Full wwPDB X-ray Structure Validation Report (i)

Jul 28, 2016 – 04:45 PM EDT

PDB ID	:	5A5J
Title	:	Cytochrome 2C9 P450 inhibitor complex
Authors	:	Skerratt, S.E.; de Groot, M.J.; Phillips, C.
Deposited on	:	2015-06-18
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

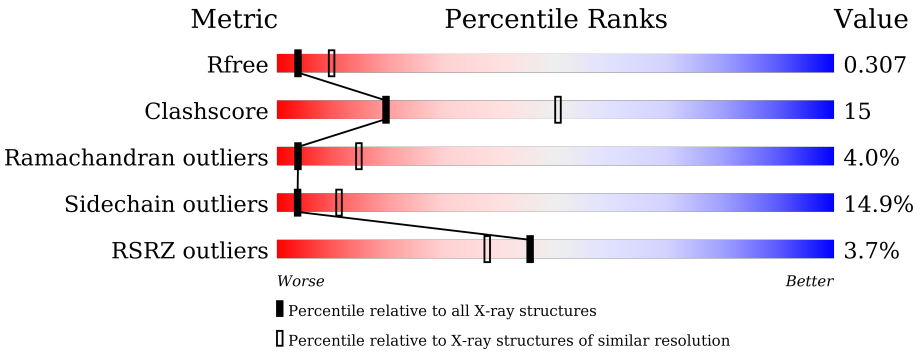
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	477	4% 57% 30% 8% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3717 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.

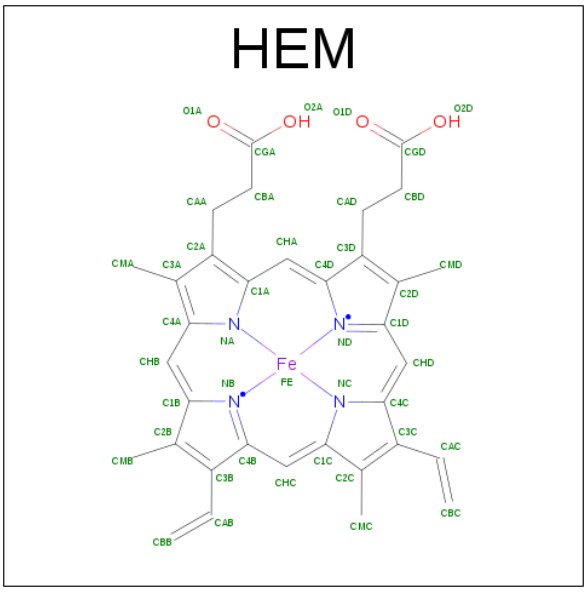
- Molecule 1 is a protein called CYTOCHROME P450 2C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3646	2353	614	656	23			

There are 10 discrepancies between the modelled and reference sequences:

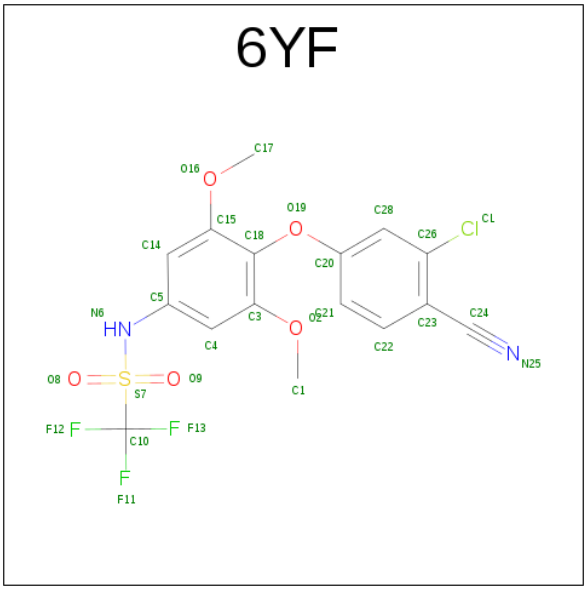
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	EXPRESSION TAG	UNP P11712
A	19	ALA	-	EXPRESSION TAG	UNP P11712
A	20	LYS	-	EXPRESSION TAG	UNP P11712
A	21	LYS	-	EXPRESSION TAG	UNP P11712
A	22	THR	-	EXPRESSION TAG	UNP P11712
A	490	ILE	-	EXPRESSION TAG	UNP P11712
A	491	HIS	-	EXPRESSION TAG	UNP P11712
A	492	HIS	-	EXPRESSION TAG	UNP P11712
A	493	HIS	-	EXPRESSION TAG	UNP P11712
A	494	HIS	-	EXPRESSION TAG	UNP P11712

