



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 05:40 AM EDT

PDB ID : 3T3Z
Title : Human Cytochrome P450 2E1 in complex with pilocarpine
Authors : Meneely, K.M.; DeVore, N.M.; Scott, E.E.
Deposited on : unknown
Resolution : 2.35 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

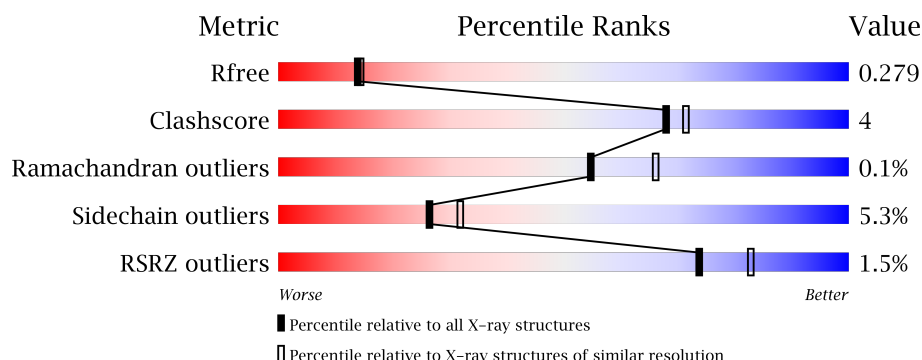
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	476	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	476	<div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	C	476	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	476	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	9PL	B	501	-	-	-	X
4	SUC	B	1	-	-	-	X
4	SUC	C	1	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16204 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 2E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	2	0
			3799	2458	651	672	18			
1	B	464	Total	C	N	O	S	0	1	0
			3793	2454	651	670	18			
1	C	464	Total	C	N	O	S	0	0	0
			3787	2450	651	668	18			
1	D	464	Total	C	N	O	S	0	0	0
			3787	2450	651	668	18			

There are 56 discrepancies between the modelled and reference sequences:

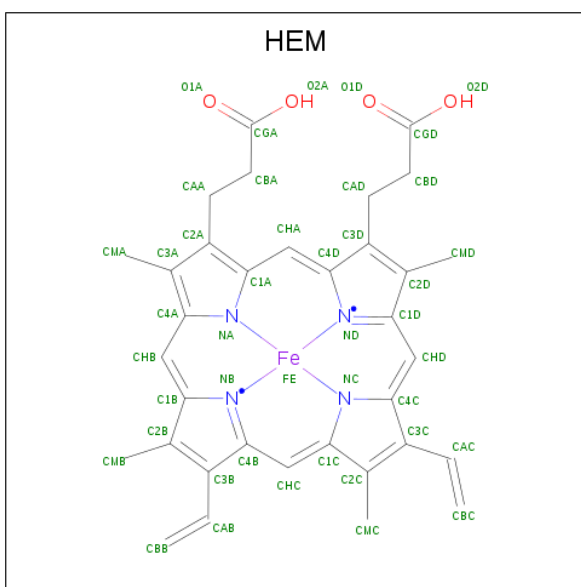
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	EXPRESSION TAG	UNP P05181
A	23	ALA	-	EXPRESSION TAG	UNP P05181
A	24	LYS	-	EXPRESSION TAG	UNP P05181
A	25	LYS	-	EXPRESSION TAG	UNP P05181
A	26	THR	-	EXPRESSION TAG	UNP P05181
A	27	SER	-	EXPRESSION TAG	UNP P05181
A	28	SER	-	EXPRESSION TAG	UNP P05181
A	29	LYS	-	EXPRESSION TAG	UNP P05181
A	30	GLY	-	EXPRESSION TAG	UNP P05181
A	31	LYS	-	EXPRESSION TAG	UNP P05181
A	494	HIS	-	EXPRESSION TAG	UNP P05181
A	495	HIS	-	EXPRESSION TAG	UNP P05181
A	496	HIS	-	EXPRESSION TAG	UNP P05181
A	497	HIS	-	EXPRESSION TAG	UNP P05181
B	22	MET	-	EXPRESSION TAG	UNP P05181
B	23	ALA	-	EXPRESSION TAG	UNP P05181
B	24	LYS	-	EXPRESSION TAG	UNP P05181
B	25	LYS	-	EXPRESSION TAG	UNP P05181
B	26	THR	-	EXPRESSION TAG	UNP P05181
B	27	SER	-	EXPRESSION TAG	UNP P05181
B	28	SER	-	EXPRESSION TAG	UNP P05181

