WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID	:	3ZK5
Title	:	PikC D50N mutant bound to the 10-DML analog with the 3-(N,N-dimethylamino)ethanoate anchoring group
Authors	:	Podust, L.M.
Deposited on	:	2013-01-21
Resolution	:	1.89 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (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 (i)

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

The reported resolution of this entry is 1.89 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		0.267
Clashscore		12
Ramachandran outliers		0.5%
Sidechain outliers		3.9%
RSRZ outliers		1.0%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
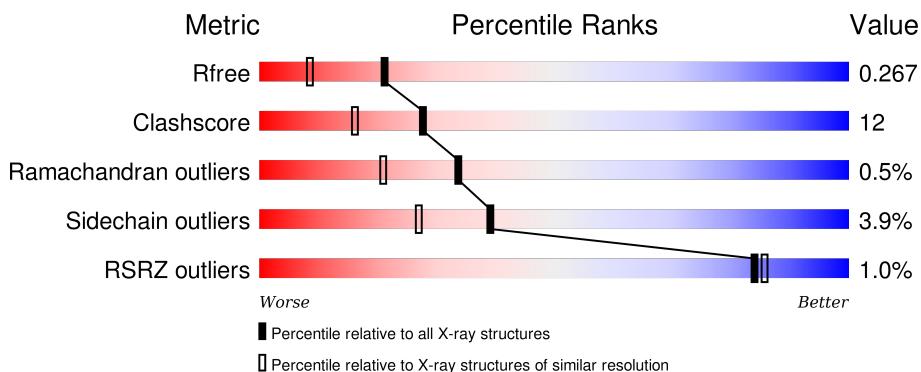
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	436	72% 18% • 9%
1	B	436	71% 17% • 10%
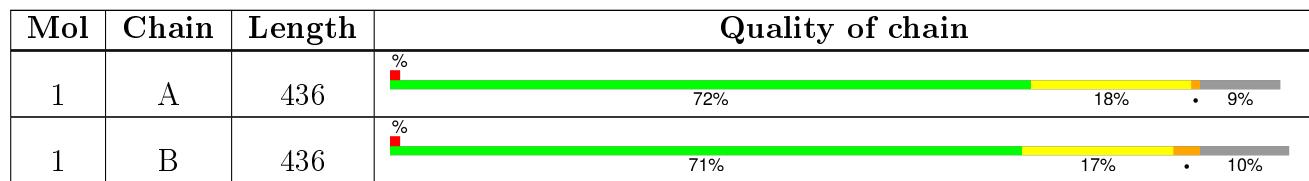
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6821 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 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	2	0
			3079	1943	551	572	13			
1	B	394	Total	C	N	O	S	0	2	0
			3078	1945	550	570	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O87605
A	-18	GLY	-	EXPRESSION TAG	UNP O87605
A	-17	SER	-	EXPRESSION TAG	UNP O87605
A	-16	SER	-	EXPRESSION TAG	UNP O87605
A	-15	HIS	-	EXPRESSION TAG	UNP O87605
A	-14	HIS	-	EXPRESSION TAG	UNP O87605
A	-13	HIS	-	EXPRESSION TAG	UNP O87605
A	-12	HIS	-	EXPRESSION TAG	UNP O87605
A	-11	HIS	-	EXPRESSION TAG	UNP O87605
A	-10	HIS	-	EXPRESSION TAG	UNP O87605
A	-9	SER	-	EXPRESSION TAG	UNP O87605
A	-8	SER	-	EXPRESSION TAG	UNP O87605
A	-7	GLY	-	EXPRESSION TAG	UNP O87605
A	-6	LEU	-	EXPRESSION TAG	UNP O87605
A	-5	VAL	-	EXPRESSION TAG	UNP O87605
A	-4	PRO	-	EXPRESSION TAG	UNP O87605
A	-3	ARG	-	EXPRESSION TAG	UNP O87605
A	-2	GLY	-	EXPRESSION TAG	UNP O87605
A	-1	SER	-	EXPRESSION TAG	UNP O87605
