Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:21 PM GMT

PDB ID	:	3QU8
Title	:	Crystal structure of a human cytochrome P450 2B6 (Y226H/K262R) in complex with the inhibitor 4-(4-Nitrobenzyl)pyridine.
Authors	:	Shah, M.B.; Pascual, J.; Stout, C.D.; Halpert, J.R.
Deposited on	:	2011-02-23
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

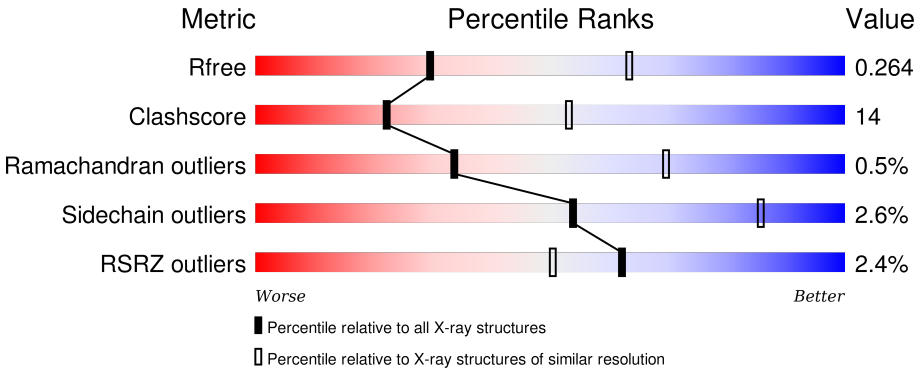
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	476	76% 18%
1	B	476	% 77% 17%
1	C	476	76% 19%
1	D	476	% 76% 20%
1	E	476	% 73% 22%

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Mol	Chain	Length	Quality of chain
1	F	476	10% 71% 22% 5%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3QU	A	501	-	-	-	X
3	3QU	B	501	-	-	-	X
3	3QU	D	501	-	-	-	X
3	3QU	E	501	-	-	-	X
4	CM5	B	602	-	-	-	X
4	CM5	C	603	-	-	-	X
4	CM5	D	604	X	-	-	-
4	CM5	D	607	-	-	-	X
4	CM5	F	606	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22964 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 2B6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3732	2416	641	658	17			
1	B	459	Total	C	N	O	S	0	0	0
			3713	2403	639	655	16			
1	C	462	Total	C	N	O	S	0	0	0
			3724	2408	642	658	16			
1	D	458	Total	C	N	O	S	0	0	0
			3693	2389	635	653	16			
1	E	459	Total	C	N	O	S	0	0	0
			3717	2406	640	655	16			
1	F	453	Total	C	N	O	S	0	0	0
			3649	2359	625	649	16			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
A	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
A	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
A	26	SER	THR	ENGINEERED MUTATION	UNP P20813
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
A	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
A	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
A	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
A	492	HIS	-	EXPRESSION TAG	UNP P20813
A	493	HIS	-	EXPRESSION TAG	UNP P20813
A	494	HIS	-	EXPRESSION TAG	UNP P20813
A	495	HIS	-	EXPRESSION TAG	UNP P20813
B	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
B	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
B	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
B	26	SER	THR	ENGINEERED MUTATION	UNP P20813
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
B	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
B	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
B	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
B	492	HIS	-	EXPRESSION TAG	UNP P20813
B	493	HIS	-	EXPRESSION TAG	UNP P20813
B	494	HIS	-	EXPRESSION TAG	UNP P20813
B	495	HIS	-	EXPRESSION TAG	UNP P20813
C	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
C	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
C	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
C	26	SER	THR	ENGINEERED MUTATION	UNP P20813
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
C	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
C	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
C	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
C	492	HIS	-	EXPRESSION TAG	UNP P20813
C	493	HIS	-	EXPRESSION TAG	UNP P20813
C	494	HIS	-	EXPRESSION TAG	UNP P20813
C	495	HIS	-	EXPRESSION TAG	UNP P20813
D	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
D	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
D	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
D	26	SER	THR	ENGINEERED MUTATION	UNP P20813
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
D	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
D	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
D	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
D	492	HIS	-	EXPRESSION TAG	UNP P20813
D	493	HIS	-	EXPRESSION TAG	UNP P20813
D	494	HIS	-	EXPRESSION TAG	UNP P20813

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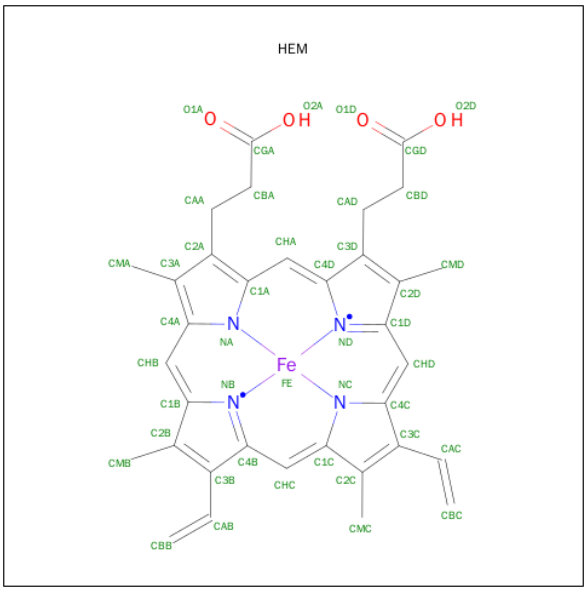
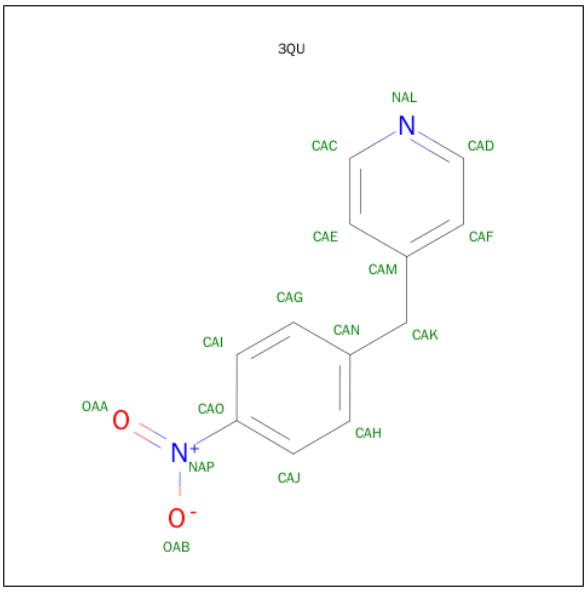
Chain	Residue	Modelled	Actual	Comment	Reference
D	495	HIS	-	EXPRESSION TAG	UNP P20813
E	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
E	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
E	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
E	26	SER	THR	ENGINEERED MUTATION	UNP P20813
E	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
E	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
E	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
E	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
E	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
E	492	HIS	-	EXPRESSION TAG	UNP P20813
E	493	HIS	-	EXPRESSION TAG	UNP P20813
E	494	HIS	-	EXPRESSION TAG	UNP P20813
E	495	HIS	-	EXPRESSION TAG	UNP P20813
F	2	ALA	GLU	ENGINEERED MUTATION	UNP P20813
F	22	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	23	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	24	THR	PRO	ENGINEERED MUTATION	UNP P20813
F	25	SER	ASN	ENGINEERED MUTATION	UNP P20813
F	26	SER	THR	ENGINEERED MUTATION	UNP P20813
F	27	LYS	HIS	ENGINEERED MUTATION	UNP P20813
F	28	GLY	ASP	ENGINEERED MUTATION	UNP P20813
F	29	LYS	ARG	ENGINEERED MUTATION	UNP P20813
F	226	HIS	TYR	ENGINEERED MUTATION	UNP P20813
F	262	ARG	LYS	ENGINEERED MUTATION	UNP P20813
F	492	HIS	-	EXPRESSION TAG	UNP P20813
F	493	HIS	-	EXPRESSION TAG	UNP P20813
F	494	HIS	-	EXPRESSION TAG	UNP P20813
F	495	HIS	-	EXPRESSION TAG	UNP P20813

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



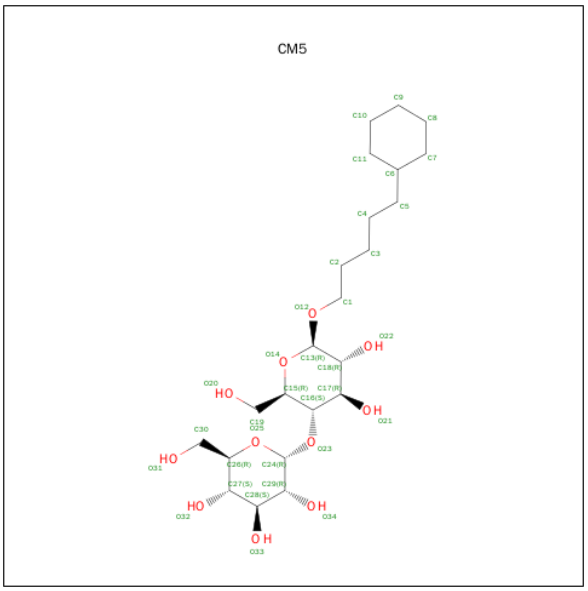
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-(4-NITROBENZYL)PYRIDINE (three-letter code: 3QU) (formula: $C_{12}H_{10}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 7 6 1	0	0
3	B	1	Total C N O 16 12 2 2	0	0
3	C	1	Total C N 7 6 1	0	0
3	D	1	Total C N 13 12 1	0	0
3	E	1	Total C N 13 12 1	0	0

- Molecule 4 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	B	1	Total C O 34 23 11	0	0
4	C	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	D	1	Total C O 34 23 11	0	0
4	E	1	Total C O 34 23 11	0	0
4	F	1	Total C O 34 23 11	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	B	23	Total O 23 23	0	0
5	C	29	Total O 29 29	0	0
5	D	38	Total O 38 38	0	0

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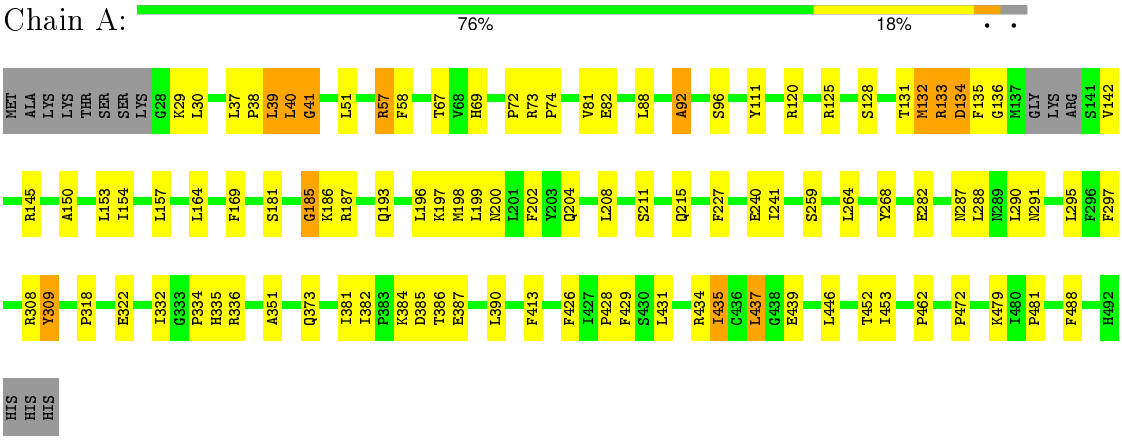
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	23	Total O 23 23	0	0
5	F	12	Total O 12 12	0	0

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.

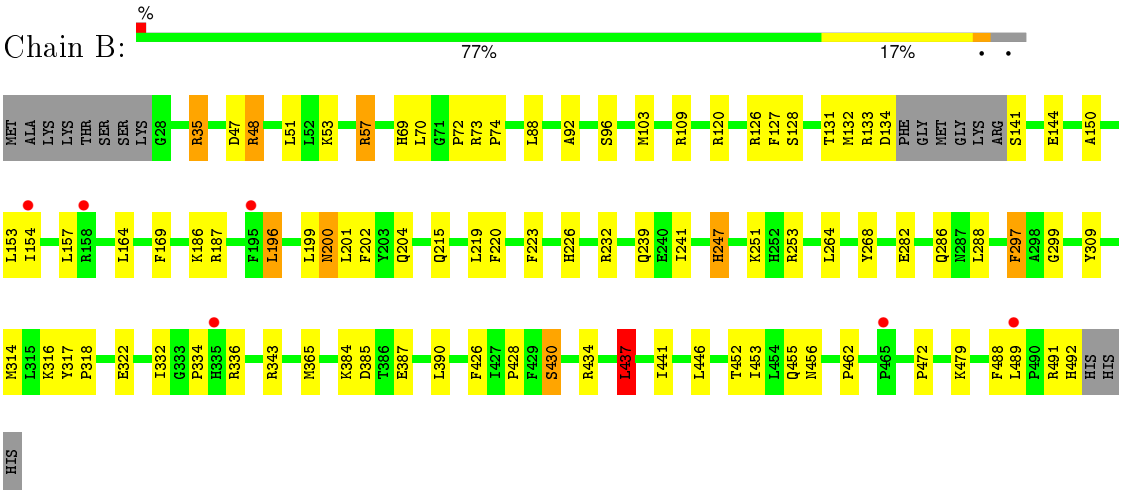
- Molecule 1: Cytochrome P450 2B6

Chain A:



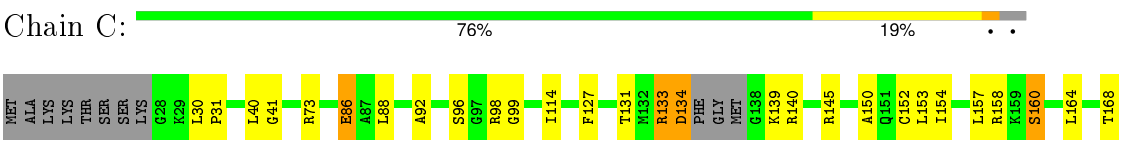
- Molecule 1: Cytochrome P450 2B6

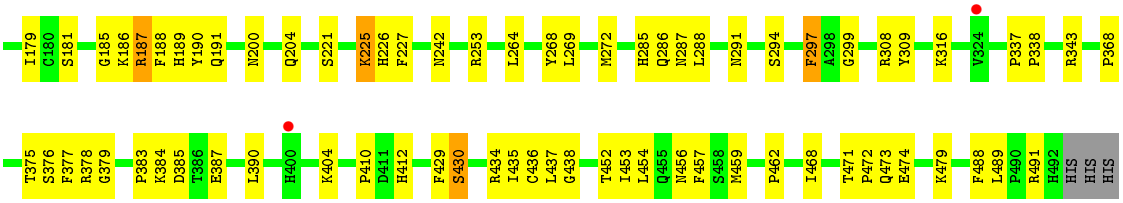
Chain B:



- Molecule 1: Cytochrome P450 2B6

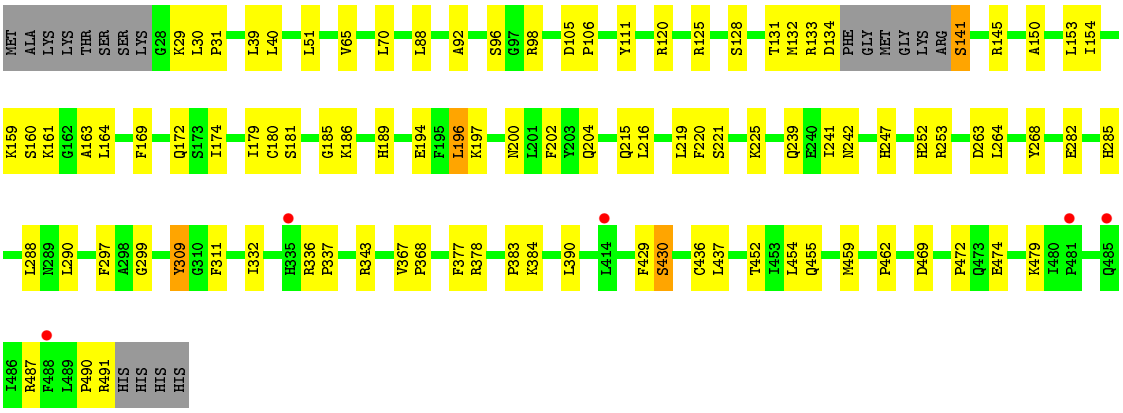
Chain C:





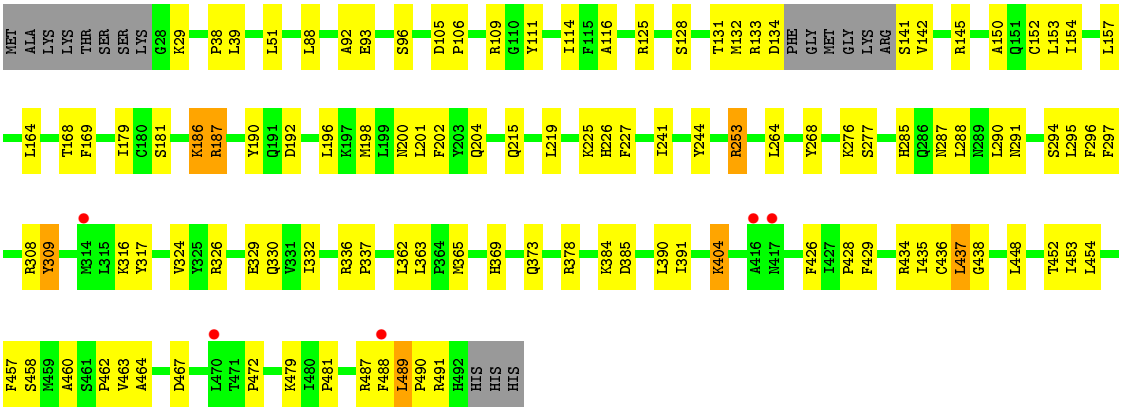
• Molecule 1: Cytochrome P450 2B6

Chain D:



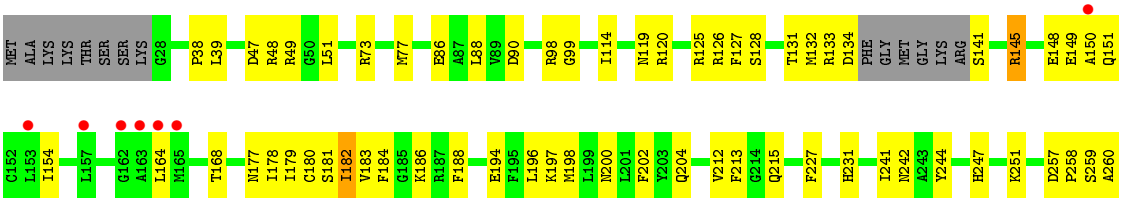
• Molecule 1: Cytochrome P450 2B6

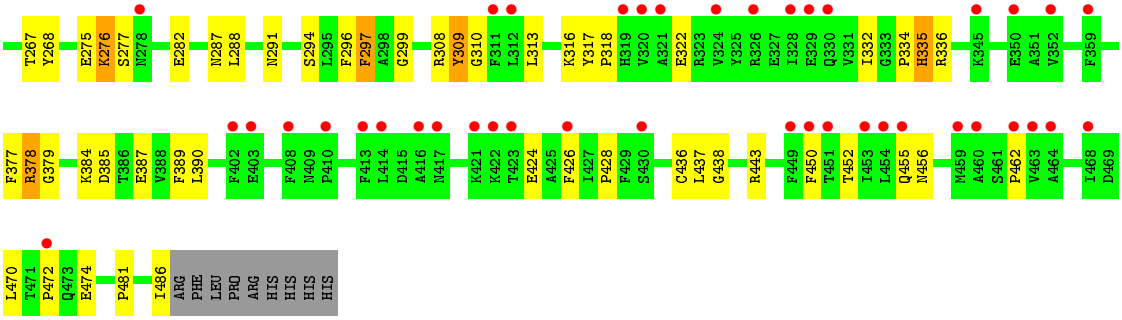
Chain E:



• Molecule 1: Cytochrome P450 2B6

Chain F:




T267 Y268 E275 K276 S277 N278 E282 N287 L288 N291 S294 L295 F296 F297 A298 G299 R308 Y309 G310 F311 L312 L313 K316 Y317 P318 H319 V320 A321 E322 R323 V324 Y325 R326 E327 I328 E329 Q330 V331 I332 G333 P334 H335 R336 K345 E350 A351 V352 F359
F377 R378 G379 K384 D385 T386 E387 V388 F389 L390 F402 E403 F408 N409 P410 F413 L414 D415 A416 N417 K421 K422 T423 E424 A425 F426 I427 P428 F429 S430 C436 L437 G438 R443 F449 P450 T451 T452 I453 L454 Q455 N456 N459 A460 S461 P462 V463 A464 I468 D469
L470 T471 P472 Q473 E474 P481 I486 ARG PHE LEU PRO ARG HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	101.88Å 101.88Å 299.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.51 – 2.80 50.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (50.51-2.80) 88.9 (50.22-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.218 , 0.259 0.226 , 0.264	Depositor DCC
R_{free} test set	3810 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.4	EDS
Estimated twinning fraction	0.043 for -h,-k,l 0.149 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 76006 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22964	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, CM5, 3QU

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	0.84	0/3833	0.75	1/5185 (0.0%)
1	B	0.83	0/3813	0.78	4/5158 (0.1%)
1	C	0.90	2/3822 (0.1%)	0.76	1/5167 (0.0%)
1	D	0.83	0/3791	0.78	2/5129 (0.0%)
1	E	0.82	0/3817	0.75	0/5162
1	F	0.95	1/3745 (0.0%)	0.78	0/5067
All	All	0.86	3/22821 (0.0%)	0.77	8/30868 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	450	PHE	CE2-CZ	5.42	1.47	1.37
1	C	152	CYS	CB-SG	-5.35	1.73	1.81
1	C	86	GLU	CG-CD	5.07	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	474	GLU	CB-CA-C	-5.88	98.64	110.40
1	A	185	GLY	N-CA-C	5.46	126.76	113.10
1	C	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	343	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	103	MET	CG-SD-CE	-5.40	91.57	100.20
1	B	35	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	437	LEU	CA-CB-CG	5.28	127.43	115.30
1	D	343	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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	3732	0	3712	103	0
1	B	3713	0	3702	93	0
1	C	3724	0	3711	83	0
1	D	3693	0	3682	97	0
1	E	3717	0	3713	117	0
1	F	3649	0	3635	100	0
2	A	43	0	30	10	0
2	B	43	0	30	4	0
2	C	43	0	30	9	0
2	D	43	0	30	12	0
2	E	43	0	30	9	0
2	F	43	0	30	18	0
3	A	7	0	4	0	0
3	B	16	0	10	0	0
3	C	7	0	4	0	0
3	D	13	0	10	0	0
3	E	13	0	10	1	0
4	A	34	0	35	1	0
4	B	68	0	77	34	0
4	C	34	0	40	5	0
4	D	68	0	78	12	0
4	E	34	0	40	3	0
4	F	34	0	38	5	0
5	A	25	0	0	1	0
5	B	23	0	0	12	0
5	C	29	0	0	2	0
5	D	38	0	0	5	0
5	E	23	0	0	5	0
5	F	12	0	0	5	0
All	All	22964	0	22681	629	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 14.