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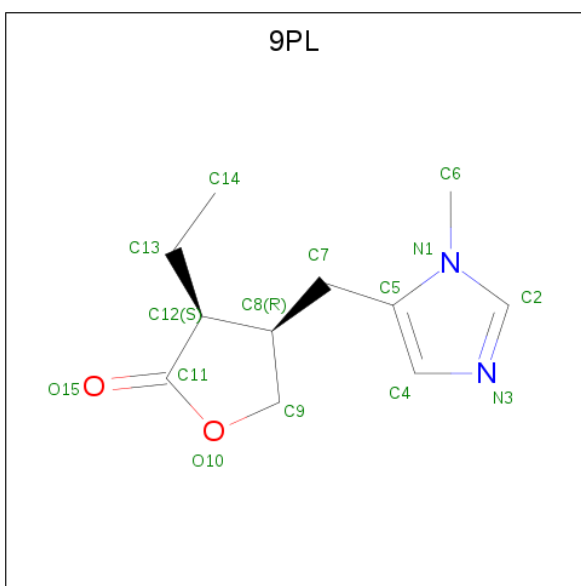
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	LYS	-	EXPRESSION TAG	UNP P05181
B	30	GLY	-	EXPRESSION TAG	UNP P05181
B	31	LYS	-	EXPRESSION TAG	UNP P05181
B	494	HIS	-	EXPRESSION TAG	UNP P05181
B	495	HIS	-	EXPRESSION TAG	UNP P05181
B	496	HIS	-	EXPRESSION TAG	UNP P05181
B	497	HIS	-	EXPRESSION TAG	UNP P05181
C	22	MET	-	EXPRESSION TAG	UNP P05181
C	23	ALA	-	EXPRESSION TAG	UNP P05181
C	24	LYS	-	EXPRESSION TAG	UNP P05181
C	25	LYS	-	EXPRESSION TAG	UNP P05181
C	26	THR	-	EXPRESSION TAG	UNP P05181
C	27	SER	-	EXPRESSION TAG	UNP P05181
C	28	SER	-	EXPRESSION TAG	UNP P05181
C	29	LYS	-	EXPRESSION TAG	UNP P05181
C	30	GLY	-	EXPRESSION TAG	UNP P05181
C	31	LYS	-	EXPRESSION TAG	UNP P05181
C	494	HIS	-	EXPRESSION TAG	UNP P05181
C	495	HIS	-	EXPRESSION TAG	UNP P05181
C	496	HIS	-	EXPRESSION TAG	UNP P05181
C	497	HIS	-	EXPRESSION TAG	UNP P05181
D	22	MET	-	EXPRESSION TAG	UNP P05181
D	23	ALA	-	EXPRESSION TAG	UNP P05181
D	24	LYS	-	EXPRESSION TAG	UNP P05181
D	25	LYS	-	EXPRESSION TAG	UNP P05181
D	26	THR	-	EXPRESSION TAG	UNP P05181
D	27	SER	-	EXPRESSION TAG	UNP P05181
D	28	SER	-	EXPRESSION TAG	UNP P05181
D	29	LYS	-	EXPRESSION TAG	UNP P05181
D	30	GLY	-	EXPRESSION TAG	UNP P05181
D	31	LYS	-	EXPRESSION TAG	UNP P05181
D	494	HIS	-	EXPRESSION TAG	UNP P05181
D	495	HIS	-	EXPRESSION TAG	UNP P05181
D	496	HIS	-	EXPRESSION TAG	UNP P05181
D	497	HIS	-	EXPRESSION TAG	UNP P05181

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



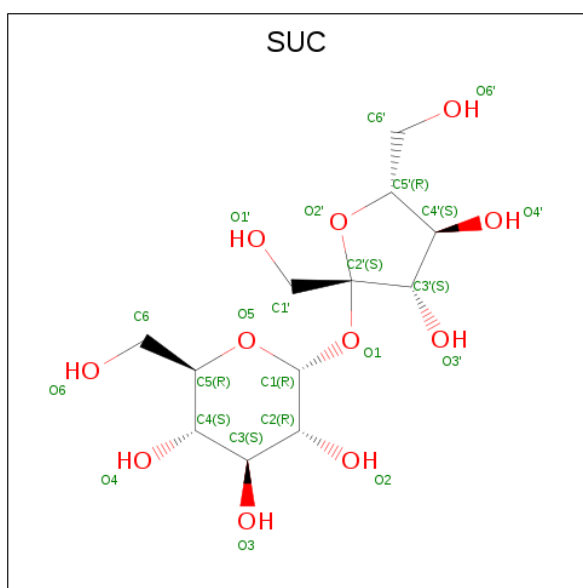
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (3S,4R)-3-ethyl-4-[(1-methyl-1H-imidazol-5-yl)methyl]dihydrofuran-2(3H)-one (three-letter code: 9PL) (formula: C₁₁H₁₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is SUCROSE (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		
4	B	1	Total	C	O	0	0
			23	12	11		
4	C	1	Total	C	O	0	0
			23	12	11		
4	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		
5	B	202	Total	O	0	0
			202	202		

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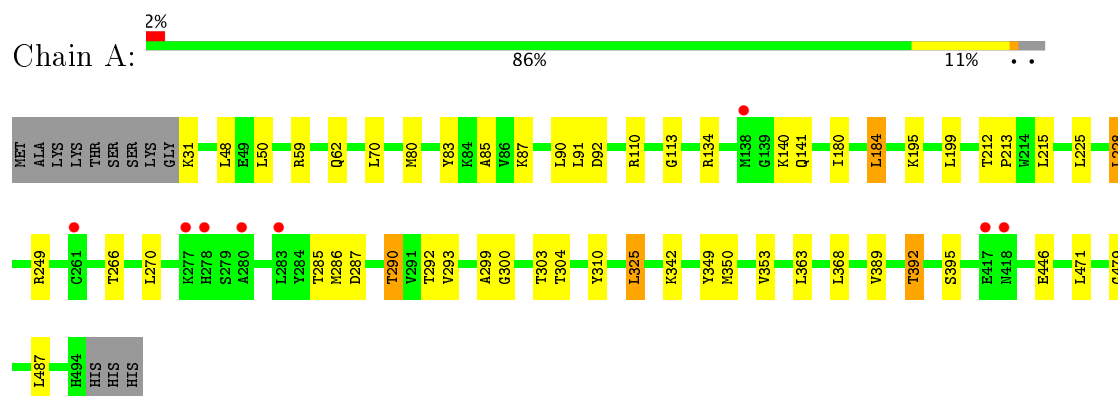
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	151	Total 151	O 151	0	0
5	D	159	Total 159	O 159	0	0

