



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1W0G
Title : CRYSTAL STRUCTURE OF HUMAN CYTOCHROME P450 3A4
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Deposited on : 2004-06-03
Resolution : 2.73 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

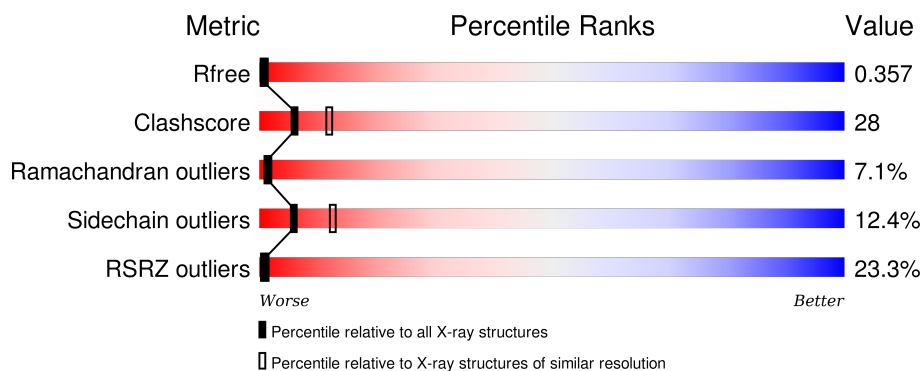
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	485	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3741 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.

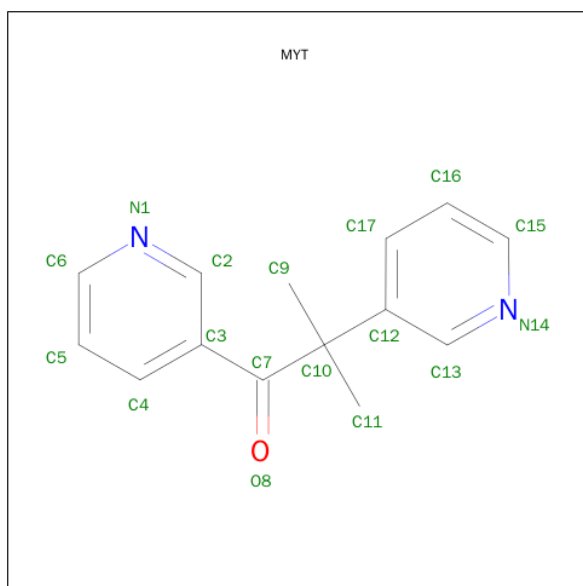
- Molecule 1 is a protein called CYTOCHROME P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3652	2382	597	649	24			

There is a discrepancy between the modelled and reference sequences:

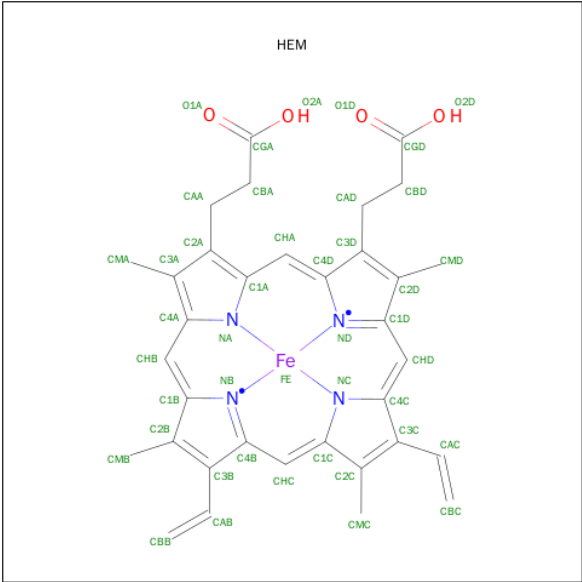
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	VAL	TRP	CONFLICT SEE REMARK 9	UNP P08684

- Molecule 2 is METYRAPONE (three-letter code: MYT) (formula: $C_{14}H_{14}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

