Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:02 PM GMT

PDB ID	:	4NKW
Title	:	Human steroidogenic cytochrome P450 17A1 mutant A105L with substrate pregnenolone
Authors	:	Scott, E.E.; Petrunak, E.P.
Deposited on	:	2013-11-13
Resolution	:	2.50 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:

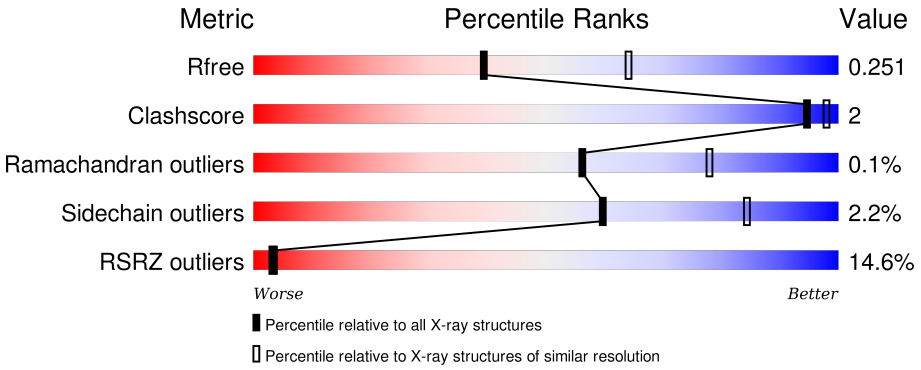
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	494	10% 89% 5% 6%
1	B	494	11% 90% • 6%
1	C	494	20% 88% 7% 5%
1	D	494	15% 88% 6% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30612 atoms, of which 15409 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	464	Total	C	H	N	O	S	0	0	0
			7487	2379	3784	640	669	15			
1	B	464	Total	C	H	N	O	S	0	0	0
			7494	2379	3791	640	669	15			
1	C	467	Total	C	H	N	O	S	0	0	0
			7520	2389	3797	644	675	15			
1	D	467	Total	C	H	N	O	S	0	0	0
			7512	2389	3789	644	675	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP P05093
A	20	ALA	-	EXPRESSION TAG	UNP P05093
A	21	LYS	-	EXPRESSION TAG	UNP P05093
A	22	LYS	-	EXPRESSION TAG	UNP P05093
A	23	THR	-	EXPRESSION TAG	UNP P05093
A	105	LEU	ALA	ENGINEERED MUTATION	UNP P05093
A	509	HIS	-	EXPRESSION TAG	UNP P05093
A	510	HIS	-	EXPRESSION TAG	UNP P05093
A	511	HIS	-	EXPRESSION TAG	UNP P05093
A	512	HIS	-	EXPRESSION TAG	UNP P05093
B	19	MET	-	EXPRESSION TAG	UNP P05093
B	20	ALA	-	EXPRESSION TAG	UNP P05093
B	21	LYS	-	EXPRESSION TAG	UNP P05093
B	22	LYS	-	EXPRESSION TAG	UNP P05093
B	23	THR	-	EXPRESSION TAG	UNP P05093
B	105	LEU	ALA	ENGINEERED MUTATION	UNP P05093
B	509	HIS	-	EXPRESSION TAG	UNP P05093
B	510	HIS	-	EXPRESSION TAG	UNP P05093
B	511	HIS	-	EXPRESSION TAG	UNP P05093
B	512	HIS	-	EXPRESSION TAG	UNP P05093
C	19	MET	-	EXPRESSION TAG	UNP P05093

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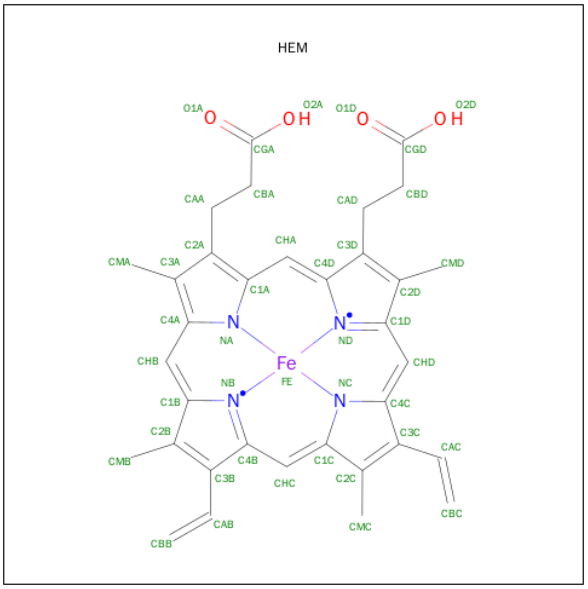
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	EXPRESSION TAG	UNP P05093
C	21	LYS	-	EXPRESSION TAG	UNP P05093
C	22	LYS	-	EXPRESSION TAG	UNP P05093
C	23	THR	-	EXPRESSION TAG	UNP P05093
C	105	LEU	ALA	ENGINEERED MUTATION	UNP P05093
C	509	HIS	-	EXPRESSION TAG	UNP P05093
C	510	HIS	-	EXPRESSION TAG	UNP P05093
C	511	HIS	-	EXPRESSION TAG	UNP P05093
C	512	HIS	-	EXPRESSION TAG	UNP P05093
D	19	MET	-	EXPRESSION TAG	UNP P05093
D	20	ALA	-	EXPRESSION TAG	UNP P05093
D	21	LYS	-	EXPRESSION TAG	UNP P05093
D	22	LYS	-	EXPRESSION TAG	UNP P05093
D	23	THR	-	EXPRESSION TAG	UNP P05093
D	105	LEU	ALA	ENGINEERED MUTATION	UNP P05093
D	509	HIS	-	EXPRESSION TAG	UNP P05093
D	510	HIS	-	EXPRESSION TAG	UNP P05093
D	511	HIS	-	EXPRESSION TAG	UNP P05093
D	512	HIS	-	EXPRESSION TAG	UNP P05093