- 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		

- Molecule 3 is N-[4-(3-CHLORANYL-4-CYANO-PHENOXY)-3,5-DIMETHOXY-PHENYL]-1,1,1-TRIS(FLUORANYL)METHANESULFONAMIDE (three-letter code: 6YF) (formula: $C_{16}H_{12}ClF_3N_2O_5S$).



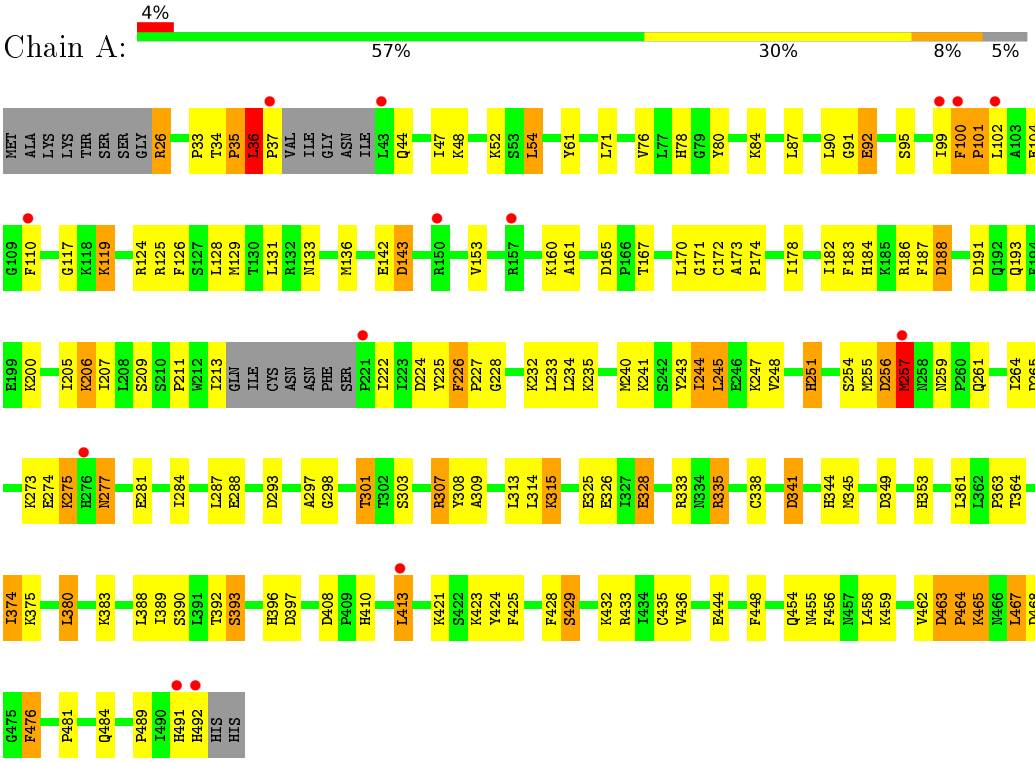
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			28	16	1	3	2	5	1		

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 (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 2C9

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	91.29Å 91.29Å 169.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.74 – 2.90 29.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.74-2.90) 99.8 (29.43-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.288 0.221 , 0.307	Depositor DCC
R_{free} test set	555 reflections (4.77%)	DCC
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3717	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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, 6YF

