



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:44 PM UTC

PDB ID : 4EGP / pdb_00004egp
Title : The X-ray crystal structure of CYP19A4 in complex with 2-naphthoic acid
Authors : Zhou, W.; Bell, S.G.; Yang, W.; Zhou, R.M.; Tan, A.B.H.; Wong, L.-L.
Deposited on : 2012-03-31
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

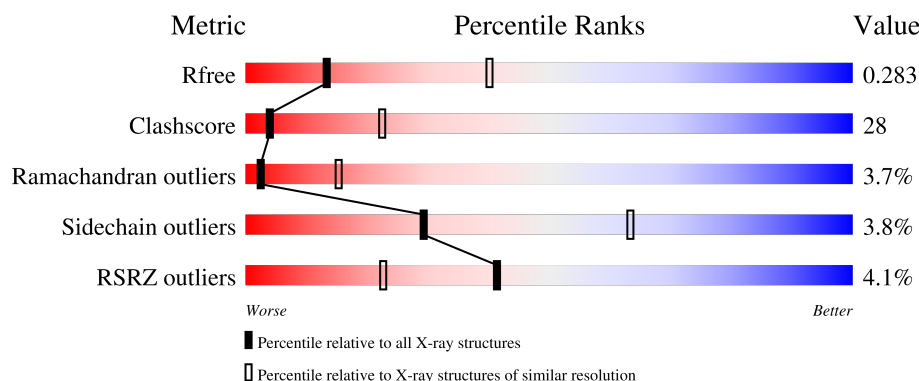
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	410	 64% 29% . .
1	B	410	 8% 47% 42% 6% .

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
3	FIV	A	502	-	-	X	-

2 Entry composition [i](#)

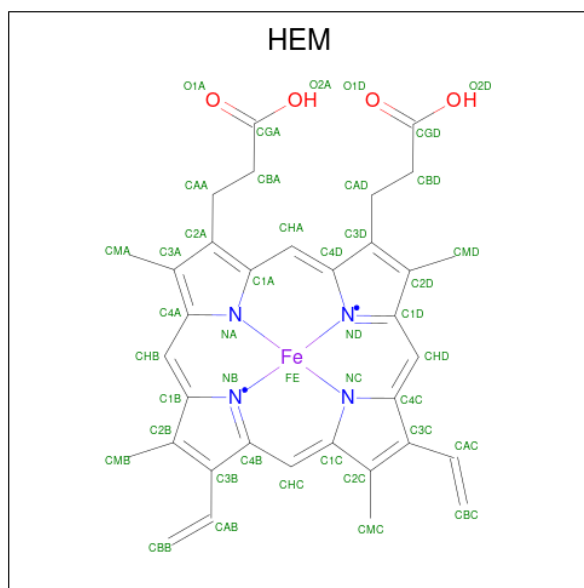
There are 7 unique types of molecules in this entry. The entry contains 6211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

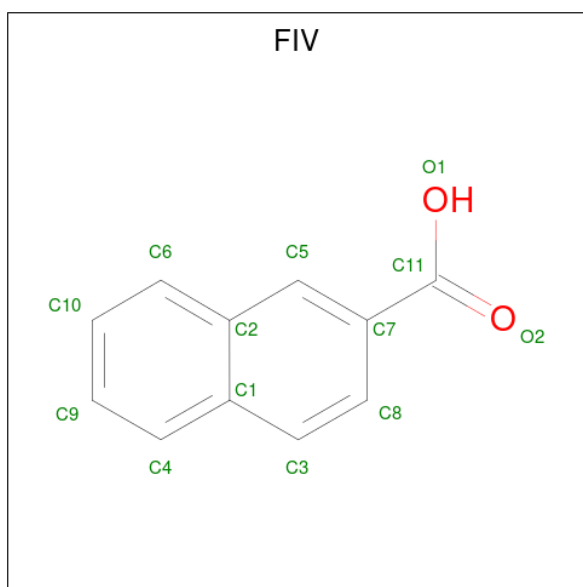
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3024	1914	534	564	12			
1	B	393	Total	C	N	O	S	0	0	0
			3021	1912	534	564	11			

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



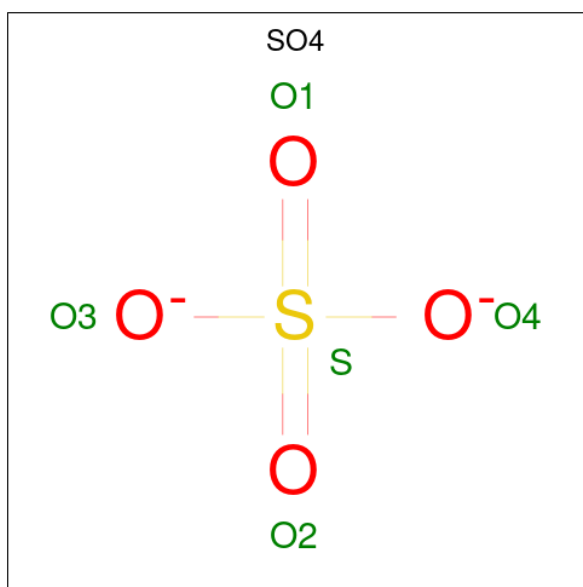
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is naphthalene-2-carboxylic acid (CCD ID: FIV) (formula: $C_{11}H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			13	11	2		
3	B	1	Total	C	O	0	0
			13	11	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



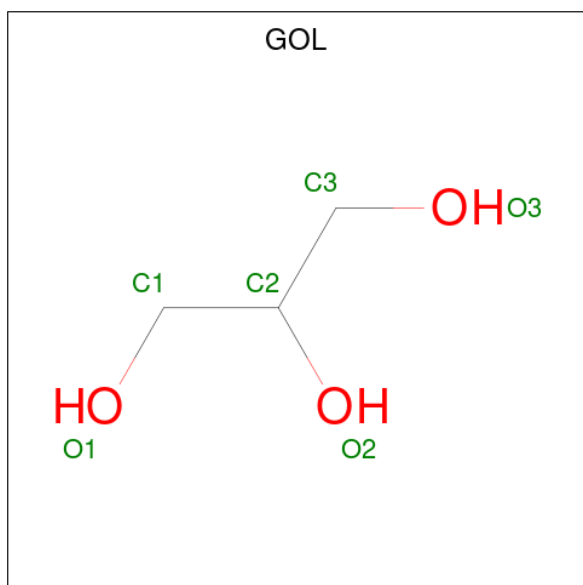
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

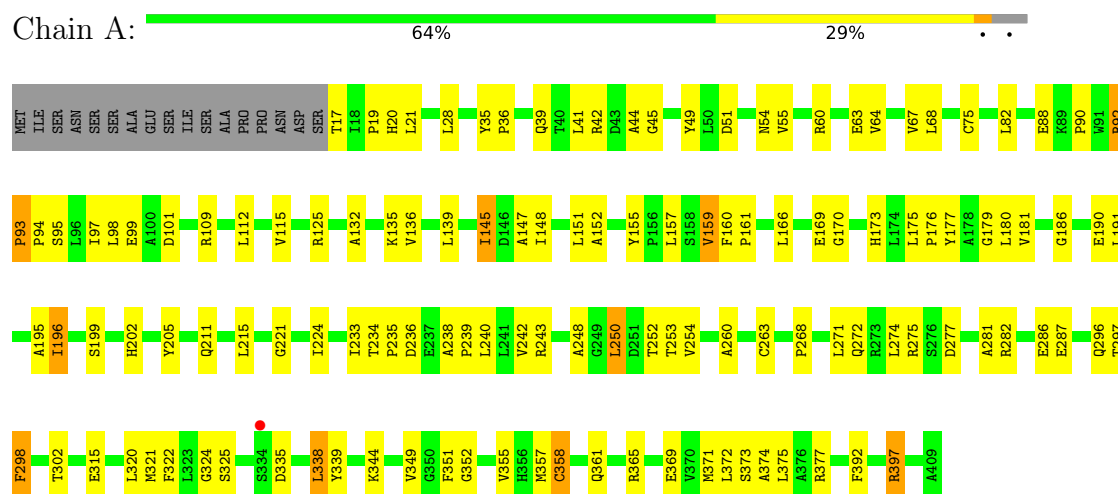
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	8	Total	O	0	0
			8	8		