- 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	H	N	O	0	0
			73	34	1	30	4	4		

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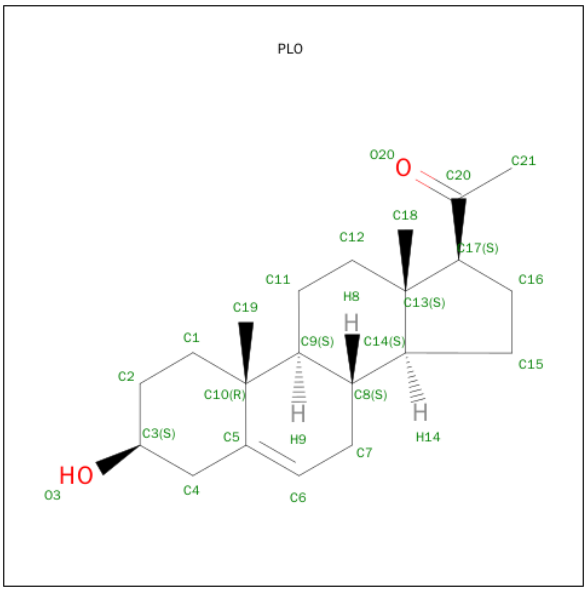
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is (3BETA)-3-HYDROXYPREGN-5-EN-20-ONE (three-letter code: PLO) (formula: $C_{21}H_{32}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			55	21	32	2		
3	B	1	Total	C	H	O	0	0
			55	21	32	2		
3	C	1	Total	C	H	O	0	0
			55	21	32	2		
3	D	1	Total	C	H	O	0	0
			55	21	32	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	20	Total	O	0	0
			20	20		

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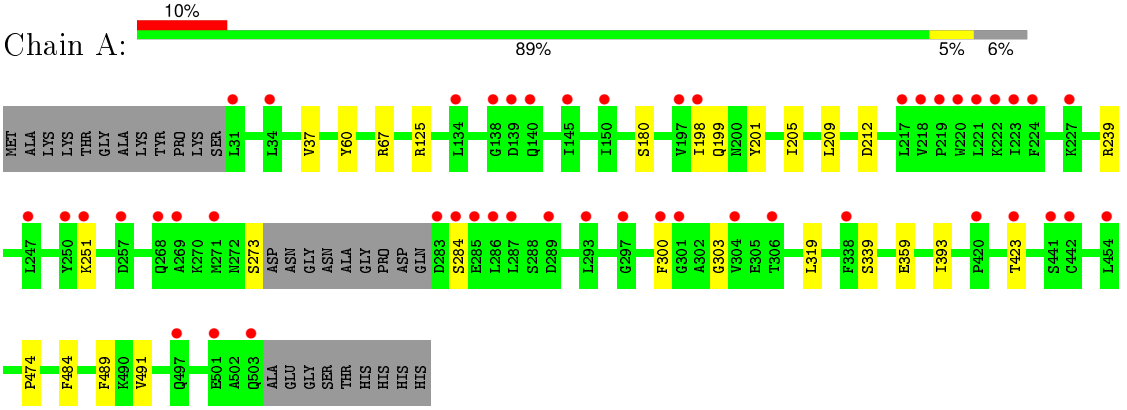
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	17	Total O 17 17	0	0
4	D	21	Total O 21 21	0	0

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.

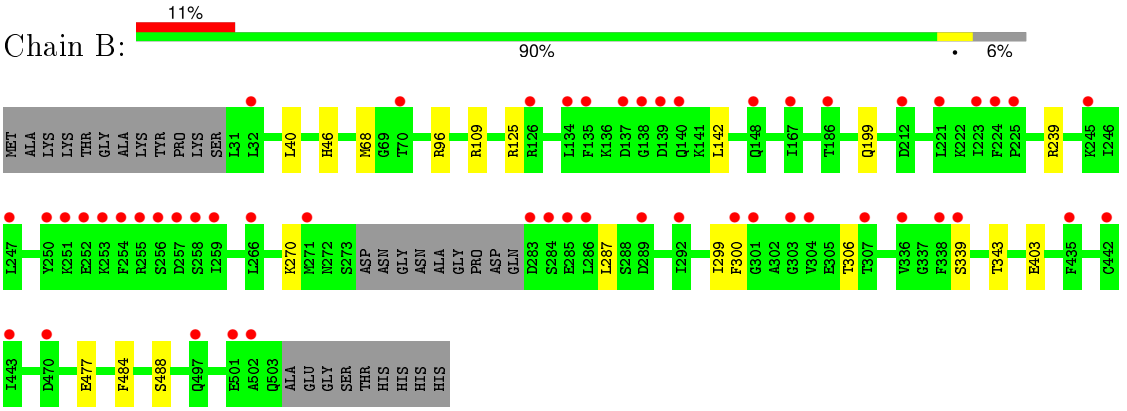
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain A:



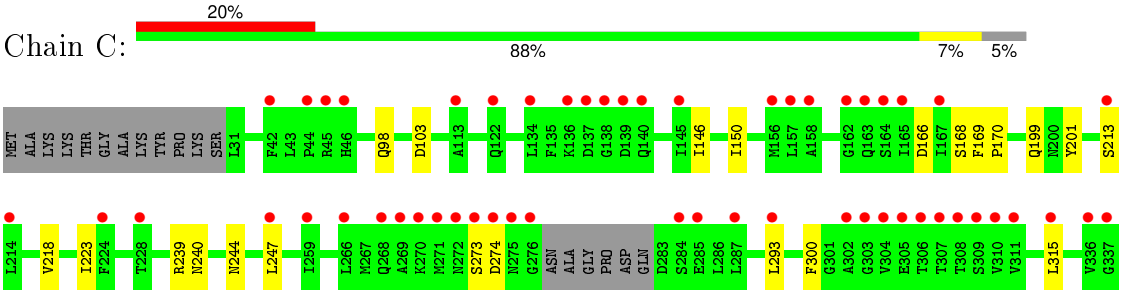
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