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	1.01	4/3735 (0.1%)	1.06	16/5047 (0.3%)

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	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	LYS	CD-CE	5.95	1.66	1.51
1	A	423	LYS	CD-CE	5.66	1.65	1.51
1	A	269	MET	SD-CE	5.07	2.06	1.77
1	A	257	MET	SD-CE	5.01	2.06	1.77

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	397	ASP	CB-CG-OD2	7.84	125.35	118.30
1	A	265	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	256	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	408	ASP	CB-CG-OD1	7.13	124.71	118.30
1	A	341	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	372	CYS	CA-CB-SG	-6.38	102.52	114.00
1	A	349	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	463	ASP	CB-CG-OD1	6.08	123.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	335	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	188	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	380	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	191	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	26	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	293	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	165	ASP	CB-CG-OD1	5.31	123.08	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	PRO	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	3646	0	3678	109	0
2	A	43	0	30	7	0
3	A	28	0	0	1	0
All	All	3717	0	3708	111	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 15.

All (111) 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:257:MET:CE	1:A:257:MET:SD	2.05	1.43
1:A:269:MET:CE	1:A:269:MET:SD	2.06	1.42
1:A:193:GLN:NE2	1:A:247:LYS:HZ2	1.70	0.89
1:A:245:LEU:HD22	1:A:288:GLU:OE2	1.80	0.81
1:A:353:HIS:HD2	1:A:425:PHE:CZ	1.99	0.80
1:A:193:GLN:NE2	1:A:247:LYS:NZ	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG23	1:A:363:PRO:HG2	1.67	0.77
1:A:209:SER:HB2	1:A:474:ASN:HD21	1.49	0.76
1:A:491:HIS:C	1:A:492:HIS:ND1	2.42	0.73
1:A:36:LEU:N	1:A:37:PRO:HD3	2.05	0.72
1:A:178:ILE:HG22	1:A:182:ILE:HD12	1.70	0.71
1:A:209:SER:HB2	1:A:474:ASN:ND2	2.06	0.70
1:A:90:LEU:HD22	1:A:374:ILE:HD11	1.77	0.67
1:A:35:PRO:C	1:A:37:PRO:HD3	2.15	0.67
1:A:92:GLU:HG2	1:A:432:LYS:NZ	2.10	0.67
1:A:353:HIS:HD2	1:A:425:PHE:CE2	2.15	0.65
1:A:368:HIS:HD2	1:A:389:ILE:HD13	1.61	0.65
1:A:119:LYS:HG3	1:A:281:GLU:OE1	1.97	0.64
1:A:454:GLN:HB3	1:A:455:ASN:ND2	2.13	0.63
1:A:211:PRO:O	1:A:224:ASP:HB2	1.99	0.63
1:A:309:ALA:O	1:A:313:LEU:HG	1.99	0.62
3:A:1494:6YF:C14	3:A:1494:6YF:O8	2.47	0.62
1:A:267:PHE:CG	1:A:287:LEU:HD13	2.36	0.61
1:A:78:HIS:CD2	1:A:393:SER:HB2	2.36	0.61
1:A:251:HIS:CD2	1:A:264:ILE:HB	2.37	0.60
1:A:193:GLN:HE21	1:A:247:LYS:NZ	2.02	0.58
1:A:389:ILE:N	1:A:389:ILE:HD12	2.18	0.58
1:A:100:PHE:CG	1:A:101:PRO:HD2	2.38	0.58
1:A:492:HIS:N	1:A:492:HIS:ND1	2.52	0.57
1:A:90:LEU:HD22	1:A:374:ILE:CD1	2.35	0.56
1:A:183:PHE:O	1:A:184:HIS:HB3	2.06	0.56
1:A:364:THR:HA	1:A:389:ILE:O	2.05	0.56
1:A:125:ARG:O	1:A:129:MET:HG2	2.06	0.56
1:A:183:PHE:O	1:A:184:HIS:CB	2.54	0.56
1:A:80:TYR:HB2	1:A:424:TYR:CE2	2.42	0.55
2:A:1493:HEM:HBB2	2:A:1493:HEM:HMB2	1.89	0.55
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.88	0.54
1:A:207:ILE:HG21	1:A:233:LEU:HD13	1.89	0.54
1:A:353:HIS:CD2	1:A:425:PHE:CE2	2.96	0.54
1:A:244:ILE:O	1:A:248:VAL:HG23	2.08	0.54
1:A:275:LYS:C	1:A:277:ASN:H	2.12	0.53