All (629) 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)
4:B:608:CM5:C16	4:B:608:CM5:O23	1.64	1.42
4:B:608:CM5:H17	4:B:608:CM5:C24	1.61	1.28
1:A:381:ILE:HG21	1:B:239:GLN:CG	1.65	1.25
1:A:136:GLY:HA2	1:A:142:VAL:CG2	1.65	1.24
1:B:232:ARG:HH12	4:B:602:CM5:C19	1.48	1.24
1:F:148:GLU:HG2	5:F:506:HOH:O	1.36	1.21
1:B:232:ARG:NH1	4:B:602:CM5:H191	1.54	1.19
1:A:381:ILE:HG21	1:B:239:GLN:HG2	1.24	1.16
1:E:384:LYS:O	1:E:385:ASP:HB2	1.46	1.15
1:E:362:LEU:O	1:E:363:LEU:HD23	1.48	1.10
1:E:253:ARG:HH11	1:E:253:ARG:CG	1.65	1.09
1:E:253:ARG:HG3	1:E:253:ARG:NH1	1.50	1.08
4:B:608:CM5:C24	4:B:608:CM5:C17	2.31	1.06
1:F:437:LEU:HD21	2:F:500:HEM:HMD1	1.36	1.03
4:B:608:CM5:O23	4:B:608:CM5:C17	2.06	1.02
4:B:608:CM5:H191	4:B:608:CM5:H12	1.41	1.01
4:B:602:CM5:H11	4:B:602:CM5:O22	1.60	1.00
1:E:198:MET:HE2	1:E:244:TYR:CD2	1.97	1.00
1:A:136:GLY:CA	1:A:142:VAL:CG2	2.41	0.98
2:A:500:HEM:HBC2	2:A:500:HEM:HHD	1.46	0.97
1:E:225:LYS:HE2	1:E:226:HIS:CE1	2.00	0.96
1:D:454:LEU:HD23	1:D:459:MET:CE	1.95	0.96
1:F:437:LEU:HD21	2:F:500:HEM:CMD	1.96	0.95
1:B:437:LEU:O	1:B:437:LEU:HD23	1.65	0.94
1:B:226:HIS:HB3	4:B:602:CM5:H32A	1.45	0.94
4:C:603:CM5:H301	4:C:603:CM5:H191	1.47	0.94
1:C:375:THR:C	1:C:376:SER:CA	2.37	0.93
1:B:232:ARG:HH12	4:B:602:CM5:H191	0.76	0.92
2:E:500:HEM:HHD	2:E:500:HEM:HBC2	1.53	0.91
1:D:253:ARG:HH12	1:D:285:HIS:CE1	1.88	0.91
1:E:437:LEU:C	1:E:437:LEU:HD23	1.92	0.90
1:F:437:LEU:CD2	2:F:500:HEM:HMD1	2.02	0.89
1:D:40:LEU:CD2	4:D:607:CM5:H102	2.02	0.88
1:A:136:GLY:HA2	1:A:142:VAL:HG22	1.54	0.88
1:E:128:SER:O	1:E:132:MET:HG2	1.74	0.87
1:A:381:ILE:HG12	1:B:239:GLN:HG3	1.55	0.87
1:A:437:LEU:O	1:A:437:LEU:HD12	1.74	0.87
1:A:88:LEU:HD11	1:A:390:LEU:HD13	1.54	0.87
1:A:88:LEU:HD21	1:A:390:LEU:HD11	1.56	0.87
1:A:88:LEU:HD11	1:A:390:LEU:CD1	2.05	0.86
1:D:39:LEU:CD2	4:F:606:CM5:H111	2.06	0.86
1:F:141:SER:O	1:F:145:ARG:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:LEU:CD2	1:D:459:MET:CE	2.55	0.85
1:A:437:LEU:C	1:A:437:LEU:HD12	1.96	0.85
1:A:134:ASP:OD2	1:A:134:ASP:C	2.14	0.85
1:A:336:ARG:HG2	1:A:336:ARG:HH11	1.42	0.85
1:A:381:ILE:HG21	1:B:239:GLN:HG3	1.58	0.84
4:B:608:CM5:H191	4:B:608:CM5:C1	2.05	0.84
1:A:136:GLY:O	1:A:142:VAL:HG23	1.78	0.84
1:A:384:LYS:O	1:A:385:ASP:HB2	1.77	0.83
1:D:454:LEU:HD23	1:D:459:MET:HE3	1.57	0.83
1:C:473:GLN:O	1:C:474:GLU:HG2	1.78	0.82
1:E:326:ARG:O	1:E:330:GLN:HG2	1.80	0.82
1:C:437:LEU:O	1:C:437:LEU:HD12	1.81	0.81
1:E:198:MET:CE	1:E:244:TYR:CD2	2.63	0.81
4:E:605:CM5:O20	4:E:605:CM5:O25	1.99	0.81
1:B:437:LEU:HD23	1:B:437:LEU:C	2.01	0.80
1:D:454:LEU:CD2	1:D:459:MET:HE1	2.11	0.80
1:D:454:LEU:HD23	1:D:459:MET:HE1	1.63	0.80
1:A:198:MET:HE1	1:A:241:ILE:HA	1.61	0.80
1:A:136:GLY:HA2	1:A:142:VAL:HG21	1.62	0.79
1:B:384:LYS:O	1:B:385:ASP:HB2	1.80	0.79
1:D:436:CYS:HB2	2:D:500:HEM:NA	1.95	0.79
1:F:128:SER:O	1:F:132:MET:HG2	1.82	0.79
1:F:384:LYS:O	1:F:385:ASP:HB2	1.83	0.79
1:E:157:LEU:HD22	1:E:488:PHE:CD2	2.18	0.78
1:A:437:LEU:CD1	1:A:437:LEU:O	2.31	0.78
1:F:88:LEU:HD11	1:F:390:LEU:CD1	2.14	0.78
1:E:436:CYS:HB2	2:E:500:HEM:NA	1.97	0.78
1:B:141:SER:HB3	1:B:144:GLU:HB2	1.65	0.77
1:E:152:CYS:HB3	5:E:508:HOH:O	1.83	0.77
1:A:136:GLY:C	1:A:142:VAL:HG23	2.04	0.77
1:A:136:GLY:C	1:A:142:VAL:CG2	2.53	0.77
1:D:253:ARG:NH1	1:D:285:HIS:NE2	2.32	0.77
4:B:608:CM5:C16	4:B:608:CM5:C24	2.63	0.76
1:F:299:GLY:N	2:F:500:HEM:HBC2	2.00	0.76
1:F:88:LEU:HD21	1:F:390:LEU:HD11	1.67	0.76
4:B:602:CM5:C1	4:B:602:CM5:O22	2.30	0.76
1:B:365:MET:HB2	5:B:506:HOH:O	1.84	0.76
1:A:136:GLY:CA	1:A:142:VAL:HG23	2.15	0.76
1:E:253:ARG:HH22	1:E:285:HIS:CE1	2.03	0.76
2:F:500:HEM:HMB1	2:F:500:HEM:HBB2	1.67	0.75
1:E:436:CYS:HB2	2:E:500:HEM:C1A	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:LEU:HD11	1:F:390:LEU:HD12	1.69	0.74
1:D:164:LEU:HD23	1:D:487:ARG:HG3	1.68	0.74
4:C:603:CM5:O25	4:C:603:CM5:C19	2.35	0.74
1:A:133:ARG:O	1:A:136:GLY:N	2.21	0.73
1:E:489:LEU:N	1:E:489:LEU:HD23	2.02	0.73
1:B:169:PHE:CE1	1:B:196:LEU:HG	2.24	0.72
2:F:500:HEM:HBB2	2:F:500:HEM:CMB	2.18	0.72
1:F:242:ASN:HB3	5:F:499:HOH:O	1.88	0.72
1:C:299:GLY:HA2	2:C:500:HEM:HBC2	1.72	0.72
1:F:131:THR:HG21	1:F:267:THR:HG21	1.72	0.72
1:D:39:LEU:HA	5:D:509:HOH:O	1.89	0.72
1:F:154:ILE:HD11	1:F:452:THR:HG22	1.71	0.72
4:C:603:CM5:O25	4:C:603:CM5:H191	1.91	0.71
1:A:336:ARG:HG2	1:A:336:ARG:NH1	2.03	0.71
4:B:608:CM5:H17	4:B:608:CM5:O25	1.90	0.71
1:D:39:LEU:HD21	4:F:606:CM5:H111	1.71	0.71
1:F:125:ARG:NH1	2:F:500:HEM:O1D	2.24	0.70
1:B:223:PHE:HA	4:B:602:CM5:H102	1.72	0.70
1:C:437:LEU:HD21	2:C:500:HEM:HMD1	1.74	0.70
1:A:136:GLY:CA	1:A:142:VAL:HG21	2.19	0.70
1:C:437:LEU:CD2	2:C:500:HEM:HMD1	2.21	0.69
1:B:128:SER:O	1:B:132:MET:HG2	1.92	0.69
1:F:437:LEU:CD2	2:F:500:HEM:CMD	2.68	0.69
1:E:253:ARG:HH11	1:E:253:ARG:HG3	0.70	0.69
1:D:40:LEU:CD2	4:D:607:CM5:C10	2.70	0.69
1:B:491:ARG:O	1:B:492:HIS:CB	2.41	0.69
1:C:73:ARG:HD2	1:C:387:GLU:OE1	1.93	0.69
1:F:437:LEU:O	1:F:437:LEU:HD12	1.93	0.69
1:E:488:PHE:O	1:E:490:PRO:HD3	1.93	0.69
1:D:252:HIS:NE2	1:D:263:ASP:OD2	2.26	0.68
1:C:179:ILE:HD11	2:C:500:HEM:HBC1	1.73	0.68
1:C:253:ARG:NH1	5:C:521:HOH:O	2.26	0.68
1:E:226:HIS:O	1:E:227:PHE:CG	2.47	0.68
1:C:456:ASN:O	1:C:491:ARG:N	2.20	0.67
1:E:384:LYS:O	1:E:385:ASP:CB	2.31	0.67
4:B:608:CM5:C19	4:B:608:CM5:C1	2.64	0.67
2:A:500:HEM:HBA1	2:A:500:HEM:HMA1	1.76	0.66
1:D:437:LEU:HD12	1:D:437:LEU:C	2.16	0.66
1:D:299:GLY:CA	2:D:500:HEM:HBC2	2.26	0.66
4:B:608:CM5:H191	4:B:608:CM5:H31A	1.77	0.66
1:A:136:GLY:HA2	1:A:142:VAL:HG23	1.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ILE:HG21	1:F:296:PHE:HA	1.77	0.66
1:B:200:ASN:O	1:B:204:GLN:HG2	1.94	0.66
2:C:500:HEM:HBB2	2:C:500:HEM:HMB2	1.75	0.66
1:E:332:ILE:HA	1:E:336:ARG:HH21	1.60	0.66
1:B:72:PRO:HB3	5:B:517:HOH:O	1.94	0.66
4:B:602:CM5:O20	4:B:602:CM5:O25	2.13	0.65
1:E:454:LEU:O	1:E:491:ARG:NH1	2.28	0.65
1:B:92:ALA:O	1:B:96:SER:HB3	1.97	0.65
1:F:181:SER:OG	1:F:182:ILE:N	2.30	0.65
1:D:128:SER:O	1:D:132:MET:HG2	1.96	0.65
1:E:458:SER:HB3	1:E:489:LEU:HB2	1.78	0.65
1:F:227:PHE:HA	4:F:606:CM5:O22	1.96	0.65
1:E:154:ILE:HD11	1:E:452:THR:HG22	1.78	0.65
1:D:437:LEU:O	1:D:437:LEU:HD12	1.97	0.65
1:F:377:PHE:O	1:F:378:ARG:C	2.32	0.64
1:F:299:GLY:CA	2:F:500:HEM:HBC2	2.27	0.64
1:C:227:PHE:HA	4:C:603:CM5:O22	1.97	0.64
1:A:198:MET:CE	1:A:241:ILE:HA	2.26	0.64
1:B:316:LYS:HG2	1:B:317:TYR:CE1	2.32	0.64
1:F:178:ILE:O	1:F:182:ILE:HG13	1.97	0.64
1:C:377:PHE:O	1:C:378:ARG:C	2.35	0.64
4:B:608:CM5:O12	4:B:608:CM5:H192	1.97	0.64
1:C:200:ASN:O	1:C:204:GLN:HG2	1.98	0.64
1:A:73:ARG:HD2	1:A:387:GLU:OE1	1.97	0.63
1:B:35:ARG:HB2	5:B:508:HOH:O	1.98	0.63
4:B:608:CM5:O22	4:B:608:CM5:H301	1.98	0.63
1:A:88:LEU:CD1	1:A:390:LEU:HD13	2.25	0.63
1:A:334:PRO:HD2	1:A:335:HIS:CD2	2.33	0.63
1:E:169:PHE:CE2	1:E:196:LEU:HG	2.34	0.63
1:A:128:SER:O	1:A:132:MET:CG	2.47	0.63
1:C:73:ARG:NE	1:C:387:GLU:OE1	2.32	0.63
1:F:47:ASP:CG	1:F:49:ARG:HH21	2.03	0.62
1:E:316:LYS:HG2	1:E:316:LYS:O	1.99	0.62
1:E:88:LEU:HD21	1:E:390:LEU:HD11	1.79	0.62
1:E:164:LEU:HD21	1:E:462:PRO:HD3	1.80	0.62
1:A:92:ALA:O	1:A:96:SER:HB3	1.98	0.62
1:B:133:ARG:O	1:B:134:ASP:C	2.38	0.62
1:F:141:SER:O	1:F:145:ARG:CG	2.46	0.62
1:C:384:LYS:O	1:C:385:ASP:HB2	1.99	0.62
1:D:181:SER:HA	1:D:186:LYS:H	1.64	0.62
1:E:198:MET:HE2	1:E:244:TYR:CG	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:LEU:HD22	4:F:606:CM5:H52	1.82	0.61
1:C:133:ARG:HG2	1:C:134:ASP:N	2.14	0.61
1:A:136:GLY:C	1:A:142:VAL:HG21	2.21	0.61
1:E:198:MET:CE	1:E:244:TYR:HD2	2.10	0.61
1:A:437:LEU:C	1:A:437:LEU:CD1	2.68	0.61
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.31	0.61
1:C:154:ILE:HD11	1:C:452:THR:HG22	1.83	0.61
1:B:154:ILE:HD11	1:B:452:THR:HG22	1.83	0.61
1:D:88:LEU:HD21	1:D:390:LEU:HD11	1.82	0.61
4:B:608:CM5:C18	4:B:608:CM5:H192	2.31	0.61
1:C:134:ASP:O	1:C:134:ASP:CG	2.40	0.60
1:B:232:ARG:NH1	4:B:602:CM5:C19	2.31	0.60
1:E:157:LEU:HD22	1:E:488:PHE:CE2	2.37	0.60
1:E:464:ALA:HB3	1:E:467:ASP:HB2	1.82	0.60
1:F:299:GLY:HA2	2:F:500:HEM:HMC3	1.82	0.60
1:C:73:ARG:CD	1:C:387:GLU:OE1	2.50	0.60
1:E:192:ASP:O	1:E:196:LEU:HD13	2.01	0.60
1:A:164:LEU:HD21	1:A:462:PRO:HD3	1.84	0.60
1:E:150:ALA:O	1:E:154:ILE:HG12	2.02	0.60
1:A:308:ARG:HH11	1:A:481:PRO:HG2	1.66	0.60
1:B:472:PRO:HG3	1:B:479:LYS:HE3	1.84	0.60
1:B:132:MET:HB3	5:B:503:HOH:O	2.01	0.59
1:F:316:LYS:HG2	1:F:317:TYR:CE1	2.37	0.59
2:A:500:HEM:CBA	2:A:500:HEM:CMA	2.80	0.59
1:B:491:ARG:O	1:B:492:HIS:HB3	2.02	0.59
1:C:133:ARG:O	1:C:134:ASP:C	2.41	0.59
1:E:268:TYR:CE1	1:E:288:LEU:HB2	2.37	0.59
1:D:141:SER:O	1:D:145:ARG:HD2	2.03	0.59
1:F:247:HIS:NE2	1:F:251:LYS:HE3	2.18	0.59
1:F:73:ARG:HD2	1:F:387:GLU:OE1	2.02	0.59
1:A:309:TYR:CD1	1:A:481:PRO:HB3	2.38	0.59
1:C:131:THR:HB	1:C:264:LEU:HD12	1.84	0.59
1:C:473:GLN:HG3	1:C:474:GLU:HG2	1.84	0.59
1:B:332:ILE:HA	1:B:336:ARG:NH2	2.16	0.59
1:D:454:LEU:CD2	1:D:459:MET:HE3	2.29	0.59
1:E:437:LEU:C	1:E:437:LEU:CD2	2.66	0.59
4:B:608:CM5:H191	4:B:608:CM5:C3	2.33	0.58
1:C:140:ARG:NH1	1:C:145:ARG:HG2	2.19	0.58
1:D:332:ILE:HA	1:D:336:ARG:HH21	1.69	0.58
1:D:40:LEU:HD23	4:D:607:CM5:H102	1.82	0.58
1:F:377:PHE:O	1:F:379:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:ILE:HA	1:F:336:ARG:HH21	1.69	0.58
1:F:164:LEU:HD21	1:F:462:PRO:HD3	1.85	0.58
1:B:226:HIS:CB	4:B:602:CM5:H32A	2.27	0.58
1:E:186:LYS:HG2	1:E:187:ARG:N	2.17	0.58
