Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:36 AM EDT

PDB ID	:	3K9V
Title	:	Crystal structure of rat mitochondrial P450 24A1 S57D in complex with CHAPS
Authors	:	Annalora, A.J.; Goodin, D.B.; Hong, W.; Zhang, Q.; Johnson, E.F.; Stout, C.D.
Deposited on	:	2009-10-16
Resolution	:	2.50 Å(reported)

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

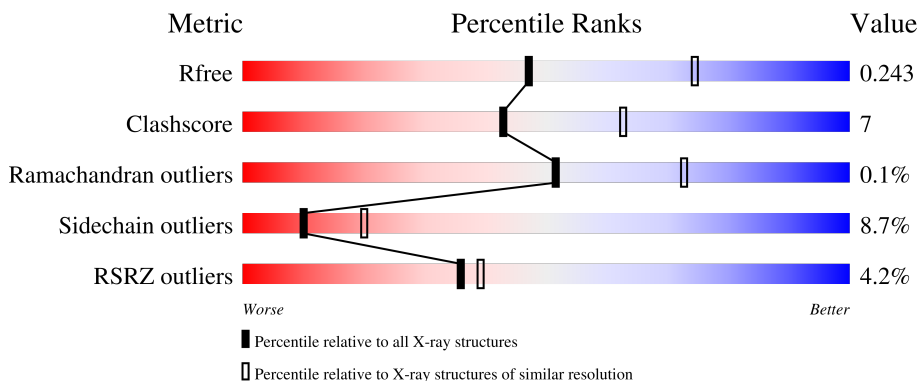|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
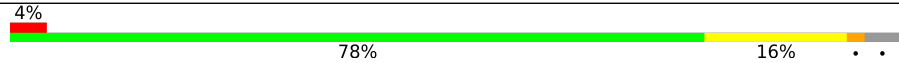*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.243
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		8.7%
RSRZ outliers		4.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	482	5% 75% 19% • •
1	B	482	4% 78% 16% • •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8157 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 1,25-dihydroxyvitamin D(3) 24-hydroxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3797	2430	662	684	21			
1	B	464	Total	C	N	O	S	0	0	0
			3797	2430	662	684	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP Q09128
A	57	ASP	SER	engineered mutation	UNP Q09128
B	33	MET	-	expression tag	UNP Q09128
B	57	ASP	SER	engineered mutation	UNP Q09128

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: $C_{32}H_{58}N_2O_7S$).
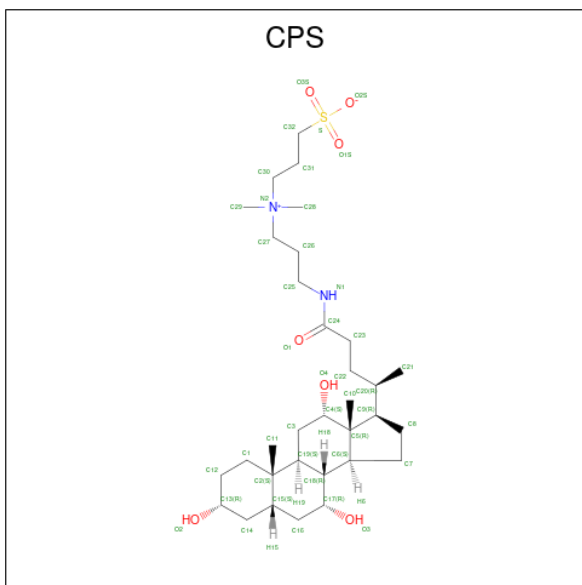
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	A	1	Total	C	N	O		0	0
			32	27	1	4			
3	A	1	Total	C	N	O		0	0
			32	27	1	4			
3	B	1	Total	C	N	O	S	0	0
			42	32	2	7	1		
3	B	1	Total	C	N	O		0	0
			32	27	1	4			
3	B	1	Total	C	N	O		0	0
			32	27	1	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	147	Total	O	0	0
			147	147		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	118	Total O 118 118		0	0

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: 1,25-dihydroxyvitamin D(3) 24-hydroxylase, mitochondrial
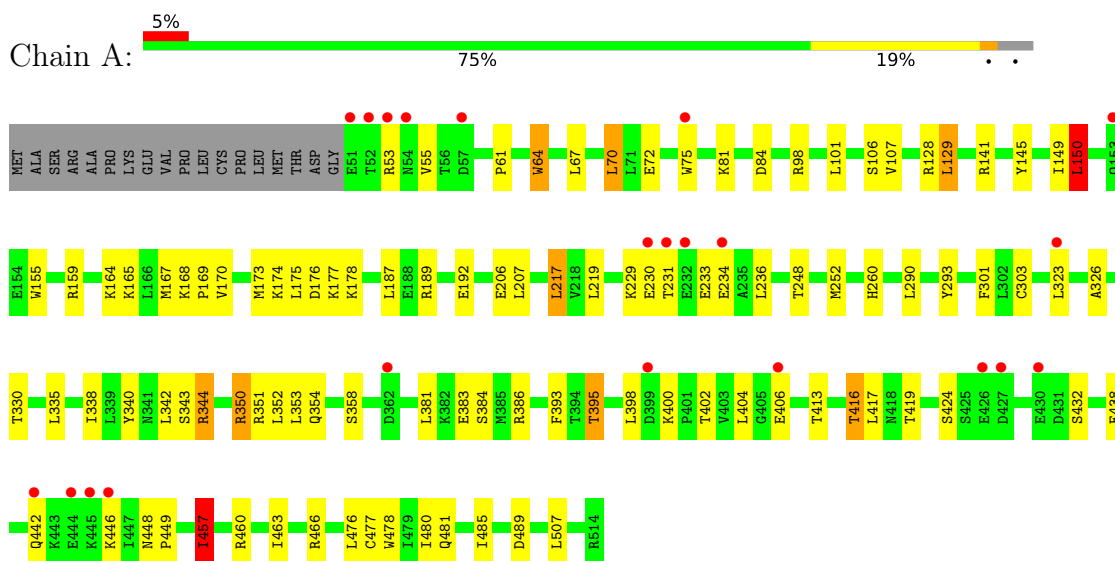
• Molecule 1: 1,25-dihydroxyvitamin D(3) 24-hydroxylase, mitochondrial
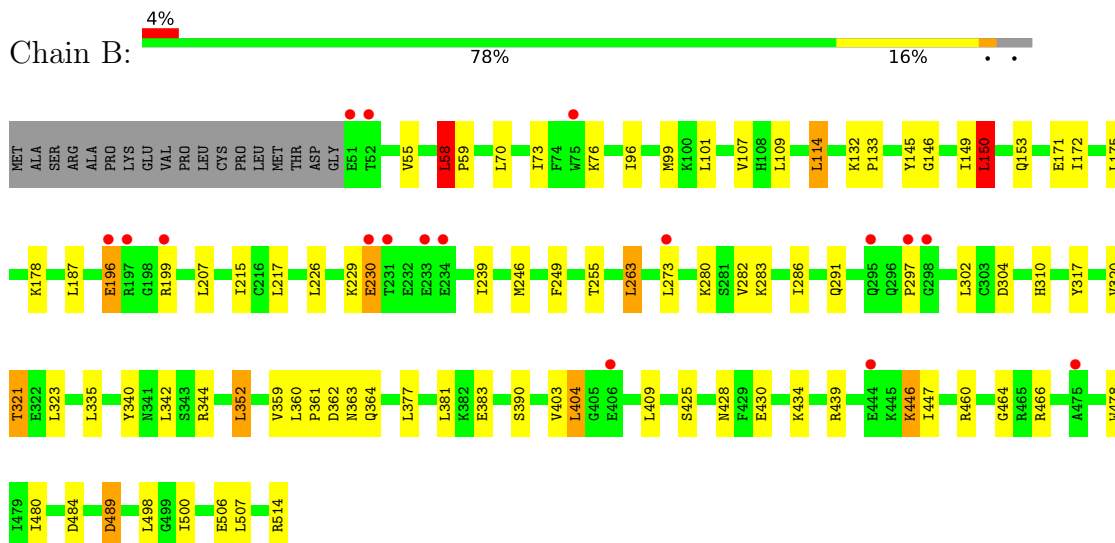
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.61Å 81.65Å 108.70Å 90.00° 122.89° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.50) 97.4 (30.00-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	6.04 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072, CNS 1.0	Depositor
R, R_{free}	0.206 , 0.252 0.199 , 0.243	Depositor DCC
R_{free} test set	2287 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å²)	37.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.36 , 49.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8157	wwPDB-VP
Average B, all atoms (Å²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CPS