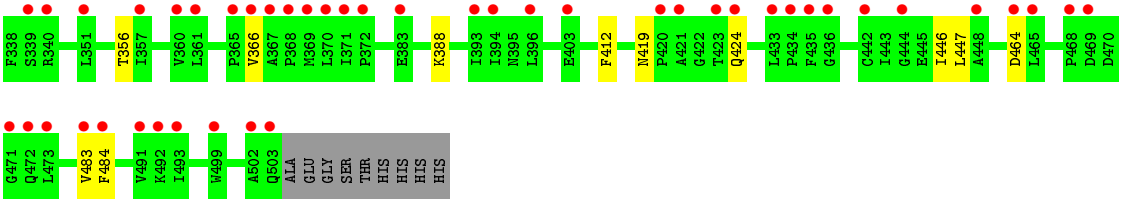
Chain B:



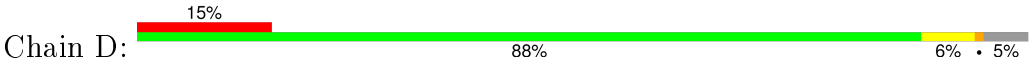
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

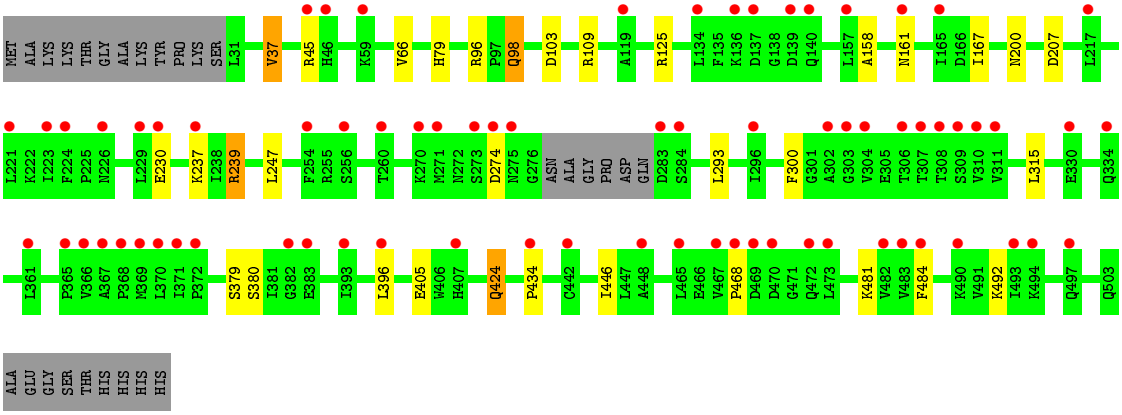
Chain C:





• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.07Å 152.63Å 173.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 2.50 39.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.11-2.50) 99.2 (39.11-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.245 0.206 , 0.251	Depositor DCC
R_{free} test set	3978 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 79261 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30612	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.27 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3453e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.40	0/3783	0.55	0/5121
1	B	0.40	0/3783	0.53	0/5121
1	C	0.38	0/3803	0.56	0/5148
1	D	0.39	0/3803	0.53	0/5148
All	All	0.39	0/15172	0.54	0/20538

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	3703	3784	3781	14	0
1	B	3703	3791	3781	8	0
1	C	3723	3797	3794	12	0
1	D	3723	3789	3794	19	0
2	A	43	30	30	2	0
2	B	43	30	30	4	0
2	C	43	30	30	1	0
2	D	43	30	30	3	0
3	A	23	32	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	23	32	32	1	0
3	C	23	32	32	0	0
3	D	23	32	32	0	0
4	A	29	0	0	2	0
4	B	20	0	0	1	0
4	C	17	0	0	0	0
4	D	21	0	0	1	0
All	All	15203	15409	15398	53	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 2.

