Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:02 PM GMT

PDB ID	:	4NKY
Title	:	Human steroidogenic cytochrome P450 17A1 mutant A105L with substrate 17alpha-hydroxyprogesterone
Authors	:	Scott, E.E.; Petrunak, E.M.
Deposited on	:	2013-11-13
Resolution	:	2.55 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:

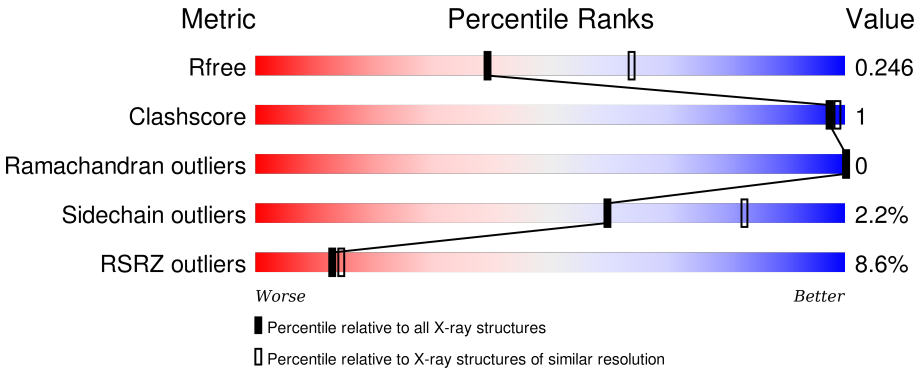
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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% • 6%
1	B	494	7% 88% 5% 6%
1	C	494	7% 90% • 5%
1	D	494	7% 91% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30605 atoms, of which 15344 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	462	Total	C	H	N	O	S	0	0	0
			7473	2373	3782	638	665	15			
1	B	464	Total	C	H	N	O	S	0	0	0
			7496	2379	3793	640	669	15			
1	C	467	Total	C	H	N	O	S	0	0	0
			7466	2393	3739	645	674	15			
1	D	465	Total	C	H	N	O	S	0	0	0
			7501	2383	3790	641	672	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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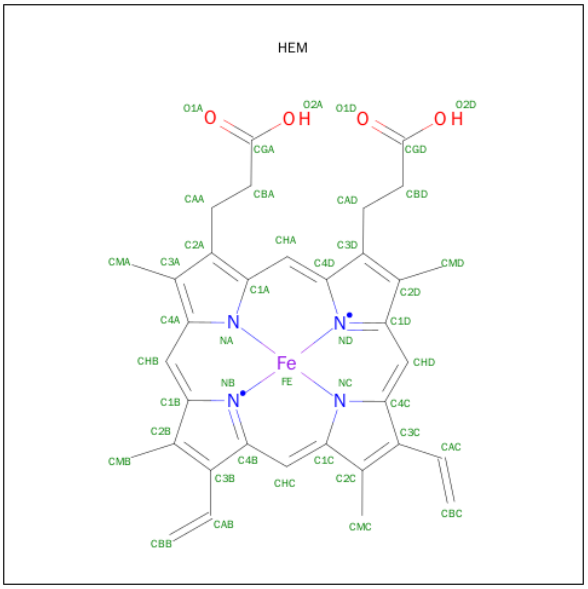
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	EXPRESSION TAG	UNP P05093
C	21	LYS	-	EXPRESSION TAG	UNP P05093
C	22	LYS	-	EXPRESSION TAG	UNP P05093
C	23	THR	-	EXPRESSION TAG	UNP P05093
C	105	LEU	ALA	ENGINEERED MUTATION	UNP P05093
C	509	HIS	-	EXPRESSION TAG	UNP P05093
C	510	HIS	-	EXPRESSION 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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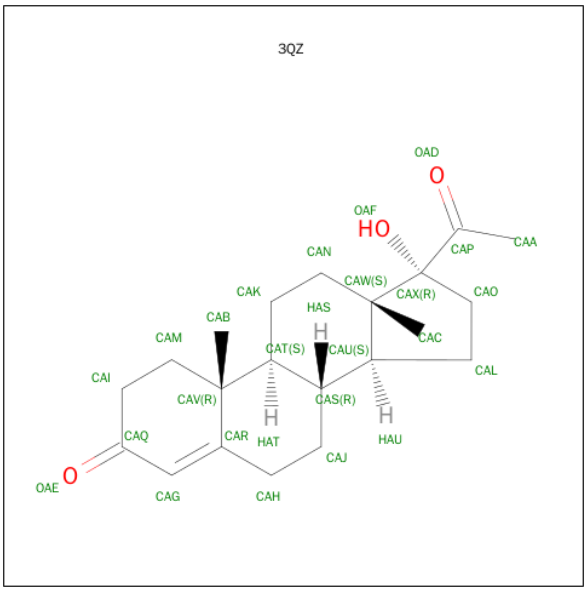
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is (9BETA)-17-HYDROXYPREGN-4-ENE-3,20-DIONE (three-letter code: 3QZ) (formula: $C_{21}H_{30}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			54	21	30	3		
3	B	1	Total	C	H	O	0	0
			54	21	30	3		
3	C	1	Total	C	H	O	0	0
			54	21	30	3		
3	D	1	Total	C	H	O	0	0
			54	21	30	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	36	Total	O	0	0
			36	36		