A	0	HIS	-	EXPRESSION TAG	UNP O87605
A	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605
B	-19	MET	-	EXPRESSION TAG	UNP O87605
B	-18	GLY	-	EXPRESSION TAG	UNP O87605
B	-17	SER	-	EXPRESSION TAG	UNP O87605
B	-16	SER	-	EXPRESSION TAG	UNP O87605

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP O87605
B	-14	HIS	-	EXPRESSION TAG	UNP O87605
B	-13	HIS	-	EXPRESSION TAG	UNP O87605
B	-12	HIS	-	EXPRESSION TAG	UNP O87605
B	-11	HIS	-	EXPRESSION TAG	UNP O87605
B	-10	HIS	-	EXPRESSION TAG	UNP O87605
B	-9	SER	-	EXPRESSION TAG	UNP O87605
B	-8	SER	-	EXPRESSION TAG	UNP O87605
B	-7	GLY	-	EXPRESSION TAG	UNP O87605
B	-6	LEU	-	EXPRESSION TAG	UNP O87605
B	-5	VAL	-	EXPRESSION TAG	UNP O87605
B	-4	PRO	-	EXPRESSION TAG	UNP O87605
B	-3	ARG	-	EXPRESSION TAG	UNP O87605
B	-2	GLY	-	EXPRESSION TAG	UNP O87605
B	-1	SER	-	EXPRESSION TAG	UNP O87605
B	0	HIS	-	EXPRESSION TAG	UNP O87605
B	50	ASN	ASP	ENGINEERED MUTATION	UNP O87605

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
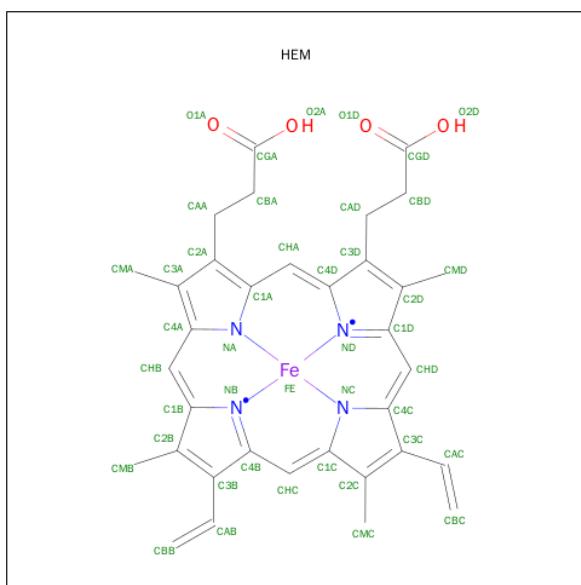
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (3R,4S,5S,7R,9E,11R,12R)-12-ETHYL-3,5,7,11-TETRAMETHYL-2,8-DIO
  XOOXACYCLODODEC-9-EN-4-YL N,N-DIMETHYLGLYCINATE (three-letter code:
  Z18) (formula: $C_{21}H_{35}NO_5$).
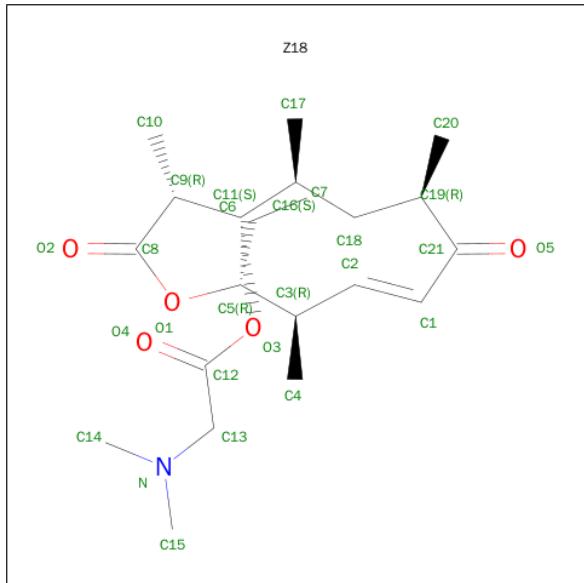
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 27	C 21	N 1	O 5	0	0
3	B	1	Total 27	C 21	N 1	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total 278	O 278	0	0
4	B	246	Total 246	O 246	0	0

3 Residue-property plots ⓘ

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 (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 HYDROXYLASE PIKC
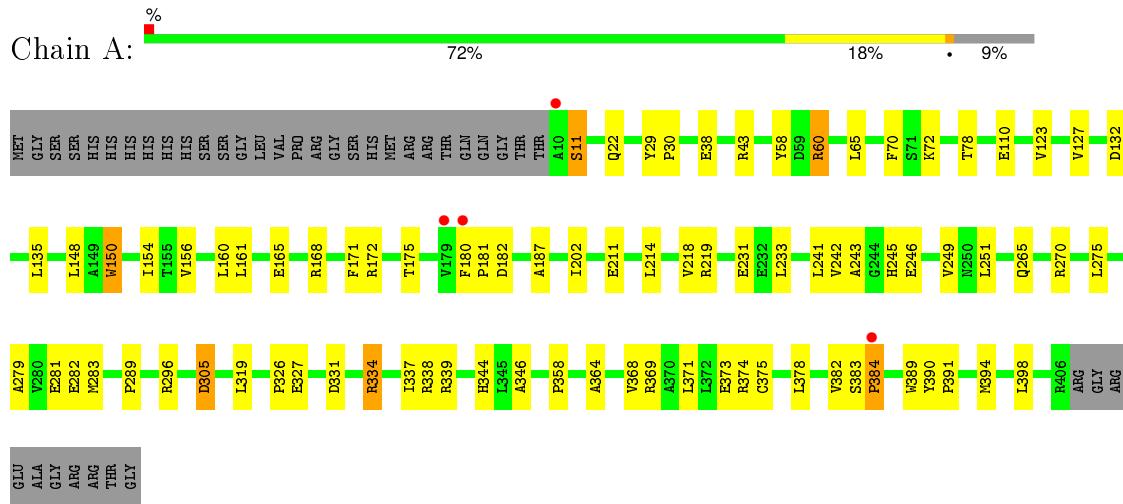
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC
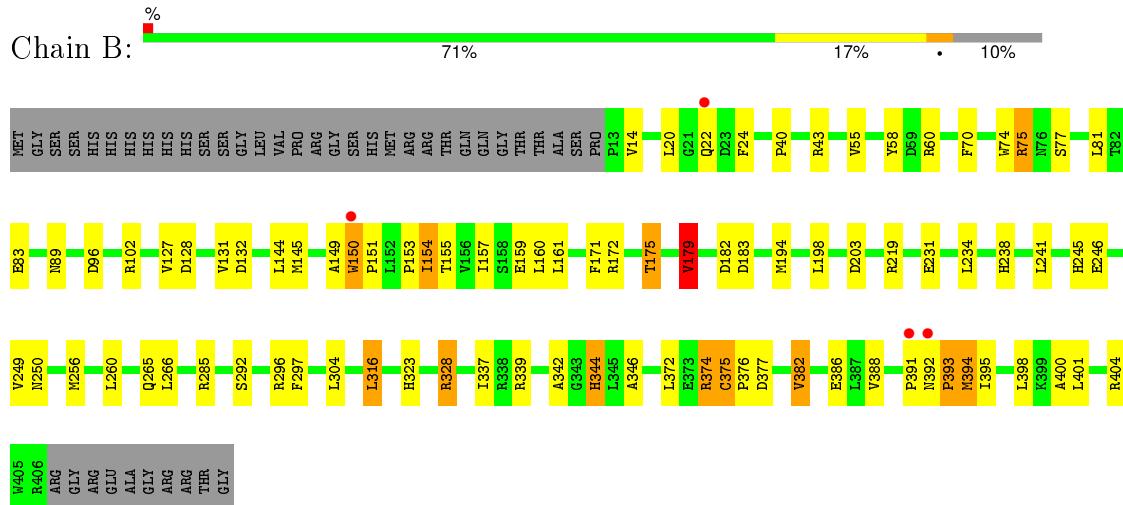