1:A:381:ILE:CG2	1:B:239:GLN:HG2	2.16	0.58
1:E:253:ARG:NH2	1:E:285:HIS:CE1	2.71	0.57
4:B:602:CM5:O20	4:B:602:CM5:C24	2.52	0.57
1:D:454:LEU:HD21	1:D:459:MET:HE1	1.85	0.57
1:B:437:LEU:CD2	1:B:437:LEU:C	2.73	0.57
1:D:164:LEU:HD21	1:D:462:PRO:HD3	1.87	0.57
1:A:69:HIS:NE2	1:A:74:PRO:HG3	2.18	0.57
1:F:299:GLY:H	2:F:500:HEM:HBC2	1.70	0.57
1:F:73:ARG:NE	1:F:387:GLU:OE1	2.37	0.57
1:D:154:ILE:HD11	1:D:452:THR:HG22	1.85	0.57
1:B:69:HIS:HA	1:B:73:ARG:O	2.04	0.57
1:C:436:CYS:HB2	2:C:500:HEM:NA	2.18	0.57
1:E:88:LEU:HD21	1:E:390:LEU:CD1	2.35	0.57
1:B:247:HIS:C	1:B:247:HIS:CD2	2.77	0.57
1:B:316:LYS:O	1:B:316:LYS:HG3	2.04	0.57
1:C:383:PRO:O	1:C:384:LYS:C	2.43	0.57
1:D:40:LEU:HD23	4:D:607:CM5:C11	2.35	0.56
4:B:608:CM5:H17	4:B:608:CM5:C26	2.35	0.56
1:A:202:PHE:CE2	1:A:241:ILE:HD13	2.40	0.56
1:F:47:ASP:OD2	1:F:49:ARG:NH2	2.36	0.56
1:E:141:SER:O	1:E:145:ARG:HG3	2.06	0.56
1:D:164:LEU:HG	1:D:487:ARG:CZ	2.35	0.56
1:A:198:MET:HE1	1:A:241:ILE:HG12	1.87	0.56
1:D:299:GLY:N	2:D:500:HEM:HBC2	2.21	0.56
1:B:247:HIS:NE2	1:B:251:LYS:HE3	2.20	0.56
1:A:198:MET:CE	1:A:241:ILE:HG23	2.35	0.56
1:A:128:SER:O	1:A:132:MET:HG2	2.06	0.56
1:A:38:PRO:O	1:A:39:LEU:HB2	2.06	0.55
1:B:430:SER:CB	2:B:500:HEM:HBA1	2.35	0.55
1:D:88:LEU:HD11	1:D:390:LEU:CD1	2.36	0.55
1:F:287:ASN:O	1:F:291:ASN:HB2	2.06	0.55
1:F:268:TYR:CG	1:F:288:LEU:HD13	2.41	0.55
1:B:223:PHE:CD1	4:B:608:CM5:H112	2.42	0.55
1:A:40:LEU:O	1:A:41:GLY:C	2.45	0.55
1:D:31:PRO:HB3	1:D:65:VAL:HG12	1.89	0.55
1:B:164:LEU:HD21	1:B:462:PRO:HD3	1.87	0.55
1:E:488:PHE:C	1:E:489:LEU:HD23	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ILE:HG22	1:F:182:ILE:O	2.06	0.55
1:B:126:ARG:CD	5:B:515:HOH:O	2.54	0.55
1:E:133:ARG:O	1:E:134:ASP:C	2.45	0.55
1:F:133:ARG:O	1:F:134:ASP:C	2.45	0.55
2:A:500:HEM:CBA	2:A:500:HEM:HMA1	2.37	0.55
1:A:227:PHE:CE1	4:A:601:CM5:H22A	2.42	0.55
1:F:275:GLU:O	1:F:277:SER:N	2.40	0.54
1:E:169:PHE:HZ	1:E:190:TYR:O	1.90	0.54
1:A:131:THR:HB	1:A:264:LEU:HD12	1.88	0.54
1:A:135:PHE:HB3	1:A:145:ARG:HH12	1.71	0.54
1:A:154:ILE:HD11	1:A:452:THR:HG22	1.89	0.54
1:A:382:ILE:HG22	1:A:386:THR:HB	1.89	0.54
1:D:179:ILE:HD11	2:D:500:HEM:HBC1	1.89	0.54
1:A:373:GLN:HA	1:A:384:LYS:HG3	1.88	0.54
1:C:86:GLU:OE2	1:C:378:ARG:NH2	2.25	0.54
1:C:88:LEU:HD11	1:C:390:LEU:HD13	1.89	0.54
1:E:435:ILE:HG12	1:E:436:CYS:N	2.22	0.54
1:A:197:LYS:HE2	1:A:240:GLU:OE1	2.07	0.54
1:A:381:ILE:CG2	1:B:239:GLN:CG	2.61	0.53
1:D:92:ALA:O	1:D:96:SER:HB3	2.09	0.53
1:E:253:ARG:NH1	1:E:253:ARG:CG	2.37	0.53
1:F:150:ALA:HB1	1:F:452:THR:HG21	1.90	0.53
1:E:92:ALA:O	1:E:96:SER:HB3	2.08	0.53
1:E:114:ILE:HG13	1:E:294:SER:HB3	1.89	0.53
1:E:404:LYS:HA	1:E:404:LYS:HE3	1.90	0.53
1:C:164:LEU:HD21	1:C:462:PRO:HD3	1.91	0.53
1:D:40:LEU:HD23	4:D:607:CM5:C10	2.38	0.53
1:C:473:GLN:C	1:C:474:GLU:HG2	2.26	0.53
1:C:473:GLN:O	1:C:474:GLU:CG	2.54	0.53
1:A:429:PHE:CD1	1:A:439:GLU:HB2	2.44	0.53
1:B:202:PHE:CE2	1:B:241:ILE:HD13	2.43	0.53
1:C:472:PRO:HG3	1:C:479:LYS:HE3	1.91	0.53
2:F:500:HEM:HMB1	2:F:500:HEM:CBB	2.36	0.53
1:F:168:THR:OG1	1:F:308:ARG:HD3	2.07	0.53
1:A:133:ARG:O	1:A:136:GLY:CA	2.56	0.53
1:C:92:ALA:O	1:C:96:SER:HB3	2.09	0.53
1:E:332:ILE:HA	1:E:336:ARG:NH2	2.23	0.52
1:C:140:ARG:NH1	1:C:145:ARG:CG	2.72	0.52
1:F:275:GLU:C	1:F:277:SER:H	2.12	0.52
1:E:472:PRO:HG3	1:E:479:LYS:HE3	1.91	0.52
1:E:88:LEU:HD11	1:E:390:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:HG21	1:A:74:PRO:HB3	1.91	0.52
1:B:126:ARG:HD2	5:B:515:HOH:O	2.08	0.52
1:A:37:LEU:HD12	5:A:508:HOH:O	2.08	0.52
1:A:434:ARG:O	1:A:435:ILE:C	2.47	0.52
1:D:311:PHE:HE1	1:D:459:MET:HE1	1.75	0.52
1:D:332:ILE:HA	1:D:336:ARG:NH2	2.25	0.52
1:C:158:ARG:C	1:C:160:SER:H	2.12	0.52
1:E:116:ALA:O	1:E:434:ARG:NH2	2.30	0.51
1:D:133:ARG:O	1:D:134:ASP:C	2.47	0.51
1:C:434:ARG:O	1:C:435:ILE:C	2.46	0.51
1:D:120:ARG:HA	1:D:282:GLU:HG3	1.91	0.51
1:F:257:ASP:O	1:F:260:ALA:N	2.36	0.51
1:E:463:VAL:HG12	1:E:464:ALA:N	2.25	0.51
1:A:381:ILE:CG2	1:B:239:GLN:HG3	2.37	0.51
1:E:437:LEU:HD23	1:E:438:GLY:N	2.26	0.51
2:D:500:HEM:HBB2	2:D:500:HEM:HMB2	1.91	0.51
1:F:437:LEU:HD21	2:F:500:HEM:HMD2	1.87	0.51
1:F:73:ARG:CD	1:F:387:GLU:OE1	2.58	0.51
1:E:51:LEU:HG	1:E:215:GLN:HB3	1.92	0.51
1:E:326:ARG:O	1:E:330:GLN:CG	2.55	0.51
1:B:318:PRO:O	1:B:322:GLU:HG2	2.11	0.51
1:F:437:LEU:C	1:F:437:LEU:HD12	2.31	0.51
1:B:70:LEU:HB3	1:B:219:LEU:HD12	1.93	0.51
1:D:220:PHE:CE1	4:D:607:CM5:H112	2.46	0.50
1:F:180:CYS:HA	1:F:184:PHE:HD2	1.77	0.50
1:E:168:THR:OG1	1:E:308:ARG:HD3	2.11	0.50
1:D:472:PRO:HG3	1:D:479:LYS:HE3	1.93	0.50
1:F:299:GLY:CA	2:F:500:HEM:CBC	2.89	0.50
1:C:225:LYS:CG	1:C:225:LYS:O	2.58	0.50
1:C:429:PHE:O	1:C:430:SER:CB	2.59	0.50
1:F:179:ILE:HG12	1:F:299:GLY:HA3	1.93	0.50
1:D:430:SER:CB	2:D:500:HEM:HBA1	2.42	0.50
1:E:457:PHE:HA	1:E:490:PRO:HA	1.93	0.50
1:F:38:PRO:O	1:F:39:LEU:HB2	2.10	0.50
1:C:410:PRO:C	1:C:412:HIS:H	2.13	0.50
1:C:299:GLY:CA	2:C:500:HEM:HBC2	2.40	0.50
1:D:181:SER:O	1:D:185:GLY:HA2	2.11	0.50
1:D:70:LEU:HB3	1:D:219:LEU:HD12	1.93	0.50
1:B:247:HIS:O	1:B:247:HIS:CD2	2.64	0.50
1:C:134:ASP:OD2	1:C:134:ASP:O	2.30	0.50
1:D:125:ARG:NH1	2:D:500:HEM:O1D	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASP:OD2	1:F:49:ARG:NE	2.45	0.50
1:E:202:PHE:CE2	1:E:241:ILE:HD13	2.46	0.50
1:C:286:GLN:HG3	1:E:384:LYS:HD2	1.93	0.50
1:E:125:ARG:NH1	1:E:435:ILE:O	2.43	0.50
1:E:131:THR:HB	1:E:264:LEU:HD12	1.93	0.50
1:E:227:PHE:HA	4:E:605:CM5:O22	2.12	0.49
1:E:472:PRO:CG	1:E:479:LYS:HE3	2.42	0.49
2:A:500:HEM:CHD	2:A:500:HEM:HBC2	2.25	0.49
1:C:40:LEU:O	1:C:41:GLY:C	2.50	0.49
1:B:169:PHE:CD1	1:B:196:LEU:HG	2.47	0.49
1:D:150:ALA:O	1:D:154:ILE:HG12	2.12	0.49
1:B:268:TYR:CG	1:B:288:LEU:HD13	2.47	0.49
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.94	0.49
1:B:169:PHE:CD1	1:B:199:LEU:HD12	2.48	0.49
1:D:185:GLY:O	1:D:186:LYS:HB3	2.12	0.49
1:D:88:LEU:HD21	1:D:390:LEU:CD1	2.42	0.49
1:C:287:ASN:O	1:C:291:ASN:CB	2.61	0.49
1:C:268:TYR:CE1	1:C:288:LEU:HB2	2.48	0.49
1:F:120:ARG:HA	1:F:282:GLU:HG3	1.95	0.49
1:D:469:ASP:HB3	5:D:527:HOH:O	2.13	0.49
1:A:373:GLN:CA	1:A:384:LYS:HG3	2.42	0.49
1:C:150:ALA:O	1:C:154:ILE:HG12	2.12	0.49
1:F:149:GLU:OE2	1:F:177:ASN:ND2	2.45	0.49
1:F:310:GLY:O	1:F:313:LEU:HB2	2.13	0.49
1:D:268:TYR:CE1	1:D:288:LEU:HB2	2.48	0.49
1:D:429:PHE:O	1:D:430:SER:HB3	2.13	0.49
2:F:500:HEM:HBD1	2:F:500:HEM:HHA	1.94	0.48
1:A:384:LYS:HD2	1:B:286:GLN:HG3	1.95	0.48
1:C:133:ARG:CG	1:C:134:ASP:N	2.76	0.48
1:B:150:ALA:O	1:B:154:ILE:HG12	2.14	0.48
1:C:436:CYS:HB2	2:C:500:HEM:C4A	2.48	0.48
1:F:486:ILE:C	5:F:497:HOH:O	2.52	0.48
1:A:318:PRO:O	1:A:322:GLU:HG2	2.13	0.48
1:F:150:ALA:O	1:F:154:ILE:HG12	2.12	0.48
1:B:47:ASP:OD1	1:B:48:ARG:N	2.46	0.48
1:C:189:HIS:CD2	1:C:191:GLN:OE1	2.66	0.48
1:B:297:PHE:C	1:B:297:PHE:HD2	2.17	0.48
1:C:153:LEU:HD21	1:C:453:ILE:HD11	1.95	0.48
1:F:114:ILE:HG13	1:F:294:SER:HB3	1.95	0.48
4:D:604:CM5:O32	4:D:604:CM5:O31	2.19	0.48
1:B:430:SER:HB2	2:B:500:HEM:HBA1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:LEU:O	1:F:472:PRO:HD3	2.14	0.48
1:D:88:LEU:HD11	1:D:390:LEU:HD12	1.94	0.48
1:A:309:TYR:OH	1:A:472:PRO:HG3	2.13	0.48
1:D:472:PRO:CG	1:D:479:LYS:HE3	2.44	0.48
1:D:309:TYR:OH	1:D:472:PRO:HG3	2.14	0.48
1:B:120:ARG:HA	1:B:282:GLU:HG3	1.96	0.47
1:E:38:PRO:O	1:E:39:LEU:HB2	2.14	0.47
1:B:297:PHE:C	1:B:297:PHE:CD2	2.87	0.47
1:E:226:HIS:C	1:E:227:PHE:CG	2.88	0.47
1:E:435:ILE:CG1	1:E:436:CYS:H	2.27	0.47
1:E:458:SER:O	1:E:489:LEU:N	2.38	0.47
1:F:332:ILE:HA	1:F:336:ARG:NH2	2.29	0.47
1:F:443:ARG:HB3	5:F:508:HOH:O	2.14	0.47
1:F:436:CYS:HB2	2:F:500:HEM:NA	2.29	0.47
1:A:150:ALA:O	1:A:154:ILE:HG12	2.14	0.47
1:A:111:TYR:HB2	1:A:290:LEU:HD12	1.95	0.47
1:E:219:LEU:N	1:E:219:LEU:CD1	2.78	0.47
1:D:40:LEU:HD22	4:D:607:CM5:H102	1.95	0.47
1:D:163:ALA:HA	1:D:487:ARG:NH1	2.28	0.47
1:B:268:TYR:CE1	1:B:288:LEU:HB2	2.50	0.47
1:A:431:LEU:HA	1:A:435:ILE:HD12	1.96	0.47
2:A:500:HEM:CBC	2:A:500:HEM:HHD	2.33	0.47
2:E:500:HEM:HHD	2:E:500:HEM:CBC	2.35	0.47
1:F:88:LEU:CD1	1:F:390:LEU:CD1	2.90	0.47
1:B:365:MET:N	5:B:506:HOH:O	2.33	0.47
1:F:257:ASP:HB3	1:F:260:ALA:HB3	1.96	0.47
1:A:169:PHE:CE1	1:A:199:LEU:HD12	2.49	0.47
1:D:153:LEU:HD22	1:D:174:ILE:HD13	1.96	0.47
1:A:134:ASP:OD2	1:A:135:PHE:N	2.48	0.47
1:E:309:TYR:OH	1:E:472:PRO:HG3	2.15	0.47
1:A:434:ARG:NH1	2:A:500:HEM:O2D	2.47	0.47
1:E:462:PRO:HB2	5:E:520:HOH:O	2.15	0.47
1:E:435:ILE:CG1	1:E:436:CYS:N	2.78	0.47
1:E:316:LYS:HD3	1:E:317:TYR:CE1	2.50	0.47
1:E:287:ASN:O	1:E:291:ASN:CB	2.64	0.47
1:F:86:GLU:O	1:F:90:ASP:HB2	2.14	0.47
1:A:268:TYR:CE1	1:A:288:LEU:HB2	2.50	0.46
1:F:200:ASN:O	1:F:204:GLN:HG2	2.15	0.46
1:E:429:PHE:HB2	5:E:511:HOH:O	2.15	0.46
1:D:437:LEU:O	1:D:437:LEU:CD1	2.63	0.46
1:F:287:ASN:O	1:F:291:ASN:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASN:HB3	5:C:508:HOH:O	2.15	0.46
1:F:51:LEU:HG	1:F:215:GLN:HB3	1.97	0.46
1:D:454:LEU:HD21	1:D:459:MET:CE	2.43	0.46
1:B:57:ARG:HB3	1:B:57:ARG:HE	1.37	0.46
1:D:200:ASN:O	1:D:204:GLN:HG2	2.15	0.46
1:D:383:PRO:O	1:D:384:LYS:C	2.54	0.46
1:C:158:ARG:C	1:C:160:SER:N	2.69	0.46
1:F:183:VAL:HG12	1:F:184:PHE:N	2.28	0.46
1:A:429:PHE:CE1	1:A:439:GLU:HA	2.50	0.46
1:B:314:MET:O	5:B:513:HOH:O	2.21	0.46
1:D:40:LEU:HD21	4:D:607:CM5:C10	2.45	0.46
2:D:500:HEM:HMB2	2:D:500:HEM:CBB	2.46	0.46
1:E:200:ASN:O	1:E:204:GLN:HG2	2.15	0.46