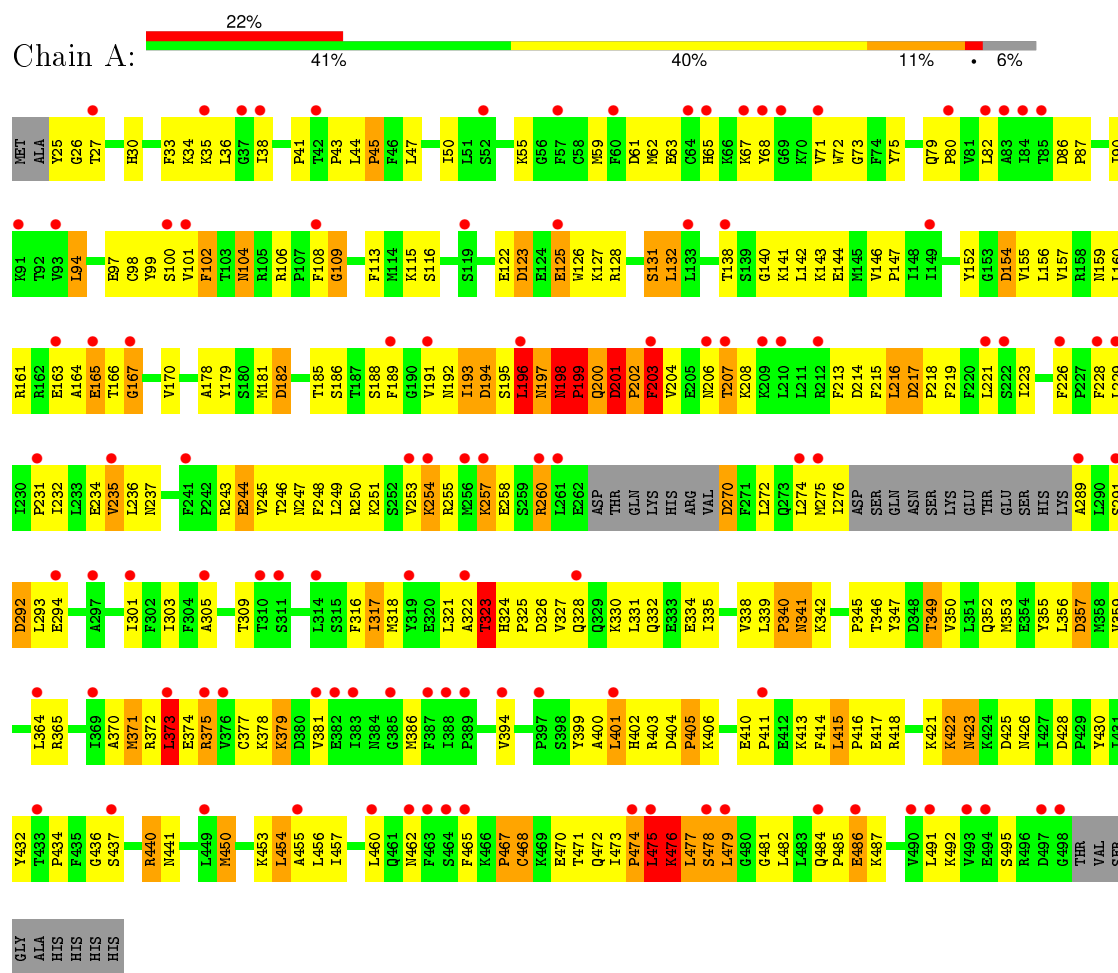
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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 3A4



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	77.94Å 100.91Å 131.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.73 40.08 – 2.71	Depositor EDS
% Data completeness (in resolution range)	93.9 (81.65-2.73) 91.8 (40.08-2.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0003A	Depositor
R, R_{free}	0.234 , 0.318 0.375 , 0.357	Depositor DCC
R_{free} test set	650 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13174 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MYT

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	0.76	0/3742	0.95	18/5063 (0.4%)

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	1	4

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	214	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	217	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	475	LEU	CA-CB-CG	7.45	132.44	115.30
1	A	61	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	123	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	357	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	86	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	182	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	326	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	194	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	154	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	270	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	201	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	292	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	196	LEU	CA-CB-CG	5.47	127.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	373	LEU	N-CA-C	-5.21	96.92	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	421	LYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	PRO	Peptide
1	A	322	ALA	Peptide
1	A	323	THR	Peptide
1	A	33	PHE	Peptide

5.2 Too-close contacts [i](#)

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	3652	0	3728	210	5
2	A	17	0	14	5	0
3	A	43	0	30	4	0
4	A	29	0	0	5	0
All	All	3741	0	3772	213	5

