Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 10:33 PM GMT

PDB ID	:	4Y8W
Title	:	Crystal Structure of Human Cytochrome P450 21A2 Progesterone Complex
Authors	:	Pallan, P.S.; Lei, L.; Egli, M.
Deposited on	:	2015-02-16
Resolution	:	2.64 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:

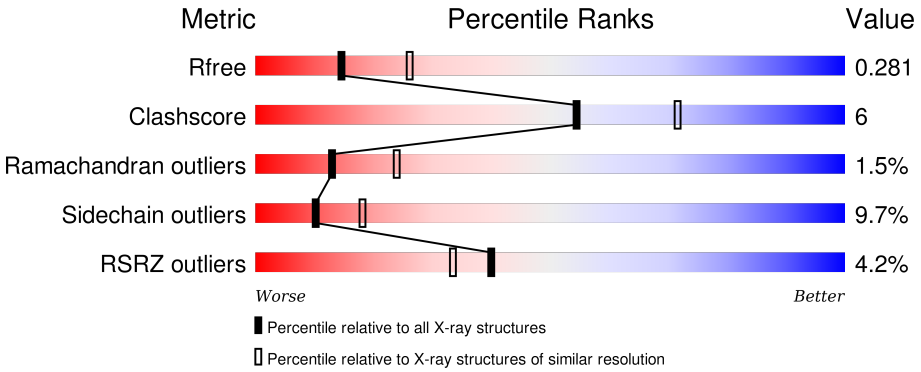
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.64 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	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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	482	5% 69% 18% • 9%
1	B	482	5% 70% 18% • 9%
1	C	482	2% 75% 15% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10832 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 21-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3493	2258	606	612	17			
1	B	440	Total	C	N	O	S	0	0	0
			3513	2270	611	615	17			
1	C	442	Total	C	N	O	S	0	0	0
			3531	2279	617	618	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q16874
A	21	ALA	-	expression tag	UNP Q16874
A	22	LYS	-	expression tag	UNP Q16874
A	23	LYS	-	expression tag	UNP Q16874
A	24	THR	-	expression tag	UNP Q16874
A	25	SER	-	expression tag	UNP Q16874
A	26	SER	-	expression tag	UNP Q16874
A	27	LYS	-	expression tag	UNP Q16874
A	28	GLY	-	expression tag	UNP Q16874
A	29	LYS	-	expression tag	UNP Q16874
A	496	HIS	-	expression tag	UNP Q16874
A	497	HIS	-	expression tag	UNP Q16874
A	498	HIS	-	expression tag	UNP Q16874
A	499	HIS	-	expression tag	UNP Q16874
A	500	HIS	-	expression tag	UNP Q16874
A	501	HIS	-	expression tag	UNP Q16874
B	20	MET	-	initiating methionine	UNP Q16874
B	21	ALA	-	expression tag	UNP Q16874
B	22	LYS	-	expression tag	UNP Q16874
B	23	LYS	-	expression tag	UNP Q16874
B	24	THR	-	expression tag	UNP Q16874
B	25	SER	-	expression tag	UNP Q16874
B	26	SER	-	expression tag	UNP Q16874

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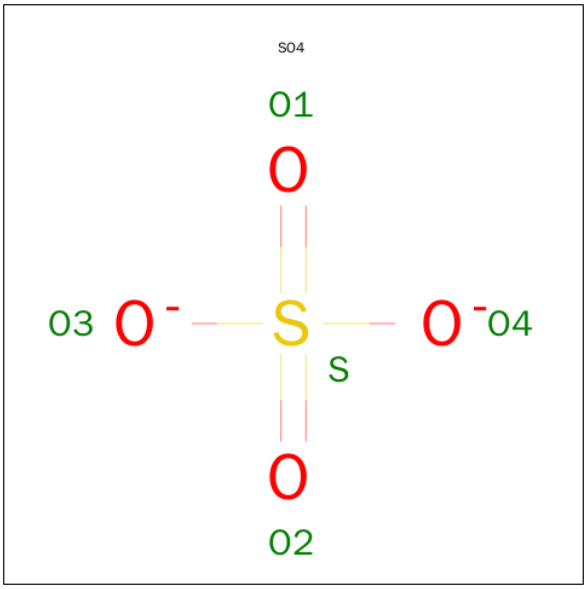
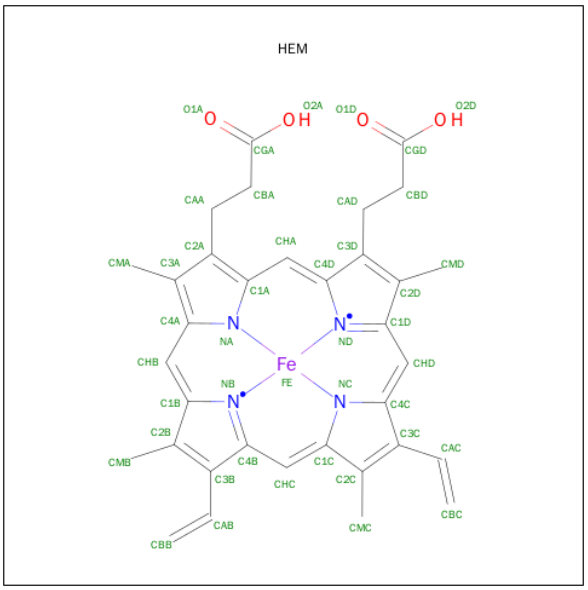
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LYS	-	expression tag	UNP Q16874
B	28	GLY	-	expression tag	UNP Q16874
B	29	LYS	-	expression tag	UNP Q16874
B	496	HIS	-	expression tag	UNP Q16874
B	497	HIS	-	expression tag	UNP Q16874
B	498	HIS	-	expression tag	UNP Q16874
B	499	HIS	-	expression tag	UNP Q16874
B	500	HIS	-	expression tag	UNP Q16874
B	501	HIS	-	expression tag	UNP Q16874
C	20	MET	-	initiating methionine	UNP Q16874
C	21	ALA	-	expression tag	UNP Q16874
C	22	LYS	-	expression tag	UNP Q16874
C	23	LYS	-	expression tag	UNP Q16874
C	24	THR	-	expression tag	UNP Q16874
C	25	SER	-	expression tag	UNP Q16874
C	26	SER	-	expression tag	UNP Q16874
C	27	LYS	-	expression tag	UNP Q16874
C	28	GLY	-	expression tag	UNP Q16874
C	29	LYS	-	expression tag	UNP Q16874
C	496	HIS	-	expression tag	UNP Q16874
C	497	HIS	-	expression tag	UNP Q16874
C	498	HIS	-	expression tag	UNP Q16874
C	499	HIS	-	expression tag	UNP Q16874
C	500	HIS	-	expression tag	UNP Q16874
C	501	HIS	-	expression tag	UNP Q16874