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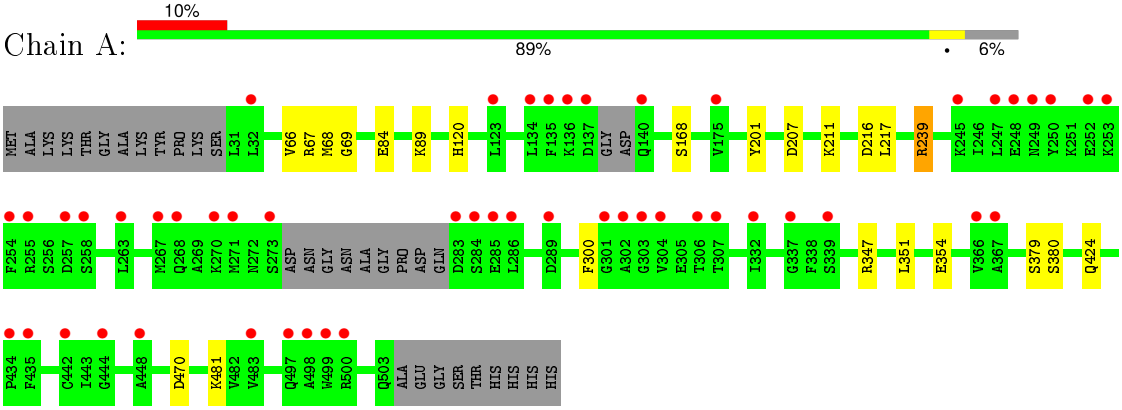
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	53	Total O 53 53	0	0
4	D	32	Total O 32 32	0	0

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.

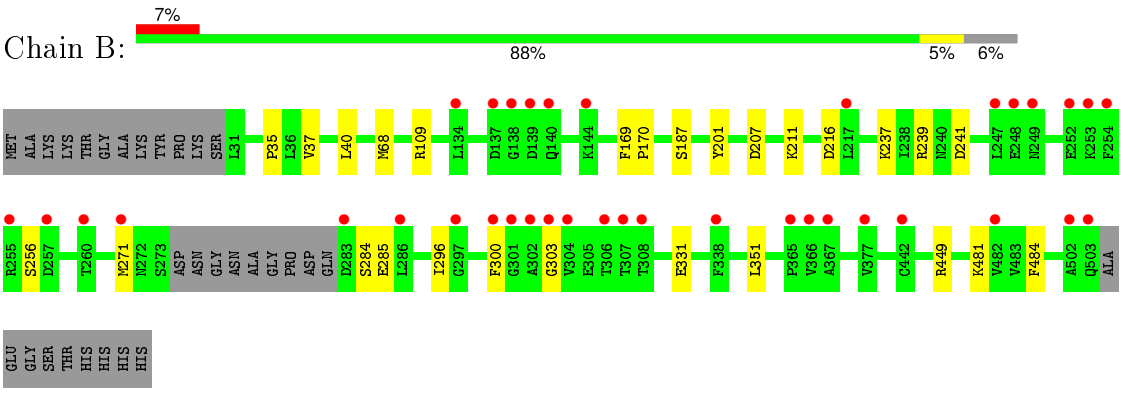
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain A:



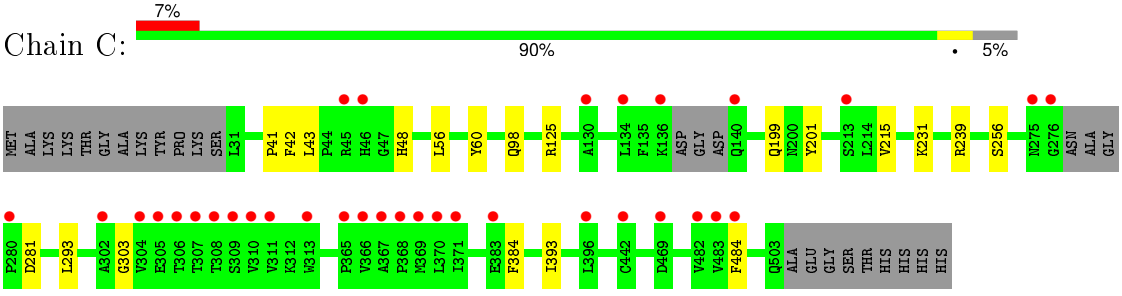
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain B:



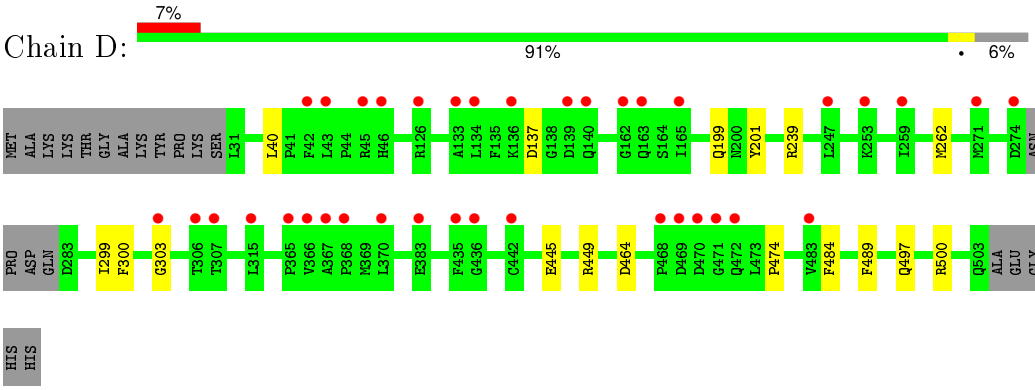
- Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain C:



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

Chain D:


7%
91%
6%
MET ALA LYS LYS THR GLY ALA LYS TYR PRO LYS SER L31 L40 P41 F42 L43 P44 R45 H46 R126 A133 L134 F135 K136 D137 G138 D139 Q140 G162 Q163 S164 I165 Q199 N200 Y201 R239 L247 K253 I259 M262 M271 D274 ASN GLY ASN ALA GLY
PRO ASP GLN D283 I299 F300 G303 T306 T307 L315 P365 V366 A367 P368 M369 L370 E383 F435 G436 C442 E445 R449 D464 P468 D469 D470 G471 Q472 L473 P474 V483 F484 F489 Q497 R500 Q503 ALA GLU GLY SER THR HIS HIS
HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.28Å 151.78Å 168.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.15 – 2.55 39.15 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.15-2.55) 98.8 (39.15-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.178 , 0.244 0.191 , 0.246	Depositor DCC
R_{free} test set	3806 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 75848 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30605	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3QZ, 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	0.35	0/3770	0.51	0/5102
1	B	0.37	0/3783	0.51	0/5121
1	C	0.39	0/3807	0.52	0/5152
1	D	0.37	0/3791	0.51	0/5132
All	All	0.37	0/15151	0.52	0/20507

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	3691	3782	3773	9	0
1	B	3703	3793	3781	9	0
1	C	3727	3739	3802	9	0
1	D	3711	3790	3785	6	0
2	A	43	30	30	2	0
2	B	43	30	30	1	0
2	C	43	30	30	2	0
2	D	43	30	30	2	0
3	A	24	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	30	30	0	0
3	C	24	30	30	0	0
3	D	24	30	30	0	0
4	A	40	0	0	1	0
4	B	36	0	0	0	0
4	C	53	0	0	1	0
4	D	32	0	0	0	0
All	All	15261	15344	15381	35	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 1.

All (35) 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)
3:A:601:3QZ:HAN	3:A:601:3QZ:HAA	1.70	0.71
1:D:445:GLU:OE2	1:D:449:ARG:NH2	2.29	0.65
1:A:239:ARG:NH2	4:A:733:HOH:O	2.29	0.65
1:A:84:GLU:OE2	1:A:89:LYS:NZ	2.31	0.64
2:A:600:HEM:HHC	2:A:600:HEM:HBB2	1.80	0.62
2:A:600:HEM:HHD	2:A:600:HEM:HBC2	1.82	0.61
1:C:42:PHE:O	1:C:43:LEU:HG	2.03	0.59
1:B:303:GLY:HA2	2:B:600:HEM:HMC2	1.85	0.58
1:C:125:ARG:NH1	2:C:600:HEM:O1D	2.37	0.58
3:A:601:3QZ:CAN	3:A:601:3QZ:HAA	2.35	0.57
1:A:470:ASP:O	1:C:231:LYS:NZ	2.35	0.54
1:D:497:GLN:OE1	1:D:500:ARG:NH1	2.42	0.52
1:B:40:LEU:HD21	1:B:68:MET:HE1	1.92	0.51
1:A:347:ARG:NH2	1:A:354:GLU:OE1	2.44	0.51
1:C:48:HIS:HD2	4:C:734:HOH:O	1.94	0.51
1:D:474:PRO:HB3	1:D:489:PHE:CG	2.48	0.48
1:D:262:MET:SD	1:D:299:ILE:HD13	2.54	0.47
1:A:211:LYS:O	1:A:481:LYS:NZ	2.34	0.47
1:B:256:SER:OG	1:B:271:MET:SD	2.73	0.47
1:B:211:LYS:O	1:B:481:LYS:NZ	2.39	0.47
1:D:137:ASP:OD1	1:D:137:ASP:N	2.49	0.46
1:B:237:LYS:NZ	1:B:241:ASP:OD2	2.50	0.44
1:A:66:VAL:HG12	1:A:68:MET:HE2	1.99	0.44
1:A:351:LEU:HD13	1:A:424:GLN:HA	2.00	0.43
1:A:379:SER:OG	1:A:380:SER:N	2.49	0.43
1:B:169:PHE:HB3	1:B:170:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLY:HA2	2:D:600:HEM:HMC2	1.99	0.43
1:A:67:ARG:NH1	1:A:69:GLY:O	2.52	0.43
1:B:37:VAL:O	1:C:41:PRO:HD2	2.20	0.42
1:C:42:PHE:HE2	1:C:60:TYR:HH	1.67	0.41
1:C:303:GLY:HA2	2:C:600:HEM:HMC2	2.02	0.41
1:B:331:GLU:OE2	1:B:351:LEU:N	2.54	0.41
1:B:35:PRO:HD3	1:C:384:PHE:CE1	2.55	0.41
1:C:215:VAL:HG13	1:C:393:ILE:CD1	2.52	0.40
2:D:600:HEM:HMC2	2:D:600:HEM:HBC2	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	456/494 (92%)	441 (97%)	15 (3%)	0	100	100
1	B	460/494 (93%)	442 (96%)	18 (4%)	0	100	100
1	C	461/494 (93%)	450 (98%)	11 (2%)	0	100	100
1	D	461/494 (93%)	440 (95%)	21 (5%)	0	100	100
All	All	1838/1976 (93%)	1773 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	414/437 (95%)	406 (98%)	8 (2%)	65 86
1	B	415/437 (95%)	403 (97%)	12 (3%)	50 75
1	C	418/437 (96%)	409 (98%)	9 (2%)	60 83
1	D	416/437 (95%)	409 (98%)	7 (2%)	68 88
All	All	1663/1748 (95%)	1627 (98%)	36 (2%)	60 83