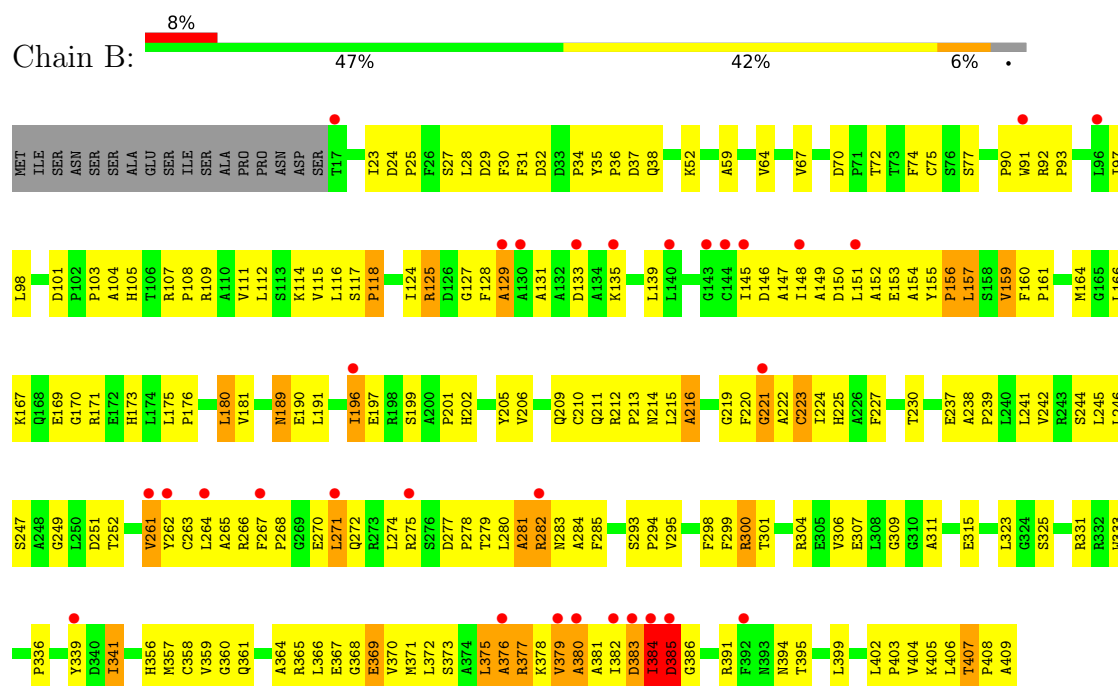
3 Residue-property plots [i](#)

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

• Molecule 1: Cytochrome P450



• Molecule 1: Cytochrome P450



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	143.54Å 172.21Å 106.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 3.00 48.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.94-3.00) 99.4 (48.94-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.287 0.234 , 0.283	Depositor DCC
R_{free} test set	1346 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6211	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: GOL, CL, SO4, HEM, FIV

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	0.84	0/3099	1.15	15/4217 (0.4%)
1	B	0.89	0/3093	1.18	19/4209 (0.5%)
All	All	0.86	0/6192	1.16	34/8426 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	ASP	N-CA-CB	-11.61	90.87	110.49
1	B	261	VAL	N-CA-C	9.08	119.63	110.82
1	B	129	ALA	N-CA-C	8.47	121.35	111.02
1	A	281	ALA	N-CA-C	7.66	123.93	111.37
1	B	407	THR	CB-CA-C	7.62	120.36	108.63
1	B	283	ASN	N-CA-C	-7.60	103.27	112.54
1	A	281	ALA	CB-CA-C	-7.55	98.31	110.84
1	A	45	GLY	CA-C-N	-7.52	111.92	120.04
1	A	45	GLY	C-N-CA	-7.52	111.92	120.04
1	B	189	ASN	N-CA-C	7.40	117.65	107.73
1	A	17	THR	CA-C-N	-7.35	117.60	122.60
1	A	17	THR	C-N-CA	-7.35	117.60	122.60
1	B	261	VAL	CB-CA-C	-7.17	102.65	112.04
1	B	293	SER	N-CA-C	7.16	125.64	109.81
1	B	384	ILE	CB-CA-C	-6.85	100.05	111.29
1	B	282	ARG	N-CA-C	6.28	124.19	110.80
1	A	324	GLY	N-CA-C	-6.15	105.05	112.49
1	B	223	CYS	N-CA-C	-6.12	104.67	111.71
1	A	93	PRO	CA-C-N	6.05	126.39	119.92
1	A	93	PRO	C-N-CA	6.05	126.39	119.92
1	B	407	THR	CA-C-N	5.74	127.02	119.84
1	B	407	THR	C-N-CA	5.74	127.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	VAL	N-CA-C	5.72	116.77	111.45
1	B	29	ASP	N-CA-C	-5.61	105.07	111.07
1	A	355	VAL	N-CA-C	5.23	117.63	111.09
1	A	186	GLY	CA-C-N	5.23	125.77	120.38
1	A	186	GLY	C-N-CA	5.23	125.77	120.38
1	B	251	ASP	CB-CA-C	-5.21	100.06	110.42
1	B	70	ASP	CA-C-N	5.17	124.96	119.28
1	B	70	ASP	C-N-CA	5.17	124.96	119.28
1	B	300	ARG	N-CA-C	-5.12	101.62	109.41
1	A	92	ARG	CA-C-N	-5.07	115.16	120.38
1	A	92	ARG	C-N-CA	-5.07	115.16	120.38
1	B	282	ARG	CB-CA-C	-5.01	100.45	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	3024	0	2998	105	0
1	B	3021	0	2993	238	0
2	A	43	0	30	3	0
2	B	43	0	30	8	0
3	A	26	0	14	7	0
3	B	13	0	7	4	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	6	0	8	0	0
6	A	1	0	0	0	0
7	A	11	0	0	1	0
7	B	8	0	0	1	0
All	All	6211	0	6080	344	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 28.