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



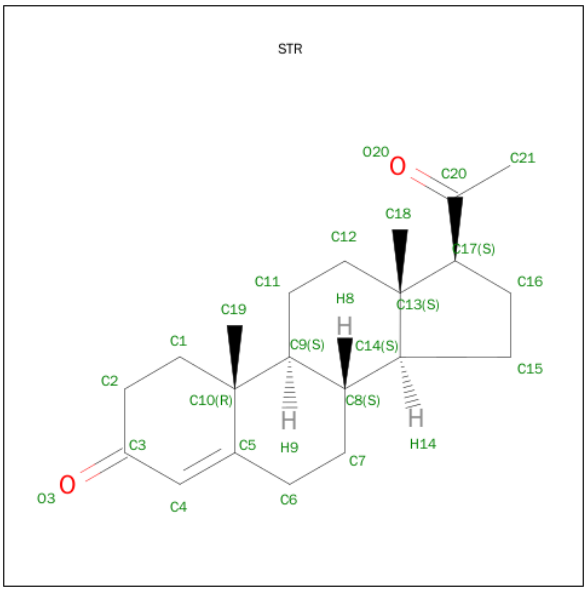
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is PROGESTERONE (three-letter code: STR) (formula: $C_{21}H_{30}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 23 21 2	0	0
4	B	1	Total C O 23 21 2	0	0
4	C	1	Total C O 23 21 2	0	0

- Molecule 5 is water.

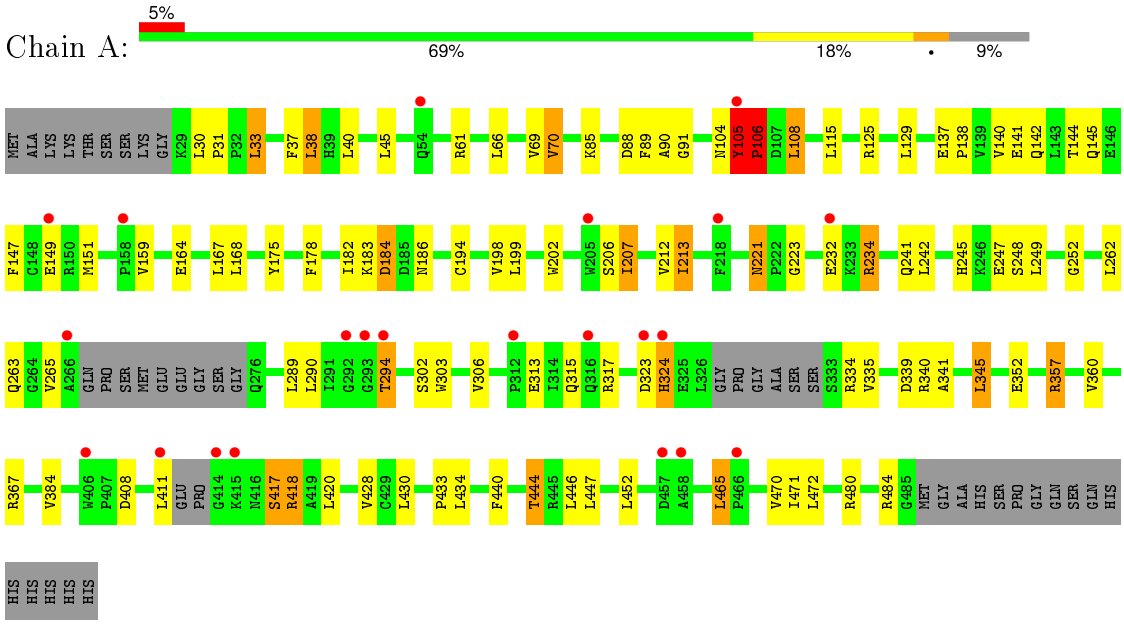
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	25	Total O 25 25	0	0
5	C	30	Total O 30 30	0	0

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.