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 (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HB2	1:A:476:LYS:HZ1	1.37	0.90
1:A:178:ALA:HB3	1:A:196:LEU:HD12	1.55	0.88
1:A:104:ASN:ND2	1:A:123:ASP:OD1	2.09	0.86
1:A:178:ALA:HB1	1:A:196:LEU:HA	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HE22	1:A:487:LYS:NZ	1.78	0.81
1:A:25:TYR:HB3	4:A:2001:HOH:O	1.82	0.79
1:A:472:GLN:HE22	1:A:487:LYS:HZ3	1.30	0.77
1:A:332:GLN:HA	1:A:335:ILE:HD12	1.69	0.74
1:A:373:LEU:HD21	1:A:436:GLY:HA2	1.69	0.74
1:A:413:LYS:HB2	1:A:415:LEU:HD11	1.70	0.73
1:A:198:ASN:O	1:A:200:GLN:N	2.22	0.72
1:A:276:ILE:N	1:A:276:ILE:HD12	2.05	0.71
1:A:101:VAL:HA	1:A:378:LYS:HG3	1.72	0.71
1:A:146:VAL:HG13	1:A:454:LEU:HD21	1.73	0.70
1:A:178:ALA:CB	1:A:196:LEU:HA	2.21	0.70
1:A:472:GLN:HB2	1:A:476:LYS:NZ	2.05	0.70
1:A:101:VAL:HG22	1:A:102:PHE:CD1	2.26	0.70
1:A:323:THR:O	1:A:324:HIS:CD2	2.47	0.68
1:A:330:LYS:HB3	1:A:355:TYR:CE1	2.30	0.67
1:A:477:LEU:N	1:A:485:PRO:O	2.24	0.67
1:A:345:PRO:HG3	1:A:457:ILE:HG21	1.75	0.67
1:A:357:ASP:HA	1:A:453:LYS:HZ1	1.58	0.66
1:A:479:LEU:HD23	1:A:479:LEU:H	1.60	0.66
1:A:201:ASP:H	1:A:202:PRO:HD3	1.59	0.66
1:A:201:ASP:N	1:A:202:PRO:HD3	2.11	0.66
1:A:55:LYS:HB3	1:A:59:MET:HB2	1.76	0.66
1:A:377:CYS:SG	1:A:379:LYS:O	2.53	0.65
1:A:181:MET:O	1:A:185:THR:HG23	1.97	0.65
1:A:179:TYR:CE1	1:A:455:ALA:HB2	2.31	0.64
1:A:251:LYS:O	1:A:254:LYS:HB3	1.97	0.63
1:A:309:THR:HG21	2:A:1499:MYT:H16	1.79	0.63
1:A:370:ALA:O	1:A:372:ARG:N	2.32	0.63
1:A:185:THR:HG21	1:A:193:ILE:HD11	1.81	0.63
1:A:155:VAL:HG12	1:A:196:LEU:HD22	1.82	0.62
1:A:101:VAL:HG23	1:A:378:LYS:HB2	1.81	0.62
1:A:99:TYR:HD2	1:A:127:LYS:CE	2.13	0.62
1:A:194:ASP:OD2	1:A:198:ASN:ND2	2.27	0.60
1:A:123:ASP:OD1	1:A:378:LYS:NZ	2.31	0.60
1:A:423:ASN:O	1:A:426:ASN:ND2	2.34	0.60
1:A:318:MET:CE	1:A:465:PHE:CD2	2.84	0.60
1:A:62:MET:O	1:A:65:HIS:N	2.35	0.60
1:A:140:GLY:O	1:A:144:GLU:HB2	2.03	0.59
1:A:99:TYR:HD2	1:A:127:LYS:HE2	1.68	0.58
1:A:321:LEU:HD21	1:A:359:VAL:HG11	1.86	0.57
1:A:101:VAL:O	1:A:102:PHE:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:HB3	1:A:476:LYS:HE3	1.85	0.57
1:A:357:ASP:HA	1:A:453:LYS:NZ	2.20	0.57
1:A:415:LEU:HD12	1:A:415:LEU:N	2.21	0.56
1:A:178:ALA:HB1	1:A:196:LEU:CA	2.32	0.56
1:A:253:VAL:HG13	1:A:272:LEU:HD21	1.88	0.56
1:A:472:GLN:CB	1:A:476:LYS:HE3	2.37	0.55
1:A:475:LEU:C	1:A:476:LYS:HD3	2.26	0.55