All (344) 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:381:ALA:CB	1:B:407:THR:HB	1.34	1.54
1:B:376:ALA:O	1:B:377:ARG:HG3	1.36	1.25
1:B:381:ALA:CB	1:B:407:THR:CB	2.20	1.17
1:B:381:ALA:HB3	1:B:407:THR:HB	1.30	1.13
1:B:384:ILE:HG13	1:B:385:ASP:N	1.58	1.10
1:B:379:VAL:HG22	1:B:380:ALA:H	1.05	1.09
1:B:151:LEU:HD21	1:B:371:MET:HE3	1.21	1.09
1:B:381:ALA:HB3	1:B:407:THR:CB	1.85	1.05
1:B:384:ILE:CG1	1:B:385:ASP:H	1.66	1.04
1:B:379:VAL:HG22	1:B:380:ALA:N	1.67	1.04
1:B:244:SER:HB2	3:B:502:FIV:H2	1.36	1.03
1:B:381:ALA:HB1	1:B:407:THR:CB	1.85	1.03
1:B:384:ILE:O	1:B:385:ASP:HB2	1.23	1.03
1:B:384:ILE:HD12	1:B:403:PRO:O	1.56	1.02
1:B:384:ILE:O	1:B:385:ASP:CB	2.11	0.99
1:B:281:ALA:O	1:B:372:LEU:HD22	1.67	0.95
1:B:384:ILE:HG13	1:B:385:ASP:H	0.78	0.93
1:B:384:ILE:N	1:B:404:VAL:HG13	1.84	0.92
1:B:381:ALA:HB1	1:B:407:THR:HB	0.92	0.92
1:B:244:SER:HB2	3:B:502:FIV:C8	2.00	0.92
1:A:92:ARG:HH22	3:A:502:FIV:H2	1.34	0.92
1:B:379:VAL:HA	1:B:409:ALA:HB2	1.52	0.91
1:B:382:ILE:O	1:B:383:ASP:HB2	1.70	0.90
1:B:379:VAL:CG2	1:B:380:ALA:H	1.85	0.89
1:B:376:ALA:O	1:B:377:ARG:CG	2.19	0.89
1:B:281:ALA:O	1:B:372:LEU:CD2	2.21	0.88
1:B:383:ASP:O	1:B:384:ILE:HB	1.73	0.87
1:B:382:ILE:HG23	1:B:404:VAL:HG11	1.55	0.87
1:B:147:ALA:HB3	1:B:402:LEU:O	1.75	0.85
1:B:282:ARG:HH22	1:B:365:ARG:HH11	1.24	0.84
1:B:151:LEU:CD2	1:B:371:MET:HE3	2.07	0.83
1:B:24:ASP:OD2	1:B:52:LYS:HE3	1.77	0.83
1:B:381:ALA:HB3	1:B:407:THR:CA	2.08	0.83
1:B:167:LYS:HE3	1:B:209:GLN:HE22	1.44	0.81
1:A:75:CYS:HB2	1:A:101:ASP:OD2	1.81	0.80
1:A:39:GLN:HA	1:A:42:ARG:HH21	1.46	0.80
1:B:384:ILE:HA	1:B:404:VAL:HA	1.64	0.80
1:B:270:GLU:HB3	1:B:341:ILE:HG12	1.62	0.80
1:A:236:ASP:O	1:A:240:LEU:HD13	1.81	0.80
1:B:383:ASP:O	1:B:384:ILE:CB	2.30	0.79
1:B:282:ARG:NH2	1:B:365:ARG:HH11	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LEU:HD22	1:B:209:GLN:HE21	1.46	0.78
1:B:277:ASP:O	1:B:280:LEU:HD12	1.83	0.78
1:A:20:HIS:HD2	1:A:49:TYR:CD2	2.02	0.77
1:B:384:ILE:H	1:B:404:VAL:HG13	1.49	0.77
1:A:20:HIS:CD2	1:A:49:TYR:CD2	2.73	0.76
1:B:265:ALA:HB1	1:B:383:ASP:HA	1.66	0.75
1:A:240:LEU:HD12	1:A:240:LEU:N	2.02	0.75
1:B:265:ALA:HB2	1:B:382:ILE:HG22	1.68	0.74
1:B:278:PRO:C	1:B:280:LEU:H	1.95	0.74
1:B:127:GLY:O	1:B:131:ALA:HB3	1.87	0.73
1:A:135:LYS:O	1:A:139:LEU:HG	1.89	0.73
1:B:220:PHE:O	1:B:221:GLY:C	2.29	0.73
1:B:274:LEU:HD11	1:B:281:ALA:H	1.54	0.72
1:B:155:TYR:N	1:B:156:PRO:HD2	2.05	0.72
1:B:210:CYS:O	1:B:215:LEU:HD11	1.89	0.72
1:B:376:ALA:C	1:B:377:ARG:HG3	2.14	0.71
1:B:161:PRO:HA	1:B:164:MET:HB2	1.73	0.71
1:A:397:ARG:CG	1:A:397:ARG:HH11	2.03	0.71
1:B:117:SER:HB2	1:B:118:PRO:HD2	1.73	0.71
1:B:378:LYS:HG2	1:B:378:LYS:O	1.90	0.70
1:B:381:ALA:HB3	1:B:407:THR:C	2.17	0.70
1:B:196:ILE:HG22	1:B:197:GLU:HG3	1.74	0.69
1:B:145:ILE:HD13	1:B:406:LEU:HD11	1.73	0.69
1:B:252:THR:HB	2:B:501:HEM:HBB2	1.74	0.69
1:B:265:ALA:HB2	1:B:382:ILE:CG2	2.23	0.69
1:B:384:ILE:CD1	1:B:403:PRO:O	2.37	0.69
1:A:151:LEU:HD11	1:A:371:MET:SD	2.34	0.68
1:B:384:ILE:CA	1:B:404:VAL:HA	2.23	0.68
1:B:215:LEU:O	1:B:216:ALA:C	2.36	0.68
1:A:20:HIS:CD2	1:A:51:ASP:OD1	2.46	0.68
1:B:156:PRO:HG2	1:B:157:LEU:H	1.59	0.68
1:B:267:PHE:N	1:B:268:PRO:HD3	2.10	0.67
1:A:19:PRO:HG3	1:A:44:ALA:O	1.94	0.66
1:B:285:PHE:HB2	1:B:372:LEU:HD11	1.77	0.66
1:B:280:LEU:O	1:B:282:ARG:N	2.29	0.66
1:B:157:LEU:HD11	1:B:175:LEU:HD11	1.77	0.66
1:B:382:ILE:O	1:B:383:ASP:CB	2.39	0.66
1:B:220:PHE:O	1:B:224:ILE:N	2.20	0.65
1:B:114:LYS:O	1:B:117:SER:HB3	1.95	0.65
1:B:373:SER:HB3	1:B:377:ARG:HH21	1.62	0.65
1:B:145:ILE:CD1	1:B:406:LEU:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASP:HB3	1:B:378:LYS:NZ	2.12	0.65
1:B:220:PHE:O	1:B:222:ALA:N	2.30	0.64
1:B:129:ALA:HB2	1:B:370:VAL:HG11	1.78	0.64
1:B:282:ARG:NH2	1:B:365:ARG:NH1	2.45	0.64
1:B:220:PHE:O	1:B:223:CYS:N	2.31	0.64
1:B:125:ARG:HB3	7:B:606:HOH:O	1.99	0.63
1:A:20:HIS:HD2	1:A:51:ASP:OD1	1.80	0.63
1:B:373:SER:HB3	1:B:377:ARG:NH2	2.14	0.63
1:A:173:HIS:C	1:A:176:PRO:HD2	2.24	0.62
1:B:111:VAL:O	1:B:115:VAL:HG23	1.98	0.62
1:B:146:ASP:O	1:B:148:ILE:N	2.30	0.62
1:A:21:LEU:HD13	1:A:41:LEU:HD23	1.82	0.62
1:B:35:TYR:HD2	1:B:38:GLN:OE1	1.82	0.61
1:B:282:ARG:HH22	1:B:365:ARG:NH1	1.96	0.61
1:B:77:SER:HB3	1:B:101:ASP:CG	2.25	0.61
1:A:240:LEU:N	1:A:240:LEU:CD1	2.62	0.61
1:B:212:ARG:N	1:B:213:PRO:HD2	2.14	0.61
1:B:381:ALA:CB	1:B:407:THR:CG2	2.79	0.61
1:A:320:LEU:HD12	1:A:321:MET:H	1.66	0.61
1:A:215:LEU:HD22	1:A:221:GLY:HA3	1.82	0.60
1:B:379:VAL:O	1:B:380:ALA:HB2	2.01	0.60
1:A:28:LEU:HD22	1:A:392:PHE:CD1	2.37	0.60
1:A:238:ALA:HB3	1:A:239:PRO:HD3	1.84	0.60
1:B:105:HIS:HE1	2:B:501:HEM:O1D	1.85	0.60
1:A:139:LEU:HD13	1:A:145:ILE:HD13	1.83	0.60
1:A:157:LEU:O	1:A:161:PRO:HD2	2.01	0.60
1:A:97:ILE:HD13	1:A:112:LEU:HD12	1.84	0.59
1:A:180:LEU:HD21	1:A:199:SER:HB2	1.84	0.59
1:B:155:TYR:N	1:B:156:PRO:CD	2.65	0.59
1:B:384:ILE:HG23	1:B:385:ASP:N	2.18	0.59
1:A:181:VAL:HG11	3:A:502:FIV:H3	1.83	0.59
1:B:268:PRO:HA	1:B:271:LEU:HD23	1.85	0.59
1:B:368:GLY:O	1:B:372:LEU:HD13	2.03	0.59
1:A:39:GLN:CA	1:A:42:ARG:HH21	2.13	0.58