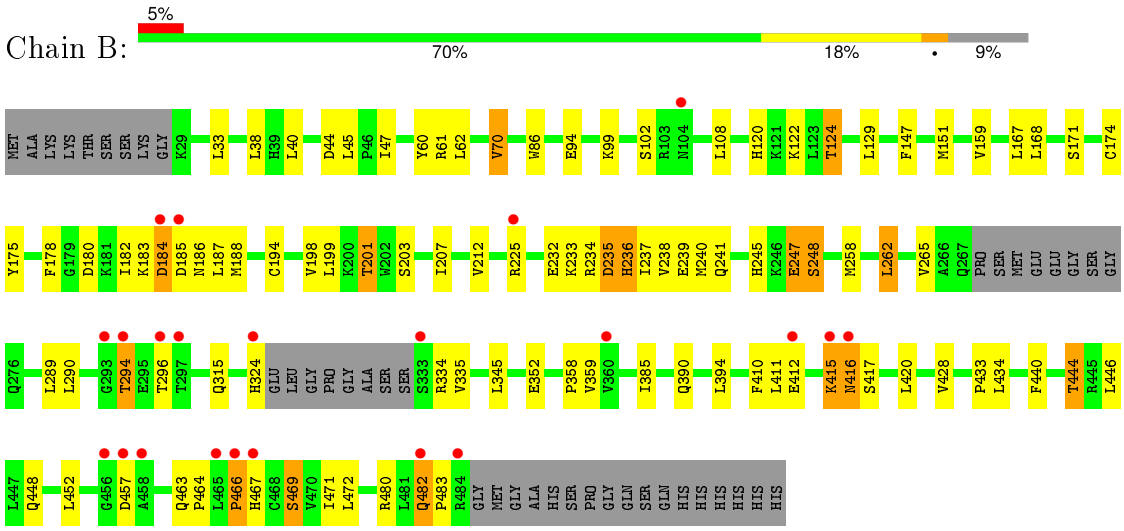
- Molecule 1: Cytochrome P450 21-hydroxylase

Chain A:



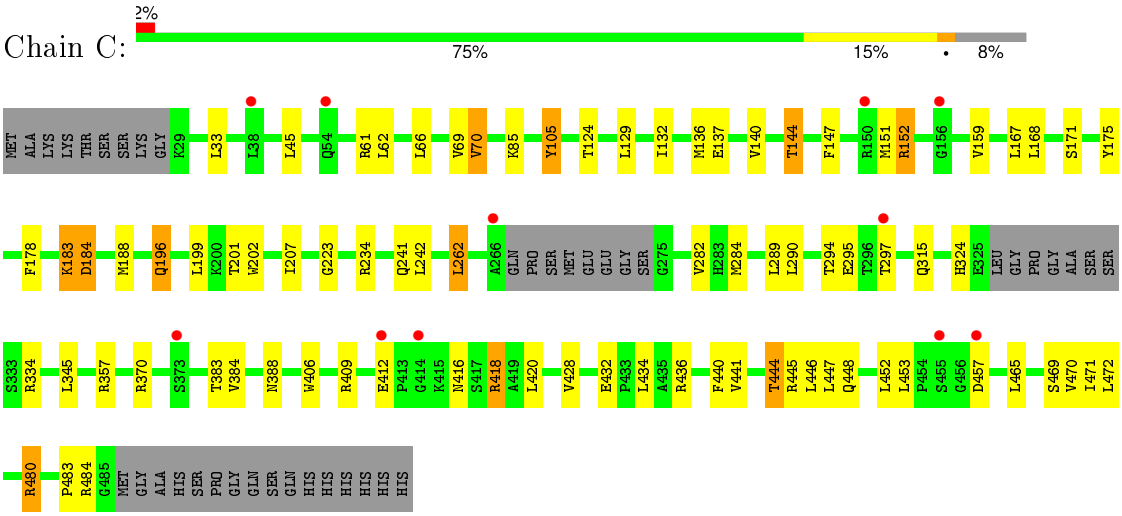
- Molecule 1: Cytochrome P450 21-hydroxylase

Chain B:



- Molecule 1: Cytochrome P450 21-hydroxylase

Chain C:


2%
75%
15%
8%
MET ALA LYS LYS THR SER SER LYS GLY R29 L33 L38 L45 Q54 R61 L62 L66 V69 V70 K85 Y105 T124 L129 I132 M136 E137 V140 T144 F147 R150 M151 R152 G156 V159 L167 L168 S171 Y175
F178 K183 D184 M188 Q196 L199 K200 T201 W202 I207 G223 R234 Q241 L242 L262 A266 GLN PRO SER MET GLU GLU GLY SER G275 V282 H283 M284 L289 L290 T294 E295 T296 T297 Q315 H324 E325 LEU GLY PRO GLY ALA SER SER
S333 R334 L345 R357 R370 S373 T383 V384 N388 W406 R409 E412 P413 G414 K415 N416 S417 R418 A419 L420 V428 E432 P433 L434 A435 R436 F440 V441 T444 R445 L446 L447 Q448 L452 L453 P454 S455 G456 D457 L465 S469 V470 I471 L472
R480 P483 R484 G485 MET GLY ALA HIS SER PRO GLY GLN SER GLN HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.38Å 86.86Å 108.92Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.64 29.63 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.64) 99.6 (29.63-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.231 , 0.281 0.231 , 0.281	Depositor DCC
R_{free} test set	3087 reflections (8.30%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 40297 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10832	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: HEM, SO4, STR