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	0.47	0/3885	0.62	2/5252 (0.0%)
1	B	0.46	0/3885	0.61	3/5252 (0.1%)
All	All	0.47	0/7770	0.62	5/10504 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	457	ILE	CB-CA-C	-5.26	101.08	111.60
1	B	263	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	150	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	58	LEU	CA-CB-CG	5.01	126.81	115.30

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	3797	0	3853	56	0
1	B	3797	0	3853	51	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	106	0	146	1	0
3	B	106	0	146	3	0
4	A	147	0	0	2	0
4	B	118	0	0	1	0
All	All	8157	0	8058	109	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 (109) 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:317:TYR:O	1:B:321:THR:HG23	1.70	0.91
1:B:229:LYS:O	1:B:230:GLU:HB2	1.72	0.87
1:A:293:TYR:HB2	1:A:303:CYS:SG	2.18	0.84
1:A:145:TYR:HB2	1:A:150:LEU:HD13	1.57	0.83
1:A:466:ARG:HH11	1:A:466:ARG:HG3	1.41	0.83
1:B:404:LEU:HD21	1:B:409:LEU:HD12	1.63	0.80
1:B:145:TYR:HB2	1:B:150:LEU:HD13	1.64	0.80
1:A:383:GLU:CD	1:A:386:ARG:HH12	1.84	0.80
1:B:430:GLU:O	1:B:439:ARG:NH2	2.15	0.79
1:A:344:ARG:NH2	1:A:489:ASP:O	2.19	0.74
1:B:282:VAL:HG11	1:B:321:THR:HG22	1.69	0.73
1:A:460:ARG:HD2	2:A:520:HEM:O2D	1.89	0.72
1:A:417:LEU:CD1	1:A:457:ILE:HD11	2.20	0.71
1:A:187:LEU:HD22	1:A:478:TRP:HE3	1.56	0.71
1:B:460:ARG:HD2	2:B:520:HEM:O2D	1.91	0.70
1:A:460:ARG:O	1:A:460:ARG:HG3	1.92	0.69
1:B:484:ASP:HB2	1:B:514:ARG:HH12	1.60	0.67
1:A:164:LYS:O	1:A:168:LYS:HG3	1.95	0.67
1:B:460:ARG:O	1:B:460:ARG:HG3	1.95	0.66
1:A:229:LYS:O	1:A:230:GLU:HB2	1.96	0.65
1:A:466:ARG:HG3	1:A:466:ARG:NH1	2.08	0.64
1:A:129:LEU:HB2	1:A:395:THR:HG21	1.79	0.64
1:A:383:GLU:CD	1:A:386:ARG:NH1	2.51	0.64
1:A:170:VAL:HA	1:A:173:MET:HE2	1.83	0.61
1:B:99:MET:HE1	1:B:101:LEU:HD21	1.82	0.60
1:A:64:TRP:HZ3	1:A:72:GLU:OE1	1.84	0.60
1:B:361:PRO:O	1:B:362:ASP:HB3	2.02	0.59
1:B:226:LEU:HD11	1:B:239:ILE:HD11	1.86	0.58
1:B:446:LYS:HE3	1:B:447:ILE:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:HD12	1:A:457:ILE:HD11	1.86	0.58
1:A:383:GLU:OE1	1:A:386:ARG:NH1	2.38	0.57
1:B:484:ASP:HB2	1:B:514:ARG:NH1	2.18	0.57
1:B:446:LYS:HE3	1:B:447:ILE:N	2.20	0.56
1:B:229:LYS:O	1:B:230:GLU:CB	2.48	0.55
1:B:352:LEU:HD21	1:B:377:LEU:HD13	1.88	0.55
1:B:489:ASP:C	1:B:489:ASP:OD1	2.45	0.54
1:B:145:TYR:HB3	1:B:149:ILE:HG13	1.90	0.54
1:A:170:VAL:HA	1:A:173:MET:CE	2.38	0.53
1:A:398:LEU:HD12	1:A:413:THR:HB	1.89	0.53
1:A:448:ASN:HD22	1:A:449:PRO:HD2	1.73	0.53
1:B:352:LEU:HD13	1:B:480:ILE:HG13	1.88	0.53
1:A:81:LYS:HE2	1:A:84:ASP:OD2	2.08	0.53
1:A:398:LEU:HD22	1:A:402:THR:HG21	1.91	0.52
1:B:187:LEU:HD22	1:B:478:TRP:HE3	1.74	0.52
1:A:189:ARG:NH1	1:A:206:GLU:OE1	2.43	0.52
1:A:70:LEU:HD13	1:A:101:LEU:HB3	1.92	0.51
1:A:169:PRO:O	1:A:173:MET:HG3	2.11	0.51
1:A:67:LEU:O	1:A:70:LEU:HB2	2.11	0.50
1:B:178:LYS:NZ	4:B:594:HOH:O	2.43	0.50
1:A:150:LEU:HB3	1:A:155:TRP:HB2	1.93	0.50
1:A:176:ASP:OD2	1:A:177:LYS:N	2.45	0.50
1:B:484:ASP:CB	1:B:514:ARG:HH12	2.25	0.49
1:B:340:TYR:HB2	1:B:507:LEU:HD21	1.95	0.48
1:B:464:GLY:HA3	2:B:520:HEM:C3C	2.48	0.48
1:A:165:LYS:HD2	1:A:301:PHE:HB2	1.95	0.47
1:B:196:GLU:CD	1:B:196:GLU:H	2.16	0.47
1:B:425:SER:OG	1:B:428:ASN:OD1	2.31	0.47
1:A:340:TYR:HB2	1:A:507:LEU:HD21	1.97	0.47
1:A:338:ILE:HD13	1:A:384:SER:HB2	1.96	0.47
1:B:145:TYR:CB	1:B:150:LEU:HD13	2.40	0.47
1:A:424:SER:HA	1:A:432:SER:HB2	1.98	0.46
1:A:231:THR:O	1:A:234:GLU:HG2	2.15	0.46
1:B:187:LEU:HD22	1:B:478:TRP:CE3	2.50	0.46
1:A:419:THR:HG23	4:A:533:HOH:O	2.16	0.45
1:A:129:LEU:HG	3:A:601:CPS:H21B	1.98	0.45
1:A:393:PHE:HA	1:A:419:THR:HG22	1.98	0.45
1:B:146:GLY:C	1:B:150:LEU:HD22	2.37	0.45
1:B:390:SER:HB3	1:B:500:ILE:HD11	1.98	0.45
1:B:70:LEU:HD13	1:B:101:LEU:HB3	2.00	0.44
1:A:343:SER:HB3	1:A:485:ILE:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:701:CPS:H4	3:B:701:CPS:H21A	2.00	0.44
1:A:476:LEU:HD23	1:A:476:LEU:HA	1.61	0.44
1:A:383:GLU:OE1	1:A:383:GLU:HA	2.17	0.44
1:A:477:CYS:O	1:A:481:GLN:HB2	2.17	0.44
1:B:286:ILE:HD11	1:B:320:VAL:HB	2.00	0.43
1:B:383:GLU:HA	1:B:383:GLU:OE1	2.17	0.43
1:A:145:TYR:HB3	1:A:149:ILE:HG13	2.00	0.43
3:B:702:CPS:H22A	3:B:702:CPS:H8A	1.79	0.43
1:A:128:ARG:HG2	1:A:395:THR:O	2.19	0.43
1:A:178:LYS:HB3	1:A:217:LEU:HD13	2.01	0.43
1:A:252:MET:HG2	1:A:260:HIS:CD2	2.53	0.43
1:B:146:GLY:O	1:B:150:LEU:HD22	2.19	0.43
1:B:187:LEU:HD21	1:B:478:TRP:HB3	2.00	0.43
1:B:73:ILE:HD13	1:B:73:ILE:HA	1.95	0.42
1:B:96:ILE:HB	1:B:114:LEU:HD21	2.02	0.42
1:B:58:LEU:HD12	1:B:59:PRO:HD2	2.02	0.42
1:B:246:MET:HE2	3:B:700:CPS:H22	2.00	0.42
1:A:167:MET:SD	1:A:466:ARG:HG2	2.60	0.42
1:A:438:GLU:H	1:A:438:GLU:CD	2.23	0.42
1:B:145:TYR:HB2	1:B:150:LEU:CD1	2.43	0.42
1:B:362:ASP:CG	1:B:363:ASN:N	2.73	0.42
1:B:297:PRO:O	1:B:304:ASP:OD1	2.37	0.42
1:B:187:LEU:CD2	1:B:478:TRP:HB3	2.49	0.41
1:B:404:LEU:HD21	1:B:409:LEU:CD1	2.40	0.41
1:A:159:ARG:HD2	1:A:463:ILE:HD12	2.02	0.41
1:B:132:LYS:N	1:B:133:PRO:CD	2.83	0.41
1:B:359:VAL:HG23	1:B:360:LEU:HG	2.03	0.41
1:B:498:LEU:C	1:B:500:ILE:H	2.24	0.41
1:A:350:ARG:NH2	1:A:354:GLN:OE1	2.53	0.41
1:A:106:SER:OG	1:A:416:THR:HG23	2.21	0.41
1:A:229:LYS:O	1:A:230:GLU:CB	2.65	0.41
1:A:233:GLU:HG3	1:A:236:LEU:HD22	2.02	0.41
1:A:338:ILE:HG12	1:A:476:LEU:HD11	2.03	0.41
1:B:283:LYS:HG2	1:B:317:TYR:CE1	2.56	0.41
1:A:164:LYS:HD3	1:A:164:LYS:HA	1.51	0.40
1:A:326:ALA:O	1:A:330:THR:HG22	2.22	0.40
1:A:61:PRO:HB2	4:A:569:HOH:O	2.20	0.40
1:B:172:ILE:HD13	1:B:466:ARG:HB3	2.04	0.40
1:B:360:LEU:HB3	1:B:364:GLN:HB3	2.04	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	462/482 (96%)	446 (96%)	16 (4%)	0	100	100
1	B	462/482 (96%)	448 (97%)	13 (3%)	1 (0%)	47	68
All	All	924/964 (96%)	894 (97%)	29 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	GLU

