



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:00 AM GMT

PDB ID : 3R1B
Title : Open crystal structure of cytochrome P450 2B4 covalently bound to the mechanism-based inactivator tert-butylphenylacetylene
Authors : Gay, S.C.; Zhang, H.; Stout, C.D.; Hollenberg, P.F.; Halpert, J.R.
Deposited on : 2011-03-09
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

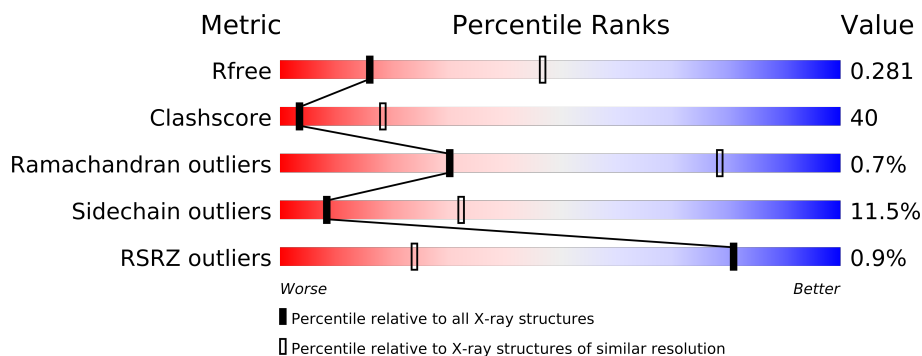
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	
1	C	476	
1	D	476	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CM5	A	605	-	X
5	CM5	A	608	-	X
5	CM5	D	610	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14499 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2B4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	2	0	0
			3583	2294	619	659	11			
1	B	465	Total	C	N	O	S	2	0	0
			3589	2308	615	656	10			
1	C	456	Total	C	N	O	S	1	0	0
			3406	2171	589	638	8			
1	D	464	Total	C	N	O	S	0	0	0
			3445	2199	598	640	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	SER	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	ALA	DELETION	UNP P00178
A	?	-	GLY	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	LEU	DELETION	UNP P00178
A	?	-	PHE	DELETION	UNP P00178
A	?	-	ARG	DELETION	UNP P00178
A	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
A	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
A	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
A	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
A	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
A	221	SER	PRO	CONFLICT	UNP P00178
A	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
A	492	HIS	-	EXPRESSION TAG	UNP P00178
A	493	HIS	-	EXPRESSION TAG	UNP P00178
A	494	HIS	-	EXPRESSION TAG	UNP P00178
A	495	HIS	-	EXPRESSION TAG	UNP P00178
B	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	SER	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	ALA	DELETION	UNP P00178
B	?	-	GLY	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	LEU	DELETION	UNP P00178
B	?	-	PHE	DELETION	UNP P00178
B	?	-	ARG	DELETION	UNP P00178
B	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
B	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
B	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
B	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
B	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
B	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
B	221	SER	PRO	CONFLICT	UNP P00178
B	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
B	492	HIS	-	EXPRESSION TAG	UNP P00178

Continued on next page...

Continued from previous page...

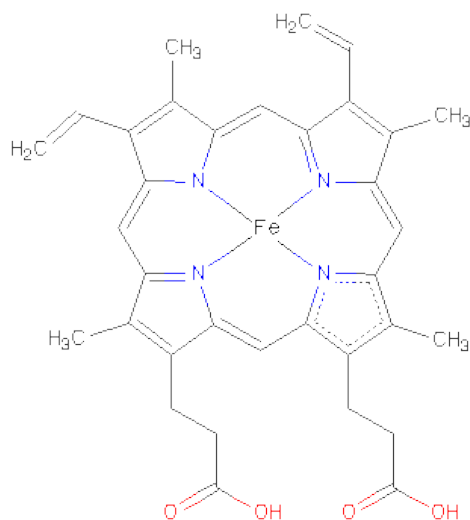
Chain	Residue	Modelled	Actual	Comment	Reference
B	493	HIS	-	EXPRESSION TAG	UNP P00178
B	494	HIS	-	EXPRESSION TAG	UNP P00178
B	495	HIS	-	EXPRESSION TAG	UNP P00178
C	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	SER	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	ALA	DELETION	UNP P00178
C	?	-	GLY	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	LEU	DELETION	UNP P00178
C	?	-	PHE	DELETION	UNP P00178
C	?	-	ARG	DELETION	UNP P00178
C	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
C	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
C	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
C	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
C	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
C	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
C	221	SER	PRO	CONFLICT	UNP P00178
C	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
C	492	HIS	-	EXPRESSION TAG	UNP P00178
C	493	HIS	-	EXPRESSION TAG	UNP P00178
C	494	HIS	-	EXPRESSION TAG	UNP P00178
C	495	HIS	-	EXPRESSION TAG	UNP P00178
D	21	ALA	GLU	ENGINEERED MUTATION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	SER	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178

Continued on next page...

Continued from previous page...