1:B:379:VAL:HG23	1:B:407:THR:O	2.03	0.58
1:A:240:LEU:CD1	1:A:240:LEU:H	2.15	0.58
1:B:154:ALA:N	1:B:156:PRO:HD2	2.19	0.58
1:B:166:LEU:HD22	1:B:209:GLN:NE2	2.19	0.58
1:A:125:ARG:HH22	1:A:369:GLU:CD	2.11	0.57
1:B:381:ALA:O	1:B:407:THR:N	2.34	0.57
1:B:281:ALA:O	1:B:284:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:CG2	1:B:407:THR:O	2.53	0.57
1:B:34:PRO:O	1:B:38:GLN:HG3	2.05	0.57
1:A:196:ILE:O	1:A:199:SER:HB3	2.05	0.56
1:A:272:GLN:HE22	1:A:275:ARG:HH11	1.53	0.56
1:B:225:HIS:C	1:B:227:PHE:H	2.13	0.56
1:A:335:ASP:HB3	1:A:338:LEU:HG	1.86	0.56
1:B:366:LEU:C	1:B:368:GLY:H	2.14	0.56
1:B:97:ILE:HG23	1:B:98:LEU:H	1.71	0.56
1:A:268:PRO:O	1:A:271:LEU:HB3	2.04	0.56
1:B:295:VAL:HG11	1:B:298:PHE:CE1	2.40	0.56
1:B:384:ILE:HA	1:B:404:VAL:HG22	1.87	0.56
1:A:250:LEU:HD12	1:A:254:VAL:HG23	1.88	0.56
1:B:369:GLU:HG2	1:B:369:GLU:O	2.05	0.55
1:A:211:GLN:NE2	7:A:606:HOH:O	2.37	0.55
1:B:278:PRO:C	1:B:280:LEU:N	2.63	0.55
1:A:351:PHE:HB3	1:A:358:CYS:HB3	1.89	0.55
1:B:278:PRO:HB3	1:B:376:ALA:HB1	1.88	0.55
1:B:153:GLU:C	1:B:157:LEU:HD13	2.32	0.55
1:B:148:ILE:HG12	1:B:402:LEU:HB3	1.88	0.55
1:A:95:SER:HB3	1:A:98:LEU:H	1.72	0.55
1:B:219:GLY:O	1:B:220:PHE:HD1	1.89	0.55
1:B:124:ILE:HG13	1:B:125:ARG:N	2.22	0.54
1:B:378:LYS:O	1:B:378:LYS:CG	2.55	0.54
1:B:170:GLY:HA3	1:B:205:TYR:CZ	2.42	0.54
1:A:177:TYR:O	1:A:180:LEU:HB3	2.08	0.54
1:A:260:ALA:O	1:A:263:CYS:HB2	2.07	0.54
1:B:91:TRP:CE3	1:B:92:ARG:HB3	2.42	0.54
1:B:304:ARG:O	1:B:315:GLU:HA	2.08	0.54
1:A:139:LEU:HB3	1:A:145:ILE:HG21	1.89	0.54
1:B:128:PHE:CE1	1:B:159:VAL:HG13	2.43	0.54
1:B:274:LEU:HD12	1:B:280:LEU:HB2	1.90	0.53
1:B:265:ALA:CB	1:B:382:ILE:HG22	2.38	0.53
1:A:68:LEU:HD21	1:A:321:MET:HE1	1.90	0.53
1:B:107:ARG:HB3	1:B:108:PRO:CD	2.38	0.53
1:B:153:GLU:O	1:B:157:LEU:HD22	2.09	0.53
1:B:238:ALA:N	1:B:239:PRO:HD2	2.24	0.53
1:A:63:GLU:O	1:A:67:VAL:HG23	2.08	0.53
1:B:164:MET:HE2	1:B:246:LEU:HD21	1.89	0.53
1:B:285:PHE:HB2	1:B:372:LEU:CD1	2.38	0.53
1:A:97:ILE:HD12	1:A:109:ARG:HA	1.90	0.53
1:A:49:TYR:HE2	1:A:51:ASP:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HB2	1:A:99:GLU:HG3	1.91	0.53
1:B:379:VAL:CA	1:B:409:ALA:HB2	2.32	0.53
1:A:397:ARG:HH11	1:A:397:ARG:HG3	1.74	0.52
1:B:391:ARG:H	1:B:399:LEU:HA	1.73	0.52
1:B:356:HIS:HD1	2:B:501:HEM:CGD	2.23	0.52
1:A:320:LEU:HD12	1:A:321:MET:N	2.25	0.52
1:B:97:ILE:HG23	1:B:98:LEU:N	2.25	0.51
1:A:49:TYR:CE2	1:A:51:ASP:HA	2.45	0.51
1:B:261:VAL:C	1:B:263:CYS:H	2.17	0.51
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.74	0.51
1:B:219:GLY:C	1:B:220:PHE:CD1	2.89	0.51
1:B:149:ALA:HA	1:B:153:GLU:HB2	1.92	0.51
1:B:220:PHE:C	1:B:222:ALA:N	2.65	0.51
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.93	0.51
1:B:275:ARG:NH1	1:B:380:ALA:CB	2.74	0.51
1:B:152:ALA:O	1:B:156:PRO:HG3	2.10	0.51
1:B:307:GLU:HA	1:B:311:ALA:O	2.11	0.51
1:A:95:SER:HG	3:A:502:FIV:C11	2.24	0.51
1:B:153:GLU:O	1:B:157:LEU:HD13	2.10	0.51
1:B:373:SER:C	1:B:375:LEU:H	2.19	0.51
1:B:375:LEU:C	1:B:377:ARG:H	2.19	0.50
1:B:384:ILE:C	1:B:404:VAL:HA	2.35	0.50
1:A:374:ALA:O	1:A:375:LEU:C	2.51	0.50
1:B:148:ILE:HG12	1:B:402:LEU:CB	2.41	0.50
1:B:219:GLY:C	1:B:220:PHE:HD1	2.20	0.50
1:B:263:CYS:O	1:B:267:PHE:HD2	1.93	0.50
1:A:242:VAL:O	1:A:243:ARG:C	2.55	0.50
1:B:35:TYR:CD2	1:B:38:GLN:OE1	2.63	0.50
1:B:146:ASP:O	1:B:146:ASP:OD2	2.30	0.50
1:B:384:ILE:CG1	1:B:385:ASP:N	2.32	0.50
1:A:173:HIS:O	1:A:176:PRO:HD2	2.11	0.50
1:B:147:ALA:CB	1:B:402:LEU:O	2.52	0.49
1:B:173:HIS:ND1	1:B:201:PRO:O	2.45	0.49
1:B:281:ALA:O	1:B:372:LEU:HD23	2.08	0.49
1:B:357:MET:HG2	1:B:361:GLN:HE22	1.76	0.49
1:B:75:CYS:HB2	1:B:101:ASP:OD2	2.13	0.49
1:B:221:GLY:HA2	1:B:242:VAL:HG22	1.93	0.49
1:B:223:CYS:O	1:B:227:PHE:HD1	1.96	0.49
1:B:274:LEU:HD11	1:B:281:ALA:N	2.26	0.49
1:A:97:ILE:CD1	1:A:109:ARG:HA	2.43	0.49
1:A:148:ILE:HA	1:A:152:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:CYS:HA	2:A:501:HEM:CHA	2.43	0.49
1:B:215:LEU:O	1:B:216:ALA:O	2.30	0.49
1:A:180:LEU:CD2	1:A:199:SER:HB2	2.43	0.48
1:A:282:ARG:HD2	1:A:369:GLU:OE1	2.13	0.48
1:A:179:GLY:HA3	3:A:503:FIV:H4	1.96	0.48
1:A:115:VAL:HG21	1:A:224:ILE:HG13	1.96	0.48
1:B:109:ARG:NH1	1:B:357:MET:O	2.44	0.48
1:B:214:ASN:C	1:B:215:LEU:HG	2.39	0.48
1:B:264:LEU:HD21	1:B:339:TYR:HE2	1.78	0.48
1:B:300:ARG:HH22	2:B:501:HEM:CGA	2.26	0.48
1:A:176:PRO:HB2	1:A:202:HIS:CE1	2.49	0.47
1:B:274:LEU:CD1	1:B:281:ALA:H	2.23	0.47
1:B:285:PHE:HB2	1:B:372:LEU:HD21	1.96	0.47
1:A:95:SER:OG	3:A:502:FIV:C11	2.61	0.47
1:A:272:GLN:HE22	1:A:275:ARG:NH1	2.11	0.47
1:B:97:ILE:HD13	1:B:112:LEU:HD12	1.96	0.47
1:A:349:VAL:O	1:A:352:GLY:N	2.43	0.47
1:A:175:LEU:N	1:A:176:PRO:CD	2.78	0.47
1:B:267:PHE:N	1:B:268:PRO:CD	2.77	0.47
1:A:252:THR:HB	2:A:501:HEM:C3B	2.49	0.47
1:A:180:LEU:CD1	1:A:195:ALA:O	2.63	0.47
1:B:383:ASP:O	1:B:384:ILE:CG2	2.63	0.47
1:B:124:ILE:O	1:B:125:ARG:C	2.58	0.46
1:B:264:LEU:CD2	1:B:339:TYR:HE2	2.27	0.46
1:B:368:GLY:C	1:B:370:VAL:H	2.23	0.46
1:B:384:ILE:O	1:B:405:LYS:N	2.49	0.46
1:A:274:LEU:O	1:A:277:ASP:C	2.58	0.46