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	418/433 (96%)	381 (91%)	37 (9%)	9	19
1	B	418/433 (96%)	382 (91%)	36 (9%)	10	20
All	All	836/866 (96%)	763 (91%)	73 (9%)	10	20

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	55	VAL
1	A	64	TRP
1	A	70	LEU
1	A	75	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	98	ARG
1	A	107	VAL
1	A	129	LEU
1	A	141	ARG
1	A	150	LEU
1	A	174	LYS
1	A	175	LEU
1	A	192	GLU
1	A	207	LEU
1	A	217	LEU
1	A	219	LEU
1	A	248	THR
1	A	290	LEU
1	A	323	LEU
1	A	335	LEU
1	A	342	LEU
1	A	344	ARG
1	A	350	ARG
1	A	351	ARG
1	A	352	LEU
1	A	353	LEU
1	A	358	SER
1	A	381	LEU
1	A	395	THR
1	A	400	LYS
1	A	404	LEU
1	A	406	GLU
1	A	416	THR
1	A	442	GLN
1	A	446	LYS
1	A	457	ILE
1	A	480	ILE
1	B	55	VAL
1	B	58	LEU
1	B	76	LYS
1	B	107	VAL
1	B	109	LEU
1	B	114	LEU
1	B	150	LEU
1	B	153	GLN
1	B	171	GLU
1	B	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	196	GLU
1	B	199	ARG
1	B	207	LEU
1	B	215	ILE
1	B	217	LEU
1	B	249	PHE
1	B	255	THR
1	B	263	LEU
1	B	273	LEU
1	B	280	LYS
1	B	291	GLN
1	B	302	LEU
1	B	310	HIS
1	B	321	THR
1	B	323	LEU
1	B	335	LEU
1	B	342	LEU
1	B	344	ARG
1	B	352	LEU
1	B	381	LEU
1	B	403	VAL
1	B	404	LEU
1	B	434	LYS
1	B	446	LYS
1	B	489	ASP
1	B	506	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	373	ASN
1	A	428	ASN
1	A	448	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