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	0/3581	0.76	8/4875 (0.2%)
1	B	0.41	0/3603	0.73	2/4905 (0.0%)
1	C	0.41	0/3621	0.68	0/4927
All	All	0.42	0/10805	0.72	10/14707 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	465	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	108	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	106	PRO	CA-N-CD	-5.84	103.32	111.50
1	A	38	LEU	CA-CB-CG	5.83	128.70	115.30
1	B	38	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	33	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	242	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	234	ARG	N-CA-C	5.17	124.94	111.00
1	B	247	GLU	C-N-CA	5.08	134.41	121.70
1	A	105	TYR	CA-CB-CG	5.07	123.03	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLU	Peptide
1	B	235	ASP	Peptide
1	B	466	PRO	Peptide

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	3493	0	3528	55	0
1	B	3513	0	3563	46	0
1	C	3531	0	3586	35	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	0	0
3	C	43	0	30	2	0
4	A	23	0	30	1	0
4	B	23	0	30	1	0
4	C	23	0	30	0	0
5	A	22	0	0	0	0
5	B	25	0	0	0	0
5	C	30	0	0	0	0
All	All	10832	0	10857	138	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 6.

All (138) 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:178:PHE:HB2	1:A:182:ILE:HD11	1.42	0.96
1:B:315:GLN:HE22	1:B:452:LEU:H	1.14	0.92
1:A:315:GLN:HE22	1:A:452:LEU:H	1.16	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HD2	1:A:418:ARG:H	1.43	0.84
1:C:315:GLN:HE22	1:C:452:LEU:H	1.31	0.79
1:A:105:TYR:HB3	1:A:106:PRO:CA	2.14	0.78
1:C:178:PHE:CD1	1:C:241:GLN:HG2	2.18	0.77
1:B:70:VAL:HG22	1:B:385:ILE:HG12	1.70	0.74
1:C:61:ARG:HG2	1:C:70:VAL:HG12	1.70	0.73
1:B:174:CYS:HB2	1:B:188:MET:HE1	1.73	0.70
1:B:315:GLN:HE22	1:B:452:LEU:N	1.90	0.69
1:A:151:MET:HE1	1:A:159:VAL:HG11	1.74	0.69
1:B:315:GLN:NE2	1:B:452:LEU:H	1.90	0.68
1:A:252:GLY:H	1:A:263:GLN:HE22	1.40	0.67
1:A:105:TYR:HB3	1:A:106:PRO:HA	1.76	0.66
1:B:236:HIS:O	1:B:238:VAL:N	2.29	0.66
1:B:415:LYS:HB2	1:B:416:ASN:HB3	1.78	0.66
1:B:440:PHE:O	1:B:444:THR:HB	1.96	0.65
1:B:290:LEU:O	1:B:294:THR:HG23	1.97	0.65
1:A:151:MET:CE	1:A:159:VAL:HG11	2.28	0.63
1:C:440:PHE:O	1:C:444:THR:HB	2.00	0.62
1:B:171:SER:HA	1:B:188:MET:HE1	1.82	0.62
1:C:140:VAL:O	1:C:144:THR:HG22	1.98	0.62
1:B:194:CYS:O	1:B:198:VAL:HG23	1.99	0.62
1:C:196:GLN:HA	1:C:196:GLN:HE21	1.65	0.61
1:A:178:PHE:CD1	1:A:241:GLN:HG2	2.35	0.61
1:B:247:GLU:H	1:B:248:SER:HB3	1.66	0.60
1:A:184:ASP:H	1:A:186:ASN:H	1.50	0.60
1:C:151:MET:HE1	1:C:159:VAL:HG11	1.82	0.60
1:B:296:THR:HA	1:B:359:VAL:HG11	1.84	0.59
1:C:406:TRP:O	1:C:409:ARG:HB3	2.03	0.58
1:B:203:SER:HB2	1:B:469:SER:HB2	1.86	0.58
1:A:138:PRO:HA	1:A:141:GLU:HG2	1.86	0.57
1:A:202:TRP:HZ3	1:A:470:VAL:HG21	1.69	0.57
1:A:290:LEU:O	1:A:294:THR:HG23	2.03	0.57
1:C:188:MET:HE2	1:C:188:MET:HA	1.87	0.57
1:B:175:TYR:OH	1:B:183:LYS:HB2	2.04	0.56
1:A:105:TYR:HB3	1:A:106:PRO:CB	2.36	0.55
3:A:603:HEM:HMC2	3:A:603:HEM:HBC2	1.89	0.55
1:C:290:LEU:O	1:C:294:THR:HG23	2.07	0.54
1:B:178:PHE:CD1	1:B:241:GLN:HG2	2.42	0.54
1:C:201:THR:O	1:C:207:ILE:HD12	2.07	0.54
1:B:40:LEU:HD11	1:B:212:VAL:HG11	1.90	0.53
1:A:61:ARG:HG2	1:A:70:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:MET:HA	1:C:188:MET:CE	2.39	0.53
1:B:178:PHE:CG	1:B:241:GLN:HG2	2.43	0.53
1:A:418:ARG:CD	1:A:418:ARG:H	2.17	0.52
1:B:182:ILE:HA	1:B:187:LEU:HD12	1.90	0.52
1:C:69:VAL:HG22	1:C:384:VAL:HB	1.91	0.51
1:A:339:ASP:O	1:A:341:ALA:N	2.43	0.51
1:C:406:TRP:CE3	1:C:409:ARG:HB2	2.45	0.51
1:C:171:SER:O	1:C:175:TYR:HD1	1.93	0.51
1:C:178:PHE:CG	1:C:241:GLN:HG2	2.47	0.50
1:B:415:LYS:HD3	1:B:416:ASN:HB3	1.93	0.50
1:C:418:ARG:H	1:C:418:ARG:HD3	1.77	0.50
1:A:252:GLY:H	1:A:263:GLN:NE2	2.07	0.50
1:A:105:TYR:HB3	1:A:106:PRO:HB3	1.94	0.50
1:B:184:ASP:H	1:B:186:ASN:H	1.60	0.50
1:A:212:VAL:HG23	1:A:213:ILE:HG13	1.94	0.49