1:B:107:ARG:O	1:B:111:VAL:HG23	2.16	0.46
1:A:180:LEU:HD13	1:A:195:ALA:O	2.16	0.46
1:B:407:THR:HG23	1:B:408:PRO:HD2	1.97	0.46
1:A:263:CYS:HB3	1:A:339:TYR:CD2	2.51	0.46
1:B:59:ALA:HB1	1:B:325:SER:OG	2.16	0.46
1:B:366:LEU:C	1:B:368:GLY:N	2.74	0.46
1:B:77:SER:HB3	1:B:101:ASP:OD2	2.16	0.45
1:B:180:LEU:HD22	1:B:199:SER:HB2	1.98	0.45
1:B:333:TRP:HB2	1:B:336:PRO:HB3	1.98	0.45
1:B:364:ALA:C	1:B:366:LEU:H	2.24	0.45
1:A:302:THR:OG1	1:A:315:GLU:HA	2.17	0.45
1:A:42:ARG:HG2	1:A:60:ARG:HG2	1.98	0.45
1:B:156:PRO:CG	1:B:157:LEU:H	2.28	0.45
1:B:275:ARG:HH11	1:B:380:ALA:CB	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASP:H	1:B:404:VAL:CG1	2.30	0.45
1:B:190:GLU:HB3	1:B:191:LEU:HD12	1.97	0.45
1:B:358:CYS:SG	2:B:501:HEM:C1C	3.09	0.45
1:A:373:SER:C	1:A:377:ARG:HH21	2.24	0.45
1:B:382:ILE:HG22	1:B:383:ASP:N	2.32	0.45
1:B:175:LEU:HB2	1:B:176:PRO:HD3	1.99	0.44
1:B:249:GLY:HA2	2:B:501:HEM:C2C	2.53	0.44
1:B:382:ILE:CG2	1:B:404:VAL:HG11	2.37	0.44
1:A:248:ALA:HB2	3:A:502:FIV:C6	2.46	0.44
1:A:55:VAL:HG21	1:A:82:LEU:CD1	2.48	0.44
1:A:234:THR:HB	1:A:235:PRO:HD2	1.99	0.44
1:B:285:PHE:HB2	1:B:372:LEU:CD2	2.48	0.44
1:B:154:ALA:H	1:B:156:PRO:HD2	1.82	0.44
1:B:241:LEU:HA	1:B:241:LEU:HD23	1.85	0.44
1:B:225:HIS:C	1:B:227:PHE:N	2.75	0.44
1:A:132:ALA:O	1:A:136:VAL:HG23	2.18	0.44
1:B:139:LEU:HD21	1:B:150:ASP:O	2.18	0.44
1:B:224:ILE:O	1:B:224:ILE:HG22	2.17	0.44
1:B:139:LEU:HD22	1:B:150:ASP:HB3	2.00	0.43
1:B:135:LYS:HD2	1:B:135:LYS:HA	1.83	0.43
1:A:160:PHE:HB3	1:A:161:PRO:HD3	2.00	0.43
1:B:139:LEU:CD2	1:B:150:ASP:HB3	2.48	0.43
1:B:384:ILE:HG13	1:B:386:GLY:H	1.82	0.43
1:A:238:ALA:O	1:A:242:VAL:HG23	2.18	0.43
1:B:92:ARG:HG3	1:B:93:PRO:O	2.19	0.43
1:A:253:THR:O	1:A:254:VAL:C	2.60	0.43
1:B:24:ASP:HA	1:B:25:PRO:HD3	1.82	0.43
1:B:164:MET:HE2	1:B:246:LEU:CD2	2.48	0.43
1:A:297:THR:HB	1:A:320:LEU:HD11	2.01	0.43
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.75	0.43
1:A:297:THR:HA	1:A:321:MET:O	2.18	0.43
1:A:181:VAL:CG1	3:A:502:FIV:H3	2.48	0.43
1:B:67:VAL:HG13	1:B:74:PHE:CG	2.54	0.43
1:B:202:HIS:O	1:B:206:VAL:HG23	2.19	0.43
1:B:295:VAL:HG11	1:B:298:PHE:HE1	1.84	0.43
1:A:55:VAL:HG21	1:A:82:LEU:HD11	2.00	0.42
1:B:115:VAL:HG11	1:B:224:ILE:CG1	2.49	0.42
1:B:146:ASP:C	1:B:148:ILE:H	2.21	0.42
1:A:357:MET:O	1:A:358:CYS:C	2.61	0.42
1:B:27:SER:O	1:B:31:PHE:CD1	2.72	0.42
1:B:383:ASP:O	1:B:383:ASP:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:HG3	1:A:339:TYR:CD1	2.53	0.42
1:A:397:ARG:CG	1:A:397:ARG:NH1	2.71	0.42
1:B:30:PHE:HE1	1:B:37:ASP:HB2	1.84	0.42
1:B:368:GLY:O	1:B:370:VAL:N	2.52	0.42
1:A:88:GLU:O	1:A:90:PRO:HD3	2.19	0.42
1:B:117:SER:CB	1:B:118:PRO:HD2	2.42	0.42
1:A:147:ALA:O	1:A:151:LEU:HB3	2.20	0.42
1:B:133:ASP:HB3	1:B:378:LYS:HZ2	1.81	0.42
1:B:224:ILE:O	1:B:224:ILE:CG2	2.67	0.42
1:B:280:LEU:O	1:B:281:ALA:C	2.63	0.42
1:B:368:GLY:C	1:B:370:VAL:N	2.77	0.42
1:B:379:VAL:HG22	1:B:381:ALA:H	1.83	0.42
1:A:92:ARG:HD2	1:A:243:ARG:NH2	2.34	0.42
1:B:383:ASP:H	1:B:404:VAL:HG13	1.84	0.42
1:A:35:TYR:N	1:A:36:PRO:HD2	2.34	0.42
1:A:322:PHE:O	1:A:325:SER:HB3	2.20	0.42
1:B:211:GLN:HA	1:B:211:GLN:NE2	2.35	0.42
1:B:278:PRO:O	1:B:280:LEU:N	2.53	0.42
1:A:97:ILE:HG12	2:A:501:HEM:CGD	2.50	0.42
1:A:298:PHE:O	1:A:321:MET:HB2	2.20	0.42
1:B:379:VAL:CG2	1:B:380:ALA:N	2.42	0.42
1:A:236:ASP:O	1:A:240:LEU:CD1	2.62	0.41
1:A:296:GLN:CG	1:A:397:ARG:HB2	2.50	0.41
1:B:299:PHE:CD1	1:B:299:PHE:N	2.89	0.41
1:B:111:VAL:HG13	1:B:227:PHE:CD2	2.55	0.41
1:B:103:PRO:O	1:B:104:ALA:C	2.63	0.41
1:B:364:ALA:C	1:B:366:LEU:N	2.78	0.41
1:B:128:PHE:CD1	1:B:159:VAL:HG13	2.55	0.41
1:B:366:LEU:O	1:B:370:VAL:HG22	2.21	0.41
1:B:145:ILE:HD12	1:B:147:ALA:HA	2.02	0.41
1:B:189:ASN:OD1	1:B:189:ASN:C	2.63	0.41
1:B:268:PRO:O	1:B:272:GLN:HG2	2.20	0.41
1:B:360:GLY:HA3	2:B:501:HEM:C3C	2.56	0.41
1:A:49:TYR:OH	1:A:54:ASN:ND2	2.38	0.41
1:B:28:LEU:O	1:B:32:ASP:HB2	2.20	0.41
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.90	0.41
1:A:170:GLY:HA3	1:A:205:TYR:CE1	2.56	0.41
1:B:244:SER:CB	3:B:502:FIV:H2	2.27	0.41
1:A:20:HIS:HB3	1:A:51:ASP:CG	2.46	0.41
1:A:286:GLU:OE2	1:A:365:ARG:NE	2.54	0.41
1:B:91:TRP:CZ3	1:B:92:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:VAL:HG21	1:B:247:SER:HB3	2.02	0.41
1:B:191:LEU:HD12	1:B:191:LEU:N	2.36	0.41
1:B:222:ALA:O	1:B:223:CYS:C	2.63	0.41
1:B:275:ARG:NH1	1:B:380:ALA:HB3	2.36	0.41
2:B:501:HEM:C3D	3:B:502:FIV:H8	2.56	0.41
1:A:233:ILE:HD12	1:A:238:ALA:HA	2.02	0.41
1:B:264:LEU:C	1:B:266:ARG:H	2.29	0.41
1:A:20:HIS:O	1:A:21:LEU:HG	2.22	0.40
1:B:23:ILE:HG22	1:B:24:ASP:N	2.36	0.40
1:B:223:CYS:O	1:B:227:PHE:CD1	2.75	0.40
1:B:237:GLU:C	1:B:239:PRO:HD2	2.46	0.40
1:B:383:ASP:O	1:B:384:ILE:HG22	2.21	0.40
1:B:116:LEU:HD12	1:B:359:VAL:HG22	2.03	0.40
1:B:404:VAL:HG12	1:B:405:LYS:N	2.36	0.40
1:A:155:TYR:O	1:A:159:VAL:HG22	2.22	0.40
1:A:190:GLU:O	1:A:191:LEU:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/410 (96%)	347 (88%)	42 (11%)	3 (1%)	16	50
1	B	391/410 (95%)	299 (76%)	66 (17%)	26 (7%)	1	5
All	All	783/820 (96%)	646 (82%)	108 (14%)	29 (4%)	2	15

