



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:14 AM GMT

PDB ID : 3LD6  
Title : Crystal structure of human lanosterol 14alpha-demethylase (CYP51) in complex with ketoconazole  
Authors : Strushkevich, N.; Tempel, W.; MacKenzie, F.; Arrowsmith, C.H.; Edwards, A.M; Bountra, C.; Weigelt, J.; Park, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2010-01-12  
Resolution : 2.80 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](mailto: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.

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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

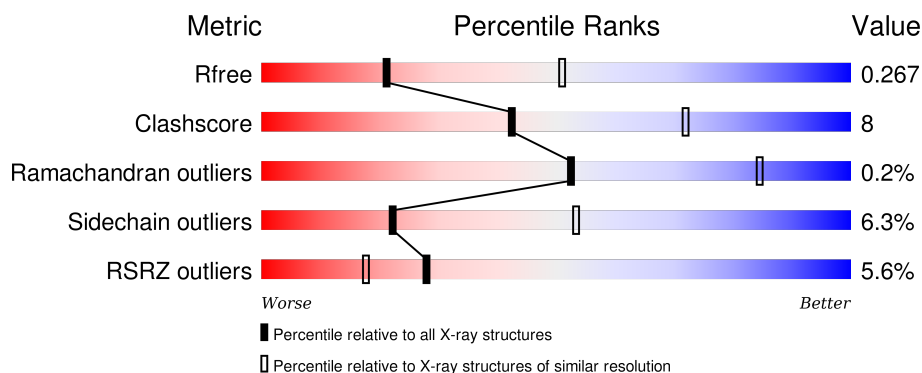
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	461	
1	B	461	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7522 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 Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3589	2310	611	652	16			
1	B	444	Total	C	N	O	S	0	0	0
			3583	2307	610	650	16			

There are 24 discrepancies between the modelled and reference sequences:

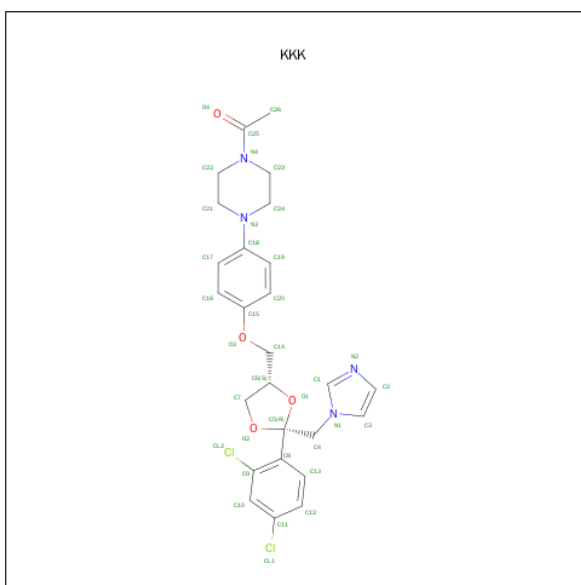
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	MET	-	EXPRESSION TAG	UNP Q16850
A	50	ALA	-	EXPRESSION TAG	UNP Q16850
A	51	LYS	-	EXPRESSION TAG	UNP Q16850
A	52	LYS	-	EXPRESSION TAG	UNP Q16850
A	53	THR	-	EXPRESSION TAG	UNP Q16850
A	503	THR	-	EXPRESSION TAG	UNP Q16850
A	504	HIS	-	EXPRESSION TAG	UNP Q16850
A	505	HIS	-	EXPRESSION TAG	UNP Q16850
A	506	HIS	-	EXPRESSION TAG	UNP Q16850
A	507	HIS	-	EXPRESSION TAG	UNP Q16850
A	508	HIS	-	EXPRESSION TAG	UNP Q16850
A	509	HIS	-	EXPRESSION TAG	UNP Q16850
B	49	MET	-	EXPRESSION TAG	UNP Q16850
B	50	ALA	-	EXPRESSION TAG	UNP Q16850
B	51	LYS	-	EXPRESSION TAG	UNP Q16850
B	52	LYS	-	EXPRESSION TAG	UNP Q16850
B	53	THR	-	EXPRESSION TAG	UNP Q16850
B	503	THR	-	EXPRESSION TAG	UNP Q16850
B	504	HIS	-	EXPRESSION TAG	UNP Q16850
B	505	HIS	-	EXPRESSION TAG	UNP Q16850
B	506	HIS	-	EXPRESSION TAG	UNP Q16850
B	507	HIS	-	EXPRESSION TAG	UNP Q16850
B	508	HIS	-	EXPRESSION TAG	UNP Q16850
B	509	HIS	-	EXPRESSION TAG	UNP Q16850