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

Mol	Chain	Res	Type
1	A	120	HIS
1	A	168	SER
1	A	201	TYR
1	A	207	ASP
1	A	216	ASP
1	A	217	LEU
1	A	239	ARG
1	A	300	PHE
1	B	109	ARG
1	B	187	SER
1	B	201	TYR
1	B	207	ASP
1	B	216	ASP
1	B	239	ARG
1	B	284	SER
1	B	285	GLU
1	B	296	ILE
1	B	300	PHE
1	B	449	ARG
1	B	484	PHE
1	C	56	LEU
1	C	98	GLN
1	C	199	GLN
1	C	201	TYR
1	C	239	ARG
1	C	256	SER
1	C	281	ASP
1	C	293	LEU
1	C	484	PHE
1	D	40	LEU
1	D	199	GLN
1	D	201	TYR
1	D	239	ARG

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Mol	Chain	Res	Type
1	D	300	PHE
1	D	464	ASP
1	D	484	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	B	50	HIS
1	B	140	GLN
1	B	202	ASN
1	B	407	HIS
1	C	50	HIS
1	C	202	ASN
1	D	50	HIS
1	D	160	HIS
1	D	202	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

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	2.10	10 (33%)	24,82,82	2.44	10 (41%)
3	3QZ	A	601	-	27,27,27	4.04	17 (62%)	42,45,45	5.27	16 (38%)
2	HEM	B	600	1	30,50,50	2.19	7 (23%)	24,82,82	2.69	8 (33%)
3	3QZ	B	601	-	27,27,27	4.04	17 (62%)	42,45,45	5.20	20 (47%)
2	HEM	C	600	1	30,50,50	2.13	8 (26%)	24,82,82	2.58	10 (41%)
3	3QZ	C	601	-	27,27,27	4.05	18 (66%)	42,45,45	5.21	17 (40%)
2	HEM	D	600	1	30,50,50	2.21	8 (26%)	24,82,82	2.50	7 (29%)
3	3QZ	D	601	-	27,27,27	4.13	18 (66%)	42,45,45	5.11	19 (45%)

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	3QZ	A	601	-	-	2/6/68/68	0/4/4/4
2	HEM	B	600	1	-	0/10/54/54	0/0/8/8
3	3QZ	B	601	-	-	0/6/68/68	0/4/4/4
2	HEM	C	600	1	-	0/10/54/54	0/0/8/8
3	3QZ	C	601	-	-	0/6/68/68	0/4/4/4
2	HEM	D	600	1	-	0/10/54/54	0/0/8/8
3	3QZ	D	601	-	-	0/6/68/68	0/4/4/4

