



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:57 AM GMT

PDB ID : 3GPH
Title : Human cytochrome P450 2E1 in complex with omega-imidazolyl-decanoic acid
Authors : Porubsky, P.R.; Battaile, K.P.; Scott, E.E.
Deposited on : 2009-03-23
Resolution : 2.70 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

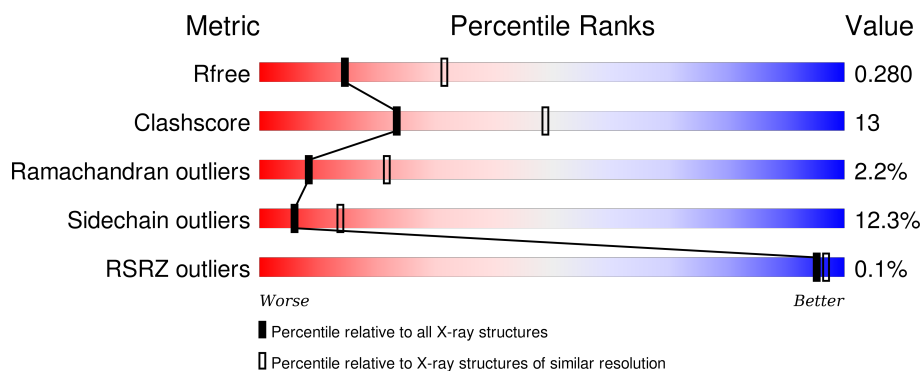
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	476	 69% 23% 5% .
1	B	476	 63% 26% 6% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OID	A	501	-	-	-	X
3	OID	B	501	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7682 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 2E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	1	0
			3772	2442	648	665	17			
1	B	461	Total	C	N	O	S	0	0	0
			3765	2437	646	665	17			

There are 28 discrepancies between the modelled and reference sequences:

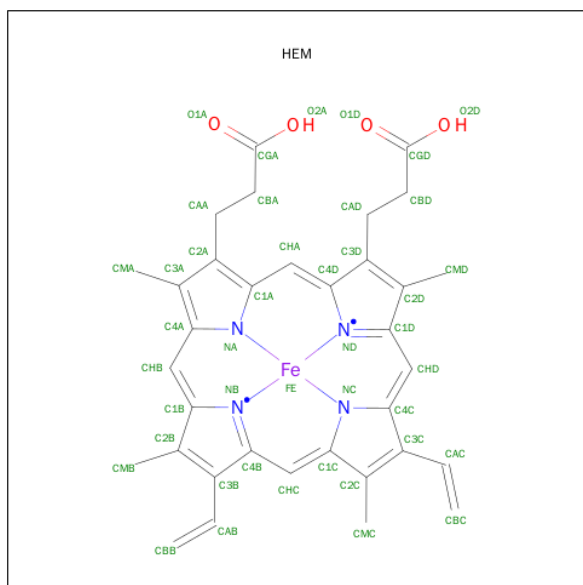
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	EXPRESSION TAG	UNP P05181
A	23	ALA	-	EXPRESSION TAG	UNP P05181
A	24	LYS	-	EXPRESSION TAG	UNP P05181
A	25	LYS	-	EXPRESSION TAG	UNP P05181
A	26	THR	-	EXPRESSION TAG	UNP P05181
A	27	SER	-	EXPRESSION TAG	UNP P05181
A	28	SER	-	EXPRESSION TAG	UNP P05181
A	29	LYS	-	EXPRESSION TAG	UNP P05181
A	30	GLY	-	EXPRESSION TAG	UNP P05181
A	31	LYS	-	EXPRESSION TAG	UNP P05181
A	494	HIS	-	EXPRESSION TAG	UNP P05181
A	495	HIS	-	EXPRESSION TAG	UNP P05181
A	496	HIS	-	EXPRESSION TAG	UNP P05181
A	497	HIS	-	EXPRESSION TAG	UNP P05181
B	22	MET	-	EXPRESSION TAG	UNP P05181
B	23	ALA	-	EXPRESSION TAG	UNP P05181
B	24	LYS	-	EXPRESSION TAG	UNP P05181
B	25	LYS	-	EXPRESSION TAG	UNP P05181
B	26	THR	-	EXPRESSION TAG	UNP P05181
B	27	SER	-	EXPRESSION TAG	UNP P05181
B	28	SER	-	EXPRESSION TAG	UNP P05181
B	29	LYS	-	EXPRESSION TAG	UNP P05181
B	30	GLY	-	EXPRESSION TAG	UNP P05181
B	31	LYS	-	EXPRESSION TAG	UNP P05181
B	494	HIS	-	EXPRESSION TAG	UNP P05181

Continued on next page...