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



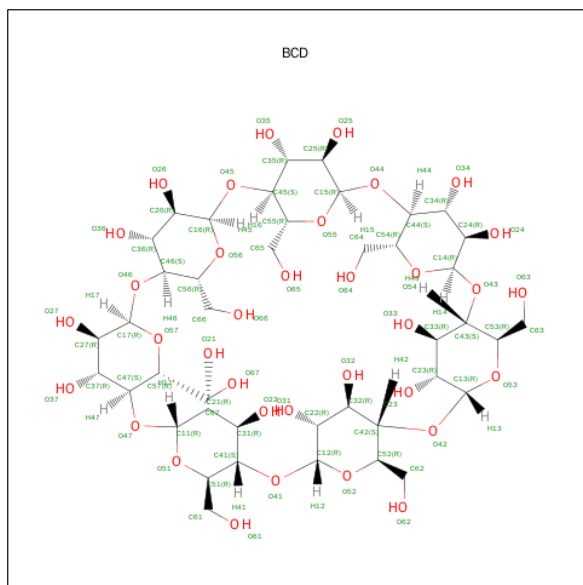
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-ACETYL-4-(4-{[(2R,4S)-2-(2,4-DICHLOROPHENYL)-2-(1H-IMIDAZOL-1-YLMETHYL)-1,3-DIOXOLAN-4-YL]METHOXY}PHENYL)PIPERAZINE (three-letter code: KKK) (formula:  $C_{26}H_{28}Cl_2N_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			36	26	2	4	4	
3	B	1	Total	C	Cl	N	O	0
			36	26	2	4	4	

- Molecule 4 is SUGAR (BETA-CYCLODEXTRIN) (three-letter code: BCD) (formula:  $C_{42}H_{70}O_{35}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			77	42	35		
4	B	1	Total	C	O	0	0
			77	42	35		

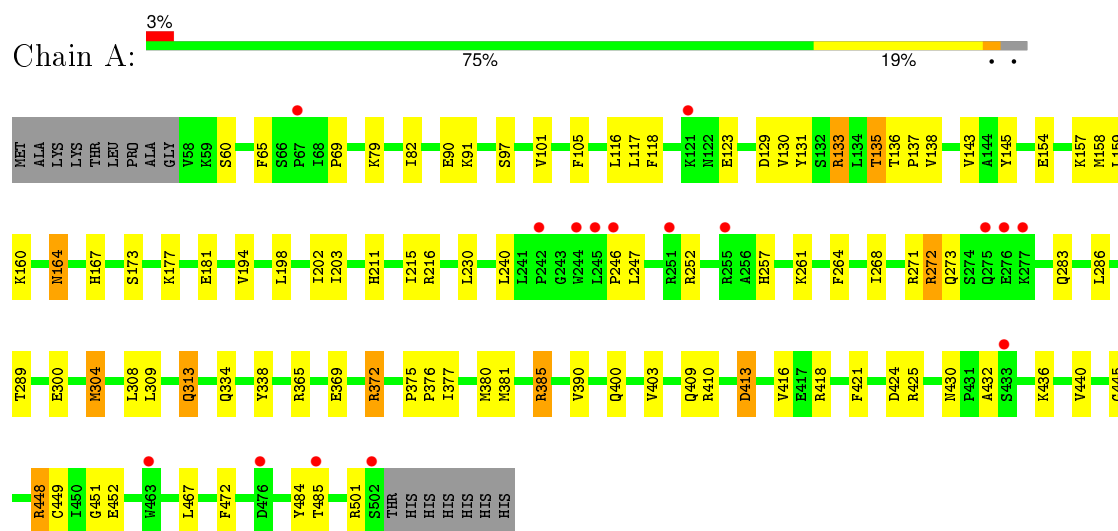
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	12	Total	O	0	0
			12	12		