All (53) 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:D:96:ARG:O	1:D:109:ARG:NH2	2.31	0.62
2:C:600:HEM:HBB2	2:C:600:HEM:HHC	1.80	0.62
1:B:199:GLN:NE2	4:B:716:HOH:O	2.24	0.61
2:D:600:HEM:HHD	2:D:600:HEM:HBC2	1.82	0.60
2:B:600:HEM:HBC2	2:B:600:HEM:HHD	1.83	0.59
1:C:388:LYS:NZ	1:D:274:ASP:OD1	2.35	0.59
1:B:125:ARG:NH1	2:B:600:HEM:O1D	2.37	0.57
2:D:600:HEM:HHC	2:D:600:HEM:HBB2	1.86	0.56
1:A:37:VAL:CG2	1:D:66:VAL:HG22	2.40	0.52
1:A:37:VAL:HG22	1:D:66:VAL:HG22	1.93	0.51
1:C:166:ASP:OD1	1:C:168:SER:OG	2.21	0.50
1:D:247:LEU:HB2	1:D:293:LEU:HD21	1.93	0.50
1:B:299:ILE:HG23	2:B:600:HEM:HBC1	1.92	0.49
1:C:240:ASN:O	1:C:244:ASN:ND2	2.45	0.49
1:A:201:TYR:OH	4:A:727:HOH:O	2.20	0.49
1:D:379:SER:OG	1:D:380:SER:N	2.46	0.49
1:A:319:LEU:HD11	1:A:491:VAL:HG12	1.95	0.49
1:D:207:ASP:HA	1:D:481:LYS:HE2	1.93	0.49
1:D:98:GLN:NE2	1:D:103:ASP:OD2	2.47	0.48
1:C:218:VAL:CG1	1:C:223:ILE:HD11	2.45	0.47
1:C:446:ILE:HG22	1:C:447:LEU:N	2.31	0.45
1:C:356:THR:HG23	1:C:412:PHE:HZ	1.82	0.45
2:B:600:HEM:HHC	2:B:600:HEM:HBB2	1.97	0.45
1:C:146:ILE:O	1:C:150:ILE:HG12	2.16	0.45
1:C:247:LEU:HB2	1:C:293:LEU:HD21	1.99	0.44
1:A:125:ARG:NH1	2:A:600:HEM:O1D	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:TYR:CD2	1:D:37:VAL:HG21	2.53	0.44
1:C:419:ASN:ND2	1:C:424:GLN:HG2	2.33	0.44
1:C:98:GLN:NE2	1:C:103:ASP:OD2	2.50	0.44
1:A:251:LYS:NZ	4:A:720:HOH:O	2.51	0.44
1:B:96:ARG:O	1:B:109:ARG:NH1	2.50	0.44
1:B:477:GLU:OE1	1:D:237:LYS:NZ	2.44	0.44
1:D:468:PRO:HA	1:D:492:LYS:HB2	2.00	0.44
1:A:474:PRO:HB3	1:A:489:PHE:CG	2.53	0.43
1:B:306:THR:HG21	3:B:601:PLO:H213	2.00	0.43
1:A:303:GLY:HA2	2:A:600:HEM:HMC2	2.01	0.43
1:A:359:GLU:OE1	1:A:359:GLU:HA	2.19	0.42
1:C:169:PHE:N	1:C:170:PRO:HD2	2.34	0.42
1:D:79:HIS:NE2	1:D:405:GLU:OE2	2.52	0.42
1:B:40:LEU:HD21	1:B:68:MET:HE2	2.01	0.42
1:D:239:ARG:NH2	4:D:718:HOH:O	2.53	0.42
1:C:366:VAL:HG13	1:C:483:VAL:HG13	2.01	0.42
1:A:273:SER:O	1:A:284:SER:OG	2.37	0.41
1:D:167:ILE:HD11	1:D:315:LEU:CD1	2.50	0.41
1:D:98:GLN:HG2	1:D:109:ARG:HD2	2.02	0.41
1:D:158:ALA:O	1:D:161:ASN:HB2	2.20	0.41
1:A:198:ILE:HA	1:A:201:TYR:CE2	2.56	0.41
1:A:205:ILE:O	1:A:209:LEU:HB2	2.21	0.41
1:D:396:LEU:HD21	1:D:434:PRO:HA	2.02	0.41
1:B:270:LYS:HA	1:B:287:LEU:HD13	2.03	0.41
1:A:393:ILE:N	1:A:393:ILE:HD12	2.36	0.40
1:D:125:ARG:NH1	2:D:600:HEM:O1D	2.54	0.40
1:D:45:ARG:HA	1:D:45:ARG:HD3	1.83	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	460/494 (93%)	440 (96%)	19 (4%)	1 (0%)	52 75
1	B	460/494 (93%)	442 (96%)	18 (4%)	0	100 100
1	C	463/494 (94%)	442 (96%)	21 (4%)	0	100 100
1	D	463/494 (94%)	439 (95%)	23 (5%)	1 (0%)	52 75
All	All	1846/1976 (93%)	1763 (96%)	81 (4%)	2 (0%)	56 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ASP
1	D	424	GLN

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	415/437 (95%)	407 (98%)	8 (2%)	65 87
1	B	415/437 (95%)	406 (98%)	9 (2%)	60 84
1	C	417/437 (95%)	407 (98%)	10 (2%)	57 82
1	D	417/437 (95%)	408 (98%)	9 (2%)	60 84
All	All	1664/1748 (95%)	1628 (98%)	36 (2%)	60 84

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	180	SER
1	A	199	GLN
1	A	239	ARG
1	A	300	PHE
1	A	339	SER
1	A	423	THR
1	A	484	PHE
1	B	46	HIS

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Mol	Chain	Res	Type
1	B	142	LEU
1	B	239	ARG
1	B	300	PHE
1	B	339	SER
1	B	343	THR
1	B	403	GLU
1	B	484	PHE
1	B	488	SER
1	C	199	GLN
1	C	201	TYR
1	C	213	SER
1	C	239	ARG
1	C	273	SER
1	C	274	ASP
1	C	300	PHE
1	C	315	LEU
1	C	464	ASP
1	C	484	PHE
1	D	37	VAL
1	D	98	GLN
1	D	200	ASN
1	D	230	GLU
1	D	239	ARG
1	D	300	PHE
1	D	424	GLN
1	D	446	ILE
1	D	484	PHE

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	50	HIS
1	B	50	HIS
1	C	50	HIS
1	C	291	HIS
1	D	46	HIS
1	D	50	HIS

5.3.3 RNA

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)

8 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	600	1	30,50,50	2.11	7 (23%)	24,82,82	2.58	8 (33%)
3	PLO	A	601	-	26,26,26	2.06	9 (34%)	42,42,42	2.28	13 (30%)
2	HEM	B	600	1	30,50,50	2.17	6 (20%)	24,82,82	2.28	8 (33%)
3	PLO	B	601	-	26,26,26	2.18	10 (38%)	42,42,42	2.10	13 (30%)
2	HEM	C	600	1	30,50,50	2.17	7 (23%)	24,82,82	2.51	9 (37%)
3	PLO	C	601	-	26,26,26	2.09	8 (30%)	42,42,42	1.95	9 (21%)
2	HEM	D	600	1	30,50,50	2.19	11 (36%)	24,82,82	2.35	10 (41%)
3	PLO	D	601	-	26,26,26	2.05	9 (34%)	42,42,42	2.16	13 (30%)