Continued from previous page...

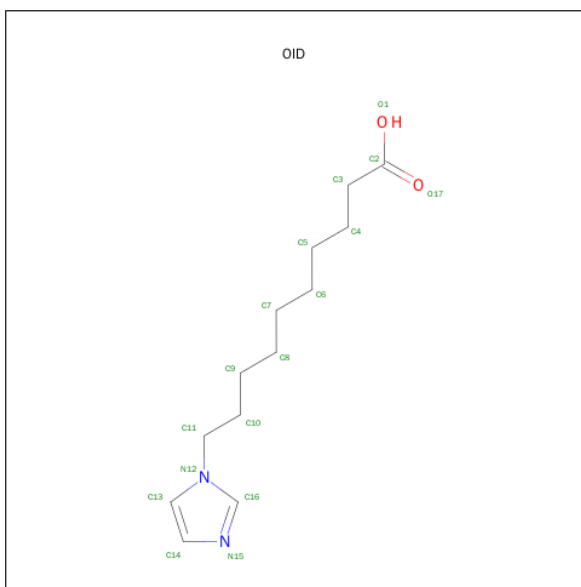
Chain	Residue	Modelled	Actual	Comment	Reference
B	495	HIS	-	EXPRESSION TAG	UNP P05181
B	496	HIS	-	EXPRESSION TAG	UNP P05181
B	497	HIS	-	EXPRESSION TAG	UNP P05181

- 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 10-(1H-IMIDAZOL-1-YL)DECANOIC ACID (three-letter code: OID) (formula: $C_{13}H_{22}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	13	2	2		
3	B	1	Total	C	N	O	0	0
			17	13	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	10	Total	O	0	0
			10	10		

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.

Chain A:

Chain A	Chain B	Chain C	Chain D	Chain E	Chain F	Chain G	Chain H	Chain I	Chain J	Chain K	Chain L	Chain M	Chain N	Chain O	Chain P	Chain Q	Chain R	Chain S	Chain T	Chain U	Chain V	Chain W	Chain X	Chain Y	Chain Z																	
Met	ALA	LVS	THR	SER	SER	LVS	GLY	K31	L32	F46	L50	I53	P54	T58	Q62	R63	L70	G73	S74	M77	V78	M80	H81	G82	Y83	K87	L90	K94	D95	E96	R110	D111	R112	G113	I114	N117	N118	T121	K123	R126	R127	
R134	G137	Met	GLY	K140	Q141	G142	S145	A157	K160	L171	T180	L184	F185	R186	D193	E194	K195	L199	M200	M206	F207	L217	L225	R233	K234	V235	V239	V246	R249	C261	T266	L270	E274	K275	K277	H278	G279					
K280	E281	R282	L283	V284	T285	K286	T289	T290	V293	F298	E302	T303	T304	L308	K309	Y310	G311	L312	L313	K317	Y318	T321	H326	E327	E328	R331	K342	P348	V349	H350	V354	I357	T361	V364	N367	L368	E371	R374	D375	T376		
R379	T387	V388	V389	V390	P391	Q401	K410	F411	E412	H413	N416	E417	N418	G419	K420	D425	V436	G439	E446	L450	L455	K461	V464	D465	L471	P482	Y485	K486	L487	C488	V489	L490	P491	A492	S493	HIS	HIS	HIS	HIS			

Chain B:

63% 26% 6% 5%

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	70.71Å 70.71Å 222.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.31 – 2.70 30.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.31-2.70) 95.5 (30.42-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.283 0.210 , 0.280	Depositor DCC
R_{free} test set	1442 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -6.6	EDS
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 28481 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7682	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.86	1/3880 (0.0%)	0.91	2/5254 (0.0%)
1	B	0.91	4/3869 (0.1%)	0.93	3/5239 (0.1%)
All	All	0.88	5/7749 (0.1%)	0.92	5/10493 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	412	GLU	CG-CD	5.87	1.60	1.51
1	B	219	ASN	CB-CG	5.50	1.63	1.51
1	B	244	GLU	CG-CD	5.34	1.59	1.51
1	B	214	TRP	CB-CG	5.15	1.59	1.50
1	A	261	CYS	CB-SG	-5.02	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	LEU	CA-CB-CG	-7.08	99.03	115.30
1	B	70	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	447	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	73	GLY	N-CA-C	-5.39	99.62	113.10
1	A	465	ASP	CB-CG-OD1	5.01	122.81	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	3772	0	3775	82	0
1	B	3765	0	3768	121	0
2	A	43	0	30	12	0
2	B	43	0	30	7	0
3	A	17	0	21	3	0
3	B	17	0	21	1	0
4	A	15	0	0	3	0
4	B	10	0	0	1	0
All	All	7682	0	7645	204	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 13.