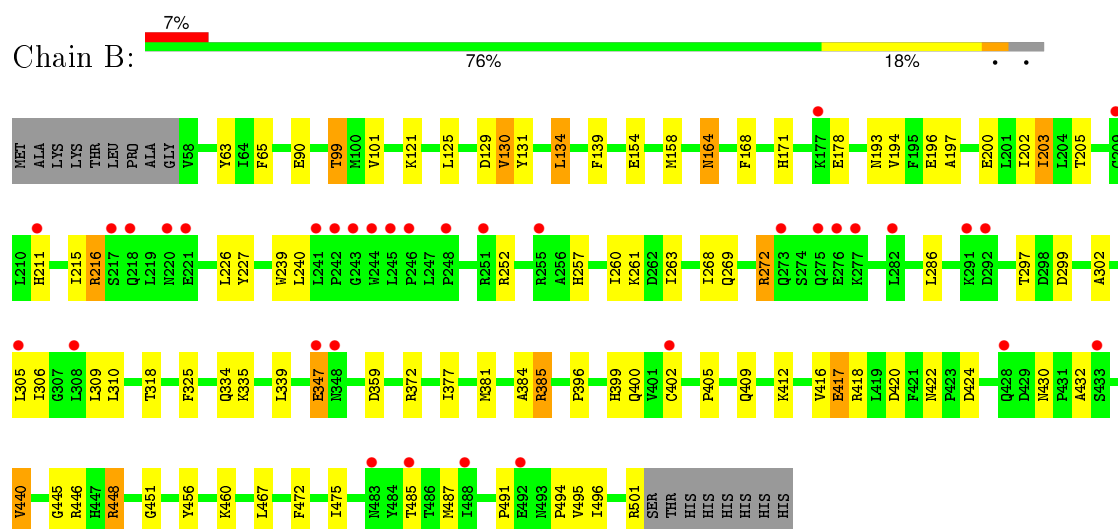
### 3 Residue-property plots

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: Lanosterol 14-alpha demethylase



- Molecule 1: Lanosterol 14-alpha demethylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.73 Å   145.73 Å   110.34 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	24.29 – 2.80 24.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (24.29-2.80) 98.9 (24.29-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.95 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.212   ,   0.275 0.210   ,   0.267	Depositor DCC
$R_{free}$ test set	1491 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 29474 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BCD, HEM, KKK

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	0.45	0/3682	0.58	0/4988
1	B	0.42	0/3676	0.54	0/4980
All	All	0.44	0/7358	0.56	0/9968

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3589	0	3581	60	0
1	B	3583	0	3576	57	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	36	0	28	2	0
3	B	36	0	28	6	0
4	A	77	0	70	2	0
4	B	77	0	70	2	0
5	A	26	0	0	2	0
5	B	12	0	0	1	0
All	All	7522	0	7413	123	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 8.