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	600	1	-	0/10/54/54	0/0/8/8
3	PLO	A	601	-	-	0/4/62/62	0/4/4/4
2	HEM	B	600	1	-	0/10/54/54	0/0/8/8
3	PLO	B	601	-	-	0/4/62/62	0/4/4/4
2	HEM	C	600	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLO	C	601	-	-	0/4/62/62	0/4/4/4
2	HEM	D	600	1	-	0/10/54/54	0/0/8/8
3	PLO	D	601	-	-	0/4/62/62	0/4/4/4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	C3B-C4B	-6.97	1.45	1.51
2	D	600	HEM	C3B-C4B	-6.03	1.46	1.51
2	C	600	HEM	C3D-C4D	-6.00	1.43	1.51
3	B	601	PLO	C1-C10	-5.95	1.43	1.54
2	B	600	HEM	C3B-C4B	-5.93	1.46	1.51
2	C	600	HEM	C3B-C4B	-5.83	1.46	1.51
2	D	600	HEM	C3D-C4D	-5.79	1.44	1.51
2	B	600	HEM	C3D-C4D	-5.72	1.44	1.51
3	C	601	PLO	C1-C10	-5.67	1.43	1.54
3	A	601	PLO	C1-C10	-5.54	1.44	1.54
3	D	601	PLO	C1-C10	-5.51	1.44	1.54
2	A	600	HEM	C3D-C4D	-4.64	1.45	1.51
2	B	600	HEM	C2C-C1C	-4.33	1.44	1.52
2	A	600	HEM	C2C-C1C	-4.18	1.44	1.52
2	D	600	HEM	C2C-C1C	-4.08	1.44	1.52
2	C	600	HEM	C2C-C1C	-3.66	1.45	1.52
3	B	601	PLO	C7-C8	-3.52	1.47	1.53
3	D	601	PLO	C7-C8	-3.52	1.47	1.53
3	C	601	PLO	C7-C8	-3.40	1.47	1.53
3	A	601	PLO	C13-C14	-3.22	1.48	1.55
3	A	601	PLO	C7-C8	-3.06	1.48	1.53
3	B	601	PLO	C13-C14	-2.86	1.49	1.55
3	D	601	PLO	C13-C14	-2.80	1.49	1.55
3	C	601	PLO	C13-C14	-2.66	1.49	1.55
2	C	600	HEM	C2B-C1B	-2.47	1.43	1.51
3	B	601	PLO	C15-C14	-2.45	1.48	1.54
3	D	601	PLO	C15-C14	-2.30	1.49	1.54
2	A	600	HEM	C2D-C1D	-2.30	1.44	1.51
3	A	601	PLO	C13-C17	-2.22	1.52	1.56
3	B	601	PLO	C13-C17	-2.22	1.52	1.56
3	C	601	PLO	C15-C14	-2.15	1.49	1.54
2	C	600	HEM	C2D-C1D	-2.13	1.44	1.51
2	D	600	HEM	C2D-C1D	-2.10	1.45	1.51
2	D	600	HEM	C2B-C1B	-2.09	1.45	1.51
3	A	601	PLO	C15-C14	-2.04	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	PLO	C11-C9	-2.02	1.50	1.53
3	D	601	PLO	C8-C9	-2.01	1.49	1.53
2	A	600	HEM	FE-NB	2.01	2.08	1.97
3	C	601	PLO	C8-C14	2.04	1.57	1.53
2	D	600	HEM	FE-NC	2.05	2.03	1.95
2	D	600	HEM	FE-NB	2.07	2.08	1.97
3	D	601	PLO	C8-C14	2.09	1.57	1.53
2	D	600	HEM	C3C-CAC	2.17	1.55	1.51
2	D	600	HEM	C1C-NC	2.17	1.38	1.36
3	A	601	PLO	C8-C14	2.18	1.57	1.53
2	B	600	HEM	C3C-CAC	2.22	1.55	1.51
3	B	601	PLO	C10-C5	2.24	1.57	1.52
3	A	601	PLO	C10-C5	2.28	1.57	1.52
2	D	600	HEM	C3B-CAB	2.38	1.55	1.51
2	A	600	HEM	FE-ND	2.45	2.10	1.97
2	C	600	HEM	C3C-CAC	2.47	1.56	1.51
2	A	600	HEM	C3C-CAC	2.48	1.56	1.51
3	C	601	PLO	C10-C5	2.54	1.58	1.52
3	D	601	PLO	C10-C5	2.55	1.58	1.52
3	B	601	PLO	C6-C5	2.66	1.39	1.33
2	B	600	HEM	FE-NB	2.76	2.12	1.97
2	D	600	HEM	C4C-NC	2.85	1.39	1.36
3	B	601	PLO	C8-C14	2.86	1.59	1.53
3	D	601	PLO	C6-C5	2.91	1.40	1.33
3	C	601	PLO	C6-C5	2.98	1.40	1.33
3	A	601	PLO	C6-C5	3.16	1.40	1.33
3	D	601	PLO	C4-C5	3.24	1.59	1.51
3	B	601	PLO	C4-C5	3.31	1.59	1.51
2	B	600	HEM	FE-NC	3.41	2.09	1.95
2	C	600	HEM	FE-NC	3.42	2.09	1.95
3	C	601	PLO	C4-C5	3.49	1.60	1.51
3	A	601	PLO	C4-C5	3.60	1.60	1.51