All (204) 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:142:GLY:HA2	4:A:18:HOH:O	1.28	1.27
1:A:303:THR:HG21	2:A:500:HEM:CHC	1.80	1.12
1:B:63:ARG:HH21	1:B:63:ARG:HG2	1.22	1.03
1:B:94:LYS:HB2	1:B:434:LYS:HG2	1.42	1.01
1:A:303:THR:HG23	2:A:500:HEM:HBB2	1.46	0.97
1:B:257:LEU:HG	1:B:258:ASP:H	1.33	0.90
1:A:303:THR:HG21	2:A:500:HEM:HHC	1.54	0.90
1:B:94:LYS:HB2	1:B:434:LYS:CG	2.03	0.88
1:A:137:GLY:O	1:A:140:LYS:HB3	1.74	0.88
1:B:63:ARG:HH21	1:B:63:ARG:CG	1.87	0.87
1:B:432:THR:HA	1:B:436:VAL:HG13	1.54	0.86
1:B:112:ARG:HH11	1:B:112:ARG:HG2	1.41	0.85
1:A:96:GLU:HG2	1:A:376:THR:HG21	1.58	0.84
1:B:114:ILE:HD12	1:B:126:ARG:HG3	1.56	0.84
1:B:359:ARG:NH2	1:B:406:PRO:O	2.11	0.84
1:A:73:GLY:HA3	4:A:502:HOH:O	1.80	0.82
1:A:303:THR:HG23	2:A:500:HEM:CBB	2.10	0.81
1:A:303:THR:CG2	2:A:500:HEM:CHC	2.59	0.80
1:A:303:THR:CG2	2:A:500:HEM:HHC	2.13	0.78
1:A:286:MET:O	1:A:290:THR:HG23	1.84	0.77
1:B:432:THR:HA	1:B:436:VAL:CG1	2.14	0.76
1:B:112:ARG:HD3	1:B:112:ARG:N	2.02	0.74
1:A:157:ALA:HB1	1:A:171:LEU:HD11	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PRO:O	1:B:406:PRO:HD3	1.87	0.74
1:A:123:LYS:HE3	1:A:127:ARG:HH22	1.51	0.74
1:B:137:GLY:HA3	1:B:143:ASN:HB2	1.70	0.72
1:B:63:ARG:NH2	1:B:63:ARG:CG	2.49	0.70
1:B:114:ILE:HG12	2:B:500:HEM:HAD1	1.74	0.68
1:B:140:LYS:HG2	1:B:141:GLN:H	1.58	0.68
1:B:127:ARG:CZ	1:B:127:ARG:HB3	2.22	0.68
1:B:257:LEU:CG	1:B:258:ASP:H	2.07	0.67
1:B:278:HIS:HA	4:B:2:HOH:O	1.93	0.67
1:A:235:VAL:O	1:A:239:VAL:HG23	1.95	0.66
1:A:142:GLY:CA	4:A:18:HOH:O	2.06	0.66
1:B:274:GLU:C	1:B:276:GLU:H	1.98	0.65
1:B:180:ILE:HG13	1:B:184:LEU:HD22	1.78	0.65
1:A:111:ASP:HA	1:A:117:ASN:HB2	1.79	0.65
1:A:318:TYR:HB3	1:A:321:ILE:HD12	1.78	0.64
1:A:112:ARG:O	1:A:117:ASN:HB3	1.98	0.63
1:B:356:GLU:OE2	1:B:359:ARG:NH1	2.33	0.62
1:A:416:ASN:C	1:A:418:ASN:H	2.01	0.62
1:B:317:LYS:HD3	1:B:471:LEU:HD22	1.81	0.61
1:B:114:ILE:CD1	1:B:126:ARG:HG3	2.27	0.60
1:A:53:ILE:HB	1:A:54:PRO:HD3	1.82	0.60
1:B:215:LEU:HD11	1:B:231:SER:HB3	1.83	0.60
1:B:31:LYS:HG3	1:B:382:LEU:HB2	1.84	0.60
1:B:112:ARG:HG2	1:B:112:ARG:NH1	2.13	0.60
1:A:303:THR:HG22	1:A:304:THR:H	1.67	0.59
1:B:257:LEU:HG	1:B:258:ASP:N	2.13	0.59
1:B:110:ARG:O	1:B:112:ARG:HD3	2.02	0.59
1:B:104:PRO:HG2	1:B:222:PRO:HG3	1.85	0.59
1:A:282:ARG:HH21	1:A:284:TYR:HB2	1.68	0.59
1:B:327:GLU:OE1	1:B:331:ARG:NH2	2.35	0.59
1:A:114:ILE:CD1	1:A:126:ARG:HG3	2.33	0.58
1:B:235:VAL:O	1:B:239:VAL:HG23	2.03	0.58
1:B:298:PHE:CD1	3:B:501:OID:H6A	2.38	0.58
1:B:403:PHE:O	1:B:404:PRO:C	2.41	0.58
1:A:111:ASP:CA	1:A:117:ASN:HB2	2.33	0.57
1:A:303:THR:HG21	2:A:500:HEM:C1C	2.38	0.57
1:B:448:PHE:HD2	1:B:449:LEU:HD23	1.70	0.56
1:B:448:PHE:CD2	1:B:449:LEU:HD23	2.40	0.56
1:B:342:LYS:O	1:B:345:GLN:HG2	2.06	0.56
1:B:461:LYS:HB3	1:B:488:CYS:HB2	1.88	0.56
1:B:59:ARG:O	1:B:62:GLN:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:THR:CA	1:B:436:VAL:HG13	2.31	0.55
1:B:356:GLU:CD	1:B:359:ARG:HH11	2.09	0.55
1:A:94:LYS:HE3	1:A:95:ASP:OD2	2.05	0.55
1:B:356:GLU:HG3	1:B:409:PHE:CE1	2.41	0.55
1:B:112:ARG:NH1	1:B:287:ASP:OD2	2.40	0.55