1:A:291:SER:HB3	1:A:294:GLU:CD	2.27	0.55
1:A:164:ALA:O	1:A:167:GLY:N	2.39	0.54
1:A:195:SER:O	1:A:197:ASN:N	2.40	0.54
1:A:228:PHE:O	1:A:231:PRO:HD2	2.08	0.54
1:A:178:ALA:CB	1:A:196:LEU:HD12	2.34	0.54
1:A:482:LEU:HB2	1:A:484:GLN:OE1	2.07	0.54
1:A:25:TYR:CB	4:A:2001:HOH:O	2.49	0.54
1:A:25:TYR:CD1	4:A:2001:HOH:O	2.53	0.54
1:A:47:LEU:HD22	1:A:50:ILE:HD11	1.90	0.54
1:A:400:ALA:O	1:A:401:LEU:C	2.46	0.53
1:A:159:ASN:HD22	1:A:196:LEU:HD23	1.73	0.53
1:A:154:ASP:O	1:A:157:VAL:HG22	2.09	0.53
1:A:189:PHE:O	1:A:260:ARG:NH2	2.42	0.52
1:A:26:GLY:O	1:A:45:PRO:O	2.28	0.52
1:A:94:LEU:HD21	1:A:373:LEU:HD23	1.92	0.52
1:A:146:VAL:N	1:A:147:PRO:CD	2.72	0.52
1:A:138:THR:OG1	1:A:141:LYS:HD3	2.09	0.52
1:A:328:GLN:O	1:A:332:GLN:HG3	2.10	0.52
1:A:485:PRO:O	1:A:486:GLU:CB	2.58	0.52
1:A:156:LEU:HA	1:A:196:LEU:HD21	1.90	0.51
1:A:327:VAL:HG22	1:A:355:TYR:OH	2.10	0.51
1:A:206:ASN:ND2	1:A:248:PHE:CD1	2.78	0.51
1:A:170:VAL:N	1:A:491:LEU:O	2.43	0.51
1:A:338:VAL:HG12	1:A:349:THR:HG22	1.92	0.51
1:A:467:PRO:O	1:A:468:CYS:HB3	2.10	0.51
1:A:272:LEU:HD13	1:A:272:LEU:C	2.31	0.51
1:A:201:ASP:N	1:A:202:PRO:CD	2.74	0.51
1:A:181:MET:SD	1:A:207:THR:HB	2.51	0.50
1:A:243:ARG:HD2	4:A:2017:HOH:O	2.11	0.50
1:A:346:THR:HB	1:A:349:THR:OG1	2.10	0.50
1:A:97:GLU:O	1:A:99:TYR:N	2.45	0.50
1:A:25:TYR:HD1	4:A:2001:HOH:O	1.94	0.50
1:A:97:GLU:HB3	1:A:101:VAL:CG1	2.42	0.50
1:A:404:ASP:O	1:A:406:LYS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG21	1:A:193:ILE:CD1	2.42	0.50
1:A:126:TRP:CZ2	1:A:440:ARG:HG2	2.47	0.49
1:A:460:LEU:C	1:A:462:ASN:H	2.15	0.49
1:A:106:ARG:HD2	1:A:374:GLU:OE2	2.12	0.49
1:A:243:ARG:HA	1:A:246:THR:OG1	2.12	0.49
1:A:226:PHE:HB2	1:A:229:LEU:HD22	1.94	0.49
1:A:216:LEU:HD22	1:A:481:GLY:CA	2.42	0.49
1:A:472:GLN:CB	1:A:476:LYS:CE	2.90	0.49
1:A:353:MET:O	1:A:356:LEU:HB3	2.13	0.49
1:A:128:ARG:NH1	1:A:289:ALA:O	2.46	0.49
1:A:198:ASN:CB	1:A:199:PRO:HD2	2.43	0.49
2:A:1499:MYT:H4	2:A:1499:MYT:C17	2.43	0.49
1:A:108:PHE:O	1:A:109:GLY:O	2.30	0.49
1:A:160:LEU:HD12	1:A:163:GLU:HB2	1.95	0.49
1:A:159:ASN:ND2	1:A:196:LEU:HD23	2.27	0.49
1:A:101:VAL:HG11	1:A:381:VAL:HG21	1.95	0.49
1:A:359:VAL:HG13	1:A:414:PHE:HZ	1.78	0.49
1:A:178:ALA:O	1:A:182:ASP:CG	2.51	0.48
1:A:441:ASN:HA	3:A:1501:HEM:HBA2	1.95	0.48
1:A:194:ASP:OD1	1:A:196:LEU:HB3	2.13	0.48
1:A:340:PRO:O	1:A:341:ASN:O	2.30	0.48
1:A:471:THR:HG21	1:A:491:LEU:HD23	1.96	0.48
1:A:346:THR:O	1:A:350:VAL:HG23	2.14	0.48