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.42Å 92.38Å 69.25Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	69.25 – 1.89 69.25 – 1.89	Depositor EDS
% Data completeness (in resolution range)	89.2 (69.25-1.89) 87.9 (69.25-1.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.76 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.267 0.198 , 0.267	Depositor DCC
R_{free} test set	2753 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 17.4	EDS
Estimated twinning fraction	0.267 for h,-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.41, <L^2> = 0.23$	Xtriage
Outliers	0 of 54264 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, Z18

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	0.97	2/3152 (0.1%)	0.97	2/4305 (0.0%)
1	B	0.95	2/3152 (0.1%)	0.95	9/4304 (0.2%)
All	All	0.96	4/6304 (0.1%)	0.96	11/8609 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	GLU	CB-CG	-5.82	1.41	1.52
1	B	375	CYS	CB-SG	-5.42	1.73	1.81
1	B	400	ALA	CA-CB	5.22	1.63	1.52
1	A	211	GLU	CG-CD	5.09	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	A	219	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	219	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	316	LEU	CA-CB-CG	5.92	128.91	115.30
1	B	102	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	219	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	179	VAL	CB-CA-C	-5.53	100.89	111.40
1	B	328	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	398	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	B	374	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	96	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3079	0	3027	61	0
1	B	3078	0	3039	77	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	27	0	35	8	0
3	B	27	0	35	6	0
4	A	278	0	0	7	0
4	B	246	0	0	7	0
All	All	6821	0	6196	147	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 12.