1:A:357:ILE:O	1:A:361:ILE:HG12	2.06	0.55
1:B:440:GLU:O	1:B:444:ARG:HG2	2.06	0.55
1:B:274:GLU:C	1:B:276:GLU:N	2.61	0.54
1:A:303:THR:CG2	2:A:500:HEM:HBB2	2.28	0.54
1:B:274:GLU:O	1:B:276:GLU:N	2.40	0.54
1:A:180:ILE:HG13	1:A:184:LEU:HD22	1.88	0.54
1:A:318:TYR:CB	1:A:321:ILE:HD12	2.38	0.54
1:A:118:ASN:ND2	1:A:371:GLU:OE2	2.39	0.54
1:B:36:PRO:O	1:B:38:PRO:HD3	2.07	0.54
1:B:400:ASN:HB3	1:B:406:PRO:HG3	1.89	0.54
1:B:94:LYS:HB2	1:B:434:LYS:HG3	1.89	0.54
1:B:156:GLU:O	1:B:160:LYS:HB2	2.07	0.53
1:B:147:ILE:HD12	1:B:445:MET:HG3	1.89	0.53
1:A:416:ASN:OD1	1:A:418:ASN:HB3	2.09	0.53
1:B:53:ILE:HG13	1:B:216:GLN:NE2	2.24	0.53
1:B:137:GLY:HA2	1:B:140:LYS:HB3	1.90	0.53
2:A:500:HEM:HHC	2:A:500:HEM:HBB2	1.91	0.52
1:B:281:GLU:O	1:B:281:GLU:HG2	2.10	0.52
1:A:266:THR:HG22	1:A:270:LEU:HD22	1.91	0.52
1:B:286:MET:O	1:B:290:THR:HG23	2.09	0.52
1:A:342:LYS:HB3	1:B:281:GLU:OE1	2.09	0.52
1:A:374:ARG:NH1	1:A:375:ASP:H	2.08	0.52
1:A:114:ILE:HD12	1:A:126:ARG:HG3	1.92	0.52
1:B:338:ILE:HD12	1:B:338:ILE:H	1.75	0.52
1:A:303:THR:CG2	1:A:304:THR:N	2.73	0.51
1:B:249:ARG:NE	1:B:249:ARG:HA	2.26	0.51
1:A:461:LYS:HB3	1:A:488:CYS:HB2	1.93	0.51
1:B:433:GLY:O	1:B:436:VAL:HG22	2.11	0.51
1:B:73:GLY:HA2	1:B:221:PHE:CE1	2.45	0.51
1:A:298:PHE:C	1:A:298:PHE:CD1	2.83	0.51
1:A:446:GLU:O	1:A:450:LEU:HB2	2.10	0.51
1:B:214:TRP:CD1	1:B:231:SER:HB2	2.45	0.50
1:B:303:THR:HB	2:B:500:HEM:HBB2	1.94	0.50
1:A:412:GLU:H	1:A:412:GLU:CD	2.15	0.50
1:B:436:VAL:O	1:B:437:CYS:C	2.48	0.49
1:B:110:ARG:O	1:B:112:ARG:CD	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HD22	1:B:284:TYR:HE1	1.77	0.49
1:A:270:LEU:O	1:A:274:GLU:HG2	2.12	0.49
1:B:173:GLY:O	1:B:177:CYS:HB2	2.13	0.49
1:B:363:LEU:O	1:B:479:GLY:HA2	2.13	0.49
1:B:53:ILE:HG13	1:B:216:GLN:HE21	1.78	0.49
1:B:147:ILE:CD1	1:B:445:MET:HG3	2.43	0.49
1:A:96:GLU:HG2	1:A:376:THR:CG2	2.37	0.49
1:A:289:ILE:O	1:A:293:VAL:HG23	2.13	0.49
1:B:209:LEU:O	1:B:215:LEU:HD13	2.13	0.48
1:B:215:LEU:CD1	1:B:231:SER:HB3	2.43	0.48
1:B:48:LEU:HD13	1:B:53:ILE:HD13	1.96	0.48
1:B:137:GLY:CA	1:B:140:LYS:HB3	2.44	0.48
1:B:130:LEU:O	1:B:134:ARG:HG3	2.14	0.48
1:B:484:ARG:HH11	1:B:484:ARG:HG2	1.78	0.48
1:A:303:THR:HG22	1:A:304:THR:N	2.28	0.48
1:A:78:VAL:HG23	1:A:387:THR:HG21	1.96	0.48
1:B:410:LYS:HB2	1:B:413:HIS:CE1	2.49	0.48
1:A:368:LEU:HB2	2:A:500:HEM:HAA1	1.95	0.47
1:B:137:GLY:CA	1:B:143:ASN:HB2	2.41	0.47
1:B:300:GLY:HA2	2:B:500:HEM:HMC2	1.97	0.47
1:B:31:LYS:O	1:B:381:TYR:HB3	2.15	0.47
1:B:368:LEU:HB2	2:B:500:HEM:HAA2	1.95	0.47
1:A:50:LEU:HD11	1:A:217:LEU:HD13	1.97	0.47
1:A:302:GLU:OE2	1:A:302:GLU:HA	2.14	0.47
1:B:306:THR:HA	1:B:309:ARG:NH2	2.30	0.46
1:B:205:GLU:OE1	1:B:238:ASN:ND2	2.42	0.46
1:A:276:GLU:HB3	1:A:282:ARG:CZ	2.46	0.46
1:A:246:VAL:HG11	1:A:290:THR:O	2.15	0.46
1:A:195:LYS:O	1:A:199:LEU:HD22	2.16	0.46
1:B:186:ARG:HG2	1:B:263:ARG:HB3	1.96	0.46
1:B:100:ARG:HG2	1:B:115:ILE:O	2.15	0.45
1:B:252:GLU:O	1:B:256:SER:HB3	2.17	0.45
1:B:303:THR:CB	2:B:500:HEM:HBB2	2.46	0.45
1:B:180:ILE:O	1:B:184:LEU:HB2	2.17	0.45
1:A:439:GLY:HA3	2:A:500:HEM:C3C	2.52	0.45