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	PLO	C3-C4-C5	-6.42	98.58	111.82
3	A	601	PLO	C16-C17-C13	-6.15	98.64	104.21
3	B	601	PLO	C16-C17-C13	-5.94	98.83	104.21
3	A	601	PLO	C3-C4-C5	-5.78	99.90	111.82
3	B	601	PLO	C3-C4-C5	-5.34	100.82	111.82
3	D	601	PLO	C3-C4-C5	-5.29	100.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	CAA-CBA-CGA	-4.49	104.52	112.75
3	A	601	PLO	C14-C8-C9	-4.30	103.41	109.06
3	A	601	PLO	C12-C13-C17	-4.19	111.96	116.20
3	D	601	PLO	C7-C8-C14	-3.88	104.80	110.86
3	B	601	PLO	C14-C8-C9	-3.84	104.01	109.06
3	D	601	PLO	C14-C8-C9	-3.84	104.01	109.06
3	D	601	PLO	C16-C17-C13	-3.84	100.73	104.21
3	C	601	PLO	C7-C8-C14	-3.74	105.02	110.86
3	C	601	PLO	C14-C8-C9	-3.72	104.17	109.06
3	B	601	PLO	C12-C13-C17	-3.68	112.48	116.20
3	A	601	PLO	C7-C8-C14	-3.39	105.57	110.86
3	C	601	PLO	C16-C17-C13	-3.32	101.20	104.21
3	D	601	PLO	C15-C14-C8	-3.30	113.81	119.03
3	C	601	PLO	C15-C14-C8	-3.22	113.93	119.03
3	A	601	PLO	C19-C10-C5	-3.10	103.56	108.36
3	B	601	PLO	C11-C12-C13	-3.01	107.45	112.84
2	C	600	HEM	CAA-CBA-CGA	-2.87	107.49	112.75
2	D	600	HEM	CAA-C2A-C1A	-2.80	123.97	127.01
3	B	601	PLO	C11-C9-C8	-2.72	107.80	111.74
3	B	601	PLO	C7-C8-C14	-2.67	106.69	110.86
2	D	600	HEM	CMA-C3A-C4A	-2.62	124.03	128.36
3	A	601	PLO	C15-C14-C8	-2.58	114.95	119.03
3	C	601	PLO	C16-C15-C14	-2.57	99.95	105.12
3	D	601	PLO	C16-C15-C14	-2.56	99.97	105.12
2	B	600	HEM	CAA-C2A-C1A	-2.52	124.27	127.01
3	B	601	PLO	C15-C14-C8	-2.51	115.07	119.03
3	B	601	PLO	C16-C15-C14	-2.41	100.27	105.12
3	C	601	PLO	C11-C12-C13	-2.40	108.54	112.84
2	B	600	HEM	CAA-CBA-CGA	-2.34	108.46	112.75
2	A	600	HEM	CAA-C2A-C1A	-2.33	124.48	127.01
2	D	600	HEM	CAA-CBA-CGA	-2.27	108.59	112.75
3	D	601	PLO	C18-C13-C12	-2.24	106.72	110.54
2	C	600	HEM	C3B-C4B-NB	-2.24	107.35	111.63
3	C	601	PLO	C12-C13-C17	-2.16	114.02	116.20
3	A	601	PLO	C16-C15-C14	-2.14	100.82	105.12
3	A	601	PLO	C2-C3-C4	2.01	113.90	110.32
3	B	601	PLO	C13-C17-C20	2.04	117.70	115.13
3	B	601	PLO	C4-C5-C10	2.24	119.69	116.43
2	A	600	HEM	C3B-C4B-CHC	2.40	126.54	123.16
3	D	601	PLO	C1-C2-C3	2.42	114.36	110.43
3	D	601	PLO	C12-C11-C9	2.54	117.38	113.10
2	D	600	HEM	CMD-C2D-C3D	2.54	125.60	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	HEM	CMD-C2D-C3D	2.58	125.78	114.35
3	A	601	PLO	C7-C8-C9	2.64	113.31	109.71
2	C	600	HEM	C2D-C3D-C4D	2.68	106.03	101.50
2	D	600	HEM	C2D-C3D-C4D	2.79	106.23	101.50
2	C	600	HEM	CMD-C2D-C3D	2.81	126.79	114.35
3	D	601	PLO	C4-C5-C10	2.82	120.53	116.43
2	B	600	HEM	C3B-C4B-CHC	3.00	127.39	123.16
2	A	600	HEM	CMD-C2D-C3D	3.04	127.81	114.35
3	B	601	PLO	C21-C20-C17	3.14	121.93	117.53
3	A	601	PLO	C13-C17-C20	3.22	119.18	115.13
3	A	601	PLO	C12-C11-C9	3.28	118.63	113.10
3	D	601	PLO	C21-C20-C17	3.36	122.22	117.53
3	A	601	PLO	C1-C2-C3	3.39	115.93	110.43
2	B	600	HEM	CMB-C2B-C3B	3.48	125.23	116.53
3	C	601	PLO	C7-C8-C9	3.54	114.54	109.71
2	D	600	HEM	C3B-C4B-CHC	3.63	128.27	123.16
3	B	601	PLO	C7-C8-C9	3.63	114.66	109.71
2	B	600	HEM	CMC-C2C-C3C	3.75	125.90	116.53
2	D	600	HEM	CMB-C2B-C3B	3.81	126.05	116.53
3	D	601	PLO	C13-C17-C20	3.90	120.04	115.13
3	D	601	PLO	C7-C8-C9	3.96	115.11	109.71
2	C	600	HEM	C3B-C4B-CHC	4.02	128.82	123.16