All (147) 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:132:ASP:OD1	1:B:374:ARG:NH2	1.77	1.16
2:B:1407:HEM:HBC2	2:B:1407:HEM:HHD	1.27	1.16
1:A:245:HIS:HA	4:A:2211:HOH:O	1.46	1.15
1:A:156:VAL:O	1:A:160:LEU:HD13	1.61	0.99
1:B:175:THR:HG21	1:B:245:HIS:CD2	2.02	0.94
1:A:175:THR:HG21	1:A:245:HIS:HD2	1.32	0.93
1:B:145:MET:HG3	1:B:150[B]:TRP:CD1	2.03	0.92
3:A:1408:Z18:H16	3:A:1408:Z18:H2	1.51	0.89
1:A:60:ARG:NH2	1:A:305:ASP:HB2	1.87	0.89
1:B:175:THR:HG21	1:B:245:HIS:HD2	1.36	0.88
1:A:132:ASP:OD1	1:A:374:ARG:NH2	2.08	0.87
1:B:150[A]:TRP:CZ3	1:B:172:ARG:HB2	2.09	0.87
1:B:150[B]:TRP:HZ3	1:B:245:HIS:HE2	1.21	0.86
1:B:344:HIS:HD2	1:B:346:ALA:H	1.24	0.84
1:B:75:ARG:HB3	1:B:75:ARG:HH11	1.39	0.84
1:A:22:GLN:HE22	1:A:389:TRP:H	1.26	0.82
1:A:38:GLU:OE2	4:A:2031:HOH:O	1.97	0.82
1:B:150[B]:TRP:HZ3	1:B:245:HIS:NE2	1.76	0.82
1:B:150[B]:TRP:CZ3	1:B:245:HIS:NE2	2.49	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ASP:CG	1:B:374:ARG:HH22	1.85	0.80
1:B:161:LEU:CD1	1:B:241:LEU:HG	2.13	0.79
1:A:265:GLN:NE2	1:A:337:ILE:H	1.79	0.78
2:B:1407:HEM:HBC2	2:B:1407:HEM:CHD	2.00	0.78
1:B:161:LEU:HD12	1:B:241:LEU:HG	1.67	0.76
3:A:1408:Z18:H7B	3:A:1408:Z18:H4	1.66	0.75
1:A:338:ARG:NH1	4:A:2253:HOH:O	2.20	0.74
1:B:150[B]:TRP:HZ2	4:B:2129:HOH:O	1.71	0.74
1:B:161:LEU:HD12	1:B:241:LEU:CG	2.19	0.73
1:A:60:ARG:HH22	1:A:305:ASP:HB2	1.51	0.73
1:B:75:ARG:HB3	1:B:75:ARG:NH1	2.04	0.72
1:B:149:ALA:O	1:B:249:VAL:HG22	1.90	0.71
1:B:179:VAL:HG13	3:B:1408:Z18:H20	1.71	0.71
1:A:175:THR:HG21	1:A:245:HIS:CD2	2.21	0.71
3:A:1408:Z18:C16	3:A:1408:Z18:H2	2.23	0.69
1:A:265:GLN:HE21	1:A:337:ILE:H	1.41	0.69
1:B:22:GLN:HG3	1:B:22:GLN:O	1.93	0.69
1:B:75:ARG:CB	1:B:75:ARG:HH11	2.05	0.68
1:B:150[A]:TRP:CH2	1:B:172:ARG:HB2	2.28	0.68
1:B:150[A]:TRP:CZ3	1:B:154:ILE:HG12	2.29	0.68
1:B:150[B]:TRP:CZ2	4:B:2129:HOH:O	2.46	0.68
1:A:281:GLU:OE1	1:A:344:HIS:HE1	1.78	0.67
2:B:1407:HEM:CBC	2:B:1407:HEM:HHD	2.15	0.67
1:A:181:PRO:HB3	1:A:187:ALA:HB2	1.75	0.67
1:B:266:LEU:HD11	1:B:372:LEU:HD21	1.77	0.66
1:B:60:ARG:HD2	1:B:304:LEU:HD22	1.77	0.66
1:B:145:MET:HG3	1:B:150[B]:TRP:HD1	1.63	0.63
1:B:89:ASN:ND2	4:B:2074:HOH:O	2.31	0.63
1:B:161:LEU:HD12	1:B:241:LEU:CD2	2.29	0.63
1:A:60:ARG:HH22	1:A:305:ASP:CB	2.12	0.62
1:B:145:MET:HA	1:B:149:ALA:HB3	1.81	0.62