1:B:356:GLU:OE1	1:B:359:ARG:HD3	2.17	0.45
1:A:79:VAL:HG22	1:A:390:VAL:HB	1.98	0.45
1:B:161:THR:C	1:B:162:GLN:HG2	2.37	0.45
1:A:110:ARG:O	1:A:112:ARG:NE	2.47	0.45
1:B:189:PHE:CG	1:B:196:PHE:CD1	3.04	0.45
1:B:463:LEU:HD12	1:B:486:LYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TRP:CZ2	1:B:435:ARG:HG2	2.53	0.44
1:B:326:HIS:HB3	1:B:492:ARG:HH22	1.82	0.44
1:A:326:HIS:CE1	1:A:455:LEU:O	2.70	0.44
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	2.00	0.44
1:A:389:VAL:O	1:A:391:PRO:HD3	2.16	0.44
1:B:206:ASN:O	1:B:210:LEU:HG	2.18	0.44
1:B:110:ARG:O	1:B:112:ARG:NE	2.50	0.44
1:B:127:ARG:NH1	1:B:127:ARG:HB3	2.33	0.44
1:A:207:PHE:CE1	3:A:501:OID:H9A	2.52	0.44
1:B:137:GLY:C	1:B:140:LYS:HB3	2.38	0.44
1:B:53:ILE:HB	1:B:54:PRO:HD3	1.99	0.44
1:A:350:MET:HE2	1:A:354:VAL:HG23	1.99	0.43
1:B:316:MET:SD	1:B:487:LEU:HD23	2.58	0.43
1:B:212:THR:O	1:B:213:PRO:C	2.55	0.43
1:B:112:ARG:CG	1:B:112:ARG:HH11	2.17	0.43
1:B:274:GLU:OE1	1:B:277:LYS:HD3	2.18	0.43
1:A:410:LYS:HB2	1:A:413:HIS:CE1	2.53	0.43
1:A:277:LYS:O	1:A:279:SER:N	2.45	0.43
1:A:416:ASN:C	1:A:418:ASN:N	2.69	0.43
1:B:248:GLU:O	1:B:252:GLU:HG3	2.18	0.43
1:A:317:LYS:HG2	1:A:471:LEU:HD22	2.01	0.43
1:A:58:THR:HG23	1:A:81:HIS:CE1	2.54	0.43
1:A:310:TYR:CD1	1:A:482:PRO:HB3	2.54	0.43
1:A:266:THR:HG22	1:A:270:LEU:CD2	2.48	0.43
1:A:328:GLU:OE1	1:A:348:PRO:HD2	2.17	0.43
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.91	0.43
1:B:397:LEU:HD21	1:B:428:LYS:H	1.84	0.42
1:A:328:GLU:HG3	1:A:331:ARG:HH12	1.84	0.42
1:A:401:GLN:HA	1:A:401:GLN:NE2	2.34	0.42
1:B:303:THR:HB	2:B:500:HEM:CBB	2.49	0.42
1:A:416:ASN:O	1:A:418:ASN:N	2.43	0.42
1:A:83:TYR:OH	1:A:425:ASP:OD1	2.26	0.42
1:A:282:ARG:CZ	1:A:283:LEU:H	2.32	0.42
1:B:189:PHE:CD1	1:B:196:PHE:HB2	2.55	0.42
1:A:490:ILE:HA	1:A:491:PRO:HD2	1.85	0.42
1:A:206:ASN:ND2	3:A:501:OID:O1	2.47	0.42
1:A:367:ASN:OD1	2:A:500:HEM:HAA2	2.20	0.41
1:B:189:PHE:CD2	1:B:196:PHE:CD1	3.08	0.41
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.85	0.41
1:A:83:TYR:O	1:A:87:LYS:HB2	2.20	0.41
1:A:308:LEU:HA	1:A:308:LEU:HD23	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:HE2	1:B:275:LYS:HB3	1.89	0.41
1:B:127:ARG:NH1	1:B:127:ARG:CB	2.84	0.41
1:B:149:ARG:HD2	1:B:149:ARG:HA	1.86	0.41
1:A:77:MET:HB3	1:A:388:VAL:HB	2.02	0.41
1:B:31:LYS:HA	1:B:31:LYS:HD3	1.84	0.41
1:A:298:PHE:CD1	3:A:501:OID:H5	2.56	0.41
1:A:313:LEU:HB2	1:A:485:TYR:CE2	2.56	0.41
1:B:137:GLY:HA2	1:B:140:LYS:HD3	2.02	0.41
1:B:127:ARG:CZ	1:B:127:ARG:CB	2.97	0.41
1:B:100:ARG:HD3	1:B:369:PRO:O	2.21	0.41
1:B:114:ILE:HD12	1:B:126:ARG:CG	2.41	0.41
1:B:356:GLU:CD	1:B:359:ARG:NH1	2.73	0.41
1:B:393:LEU:O	1:B:397:LEU:HG	2.21	0.40
1:A:90:LEU:HD11	1:A:391:PRO:HG2	2.03	0.40
1:A:112:ARG:O	1:A:117:ASN:CB	2.66	0.40
1:B:93:TYR:CE2	1:B:378:PHE:CD1	3.09	0.40
1:B:47:GLN:HG2	1:B:60:LEU:HD21	2.03	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	458/476 (96%)	418 (91%)	33 (7%)	7 (2%)	13	32
1	B	457/476 (96%)	409 (90%)	35 (8%)	13 (3%)	6	15
All	All	915/952 (96%)	827 (90%)	68 (7%)	20 (2%)	8	22