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	C3B-C4B	-7.76	1.44	1.51
2	C	600	HEM	C3B-C4B	-6.82	1.45	1.51
2	D	600	HEM	C3B-C4B	-6.79	1.45	1.51
3	D	601	3QZ	CAV-CAT	-5.85	1.45	1.56
2	A	600	HEM	C3B-C4B	-5.80	1.46	1.51
2	D	600	HEM	C3D-C4D	-5.40	1.44	1.51
3	C	601	3QZ	CAV-CAT	-5.40	1.46	1.56
3	A	601	3QZ	CAV-CAT	-5.38	1.46	1.56
2	C	600	HEM	C3D-C4D	-5.18	1.44	1.51
3	A	601	3QZ	CAW-CAU	-5.04	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	3QZ	CAV-CAT	-4.97	1.47	1.56
2	A	600	HEM	C3D-C4D	-4.91	1.45	1.51
2	B	600	HEM	C3D-C4D	-4.80	1.45	1.51
3	D	601	3QZ	CAW-CAU	-4.65	1.46	1.54
3	C	601	3QZ	CAW-CAU	-4.56	1.46	1.54
3	B	601	3QZ	CAW-CAU	-4.35	1.47	1.54
2	B	600	HEM	C2C-C1C	-4.20	1.44	1.52
2	A	600	HEM	C2C-C1C	-3.91	1.45	1.52
2	C	600	HEM	C2C-C1C	-3.73	1.45	1.52
2	D	600	HEM	C2C-C1C	-3.65	1.45	1.52
3	C	601	3QZ	CAV-CAR	-3.51	1.45	1.52
3	D	601	3QZ	CAV-CAR	-3.49	1.45	1.52
3	D	601	3QZ	CAS-CAT	-3.44	1.46	1.53
3	C	601	3QZ	CAS-CAT	-3.42	1.46	1.53
3	A	601	3QZ	CAS-CAT	-3.39	1.46	1.53
3	A	601	3QZ	CAV-CAR	-3.29	1.45	1.52
3	B	601	3QZ	CAV-CAR	-3.15	1.46	1.52
3	B	601	3QZ	CAS-CAT	-3.13	1.47	1.53
3	C	601	3QZ	CAN-CAW	-2.93	1.48	1.54
3	A	601	3QZ	CAN-CAW	-2.79	1.49	1.54
3	D	601	3QZ	CAN-CAW	-2.72	1.49	1.54
3	D	601	3QZ	CAX-CAP	-2.28	1.49	1.53
3	B	601	3QZ	CAN-CAW	-2.27	1.50	1.54
3	A	601	3QZ	CAX-CAP	-2.25	1.49	1.53
3	C	601	3QZ	CAX-CAP	-2.10	1.49	1.53
2	B	600	HEM	C2D-C1D	-2.09	1.45	1.51
2	C	600	HEM	C2D-C1D	-2.08	1.45	1.51
2	A	600	HEM	C2B-C1B	-2.03	1.45	1.51
3	D	601	3QZ	CAS-CAU	-2.01	1.49	1.53
2	A	600	HEM	CAA-C2A	2.04	1.55	1.52
2	C	600	HEM	CAA-C2A	2.05	1.55	1.52
2	D	600	HEM	C1C-NC	2.09	1.38	1.36
3	B	601	3QZ	CAA-CAP	2.12	1.56	1.49
3	B	601	3QZ	CAM-CAI	2.14	1.57	1.53
2	B	600	HEM	FE-NC	2.19	2.04	1.95
3	C	601	3QZ	CAA-CAP	2.21	1.56	1.49
2	B	600	HEM	C3B-CAB	2.25	1.55	1.51
2	C	600	HEM	C3C-CAC	2.29	1.55	1.51
2	A	600	HEM	FE-ND	2.34	2.09	1.97
3	A	601	3QZ	CAM-CAI	2.36	1.58	1.53
2	C	600	HEM	FE-ND	2.37	2.10	1.97
2	B	600	HEM	FE-ND	2.37	2.10	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	3QZ	CAO-CAL	2.38	1.62	1.54
3	C	601	3QZ	CAM-CAI	2.41	1.58	1.53
2	D	600	HEM	C3C-CAC	2.42	1.55	1.51
3	D	601	3QZ	CAO-CAL	2.43	1.62	1.54
2	D	600	HEM	C3B-CAB	2.43	1.55	1.51
2	C	600	HEM	FE-NC	2.44	2.05	1.95
2	A	600	HEM	C4C-NC	2.45	1.39	1.36
3	B	601	3QZ	CAO-CAL	2.48	1.62	1.54
2	A	600	HEM	C3B-CAB	2.50	1.56	1.51
2	A	600	HEM	FE-NB	2.52	2.10	1.97
3	A	601	3QZ	CAO-CAL	2.53	1.62	1.54
2	A	600	HEM	C3C-CAC	2.61	1.56	1.51
3	D	601	3QZ	CAM-CAI	2.64	1.59	1.53
2	D	600	HEM	FE-NC	2.88	2.07	1.95
2	D	600	HEM	FE-ND	3.05	2.13	1.97
3	D	601	3QZ	CAG-CAQ	3.07	1.52	1.45
3	A	601	3QZ	CAI-CAQ	3.15	1.56	1.49
3	A	601	3QZ	CAG-CAQ	3.33	1.52	1.45
3	C	601	3QZ	CAG-CAQ	3.33	1.52	1.45
3	C	601	3QZ	CAI-CAQ	3.34	1.57	1.49
3	C	601	3QZ	CAM-CAV	3.52	1.60	1.54
3	B	601	3QZ	CAG-CAQ	3.53	1.53	1.45
3	B	601	3QZ	CAI-CAQ	3.57	1.57	1.49
3	B	601	3QZ	CAM-CAV	3.63	1.60	1.54
3	D	601	3QZ	CAI-CAQ	3.92	1.58	1.49
3	D	601	3QZ	CAM-CAV	3.99	1.61	1.54
3	A	601	3QZ	CAM-CAV	4.01	1.61	1.54
3	C	601	3QZ	CAH-CAR	4.26	1.57	1.50
3	C	601	3QZ	CAJ-CAS	4.32	1.61	1.53
3	D	601	3QZ	CAH-CAR	4.38	1.57	1.50
3	A	601	3QZ	CAH-CAR	4.40	1.57	1.50
3	B	601	3QZ	CAH-CAR	4.47	1.57	1.50
3	B	601	3QZ	CAJ-CAS	4.51	1.61	1.53
3	A	601	3QZ	CAJ-CAS	4.52	1.61	1.53
3	D	601	3QZ	CAJ-CAS	4.80	1.62	1.53
3	B	601	3QZ	CAJ-CAH	5.27	1.65	1.52
3	C	601	3QZ	CAJ-CAH	5.60	1.65	1.52
3	D	601	3QZ	CAJ-CAH	5.79	1.66	1.52
3	A	601	3QZ	CAJ-CAH	5.81	1.66	1.52
3	A	601	3QZ	CAN-CAK	7.68	1.70	1.53
3	B	601	3QZ	CAN-CAK	7.74	1.70	1.53
3	C	601	3QZ	CAN-CAK	7.83	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	3QZ	CAN-CAK	7.95	1.71	1.53
3	C	601	3QZ	CAO-CAX	8.29	1.67	1.54
3	D	601	3QZ	CAO-CAX	8.35	1.68	1.54
3	A	601	3QZ	CAO-CAX	8.55	1.68	1.54
3	B	601	3QZ	CAO-CAX	9.03	1.69	1.54
3	A	601	3QZ	CAK-CAT	9.43	1.70	1.53
3	D	601	3QZ	CAK-CAT	9.61	1.70	1.53
3	B	601	3QZ	CAK-CAT	9.97	1.71	1.53
3	C	601	3QZ	CAK-CAT	9.97	1.71	1.53