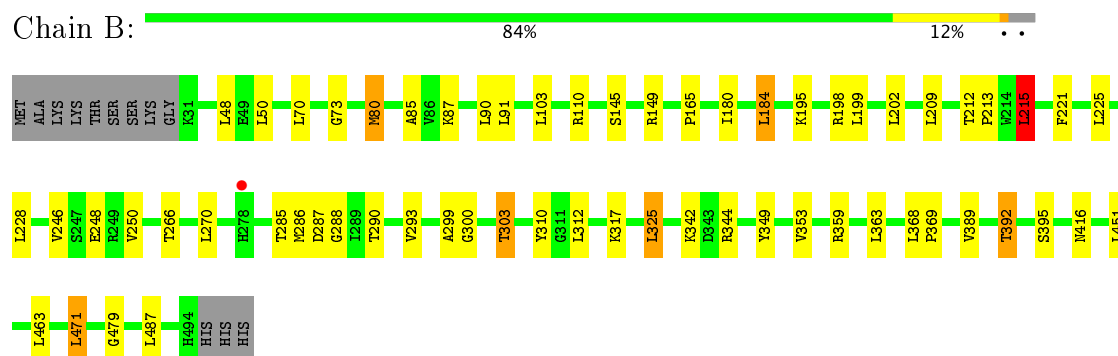
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

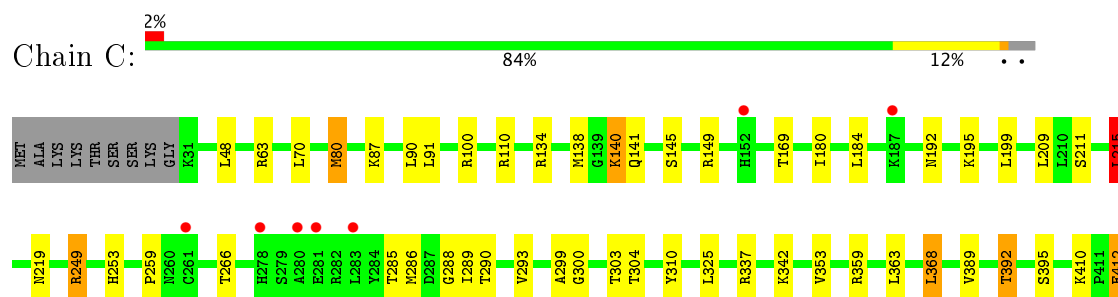
• Molecule 1: Cytochrome P450 2E1



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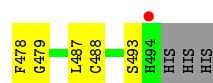
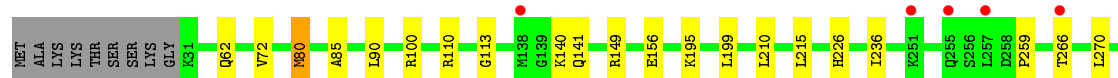
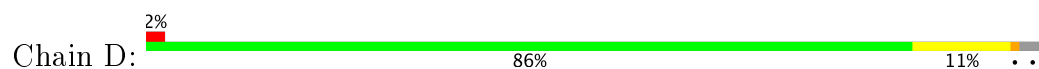


• Molecule 1: Cytochrome P450 2E1





● Molecule 1: Cytochrome P450 2E1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	100.64Å 100.64Å 259.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.98 – 2.35 36.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.9 (36.98-2.35) 95.9 (36.98-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.34Å)	Xtriage
Refinement program	REFMAC 6.1.13	Depositor
R, R_{free}	0.217 , 0.281 0.222 , 0.279	Depositor DCC
R_{free} test set	5096 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16204	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 72.68 % 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 2.1083e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SUC, 9PL

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	0.48	0/3911	0.59	0/5296
1	B	0.48	0/3902	0.60	1/5284 (0.0%)
1	C	0.47	0/3893	0.58	2/5272 (0.0%)
1	D	0.46	0/3893	0.57	0/5272
All	All	0.47	0/15599	0.59	3/21124 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	LEU	CA-CB-CG	-5.74	102.09	115.30
1	C	215	LEU	CA-CB-CG	-5.38	102.92	115.30
1	C	487	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3799	0	3800	29	0
1	B	3793	0	3794	39	0
1	C	3787	0	3788	33	0
1	D	3787	0	3788	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	7	0
2	D	43	0	30	4	0
3	A	15	0	16	2	0
3	B	15	0	16	3	0
3	C	15	0	16	2	0
3	D	15	0	16	2	0
4	A	23	0	22	0	0
4	B	23	0	22	0	0
4	C	23	0	22	0	0
4	D	23	0	22	1	0
5	A	202	0	0	1	0
5	B	202	0	0	3	0
5	C	151	0	0	4	0
5	D	159	0	0	0	0
All	All	16204	0	15442	136	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 4.