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	ARG
1	B	231	SER
1	B	404	PRO
1	A	186	ARG
1	A	278	HIS
1	B	160	LYS
1	B	257	LEU
1	B	260	ASN
1	B	275	LYS
1	A	141	GLN
1	A	417	GLU
1	B	264	ASP
1	B	258	ASP
1	A	94	LYS
1	A	379	ARG
1	B	362	THR
1	B	419	GLY
1	B	454	ILE
1	A	436	VAL

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	417/428 (97%)	369 (88%)	48 (12%)	7	16
1	B	416/428 (97%)	362 (87%)	54 (13%)	5	12
All	All	833/856 (97%)	731 (88%)	102 (12%)	6	14

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	32	LEU
1	A	46	PHE
1	A	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	63	ARG
1	A	70	LEU
1	A	74	SER
1	A	90	LEU
1	A	94	LYS
1	A	112	ARG
1	A	114	ILE
1	A	117	ASN
1	A	121	THR
1	A	134	ARG
1	A	140	LYS
1	A	141	GLN
1	A	145	SER
1	A	160	LYS
1	A	184	LEU
1	A	186	ARG
1	A	193	ASP
1	A	199	LEU
1	A	200	MET
1	A	225	LEU
1	A	233	ARG
1	A	249	ARG
1	A	261	CYS
1	A	270	LEU
1	A	279	SER
1	A	281	GLU
1	A	285	THR
1	A	298	PHE
1	A	303	THR
1	A	310	TYR
1	A	312	LEU
1	A	327	GLU
1	A	364	VAL
1	A	368	LEU
1	A	374	ARG
1	A	376	THR
1	A	412	GLU
1	A	416	ASN
1	A	420	LYS
1	A	450	LEU
1	A	464	VAL
1	A	471	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	486	LYS
1	A	487	LEU
1	B	31	LYS
1	B	32	LEU
1	B	41	ILE
1	B	51	LYS
1	B	53	ILE
1	B	59	ARG
1	B	63	ARG
1	B	90	LEU
1	B	91	LEU
1	B	94	LYS
1	B	112	ARG
1	B	114	ILE
1	B	117	ASN
1	B	121	THR
1	B	127	ARG
1	B	160	LYS
1	B	162	GLN
1	B	184	LEU
1	B	186	ARG
1	B	195	LYS
1	B	199	LEU
1	B	215	LEU
1	B	231	SER
1	B	237	LYS
1	B	244	GLU
1	B	256	SER
1	B	261	CYS
1	B	275	LYS
1	B	278	HIS
1	B	297	PHE
1	B	308	LEU
1	B	310	TYR
1	B	312	LEU
1	B	325	LEU
1	B	327	GLU
1	B	338	ILE
1	B	342	LYS
1	B	346	GLU
1	B	359	ARG
1	B	368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	ARG
1	B	375	ASP
1	B	376	THR
1	B	382	LEU
1	B	407	GLU
1	B	418	ASN
1	B	428	LYS
1	B	436	VAL
1	B	445	MET
1	B	464	VAL
1	B	465	ASP
1	B	471	LEU
1	B	487	LEU
1	B	493	SER