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	3QZ	OAF-CAX-CAP	-20.43	74.73	107.65
3	C	601	3QZ	OAF-CAX-CAP	-19.16	76.79	107.65
3	B	601	3QZ	OAF-CAX-CAP	-19.09	76.90	107.65
3	D	601	3QZ	OAF-CAX-CAP	-17.36	79.68	107.65
3	B	601	3QZ	OAF-CAX-CAO	-8.57	90.79	110.65
3	C	601	3QZ	OAF-CAX-CAO	-8.50	90.95	110.65
3	D	601	3QZ	OAF-CAX-CAO	-8.36	91.28	110.65
3	D	601	3QZ	OAF-CAX-CAW	-8.02	90.97	107.92
3	A	601	3QZ	OAF-CAX-CAW	-7.69	91.65	107.92
3	D	601	3QZ	CAH-CAR-CAG	-7.54	111.32	120.89
3	A	601	3QZ	OAF-CAX-CAO	-7.20	93.96	110.65
3	D	601	3QZ	CAC-CAW-CAX	-7.04	100.95	109.13
3	C	601	3QZ	CAC-CAW-CAX	-7.02	100.97	109.13
3	A	601	3QZ	CAM-CAI-CAQ	-6.90	97.62	111.64
3	B	601	3QZ	OAF-CAX-CAW	-6.78	93.59	107.92
3	C	601	3QZ	OAF-CAX-CAW	-6.60	93.96	107.92
3	C	601	3QZ	CAM-CAI-CAQ	-6.29	98.86	111.64
3	B	601	3QZ	CAC-CAW-CAX	-5.86	102.32	109.13
3	B	601	3QZ	CAM-CAI-CAQ	-5.82	99.82	111.64
3	A	601	3QZ	CAC-CAW-CAX	-5.29	102.98	109.13
3	B	601	3QZ	CAL-CAU-CAS	-5.27	110.70	119.03
3	C	601	3QZ	CAL-CAU-CAS	-5.24	110.75	119.03
3	C	601	3QZ	CAH-CAR-CAG	-5.22	114.27	120.89
3	A	601	3QZ	CAH-CAR-CAG	-5.08	114.44	120.89
3	A	601	3QZ	CAL-CAU-CAS	-5.03	111.08	119.03
3	D	601	3QZ	CAL-CAU-CAS	-5.01	111.12	119.03
3	B	601	3QZ	CAJ-CAH-CAR	-4.49	103.61	111.90
3	D	601	3QZ	CAM-CAI-CAQ	-4.45	102.60	111.64
3	B	601	3QZ	CAH-CAR-CAG	-4.17	115.60	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	HEM	CAA-CBA-CGA	-3.98	105.44	112.75
2	A	600	HEM	CAA-C2A-C1A	-3.61	123.09	127.01
3	B	601	3QZ	CAH-CAJ-CAS	-3.60	105.64	111.67
2	B	600	HEM	CAA-C2A-C1A	-3.55	123.16	127.01
3	C	601	3QZ	CAK-CAN-CAW	-3.30	107.18	112.80
3	B	601	3QZ	CAI-CAM-CAV	-3.27	108.80	113.41
3	A	601	3QZ	CAJ-CAH-CAR	-2.96	106.45	111.90
3	C	601	3QZ	CAJ-CAH-CAR	-2.95	106.45	111.90
3	A	601	3QZ	CAK-CAN-CAW	-2.85	107.94	112.80
3	B	601	3QZ	CAJ-CAS-CAT	-2.81	107.09	110.46
3	D	601	3QZ	CAK-CAN-CAW	-2.79	108.05	112.80
2	D	600	HEM	CAA-C2A-C1A	-2.63	124.15	127.01
3	B	601	3QZ	CAK-CAN-CAW	-2.52	108.51	112.80
3	A	601	3QZ	CAI-CAM-CAV	-2.49	109.90	113.41
2	A	600	HEM	CAA-CBA-CGA	-2.39	108.37	112.75
3	C	601	3QZ	CAI-CAM-CAV	-2.34	110.11	113.41
3	D	601	3QZ	CAK-CAT-CAS	-2.30	108.40	111.74
3	C	601	3QZ	CAJ-CAS-CAU	-2.29	108.23	112.02
3	B	601	3QZ	CAM-CAV-CAT	-2.29	105.71	108.64
2	C	600	HEM	CBA-CAA-C2A	-2.24	108.51	112.53
3	A	601	3QZ	CAK-CAT-CAS	-2.23	108.50	111.74
3	D	601	3QZ	CAC-CAW-CAN	-2.18	106.60	109.80
3	B	601	3QZ	OAD-CAP-CAA	-2.16	117.03	121.41
2	A	600	HEM	CMA-C3A-C4A	-2.16	124.80	128.36