1:A:208:LEU:O	1:A:211:SER:OG	2.25	0.46
1:E:111:TYR:HB2	1:E:290:LEU:HD12	1.98	0.46
1:C:286:GLN:HG2	1:E:373:GLN:CB	2.45	0.46
1:C:437:LEU:HD21	2:C:500:HEM:CMD	2.44	0.46
1:B:150:ALA:HB1	1:B:452:THR:HG21	1.97	0.46
1:B:299:GLY:HA2	2:B:500:HEM:HMC3	1.97	0.45
1:F:212:VAL:O	1:F:213:PHE:C	2.50	0.45
1:A:128:SER:O	1:A:132:MET:HG3	2.16	0.45
1:F:309:TYR:OH	1:F:472:PRO:HG3	2.16	0.45
1:C:316:LYS:HD2	1:C:468:ILE:HB	1.98	0.45
1:E:436:CYS:CB	2:E:500:HEM:NA	2.69	0.45
1:D:39:LEU:N	5:D:509:HOH:O	2.49	0.45
1:E:226:HIS:O	1:E:227:PHE:CD1	2.70	0.45
1:E:169:PHE:CZ	1:E:190:TYR:O	2.68	0.45
1:B:73:ARG:HD2	1:B:387:GLU:OE1	2.17	0.45
1:D:131:THR:HB	1:D:264:LEU:HD12	1.99	0.45
1:E:437:LEU:O	1:E:437:LEU:HG	2.17	0.45
1:F:318:PRO:O	1:F:322:GLU:HG2	2.16	0.45
1:E:105:ASP:O	1:E:109:ARG:HG2	2.17	0.45
1:A:287:ASN:O	1:A:291:ASN:CB	2.65	0.45
4:D:604:CM5:C30	4:D:604:CM5:O21	2.65	0.45
1:F:443:ARG:C	5:F:508:HOH:O	2.55	0.45
4:B:608:CM5:H18	4:B:608:CM5:H192	1.98	0.45
1:A:135:PHE:O	1:A:145:ARG:NH1	2.49	0.45
1:D:164:LEU:H	1:D:487:ARG:NH1	2.15	0.45
1:F:182:ILE:CG2	1:F:182:ILE:O	2.64	0.45
1:F:275:GLU:C	1:F:277:SER:N	2.71	0.45
1:E:308:ARG:NH1	1:E:481:PRO:HG2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HD1	4:B:608:CM5:H22A	1.82	0.44
1:F:299:GLY:HA2	2:F:500:HEM:CMC	2.46	0.44
1:E:458:SER:CB	1:E:489:LEU:O	2.64	0.44
1:B:253:ARG:HH11	1:B:253:ARG:HG3	1.81	0.44
1:D:436:CYS:HB2	2:D:500:HEM:C1A	2.52	0.44
1:C:189:HIS:O	1:C:191:GLN:N	2.51	0.44
1:E:153:LEU:HD21	1:E:453:ILE:HD11	2.00	0.44
1:B:51:LEU:HG	1:B:215:GLN:HB3	1.98	0.44
1:E:268:TYR:CG	1:E:288:LEU:HD13	2.53	0.44
1:E:219:LEU:N	1:E:219:LEU:HD12	2.32	0.44
1:A:200:ASN:O	1:A:204:GLN:HG2	2.18	0.44
1:D:164:LEU:N	1:D:487:ARG:HG2	2.32	0.44
1:F:257:ASP:HA	1:F:258:PRO:HD2	1.86	0.44
1:C:221:SER:O	1:C:225:LYS:HB3	2.17	0.44
1:D:196:LEU:O	1:D:197:LYS:C	2.54	0.44
1:B:88:LEU:HD11	1:B:390:LEU:HD13	1.99	0.44
1:A:332:ILE:HA	1:A:336:ARG:NH2	2.33	0.44
1:F:47:ASP:OD2	1:F:49:ARG:HB2	2.18	0.44
1:E:201:LEU:HA	1:E:201:LEU:HD23	1.69	0.44
1:D:29:LYS:HB3	1:D:30:LEU:H	1.58	0.44
1:A:426:PHE:CZ	1:A:428:PRO:HG3	2.53	0.44
1:E:227:PHE:CZ	4:E:605:CM5:H52	2.53	0.44
1:C:436:CYS:C	1:C:438:GLY:H	2.21	0.44
1:C:98:ARG:HD3	1:C:368:PRO:O	2.18	0.44
1:B:127:PHE:O	1:B:131:THR:HG22	2.17	0.44
1:E:157:LEU:CD2	1:E:488:PHE:CE2	3.01	0.44
1:B:365:MET:CA	5:B:506:HOH:O	2.65	0.44
1:B:223:PHE:HD2	4:B:602:CM5:H92	1.83	0.43
1:B:437:LEU:HD13	2:B:500:HEM:HMD1	1.99	0.43
1:E:436:CYS:HA	2:E:500:HEM:CHA	2.48	0.43
1:A:132:MET:HE2	1:A:132:MET:HB3	1.72	0.43
1:E:181:SER:HA	1:E:186:LYS:H	1.83	0.43
1:F:231:HIS:H	1:F:231:HIS:CD2	2.36	0.43
1:F:437:LEU:HG	2:F:500:HEM:C2D	2.52	0.43
2:D:500:HEM:CMB	2:D:500:HEM:CBB	2.97	0.43
1:D:436:CYS:HB2	2:D:500:HEM:C4A	2.53	0.43
1:D:39:LEU:HD22	4:F:606:CM5:H111	1.93	0.43
1:B:169:PHE:CE1	1:B:196:LEU:CD1	3.01	0.43
1:A:51:LEU:HG	1:A:215:GLN:HB3	2.00	0.43
1:A:309:TYR:CG	1:A:481:PRO:HB3	2.53	0.43
1:C:285:HIS:CE1	1:E:93:GLU:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:PHE:CZ	1:E:428:PRO:HG3	2.54	0.43
1:B:53:LYS:HA	1:B:53:LYS:HD3	1.81	0.43
1:B:441:ILE:HD11	5:B:503:HOH:O	2.18	0.43
1:C:287:ASN:O	1:C:291:ASN:HB2	2.19	0.43
1:C:168:THR:OG1	1:C:308:ARG:HD3	2.18	0.43
1:A:153:LEU:HD21	1:A:453:ILE:HD11	2.00	0.43
2:E:500:HEM:C1A	3:E:501:3QU:HAC	2.54	0.43
1:F:178:ILE:O	1:F:181:SER:OG	2.36	0.43
1:A:446:LEU:HD23	1:A:446:LEU:HA	1.87	0.43
1:C:457:PHE:HA	1:C:489:LEU:O	2.18	0.43
1:C:253:ARG:HG2	1:C:253:ARG:NH1	2.33	0.43
1:E:460:ALA:O	1:E:487:ARG:HB2	2.19	0.43
1:D:98:ARG:HD3	1:D:368:PRO:O	2.19	0.43
1:F:98:ARG:HG3	1:F:99:GLY:O	2.19	0.43
1:E:437:LEU:O	1:E:437:LEU:CG	2.66	0.43
1:F:119:ASN:O	1:F:120:ARG:C	2.56	0.43
1:E:296:PHE:O	1:E:296:PHE:CD1	2.72	0.43
1:F:276:LYS:O	1:F:276:LYS:HG3	2.18	0.43
1:E:226:HIS:C	1:E:227:PHE:CD2	2.93	0.43
1:A:67:THR:CG2	1:A:74:PRO:HB3	2.47	0.43
1:B:127:PHE:HE1	1:B:264:LEU:HD21	1.83	0.43
1:C:454:LEU:HD21	1:C:459:MET:HE1	2.01	0.43
1:F:202:PHE:CE2	1:F:241:ILE:HD13	2.53	0.43
1:B:226:HIS:CE1	4:B:602:CM5:H101	2.53	0.42
4:D:604:CM5:O20	4:D:604:CM5:O23	2.24	0.42
1:D:202:PHE:CE2	1:D:241:ILE:HD13	2.54	0.42
1:D:39:LEU:CA	5:D:509:HOH:O	2.57	0.42
1:E:463:VAL:CG1	1:E:464:ALA:N	2.82	0.42
1:B:73:ARG:NE	1:B:387:GLU:OE1	2.51	0.42
1:B:297:PHE:O	1:B:297:PHE:HD2	2.02	0.42
1:F:455:GLN:HB3	1:F:456:ASN:HD22	1.85	0.42
1:F:88:LEU:HG	1:F:390:LEU:HD13	2.01	0.42
1:A:132:MET:SD	1:A:295:LEU:HD22	2.59	0.42
1:E:225:LYS:HE2	1:E:226:HIS:NE2	2.32	0.42
1:E:324:VAL:HG11	1:E:454:LEU:HD12	2.01	0.42
1:C:127:PHE:CZ	1:C:131:THR:HG21	2.55	0.42
1:F:309:TYR:CE2	1:F:481:PRO:HB3	2.55	0.42
1:A:57:ARG:O	1:A:58:PHE:C	2.56	0.42
1:E:142:VAL:HG21	5:E:517:HOH:O	2.19	0.42
1:D:247:HIS:C	1:D:247:HIS:CD2	2.92	0.42
1:D:437:LEU:CD1	1:D:437:LEU:C	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:CG	1:A:288:LEU:HD13	2.55	0.42
1:D:98:ARG:NH1	1:D:367:VAL:HG12	2.34	0.42
1:F:474:GLU:HA	1:F:474:GLU:OE1	2.19	0.42
1:C:157:LEU:HD22	1:C:488:PHE:CD2	2.55	0.42
1:E:365:MET:HG2	1:E:391:ILE:HD12	2.02	0.42
1:A:429:PHE:CG	1:A:439:GLU:HB2	2.55	0.42
1:E:179:ILE:HG21	1:E:296:PHE:HA	2.02	0.42
1:C:297:PHE:C	1:C:297:PHE:CD2	2.93	0.42
1:D:429:PHE:O	1:D:430:SER:CB	2.68	0.42
1:A:308:ARG:HH12	1:A:481:PRO:HD2	1.85	0.42
1:C:268:TYR:CG	1:C:288:LEU:HD13	2.54	0.42
1:C:337:PRO:O	1:C:338:PRO:C	2.57	0.42
1:C:114:ILE:HG13	1:C:294:SER:HB3	2.02	0.42
1:B:220:PHE:CD1	4:B:608:CM5:H22A	2.54	0.42
1:F:268:TYR:CE1	1:F:288:LEU:HB2	2.54	0.42
1:C:410:PRO:C	1:C:412:HIS:N	2.73	0.42
1:A:181:SER:O	1:A:185:GLY:HA2	2.20	0.42
1:D:169:PHE:O	1:D:172:GLN:HB2	2.19	0.42
1:D:51:LEU:HG	1:D:215:GLN:HB3	2.02	0.42
1:B:126:ARG:NE	5:B:515:HOH:O	2.53	0.42
1:A:120:ARG:HA	1:A:282:GLU:HG3	2.02	0.42
1:A:193:GLN:H	1:A:193:GLN:HG3	1.65	0.42
2:A:500:HEM:HBA1	2:A:500:HEM:CMA	2.45	0.41
1:A:125:ARG:NH1	2:A:500:HEM:O1D	2.53	0.41
1:A:373:GLN:HA	1:B:286:GLN:HG2	2.02	0.41
1:B:153:LEU:HD21	1:B:453:ILE:HD11	2.02	0.41
1:D:159:LYS:O	1:D:161:LYS:HG3	2.19	0.41
1:C:185:GLY:O	1:C:186:LYS:HB3	2.20	0.41
1:F:436:CYS:C	1:F:438:GLY:H	2.23	0.41
1:C:131:THR:CB	1:C:264:LEU:HD12	2.48	0.41
1:D:216:LEU:HA	1:D:216:LEU:HD12	1.89	0.41
1:F:297:PHE:CD2	1:F:297:PHE:C	2.93	0.41
1:D:239:GLN:OE1	1:D:239:GLN:HA	2.20	0.41
1:A:157:LEU:HD22	1:A:488:PHE:CD2	2.55	0.41
1:E:435:ILE:HG12	1:E:436:CYS:H	1.83	0.41
1:B:434:ARG:HB2	5:B:505:HOH:O	2.20	0.41
1:C:269:LEU:O	1:C:272:MET:HB3	2.21	0.41
1:C:187:ARG:HG3	1:C:188:PHE:N	2.35	0.41
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.91	0.41
1:E:369:HIS:HE2	2:E:500:HEM:CGA	2.33	0.41
1:E:436:CYS:HB2	2:E:500:HEM:C4A	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:THR:HA	1:C:472:PRO:HD3	1.94	0.41
1:B:455:GLN:HB3	1:B:456:ASN:HD22	1.85	0.41
1:E:362:LEU:C	1:E:363:LEU:HD23	2.34	0.41
1:E:226:HIS:O	1:E:227:PHE:CD2	2.73	0.41
1:D:179:ILE:CG2	1:D:180:CYS:N	2.82	0.41
1:E:458:SER:N	1:E:489:LEU:O	2.53	0.41
1:A:181:SER:HA	1:A:186:LYS:O	2.21	0.41
1:F:196:LEU:O	1:F:197:LYS:C	2.58	0.41
1:B:157:LEU:HD22	1:B:488:PHE:CD2	2.55	0.41
1:E:448:LEU:HA	1:E:448:LEU:HD23	1.90	0.41
1:F:188:PHE:HZ	1:F:244:TYR:HH	1.67	0.41
1:C:377:PHE:O	1:C:379:GLY:N	2.52	0.41
1:B:47:ASP:C	1:B:47:ASP:OD1	2.59	0.41
1:F:309:TYR:CD2	1:F:481:PRO:HB3	2.55	0.41
1:C:226:HIS:CG	4:C:603:CM5:H71	2.55	0.41
1:E:105:ASP:N	1:E:106:PRO:CD	2.84	0.41
1:C:99:GLY:HA3	1:C:368:PRO:HB2	2.02	0.41
1:B:426:PHE:CZ	1:B:428:PRO:HG3	2.56	0.41
1:E:336:ARG:HA	1:E:337:PRO:HD2	1.93	0.41
1:E:88:LEU:HD11	1:E:390:LEU:HD12	2.02	0.41
1:F:194:GLU:O	1:F:198:MET:HG2	2.21	0.41
4:B:608:CM5:O22	4:B:608:CM5:C30	2.67	0.41
4:D:604:CM5:H301	4:D:604:CM5:O21	2.21	0.41
1:D:247:HIS:CD2	1:D:247:HIS:O	2.74	0.41
1:D:160:SER:O	1:D:161:LYS:C	2.58	0.41
1:F:77:MET:SD	1:F:389:PHE:HB2	2.61	0.41
1:D:221:SER:O	1:D:225:LYS:HB3	2.21	0.41
1:B:201:LEU:HA	1:B:201:LEU:HD23	1.88	0.41
1:D:455:GLN:O	1:D:491:ARG:HD2	2.21	0.41
1:F:426:PHE:CZ	1:F:428:PRO:HG3	2.56	0.41
1:D:336:ARG:HA	1:D:337:PRO:HD2	1.85	0.41
1:F:126:ARG:O	1:F:127:PHE:C	2.58	0.41
1:A:88:LEU:HD21	1:A:390:LEU:CD1	2.40	0.40
1:A:332:ILE:HG23	1:A:336:ARG:NH1	2.36	0.40
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.85	0.40
1:A:351:ALA:HB1	1:A:413:PHE:HB2	2.02	0.40
1:A:29:LYS:O	1:A:30:LEU:C	2.59	0.40
1:D:105:ASP:N	1:D:106:PRO:CD	2.84	0.40
1:C:286:GLN:HG2	1:E:373:GLN:HA	2.03	0.40
1:E:190:TYR:HB2	5:E:518:HOH:O	2.21	0.40
1:C:181:SER:HA	1:C:186:LYS:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:TYR:HB2	1:D:290:LEU:HD12	2.03	0.40
1:D:242:ASN:HB3	5:D:523:HOH:O	2.20	0.40
1:F:334:PRO:C	1:F:335:HIS:HD1	2.25	0.40
1:D:377:PHE:O	1:D:378:ARG:C	2.60	0.40
1:D:179:ILE:HG22	1:D:180:CYS:N	2.36	0.40
1:D:263:ASP:OD1	1:D:263:ASP:C	2.59	0.40
1:A:81:VAL:O	1:A:82:GLU:C	2.60	0.40
1:B:226:HIS:ND1	4:B:602:CM5:H101	2.36	0.40
2:A:500:HEM:CMB	2:A:500:HEM:HBB2	2.51	0.40
1:A:308:ARG:NH1	1:A:481:PRO:HD2	2.37	0.40
1:B:316:LYS:HG2	1:B:317:TYR:CZ	2.56	0.40
1:A:472:PRO:HG3	1:A:479:LYS:HE3	2.04	0.40
1:B:131:THR:HG23	1:B:264:LEU:CD1	2.52	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	458/476 (96%)	436 (95%)	18 (4%)	4 (1%)	21	55
1	B	455/476 (96%)	431 (95%)	21 (5%)	3 (1%)	26	62
1	C	456/476 (96%)	424 (93%)	30 (7%)	2 (0%)	39	74
1	D	454/476 (95%)	424 (93%)	28 (6%)	2 (0%)	39	74
1	E	455/476 (96%)	433 (95%)	22 (5%)	0	100	100
1	F	449/476 (94%)	417 (93%)	29 (6%)	3 (1%)	26	62
All	All	2727/2856 (96%)	2565 (94%)	148 (5%)	14 (0%)	34	69