1:A:403:ARG:O	1:A:405:PRO:HD3	2.14	0.48
1:A:475:LEU:O	1:A:476:LYS:HB2	2.14	0.48
1:A:101:VAL:HG22	1:A:102:PHE:HD1	1.78	0.47
1:A:450:MET:SD	1:A:454:LEU:HD22	2.53	0.47
1:A:472:GLN:HB2	1:A:476:LYS:CE	2.44	0.47
1:A:97:GLU:HB3	1:A:101:VAL:HG12	1.96	0.47
1:A:102:PHE:CE2	1:A:394:VAL:HG21	2.50	0.47
1:A:357:ASP:CA	1:A:453:LYS:HZ1	2.25	0.47
1:A:71:VAL:HG13	1:A:82:LEU:HD21	1.96	0.47
1:A:217:ASP:HB2	1:A:218:PRO:CD	2.45	0.47
1:A:415:LEU:CD1	1:A:418:ARG:NH1	2.78	0.46
1:A:338:VAL:HG12	1:A:349:THR:CG2	2.45	0.46
1:A:125:GLU:HA	1:A:125:GLU:OE1	2.15	0.46
1:A:142:LEU:HD11	1:A:450:MET:HG3	1.98	0.46
2:A:1499:MYT:H13	3:A:1501:HEM:C4D	2.50	0.46
1:A:276:ILE:N	1:A:276:ILE:CD1	2.72	0.46
1:A:202:PRO:HB2	1:A:203:PHE:CB	2.46	0.46
1:A:323:THR:O	1:A:324:HIS:CG	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLU:OE1	1:A:355:TYR:HB3	2.16	0.46
1:A:478:SER:HB2	1:A:484:GLN:HG2	1.97	0.46
1:A:257:LYS:HD2	1:A:257:LYS:C	2.36	0.46
1:A:213:PHE:HB2	1:A:215:PHE:CE1	2.50	0.45
1:A:213:PHE:O	1:A:482:LEU:HD21	2.16	0.45
1:A:356:LEU:HD21	1:A:453:LYS:HB3	1.98	0.45
1:A:476:LYS:N	1:A:476:LYS:CD	2.79	0.45
1:A:321:LEU:O	1:A:328:GLN:NE2	2.49	0.45
1:A:318:MET:HE1	1:A:465:PHE:CD2	2.51	0.45
1:A:41:PRO:HD2	1:A:73:GLY:O	2.17	0.45
1:A:305:ALA:HB1	2:A:1499:MYT:N14	2.32	0.45
1:A:421:LYS:O	1:A:422:LYS:CB	2.65	0.45
1:A:340:PRO:O	1:A:341:ASN:C	2.55	0.45
1:A:204:VAL:O	1:A:208:LYS:HB2	2.17	0.45
1:A:339:LEU:O	1:A:340:PRO:C	2.55	0.45
1:A:316:PHE:O	1:A:317:ILE:C	2.54	0.45
1:A:335:ILE:HG12	1:A:353:MET:HE1	1.99	0.44
1:A:59:MET:O	1:A:63:GLU:HG3	2.16	0.44
1:A:62:MET:O	1:A:63:GLU:C	2.56	0.44
1:A:87:PRO:HA	1:A:90:ILE:HB	1.99	0.44
1:A:75:TYR:HA	1:A:79:GLN:O	2.17	0.44
1:A:226:PHE:O	1:A:229:LEU:HB2	2.17	0.44
1:A:131:SER:O	1:A:132:LEU:HB2	2.17	0.44
1:A:260:ARG:HH12	1:A:272:LEU:HD12	1.83	0.44
1:A:386:MET:HE3	1:A:386:MET:HA	2.00	0.44
1:A:203:PHE:O	1:A:203:PHE:HD1	2.01	0.44
1:A:356:LEU:O	1:A:357:ASP:C	2.54	0.44
1:A:460:LEU:O	1:A:462:ASN:N	2.51	0.44
1:A:235:VAL:HG12	1:A:236:LEU:HD22	2.00	0.43
1:A:432:TYR:CZ	1:A:434:PRO:HG3	2.53	0.43
1:A:472:GLN:NE2	1:A:487:LYS:NZ	2.56	0.43
1:A:470:GLU:O	1:A:472:GLN:HG3	2.19	0.43
1:A:75:TYR:CE2	1:A:80:PRO:HB3	2.54	0.43
1:A:223:ILE:O	1:A:223:ILE:HG22	2.17	0.43
1:A:291:SER:HB3	1:A:294:GLU:CG	2.48	0.43
1:A:27:THR:HG22	1:A:45:PRO:HA	1.99	0.43
1:A:470:GLU:O	1:A:472:GLN:N	2.52	0.43
1:A:415:LEU:HD11	1:A:418:ARG:NH1	2.33	0.43