2	C	600	HEM	CAA-C2A-C1A	-2.09	124.74	127.01
2	A	600	HEM	C3B-C4B-NB	-2.08	107.64	111.63
2	C	600	HEM	CMA-C3A-C4A	-2.08	124.92	128.36
3	C	601	3QZ	CAK-CAT-CAS	-2.06	108.75	111.74
2	B	600	HEM	CBD-CAD-C3D	-2.03	107.65	113.55
3	D	601	3QZ	CAL-CAO-CAX	-2.01	102.45	105.96
3	D	601	3QZ	CAO-CAX-CAW	2.01	105.14	103.20
2	D	600	HEM	C2D-C3D-C4D	2.02	104.92	101.50
3	D	601	3QZ	CAH-CAJ-CAS	2.04	115.08	111.67
3	D	601	3QZ	CAC-CAW-CAU	2.10	115.96	111.81
2	C	600	HEM	C3B-C4B-CHC	2.32	126.43	123.16
2	C	600	HEM	C2D-C3D-C4D	2.36	105.50	101.50
2	D	600	HEM	CMD-C2D-C3D	2.61	125.89	114.35
2	A	600	HEM	CMD-C2D-C3D	2.93	127.29	114.35
2	B	600	HEM	CMD-C2D-C3D	3.00	127.63	114.35
2	C	600	HEM	CMD-C2D-C3D	3.11	128.10	114.35
3	B	601	3QZ	CAT-CAV-CAR	3.26	114.74	109.67
3	A	601	3QZ	CAL-CAU-CAW	3.46	108.23	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	C3B-C4B-CHC	3.88	128.62	123.16
2	A	600	HEM	CAD-C3D-C4D	3.97	126.46	112.47
2	C	600	HEM	CAD-C3D-C4D	3.99	126.55	112.47
2	A	600	HEM	CMC-C2C-C3C	4.00	126.52	116.53
2	B	600	HEM	CAD-C3D-C4D	4.05	126.77	112.47
3	B	601	3QZ	CAL-CAU-CAW	4.13	109.10	103.75
2	A	600	HEM	CMB-C2B-C3B	4.18	126.95	116.53
3	C	601	3QZ	CAL-CAU-CAW	4.26	109.27	103.75
2	D	600	HEM	CAD-C3D-C4D	4.37	127.89	112.47
3	D	601	3QZ	CAL-CAU-CAW	4.50	109.58	103.75
2	D	600	HEM	CAD-C3D-C2D	4.86	127.19	113.22
3	B	601	3QZ	CAH-CAR-CAV	5.11	122.52	116.71
2	C	600	HEM	CAD-C3D-C2D	5.13	127.95	113.22
2	B	600	HEM	CAD-C3D-C2D	5.40	128.75	113.22
2	A	600	HEM	CAD-C3D-C2D	5.48	128.97	113.22
3	C	601	3QZ	CAH-CAR-CAV	5.71	123.20	116.71
3	A	601	3QZ	CAH-CAR-CAV	5.76	123.25	116.71
2	C	600	HEM	CMB-C2B-C3B	5.85	131.14	116.53
2	D	600	HEM	CMB-C2B-C3B	5.95	131.39	116.53
2	B	600	HEM	CMB-C2B-C3B	5.98	131.46	116.53
2	D	600	HEM	CMC-C2C-C3C	6.02	131.55	116.53
2	C	600	HEM	CMC-C2C-C3C	6.18	131.95	116.53
2	B	600	HEM	CMC-C2C-C3C	6.19	131.99	116.53
3	D	601	3QZ	CAX-CAW-CAU	6.46	107.11	99.81
3	B	601	3QZ	CAX-CAW-CAU	6.60	107.26	99.81
3	C	601	3QZ	CAX-CAW-CAU	7.23	107.97	99.81
3	A	601	3QZ	CAX-CAW-CAU	7.69	108.50	99.81
3	D	601	3QZ	CAH-CAR-CAV	7.77	125.54	116.71
3	A	601	3QZ	CAO-CAX-CAP	10.25	125.31	113.70
3	D	601	3QZ	CAO-CAX-CAP	10.37	125.45	113.70
3	C	601	3QZ	CAO-CAX-CAP	10.46	125.56	113.70
3	B	601	3QZ	CAO-CAX-CAP	11.42	126.64	113.70
3	D	601	3QZ	CAW-CAX-CAP	14.61	128.45	112.93
3	B	601	3QZ	CAW-CAX-CAP	14.90	128.76	112.93
3	C	601	3QZ	CAW-CAX-CAP	15.39	129.29	112.93
3	A	601	3QZ	CAW-CAX-CAP	15.80	129.72	112.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	3QZ	OAD-CAP-CAX-CAW