2	C	600	HEM	CAD-C3D-C4D	4.07	126.83	112.47
2	D	600	HEM	CMC-C2C-C3C	4.08	126.71	116.53
2	D	600	HEM	CAD-C3D-C4D	4.16	127.14	112.47
2	B	600	HEM	CAD-C3D-C4D	4.21	127.33	112.47
2	A	600	HEM	CAD-C3D-C4D	4.45	128.17	112.47
2	D	600	HEM	CAD-C3D-C2D	4.66	126.62	113.22
2	C	600	HEM	CMB-C2B-C3B	4.71	128.29	116.53
2	C	600	HEM	CAD-C3D-C2D	4.84	127.13	113.22
2	A	600	HEM	CAD-C3D-C2D	5.04	127.72	113.22
2	B	600	HEM	CAD-C3D-C2D	5.19	128.13	113.22
2	C	600	HEM	CMC-C2C-C3C	5.25	129.63	116.53
2	A	600	HEM	CMC-C2C-C3C	5.28	129.71	116.53
2	A	600	HEM	CMB-C2B-C3B	5.56	130.41	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
2	B	600	HEM	4	0
3	B	601	PLO	1	0
2	C	600	HEM	1	0
2	D	600	HEM	3	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	464/494 (93%)	0.77	47 (10%)	9 9	38, 59, 93, 123	0
1	B	464/494 (93%)	0.72	52 (11%)	7 7	39, 59, 92, 123	0
1	C	467/494 (94%)	1.10	99 (21%)	1 1	37, 64, 98, 114	0
1	D	467/494 (94%)	0.92	73 (15%)	3 2	40, 64, 95, 125	0
All	All	1862/1976 (94%)	0.88	271 (14%)	3 3	37, 62, 96, 125	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	9.0
1	C	473	LEU	7.0
1	A	223	ILE	6.4
1	A	220	TRP	6.2
1	A	217	LEU	6.2
1	C	274	ASP	5.8
1	C	45	ARG	5.7
1	A	286	LEU	5.6
1	A	139	ASP	5.4
1	C	493	ILE	5.3
1	A	271	MET	5.2
1	C	469	ASP	5.1
1	C	46	HIS	4.9
1	C	139	ASP	4.9
1	D	136	LYS	4.9
1	C	336	VAL	4.9
1	B	247	LEU	4.9
1	C	157	LEU	4.9
1	A	140	GLN	4.8
1	B	251	LYS	4.8
1	D	139	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	383	GLU	4.8
1	C	442	CYS	4.7
1	B	283	ASP	4.7
1	C	306	THR	4.7
1	C	136	LYS	4.5
1	C	471	GLY	4.5
1	A	31	LEU	4.4
1	D	273	SER	4.3
1	D	367	ALA	4.3
1	B	252	GLU	4.3
1	A	251	LYS	4.3
1	B	286	LEU	4.2
1	C	434	PRO	4.2
1	D	306	THR	4.2
1	D	221	LEU	4.2
1	B	258	SER	4.1
1	B	501	GLU	4.1
1	D	45	ARG	4.1
1	C	137	ASP	4.1
1	A	284	SER	4.1
1	D	140	GLN	4.0
1	C	340	ARG	4.0
1	D	274	ASP	4.0
1	B	502	ALA	4.0
1	C	367	ALA	4.0
1	D	493	ILE	4.0
1	C	273	SER	4.0
1	D	223	ILE	4.0
1	C	302	ALA	3.9
1	D	307	THR	3.9
1	D	442	CYS	3.9
1	C	42	PHE	3.9
1	A	219	PRO	3.9
1	A	247	LEU	3.9
1	D	369	MET	3.9
1	C	259	ILE	3.8
1	B	253	LYS	3.8
1	B	140	GLN	3.8
1	D	137	ASP	3.8
1	B	134	LEU	3.7
1	D	473	LEU	3.7
1	A	285	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	308	THR	3.7
1	D	368	PRO	3.7
1	C	435	PHE	3.6
1	A	221	LEU	3.6
1	A	283	ASP	3.6
1	C	284	SER	3.6
1	C	337	GLY	3.5
1	C	465	LEU	3.5
1	D	309	SER	3.5
1	A	420	PRO	3.5
1	D	275	ASN	3.5
1	C	503	GLN	3.5
1	D	366	VAL	3.5
1	B	135	PHE	3.4
1	C	492	LYS	3.4
1	C	366	VAL	3.4
1	A	287	LEU	3.4
1	B	138	GLY	3.4
1	B	212	ASP	3.4
1	C	134	LEU	3.3
1	D	224	PHE	3.3
1	C	365	PRO	3.3
1	C	499	TRP	3.3
1	B	301	GLY	3.3
1	C	310	VAL	3.3
1	A	501	GLU	3.2
1	C	272	ASN	3.2
1	C	163	GLN	3.2
1	D	434	PRO	3.2
1	D	310	VAL	3.2
1	D	497	GLN	3.2
1	D	472	GLN	3.2
1	C	214	LEU	3.2
1	C	368	PRO	3.1
1	B	336	VAL	3.1
1	B	442	CYS	3.1
1	B	255	ARG	3.1
1	A	289	ASP	3.1
1	A	250	TYR	3.1
1	D	134	LEU	3.1
1	D	468	PRO	3.0
1	C	468	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	271	MET	3.0
1	C	158	ALA	3.0
1	C	369	MET	3.0
1	C	307	THR	3.0
1	D	119	ALA	3.0
1	D	217	LEU	3.0
1	C	304	VAL	2.9
1	A	218	VAL	2.9
1	A	134	LEU	2.9
1	B	32	LEU	2.9
1	B	221	LEU	2.9
1	B	224	PHE	2.9
1	D	46	HIS	2.9
1	A	301	GLY	2.9
1	B	137	ASP	2.9