1:A:140:VAL:O	1:A:144:THR:HG23	2.12	0.49
1:C:202:TRP:HZ3	1:C:470:VAL:HG21	1.78	0.49
1:B:171:SER:HA	1:B:188:MET:CE	2.41	0.48
1:A:89:PHE:O	1:A:91:GLY:N	2.46	0.48
1:C:175:TYR:OH	1:C:183:LYS:HB2	2.13	0.48
1:A:69:VAL:HG22	1:A:384:VAL:HB	1.96	0.48
1:C:105:TYR:HB2	1:C:284:MET:HG2	1.96	0.48
1:C:262:LEU:HD13	1:C:282:VAL:HG11	1.95	0.48
1:A:38:LEU:HD23	1:A:40:LEU:HD12	1.95	0.48
1:C:453:LEU:HB2	1:C:480:ARG:HB3	1.96	0.48
1:B:61:ARG:HG2	1:B:70:VAL:HG12	1.96	0.48
1:A:106:PRO:HD2	1:A:106:PRO:O	2.14	0.47
1:C:334:ARG:HD2	1:C:445:ARG:HH22	1.78	0.47
1:A:340:ARG:NH1	1:B:412:GLU:O	2.47	0.47
1:A:125:ARG:NH1	1:A:430:LEU:O	2.47	0.47
1:A:206:SER:O	1:A:207:ILE:HB	2.15	0.47
1:A:247:GLU:O	1:A:248:SER:HB3	2.15	0.47
1:A:315:GLN:NE2	1:A:452:LEU:H	1.98	0.47
1:C:409:ARG:HG3	1:C:416:ASN:HD21	1.80	0.47
1:A:194:CYS:O	1:A:198:VAL:HG23	2.15	0.47
1:A:175:TYR:OH	1:A:183:LYS:HB2	2.16	0.46
1:A:66:LEU:HD13	1:A:213:ILE:HG12	1.98	0.46
3:C:602:HEM:HBB2	3:C:602:HEM:HMB2	1.97	0.46
1:C:412:GLU:CD	1:C:412:GLU:H	2.20	0.45
1:B:147:PHE:O	1:B:151:MET:HG2	2.17	0.45
1:B:463:GLN:HA	1:B:464:PRO:HD3	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PHE:CG	1:A:241:GLN:HG2	2.51	0.44
1:B:198:VAL:HG12	4:B:603:STR:H21	2.00	0.44
1:A:360:VAL:HG21	4:A:604:STR:H211	1.99	0.44
1:A:199:LEU:HD21	1:A:471:ILE:HD12	1.98	0.44
1:B:258:MET:O	1:B:262:LEU:HB2	2.17	0.44
1:B:201:THR:HG22	1:B:207:ILE:CD1	2.47	0.44
3:C:602:HEM:HMC1	3:C:602:HEM:HBC2	1.99	0.44
1:A:245:HIS:O	1:A:249:LEU:HB2	2.17	0.44
1:C:202:TRP:CZ3	1:C:470:VAL:HG21	2.52	0.44
1:B:174:CYS:HB2	1:B:188:MET:CE	2.44	0.44
1:A:147:PHE:HE1	1:A:164:GLU:HB3	1.83	0.44
1:A:147:PHE:O	1:A:151:MET:HG2	2.18	0.44
1:A:440:PHE:O	1:A:444:THR:HB	2.17	0.44
1:B:108:LEU:HD22	1:B:124:THR:HG21	1.99	0.44
1:B:482:GLN:HA	1:B:483:PRO:HD3	1.86	0.44
1:A:129:LEU:HD11	1:A:433:PRO:HG2	1.99	0.44
1:B:60:TYR:HE1	1:B:62:LEU:HD22	1.81	0.44
1:A:31:PRO:HG2	1:A:61:ARG:HG3	2.00	0.43
1:A:145:GLN:O	1:A:149:GLU:HG2	2.18	0.43
1:B:247:GLU:N	1:B:248:SER:HB3	2.32	0.43
1:C:199:LEU:HD23	1:C:295:GLU:HG3	2.00	0.43
1:B:129:LEU:HD11	1:B:433:PRO:HG2	2.00	0.43
1:B:44:ASP:HB3	1:B:47:ILE:HB	2.00	0.43
1:A:207:ILE:HD11	1:A:223:GLY:O	2.19	0.43
1:C:144:THR:HG21	1:C:441:VAL:HG12	2.01	0.43
1:A:85:LYS:HB3	1:A:88:ASP:HB2	2.01	0.43
1:A:302:SER:O	1:A:306:VAL:HG23	2.19	0.42
1:A:303:TRP:CD2	1:A:357:ARG:HG2	2.54	0.42
1:C:144:THR:HA	1:C:147:PHE:HB3	2.01	0.42
1:A:221:ASN:HD22	1:A:221:ASN:C	2.22	0.42
1:B:151:MET:HE1	1:B:159:VAL:HG11	2.01	0.42
1:C:207:ILE:HD11	1:C:223:GLY:O	2.20	0.42
1:B:94:GLU:HG2	1:B:99:LYS:HD2	2.02	0.42
1:B:358:PRO:HD2	1:B:390:GLN:HG3	2.02	0.42
1:A:206:SER:HB2	1:A:221:ASN:HD21	1.85	0.42
1:C:483:PRO:HA	1:C:484:ARG:HA	1.79	0.42
1:B:199:LEU:HD21	1:B:471:ILE:HD12	2.01	0.42
1:A:104:ASN:HD22	1:A:104:ASN:H	1.68	0.42
1:C:152:ARG:O	1:C:152:ARG:HD2	2.19	0.41
1:C:432:GLU:O	1:C:436:ARG:HG3	2.20	0.41
1:B:410:PHE:HD1	1:B:416:ASN:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:HIS:O	1:C:324:HIS:ND1	2.53	0.41
1:B:466:PRO:HB2	1:B:467:HIS:CG	2.56	0.41
1:A:178:PHE:HB2	1:A:182:ILE:CD1	2.32	0.41
1:B:183:LYS:HD3	1:B:188:MET:HB2	2.03	0.41
1:A:323:ASP:O	1:A:324:HIS:HB2	2.20	0.41
1:A:317:ARG:NH2	1:A:408:ASP:OD2	2.54	0.41
1:B:233:LYS:HA	1:B:235:ASP:N	2.36	0.41
1:C:132:ILE:HD12	1:C:136:MET:HB2	2.02	0.41
1:B:241:GLN:HG3	1:B:245:HIS:CE1	2.57	0.40
1:A:37:PHE:HD2	1:A:38:LEU:HD12	1.87	0.40
1:A:345:LEU:HD23	1:A:411:LEU:HD11	2.03	0.40
1:B:120:HIS:O	1:B:124:THR:HG22	2.22	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	432/482 (90%)	399 (92%)	24 (6%)	9 (2%)	9 15
1	B	434/482 (90%)	406 (94%)	20 (5%)	8 (2%)	11 19
1	C	436/482 (90%)	422 (97%)	12 (3%)	2 (0%)	34 57
All	All	1302/1446 (90%)	1227 (94%)	56 (4%)	19 (2%)	13 24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ALA
1	A	324	HIS
1	B	184	ASP
1	B	236	HIS
1	B	237	ILE