1:A:344:HIS:HD2	1:A:346:ALA:H	1.48	0.62
1:B:328:ARG:NH2	1:B:342:ALA:O	2.33	0.61
1:B:14:VAL:HG22	1:B:43:ARG:HB3	1.81	0.61
1:B:157:ILE:HG23	1:B:241:LEU:HD23	1.83	0.60
1:A:242:VAL:O	1:A:245:HIS:N	2.22	0.59
1:A:358:PRO:HD2	4:A:2119:HOH:O	2.02	0.59
1:A:241:LEU:O	1:A:245:HIS:HB2	2.02	0.59
1:B:151:PRO:HA	1:B:154:ILE:HD11	1.84	0.58
1:A:154:ILE:HB	1:A:245:HIS:HE1	1.66	0.58
1:B:128:ASP:OD2	4:B:2110:HOH:O	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD21	1:A:375:CYS:SG	2.44	0.58
1:B:194:MET:CE	1:B:238:HIS:ND1	2.66	0.57
3:A:1408:Z18:C4	3:A:1408:Z18:H7B	2.35	0.57
1:B:256:MET:O	1:B:260:LEU:HG	2.05	0.57
1:B:171:PHE:O	1:B:175:THR:HB	2.06	0.56
1:A:70:PHE:HB3	1:A:296:ARG:HB3	1.88	0.55
1:A:150:TRP:CZ3	1:A:172:ARG:HB2	2.42	0.55
1:A:243:ALA:HA	3:A:1408:Z18:H5	1.88	0.55
1:B:161:LEU:HD12	1:B:241:LEU:HD21	1.88	0.55
1:B:394:MET:HE1	3:B:1408:Z18:H1	1.90	0.54
1:A:148:LEU:HD23	1:A:371:LEU:HD11	1.89	0.53
3:A:1408:Z18:C2	3:A:1408:Z18:H16	2.32	0.53
1:A:369:ARG:O	1:A:373:GLU:HG3	2.07	0.53
3:A:1408:Z18:C18	3:A:1408:Z18:H2	2.38	0.53
1:B:394:MET:HE2	3:B:1408:Z18:H20A	1.91	0.52
1:A:245:HIS:CA	4:A:2211:HOH:O	2.27	0.52
1:B:127:VAL:O	1:B:131:VAL:HG23	2.10	0.52
1:B:179:VAL:CG1	3:B:1408:Z18:H20	2.41	0.49
1:B:43:ARG:NH1	4:B:2018:HOH:O	2.44	0.49
1:A:180:PHE:HB2	1:A:390:TYR:CD1	2.47	0.49
1:B:77:SER:HB2	1:B:297:PHE:CE1	2.47	0.49
1:B:183[B]:ASP:C	1:B:183[B]:ASP:OD1	2.51	0.49
1:B:194:MET:HE1	1:B:238:HIS:ND1	2.28	0.48
1:A:150:TRP:CH2	1:A:172:ARG:HB2	2.48	0.48
1:B:183[B]:ASP:O	1:B:183[B]:ASP:OD1	2.30	0.48
1:B:150[B]:TRP:HZ3	1:B:245:HIS:CD2	2.31	0.48
1:B:395:ILE:HD11	3:B:1408:Z18:H4B	1.95	0.48
1:B:150[B]:TRP:O	1:B:153:PRO:HD2	2.14	0.48
1:A:60:ARG:HH22	1:A:305:ASP:CG	2.17	0.48
1:B:265:GLN:NE2	1:B:337:ILE:H	2.12	0.48
1:A:202:ILE:HG12	1:A:214:LEU:HD11	1.95	0.48
1:A:364:ALA:O	1:A:368:VAL:HG23	2.14	0.47
1:B:382:VAL:HG22	1:B:386:GLU:CD	2.35	0.47
1:B:77:SER:HB2	1:B:297:PHE:CD1	2.49	0.47
1:B:376:PRO:HA	4:B:2239:HOH:O	2.14	0.47
1:A:270:ARG:HH22	1:A:378:LEU:HB3	1.80	0.47
1:A:154:ILE:HD13	1:A:245:HIS:CE1	2.50	0.47
1:A:245:HIS:O	1:A:249:VAL:HG23	2.15	0.47
1:B:198:LEU:HB2	1:B:234:LEU:CD1	2.45	0.47
1:B:266:LEU:CD1	1:B:372:LEU:HD21	2.45	0.46
1:A:202:ILE:HD13	1:A:233:LEU:HG	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.50	0.46