All (136) 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:392:THR:HG22	1:D:395:SER:OG	1.86	0.76
1:D:303:THR:HG23	3:D:501:9PL:H6B	1.71	0.72
1:B:287:ASP:HA	1:B:290:THR:HG22	1.72	0.72
1:A:80:MET:HE1	1:A:389:VAL:HG13	1.73	0.70
1:A:392:THR:HG22	1:A:395:SER:OG	1.92	0.70
2:D:500:HEM:HBC2	2:D:500:HEM:HMC2	1.74	0.69
1:D:80:MET:HE1	1:D:389:VAL:CG1	2.26	0.66
1:A:286:MET:O	1:A:290:THR:HG23	1.96	0.65
1:D:80:MET:HE1	1:D:389:VAL:HG13	1.77	0.65
1:B:299:ALA:HA	3:B:501:9PL:H6A	1.77	0.65
1:C:303:THR:HG23	3:C:501:9PL:H6B	1.78	0.65
1:A:87:LYS:HE3	1:A:91:LEU:HD12	1.79	0.65
1:A:303:THR:HG23	3:A:501:9PL:H6B	1.80	0.64
1:B:80:MET:HE1	1:B:389:VAL:HG13	1.78	0.64
1:B:392:THR:HG22	1:B:395:SER:OG	1.97	0.63
1:B:288:GLY:HA3	5:B:609:HOH:O	1.99	0.63
1:A:83:TYR:CZ	1:A:87:LYS:HD3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HG	1:A:293:VAL:HG13	1.83	0.60
2:D:500:HEM:HBB2	2:D:500:HEM:HMB2	1.82	0.60
1:B:48:LEU:HD21	1:B:70:LEU:HD21	1.82	0.59
1:C:80:MET:HE1	1:C:389:VAL:CG1	2.32	0.59
1:B:80:MET:O	1:B:392:THR:HB	2.02	0.59
1:D:299:ALA:HA	3:D:501:9PL:H6A	1.85	0.59
1:B:285:THR:HG22	1:B:287:ASP:H	1.68	0.58
1:D:266:THR:HG22	1:D:293:VAL:HG21	1.86	0.58
1:C:87:LYS:HE3	1:C:91:LEU:HD12	1.85	0.57
1:C:416:ASN:ND2	5:C:549:HOH:O	2.37	0.57
1:A:325:LEU:HD13	1:A:349:TYR:HD2	1.70	0.57
1:A:299:ALA:HA	3:A:501:9PL:H6A	1.88	0.56
1:B:300:GLY:HA2	2:B:500:HEM:HMC3	1.86	0.56
1:A:180:ILE:HG13	1:A:184:LEU:HD22	1.88	0.55
2:C:500:HEM:CMC	2:C:500:HEM:HBC2	2.36	0.55
1:B:87:LYS:HE3	1:B:91:LEU:HD12	1.89	0.55
1:B:287:ASP:HA	1:B:290:THR:CG2	2.37	0.55
1:C:325:LEU:HD11	1:C:353:VAL:HG11	1.89	0.55
1:B:184:LEU:HG	1:B:293:VAL:HG13	1.90	0.55
1:A:48:LEU:HD21	1:A:70:LEU:HD21	1.90	0.54
1:D:113:GLY:HA2	1:D:292:THR:OG1	2.07	0.54
1:B:248[B]:GLU:OE1	1:B:248[B]:GLU:HA	2.08	0.53
1:C:300:GLY:HA2	2:C:500:HEM:HMC3	1.90	0.53
1:A:266:THR:HG22	1:A:293:VAL:HG21	1.90	0.53
1:B:344:ARG:NH1	5:B:2:HOH:O	2.41	0.53
1:C:140:LYS:N	1:C:140:LYS:HD3	2.23	0.53
2:C:500:HEM:HMC1	2:C:500:HEM:HBC2	1.92	0.52
1:C:461:LYS:HB3	1:C:488:CYS:HB2	1.92	0.52
1:B:87:LYS:HE3	1:B:91:LEU:CD1	2.41	0.51
1:A:300:GLY:HA2	2:A:500:HEM:HMC2	1.91	0.51
1:A:80:MET:CE	1:A:389:VAL:HG13	2.41	0.51
1:A:80:MET:O	1:A:392:THR:HB	2.11	0.51
1:C:87:LYS:HE3	1:C:91:LEU:CD1	2.42	0.50
1:B:303:THR:HB	2:B:500:HEM:CAB	2.42	0.50
1:C:80:MET:HE1	1:C:389:VAL:HG13	1.93	0.49
1:C:289:ILE:O	1:C:293:VAL:HG23	2.11	0.49
1:A:80:MET:HG3	1:A:85:ALA:HB1	1.94	0.49
2:D:500:HEM:CMC	2:D:500:HEM:HBC2	2.41	0.49
1:B:165:PRO:HB3	1:B:463:LEU:HD11	1.93	0.49
1:B:246:VAL:O	1:B:250:VAL:HG23	2.13	0.49
1:B:287:ASP:CA	1:B:290:THR:HG22	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD13	1:A:349:TYR:CD2	2.48	0.49
1:B:285:THR:HG22	1:B:286:MET:N	2.28	0.49
1:C:140:LYS:H	1:C:140:LYS:HD3	1.78	0.49
1:C:299:ALA:HA	3:C:501:9PL:H6A	1.93	0.49
1:A:184:LEU:O	1:A:266:THR:HG23	2.13	0.48
1:A:285:THR:HG22	1:A:287:ASP:H	1.77	0.48
1:B:325:LEU:HD13	1:B:349:TYR:CD2	2.49	0.48
1:B:73:GLY:HA2	1:B:221:PHE:CE1	2.49	0.48
1:D:100:ARG:NH2	1:D:368:LEU:HB3	2.28	0.48
1:C:410:LYS:HB3	1:C:412:GLU:HG2	1.96	0.47
1:D:80:MET:HG3	1:D:85:ALA:HB1	1.97	0.47
1:B:325:LEU:HD21	1:B:353:VAL:HG11	1.96	0.47
1:A:325:LEU:HD21	1:A:353:VAL:HG11	1.96	0.47