1	D	484	PHE	2.9
1	A	300	PHE	2.9
1	D	302	ALA	2.9
1	B	470	ASP	2.9
1	A	304	VAL	2.8
1	C	266	LEU	2.8
1	C	444	GLY	2.8
1	C	309	SER	2.8
1	A	138	GLY	2.8
1	D	494	LYS	2.8
1	C	311	VAL	2.8
1	B	300	PHE	2.8
1	C	270	LYS	2.8
1	C	361	LEU	2.8
1	C	360	VAL	2.8
1	A	224	PHE	2.7
1	D	334	GLN	2.7
1	C	247	LEU	2.7
1	C	351	LEU	2.7
1	A	497	GLN	2.7
1	D	270	LYS	2.7
1	A	338	PHE	2.7
1	A	297	GLY	2.7
1	D	393	ILE	2.7
1	A	442	CYS	2.7
1	B	304	VAL	2.7
1	C	275	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	287	LEU	2.6
1	D	396	LEU	2.6
1	C	308	THR	2.6
1	D	365	PRO	2.6
1	D	161	ASN	2.6
1	B	259	ILE	2.6
1	D	165	ILE	2.6
1	D	465	LEU	2.6
1	C	424	GLN	2.6
1	D	303	GLY	2.6
1	B	285	GLU	2.6
1	D	304	VAL	2.6
1	D	370	LEU	2.6
1	D	448	ALA	2.6
1	C	164	SER	2.6
1	C	483	VAL	2.6
1	B	266	LEU	2.6
1	B	225	PRO	2.6
1	D	483	VAL	2.5
1	D	226	ASN	2.5
1	D	271	MET	2.5
1	C	502	ALA	2.5
1	B	257	ASP	2.5
1	C	383	GLU	2.5
1	D	361	LEU	2.5
1	A	423	THR	2.5
1	B	307	THR	2.5
1	C	372	PRO	2.5
1	D	311	VAL	2.5
1	C	167	ILE	2.5
1	C	113	ALA	2.5
1	B	338	PHE	2.5
1	C	140	GLN	2.5
1	C	371	ILE	2.5
1	C	276	GLY	2.5
1	C	472	GLN	2.5
1	B	303	GLY	2.5
1	A	257	ASP	2.4
1	B	289	ASP	2.4
1	A	197	VAL	2.4
1	C	448	ALA	2.4
1	C	396	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	357	ILE	2.4
1	D	59	LYS	2.4
1	D	371	ILE	2.4
1	D	470	ASP	2.4
1	B	339	SER	2.4
1	D	382	GLY	2.4
1	D	157	LEU	2.4
1	D	482	VAL	2.4
1	C	403	GLU	2.4
1	C	484	PHE	2.3
1	A	306	THR	2.3
1	A	145	ILE	2.3
1	B	292	ILE	2.3
1	B	126	ARG	2.3
1	C	44	PRO	2.3
1	C	138	GLY	2.3
1	C	436	GLY	2.3
1	A	503	GLN	2.3
1	B	245	LYS	2.3
1	B	443	ILE	2.3
1	B	256	SER	2.3
1	D	407	HIS	2.3
1	C	303	GLY	2.3
1	C	271	MET	2.3
1	C	228	THR	2.3
1	B	223	ILE	2.3
1	D	296	ILE	2.3
1	C	420	PRO	2.3
1	C	305	GLU	2.2
1	C	162	GLY	2.2
1	C	315	LEU	2.2
1	A	222	LYS	2.2
1	C	394	ILE	2.2
1	A	454	LEU	2.2
1	D	372	PRO	2.2
1	A	441	SER	2.2
1	D	256	SER	2.2
1	C	464	ASP	2.2
1	C	393	ILE	2.2
1	B	254	PHE	2.2
1	C	433	LEU	2.2
1	D	229	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	467	VAL	2.2
1	C	145	ILE	2.2
1	C	122	GLN	2.2
1	A	227	LYS	2.2
1	C	339	SER	2.1
1	A	150	ILE	2.1
1	B	167	ILE	2.1
1	D	490	LYS	2.1
1	B	284	SER	2.1
1	C	269	ALA	2.1
1	C	421	ALA	2.1
1	C	370	LEU	2.1
1	C	423	THR	2.1
1	A	269	ALA	2.1
1	C	491	VAL	2.1
1	D	254	PHE	2.1
1	B	186	THR	2.1
1	C	268	GLN	2.1
1	B	250	TYR	2.1
1	B	70	THR	2.1
1	D	330	GLU	2.1
1	D	237	LYS	2.1
1	C	156	MET	2.1
1	A	198	ILE	2.1
1	C	165	ILE	2.1
1	B	435	PHE	2.1
1	C	213	SER	2.1
1	D	284	SER	2.1
1	A	293	LEU	2.0
1	C	293	LEU	2.0
1	D	283	ASP	2.0
1	C	285	GLU	2.0
1	A	268	GLN	2.0
1	B	148	GLN	2.0
1	C	224	PHE	2.0
1	B	497	GLN	2.0
1	D	230	GLU	2.0
1	D	469	ASP	2.0
1	A	34	LEU	2.0
1	D	260	THR	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^{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
2	HEM	B	600	43/43	0.97	0.30	1.69	39,51,68,69	0
2	HEM	A	600	43/43	0.97	0.28	1.39	33,48,70,74	0
2	HEM	D	600	43/43	0.96	0.33	1.05	35,47,59,70	0
3	PLO	A	601	23/23	0.94	0.29	0.95	44,60,72,72	0
2	HEM	C	600	43/43	0.97	0.34	0.92	33,48,67,77	0
3	PLO	C	601	23/23	0.96	0.31	0.63	49,62,73,75	0
3	PLO	D	601	23/23	0.94	0.27	0.19	47,60,75,78	0
3	PLO	B	601	23/23	0.94	0.22	-0.00	43,56,72,73	0

6.5 Other polymers (i)

There are no such residues in this entry.