All (123) 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:135:THR:HG22	5:A:20:HOH:O	1.63	0.98
1:A:116:LEU:HB2	1:A:390:VAL:HG21	1.51	0.92
1:A:334:GLN:HE22	1:A:472:PHE:H	1.26	0.83
1:B:467:LEU:O	1:B:501:ARG:HD3	1.80	0.82
1:B:334:GLN:HE22	1:B:472:PHE:H	1.26	0.79
1:B:129:ASP:OD2	1:B:385:ARG:HD3	1.87	0.75
1:A:409:GLN:HE21	1:A:440:VAL:H	1.33	0.74
1:B:372:ARG:NH2	1:B:418:ARG:O	2.20	0.74
1:A:309:LEU:O	1:A:313:GLN:HB2	1.87	0.73
1:B:456:TYR:O	1:B:460:LYS:HB2	1.88	0.73
1:A:116:LEU:HB2	1:A:390:VAL:CG2	2.18	0.72
1:B:381:MET:CE	3:B:602:KKK:H21	2.20	0.71
1:A:101:VAL:O	1:A:101:VAL:HG12	1.91	0.69
1:A:131:TYR:CZ	3:A:602:KKK:H14	2.28	0.68
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.76	0.67
1:B:101:VAL:HG12	1:B:101:VAL:O	1.95	0.67
1:B:381:MET:HE1	3:B:602:KKK:H21	1.77	0.66
1:A:135:THR:HG21	1:A:145:TYR:HD1	1.60	0.66
1:B:130:VAL:HG11	1:B:381:MET:HB3	1.78	0.65
1:B:297:THR:HG22	1:B:299:ASP:H	1.62	0.65
1:A:198:LEU:O	1:A:202:ILE:HG12	1.97	0.64
1:A:133:ARG:HG3	5:A:21:HOH:O	1.97	0.64
1:B:226:LEU:HB3	1:B:260:ILE:HD11	1.81	0.62
1:A:430:ASN:ND2	1:A:432:ALA:HB3	2.15	0.62
1:A:138:VAL:HG13	1:A:230:LEU:HD22	1.83	0.61
1:A:129:ASP:OD2	1:A:385:ARG:HD3	1.99	0.60
1:B:193:ASN:HB3	1:B:196:GLU:HG2	1.83	0.59
1:B:131:TYR:CE2	3:B:602:KKK:H14	2.37	0.58
1:B:65:PHE:HD1	4:B:603:BCD:H32	1.68	0.58
1:B:154:GLU:O	1:B:158:MET:HG3	2.04	0.57
1:B:194:VAL:HB	1:B:496:ILE:CG1	2.35	0.57
1:B:131:TYR:CZ	3:B:602:KKK:H14	2.40	0.57
1:B:409:GLN:NE2	1:B:440:VAL:H	2.03	0.57
1:A:410:ARG:HG2	1:A:418:ARG:NH1	2.21	0.56
1:B:335:LYS:O	1:B:339:LEU:HG	2.05	0.56
1:A:369:GLU:OE1	1:A:372:ARG:HD3	2.05	0.56
1:A:177:LYS:O	1:A:181:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:O	1:A:425:ARG:NH2	2.39	0.56
1:A:159:LEU:HD22	1:A:308:LEU:HD21	1.87	0.55
1:A:272:ARG:NH1	1:A:286:LEU:HD22	2.21	0.55
1:B:211:HIS:HB3	1:B:215:ILE:HD12	1.88	0.55
1:B:257:HIS:CE1	1:B:261:LYS:HE3	2.41	0.55
1:A:272:ARG:HH11	1:A:286:LEU:HD22	1.72	0.55
1:B:302:ALA:HA	1:B:305:LEU:HD12	1.90	0.54
1:B:63:TYR:OH	1:B:99:THR:OG1	2.25	0.54
1:B:440:VAL:O	1:B:440:VAL:HG13	2.09	0.53
1:B:430:ASN:ND2	1:B:432:ALA:HB3	2.23	0.53
1:B:325:PHE:CE2	1:B:496:ILE:HG23	2.44	0.53
1:A:154:GLU:O	1:A:158:MET:HG3	2.08	0.52