1:D:437:CYS:HB2	2:D:500:HEM:NA	2.30	0.47
1:C:288:GLY:HA3	5:C:626:HOH:O	2.15	0.47
1:D:80:MET:O	1:D:392:THR:HB	2.15	0.47
1:A:113:GLY:HA2	1:A:292:THR:OG1	2.13	0.47
1:B:416:ASN:ND2	5:B:511:HOH:O	2.47	0.47
1:D:417:GLU:HG2	1:D:418:ASN:N	2.29	0.46
1:C:134:ARG:O	1:C:138:MET:HG3	2.16	0.46
1:D:72:VAL:HG13	1:D:72:VAL:O	2.14	0.46
1:C:180:ILE:HD13	2:C:500:HEM:HBC1	1.97	0.46
1:C:184:LEU:O	1:C:266:THR:HG23	2.15	0.46
1:B:285:THR:HB	1:B:288:GLY:H	1.82	0.45
1:C:286:MET:O	1:C:290:THR:HG23	2.16	0.45
1:B:325:LEU:HD13	1:B:349:TYR:HD2	1.81	0.45
1:C:363:LEU:O	1:C:479:GLY:HA2	2.16	0.45
1:C:209:LEU:HB3	1:C:215:LEU:HD13	1.99	0.44
1:C:304:THR:HG21	1:C:446:GLU:OE1	2.17	0.44
1:C:211:SER:HA	1:C:477:GLY:HA3	1.99	0.44
1:D:289:ILE:O	1:D:293:VAL:HG23	2.17	0.44
1:B:266:THR:HG22	1:B:293:VAL:HG21	2.00	0.44
1:B:80:MET:HG3	1:B:85:ALA:HB1	2.00	0.44
1:C:48:LEU:HD21	1:C:70:LEU:HD21	1.99	0.44
1:D:392:THR:HG23	1:D:394:ASP:OD1	2.18	0.44
1:D:226:HIS:HE1	1:D:236:ILE:HD13	1.83	0.44
1:B:209:LEU:HB3	1:B:215:LEU:HD13	1.99	0.43
1:D:405:ASP:HB3	1:D:408:LYS:HD2	2.00	0.43
1:B:145:SER:OG	1:B:149:ARG:NH2	2.51	0.43
4:D:1:SUC:O6'	4:D:1:SUC:O5	2.36	0.43
1:B:80:MET:CE	1:B:389:VAL:HG13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:THR:CG2	1:C:395:SER:OG	2.67	0.43
2:C:500:HEM:HMB2	2:C:500:HEM:HBB2	2.00	0.43
2:C:500:HEM:CMB	2:C:500:HEM:HBB2	2.48	0.43
1:A:363:LEU:O	1:A:479:GLY:HA2	2.19	0.43
1:D:304:THR:HG21	1:D:446:GLU:OE1	2.18	0.43
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	2.00	0.42
1:A:392:THR:HG22	1:A:395:SER:HG	1.85	0.42
1:B:103:LEU:HD21	1:B:369:PRO:HG3	2.02	0.42
1:D:325:LEU:HD11	1:D:353:VAL:HG11	2.00	0.42
1:A:59:ARG:NH2	5:A:583:HOH:O	2.49	0.42
1:B:180:ILE:HG13	1:B:184:LEU:HD22	2.00	0.42
1:C:249:ARG:O	1:C:253:HIS:ND1	2.48	0.42
1:D:270:LEU:HD12	1:D:289:ILE:HD13	2.01	0.42
1:A:212:THR:HB	1:A:213:PRO:HD2	2.01	0.42
1:D:363:LEU:O	1:D:479:GLY:HA2	2.19	0.42
1:B:198:ARG:O	1:B:202:LEU:HG	2.20	0.42
1:C:100:ARG:NH2	1:C:368:LEU:HB3	2.34	0.42
1:C:435:ARG:O	2:C:500:HEM:HBA2	2.20	0.42
1:C:184:LEU:HG	1:C:293:VAL:HG13	2.02	0.42
1:A:304:THR:HG21	1:A:446:GLU:OE1	2.20	0.41
1:C:490:ILE:HA	1:C:491:PRO:HD2	1.93	0.41
1:D:286:MET:O	1:D:290:THR:HG23	2.20	0.41
1:B:212:THR:HB	1:B:213:PRO:HD2	2.02	0.41
1:B:317:LYS:HD3	1:B:471:LEU:HD22	2.02	0.41
1:B:303:THR:HG23	3:B:501:9PL:H6B	2.02	0.41
1:D:461:LYS:HB3	1:D:488:CYS:HB2	2.02	0.41
1:C:219:ASN:HB2	5:C:604:HOH:O	2.21	0.41
1:C:63:ARG:NH1	5:C:571:HOH:O	2.54	0.41
1:B:184:LEU:O	1:B:266:THR:HG23	2.21	0.41
1:C:285:THR:HG22	1:C:286:MET:N	2.36	0.41
1:B:363:LEU:O	1:B:479:GLY:HA2	2.21	0.41
1:D:357:ILE:O	1:D:361:ILE:HG12	2.21	0.41
1:A:31:LYS:HB2	1:A:31:LYS:HE3	1.92	0.40
1:A:325:LEU:HD11	1:A:350:MET:HA	2.03	0.40
3:B:501:9PL:H14A	3:B:501:9PL:O15	2.20	0.40
1:A:225:LEU:HA	1:A:228:LEU:HD22	2.02	0.40
1:D:210:LEU:HD22	1:D:478:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	464/476 (98%)	447 (96%)	17 (4%)	0	100	100
1	B	463/476 (97%)	443 (96%)	20 (4%)	0	100	100
1	C	462/476 (97%)	445 (96%)	16 (4%)	1 (0%)	51	61
1	D	462/476 (97%)	447 (97%)	14 (3%)	1 (0%)	51	61
All	All	1851/1904 (97%)	1782 (96%)	67 (4%)	2 (0%)	55	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	259	PRO
1	D	259	PRO