8 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	CPS	A	602	-	35,35,45	1.03	1 (2%)	54,54,70	1.60	7 (12%)
2	HEM	B	520	1	41,50,50	2.92	19 (46%)	45,82,82	1.99	10 (22%)
3	CPS	A	601	-	35,35,45	1.07	1 (2%)	54,54,70	1.24	7 (12%)
3	CPS	B	701	-	35,35,45	1.08	1 (2%)	54,54,70	1.42	9 (16%)
3	CPS	A	600	-	45,45,45	2.36	5 (11%)	69,70,70	1.51	13 (18%)
3	CPS	B	702	-	35,35,45	1.06	1 (2%)	54,54,70	1.42	9 (16%)
2	HEM	A	520	1	41,50,50	2.92	19 (46%)	45,82,82	1.87	10 (22%)
3	CPS	B	700	-	45,45,45	2.38	5 (11%)	69,70,70	1.40	10 (14%)

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	CPS	A	602	-	-	4/13/78/90	0/4/4/4
2	HEM	B	520	1	-	1/12/54/54	-
3	CPS	A	601	-	-	3/13/78/90	0/4/4/4
3	CPS	B	701	-	-	2/13/78/90	0/4/4/4

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPS	A	600	-	-	3/25/90/90	0/4/4/4
3	CPS	B	702	-	-	8/13/78/90	0/4/4/4
2	HEM	A	520	1	-	2/12/54/54	-
3	CPS	B	700	-	-	5/25/90/90	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	CPS	O3S-S	8.79	1.71	1.45
3	A	600	CPS	O3S-S	8.73	1.70	1.45
3	A	600	CPS	O1S-S	8.69	1.70	1.45
3	B	700	CPS	O1S-S	8.66	1.70	1.45
3	B	700	CPS	O2S-S	6.60	1.70	1.47
2	A	520	HEM	C3B-C2B	6.42	1.50	1.37
3	A	600	CPS	O2S-S	6.36	1.70	1.47
2	B	520	HEM	C3B-C2B	6.18	1.49	1.37
2	A	520	HEM	C1B-C2B	-6.08	1.32	1.44
2	B	520	HEM	C3C-C2C	5.87	1.48	1.40
2	B	520	HEM	CHB-C1B	5.80	1.49	1.35
2	A	520	HEM	C3C-C2C	5.63	1.48	1.40
2	B	520	HEM	FE-NB	5.36	2.23	1.96
3	B	701	CPS	O1-C24	5.30	1.34	1.23
3	A	600	CPS	O1-C24	5.28	1.34	1.23
2	A	520	HEM	CHB-C1B	5.22	1.48	1.35
2	A	520	HEM	CAB-C3B	-5.21	1.33	1.47
3	B	702	CPS	O1-C24	5.19	1.33	1.23
3	A	602	CPS	O1-C24	5.17	1.33	1.23
2	B	520	HEM	CAB-C3B	-5.15	1.33	1.47
3	B	700	CPS	O1-C24	5.09	1.33	1.23
2	A	520	HEM	FE-NB	5.08	2.22	1.96
3	A	601	CPS	O1-C24	5.04	1.33	1.23
2	B	520	HEM	C1B-C2B	-4.99	1.34	1.44
2	B	520	HEM	C1A-NA	4.56	1.45	1.36
2	B	520	HEM	C2C-C1C	-4.53	1.32	1.42
3	B	700	CPS	C32-S	-4.36	1.71	1.77
3	A	600	CPS	C32-S	-4.33	1.71	1.77
2	A	520	HEM	CBB-CAB	4.22	1.51	1.30
2	A	520	HEM	C1A-NA	4.15	1.44	1.36
2	B	520	HEM	CBB-CAB	4.11	1.50	1.30
2	A	520	HEM	C2C-C1C	-4.09	1.33	1.42
2	A	520	HEM	C4D-ND	-3.84	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	520	HEM	C1A-CHA	3.67	1.51	1.41
2	A	520	HEM	C1B-NB	-3.49	1.34	1.40
2	B	520	HEM	C4D-ND	-3.43	1.34	1.40
2	A	520	HEM	CHD-C1D	-3.24	1.31	1.41
2	A	520	HEM	C1A-CHA	3.23	1.50	1.41
2	A	520	HEM	C4A-CHB	-3.23	1.32	1.41
2	B	520	HEM	C1D-C2D	3.20	1.50	1.44
2	A	520	HEM	C4D-C3D	3.06	1.50	1.45
2	B	520	HEM	CHC-C4B	-3.04	1.32	1.41
2	B	520	HEM	C1B-NB	-3.01	1.35	1.40
2	B	520	HEM	CHD-C1D	-2.96	1.32	1.41
2	B	520	HEM	C4A-CHB	-2.86	1.33	1.41
2	A	520	HEM	CHC-C4B	-2.82	1.32	1.41
2	B	520	HEM	C4D-C3D	2.74	1.49	1.45
2	A	520	HEM	C1D-C2D	2.44	1.49	1.44
2	B	520	HEM	C1D-ND	-2.37	1.33	1.38
2	A	520	HEM	C1D-ND	-2.31	1.34	1.38
2	B	520	HEM	C3B-C4B	2.30	1.49	1.44
2	A	520	HEM	C3B-C4B	2.08	1.49	1.44