1:B:381:MET:HE2	3:B:602:KKK:H21	1.91	0.52
1:A:300:GLU:O	1:A:304:MET:HG2	2.10	0.52
1:B:416:VAL:HG12	1:B:417:GLU:HG2	1.90	0.52
1:A:467:LEU:O	1:A:501:ARG:HD2	2.09	0.52
1:A:118:PHE:HE2	1:A:380:MET:HE1	1.76	0.51
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.39	0.51
2:B:601:HEM:C1A	3:B:602:KKK:H1	2.46	0.50
1:B:268:ILE:O	1:B:272:ARG:HB2	2.12	0.50
1:B:200:GLU:O	1:B:203:ILE:HG22	2.12	0.50
1:A:118:PHE:HE2	1:A:380:MET:CE	2.26	0.48
1:B:430:ASN:HD22	1:B:432:ALA:HB3	1.78	0.48
1:B:377:ILE:HD12	1:B:377:ILE:N	2.28	0.48
1:B:196:GLU:HG3	1:B:197:ALA:N	2.30	0.47
1:B:422:ASN:HD21	1:B:424:ASP:HB2	1.79	0.47
1:A:271:ARG:C	1:A:273:GLN:H	2.17	0.47
1:B:164:ASN:HD22	1:B:164:ASN:C	2.18	0.47
1:B:451:GLY:HA3	2:B:601:HEM:C2C	2.49	0.47
1:B:202:ILE:HA	1:B:205:THR:OG1	2.15	0.47
1:A:117:LEU:HD13	1:A:403:VAL:HG23	1.96	0.47
1:B:318:THR:HG22	5:B:9:HOH:O	2.14	0.47
4:A:603:BCD:H622	4:A:603:BCD:H13	1.98	0.46
1:A:211:HIS:HB3	1:A:215:ILE:HD12	1.98	0.46
1:B:194:VAL:HB	1:B:496:ILE:HG13	1.97	0.46
1:A:97:SER:HA	1:A:105:PHE:O	2.15	0.46
1:B:125:LEU:HD23	1:B:384:ALA:HA	1.98	0.46
1:A:101:VAL:HG11	1:A:240:LEU:HD22	1.98	0.46
1:B:260:ILE:HA	1:B:263:ILE:HD12	1.97	0.46
1:B:121:LYS:HD2	1:B:446:ARG:NH2	2.31	0.46
1:A:130:VAL:HB	1:A:381:MET:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:MET:HG2	1:B:402:CYS:SG	2.56	0.45
1:A:449:CYS:HB2	2:A:601:HEM:NA	2.31	0.45
1:A:449:CYS:HA	2:A:601:HEM:C4D	2.52	0.45
1:B:445:GLY:O	1:B:448:ARG:HB3	2.17	0.45
1:A:271:ARG:HD3	1:A:283:GLN:OE1	2.16	0.45
1:B:491:PRO:HB2	1:B:494:PRO:HB3	1.98	0.45
1:A:377:ILE:HD12	2:A:601:HEM:C4A	2.51	0.44
1:A:118:PHE:CE2	1:A:380:MET:HE1	2.51	0.44
1:B:396:PRO:HG2	1:B:399:HIS:CD2	2.53	0.44
1:B:178:GLU:OE2	1:B:216:ARG:HD2	2.18	0.44
1:A:334:GLN:HE22	1:A:472:PHE:N	2.05	0.44
1:B:168:PHE:HD1	1:B:171:HIS:HD2	1.65	0.44
1:B:134:LEU:HD22	1:B:239:TRP:HD1	1.81	0.44
1:A:65:PHE:HD1	4:A:603:BCD:H32	1.83	0.44
1:A:211:HIS:CE1	1:A:309:LEU:HB2	2.53	0.44
1:A:369:GLU:HG3	1:A:421:PHE:CD1	2.53	0.44
1:A:375:PRO:HA	1:A:376:PRO:HD3	1.85	0.43
1:A:304:MET:H	1:A:304:MET:HG2	1.67	0.43
1:B:272:ARG:HH11	1:B:286:LEU:HD22	1.83	0.43
1:A:79:LYS:HD3	1:A:79:LYS:HA	1.77	0.42
1:B:101:VAL:HG11	1:B:240:LEU:HD22	2.00	0.42