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	62	GLN
1	A	141	GLN
1	A	208	HIS
1	A	401	GLN
1	B	75	GLN
1	B	117	ASN
1	B	162	GLN
1	B	204	ASN
1	B	208	HIS
1	B	216	GLN
1	B	358	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	A	500	1,3	30,50,50	2.34	10 (33%)	24,82,82	2.79	12 (50%)
3	OID	A	501	2	13,17,17	0.75	0	14,19,19	0.66	0
2	HEM	B	500	1,3	30,50,50	2.33	7 (23%)	24,82,82	2.56	10 (41%)
3	OID	B	501	2	13,17,17	0.62	0	14,19,19	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,3	-	0/10/54/54	0/0/8/8
3	OID	A	501	2	-	0/10/12/12	0/1/1/1
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	OID	B	501	2	-	0/10/12/12	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-6.78	1.45	1.51
2	B	500	HEM	C3D-C4D	-6.53	1.43	1.51
2	A	500	HEM	C3B-C4B	-6.43	1.46	1.51
2	A	500	HEM	C3D-C4D	-4.89	1.45	1.51
2	B	500	HEM	C2C-C1C	-4.75	1.43	1.52
2	A	500	HEM	C2C-C1C	-4.75	1.43	1.52
2	A	500	HEM	C2B-C1B	-2.70	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C2D-C1D	-2.61	1.43	1.51
2	A	500	HEM	C2D-C1D	-2.25	1.44	1.51
2	A	500	HEM	C1C-NC	2.14	1.38	1.36
2	B	500	HEM	C3B-CAB	2.20	1.55	1.51
2	A	500	HEM	C3C-CAC	2.37	1.55	1.51
2	A	500	HEM	C4C-NC	2.42	1.39	1.36
2	A	500	HEM	FE-ND	2.88	2.12	1.97
2	B	500	HEM	FE-NB	3.30	2.15	1.97
2	B	500	HEM	FE-ND	3.46	2.15	1.97
2	A	500	HEM	FE-NB	4.75	2.22	1.97

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	HEM	CAA-C2A-C1A	-3.81	122.87	127.01
2	A	500	HEM	C2C-C1C-NC	-2.51	105.97	110.21
2	B	500	HEM	C2C-C1C-NC	-2.40	106.17	110.21
2	B	500	HEM	CMA-C3A-C4A	-2.32	124.52	128.36
2	A	500	HEM	CMA-C3A-C4A	-2.28	124.60	128.36
2	A	500	HEM	C3B-C4B-NB	-2.12	107.57	111.63
2	A	500	HEM	CBD-CAD-C3D	-2.06	107.55	113.55
2	B	500	HEM	C2D-C3D-C4D	2.28	105.37	101.50
2	A	500	HEM	C2D-C3D-C4D	2.49	105.72	101.50
2	A	500	HEM	C1D-CHD-C4C	2.60	130.17	125.82
2	B	500	HEM	CMD-C2D-C3D	2.77	126.58	114.35
2	A	500	HEM	CMD-C2D-C3D	2.86	127.00	114.35
2	B	500	HEM	CMB-C2B-C3B	3.74	125.86	116.53
2	B	500	HEM	C3B-C4B-CHC	3.83	128.55	123.16
2	A	500	HEM	CAD-C3D-C4D	4.34	127.78	112.47
2	B	500	HEM	CAD-C3D-C2D	4.35	125.72	113.22
2	A	500	HEM	CAD-C3D-C2D	4.62	126.50	113.22
2	B	500	HEM	CAD-C3D-C4D	4.65	128.88	112.47
2	A	500	HEM	CMB-C2B-C3B	5.14	129.37	116.53
2	A	500	HEM	C3B-C4B-CHC	5.59	131.03	123.16
2	A	500	HEM	CMC-C2C-C3C	5.70	130.77	116.53
2	B	500	HEM	CMC-C2C-C3C	5.79	130.97	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	12	0
3	A	501	OID	3	0
2	B	500	HEM	7	0
3	B	501	OID	1	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(Å ²)	Q<0.9
1	A	461/476 (96%)	-0.39	1 (0%) 95 96	13, 28, 45, 62	0
1	B	461/476 (96%)	-0.41	0 100 100	13, 27, 45, 64	0
All	All	922/952 (96%)	-0.40	1 (0%) 95 97	13, 27, 45, 64	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	HIS	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
3	OID	A	501	17/17	0.95	0.18	2.03	19,26,38,38	0
3	OID	B	501	17/17	0.96	0.17	2.01	22,25,40,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	500	43/43	0.98	0.15	0.24	15,24,31,35	0
2	HEM	B	500	43/43	0.97	0.14	0.00	13,24,29,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.