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	CPS	C9-C5-C6	-7.69	92.34	100.09
2	A	520	HEM	C4B-C3B-C2B	-6.28	102.13	107.11
2	B	520	HEM	C4B-C3B-C2B	-5.97	102.37	107.11
2	B	520	HEM	C1B-NB-C4B	5.94	111.20	105.07
2	A	520	HEM	CHC-C4B-NB	4.34	129.15	124.43
3	B	702	CPS	C9-C5-C6	-4.33	95.73	100.09
2	A	520	HEM	C1B-NB-C4B	4.23	109.44	105.07
3	A	600	CPS	C9-C5-C6	-4.19	95.87	100.09
2	B	520	HEM	CHC-C4B-NB	4.15	128.94	124.43
3	B	701	CPS	C9-C5-C6	-3.82	96.24	100.09
2	A	520	HEM	C4D-ND-C1D	3.76	108.95	105.07
3	A	600	CPS	C5-C9-C20	-3.49	115.32	119.50
3	B	700	CPS	C5-C9-C20	-3.46	115.37	119.50
3	A	600	CPS	O3S-S-C32	3.38	110.98	106.92
2	B	520	HEM	C4D-ND-C1D	3.32	108.50	105.07
3	B	701	CPS	C1-C2-C15	3.10	112.36	107.77
3	B	700	CPS	C9-C5-C4	-3.10	114.83	117.67
3	B	702	CPS	C5-C9-C20	-3.08	115.82	119.50
3	B	700	CPS	O1-C24-C23	-3.04	116.46	122.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	CPS	C9-C5-C6	-2.99	97.08	100.09
3	A	600	CPS	C10-C5-C6	2.98	115.87	111.21
2	B	520	HEM	CMA-C3A-C4A	-2.96	123.92	128.46
3	B	702	CPS	C8-C9-C20	2.86	116.58	112.15
2	B	520	HEM	CHC-C4B-C3B	-2.84	120.22	124.57
3	B	700	CPS	O2S-S-C32	2.84	110.36	105.77
3	B	702	CPS	C7-C6-C5	-2.82	100.79	103.55
3	A	601	CPS	C7-C6-C5	-2.76	100.85	103.55
3	A	600	CPS	C8-C7-C6	-2.75	99.68	105.13
3	B	700	CPS	O3S-S-C32	2.75	110.22	106.92
3	B	701	CPS	C19-C18-C17	-2.72	108.62	111.88
3	A	601	CPS	C9-C5-C4	-2.68	115.22	117.67
3	A	602	CPS	C19-C3-C4	-2.67	110.78	114.30
3	A	602	CPS	C19-C18-C17	-2.64	108.71	111.88
2	A	520	HEM	CMA-C3A-C4A	-2.64	124.41	128.46
2	A	520	HEM	O2A-CGA-CBA	2.61	122.42	114.03
3	A	600	CPS	O1-C24-C23	-2.58	117.30	122.02
2	B	520	HEM	C2C-C3C-C4C	-2.57	105.10	106.90
3	B	701	CPS	C11-C2-C1	-2.54	104.17	108.26
3	B	702	CPS	C9-C5-C4	-2.49	115.39	117.67
3	B	700	CPS	C5-C6-C18	-2.47	111.59	114.74
3	B	702	CPS	C22-C20-C9	2.45	115.35	110.28
3	A	601	CPS	O1-C24-C23	-2.44	117.56	122.02
2	A	520	HEM	O2D-CGD-O1D	-2.43	117.25	123.30
3	A	602	CPS	C14-C15-C2	2.42	115.23	112.66
3	A	602	CPS	O1-C24-C23	-2.42	117.59	122.02
3	A	601	CPS	C8-C7-C6	-2.41	100.35	105.13
3	A	600	CPS	C14-C15-C2	2.40	115.21	112.66
3	A	600	CPS	O1S-S-C32	2.39	109.80	106.92
2	A	520	HEM	O2D-CGD-CBD	2.38	121.69	114.03
3	A	600	CPS	O2S-S-C32	2.38	109.62	105.77
3	B	701	CPS	C16-C15-C2	2.31	115.11	112.66
2	B	520	HEM	CHA-C4D-ND	2.30	127.23	124.38
3	B	701	CPS	C10-C5-C6	2.30	114.81	111.21
2	B	520	HEM	O2D-CGD-CBD	2.27	121.31	114.03
3	A	601	CPS	C10-C5-C4	2.25	111.36	109.07
3	B	701	CPS	C12-C1-C2	2.24	116.62	112.78
3	A	600	CPS	O1-C24-N1	2.23	127.22	123.01
3	A	600	CPS	C22-C23-C24	-2.20	108.13	113.04
2	A	520	HEM	CHC-C4B-C3B	-2.20	121.21	124.57
3	B	702	CPS	C14-C15-C2	2.19	114.99	112.66
3	B	700	CPS	C8-C7-C6	-2.19	100.80	105.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	520	HEM	CHB-C1B-C2B	-2.18	120.69	126.72
3	A	602	CPS	C8-C7-C6	-2.18	100.82	105.13
3	A	602	CPS	C10-C5-C6	2.17	114.60	111.21
3	A	600	CPS	C19-C2-C15	2.15	111.61	108.58
2	B	520	HEM	C4A-C3A-C2A	2.13	108.47	107.00
3	B	701	CPS	C7-C6-C5	-2.12	101.47	103.55
3	B	700	CPS	C10-C5-C6	2.09	114.48	111.21
3	A	601	CPS	C3-C19-C2	-2.08	111.58	113.73
3	B	702	CPS	C21-C20-C9	-2.07	109.74	112.92
3	B	700	CPS	C22-C23-C24	-2.07	108.42	113.04
3	A	600	CPS	C26-C25-N1	-2.05	106.34	112.21
3	B	702	CPS	O1-C24-C23	-2.04	118.28	122.02
3	B	701	CPS	C14-C13-C12	-2.02	108.15	110.55
3	A	601	CPS	C11-C2-C1	-2.01	105.02	108.26

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	520	HEM	C2B-C3B-CAB-CBB
2	B	520	HEM	C2B-C3B-CAB-CBB
3	A	602	CPS	C23-C24-N1-C25
3	A	602	CPS	O1-C24-N1-C25
3	B	700	CPS	C26-C27-N2-C29
3	B	700	CPS	C26-C27-N2-C30
3	B	701	CPS	C23-C24-N1-C25
3	B	701	CPS	O1-C24-N1-C25
3	B	702	CPS	C21-C20-C9-C5
3	B	702	CPS	C22-C20-C9-C5
3	B	702	CPS	C22-C20-C9-C8
3	B	702	CPS	C23-C24-N1-C25
3	B	702	CPS	O1-C24-N1-C25
3	B	702	CPS	C21-C20-C9-C8
3	A	602	CPS	N1-C25-C26-C27
3	A	602	CPS	C20-C22-C23-C24
3	A	601	CPS	C23-C24-N1-C25
3	A	601	CPS	O1-C24-N1-C25
3	B	700	CPS	C26-C27-N2-C28
3	B	702	CPS	N1-C25-C26-C27
3	A	601	CPS	C21-C20-C22-C23
3	A	600	CPS	C22-C23-C24-O1
3	A	600	CPS	C22-C23-C24-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	700	CPS	C9-C20-C22-C23
2	A	520	HEM	C4B-C3B-CAB-CBB
3	B	702	CPS	C20-C22-C23-C24
3	A	600	CPS	C31-C32-S-O1S
3	B	700	CPS	C22-C23-C24-O1

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	520	HEM	2	0
3	A	601	CPS	1	0
3	B	701	CPS	1	0
3	B	702	CPS	1	0
2	A	520	HEM	1	0
3	B	700	CPS	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 then 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 CPS A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 520

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS B 702

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 520

Bond lengths

Bond angles

Torsions

Rings

Ligand CPS B 700

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	464/482 (96%)	0.10	22 (4%)	31	33	16, 33, 54, 75	0
1	B	464/482 (96%)	0.08	17 (3%)	41	45	15, 35, 57, 69	0
All	All	928/964 (96%)	0.09	39 (4%)	36	39	15, 34, 56, 75	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	THR	6.5
1	B	52	THR	6.4
1	A	51	GLU	6.1
1	B	230	GLU	4.9
1	A	75	TRP	4.6
1	A	444	GLU	4.3
1	A	231	THR	4.3
1	A	230	GLU	3.7
1	B	51	GLU	3.6
1	B	197	ARG	3.4
1	A	362	ASP	3.3
1	A	446	LYS	3.2
1	A	57	ASP	3.2
1	B	297	PRO	3.2
1	A	427	ASP	2.9
1	A	53	ARG	2.9
1	A	445	LYS	2.8
1	A	406	GLU	2.8
1	B	75	TRP	2.8
1	B	234	GLU	2.8
1	A	426	GLU	2.7
1	A	442	GLN	2.7
1	B	298	GLY	2.7
1	B	231	THR	2.7