5.3.2 Protein sidechains

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	420/428 (98%)	397 (94%)	23 (6%)	25	30
1	B	419/428 (98%)	397 (95%)	22 (5%)	26	32
1	C	418/428 (98%)	395 (94%)	23 (6%)	25	30
1	D	418/428 (98%)	397 (95%)	21 (5%)	28	35
All	All	1675/1712 (98%)	1586 (95%)	89 (5%)	26	32

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	62	GLN
1	A	90	LEU
1	A	92	ASP
1	A	110	ARG
1	A	134	ARG
1	A	140	LYS
1	A	141	GLN
1	A	184	LEU
1	A	195	LYS
1	A	199	LEU
1	A	215	LEU
1	A	228	LEU
1	A	249	ARG
1	A	270	LEU
1	A	290	THR
1	A	310	TYR
1	A	325	LEU
1	A	342	LYS
1	A	368	LEU
1	A	392	THR
1	A	471	LEU
1	A	487	LEU
1	B	50	LEU
1	B	80	MET
1	B	90	LEU
1	B	110	ARG
1	B	184	LEU
1	B	195	LYS
1	B	199	LEU
1	B	215	LEU
1	B	225	LEU
1	B	228	LEU
1	B	270	LEU
1	B	303	THR
1	B	310	TYR
1	B	312	LEU
1	B	325	LEU
1	B	342	LYS
1	B	359	ARG
1	B	368	LEU
1	B	392	THR
1	B	451	LEU

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Mol	Chain	Res	Type
1	B	471	LEU
1	B	487	LEU
1	C	80	MET
1	C	90	LEU
1	C	110	ARG
1	C	140	LYS
1	C	141	GLN
1	C	145	SER
1	C	149	ARG
1	C	169	THR
1	C	192	ASN
1	C	195	LYS
1	C	199	LEU
1	C	215	LEU
1	C	249	ARG
1	C	310	TYR
1	C	337	ARG
1	C	342	LYS
1	C	359	ARG
1	C	368	LEU
1	C	392	THR
1	C	412	GLU
1	C	417	GLU
1	C	471	LEU
1	C	487	LEU
1	D	62	GLN
1	D	80	MET
1	D	90	LEU
1	D	110	ARG
1	D	140	LYS
1	D	141	GLN
1	D	149	ARG
1	D	156	GLU
1	D	195	LYS
1	D	199	LEU
1	D	215	LEU
1	D	290	THR
1	D	310	TYR
1	D	342	LYS
1	D	368	LEU
1	D	392	THR
1	D	417	GLU

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Mol	Chain	Res	Type
1	D	451	LEU
1	D	471	LEU
1	D	487	LEU
1	D	493	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	141	GLN
1	B	326	HIS

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 ⓘ

12 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	$\# Z > 2$
4	SUC	A	1	-	24,24,24	0.90	1 (4%)	36,36,36	1.60	9 (25%)
2	HEM	A	500	1,3	28,50,50	2.19	8 (28%)	17,82,82	1.47	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	9PL	A	501	2	14,16,16	1.27	2 (14%)	16,22,22	1.45	3 (18%)
4	SUC	B	1	-	24,24,24	1.16	2 (8%)	36,36,36	1.54	6 (16%)
2	HEM	B	500	1,3	28,50,50	2.15	7 (25%)	17,82,82	1.58	5 (29%)
3	9PL	B	501	2	14,16,16	1.49	1 (7%)	16,22,22	1.66	3 (18%)
4	SUC	C	1	-	24,24,24	0.99	2 (8%)	36,36,36	1.43	4 (11%)
2	HEM	C	500	1,3	28,50,50	2.40	10 (35%)	17,82,82	2.14	6 (35%)
3	9PL	C	501	2	14,16,16	1.45	2 (14%)	16,22,22	1.58	2 (12%)
4	SUC	D	1	-	24,24,24	0.96	0	36,36,36	1.39	5 (13%)
2	HEM	D	500	1,3	28,50,50	2.29	11 (39%)	17,82,82	1.91	7 (41%)
3	9PL	D	501	2	14,16,16	1.39	2 (14%)	16,22,22	1.96	6 (37%)