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	ALA
1	B	377	ARG

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Mol	Chain	Res	Type
1	B	380	ALA
1	B	383	ASP
1	B	384	ILE
1	B	385	ASP
1	B	125	ARG
1	B	157	LEU
1	B	221	GLY
1	B	279	THR
1	B	379	VAL
1	A	361	GLN
1	B	309	GLY
1	B	331	ARG
1	A	358	CYS
1	B	171	ARG
1	B	262	TYR
1	B	367	GLU
1	B	90	PRO
1	B	156	PRO
1	B	369	GLU
1	B	394	ASN
1	B	216	ALA
1	B	271	LEU
1	B	376	ALA
1	A	64	VAL
1	B	36	PRO
1	B	118	PRO
1	B	294	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	320/334 (96%)	310 (97%)	10 (3%)	35	68
1	B	319/334 (96%)	305 (96%)	14 (4%)	25	60
All	All	639/668 (96%)	615 (96%)	24 (4%)	29	63

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ILE
1	A	166	LEU
1	A	169	GLU
1	A	196	ILE
1	A	250	LEU
1	A	298	PHE
1	A	338	LEU
1	A	344	LYS
1	A	372	LEU
1	A	397	ARG
1	B	64	VAL
1	B	72	THR
1	B	159	VAL
1	B	169	GLU
1	B	180	LEU
1	B	196	ILE
1	B	230	THR
1	B	245	LEU
1	B	301	THR
1	B	306	VAL
1	B	323	LEU
1	B	341	ILE
1	B	375	LEU
1	B	395	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	65	HIS
1	A	168	GLN
1	A	203	GLN
1	A	211	GLN
1	A	214	ASN
1	A	272	GLN
1	A	283	ASN
1	A	296	GLN
1	B	65	HIS
1	B	69	ASN
1	B	105	HIS
1	B	209	GLN

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Mol	Chain	Res	Type
1	B	211	GLN
1	B	225	HIS
1	B	255	ASN
1	B	272	GLN
1	B	283	ASN
1	B	296	GLN