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Mol	Chain	Res	Type
1	A	184	ASP
1	A	207	ILE
1	B	248	SER
1	B	417	SER
1	B	469	SER
1	C	184	ASP
1	A	484	ARG
1	A	105	TYR
1	B	335	VAL
1	A	417	SER
1	B	86	TRP
1	C	469	SER
1	A	335	VAL
1	A	106	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	379/421 (90%)	345 (91%)	34 (9%)	12 21
1	B	384/421 (91%)	346 (90%)	38 (10%)	10 17
1	C	386/421 (92%)	346 (90%)	40 (10%)	9 15
All	All	1149/1263 (91%)	1037 (90%)	112 (10%)	10 18

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	33	LEU
1	A	45	LEU
1	A	70	VAL
1	A	108	LEU
1	A	115	LEU
1	A	137	GLU
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	168	LEU
1	A	213	ILE
1	A	221	ASN
1	A	234	ARG
1	A	262	LEU
1	A	265	VAL
1	A	289	LEU
1	A	294	THR
1	A	313	GLU
1	A	334	ARG
1	A	345	LEU
1	A	352	GLU
1	A	357	ARG
1	A	367	ARG
1	A	417	SER
1	A	418	ARG
1	A	420	LEU
1	A	428	VAL
1	A	434	LEU
1	A	444	THR
1	A	446	LEU
1	A	447	LEU
1	A	465	LEU
1	A	472	LEU
1	A	480	ARG
1	B	33	LEU
1	B	45	LEU
1	B	70	VAL
1	B	102	SER
1	B	122	LYS
1	B	124	THR
1	B	167	LEU
1	B	168	LEU
1	B	180	ASP
1	B	185	ASP
1	B	201	THR
1	B	225	ARG
1	B	232	GLU
1	B	234	ARG
1	B	239	GLU
1	B	240	MET

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Mol	Chain	Res	Type
1	B	262	LEU
1	B	265	VAL
1	B	289	LEU
1	B	294	THR
1	B	324	HIS
1	B	334	ARG
1	B	345	LEU
1	B	352	GLU
1	B	394	LEU
1	B	411	LEU
1	B	415	LYS
1	B	416	ASN
1	B	420	LEU
1	B	428	VAL
1	B	434	LEU
1	B	444	THR
1	B	446	LEU
1	B	448	GLN
1	B	457	ASP
1	B	472	LEU
1	B	480	ARG
1	B	482	GLN
1	C	33	LEU
1	C	45	LEU
1	C	62	LEU
1	C	66	LEU
1	C	70	VAL
1	C	85	LYS
1	C	105	TYR
1	C	124	THR
1	C	129	LEU
1	C	137	GLU
1	C	144	THR
1	C	152	ARG
1	C	167	LEU
1	C	168	LEU
1	C	183	LYS
1	C	184	ASP
1	C	196	GLN
1	C	234	ARG
1	C	242	LEU
1	C	262	LEU