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	430	SER
1	F	276	LYS
1	F	378	ARG
1	B	430	SER
1	C	190	TYR
1	F	424	GLU
1	A	92	ALA
1	D	430	SER
1	B	334	PRO
1	B	74	PRO
1	A	72	PRO
1	A	435	ILE
1	D	490	PRO
1	A	41	GLY

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	404/418 (97%)	392 (97%)	12 (3%)	48 82
1	B	403/418 (96%)	391 (97%)	12 (3%)	48 82
1	C	402/418 (96%)	393 (98%)	9 (2%)	60 89
1	D	400/418 (96%)	394 (98%)	6 (2%)	72 93
1	E	404/418 (97%)	390 (96%)	14 (4%)	43 77
1	F	396/418 (95%)	387 (98%)	9 (2%)	58 88
All	All	2409/2508 (96%)	2347 (97%)	62 (3%)	54 86

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	40	LEU
1	A	57	ARG
1	A	132	MET
1	A	133	ARG

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Mol	Chain	Res	Type
1	A	134	ASP
1	A	187	ARG
1	A	196	LEU
1	A	259	SER
1	A	297	PHE
1	A	309	TYR
1	A	437	LEU
1	B	48	ARG
1	B	57	ARG
1	B	109	ARG
1	B	186	LYS
1	B	187	ARG
1	B	196	LEU
1	B	200	ASN
1	B	247	HIS
1	B	297	PHE
1	B	309	TYR
1	B	437	LEU
1	B	489	LEU
1	C	133	ARG
1	C	134	ASP
1	C	139	LYS
1	C	160	SER
1	C	187	ARG
1	C	225	LYS
1	C	297	PHE
1	C	309	TYR
1	C	404	LYS
1	D	141	SER
1	D	189	HIS
1	D	194	GLU
1	D	196	LEU
1	D	297	PHE
1	D	309	TYR
1	E	29	LYS
1	E	186	LYS
1	E	187	ARG
1	E	253	ARG
1	E	276	LYS
1	E	277	SER
1	E	295	LEU
1	E	297	PHE

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Mol	Chain	Res	Type
1	E	309	TYR
1	E	329	GLU
1	E	378	ARG
1	E	404	LYS
1	E	437	LEU
1	E	489	LEU
1	F	48	ARG
1	F	145	ARG
1	F	151	GLN
1	F	182	ILE
1	F	186	LYS
1	F	259	SER
1	F	297	PHE
1	F	309	TYR
1	F	335	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	GLN
1	B	455	GLN
1	B	456	ASN
1	C	231	HIS
1	C	285	HIS
1	E	226	HIS
1	E	286	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

19 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	500	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.30	9 (37%)
3	3QU	A	501	2	7,7,17	0.25	0	8,8,22	1.22	0
4	CM5	A	601	-	36,36,36	4.16	16 (44%)	49,49,49	5.57	27 (55%)
2	HEM	B	500	1,3	30,50,50	1.76	8 (26%)	24,82,82	2.93	13 (54%)
3	3QU	B	501	2	15,17,17	0.43	0	20,22,22	1.73	5 (25%)
4	CM5	B	602	-	36,36,36	2.83	9 (25%)	49,49,49	5.06	24 (48%)
4	CM5	B	608	-	36,36,36	3.17	14 (38%)	49,49,49	5.96	26 (53%)
2	HEM	C	500	1,3	30,50,50	3.54	14 (46%)	24,82,82	2.71	9 (37%)
3	3QU	C	501	2	7,7,17	0.26	0	8,8,22	1.21	0
4	CM5	C	603	-	36,36,36	3.38	13 (36%)	49,49,49	5.39	23 (46%)
2	HEM	D	500	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
3	3QU	D	501	2	14,14,17	0.33	0	17,17,22	0.86	0
4	CM5	D	604	-	36,36,36	4.09	16 (44%)	49,49,49	6.37	25 (51%)
4	CM5	D	607	-	36,36,36	3.52	13 (36%)	49,49,49	5.06	26 (53%)
2	HEM	E	500	1,3	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
3	3QU	E	501	2	14,14,17	0.79	0	17,17,22	0.90	1 (5%)
4	CM5	E	605	-	36,36,36	3.49	14 (38%)	49,49,49	3.19	22 (44%)
2	HEM	F	500	1	30,50,50	2.21	8 (26%)	24,82,82	2.31	9 (37%)
4	CM5	F	606	-	36,36,36	3.00	13 (36%)	49,49,49	4.70	25 (51%)

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	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	A	501	2	-	0/0/0/8	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CM5	A	601	-	-	0/17/65/65	0/3/3/3
2	HEM	B	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	B	501	2	-	0/8/8/8	0/2/2/2
4	CM5	B	602	-	-	0/17/65/65	0/3/3/3
4	CM5	B	608	-	-	0/17/65/65	0/3/3/3
2	HEM	C	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	C	501	2	-	0/0/0/8	0/1/1/2
4	CM5	C	603	-	-	0/17/65/65	0/3/3/3
2	HEM	D	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	D	501	2	-	0/4/4/8	0/2/2/2
4	CM5	D	604	-	1/1/11/11	0/17/65/65	0/3/3/3
4	CM5	D	607	-	-	0/17/65/65	0/3/3/3
2	HEM	E	500	1,3	-	0/10/54/54	0/0/8/8
3	3QU	E	501	2	-	0/4/4/8	0/2/2/2
4	CM5	E	605	-	-	0/17/65/65	0/3/3/3
2	HEM	F	500	1	-	0/10/54/54	0/0/8/8
4	CM5	F	606	-	-	0/17/65/65	0/3/3/3

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	CM5	O23-C24	-13.84	1.04	1.41
4	A	601	CM5	O21-C17	-13.35	1.11	1.43
2	C	500	HEM	C3B-C4B	-12.54	1.40	1.51
4	E	605	CM5	O23-C24	-11.46	1.10	1.41
4	D	604	CM5	C29-C28	-10.94	1.23	1.52
4	D	604	CM5	O25-C26	-10.50	1.18	1.44
4	F	606	CM5	C28-C27	-10.46	1.24	1.52
4	B	602	CM5	O25-C26	-9.48	1.20	1.44
4	A	601	CM5	C27-C26	-9.39	1.33	1.53
4	A	601	CM5	C28-C27	-9.19	1.28	1.52
4	D	607	CM5	C30-C26	-8.66	1.21	1.51
4	E	605	CM5	O33-C28	-8.27	1.23	1.43
4	D	604	CM5	C28-C27	-8.02	1.31	1.52
4	F	606	CM5	C17-C18	-7.93	1.31	1.52
4	A	601	CM5	C16-C15	-7.50	1.32	1.52
2	A	500	HEM	C3B-C4B	-7.32	1.45	1.51
2	F	500	HEM	C3B-C4B	-7.31	1.45	1.51
2	E	500	HEM	C3B-C4B	-7.27	1.45	1.51
2	D	500	HEM	C3B-C4B	-7.26	1.45	1.51
4	E	605	CM5	O14-C13	-7.16	1.23	1.41
2	C	500	HEM	C3D-C4D	-6.94	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	FE-NC	-6.89	1.68	1.95
4	D	607	CM5	O34-C29	-6.24	1.28	1.43
4	F	606	CM5	O32-C27	-6.12	1.28	1.43
4	D	604	CM5	C16-C15	-6.11	1.36	1.52
4	B	602	CM5	C27-C26	-6.02	1.40	1.53
4	D	604	CM5	C17-C18	-5.81	1.37	1.52
4	D	607	CM5	C28-C27	-5.78	1.37	1.52
2	C	500	HEM	C2C-C1C	-5.77	1.41	1.52
4	C	603	CM5	C30-C26	-5.57	1.32	1.51
4	A	601	CM5	O23-C16	-5.36	1.30	1.43
4	B	608	CM5	C13-C18	-5.33	1.36	1.52
4	A	601	CM5	C17-C18	-5.30	1.38	1.52
4	B	608	CM5	C30-C26	-5.09	1.33	1.51
2	E	500	HEM	C3D-C4D	-5.08	1.45	1.51
2	F	500	HEM	C3D-C4D	-5.08	1.45	1.51
2	D	500	HEM	C3D-C4D	-5.05	1.45	1.51
2	A	500	HEM	C3D-C4D	-5.04	1.45	1.51
4	D	604	CM5	C19-C15	-4.99	1.34	1.51
4	E	605	CM5	O12-C13	-4.84	1.31	1.40
4	E	605	CM5	C28-C27	-4.58	1.40	1.52
4	A	601	CM5	O25-C24	-4.53	1.30	1.41
2	B	500	HEM	C3B-C4B	-4.46	1.47	1.51
4	A	601	CM5	O23-C24	-4.20	1.30	1.41
4	F	606	CM5	O25-C24	-4.19	1.31	1.41
2	C	500	HEM	FE-NB	-4.06	1.76	1.97
4	E	605	CM5	C17-C18	-3.98	1.41	1.52
4	A	601	CM5	O14-C15	-3.89	1.34	1.44
2	B	500	HEM	C3D-C4D	-3.88	1.46	1.51
2	F	500	HEM	C2C-C1C	-3.81	1.45	1.52
2	A	500	HEM	C2C-C1C	-3.81	1.45	1.52
2	D	500	HEM	C2C-C1C	-3.79	1.45	1.52
2	E	500	HEM	C2C-C1C	-3.78	1.45	1.52
2	C	500	HEM	C2D-C1D	-3.65	1.39	1.51
4	C	603	CM5	C16-C15	-3.63	1.42	1.52
4	B	608	CM5	C27-C26	-3.60	1.45	1.53
4	B	602	CM5	C29-C28	-3.60	1.42	1.52
4	B	602	CM5	C17-C18	-3.56	1.43	1.52
4	A	601	CM5	C24-C29	-3.49	1.42	1.52
4	B	602	CM5	O34-C29	-3.43	1.34	1.43
4	B	602	CM5	C24-C29	-3.42	1.42	1.52
4	A	601	CM5	C29-C28	-3.20	1.44	1.52
4	D	604	CM5	O14-C15	-3.08	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C2A-C3A	-3.04	1.28	1.37
2	C	500	HEM	C2B-C1B	-2.98	1.42	1.51
2	B	500	HEM	C2D-C1D	-2.79	1.42	1.51
4	A	601	CM5	O14-C13	-2.77	1.34	1.41
4	B	608	CM5	O34-C29	-2.71	1.36	1.43
4	D	604	CM5	O14-C13	-2.69	1.34	1.41
4	D	604	CM5	O25-C24	-2.65	1.35	1.41
2	B	500	HEM	C2C-C1C	-2.62	1.47	1.52
2	C	500	HEM	CHD-C1D	-2.53	1.31	1.38
4	D	604	CM5	C30-C26	-2.47	1.43	1.51
2	C	500	HEM	CHD-C4C	-2.26	1.31	1.36
4	F	606	CM5	C19-C15	-2.24	1.44	1.51
2	C	500	HEM	C4A-CHB	-2.24	1.33	1.39
4	D	607	CM5	C17-C18	-2.22	1.46	1.52
2	C	500	HEM	CHC-C4B	-2.21	1.32	1.38
2	C	500	HEM	C2D-C3D	-2.16	1.48	1.54
2	B	500	HEM	C2B-C1B	-2.09	1.45	1.51
2	C	500	HEM	C1A-CHA	-2.09	1.34	1.39
2	E	500	HEM	C2D-C1D	-2.09	1.45	1.51
2	F	500	HEM	C2D-C1D	-2.06	1.45	1.51
2	D	500	HEM	C2D-C1D	-2.05	1.45	1.51
2	A	500	HEM	C2D-C1D	-2.04	1.45	1.51
4	E	605	CM5	O25-C26	2.02	1.49	1.44
4	F	606	CM5	C13-C18	2.06	1.58	1.52
2	B	500	HEM	FE-ND	2.08	2.08	1.97
2	F	500	HEM	C4C-NC	2.10	1.38	1.36
4	F	606	CM5	O12-C13	2.12	1.44	1.40
4	C	603	CM5	O12-C13	2.12	1.44	1.40
4	B	608	CM5	O22-C18	2.12	1.48	1.43
4	F	606	CM5	O23-C24	2.12	1.47	1.41
2	F	500	HEM	FE-ND	2.13	2.08	1.97
2	A	500	HEM	FE-ND	2.13	2.08	1.97
2	E	500	HEM	FE-ND	2.15	2.08	1.97
2	D	500	HEM	FE-ND	2.15	2.08	1.97
2	A	500	HEM	C1C-NC	2.18	1.38	1.36
2	A	500	HEM	C4C-NC	2.21	1.38	1.36
2	B	500	HEM	CMA-C3A	2.22	1.56	1.51
2	E	500	HEM	C1C-NC	2.22	1.38	1.36
2	D	500	HEM	C4C-NC	2.23	1.38	1.36
4	E	605	CM5	C29-C28	2.23	1.58	1.52
2	B	500	HEM	C3C-CAC	2.24	1.55	1.51
2	E	500	HEM	C4C-NC	2.24	1.38	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	HEM	C1C-NC	2.28	1.38	1.36
4	C	603	CM5	C13-C18	2.28	1.59	1.52
4	A	601	CM5	O22-C18	2.29	1.48	1.43
2	D	500	HEM	C1C-NC	2.32	1.38	1.36
4	F	606	CM5	C16-C15	2.34	1.59	1.52
4	E	605	CM5	O31-C30	2.37	1.52	1.42
4	D	604	CM5	C13-C18	2.42	1.59	1.52
4	C	603	CM5	O25-C24	2.43	1.48	1.41
4	F	606	CM5	O21-C17	2.43	1.48	1.43
4	C	603	CM5	O14-C15	2.44	1.50	1.44
4	D	607	CM5	C16-C15	2.52	1.59	1.52
4	B	608	CM5	C17-C18	2.52	1.59	1.52
4	D	604	CM5	O20-C19	2.55	1.53	1.42
4	A	601	CM5	O34-C29	2.60	1.49	1.43
4	B	608	CM5	O12-C13	2.72	1.45	1.40
2	F	500	HEM	FE-NC	2.80	2.06	1.95
2	A	500	HEM	FE-NC	2.81	2.06	1.95
2	E	500	HEM	FE-NC	2.81	2.06	1.95
4	C	603	CM5	C28-C27	2.82	1.59	1.52
2	D	500	HEM	FE-NC	2.83	2.07	1.95
4	B	608	CM5	C16-C15	2.89	1.60	1.52
4	D	607	CM5	O31-C30	2.96	1.55	1.42
4	E	605	CM5	O21-C17	3.00	1.50	1.43
4	F	606	CM5	O23-C16	3.02	1.51	1.43
4	D	607	CM5	C13-C18	3.06	1.61	1.52
4	C	603	CM5	C17-C18	3.20	1.60	1.52
4	D	607	CM5	C24-C29	3.44	1.62	1.52
4	A	601	CM5	C17-C16	3.55	1.62	1.52
4	C	603	CM5	C17-C16	3.74	1.63	1.52
4	D	607	CM5	C17-C16	3.84	1.63	1.52
4	D	604	CM5	C27-C26	3.87	1.61	1.53
4	E	605	CM5	O32-C27	3.89	1.52	1.43
4	B	608	CM5	C17-C16	4.04	1.63	1.52
4	B	602	CM5	O22-C18	4.04	1.52	1.43
4	B	608	CM5	O25-C24	4.10	1.52	1.41
4	E	605	CM5	O25-C24	4.10	1.52	1.41
4	F	606	CM5	O34-C29	4.42	1.53	1.43
4	F	606	CM5	O14-C13	4.58	1.53	1.41
4	B	602	CM5	O31-C30	4.61	1.62	1.42
4	C	603	CM5	O31-C30	4.84	1.63	1.42
4	E	605	CM5	O22-C18	4.98	1.54	1.43
4	B	608	CM5	O14-C15	5.72	1.58	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	CM5	O32-C27	5.82	1.56	1.43
4	D	604	CM5	O32-C27	5.92	1.57	1.43
4	E	605	CM5	O34-C29	6.32	1.58	1.43
4	C	603	CM5	O21-C17	6.45	1.58	1.43
4	D	607	CM5	O23-C16	6.73	1.60	1.43
4	B	608	CM5	O23-C24	6.89	1.60	1.41
4	D	607	CM5	O23-C24	7.02	1.60	1.41
4	C	603	CM5	O32-C27	7.02	1.59	1.43
4	B	602	CM5	O32-C27	7.18	1.60	1.43
4	D	604	CM5	O23-C24	7.26	1.61	1.41
4	D	604	CM5	O23-C16	7.56	1.62	1.43
4	D	607	CM5	O33-C28	7.93	1.61	1.43
4	B	608	CM5	O21-C17	7.98	1.62	1.43
4	B	608	CM5	O23-C16	8.06	1.64	1.43
4	D	607	CM5	O25-C24	8.40	1.63	1.41