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 ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
5	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.65	0
3	FIV	A	502	-	14,14,14	1.31	0	19,19,19	1.18	2 (10%)
2	HEM	B	501	1	50,50,50	1.70	6 (12%)	67,82,82	1.22	6 (8%)
4	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.24	0
3	FIV	B	502	-	14,14,14	1.25	1 (7%)	19,19,19	1.39	4 (21%)
4	SO4	A	505	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	501	1	50,50,50	1.72	7 (14%)	67,82,82	1.13	5 (7%)
3	FIV	A	503	-	14,14,14	1.11	0	19,19,19	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	506	-	-	2/4/4/4	-
3	FIV	A	502	-	-	0/4/4/4	0/2/2/2
2	HEM	B	501	1	-	4/14/54/54	-
3	FIV	B	502	-	-	1/4/4/4	0/2/2/2
2	HEM	A	501	1	-	6/14/54/54	-
3	FIV	A	503	-	-	0/4/4/4	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3D-C2D	7.89	1.53	1.36
2	A	501	HEM	C3D-C2D	6.91	1.51	1.36
2	A	501	HEM	FE-NB	4.66	2.09	1.94
2	A	501	HEM	CAB-C3B	3.23	1.56	1.47
2	B	501	HEM	FE-NC	2.91	2.04	1.95
2	A	501	HEM	CAC-C3C	2.91	1.55	1.47
2	B	501	HEM	FE-ND	2.74	2.03	1.94
2	B	501	HEM	CAB-C3B	2.70	1.54	1.47
2	B	501	HEM	CAC-C3C	2.62	1.54	1.47
2	A	501	HEM	FE-NC	2.58	2.03	1.95
3	B	502	FIV	C5-C7	2.38	1.41	1.37
2	B	501	HEM	C2A-C3A	-2.23	1.33	1.38
2	A	501	HEM	CMB-C2B	2.16	1.55	1.50
2	A	501	HEM	CMC-C2C	2.08	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	5.25	111.42	105.21
2	A	501	HEM	C4D-ND-C1D	3.89	109.81	105.21
2	A	501	HEM	CBD-CAD-C3D	-3.37	103.22	112.53
2	B	501	HEM	C3B-C2B-C1B	2.68	108.43	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	O2D-CGD-CBD	2.37	121.48	114.00
2	B	501	HEM	CMD-C2D-C1D	2.34	128.69	125.03
3	B	502	FIV	C4-C1-C2	2.33	122.91	118.91
3	B	502	FIV	C8-C7-C11	-2.23	115.96	120.37
2	A	501	HEM	O2D-CGD-CBD	2.20	120.94	114.00
2	A	501	HEM	C4C-C3C-C2C	2.15	108.68	106.81
3	B	502	FIV	C5-C7-C11	2.13	124.94	120.59
3	A	502	FIV	C4-C1-C2	2.10	122.51	118.91
3	B	502	FIV	C4-C1-C3	-2.09	118.23	123.01
2	A	501	HEM	O1D-CGD-CBD	-2.07	116.52	123.09
2	B	501	HEM	O1D-CGD-CBD	-2.04	116.61	123.09
3	A	502	FIV	C4-C1-C3	-2.04	118.36	123.01
2	B	501	HEM	CAA-CBA-CGA	-2.04	108.26	113.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

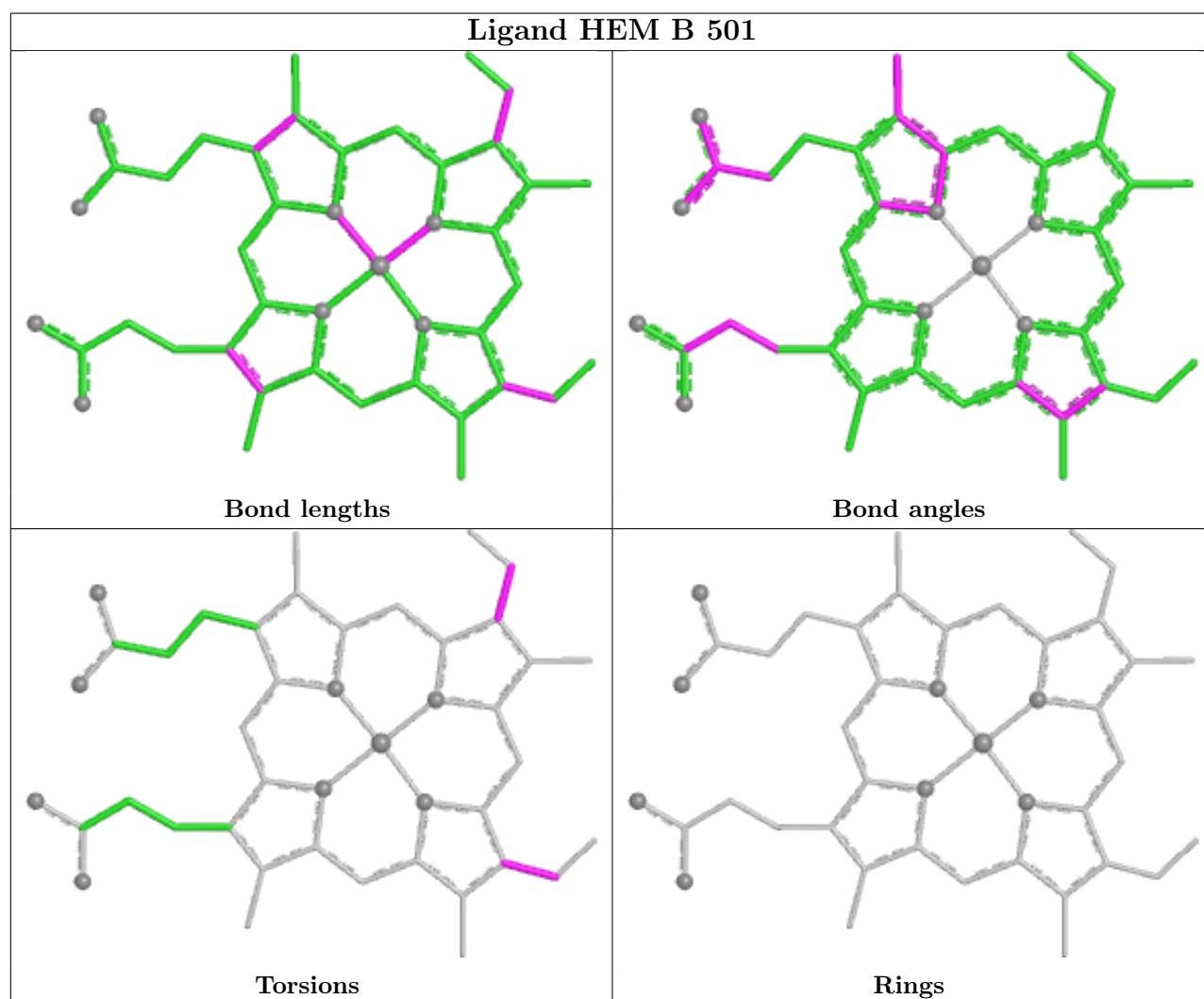
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB
5	A	506	GOL	O1-C1-C2-C3
2	A	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C2C-C3C-CAC-CBC
5	A	506	GOL	O1-C1-C2-O2
2	A	501	HEM	C4C-C3C-CAC-CBC
2	A	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4C-C3C-CAC-CBC
2	A	501	HEM	CAA-CBA-CGA-O1A
3	B	502	FIV	O2-C11-C7-C8

