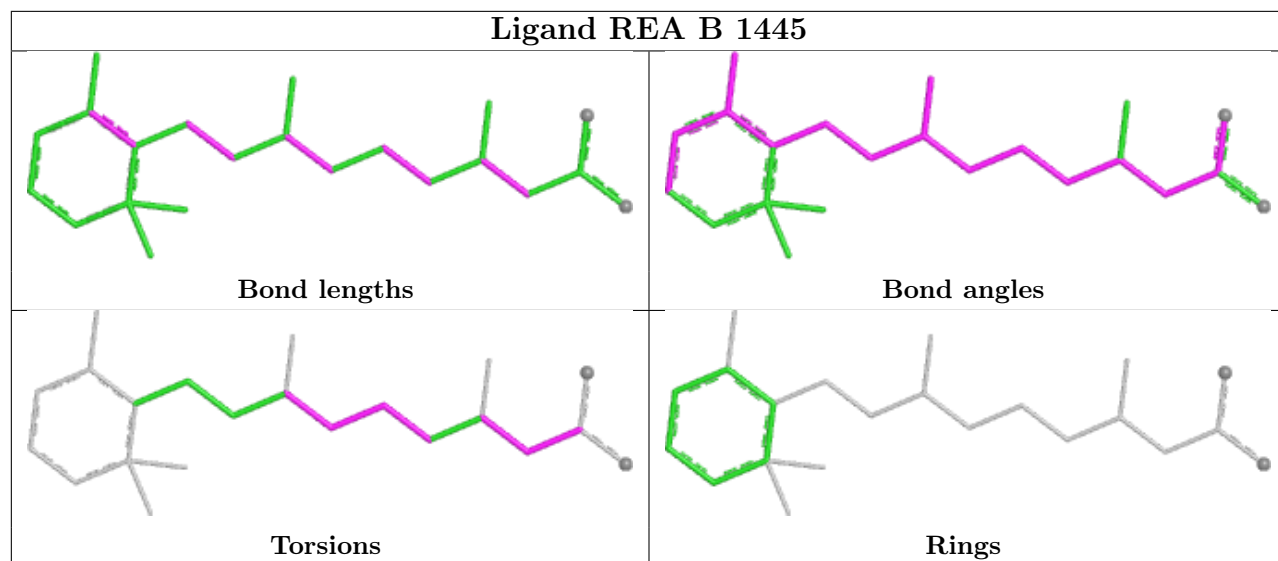
There are no ring outliers.

3 monomers are involved in 5 short contacts:

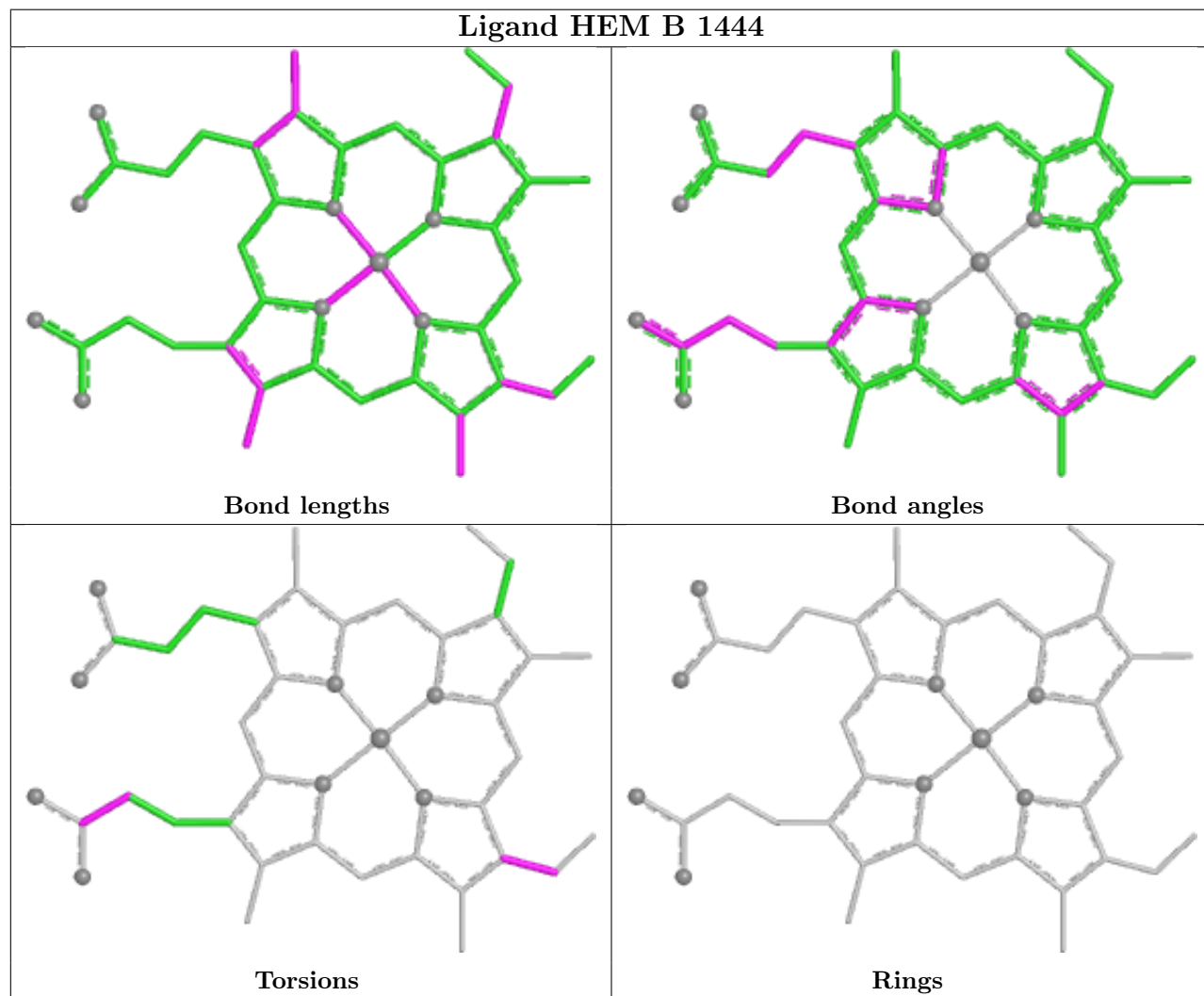
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1445	REA	1	0
2	B	1444	HEM	3	0
2	A	1444	HEM	1	0

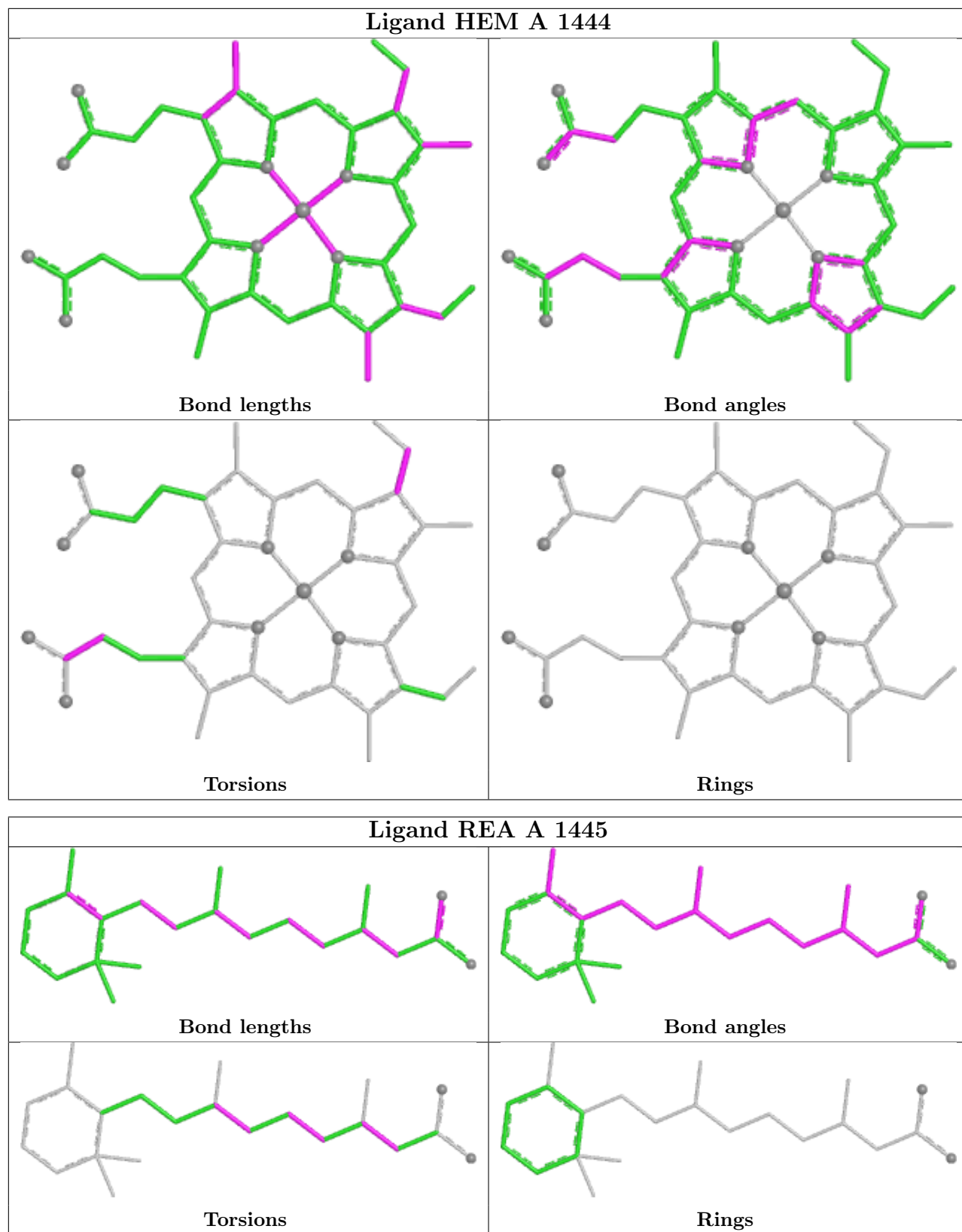
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand REA B 1445