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
4	SUC	A	1	-	-	0/12/51/51	0/2/2/2
2	HEM	A	500	1,3	-	0/6/54/54	0/0/8/8
3	9PL	A	501	2	-	0/6/19/19	0/2/2/2
4	SUC	B	1	-	-	0/12/51/51	0/2/2/2
2	HEM	B	500	1,3	-	0/6/54/54	0/0/8/8
3	9PL	B	501	2	-	0/6/19/19	0/2/2/2
4	SUC	C	1	-	-	0/12/51/51	0/2/2/2
2	HEM	C	500	1,3	-	0/6/54/54	0/0/8/8
3	9PL	C	501	2	-	0/6/19/19	0/2/2/2
4	SUC	D	1	-	-	0/12/51/51	0/2/2/2
2	HEM	D	500	1,3	-	0/6/54/54	0/0/8/8
3	9PL	D	501	2	-	0/6/19/19	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C3B-C2B	-5.51	1.33	1.40
2	B	500	HEM	C3C-C2C	-4.93	1.33	1.40
2	C	500	HEM	C3C-C2C	-4.86	1.33	1.40
2	D	500	HEM	C3C-C2C	-4.00	1.35	1.40
2	A	500	HEM	C3C-C2C	-3.64	1.35	1.40
2	D	500	HEM	C3B-C2B	-3.56	1.35	1.40
2	B	500	HEM	C3B-C2B	-3.52	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C2B	-2.78	1.36	1.40
2	A	500	HEM	C2A-C3A	-2.66	1.29	1.37
2	C	500	HEM	C4C-NC	-2.09	1.34	1.36
3	C	501	9PL	C5-N1	-2.07	1.33	1.38
3	D	501	9PL	C12-C11	-2.06	1.48	1.51
4	C	1	SUC	O2'-C5'	2.00	1.48	1.43
2	D	500	HEM	CMB-C2B	2.05	1.55	1.51
2	B	500	HEM	CAA-C2A	2.05	1.55	1.52
2	C	500	HEM	C1D-ND	2.10	1.40	1.36
4	A	1	SUC	O2'-C2'	2.11	1.47	1.42
3	A	501	9PL	C6-N1	2.17	1.52	1.47
4	C	1	SUC	O5-C1	2.18	1.47	1.41
2	D	500	HEM	C4D-ND	2.24	1.39	1.36
4	B	1	SUC	O5-C1	2.28	1.47	1.41
2	A	500	HEM	CMC-C2C	2.36	1.56	1.51
2	D	500	HEM	C1B-NB	2.42	1.39	1.36
4	B	1	SUC	O6-C6	2.54	1.53	1.42
2	B	500	HEM	CMC-C2C	2.58	1.57	1.51
2	D	500	HEM	C4B-NB	2.63	1.41	1.36
2	C	500	HEM	CMD-C2D	2.64	1.57	1.51
2	D	500	HEM	CMD-C2D	2.74	1.57	1.51
2	C	500	HEM	CMC-C2C	2.80	1.57	1.51
2	C	500	HEM	C1B-NB	2.96	1.40	1.36
2	D	500	HEM	CMC-C2C	3.43	1.58	1.51
2	B	500	HEM	C3B-CAB	3.53	1.54	1.47
3	A	501	9PL	O10-C11	3.56	1.43	1.35
2	D	500	HEM	C3B-CAB	3.59	1.55	1.47
2	A	500	HEM	C3B-CAB	3.65	1.55	1.47
2	C	500	HEM	C3B-CAB	3.77	1.55	1.47
2	A	500	HEM	C4D-ND	3.78	1.41	1.36
3	D	501	9PL	O10-C11	3.82	1.44	1.35
3	C	501	9PL	O10-C11	4.05	1.44	1.35
3	B	501	9PL	O10-C11	4.19	1.44	1.35
2	C	500	HEM	C3D-C2D	4.25	1.50	1.37
2	B	500	HEM	C3D-C2D	4.49	1.51	1.37
2	B	500	HEM	C3C-CAC	4.58	1.56	1.47
2	C	500	HEM	C3C-CAC	4.67	1.57	1.47
2	D	500	HEM	C3C-CAC	4.69	1.57	1.47
2	D	500	HEM	C3D-C2D	4.76	1.51	1.37
2	A	500	HEM	C3C-CAC	4.77	1.57	1.47
2	A	500	HEM	C3D-C2D	5.33	1.53	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C1D-C2D-C3D	-4.04	104.18	107.00
2	C	500	HEM	CAA-CBA-CGA	-3.99	105.84	112.66
4	D	1	SUC	O2-C2-C3	-3.85	101.97	110.36
4	B	1	SUC	O2-C2-C3	-3.58	102.58	110.36
4	A	1	SUC	O3-C3-C4	-3.48	102.78	110.36
4	B	1	SUC	O3-C3-C4	-3.44	102.88	110.36
4	B	1	SUC	O5-C5-C4	-3.22	103.73	109.66
2	D	500	HEM	CMA-C3A-C4A	-3.19	123.56	128.46
3	B	501	9PL	O15-C11-C12	-3.13	124.40	128.87
4	C	1	SUC	O1'-C1'-C2'	-3.02	102.29	111.74
2	D	500	HEM	CAA-CBA-CGA	-2.97	107.58	112.66
2	C	500	HEM	CBD-CAD-C3D	-2.91	106.92	112.47
4	A	1	SUC	O2-C2-C3	-2.85	104.16	110.36
2	D	500	HEM	C1D-C2D-C3D	-2.81	105.04	107.00
3	D	501	9PL	C14-C13-C12	-2.80	107.16	113.51
4	A	1	SUC	O1'-C1'-C2'	-2.79	103.02	111.74
4	D	1	SUC	O3'-C3'-C4'	-2.77	103.60	113.38
4	B	1	SUC	O1'-C1'-C2'	-2.71	103.27	111.74
4	A	1	SUC	O5-C1-C2	-2.71	105.08	110.30
2	D	500	HEM	CAD-CBD-CGD	-2.62	108.19	112.66
3	D	501	9PL	O10-C9-C8	-2.60	100.68	105.37
2	C	500	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
3	A	501	9PL	O15-C11-C12	-2.57	125.20	128.87
4	C	1	SUC	O2-C2-C3	-2.51	104.90	110.36
2	B	500	HEM	CBD-CAD-C3D	-2.46	107.77	112.47