1:A:30:HIS:CE1	1:A:43:PRO:HB2	2.54	0.43
1:A:113:PHE:C	1:A:115:LYS:N	2.71	0.43
1:A:198:ASN:CB	1:A:199:PRO:CD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HG21	1:A:456:LEU:HD11	2.01	0.43
1:A:415:LEU:CD1	1:A:418:ARG:HH11	2.32	0.43
1:A:152:TYR:HE2	1:A:186:SER:HG	1.63	0.42
1:A:479:LEU:H	1:A:479:LEU:CD2	2.31	0.42
1:A:375:ARG:NH1	3:A:1501:HEM:O2A	2.52	0.42
1:A:90:ILE:HG21	1:A:430:TYR:HB3	2.01	0.42
1:A:364:LEU:O	1:A:365:ARG:C	2.56	0.42
1:A:251:LYS:HD2	1:A:251:LYS:N	2.34	0.42
1:A:492:LYS:CB	1:A:492:LYS:NZ	2.82	0.42
1:A:472:GLN:HB3	1:A:476:LYS:CE	2.47	0.42
1:A:152:TYR:OH	1:A:192:ASN:ND2	2.22	0.42
1:A:79:GLN:NE2	1:A:80:PRO:HD2	2.34	0.42
1:A:347:TYR:C	1:A:347:TYR:CD1	2.93	0.42
1:A:143:LYS:HA	1:A:146:VAL:HG23	2.02	0.42
1:A:330:LYS:HD3	1:A:355:TYR:CE2	2.55	0.42
1:A:179:TYR:CZ	1:A:455:ALA:HB2	2.55	0.42
1:A:243:ARG:O	1:A:244:GLU:C	2.55	0.42
1:A:189:PHE:CE1	1:A:303:ILE:HD11	2.55	0.42
1:A:219:PHE:CE1	1:A:223:ILE:HD11	2.55	0.42
1:A:476:LYS:N	1:A:476:LYS:HD3	2.35	0.42
1:A:339:LEU:HD21	1:A:349:THR:HG21	2.02	0.41
1:A:166:THR:O	1:A:167:GLY:C	2.58	0.41
1:A:36:LEU:HG	1:A:38:ILE:HD12	2.02	0.41
1:A:68:TYR:HB2	1:A:72:TRP:HB3	2.02	0.41
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.56	0.41
2:A:1499:MYT:H13	3:A:1501:HEM:ND	2.35	0.41
1:A:206:ASN:HB3	1:A:245:VAL:HG13	2.01	0.41
1:A:243:ARG:HG2	1:A:247:ASN:HD21	1.85	0.41
1:A:113:PHE:C	1:A:115:LYS:H	2.23	0.41
1:A:410:GLU:N	1:A:411:PRO:HD3	2.35	0.41
1:A:198:ASN:HB3	1:A:199:PRO:HD2	2.01	0.41
1:A:104:ASN:HD22	1:A:122:GLU:HB3	1.86	0.41
1:A:275:MET:C	1:A:276:ILE:HD12	2.41	0.41
1:A:460:LEU:C	1:A:462:ASN:N	2.73	0.41
1:A:161:ARG:O	1:A:165:GLU:N	2.48	0.41
1:A:191:VAL:HG12	1:A:193:ILE:HG23	2.02	0.41
1:A:334:GLU:O	1:A:338:VAL:HG23	2.21	0.40
1:A:102:PHE:H	1:A:378:LYS:CG	2.34	0.40
1:A:198:ASN:O	1:A:199:PRO:C	2.58	0.40
1:A:292:ASP:HB3	1:A:293:LEU:HD22	2.03	0.40
1:A:476:LYS:HZ3	1:A:476:LYS:HG2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:O	1:A:486:GLU:HB2	2.21	0.40
1:A:473:ILE:N	1:A:474:PRO:CD	2.85	0.40
1:A:416:PRO:O	1:A:418:ARG:N	2.55	0.40
1:A:324:HIS:N	1:A:325:PRO:HD3	2.37	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CE2	1:A:226:PHE:CZ[2_775]	1.36	0.84
1:A:232:ILE:CD1	1:A:232:ILE:CD1[4_575]	1.73	0.47
1:A:226:PHE:CE2	1:A:226:PHE:CE2[2_775]	1.85	0.35
1:A:226:PHE:CZ	1:A:226:PHE:CZ[2_775]	2.06	0.14
1:A:228:PHE:CB	1:A:231:PRO:O[4_575]	2.10	0.10