1:B:347:GLU:H	1:B:347:GLU:HG2	1.63	0.42
1:B:130:VAL:HG13	1:B:381:MET:HE3	2.02	0.42
1:A:338:TYR:CD1	1:A:501:ARG:HD3	2.55	0.42
1:A:365:ARG:NH1	1:A:424:ASP:OD1	2.49	0.42
1:B:139:PHE:HD2	1:B:306:ILE:HG22	1.85	0.41
4:B:603:BCD:H612	4:B:603:BCD:H52	2.02	0.41
1:A:448:ARG:NH2	1:A:452:GLU:OE1	2.51	0.41
1:A:257:HIS:CE1	1:A:261:LYS:HE3	2.55	0.41
1:A:164:ASN:ND2	1:A:167:HIS:H	2.19	0.41
1:B:475:ILE:HD11	1:B:495:VAL:HG12	2.02	0.41
1:B:227:TYR:CD2	1:B:309:LEU:HD21	2.55	0.41
1:B:405:PRO:HB3	1:B:409:GLN:HE22	1.86	0.41
1:A:451:GLY:HA3	2:A:601:HEM:C2C	2.55	0.41
1:A:136:THR:HB	1:A:137:PRO:HD3	2.03	0.41
1:A:82:ILE:HD12	1:A:484:TYR:OH	2.20	0.41
1:A:377:ILE:HD12	2:A:601:HEM:CHB	2.51	0.41
1:A:449:CYS:HB2	2:A:601:HEM:C1A	2.54	0.41
1:A:413:ASP:OD1	1:A:413:ASP:N	2.54	0.41
3:A:602:KKK:O2	3:A:602:KKK:CL2	2.75	0.41
1:A:271:ARG:C	1:A:273:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:O	1:A:101:VAL:CG1	2.63	0.40
1:A:445:GLY:O	1:A:448:ARG:HB2	2.20	0.40
1:A:448:ARG:HD3	1:A:449:CYS:N	2.36	0.40
1:A:264:PHE:O	1:A:268:ILE:HG13	2.20	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	443/461 (96%)	425 (96%)	16 (4%)	2 (0%)	34	69
1	B	442/461 (96%)	415 (94%)	27 (6%)	0	100	100
All	All	885/922 (96%)	840 (95%)	43 (5%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	PRO
1	A	69	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/403 (97%)	363 (93%)	27 (7%)	19	48
1	B	389/403 (96%)	367 (94%)	22 (6%)	25	58
All	All	779/806 (97%)	730 (94%)	49 (6%)	22	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	90	GLU
1	A	91	LYS
1	A	123	GLU
1	A	133	ARG
1	A	135	THR
1	A	143	VAL
1	A	157	LYS
1	A	160	LYS
1	A	164	ASN
1	A	173	SER
1	A	194	VAL
1	A	203	ILE
1	A	216	ARG
1	A	247	LEU
1	A	252	ARG
1	A	272	ARG
1	A	289	THR
1	A	304	MET
1	A	313	GLN
1	A	372	ARG
1	A	385	ARG
1	A	400	GLN
1	A	413	ASP
1	A	436	LYS
1	A	448	ARG
1	A	485	THR
1	B	90	GLU
1	B	99	THR
1	B	130	VAL
1	B	134	LEU
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	203	ILE
1	B	216	ARG
1	B	252	ARG
1	B	269	GLN
1	B	272	ARG
1	B	310	LEU
1	B	347	GLU
1	B	359	ASP
1	B	385	ARG
1	B	400	GLN
1	B	412	LYS
1	B	417	GLU
1	B	420	ASP
1	B	440	VAL
1	B	448	ARG
1	B	485	THR
1	B	487	MET