1:A:47:ILE:HD13	1:A:476:PHE:HA	1.90	0.53
1:A:78:HIS:NE2	1:A:393:SER:HB2	2.24	0.53
1:A:171:GLY:HA2	1:A:303:SER:HB2	1.89	0.53
1:A:251:HIS:HD2	1:A:264:ILE:HB	1.73	0.53
1:A:463:ASP:O	1:A:464:PRO:C	2.47	0.53
1:A:172:CYS:SG	1:A:198:MET:HE1	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:CZ	1:A:108:ARG:HB3	2.40	0.51
1:A:226:PHE:N	1:A:227:PRO:CD	2.74	0.51
1:A:36:LEU:N	1:A:37:PRO:CD	2.73	0.51
1:A:193:GLN:HE22	1:A:247:LYS:HZ2	1.53	0.50
1:A:207:ILE:HD13	1:A:233:LEU:HD13	1.93	0.50
1:A:92:GLU:HG2	1:A:432:LYS:HZ3	1.75	0.49
1:A:462:VAL:CG2	1:A:467:LEU:HB2	2.43	0.49
1:A:100:PHE:CD1	1:A:101:PRO:HD2	2.48	0.48
1:A:454:GLN:HB3	1:A:455:ASN:HD22	1.77	0.48
1:A:78:HIS:CD2	1:A:393:SER:CB	2.97	0.48
1:A:410:HIS:HA	1:A:413:LEU:HB2	1.94	0.48
1:A:259:ASN:HD21	1:A:261:GLN:HE21	1.60	0.48
1:A:187:PHE:O	1:A:188:ASP:C	2.49	0.47
1:A:99:ILE:O	1:A:102:LEU:O	2.33	0.47
1:A:259:ASN:HD21	1:A:261:GLN:NE2	2.12	0.47
1:A:368:HIS:CD2	1:A:389:ILE:HD13	2.46	0.47
1:A:245:LEU:CD2	1:A:288:GLU:OE2	2.59	0.47
1:A:463:ASP:O	1:A:465:LYS:N	2.48	0.47
1:A:193:GLN:HE21	1:A:247:LYS:HZ1	1.63	0.47
1:A:281:GLU:OE1	1:A:281:GLU:HA	2.14	0.47
1:A:196:ASN:O	1:A:200:LYS:HG2	2.15	0.47
1:A:187:PHE:C	1:A:188:ASP:O	2.53	0.46
1:A:178:ILE:HG22	1:A:182:ILE:CD1	2.42	0.46
1:A:428:PHE:HB3	1:A:435:CYS:HB3	1.97	0.46
1:A:315:LYS:O	1:A:315:LYS:HG3	2.17	0.45
1:A:297:ALA:O	1:A:301:THR:OG1	2.34	0.45
1:A:374:ILE:HG13	1:A:375:LYS:N	2.31	0.45
1:A:275:LYS:C	1:A:277:ASN:N	2.71	0.45
1:A:128:LEU:HD23	1:A:129:MET:SD	2.58	0.44
1:A:54:LEU:N	1:A:54:LEU:HD23	2.33	0.44
1:A:142:GLU:O	1:A:143:ASP:C	2.56	0.44
1:A:298:GLY:HA2	2:A:1493:HEM:C2C	2.53	0.44
1:A:462:VAL:HG21	1:A:467:LEU:HB2	2.00	0.44
1:A:160:LYS:O	1:A:161:ALA:HB3	2.17	0.44
1:A:390:SER:HB3	1:A:393:SER:HB3	2.00	0.44
1:A:471:PRO:HA	1:A:481:PRO:HD3	2.00	0.44
1:A:170:LEU:O	1:A:174:PRO:HD3	2.19	0.43
1:A:267:PHE:CD2	1:A:287:LEU:HD13	2.53	0.43
1:A:172:CYS:HA	1:A:198:MET:SD	2.58	0.43
1:A:325:GLU:O	1:A:328:GLU:N	2.52	0.43
1:A:428:PHE:O	1:A:429:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:ND2	1:A:110:PHE:CD2	2.87	0.42
1:A:314:LEU:HD21	1:A:458:LEU:HB3	2.01	0.42
1:A:436:VAL:HG12	2:A:1493:HEM:C2D	2.54	0.42
1:A:226:PHE:CD1	1:A:227:PRO:N	2.86	0.42
1:A:436:VAL:HG12	2:A:1493:HEM:CMD	2.50	0.42
1:A:245:LEU:HD22	1:A:288:GLU:CD	2.39	0.42
1:A:301:THR:HG22	1:A:361:LEU:HD21	2.02	0.42
1:A:171:GLY:HA2	1:A:303:SER:CB	2.49	0.42
1:A:167:THR:HA	1:A:307:ARG:HD2	2.01	0.42
1:A:76:VAL:HG22	1:A:388:LEU:HB3	2.02	0.42
1:A:126:PHE:CZ	1:A:267:PHE:HA	2.55	0.42
1:A:234:LEU:O	1:A:235:LYS:C	2.58	0.42
1:A:153:VAL:HG13	1:A:456:PHE:CE2	2.54	0.42
1:A:436:VAL:HG12	2:A:1493:HEM:HMD2	2.02	0.42
1:A:353:HIS:CD2	1:A:425:PHE:CZ	2.92	0.41
1:A:444:GLU:HB3	1:A:448:PHE:CE2	2.56	0.41
1:A:436:VAL:CG1	2:A:1493:HEM:HMD2	2.51	0.41
1:A:392:THR:O	1:A:396:HIS:HB2	2.21	0.41
1:A:433:ARG:O	2:A:1493:HEM:HBA2	2.20	0.41
1:A:33:PRO:HA	1:A:61:TYR:OH	2.21	0.41
1:A:87:LEU:O	1:A:91:GLY:HA2	2.21	0.41
1:A:243:TYR:CD1	1:A:243:TYR:C	2.95	0.40
1:A:226:PHE:H	1:A:227:PRO:CD	2.34	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	449/477 (94%)	384 (86%)	47 (10%)	18 (4%)	4 15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	A	36	LEU
1	A	226	PHE
1	A	429	SER
1	A	104	GLU
1	A	107	ASN
1	A	133	ASN
1	A	257	MET
1	A	256	ASP
1	A	326	GLU
1	A	467	LEU
1	A	100	PHE
1	A	101	PRO
1	A	186	ARG
1	A	228	GLY
1	A	464	PRO
1	A	383	LYS
1	A	117	GLY