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	606	CM5	O12-C13-C18	-21.08	81.43	108.04
4	C	603	CM5	O33-C28-C27	-18.06	69.67	110.34
4	A	601	CM5	O33-C28-C29	-17.48	70.97	110.34
4	B	608	CM5	O14-C15-C19	-17.00	63.38	106.36
4	B	608	CM5	O14-C13-O12	-16.41	70.54	110.05
4	D	604	CM5	O12-C13-C18	-15.07	89.01	108.04
4	C	603	CM5	O23-C16-C15	-14.57	71.04	109.32
4	B	602	CM5	O12-C13-C18	-14.43	89.82	108.04
4	B	602	CM5	O33-C28-C27	-14.33	78.07	110.34
4	D	604	CM5	O33-C28-C29	-14.31	78.13	110.34
4	D	604	CM5	C30-C26-C27	-13.03	80.87	113.02
4	D	607	CM5	O21-C17-C16	-12.96	79.21	109.87
4	C	603	CM5	C24-O23-C16	-12.82	84.50	118.01
4	C	603	CM5	O32-C27-C26	-12.04	77.33	109.24
4	B	608	CM5	O25-C24-C29	-11.50	86.68	110.28
4	C	603	CM5	O21-C17-C18	-11.49	84.48	110.34
4	B	608	CM5	O23-C16-C17	-11.29	78.02	107.17
4	B	602	CM5	O23-C16-C17	-11.16	78.35	107.17
4	A	601	CM5	O23-C24-C29	-10.75	81.94	108.10
4	F	606	CM5	O22-C18-C13	-10.44	87.13	110.02
4	D	604	CM5	C24-O23-C16	-10.26	91.19	118.01
4	D	607	CM5	O25-C24-C29	-10.18	89.39	110.28
4	B	602	CM5	C17-C16-C15	-9.88	88.49	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	601	CM5	O32-C27-C28	-9.81	88.25	110.34
4	D	607	CM5	C17-C16-C15	-9.43	89.52	110.84
4	A	601	CM5	O34-C29-C28	-9.37	89.25	110.34
4	A	601	CM5	O22-C18-C17	-9.36	89.26	110.34
4	D	607	CM5	O14-C13-C18	-9.33	91.14	110.28
4	D	604	CM5	O14-C13-C18	-9.32	91.16	110.28
4	D	604	CM5	O32-C27-C26	-9.30	84.59	109.24
4	D	607	CM5	O12-C13-C18	-9.07	96.59	108.04
4	B	602	CM5	O22-C18-C13	-9.02	90.24	110.02
4	B	602	CM5	O32-C27-C26	-8.97	85.46	109.24
4	B	608	CM5	C17-C16-C15	-8.91	90.68	110.84
4	E	605	CM5	O32-C27-C26	-8.87	85.73	109.24
4	A	601	CM5	O14-C13-C18	-8.35	93.15	110.28
4	C	603	CM5	O23-C24-O25	-8.30	89.67	110.68
4	A	601	CM5	C18-C17-C16	-8.17	91.65	109.60
4	B	608	CM5	O21-C17-C18	-7.98	92.37	110.34
4	D	607	CM5	O23-C24-C29	-7.98	88.69	108.10
4	C	603	CM5	O32-C27-C28	-7.84	92.69	110.34
4	F	606	CM5	O23-C16-C15	-7.42	89.82	109.32
4	D	607	CM5	C30-C26-C27	-7.40	94.76	113.02
4	D	607	CM5	O23-C16-C17	-7.35	88.19	107.17
4	B	602	CM5	C28-C27-C26	-7.25	97.56	110.20
4	B	608	CM5	O12-C13-C18	-7.24	98.90	108.04
4	B	602	CM5	O14-C13-C18	-7.21	95.48	110.28
4	B	608	CM5	O21-C17-C16	-6.89	93.57	109.87
4	A	601	CM5	O23-C16-C15	-6.78	91.51	109.32
4	B	608	CM5	C19-C15-C16	-6.72	93.69	113.25
4	D	604	CM5	C28-C27-C26	-6.59	98.72	110.20
4	D	607	CM5	O32-C27-C26	-6.49	92.04	109.24
4	A	601	CM5	O32-C27-C26	-6.14	92.96	109.24
4	F	606	CM5	O32-C27-C28	-5.87	97.11	110.34
4	F	606	CM5	O14-C13-C18	-5.83	98.32	110.28
4	A	601	CM5	C13-O14-C15	-5.72	102.64	113.75
4	D	607	CM5	O31-C30-C26	-5.57	92.91	111.33
2	C	500	HEM	C4B-CHC-C1C	-5.56	116.52	125.82
4	B	602	CM5	O32-C27-C28	-5.40	98.19	110.34
4	E	605	CM5	O22-C18-C17	-5.35	98.29	110.34
4	D	607	CM5	O32-C27-C28	-5.19	98.65	110.34
4	C	603	CM5	O22-C18-C13	-5.19	98.65	110.02
4	F	606	CM5	C17-C16-C15	-5.16	99.17	110.84
4	B	602	CM5	O21-C17-C18	-5.15	98.74	110.34
2	B	500	HEM	CAA-CBA-CGA	-5.10	103.40	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	CM5	C13-O14-C15	-4.85	104.33	113.75
4	A	601	CM5	O12-C13-C18	-4.72	102.08	108.04
4	E	605	CM5	O25-C24-C29	-4.63	100.77	110.28
4	E	605	CM5	O12-C13-C18	-4.63	102.20	108.04
4	B	608	CM5	C13-O14-C15	-4.48	105.04	113.75
4	D	604	CM5	C24-C29-C28	-4.33	101.44	109.97
4	C	603	CM5	O12-C13-C18	-4.31	102.59	108.04
4	B	608	CM5	C28-C27-C26	-4.29	102.71	110.20
4	C	603	CM5	O25-C26-C30	-4.27	95.56	106.36
4	D	604	CM5	C1-O12-C13	-4.04	106.87	113.94
4	D	604	CM5	C17-C16-C15	-3.94	101.92	110.84
3	B	501	3QU	CAJ-CAO-NAP	-3.88	116.36	119.48
4	D	607	CM5	O21-C17-C18	-3.84	101.70	110.34
4	F	606	CM5	O22-C18-C17	-3.57	102.29	110.34
4	E	605	CM5	O22-C18-C13	-3.53	102.28	110.02
4	D	607	CM5	C19-C15-C16	-3.53	102.98	113.25
4	B	608	CM5	C24-O23-C16	-3.52	108.82	118.01
4	C	603	CM5	C24-O25-C26	-3.50	106.96	113.75
4	B	602	CM5	C18-C17-C16	-3.48	101.96	109.60
4	D	604	CM5	O14-C13-O12	-3.43	101.80	110.05
4	A	601	CM5	O25-C24-C29	-3.40	103.29	110.28
4	D	607	CM5	C8-C7-C6	-3.39	106.75	112.22
4	D	604	CM5	O23-C16-C15	-3.38	100.45	109.32
4	A	601	CM5	C17-C16-C15	-3.36	103.25	110.84
4	A	601	CM5	O14-C15-C16	-3.35	102.68	109.75
4	C	603	CM5	C17-C16-C15	-3.33	103.32	110.84
2	C	500	HEM	C3B-C4B-CHC	-3.23	118.62	123.16
2	C	500	HEM	CAA-CBA-CGA	-3.22	106.84	112.75
4	E	605	CM5	O31-C30-C26	-3.15	100.92	111.33
4	A	601	CM5	C1-O12-C13	-3.13	108.47	113.94
4	E	605	CM5	O23-C24-C29	-2.94	100.95	108.10
2	B	500	HEM	CMA-C3A-C4A	-2.94	123.50	128.36
4	C	603	CM5	C24-C29-C28	-2.94	104.18	109.97
2	E	500	HEM	C3C-CAC-CBC	-2.92	119.97	124.46
2	F	500	HEM	C3B-CAB-CBB	-2.92	119.98	124.46
2	A	500	HEM	C3C-CAC-CBC	-2.91	119.99	124.46
2	D	500	HEM	C3B-CAB-CBB	-2.90	120.00	124.46
2	D	500	HEM	C3C-CAC-CBC	-2.90	120.00	124.46
2	A	500	HEM	C3B-CAB-CBB	-2.90	120.01	124.46
4	A	601	CM5	C24-O25-C26	-2.89	108.13	113.75
2	F	500	HEM	C3C-CAC-CBC	-2.89	120.03	124.46
2	E	500	HEM	C3B-CAB-CBB	-2.88	120.03	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	CM5	C1-O12-C13	-2.88	108.91	113.94
4	F	606	CM5	C24-O23-C16	-2.87	110.50	118.01
4	D	607	CM5	O22-C18-C13	-2.83	103.82	110.02
4	B	602	CM5	O25-C24-C29	-2.82	104.49	110.28
4	C	603	CM5	C13-O14-C15	-2.81	108.29	113.75
4	F	606	CM5	O34-C29-C28	-2.74	104.17	110.34
4	C	603	CM5	O14-C13-C18	-2.70	104.73	110.28
4	B	608	CM5	O32-C27-C28	-2.68	104.30	110.34
4	A	601	CM5	C29-C28-C27	-2.61	105.92	110.79
4	A	601	CM5	O25-C26-C30	-2.56	99.90	106.36
4	F	606	CM5	C1-O12-C13	-2.55	109.48	113.94
4	B	608	CM5	C13-C18-C17	-2.55	104.95	109.97
4	B	608	CM5	C24-O25-C26	-2.54	108.81	113.75
4	C	603	CM5	C1-O12-C13	-2.53	109.52	113.94
4	E	605	CM5	O21-C17-C18	-2.53	104.65	110.34
3	B	501	3QU	CAG-CAI-CAO	-2.51	116.63	120.15
4	D	607	CM5	C29-C28-C27	-2.49	106.14	110.79
4	E	605	CM5	O23-C16-C17	-2.48	100.76	107.17
4	D	607	CM5	C13-O14-C15	-2.47	108.95	113.75
3	B	501	3QU	CAJ-CAH-CAN	-2.47	117.66	121.04
4	E	605	CM5	C17-C16-C15	-2.46	105.27	110.84
4	F	606	CM5	O21-C17-C16	-2.45	104.07	109.87
4	B	608	CM5	O22-C18-C17	-2.36	105.02	110.34
3	E	501	3QU	CAF-CAD-NAL	-2.34	119.57	123.64
4	E	605	CM5	C30-C26-C27	-2.31	107.32	113.02
4	B	602	CM5	O22-C18-C17	-2.24	105.28	110.34
4	F	606	CM5	O23-C16-C17	-2.23	101.41	107.17
4	D	604	CM5	O34-C29-C24	-2.21	105.19	110.02
4	E	605	CM5	O32-C27-C28	-2.19	105.41	110.34
4	A	601	CM5	C8-C7-C6	-2.18	108.70	112.22
4	E	605	CM5	C13-C18-C17	-2.18	105.68	109.97
4	F	606	CM5	O25-C26-C30	-2.18	100.86	106.36
4	D	607	CM5	C11-C6-C7	-2.17	103.81	109.26
4	B	602	CM5	O20-C19-C15	-2.12	104.31	111.33
4	D	604	CM5	O22-C18-C13	-2.08	105.46	110.02
4	C	603	CM5	O22-C18-C17	-2.05	105.73	110.34
4	B	602	CM5	C13-C18-C17	2.09	114.09	109.97
2	C	500	HEM	C2C-C1C-NC	2.12	113.79	110.21
2	E	500	HEM	C3B-C4B-CHC	2.14	126.18	123.16
2	D	500	HEM	C3B-C4B-CHC	2.15	126.19	123.16
4	E	605	CM5	O33-C28-C27	2.17	115.23	110.34
2	F	500	HEM	C3B-C4B-CHC	2.19	126.25	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C3B-C4B-CHC	2.19	126.25	123.16
2	B	500	HEM	C3B-CAB-CBB	2.24	127.89	124.46
4	B	608	CM5	O22-C18-C13	2.26	114.97	110.02
2	B	500	HEM	CAA-C2A-C1A	2.27	129.48	127.01
2	B	500	HEM	CBA-CAA-C2A	2.30	116.64	112.53
4	A	601	CM5	O22-C18-C13	2.31	115.09	110.02
2	E	500	HEM	C2D-C3D-C4D	2.32	105.43	101.50
2	B	500	HEM	C2D-C3D-C4D	2.32	105.43	101.50
2	B	500	HEM	C2C-C1C-CHC	2.33	127.22	123.68
2	D	500	HEM	C2D-C3D-C4D	2.33	105.44	101.50
4	C	603	CM5	O25-C26-C27	2.34	114.07	109.68
2	A	500	HEM	C2D-C3D-C4D	2.34	105.46	101.50
2	F	500	HEM	C2D-C3D-C4D	2.34	105.47	101.50
4	B	602	CM5	O23-C16-C15	2.39	115.60	109.32
3	B	501	3QU	CAI-CAO-NAP	2.39	121.41	119.48
3	B	501	3QU	CAG-CAN-CAH	2.48	122.11	118.13
4	D	607	CM5	O25-C26-C30	2.53	112.75	106.36
4	F	606	CM5	O21-C17-C18	2.76	116.55	110.34
4	F	606	CM5	C28-C27-C26	2.86	115.17	110.20
2	E	500	HEM	CMD-C2D-C3D	2.91	127.24	114.35
2	D	500	HEM	CMD-C2D-C3D	2.92	127.27	114.35
2	A	500	HEM	CMD-C2D-C3D	2.93	127.30	114.35
2	F	500	HEM	CMD-C2D-C3D	2.93	127.30	114.35
4	D	604	CM5	C24-O25-C26	2.98	119.53	113.75
4	D	604	CM5	C18-C17-C16	3.03	116.25	109.60
4	B	602	CM5	C29-C28-C27	3.12	116.61	110.79
4	A	601	CM5	O21-C17-C16	3.12	117.27	109.87
4	A	601	CM5	O23-C16-C17	3.13	115.24	107.17
4	F	606	CM5	O25-C26-C27	3.13	115.55	109.68
4	C	603	CM5	O34-C29-C24	3.19	117.01	110.02
2	B	500	HEM	CMD-C2D-C3D	3.22	128.58	114.35
2	C	500	HEM	CMD-C2D-C3D	3.22	128.58	114.35
4	B	608	CM5	O31-C30-C26	3.27	122.14	111.33
4	F	606	CM5	O23-C24-O25	3.29	119.01	110.68
4	E	605	CM5	C18-C17-C16	3.33	116.92	109.60
4	B	608	CM5	O25-C26-C30	3.34	114.79	106.36
4	D	607	CM5	C1-O12-C13	3.41	119.91	113.94
4	D	607	CM5	O14-C15-C16	3.46	117.05	109.75
4	B	602	CM5	O23-C24-C29	3.50	116.62	108.10
4	B	602	CM5	O34-C29-C24	3.70	118.14	110.02
2	C	500	HEM	CAD-C3D-C2D	3.73	123.94	113.22
2	A	500	HEM	CMC-C2C-C3C	3.75	125.90	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CMB-C2B-C3B	3.76	125.91	116.53
2	F	500	HEM	CMC-C2C-C3C	3.77	125.93	116.53
2	D	500	HEM	CMB-C2B-C3B	3.77	125.94	116.53
2	E	500	HEM	CMB-C2B-C3B	3.77	125.94	116.53
2	F	500	HEM	CMB-C2B-C3B	3.78	125.96	116.53
2	D	500	HEM	CMC-C2C-C3C	3.78	125.96	116.53
2	E	500	HEM	CMC-C2C-C3C	3.78	125.97	116.53
4	E	605	CM5	O25-C26-C30	3.79	115.94	106.36
2	B	500	HEM	C3B-C4B-CHC	3.82	128.55	123.16
4	F	606	CM5	O31-C30-C26	3.83	124.00	111.33
4	F	606	CM5	O32-C27-C26	3.84	119.42	109.24
4	F	606	CM5	C24-C29-C28	3.94	117.74	109.97
4	E	605	CM5	O34-C29-C28	4.09	119.54	110.34
2	C	500	HEM	CMB-C2B-C3B	4.10	126.77	116.53
2	B	500	HEM	CMC-C2C-C3C	4.12	126.81	116.53
2	A	500	HEM	CAD-C3D-C4D	4.19	127.23	112.47
2	F	500	HEM	CAD-C3D-C4D	4.20	127.28	112.47
4	E	605	CM5	C13-O14-C15	4.20	121.90	113.75
2	D	500	HEM	CAD-C3D-C4D	4.20	127.28	112.47
2	E	500	HEM	CAD-C3D-C4D	4.20	127.30	112.47
4	D	604	CM5	O31-C30-C26	4.21	125.23	111.33
4	E	605	CM5	C28-C27-C26	4.23	117.57	110.20
2	B	500	HEM	CAD-C3D-C2D	4.31	125.59	113.22
4	D	604	CM5	O23-C24-C29	4.38	118.77	108.10
2	C	500	HEM	CMC-C2C-C3C	4.48	127.71	116.53
4	D	607	CM5	C28-C27-C26	4.56	118.15	110.20
4	D	607	CM5	O22-C18-C17	4.58	120.66	110.34
2	B	500	HEM	CAD-C3D-C4D	4.68	128.97	112.47
4	C	603	CM5	C30-C26-C27	4.70	124.61	113.02
2	F	500	HEM	CAD-C3D-C2D	4.88	127.26	113.22
2	E	500	HEM	CAD-C3D-C2D	4.89	127.27	113.22
2	D	500	HEM	CAD-C3D-C2D	4.89	127.27	113.22
2	A	500	HEM	CAD-C3D-C2D	4.90	127.30	113.22
4	A	601	CM5	O21-C17-C18	5.28	122.23	110.34
4	F	606	CM5	C30-C26-C27	5.34	126.19	113.02
4	E	605	CM5	C24-O23-C16	5.36	132.00	118.01
4	D	607	CM5	C24-C29-C28	5.36	120.54	109.97
4	D	604	CM5	O20-C19-C15	5.40	129.16	111.33
4	B	608	CM5	O14-C13-C18	5.45	121.45	110.28
4	B	602	CM5	O33-C28-C29	5.59	122.92	110.34
4	F	606	CM5	O20-C19-C15	5.80	130.51	111.33
4	F	606	CM5	O14-C15-C16	5.89	122.18	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	HEM	CAD-C3D-C4D	5.99	133.59	112.47
4	B	608	CM5	C30-C26-C27	6.01	127.85	113.02
4	D	604	CM5	O33-C28-C27	6.02	123.89	110.34
4	C	603	CM5	O23-C24-C29	6.10	122.94	108.10
4	E	605	CM5	O33-C28-C29	6.34	124.61	110.34
4	B	608	CM5	O23-C24-O25	6.70	127.64	110.68
4	B	602	CM5	O25-C26-C27	6.70	122.26	109.68
2	B	500	HEM	CMB-C2B-C3B	6.72	133.30	116.53
4	C	603	CM5	O21-C17-C16	6.99	126.42	109.87
4	F	606	CM5	O23-C24-C29	7.03	125.22	108.10
4	A	601	CM5	C13-C18-C17	7.33	124.41	109.97
4	A	601	CM5	O25-C26-C27	7.38	123.53	109.68
4	C	603	CM5	O14-C15-C16	7.40	125.38	109.75
4	B	608	CM5	C18-C17-C16	7.72	126.55	109.60
4	A	601	CM5	C24-C29-C28	7.95	125.64	109.97
4	D	604	CM5	O23-C24-O25	8.03	131.01	110.68
4	D	607	CM5	C24-O23-C16	8.16	139.32	118.01
4	F	606	CM5	C18-C17-C16	9.27	129.96	109.60
4	B	602	CM5	O23-C24-O25	9.27	134.16	110.68
4	D	604	CM5	O25-C26-C30	9.66	130.77	106.36
4	B	608	CM5	O14-C15-C16	10.16	131.21	109.75
4	B	608	CM5	O23-C24-C29	10.24	133.03	108.10
4	E	605	CM5	O14-C13-O12	10.25	134.73	110.05
4	B	608	CM5	O23-C16-C15	11.22	138.81	109.32
4	D	604	CM5	C29-C28-C27	11.80	132.81	110.79
4	D	604	CM5	O34-C29-C28	12.28	137.97	110.34
4	D	607	CM5	O23-C16-C15	14.15	146.50	109.32
4	A	601	CM5	O23-C24-O25	15.33	149.48	110.68
4	D	604	CM5	O23-C16-C17	19.52	157.57	107.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	604	CM5	C16