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	449/485 (93%)	351 (78%)	66 (15%)	32 (7%)	1 1

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	196	LEU
1	A	198	ASN
1	A	199	PRO
1	A	203	PHE
1	A	237	ASN
1	A	255	ARG
1	A	323	THR

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	342	LYS
1	A	467	PRO
1	A	468	CYS
1	A	476	LYS
1	A	486	GLU
1	A	109	GLY
1	A	132	LEU
1	A	167	GLY
1	A	340	PRO
1	A	401	LEU
1	A	422	LYS
1	A	475	LEU
1	A	477	LEU
1	A	371	MET
1	A	402	HIS
1	A	474	PRO
1	A	100	SER
1	A	254	LYS
1	A	417	GLU
1	A	102	PHE
1	A	201	ASP
1	A	405	PRO
1	A	165	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	412/441 (93%)	361 (88%)	51 (12%)	6 12

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	35	LYS

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Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	PRO
1	A	67	LYS
1	A	94	LEU
1	A	104	ASN
1	A	116	SER
1	A	125	GLU
1	A	131	SER
1	A	188	SER
1	A	193	ILE
1	A	197	ASN
1	A	198	ASN
1	A	199	PRO
1	A	200	GLN
1	A	203	PHE
1	A	207	THR
1	A	216	LEU
1	A	221	LEU
1	A	234	GLU
1	A	235	VAL
1	A	244	GLU
1	A	249	LEU
1	A	250	ARG
1	A	257	LYS
1	A	258	GLU
1	A	260	ARG
1	A	270	ASP
1	A	274	LEU
1	A	301	ILE
1	A	317	ILE
1	A	331	LEU
1	A	349	THR
1	A	352	GLN
1	A	371	MET
1	A	373	LEU
1	A	375	ARG
1	A	379	LYS
1	A	399	TYR
1	A	415	LEU
1	A	423	ASN
1	A	437	SER
1	A	440	ARG

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Mol	Chain	Res	Type
1	A	450	MET
1	A	454	LEU
1	A	475	LEU
1	A	476	LYS
1	A	478	SER
1	A	479	LEU
1	A	495	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	79	GLN
1	A	104	ASN
1	A	159	ASN
1	A	192	ASN
1	A	197	ASN
1	A	206	ASN
1	A	247	ASN
1	A	324	HIS
1	A	328	GLN
1	A	451	ASN
1	A	472	GLN

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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
2	MYT	A	1499	3	17,18,18	1.09	1 (5%)	19,25,25	1.41	2 (10%)
3	HEM	A	1501	1,2	30,50,50	2.58	11 (36%)	24,82,82	2.16	9 (37%)

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
2	MYT	A	1499	3	-	0/16/16/16	0/2/2/2
3	HEM	A	1501	1,2	-	0/10/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	HEM	C3B-C4B	-8.95	1.43	1.51
3	A	1501	HEM	C3D-C4D	-6.90	1.42	1.51
3	A	1501	HEM	C2C-C1C	-3.95	1.45	1.52
2	A	1499	MYT	C10-C12	-3.45	1.50	1.53
3	A	1501	HEM	C2B-C1B	-2.57	1.43	1.51
3	A	1501	HEM	FE-NB	-2.35	1.85	1.97
3	A	1501	HEM	C2A-C3A	-2.33	1.30	1.37
3	A	1501	HEM	C2D-C1D	-2.02	1.45	1.51
3	A	1501	HEM	C3C-CAC	2.05	1.55	1.51
3	A	1501	HEM	C1C-NC	2.09	1.38	1.36
3	A	1501	HEM	C4C-NC	2.30	1.38	1.36
3	A	1501	HEM	FE-ND	2.45	2.10	1.97