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	410/430 (95%)	349 (85%)	61 (15%)	4 11

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	34	THR
1	A	36	LEU
1	A	44	GLN
1	A	48	LYS
1	A	52	LYS
1	A	54	LEU
1	A	71	LEU
1	A	84	LYS

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Mol	Chain	Res	Type
1	A	92	GLU
1	A	95	SER
1	A	105	ARG
1	A	108	ARG
1	A	119	LYS
1	A	124	ARG
1	A	131	LEU
1	A	136	MET
1	A	143	ASP
1	A	195	LEU
1	A	197	LEU
1	A	198	MET
1	A	205	ILE
1	A	206	LYS
1	A	213	ILE
1	A	222	ILE
1	A	225	TYR
1	A	232	LYS
1	A	240	MET
1	A	241	LYS
1	A	244	ILE
1	A	245	LEU
1	A	251	HIS
1	A	254	SER
1	A	255	MET
1	A	257	MET
1	A	273	LYS
1	A	274	GLU
1	A	275	LYS
1	A	277	ASN
1	A	284	ILE
1	A	301	THR
1	A	307	ARG
1	A	308	TYR
1	A	315	LYS
1	A	328	GLU
1	A	333	ARG
1	A	335	ARG
1	A	338	CYS
1	A	341	ASP
1	A	344	HIS
1	A	345	MET