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	GLU	2.6
1	B	233	GLU	2.5
1	B	444	GLU	2.4
1	B	295	GLN	2.4
1	A	234	GLU	2.4
1	A	399	ASP	2.4
1	A	54	ASN	2.3
1	A	323	LEU	2.3
1	B	273	LEU	2.3
1	A	430	GLU	2.1
1	B	199	ARG	2.1
1	A	153	GLN	2.1
1	B	475	ALA	2.1
1	B	196	GLU	2.0
1	B	406	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CPS	B	701	32/42	0.65	0.28	86,87,89,89	0
3	CPS	A	600	42/42	0.79	0.25	27,33,74,75	0
3	CPS	B	700	42/42	0.82	0.24	31,36,76,77	0
3	CPS	B	702	32/42	0.83	0.30	66,69,75,76	0
3	CPS	A	602	32/42	0.85	0.32	75,76,80,80	0
3	CPS	A	601	32/42	0.88	0.17	49,50,59,59	0
2	HEM	A	520	43/43	0.98	0.17	9,14,18,19	0
2	HEM	B	520	43/43	0.98	0.15	11,14,15,16	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.
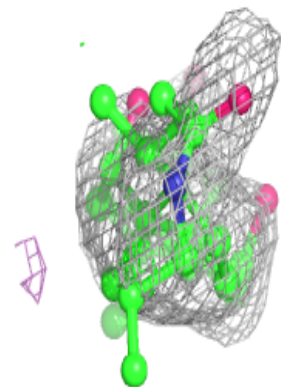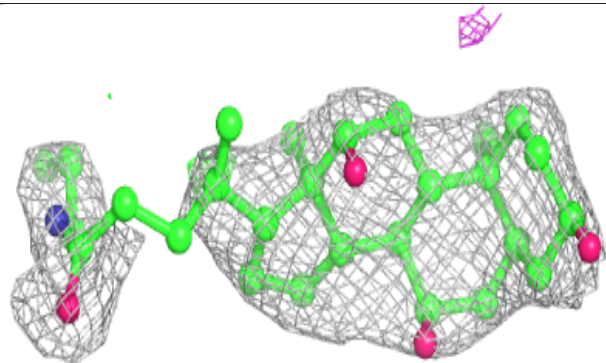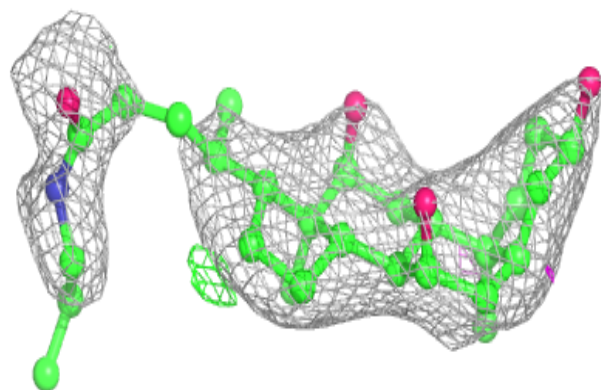