4	A	1	SUC	O3-C3-C2	-2.43	105.07	110.36
4	B	1	SUC	O4-C4-C3	-2.32	105.31	110.36
4	A	1	SUC	O1-C2'-O2'	-2.31	103.45	110.55
4	D	1	SUC	C2'-C3'-C4'	-2.29	96.53	102.06
4	D	1	SUC	O3-C3-C2	-2.26	105.43	110.36
4	A	1	SUC	O3'-C3'-C2'	-2.22	106.84	113.83
4	C	1	SUC	O2'-C2'-C3'	-2.21	100.76	105.57
2	D	500	HEM	CBD-CAD-C3D	-2.19	108.29	112.47
2	A	500	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
3	C	501	9PL	O10-C11-C12	-2.17	107.27	110.17
2	B	500	HEM	CMA-C3A-C4A	-2.14	125.17	128.46
2	A	500	HEM	CMC-C2C-C3C	2.00	128.60	124.89
3	D	501	9PL	C9-C8-C12	2.03	104.63	101.44
2	D	500	HEM	CMA-C3A-C2A	2.06	128.82	124.94
4	A	1	SUC	O1-C2'-C3'	2.08	115.05	108.11
2	C	500	HEM	CMC-C2C-C3C	2.12	128.82	124.89
2	B	500	HEM	CMB-C2B-C3B	2.13	128.85	124.89
2	B	500	HEM	CMC-C2C-C3C	2.16	128.89	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	9PL	C4-N3-C2	2.35	109.45	105.78
4	B	1	SUC	C1-C2-C3	2.53	114.68	109.98
3	B	501	9PL	C4-N3-C2	2.55	109.75	105.78
2	D	500	HEM	CMC-C2C-C3C	2.58	129.69	124.89
3	A	501	9PL	C4-N3-C2	2.60	109.83	105.78
3	A	501	9PL	O10-C11-O15	2.62	124.25	121.43
3	D	501	9PL	C6-N1-C5	2.63	127.95	124.44
2	A	500	HEM	C4A-C3A-C2A	2.68	108.86	107.00
4	D	1	SUC	O2'-C2'-C1'	2.71	115.03	108.03
2	B	500	HEM	C4C-C3C-C2C	2.76	108.83	106.90
2	A	500	HEM	CMB-C2B-C3B	2.81	130.10	124.89
4	C	1	SUC	C1-C2-C3	2.85	115.28	109.98
2	C	500	HEM	C4C-C3C-C2C	3.08	109.05	106.90
4	A	1	SUC	O2'-C2'-C1'	3.09	116.03	108.03
3	C	501	9PL	O10-C11-O15	3.54	125.23	121.43
3	B	501	9PL	O10-C11-O15	3.73	125.44	121.43
3	D	501	9PL	O10-C11-O15	3.91	125.63	121.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	2	0
3	A	501	9PL	2	0
2	B	500	HEM	2	0
3	B	501	9PL	3	0
2	C	500	HEM	7	0
3	C	501	9PL	2	0
4	D	1	SUC	1	0
2	D	500	HEM	4	0
3	D	501	9PL	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, 95th 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	464/476 (97%)	-0.10	8 (1%) 70 80	17, 28, 50, 71	0
1	B	464/476 (97%)	-0.11	1 (0%) 94 97	17, 28, 51, 69	0
1	C	464/476 (97%)	0.11	8 (1%) 70 80	17, 33, 62, 75	0
1	D	464/476 (97%)	0.09	10 (2%) 62 72	17, 32, 61, 76	0
All	All	1856/1904 (97%)	-0.00	27 (1%) 74 83	17, 30, 57, 76	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	5.2
1	D	280	ALA	5.2
1	C	281	GLU	4.0
1	D	257	LEU	3.8
1	C	494	HIS	3.4
1	D	283	LEU	3.2
1	C	283	LEU	3.1
1	C	280	ALA	2.8
1	D	255	GLN	2.8
1	A	278	HIS	2.7
1	D	494	HIS	2.7
1	A	417[A]	GLU	2.6
1	D	281	GLU	2.6
1	A	418	ASN	2.5
1	D	335	PRO	2.4
1	C	187	LYS	2.4
1	B	278	HIS	2.4
1	C	261	CYS	2.3
1	C	152	HIS	2.2
1	A	261	CYS	2.2
1	A	277	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	278	HIS	2.2
1	D	251	LYS	2.2
1	D	138	MET	2.2
1	A	283	LEU	2.2
1	D	266	THR	2.1
1	A	138	MET	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, 95th 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	SUC	B	1	23/23	0.93	0.20	3.07	25,28,32,38	0
4	SUC	C	1	23/23	0.93	0.18	2.72	26,29,32,33	0
3	9PL	B	501	15/15	0.94	0.16	2.63	20,24,26,27	0
4	SUC	D	1	23/23	0.93	0.15	0.81	25,28,30,35	0
2	HEM	C	500	43/43	0.98	0.13	0.57	13,21,24,29	0
2	HEM	D	500	43/43	0.98	0.13	0.27	17,23,27,31	0
3	9PL	A	501	15/15	0.96	0.12	0.09	18,25,31,32	0
3	9PL	C	501	15/15	0.96	0.13	0.00	24,28,34,35	0
2	HEM	B	500	43/43	0.98	0.12	-0.17	14,21,24,27	0
2	HEM	A	500	43/43	0.98	0.12	-0.18	14,22,26,26	0
4	SUC	A	1	23/23	0.95	0.13	-0.22	24,28,30,31	0
3	9PL	D	501	15/15	0.98	0.12	-0.57	19,25,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.