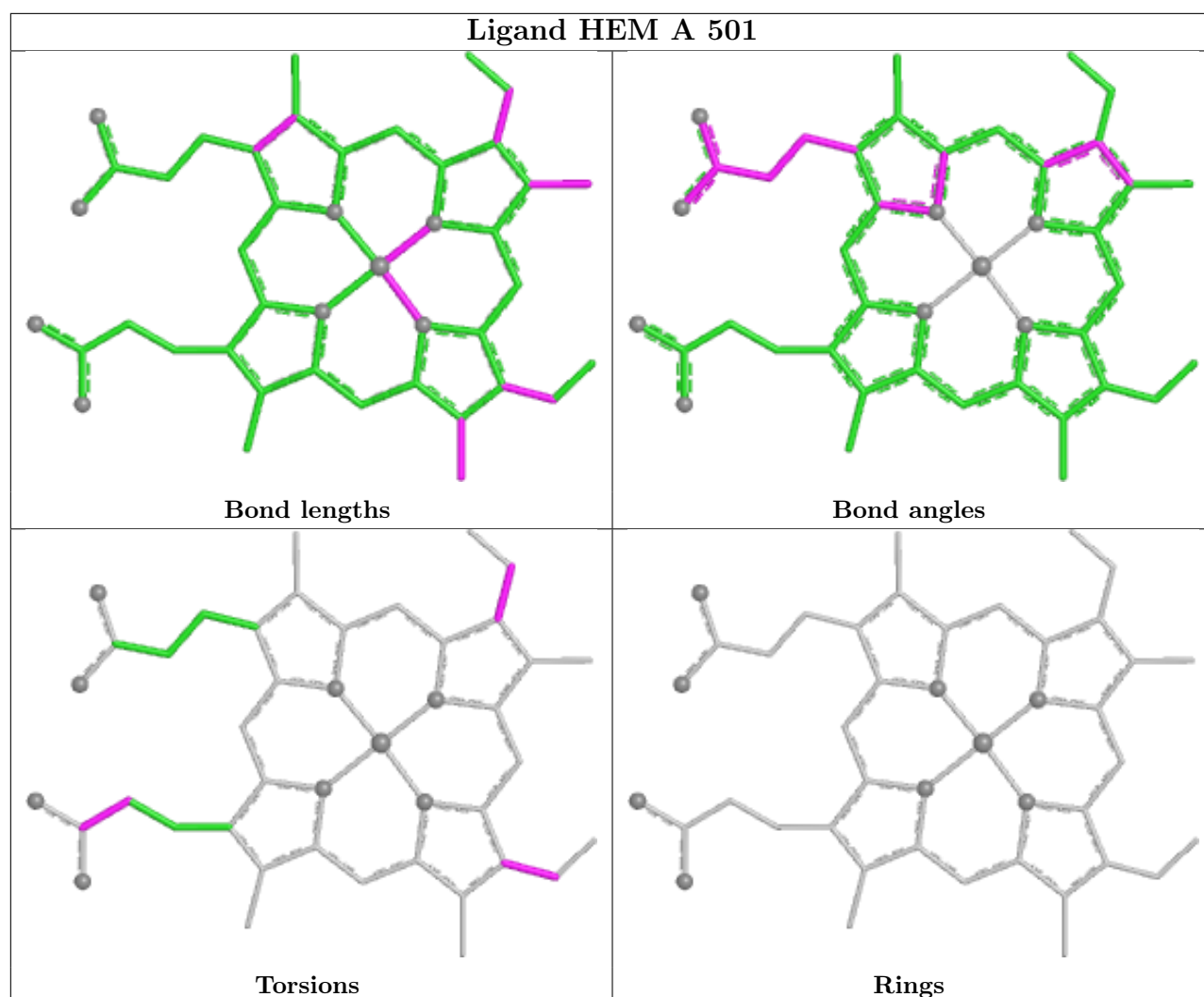
There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	FIV	6	0
2	B	501	HEM	8	0
3	B	502	FIV	4	0
2	A	501	HEM	3	0
3	A	503	FIV	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	393/410 (95%)	-0.24	1 (0%) 90 79	34, 51, 69, 80	1 (0%)
1	B	393/410 (95%)	0.46	31 (7%) 18 10	30, 69, 100, 110	0
All	All	786/820 (95%)	0.11	32 (4%) 41 23	30, 57, 97, 110	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	PHE	4.9
1	B	380	ALA	4.4
1	B	271	LEU	3.7
1	B	143	GLY	3.6
1	B	133	ASP	3.6
1	B	383	ASP	3.2
1	B	262	TYR	3.1
1	B	382	ILE	2.9
1	B	145	ILE	2.8
1	B	91	TRP	2.7
1	B	339	TYR	2.7
1	B	135	LYS	2.6
1	B	17	THR	2.5
1	B	144	CYS	2.5
1	B	385	ASP	2.4
1	B	376	ALA	2.4
1	B	129	ALA	2.4
1	B	96	LEU	2.3
1	B	130	ALA	2.3
1	B	275	ARG	2.3
1	A	334	SER	2.2
1	B	140	LEU	2.2
1	B	196	ILE	2.2
1	B	392	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	261	VAL	2.1
1	B	379	VAL	2.1
1	B	282	ARG	2.1
1	B	384	ILE	2.1
1	B	264	LEU	2.1
1	B	221	GLY	2.1
1	B	148	ILE	2.0
1	B	151	LEU	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](#)

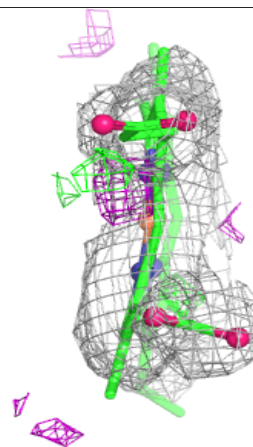
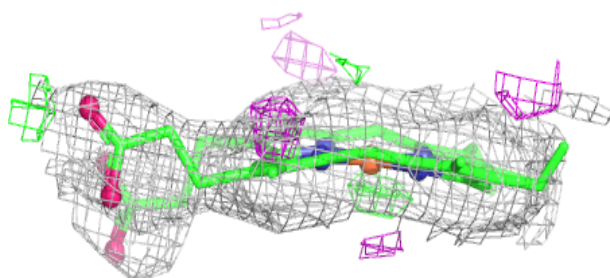
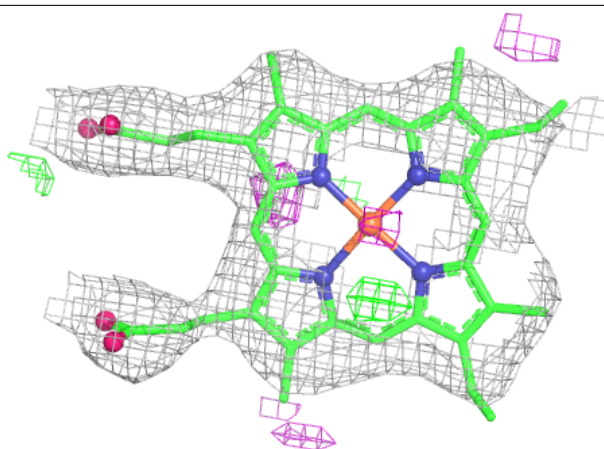
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	FIV	A	503	13/13	0.85	0.27	100,103,105,106	0
3	FIV	B	502	13/13	0.89	0.14	54,56,58,58	0
6	CL	A	507	1/1	0.91	0.11	71,71,71,71	0
4	SO4	A	504	5/5	0.92	0.10	90,90,90,90	0
4	SO4	A	505	5/5	0.94	0.10	77,79,79,79	0
4	SO4	B	503	5/5	0.94	0.08	80,80,80,81	0
5	GOL	A	506	6/6	0.94	0.09	58,61,62,65	0
3	FIV	A	502	13/13	0.94	0.10	45,48,55,56	0
2	HEM	B	501	43/43	0.96	0.12	49,56,59,60	0
2	HEM	A	501	43/43	0.98	0.07	31,36,41,43	0

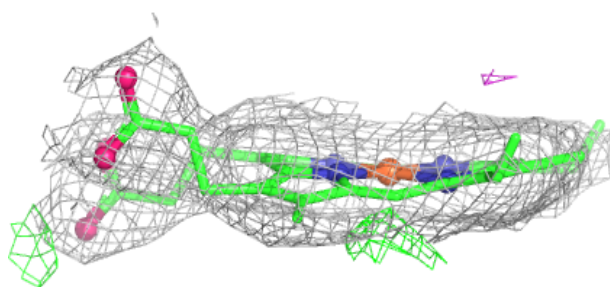
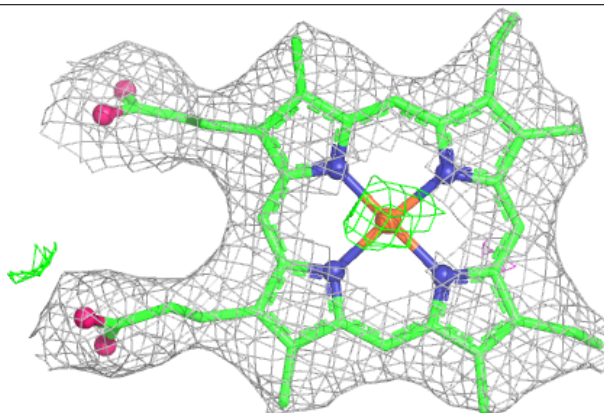
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM 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 HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.