Electron density around CPS B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
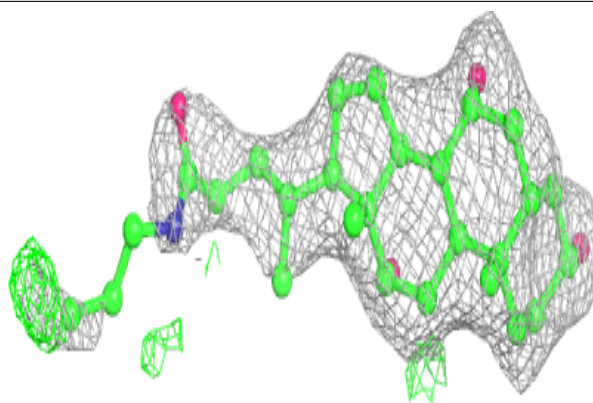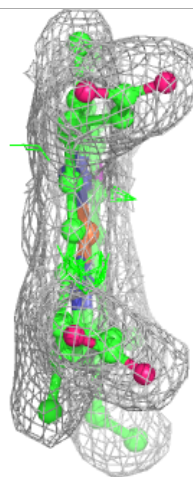mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
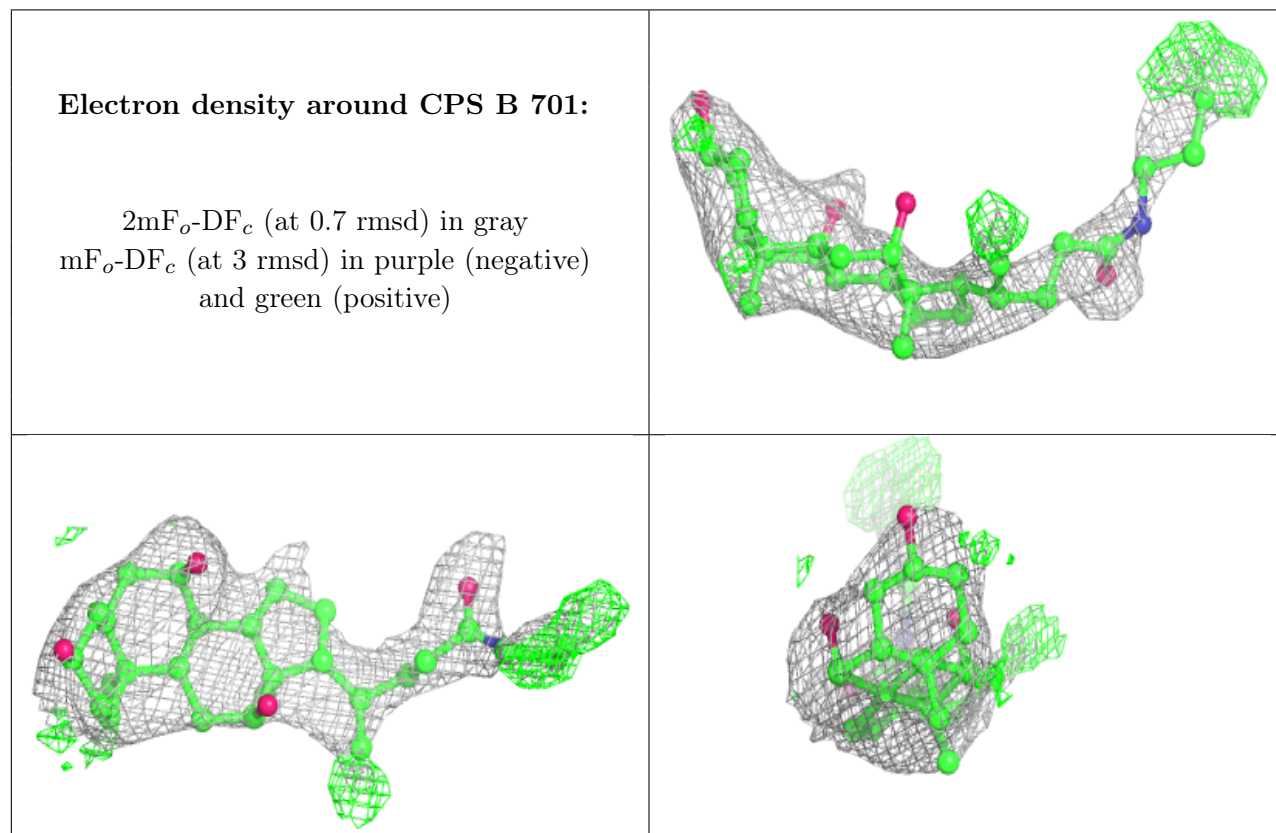
Electron density around CPS A 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
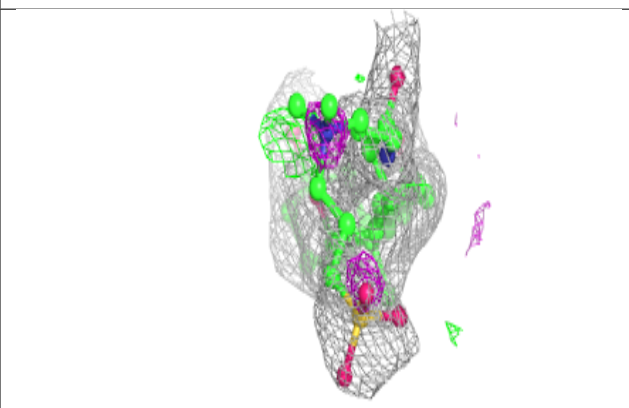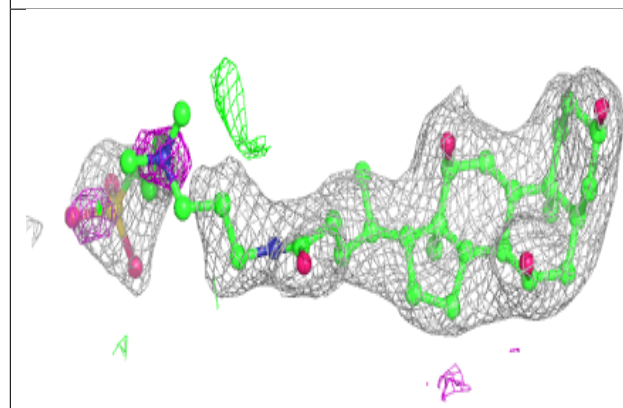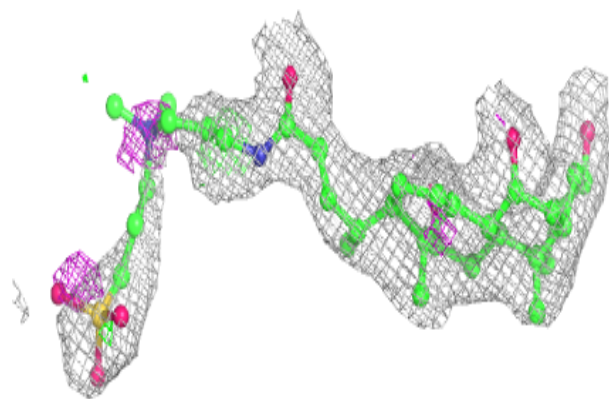
Electron density around CPS B 700:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
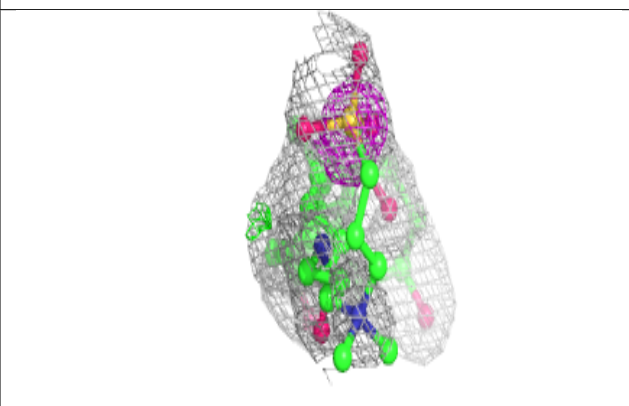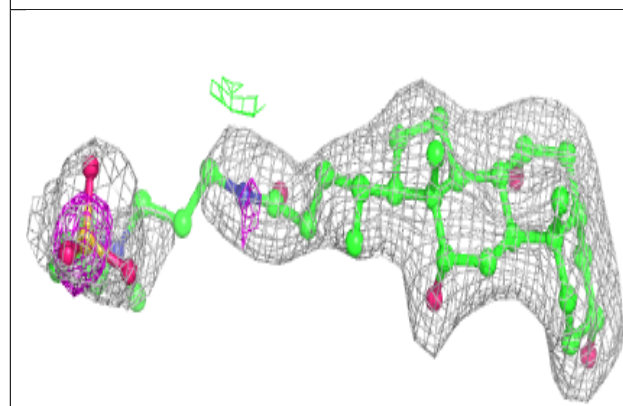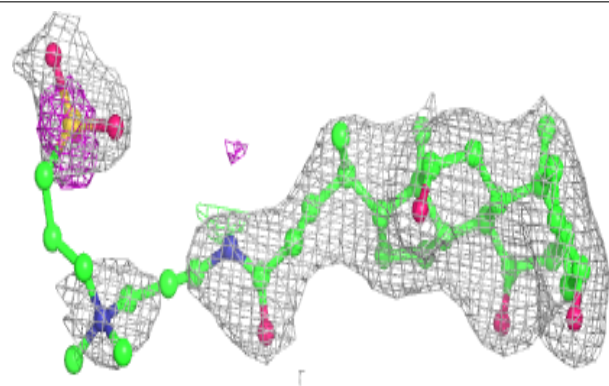
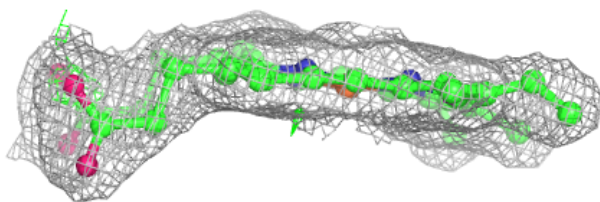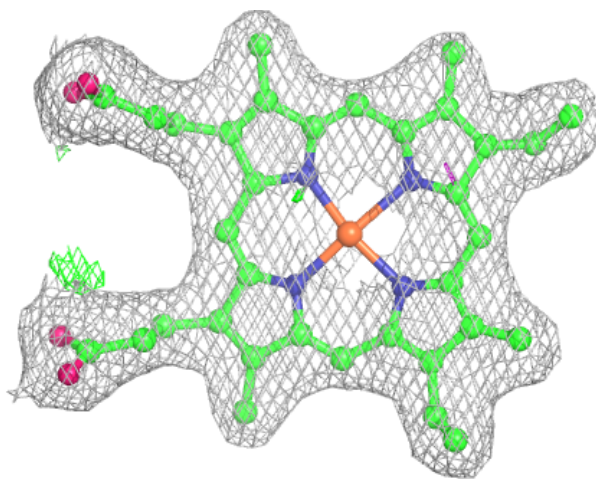**Electron density around CPS B 702:**