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Mol	Chain	Res	Type
1	A	374	ILE
1	A	380	LEU
1	A	393	SER
1	A	413	LEU
1	A	421	LYS
1	A	459	LYS
1	A	465	LYS
1	A	468	ASP
1	A	476	PHE
1	A	484	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	193	GLN
1	A	261	GLN
1	A	353	HIS
1	A	457	ASN
1	A	484	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	HEM	A	1493	1	24,50,50	2.37	7 (29%)	16,82,82	2.26	5 (31%)
3	6YF	A	1494	-	25,29,29	1.00	1 (4%)	32,43,43	2.07	9 (28%)

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	1493	1	-	0/6/54/54	0/0/8/8
3	6YF	A	1494	-	-	0/15/24/24	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1493	HEM	C3C-C2C	-6.01	1.32	1.40
2	A	1493	HEM	C3B-C2B	-5.97	1.32	1.40
2	A	1493	HEM	C1A-CHA	-2.11	1.34	1.40
2	A	1493	HEM	C3C-CAC	2.58	1.53	1.47
2	A	1493	HEM	CMA-C3A	2.77	1.57	1.51
3	A	1494	6YF	S7-N6	2.87	1.69	1.62
2	A	1493	HEM	C3B-CAB	3.10	1.54	1.47
2	A	1493	HEM	C3D-C2D	4.28	1.50	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1493	HEM	C3C-CAC-CBC	-5.21	115.92	126.40
3	A	1494	6YF	O16-C15-C14	-5.08	115.44	124.17
2	A	1493	HEM	CBD-CAD-C3D	-3.81	105.79	112.47
3	A	1494	6YF	O2-C3-C4	-3.70	117.82	124.17
3	A	1494	6YF	C28-C26-C23	-2.21	119.04	121.29
2	A	1493	HEM	CMA-C3A-C4A	-2.06	124.81	128.31
3	A	1494	6YF	O8-S7-N6	-2.03	101.47	107.49
3	A	1494	6YF	C28-C26-CL	2.13	121.91	118.46
3	A	1494	6YF	C17-O16-C15	2.86	121.69	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1493	HEM	CMB-C2B-C3B	2.91	130.77	125.09
2	A	1493	HEM	CBA-CAA-C2A	3.17	118.08	112.49
3	A	1494	6YF	O2-C3-C18	3.75	122.00	115.25
3	A	1494	6YF	C20-O19-C18	4.16	125.63	118.42
3	A	1494	6YF	O16-C15-C18	5.22	124.64	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1493	HEM	7	0
3	A	1494	6YF	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

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, 95^{th} 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	455/477 (95%)	-0.02	17 (3%) 45 38	15, 39, 66, 74	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	HIS	5.1
1	A	491	HIS	4.8
1	A	150	ARG	3.6
1	A	37	PRO	3.5
1	A	107	ASN	3.4
1	A	100	PHE	3.3
1	A	99	ILE	3.0
1	A	106	ALA	2.9
1	A	110	PHE	2.7
1	A	102	LEU	2.5
1	A	105	ARG	2.4
1	A	157	ARG	2.3
1	A	43	LEU	2.3
1	A	221	PRO	2.2
1	A	413	LEU	2.2
1	A	257	MET	2.0
1	A	276	HIS	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 carbohydrates 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. 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, 95^{th} 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	6YF	A	1494	28/28	0.82	0.26	1.73	52,57,67,68	0
2	HEM	A	1493	43/43	0.98	0.20	0.02	8,16,20,23	0

6.5 Other polymers

There are no such residues in this entry.