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1501	HEM	C4B-CHC-C1C	-2.68	121.34	125.82
3	A	1501	HEM	C3B-CAB-CBB	-2.58	120.49	124.46
2	A	1499	MYT	C16-C17-C12	-2.45	118.07	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1501	HEM	C3C-CAC-CBC	-2.36	120.83	124.46
3	A	1501	HEM	CMD-C2D-C3D	2.35	124.76	114.35
2	A	1499	MYT	C6-N1-C2	2.47	121.39	116.84
3	A	1501	HEM	C2D-C3D-C4D	2.66	106.01	101.50
3	A	1501	HEM	CMC-C2C-C3C	3.14	124.38	116.53
3	A	1501	HEM	CAD-C3D-C4D	3.95	126.40	112.47
3	A	1501	HEM	CMB-C2B-C3B	4.12	126.81	116.53
3	A	1501	HEM	CAD-C3D-C2D	5.00	127.60	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1499	MYT	5	0
3	A	1501	HEM	4	0

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	455/485 (93%)	1.33	106 (23%) 1 1	48, 81, 110, 122	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	GLY	8.1
1	A	93	VAL	6.2
1	A	275	MET	6.1
1	A	68	TYR	6.1
1	A	463	PHE	5.5
1	A	60	PHE	5.4
1	A	222	SER	4.5
1	A	257	LYS	4.2
1	A	328	GLN	4.1
1	A	206	ASN	4.1
1	A	490	VAL	4.0
1	A	37	GLY	4.0
1	A	64	CYS	4.0
1	A	387	PHE	3.9
1	A	411	PRO	3.8
1	A	71	VAL	3.8
1	A	474	PRO	3.8
1	A	491	LEU	3.7
1	A	221	LEU	3.7
1	A	291	SER	3.7
1	A	437	SER	3.7
1	A	191	VAL	3.7
1	A	35	LYS	3.6
1	A	254	LYS	3.6
1	A	52	SER	3.6
1	A	383	ILE	3.6
1	A	260	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	231	PRO	3.5
1	A	319	TYR	3.5
1	A	228	PHE	3.5
1	A	226	PHE	3.4
1	A	256	MET	3.3
1	A	381	VAL	3.3
1	A	397	PRO	3.2
1	A	84	ILE	3.2
1	A	294	GLU	3.2
1	A	57	PHE	3.1
1	A	42	THR	3.1
1	A	149	ILE	3.1
1	A	388	ILE	3.0
1	A	465	PHE	3.0
1	A	364	LEU	3.0
1	A	289	ALA	3.0
1	A	373	LEU	2.9
1	A	100	SER	2.9
1	A	460	LEU	2.9
1	A	475	LEU	2.8
1	A	455	ALA	2.8
1	A	401	LEU	2.8
1	A	433	THR	2.8
1	A	464	SER	2.8
1	A	494	GLU	2.8
1	A	462	ASN	2.8
1	A	101	VAL	2.7
1	A	235	VAL	2.7
1	A	274	LEU	2.7
1	A	189	PHE	2.7
1	A	241	PHE	2.7
1	A	486	GLU	2.7
1	A	167	GLY	2.7
1	A	210	LEU	2.6
1	A	82	LEU	2.6
1	A	314	LEU	2.6
1	A	27	THR	2.6
1	A	394	VAL	2.6
1	A	297	ALA	2.5
1	A	80	PRO	2.5
1	A	385	GLY	2.5
1	A	83	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	203	PHE	2.5
1	A	389	PRO	2.5
1	A	67	LYS	2.4
1	A	449	LEU	2.4
1	A	382	GLU	2.4
1	A	38	ILE	2.4
1	A	138	THR	2.4
1	A	209	LYS	2.4
1	A	484	GLN	2.4
1	A	165	GLU	2.4
1	A	108	PHE	2.4
1	A	163	GLU	2.4
1	A	311	SER	2.3
1	A	497	ASP	2.3
1	A	261	LEU	2.3
1	A	253	VAL	2.3
1	A	85	THR	2.3
1	A	301	ILE	2.2
1	A	369	ILE	2.2
1	A	322	ALA	2.2
1	A	478	SER	2.2
1	A	65	HIS	2.2
1	A	229	LEU	2.1
1	A	310	THR	2.1
1	A	119	SER	2.1
1	A	376	VAL	2.1
1	A	479	LEU	2.1
1	A	207	THR	2.1
1	A	493	VAL	2.1
1	A	69	GLY	2.1
1	A	133	LEU	2.1
1	A	125	GLU	2.1
1	A	305	ALA	2.1
1	A	196	LEU	2.1
1	A	91	LYS	2.0
1	A	375	ARG	2.0
1	A	212	ARG	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MYT	A	1499	17/17	0.81	0.35	1.59	67,70,75,76	0
3	HEM	A	1501	43/43	0.91	0.27	-0.48	49,59,70,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.