1:B:150[A]:TRP:CE3	1:B:172:ARG:HG3	2.51	0.46
1:A:180:PHE:CE2	1:A:182:ASP:OD1	2.69	0.45
1:A:78:THR:HG21	4:A:2085:HOH:O	2.16	0.45
1:A:326:PRO:HD2	1:A:327:GLU:OE1	2.16	0.45
1:B:394:MET:HE3	1:B:394:MET:HB3	1.76	0.45
1:B:344:HIS:CD2	1:B:346:ALA:H	2.16	0.45
1:B:20:LEU:HB3	1:B:24:PHE:HB2	1.97	0.45
1:A:279:ALA:O	1:A:283:MET:HG3	2.17	0.45
1:A:172:ARG:NH2	1:B:83:GLU:HG2	2.32	0.45
1:A:22:GLN:O	1:A:22:GLN:HG3	2.16	0.45
1:B:394:MET:CE	3:B:1408:Z18:H1	2.48	0.44
1:B:145:MET:HE2	1:B:145:MET:HB2	1.69	0.44
1:B:155:THR:O	1:B:159:GLU:HG3	2.18	0.44
1:A:110:GLU:OE2	4:A:2113:HOH:O	2.21	0.44
1:A:289:PRO:HG2	2:A:1407:HEM:HMB2	2.00	0.44
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.80	0.44
1:A:383:SER:HA	1:A:384:PRO:HD2	1.76	0.44
1:A:60:ARG:NH2	1:A:305:ASP:CB	2.68	0.43
1:A:275:LEU:HD11	1:A:338:ARG:NH1	2.34	0.43
1:B:70:PHE:HB3	1:B:296:ARG:HB3	2.00	0.43
1:A:175:THR:HG23	1:A:246:GLU:OE2	2.19	0.43
1:A:331:ASP:OD2	1:A:334:ARG:HD3	2.19	0.43
1:B:58:TYR:C	1:B:58:TYR:CD1	2.91	0.43
1:A:132:ASP:OD1	1:A:374:ARG:CZ	2.66	0.42
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.19	0.42
1:B:231:GLU:CG	4:B:2187:HOH:O	2.67	0.42
1:B:392:ASN:HA	1:B:393:PRO:HD2	1.59	0.42
1:B:40:PRO:O	1:B:55:VAL:HA	2.20	0.42
1:A:123:VAL:O	1:A:127:VAL:HG23	2.20	0.42
1:A:65:LEU:HD11	1:A:319:LEU:CD2	2.50	0.42
1:B:150[A]:TRP:O	1:B:153:PRO:HD2	2.20	0.41
1:A:165:GLU:HA	1:A:168:ARG:NE	2.35	0.41
1:B:292:SER:CB	1:B:316:LEU:HD13	2.51	0.41
1:B:285:ARG:O	1:B:323:HIS:HB3	2.20	0.41
1:B:144:LEU:HD23	1:B:401:LEU:HD23	2.02	0.41
1:A:180:PHE:CD1	1:A:391:PRO:HD2	2.56	0.41
1:A:202:ILE:HG23	1:A:218:VAL:HG22	2.03	0.41
1:A:29:TYR:N	1:A:30:PRO:CD	2.84	0.41
1:A:389:TRP:CE2	1:A:398:LEU:HD21	2.55	0.41
1:B:246:GLU:O	1:B:250:ASN:ND2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:CYS:HA	1:B:376:PRO:HD3	1.87	0.41
1:A:58:TYR:CD1	1:A:58:TYR:C	2.95	0.40
1:A:171:PHE:O	1:A:175:THR:HG22	2.21	0.40
1:A:251:LEU:HD22	2:A:1407:HEM:HBB1	2.04	0.40
3:A:1408:Z18:C21	3:A:1408:Z18:H17	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/436 (91%)	381 (96%)	14 (4%)	2 (0%)	34	21
1	B	394/436 (90%)	380 (96%)	12 (3%)	2 (0%)	34	21
All	All	791/872 (91%)	761 (96%)	26 (3%)	4 (0%)	34	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	PRO
1	A	11	SER
1	B	393	PRO
1	B	391	PRO

5.3.2 Protein sidechains (i)