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	149	ASN
1	A	164	ASN
1	A	334	GLN
1	A	409	GLN
1	A	422	ASN
1	A	430	ASN
1	B	164	ASN
1	B	334	GLN
1	B	361	ASN
1	B	409	GLN
1	B	422	ASN
1	B	430	ASN

### 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 ⓘ

6 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	601	1,3	30,50,50	2.29	7 (23%)	24,82,82	2.25	7 (29%)
3	KKK	A	602	2	39,40,40	1.17	4 (10%)	49,57,57	1.38	9 (18%)
4	BCD	A	603	-	84,84,84	0.44	0	126,126,126	1.12	7 (5%)
2	HEM	B	601	1,3	30,50,50	2.10	7 (23%)	24,82,82	2.28	6 (25%)
3	KKK	B	602	2	39,40,40	0.93	4 (10%)	49,57,57	1.24	8 (16%)
4	BCD	B	603	-	84,84,84	0.47	0	126,126,126	1.02	6 (4%)

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	601	1,3	-	0/10/54/54	0/0/8/8
3	KKK	A	602	2	-	0/24/45/45	0/5/5/5
4	BCD	A	603	-	-	0/42/182/182	0/0/8/8
2	HEM	B	601	1,3	-	0/10/54/54	0/0/8/8
3	KKK	B	602	2	-	0/24/45/45	0/5/5/5
4	BCD	B	603	-	-	0/42/182/182	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	-7.76	1.44	1.51
2	B	601	HEM	C3B-C4B	-6.95	1.45	1.51
2	A	601	HEM	C3D-C4D	-6.07	1.43	1.51
3	A	602	KKK	C5-C8	-5.01	1.50	1.53
2	B	601	HEM	C2C-C1C	-4.10	1.44	1.52
2	B	601	HEM	C3D-C4D	-4.03	1.46	1.51
2	A	601	HEM	C2C-C1C	-3.38	1.46	1.52
3	B	602	KKK	C5-C8	-2.42	1.52	1.53
2	B	601	HEM	C2D-C1D	-2.35	1.44	1.51
2	A	601	HEM	C2B-C1B	-2.20	1.44	1.51
3	A	602	KKK	C1-N2	-2.17	1.29	1.34
2	A	601	HEM	C2D-C1D	-2.09	1.45	1.51
3	B	602	KKK	C1-N2	-2.01	1.29	1.34
2	B	601	HEM	C1C-NC	2.06	1.38	1.36
3	A	602	KKK	C11-CL1	2.11	1.79	1.74
2	B	601	HEM	C3B-CAB	2.17	1.55	1.51
3	B	602	KKK	C11-CL1	2.19	1.79	1.74
2	A	601	HEM	C3B-CAB	2.35	1.55	1.51
3	A	602	KKK	C9-CL2	2.61	1.80	1.73
2	A	601	HEM	C1C-NC	2.63	1.39	1.36
3	B	602	KKK	C9-CL2	2.64	1.80	1.73
2	B	601	HEM	FE-ND	3.02	2.13	1.97