Ligand HEM B 1444





5.7 Other polymers ⓘ

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	435/444 (97%)	-1.43	0 100 100	13, 25, 44, 52	0
1	B	427/444 (96%)	-1.39	0 100 100	16, 29, 43, 51	0
All	All	862/888 (97%)	-1.41	0 100 100	13, 27, 43, 52	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

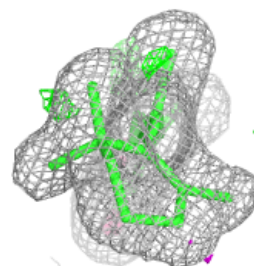
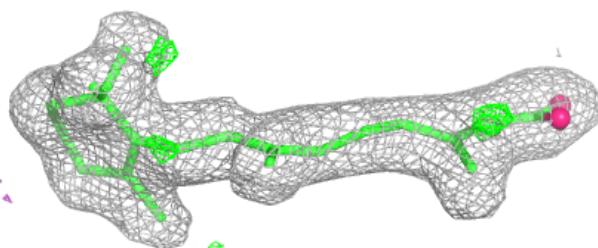
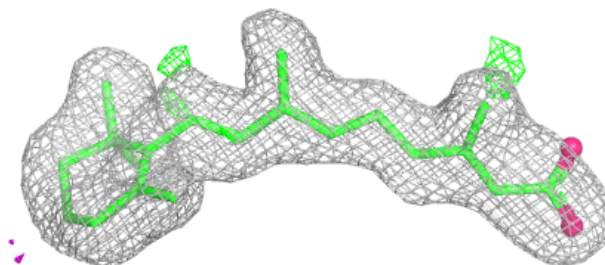
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	REA	A	1445	22/22	0.99	0.03	9,14,27,32	0
3	REA	B	1445	22/22	0.99	0.03	15,24,33,36	0
2	HEM	A	1444	43/43	1.00	0.02	10,15,20,24	0
2	HEM	B	1444	43/43	1.00	0.02	16,18,21,24	0

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

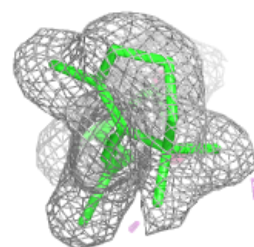
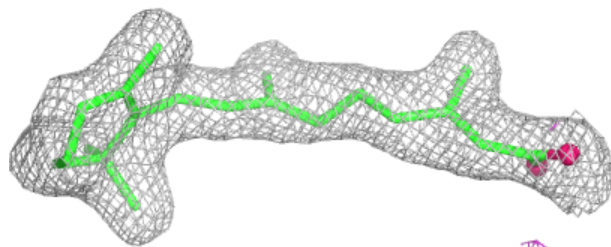
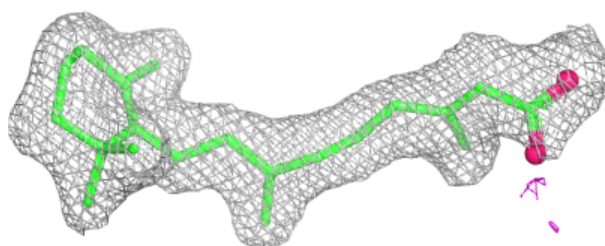
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around REA A 1445:

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

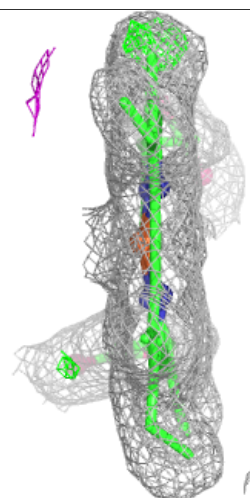
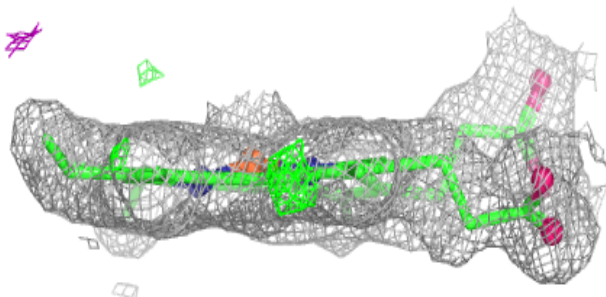
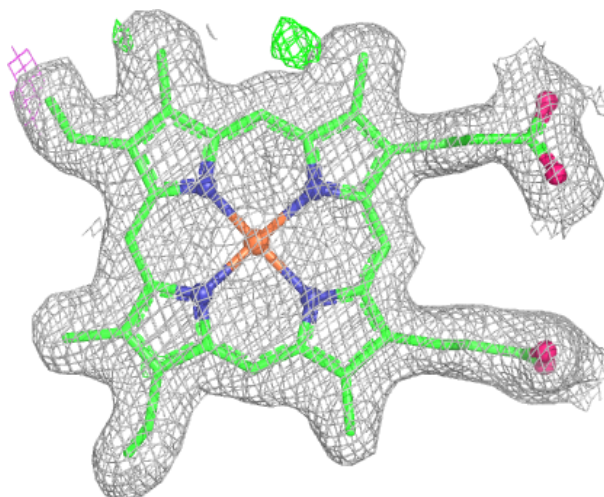
**Electron density around REA B 1445:**

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



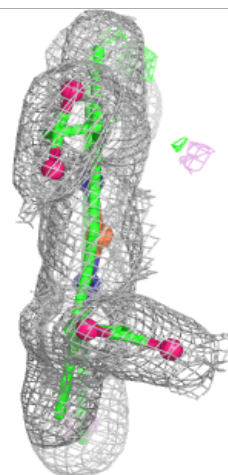
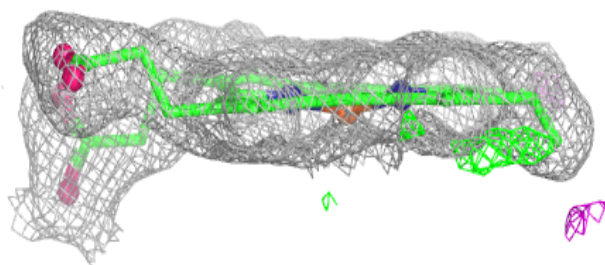
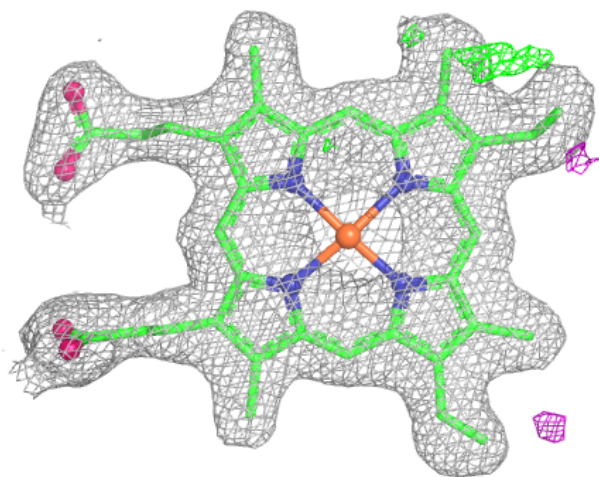
Electron density around HEM A 1444:

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



Electron density around HEM B 1444:

$2mF_o-DF_c$ (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.