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	CM5	1	0
2	B	500	HEM	4	0
4	B	602	CM5	14	0
4	B	608	CM5	20	0
2	C	500	HEM	9	0
4	C	603	CM5	5	0
2	D	500	HEM	12	0
4	D	604	CM5	4	0
4	D	607	CM5	8	0
2	E	500	HEM	9	0
3	E	501	3QU	1	0
4	E	605	CM5	3	0
2	F	500	HEM	18	0
4	F	606	CM5	5	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	462/476 (97%)	0.01	0 100 100	26, 51, 74, 82	0
1	B	459/476 (96%)	0.06	6 (1%) 79 71	28, 51, 74, 82	0
1	C	462/476 (97%)	0.04	2 (0%) 93 90	24, 50, 74, 79	0
1	D	458/476 (96%)	0.02	5 (1%) 82 74	24, 51, 74, 82	0
1	E	459/476 (96%)	0.02	5 (1%) 82 74	26, 51, 74, 87	0
1	F	453/476 (95%)	0.44	48 (10%) 8 4	24, 51, 74, 79	0
All	All	2753/2856 (96%)	0.10	66 (2%) 62 50	24, 51, 74, 87	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	463	VAL	6.9
1	F	416	ALA	5.4
1	F	460	ALA	5.1
1	F	422	LYS	4.9
1	F	153	LEU	4.6
1	F	451	THR	4.3
1	F	459	MET	4.3
1	F	408	PHE	3.9
1	F	414	LEU	3.9
1	F	423	THR	3.7
1	F	450	PHE	3.7
1	F	150	ALA	3.6
1	F	454	LEU	3.6
1	F	328	ILE	3.6
1	E	488	PHE	3.6
1	F	164	LEU	3.6
1	F	165	MET	3.4
1	F	359	PHE	3.3
1	E	470	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	335	HIS	3.1
1	D	488	PHE	3.0
1	F	464	ALA	2.9
1	E	314	MET	2.9
1	F	417	ASN	2.9
1	F	468	ILE	2.9
1	F	402	PHE	2.9
1	F	320	VAL	2.8
1	B	465	PRO	2.8
1	D	414	LEU	2.8
1	E	417	ASN	2.7
1	F	426	PHE	2.7
1	E	416	ALA	2.7
1	F	350	GLU	2.7
1	F	278	ASN	2.6
1	F	449	PHE	2.5
1	F	157	LEU	2.4
1	D	335	HIS	2.4
1	B	158	ARG	2.3
1	F	453	ILE	2.3
1	C	324	VAL	2.3
1	F	326	ARG	2.3
1	F	430	SER	2.3
1	F	162	GLY	2.3
1	F	403	GLU	2.3
1	B	195	PHE	2.3
1	B	154	ILE	2.2
1	F	462	PRO	2.2
1	F	472	PRO	2.2
1	F	311	PHE	2.2
1	D	485	GLN	2.2
1	F	330	GLN	2.2
1	F	352	VAL	2.2
1	F	413	PHE	2.2
1	F	421	LYS	2.2
1	F	324	VAL	2.2
1	F	455	GLN	2.1
1	C	400	HIS	2.1
1	F	321	ALA	2.1
1	F	410	PRO	2.1
1	F	345	LYS	2.1
1	F	329	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	312	LEU	2.1
1	F	319	HIS	2.0
1	B	489	LEU	2.0
1	D	481	PRO	2.0
1	F	163	ALA	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
3	3QU	A	501	7/16	0.92	0.29	9.59	47,50,51,52	0
3	3QU	D	501	13/16	0.93	0.25	4.88	47,49,54,54	0
4	CM5	F	606	34/34	0.78	0.33	3.83	45,62,74,76	0
3	3QU	B	501	16/16	0.94	0.27	3.23	47,51,60,66	0
4	CM5	B	602	34/34	0.78	0.30	3.20	61,72,84,85	0
4	CM5	C	603	34/34	0.81	0.27	2.45	54,63,70,71	0
4	CM5	D	607	34/34	0.80	0.23	2.43	72,97,101,103	0
3	3QU	E	501	13/16	0.96	0.24	2.25	55,57,60,63	0
3	3QU	C	501	7/16	0.93	0.25	1.54	47,50,51,52	0
4	CM5	A	601	34/34	0.92	0.24	1.45	53,60,73,74	0
4	CM5	B	608	34/34	0.81	0.23	1.30	46,84,100,100	0
4	CM5	E	605	34/34	0.86	0.26	1.22	66,73,91,92	0
2	HEM	A	500	43/43	0.97	0.21	0.62	25,31,39,43	0
2	HEM	E	500	43/43	0.97	0.20	0.51	17,28,36,40	0
4	CM5	D	604	34/34	0.89	0.20	0.32	58,67,77,79	0
2	HEM	F	500	43/43	0.95	0.22	-0.04	53,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	D	500	43/43	0.97	0.18	-0.11	23,33,38,39	0
2	HEM	B	500	43/43	0.98	0.18	-0.40	15,20,29,31	0
2	HEM	C	500	43/43	0.98	0.15	-0.94	21,27,36,46	0

6.5 Other polymers (i)

There are no such residues in this entry.