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	C3C-CAC-CBC	-3.63	118.88	124.46
4	B	603	BCD	C14-O43-C43	-3.38	109.18	118.01
3	A	602	KKK	C14-C6-C7	-3.35	106.77	113.45
3	A	602	KKK	C23-C24-N3	-2.93	104.81	110.63
4	A	603	BCD	C35-C45-C55	-2.83	104.43	110.84
3	A	602	KKK	C24-C23-N4	-2.67	104.41	110.49
3	A	602	KKK	O2-C5-C4	-2.47	105.69	109.48
3	B	602	KKK	C14-C6-C7	-2.40	108.67	113.45
3	B	602	KKK	C10-C9-CL2	-2.28	114.98	118.50
3	B	602	KKK	O2-C5-C8	-2.19	108.46	111.62
3	B	602	KKK	C23-C24-N3	-2.11	106.43	110.63
2	A	601	HEM	CAA-C2A-C1A	-2.03	124.81	127.01
3	B	602	KKK	C24-C23-N4	-2.03	105.87	110.49
3	B	602	KKK	C12-C11-CL1	2.05	122.71	119.35
3	A	602	KKK	C7-O2-C5	2.05	110.90	106.99
3	B	602	KKK	C23-N4-C22	2.05	116.36	112.56
3	A	602	KKK	C5-O1-C6	2.11	110.37	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	BCD	O52-C12-C22	2.15	114.68	110.28
3	A	602	KKK	C23-N4-C22	2.16	116.56	112.56
4	B	603	BCD	O56-C56-C46	2.22	114.44	109.75
3	B	602	KKK	C13-C8-C5	2.29	120.27	119.13
4	B	603	BCD	C17-C27-C37	2.29	114.49	109.97
3	A	602	KKK	C13-C8-C9	2.36	119.74	116.72
4	B	603	BCD	C16-O56-C56	2.44	118.49	113.75
2	A	601	HEM	C3B-C4B-CHC	2.48	126.66	123.16
4	A	603	BCD	O55-C55-C65	2.64	113.02	106.36
2	A	601	HEM	CMD-C2D-C3D	2.66	126.13	114.35
4	B	603	BCD	C26-C36-C46	2.82	115.79	109.60
4	A	603	BCD	O52-C52-C42	3.01	116.10	109.75
2	B	601	HEM	CMD-C2D-C3D	3.04	127.78	114.35
4	B	603	BCD	C27-C37-C47	3.22	116.68	109.60
3	A	602	KKK	C14-O3-C15	3.73	125.90	117.89
4	A	603	BCD	O56-C56-C46	3.99	118.17	109.75
4	A	603	BCD	C16-O56-C56	4.16	121.81	113.75
2	B	601	HEM	CMB-C2B-C3B	4.18	126.96	116.53
2	A	601	HEM	CMC-C2C-C3C	4.19	127.00	116.53
2	A	601	HEM	CAD-C3D-C4D	4.20	127.27	112.47
2	B	601	HEM	CMC-C2C-C3C	4.39	127.48	116.53
2	B	601	HEM	CAD-C3D-C2D	4.49	126.14	113.22
2	A	601	HEM	CMB-C2B-C3B	4.61	128.03	116.53
4	A	603	BCD	C12-O52-C52	4.85	123.16	113.75
2	B	601	HEM	CAD-C3D-C4D	4.86	129.60	112.47
2	A	601	HEM	CAD-C3D-C2D	5.10	127.87	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	0
3	A	602	KKK	2	0
4	A	603	BCD	2	0
2	B	601	HEM	4	0
3	B	602	KKK	6	0
4	B	603	BCD	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	445/461 (96%)	0.05	16 (3%) 46 34	32, 45, 70, 85	0
1	B	444/461 (96%)	0.36	34 (7%) 16 8	40, 61, 88, 98	0
All	All	889/922 (96%)	0.20	50 (5%) 28 18	32, 52, 84, 98	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	TRP	6.4
1	B	277	LYS	5.2
1	B	275	GLN	4.8
1	A	245	LEU	4.7
1	A	275	GLN	4.7
1	B	246	PRO	4.1
1	B	244	TRP	4.0
1	B	211	HIS	3.8
1	A	67	PRO	3.6
1	B	485	THR	3.6
1	A	277	LYS	3.6
1	B	348	ASN	3.5
1	B	243	GLY	3.5
1	B	248	PRO	3.4
1	B	241	LEU	3.3
1	A	242	PRO	3.3
1	A	276	GLU	3.1
1	B	221	GLU	3.1
1	B	251	ARG	2.9
1	A	485	THR	2.9
1	B	305	LEU	2.8
1	B	276	GLU	2.8
1	A	255	ARG	2.8
1	B	218	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	291	LYS	2.7
1	B	177	LYS	2.7
1	B	483	ASN	2.7
1	A	502	SER	2.6
1	A	251	ARG	2.6
1	B	292	ASP	2.6
1	A	433	SER	2.6
1	B	242	PRO	2.5
1	B	428	GLN	2.5
1	B	282	LEU	2.4
1	A	463	TRP	2.4
1	B	402	CYS	2.4
1	B	273	GLN	2.4
1	B	492	GLU	2.4
1	B	347	GLU	2.3
1	A	476	ASP	2.3
1	B	488	ILE	2.3
1	B	220	ASN	2.3
1	B	245	LEU	2.2
1	B	209	CYS	2.2
1	B	433	SER	2.2
1	B	255	ARG	2.1
1	A	121	LYS	2.1
1	B	217	SER	2.1
1	B	308	LEU	2.1
1	A	246	PRO	2.0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	KKK	A	602	36/36	0.93	0.19	0.11	39,50,57,58	0
4	BCD	B	603	77/77	0.89	0.18	-0.18	59,64,69,72	0
3	KKK	B	602	36/36	0.94	0.18	-0.37	53,63,66,67	0
4	BCD	A	603	77/77	0.90	0.17	-0.52	58,63,69,70	0
2	HEM	B	601	43/43	0.98	0.14	-0.86	39,43,46,49	0
2	HEM	A	601	43/43	0.98	0.12	-1.08	27,32,35,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.