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	319/355 (90%)	308 (97%)	11 (3%)	44	33
1	B	321/355 (90%)	306 (95%)	15 (5%)	32	20
All	All	640/710 (90%)	614 (96%)	26 (4%)	39	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	43	ARG
1	A	60	ARG
1	A	72	LYS
1	A	150	TRP
1	A	161	LEU
1	A	305	ASP
1	A	334	ARG
1	A	339	ARG
1	A	382	VAL
1	A	394	MET
1	B	75	ARG
1	B	150[A]	TRP
1	B	150[B]	TRP
1	B	154	ILE
1	B	175	THR
1	B	179	VAL
1	B	182	ASP
1	B	203	ASP
1	B	339	ARG
1	B	344	HIS
1	B	377	ASP
1	B	382	VAL
1	B	388	VAL
1	B	394	MET
1	B	404	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	188	GLN
1	A	245	HIS
1	A	265	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	344	HIS
1	B	22	GLN
1	B	89	ASN
1	B	188	GLN
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

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 carbohydrates in this entry.

5.6   Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
2	HEM	A	1407	1	30,50,50	2.44	8 (26%)	24,82,82	2.77	13 (54%)
3	Z18	A	1408	-	25,27,27	1.39	2 (8%)	25,37,37	1.95	5 (20%)
2	HEM	B	1407	1	30,50,50	2.40	8 (26%)	24,82,82	2.68	8 (33%)
3	Z18	B	1408	-	25,27,27	1.33	3 (12%)	25,37,37	1.76	5 (20%)

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	HEM	A	1407	1	-	0/10/54/54	0/0/8/8
3	Z18	A	1408	-	-	0/43/43/43	0/0/1/1
2	HEM	B	1407	1	-	0/10/54/54	0/0/8/8
3	Z18	B	1408	-	-	0/43/43/43	0/0/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1407	HEM	C3B-C4B	-10.07	1.42	1.51
2	B	1407	HEM	C3B-C4B	-8.90	1.43	1.51
2	B	1407	HEM	C3D-C4D	-5.27	1.44	1.51
2	A	1407	HEM	C2C-C1C	-4.01	1.45	1.52
2	B	1407	HEM	C2C-C1C	-3.80	1.45	1.52
2	A	1407	HEM	C3D-C4D	-3.70	1.46	1.51
2	A	1407	HEM	C2D-C1D	-2.50	1.43	1.51
2	B	1407	HEM	C2B-C1B	-2.34	1.44	1.51
2	A	1407	HEM	C2B-C1B	-2.13	1.44	1.51
2	B	1407	HEM	CMA-C3A	2.04	1.55	1.51
2	B	1407	HEM	CAD-C3D	2.06	1.58	1.54
3	B	1408	Z18	C18-C16	2.14	1.57	1.54
2	B	1407	HEM	CMD-C2D	2.19	1.58	1.53
2	A	1407	HEM	FE-NC	2.65	2.06	1.95
2	A	1407	HEM	CMA-C3A	2.88	1.57	1.51
2	B	1407	HEM	C1C-NC	2.94	1.39	1.36
3	B	1408	Z18	O3-C12	3.11	1.43	1.34
3	A	1408	Z18	O3-C12	3.15	1.43	1.34
2	A	1407	HEM	C3C-CAC	3.29	1.57	1.51
3	B	1408	Z18	O1-C8	4.48	1.44	1.34
3	A	1408	Z18	O1-C8	5.55	1.47	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1407	HEM	C3C-CAC-CBC	-7.28	113.28	124.46