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Mol	Chain	Res	Type	Atoms
3	A	601	3QZ	CAW-CAX-CAP-CAA

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
3	A	601	3QZ	2	0
2	B	600	HEM	1	0
2	C	600	HEM	2	0
2	D	600	HEM	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^{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	462/494 (93%)	0.51	51 (11%) 7 8	34, 50, 78, 107	0
1	B	464/494 (93%)	0.46	37 (7%) 15 17	34, 48, 76, 105	0
1	C	467/494 (94%)	0.43	34 (7%) 18 20	33, 47, 73, 92	0
1	D	465/494 (94%)	0.48	37 (7%) 15 17	34, 49, 76, 107	0
All	All	1858/1976 (94%)	0.47	159 (8%) 13 14	33, 49, 77, 107	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	MET	8.0
1	D	139	ASP	5.6
1	B	139	ASP	5.3
1	C	280	PRO	5.1
1	A	302	ALA	5.0
1	A	140	GLN	5.0
1	B	140	GLN	4.8
1	A	283	ASP	4.7
1	C	366	VAL	4.4
1	A	255	ARG	4.4
1	D	140	GLN	4.2
1	A	135	PHE	4.1
1	D	469	ASP	4.1
1	D	470	ASP	4.0
1	A	137	ASP	3.9
1	B	302	ALA	3.8
1	A	304	VAL	3.8
1	C	367	ALA	3.7
1	C	134	LEU	3.7
1	C	140	GLN	3.7
1	A	257	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	253	LYS	3.6
1	B	301	GLY	3.6
1	B	304	VAL	3.5
1	C	45	ARG	3.5
1	C	304	VAL	3.4
1	B	303	GLY	3.4
1	C	469	ASP	3.4
1	C	365	PRO	3.4
1	A	306	THR	3.3
1	C	483	VAL	3.3
1	A	134	LEU	3.3
1	A	249	ASN	3.3
1	D	43	LEU	3.3
1	B	255	ARG	3.3
1	D	42	PHE	3.3
1	C	308	THR	3.3
1	D	306	THR	3.3
1	A	245	LYS	3.3
1	C	484	PHE	3.3
1	B	366	VAL	3.2
1	C	306	THR	3.2
1	D	136	LYS	3.2
1	B	254	PHE	3.1
1	C	368	PRO	3.1
1	A	332	ILE	3.1
1	B	306	THR	3.1
1	D	365	PRO	3.1
1	A	267	MET	3.1
1	A	250	TYR	3.1
1	A	289	ASP	3.0
1	A	303	GLY	3.0
1	B	138	GLY	3.0
1	C	370	LEU	3.0
1	A	254	PHE	3.0
1	D	247	LEU	3.0
1	C	383	GLU	3.0
1	A	497	GLN	3.0
1	B	252	GLU	3.0
1	D	163	GLN	2.9
1	C	307	THR	2.9
1	B	137	ASP	2.9
1	C	482	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	442	CYS	2.8
1	D	271	MET	2.8
1	D	442	CYS	2.8
1	B	283	ASP	2.8
1	A	273	SER	2.8
1	D	46	HIS	2.8
1	A	270	LYS	2.8
1	C	309	SER	2.8
1	A	247	LEU	2.7
1	D	472	GLN	2.7
1	B	307	THR	2.7
1	A	483	VAL	2.7
1	C	369	MET	2.7
1	A	337	GLY	2.7
1	B	297	GLY	2.6
1	B	144	LYS	2.6
1	C	213	SER	2.6
1	B	367	ALA	2.6
1	C	130	ALA	2.6
1	A	136	LYS	2.6
1	C	313	TRP	2.6
1	B	300	PHE	2.6
1	C	276	GLY	2.6
1	D	370	LEU	2.6
1	A	435	PHE	2.6
1	C	136	LYS	2.5
1	A	284	SER	2.5
1	B	308	THR	2.5
1	A	500	ARG	2.5
1	D	134	LEU	2.5
1	A	367	ALA	2.5
1	B	338	PHE	2.5
1	A	258	SER	2.5
1	C	311	VAL	2.5
1	B	271	MET	2.5
1	D	436	GLY	2.5
1	C	442	CYS	2.4
1	A	252	GLU	2.4
1	A	285	GLU	2.4
1	D	45	ARG	2.4
1	A	301	GLY	2.4
1	A	434	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	217	LEU	2.4
1	A	248	GLU	2.4
1	C	310	VAL	2.4
1	B	482	VAL	2.4
1	B	248	GLU	2.4
1	A	444	GLY	2.3
1	D	435	PHE	2.3
1	B	247	LEU	2.3
1	D	483	VAL	2.3
1	C	305	GLU	2.3
1	C	46	HIS	2.3
1	D	367	ALA	2.3
1	A	499	TRP	2.3
1	D	468	PRO	2.3
1	C	396	LEU	2.3
1	A	286	LEU	2.3
1	A	253	LYS	2.3
1	C	302	ALA	2.2
1	D	165	ILE	2.2
1	B	503	GLN	2.2
1	D	471	GLY	2.2
1	D	383	GLU	2.2
1	B	365	PRO	2.2
1	D	368	PRO	2.2
1	A	498	ALA	2.2
1	B	257	ASP	2.2
1	D	133	ALA	2.2
1	D	307	THR	2.2
1	B	134	LEU	2.2
1	D	274	ASP	2.2
1	D	303	GLY	2.1
1	A	263	LEU	2.1
1	A	175	VAL	2.1
1	A	32	LEU	2.1
1	A	123	LEU	2.1
1	D	162	GLY	2.1
1	B	502	ALA	2.1
1	D	366	VAL	2.1
1	A	448	ALA	2.1
1	B	442	CYS	2.1
1	A	268	GLN	2.1
1	D	126	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	307	THR	2.1
1	B	260	THR	2.1
1	A	366	VAL	2.1
1	B	377	VAL	2.1
1	B	286	LEU	2.1
1	D	253	LYS	2.1
1	A	339	SER	2.1
1	D	259	ILE	2.0
1	B	249	ASN	2.0
1	C	371	ILE	2.0
1	D	315	LEU	2.0
1	C	275	ASN	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	D	600	43/43	0.98	0.31	1.48	31,43,53,67	0
2	HEM	A	600	43/43	0.98	0.33	1.45	29,42,55,66	0
2	HEM	C	600	43/43	0.98	0.30	1.06	31,41,52,61	0
3	3QZ	A	601	24/24	0.98	0.32	1.04	43,60,72,74	0
2	HEM	B	600	43/43	0.98	0.28	0.93	31,42,57,70	0
3	3QZ	D	601	24/24	0.96	0.26	0.70	31,44,56,58	0
3	3QZ	B	601	24/24	0.97	0.29	0.56	45,54,61,69	0
3	3QZ	C	601	24/24	0.97	0.26	0.21	35,49,58,65	0

6.5 Other polymers (i)

There are no such residues in this entry.