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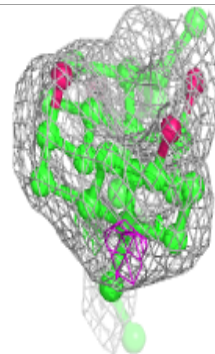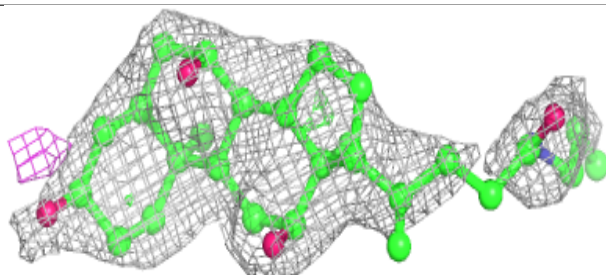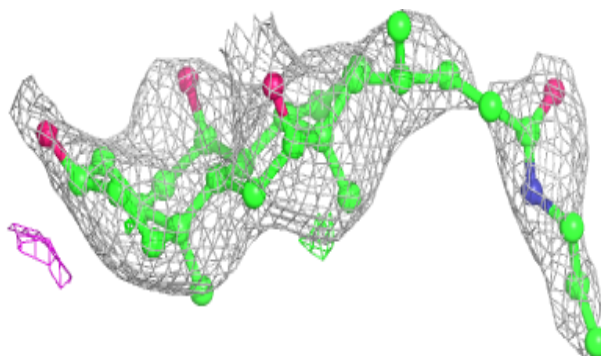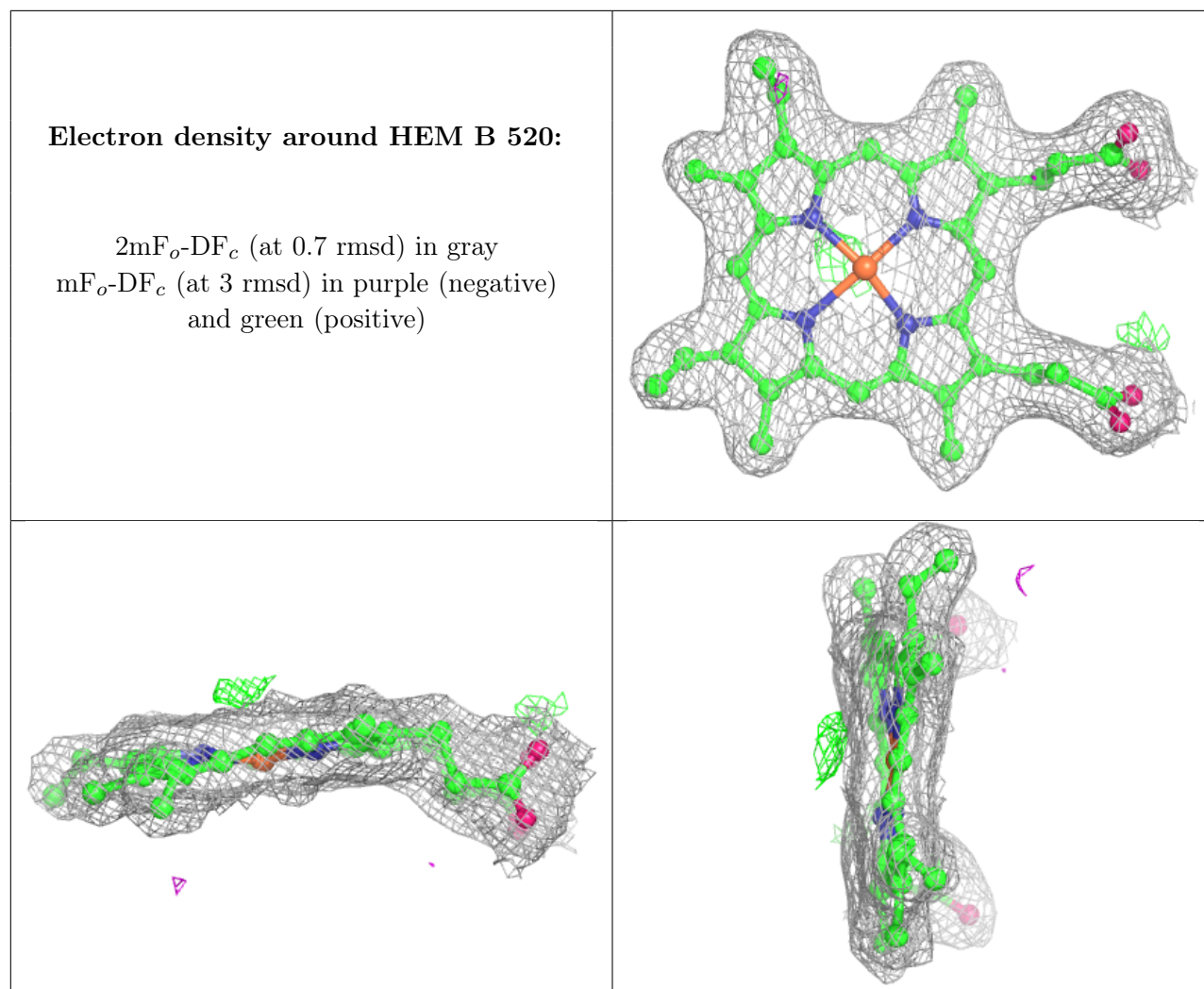

Electron density around CPS A 602:

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

Electron density around CPS A 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
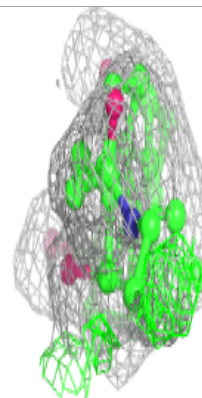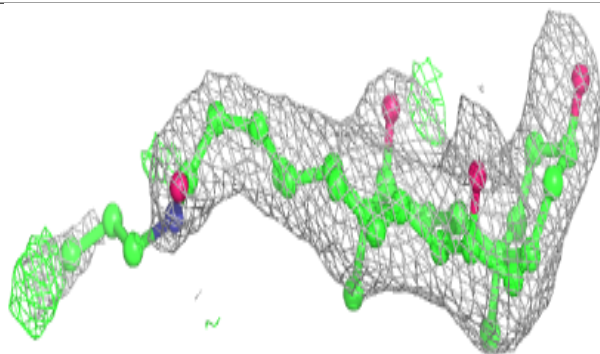
Electron density around HEM A 520:

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

Electron density around HEM B 520:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.