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Mol	Chain	Res	Type
1	C	289	LEU
1	C	297	THR
1	C	345	LEU
1	C	357	ARG
1	C	370	ARG
1	C	383	THR
1	C	388	ASN
1	C	418	ARG
1	C	420	LEU
1	C	428	VAL
1	C	434	LEU
1	C	444	THR
1	C	446	LEU
1	C	447	LEU
1	C	448	GLN
1	C	457	ASP
1	C	465	LEU
1	C	471	ILE
1	C	472	LEU
1	C	480	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	104	ASN
1	A	221	ASN
1	A	263	GLN
1	A	315	GLN
1	A	388	ASN
1	A	448	GLN
1	B	67	GLN
1	B	196	GLN
1	B	241	GLN
1	B	244	GLN
1	B	263	GLN
1	B	276	GLN
1	B	283	HIS
1	B	315	GLN
1	B	319	GLN
1	B	347	ASN
1	B	388	ASN

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Mol	Chain	Res	Type
1	B	448	GLN
1	C	196	GLN
1	C	241	GLN
1	C	263	GLN
1	C	315	GLN
1	C	319	GLN
1	C	388	ASN
1	C	448	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	SO4	A	601	2	4,4,4	0.34	0	6,6,6	0.15	0
2	SO4	A	602	2	4,4,4	0.34	0	6,6,6	0.15	0
3	HEM	A	603	1	30,50,50	2.10	7 (23%)	24,82,82	2.30	9 (37%)
4	STR	A	604	-	26,26,26	0.67	0	42,42,42	1.43	7 (16%)
2	SO4	B	601	-	4,4,4	0.32	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	B	602	1	30,50,50	2.11	7 (23%)	24,82,82	2.25	6 (25%)
4	STR	B	603	-	26,26,26	0.64	0	42,42,42	1.40	5 (11%)
2	SO4	C	601	-	4,4,4	0.29	0	6,6,6	0.15	0
3	HEM	C	602	1	30,50,50	2.11	7 (23%)	24,82,82	2.31	7 (29%)
4	STR	C	603	-	26,26,26	0.66	0	42,42,42	1.44	6 (14%)

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	SO4	A	601	2	-	0/0/0/0	0/0/0/0
2	SO4	A	602	2	-	0/0/0/0	0/0/0/0
3	HEM	A	603	1	-	0/10/54/54	0/0/8/8
4	STR	A	604	-	-	0/4/62/62	0/4/4/4
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	HEM	B	602	1	-	0/10/54/54	0/0/8/8
4	STR	B	603	-	-	0/4/62/62	0/4/4/4
2	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	HEM	C	602	1	-	0/10/54/54	0/0/8/8
4	STR	C	603	-	-	0/4/62/62	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HEM	C2D-C3D	-6.39	1.35	1.54
3	B	602	HEM	C2D-C3D	-6.32	1.35	1.54
3	A	603	HEM	C2D-C3D	-6.30	1.35	1.54
3	C	602	HEM	C2C-C1C	-5.79	1.41	1.52
3	B	602	HEM	C2C-C1C	-5.66	1.41	1.52
3	A	603	HEM	C2C-C1C	-5.57	1.42	1.52
3	A	603	HEM	C3D-C4D	-3.26	1.47	1.51
3	B	602	HEM	C3D-C4D	-2.99	1.47	1.51
3	C	602	HEM	C3D-C4D	-2.98	1.47	1.51
3	C	602	HEM	C3B-C4B	-2.94	1.49	1.51
3	B	602	HEM	C3B-C4B	-2.80	1.49	1.51
3	A	603	HEM	C3B-C4B	-2.66	1.49	1.51
3	B	602	HEM	C2B-C1B	-2.59	1.43	1.51
3	A	603	HEM	C2B-C1B	-2.55	1.43	1.51
3	C	602	HEM	C2B-C1B	-2.31	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HEM	FE-NB	2.61	2.11	1.97
3	A	603	HEM	FE-NB	2.72	2.11	1.97
3	B	602	HEM	FE-NB	2.81	2.12	1.97
3	B	602	HEM	FE-NC	3.59	2.09	1.95
3	A	603	HEM	FE-NC	3.73	2.10	1.95
3	C	602	HEM	FE-NC	3.74	2.10	1.95