3	A	1408	Z18	C2-C1-C21	-6.72	114.36	123.22
3	B	1408	Z18	C5-O1-C8	-5.40	109.61	117.92
2	A	1407	HEM	CAA-C2A-C1A	-4.27	122.37	127.01
2	B	1407	HEM	CBD-CAD-C3D	-3.21	104.22	113.55
2	A	1407	HEM	C3B-CAB-CBB	-2.82	120.14	124.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1407	HEM	CBD-CAD-C3D	-2.70	105.69	113.55
2	A	1407	HEM	CBA-CAA-C2A	-2.58	107.91	112.53
3	A	1408	Z18	O3-C12-O4	-2.53	116.88	123.67
3	A	1408	Z18	C17-C16-C18	-2.37	107.08	110.76
3	B	1408	Z18	C2-C1-C21	-2.23	120.29	123.22
3	A	1408	Z18	C5-O1-C8	-2.20	114.53	117.92
3	B	1408	Z18	C17-C16-C11	-2.03	107.70	111.27
2	A	1407	HEM	CHD-C1D-ND	2.38	130.26	124.52
3	B	1408	Z18	O1-C5-C6	2.39	110.64	106.59
2	A	1407	HEM	CMD-C2D-C3D	2.47	125.26	114.35
3	B	1408	Z18	C17-C16-C18	2.56	114.74	110.76
2	A	1407	HEM	C3B-C4B-CHC	2.61	126.84	123.16
2	B	1407	HEM	CMD-C2D-C3D	2.72	126.36	114.35
3	A	1408	Z18	O1-C8-C9	2.77	117.17	111.47
2	A	1407	HEM	CAD-C3D-C2D	2.92	121.60	113.22
2	B	1407	HEM	C2D-C3D-C4D	3.06	106.69	101.50
2	A	1407	HEM	C2D-C3D-C4D	3.37	107.21	101.50
2	A	1407	HEM	CMB-C2B-C3B	4.07	126.69	116.53
2	B	1407	HEM	CMB-C2B-C3B	4.25	127.14	116.53
2	B	1407	HEM	CAD-C3D-C4D	4.29	127.61	112.47
2	B	1407	HEM	CAD-C3D-C2D	4.34	125.70	113.22
2	B	1407	HEM	CMC-C2C-C3C	4.59	127.98	116.53
2	A	1407	HEM	C3C-CAC-CBC	4.62	131.54	124.46
2	A	1407	HEM	CAD-C3D-C4D	5.30	131.18	112.47
2	A	1407	HEM	CMC-C2C-C3C	5.61	130.54	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	HEM	2	0
3	A	1408	Z18	8	0
2	B	1407	HEM	3	0
3	B	1408	Z18	6	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	397/436 (91%)	-0.31	4 (1%)	84	86	10, 19, 32, 45	0
1	B	394/436 (90%)	-0.26	4 (1%)	84	86	11, 21, 34, 47	0
All	All	791/872 (90%)	-0.29	8 (1%)	84	86	10, 19, 34, 47	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	5.6
1	A	384	PRO	4.3
1	B	392	ASN	3.5
1	B	150[A]	TRP	3.1
1	A	180	PHE	3.1
1	B	22	GLN	2.7
1	B	391	PRO	2.5
1	A	179	VAL	2.2

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 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(Å^2)	Q<0.9
2	HEM	B	1407	43/43	0.98	0.10	1.70	9,13,17,24	0
3	Z18	A	1408	27/27	0.88	0.15	1.42	17,26,36,40	0
3	Z18	B	1408	27/27	0.94	0.11	0.29	17,21,25,27	0
2	HEM	A	1407	43/43	0.98	0.09	0.03	4,12,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.