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	604	STR	C6-C5-C4	-3.66	116.24	120.89
4	B	603	STR	C6-C5-C4	-3.33	116.66	120.89
4	C	603	STR	C6-C5-C4	-3.24	116.78	120.89
3	A	603	HEM	C3B-C4B-NB	-2.08	107.66	111.63
4	C	603	STR	O20-C20-C17	-2.05	118.75	121.83
3	A	603	HEM	CMA-C3A-C4A	-2.00	125.05	128.36
4	A	604	STR	C12-C11-C9	2.03	116.52	113.10
4	A	604	STR	C2-C3-C4	2.03	119.82	116.70
4	A	604	STR	C2-C1-C10	2.11	116.39	113.41
3	C	602	HEM	CBA-CAA-C2A	2.12	116.32	112.53
3	A	603	HEM	CBA-CAA-C2A	2.14	116.36	112.53
4	B	603	STR	C2-C3-C4	2.28	120.21	116.70
4	A	604	STR	C15-C14-C13	2.38	106.91	103.82
3	B	602	HEM	C2D-C3D-C4D	2.40	105.57	101.50
3	A	603	HEM	C2D-C3D-C4D	2.45	105.66	101.50
4	C	603	STR	C2-C3-C4	2.52	120.57	116.70
3	C	602	HEM	C2D-C3D-C4D	2.54	105.81	101.50
4	C	603	STR	C15-C14-C13	2.61	107.22	103.82
4	A	604	STR	C21-C20-C17	2.64	121.22	117.53
4	B	603	STR	C15-C14-C13	2.70	107.33	103.82
4	C	603	STR	C21-C20-C17	2.72	121.33	117.53
3	A	603	HEM	CMD-C2D-C3D	2.91	127.21	114.35
3	B	602	HEM	CMD-C2D-C3D	2.93	127.31	114.35
3	C	602	HEM	CMD-C2D-C3D	2.95	127.41	114.35
4	B	603	STR	C21-C20-C17	3.04	121.78	117.53
4	C	603	STR	C6-C5-C10	3.32	120.48	116.71
4	B	603	STR	C6-C5-C10	3.67	120.88	116.71
3	A	603	HEM	CAD-C3D-C4D	3.85	126.07	112.47
4	A	604	STR	C6-C5-C10	3.88	121.11	116.71
3	B	602	HEM	CAD-C3D-C4D	4.02	126.65	112.47
3	C	602	HEM	CAD-C3D-C4D	4.03	126.67	112.47
3	A	603	HEM	CMB-C2B-C3B	4.48	127.71	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	HEM	CMB-C2B-C3B	4.50	127.77	116.53
3	A	603	HEM	CMC-C2C-C3C	4.60	128.02	116.53
3	B	602	HEM	CMC-C2C-C3C	4.63	128.09	116.53
3	B	602	HEM	CMB-C2B-C3B	4.71	128.29	116.53
3	C	602	HEM	CMC-C2C-C3C	4.85	128.63	116.53
3	C	602	HEM	CAD-C3D-C2D	4.97	127.51	113.22
3	B	602	HEM	CAD-C3D-C2D	5.07	127.78	113.22
3	A	603	HEM	CAD-C3D-C2D	5.24	128.28	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	HEM	1	0
4	A	604	STR	1	0
4	B	603	STR	1	0
3	C	602	HEM	2	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	440/482 (91%)	0.29	22 (5%)	32	26	25, 41, 58, 81	0
1	B	440/482 (91%)	0.27	22 (5%)	32	26	28, 41, 63, 82	0
1	C	442/482 (91%)	0.24	11 (2%)	61	55	27, 43, 60, 73	0
All	All	1322/1446 (91%)	0.27	55 (4%)	40	33	25, 42, 61, 82	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	457	ASP	4.3
1	B	324	HIS	3.8
1	B	458	ALA	3.7
1	C	54	GLN	3.5
1	A	411	LEU	3.4
1	B	466	PRO	3.4
1	B	412	GLU	3.2
1	B	456	GLY	3.1
1	A	292	GLY	3.1
1	A	458	ALA	3.0
1	B	482	GLN	3.0
1	A	54	GLN	3.0
1	C	266	ALA	3.0
1	B	333	SER	2.8
1	A	312	PRO	2.8
1	A	105	TYR	2.8
1	A	323	ASP	2.8
1	B	296	THR	2.7
1	B	484	ARG	2.6
1	C	38	LEU	2.6
1	A	414	GLY	2.6
1	A	293	GLY	2.6
1	A	316	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	360	VAL	2.5
1	C	156	GLY	2.5
1	B	185	ASP	2.5
1	C	457	ASP	2.5
1	B	225	ARG	2.5
1	B	467	HIS	2.5
1	C	412	GLU	2.4
1	B	104	ASN	2.4
1	C	414	GLY	2.4
1	B	184	ASP	2.3
1	A	294	THR	2.3
1	A	232	GLU	2.3
1	A	158	PRO	2.3
1	C	373	SER	2.3
1	C	150	ARG	2.2
1	A	324	HIS	2.2
1	B	416	ASN	2.2
1	A	406	TRP	2.2
1	C	297	THR	2.2
1	B	465	LEU	2.2
1	A	218	PHE	2.2
1	A	415	LYS	2.2
1	B	415	LYS	2.2
1	A	466	PRO	2.1
1	A	205	TRP	2.1
1	B	293	GLY	2.1
1	C	455	SER	2.1
1	B	297	THR	2.1
1	B	294	THR	2.0
1	A	266	ALA	2.0
1	A	149	GLU	2.0
1	A	457	ASP	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

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
4	STR	A	604	23/23	0.90	0.23	0.45	30,30,31,32	0
4	STR	B	603	23/23	0.93	0.23	0.40	30,30,33,35	0
3	HEM	B	602	43/43	0.96	0.21	0.09	26,27,29,29	0
4	STR	C	603	23/23	0.94	0.20	0.05	34,35,36,38	0
3	HEM	A	603	43/43	0.96	0.20	-0.15	24,25,26,26	0
3	HEM	C	602	43/43	0.97	0.18	-0.33	24,25,26,26	0
2	SO4	C	601	5/5	0.99	0.13	-1.15	31,31,32,32	0
2	SO4	B	601	5/5	0.99	0.11	-2.15	41,41,42,42	0
2	SO4	A	601	5/5	0.98	0.11	-4.70	30,30,30,30	5
2	SO4	A	602	5/5	0.98	0.10	-5.33	36,36,36,37	5

6.5 Other polymers

There are no such residues in this entry.