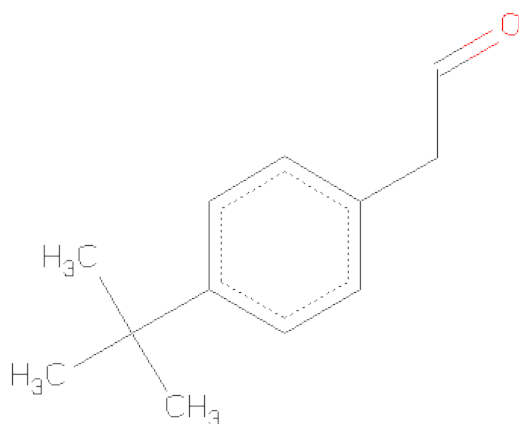
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	ALA	DELETION	UNP P00178
D	?	-	GLY	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	LEU	DELETION	UNP P00178
D	?	-	PHE	DELETION	UNP P00178
D	?	-	ARG	DELETION	UNP P00178
D	22	LYS	GLY	ENGINEERED MUTATION	UNP P00178
D	23	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	24	THR	PRO	ENGINEERED MUTATION	UNP P00178
D	25	SER	LYS	ENGINEERED MUTATION	UNP P00178
D	26	SER	ALA	ENGINEERED MUTATION	UNP P00178
D	27	LYS	HIS	ENGINEERED MUTATION	UNP P00178
D	29	LYS	ARG	ENGINEERED MUTATION	UNP P00178
D	221	SER	PRO	CONFLICT	UNP P00178
D	226	TYR	HIS	ENGINEERED MUTATION	UNP P00178
D	492	HIS	-	EXPRESSION TAG	UNP P00178
D	493	HIS	-	EXPRESSION TAG	UNP P00178
D	494	HIS	-	EXPRESSION TAG	UNP P00178
D	495	HIS	-	EXPRESSION TAG	UNP P00178

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



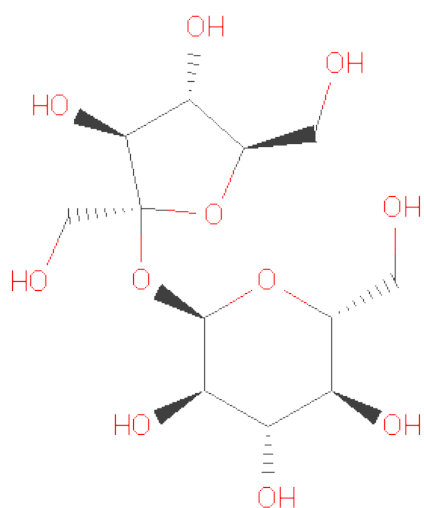
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (4-TERT-BUTYLPHENYL)ACETALDEHYDE (three-letter code: TB2) (formula: C₁₂H₁₆O).



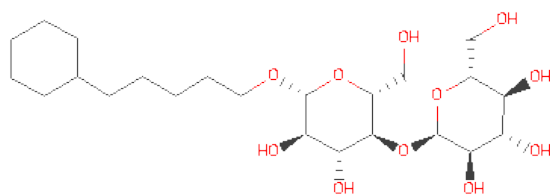
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	12	1		
3	B	1	Total	C	O	0	0
			13	12	1		
3	C	1	Total	C	O	0	0
			13	12	1		
3	D	1	Total	C	O	0	0
			13	12	1		

- Molecule 4 is SUGAR (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 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: C₂₃H₄₂O₁₁).



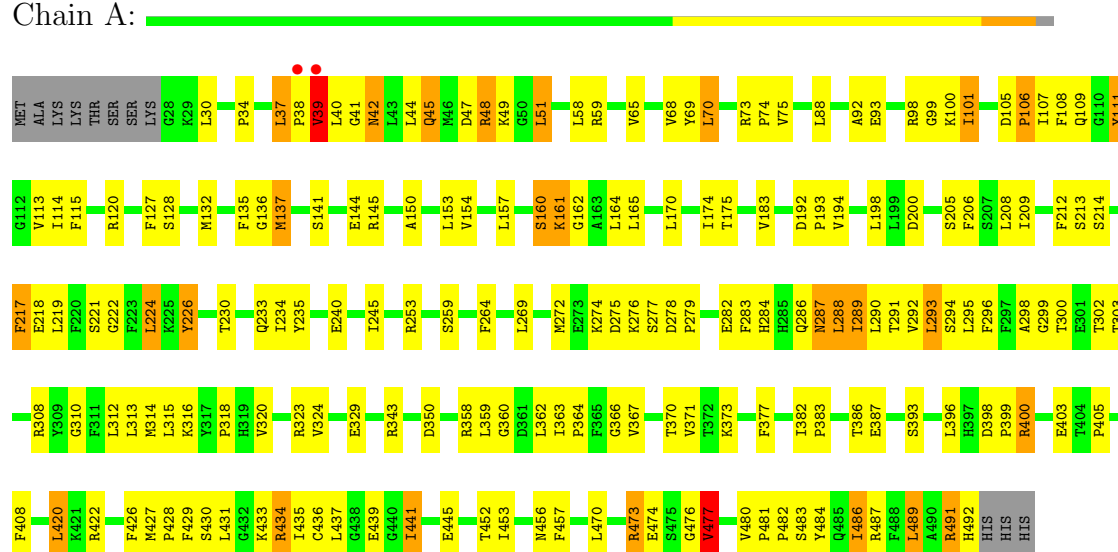
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	18	6		
5	B	1	Total	C	O	0	0
			34	23	11		
5	B	1	Total	C	O	0	0
			34	23	11		
5	A	1	Total	C	O	0	0
			34	23	11		
5	D	1	Total	C	O	0	0
			34	23	11		

3 Residue-property plots

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.

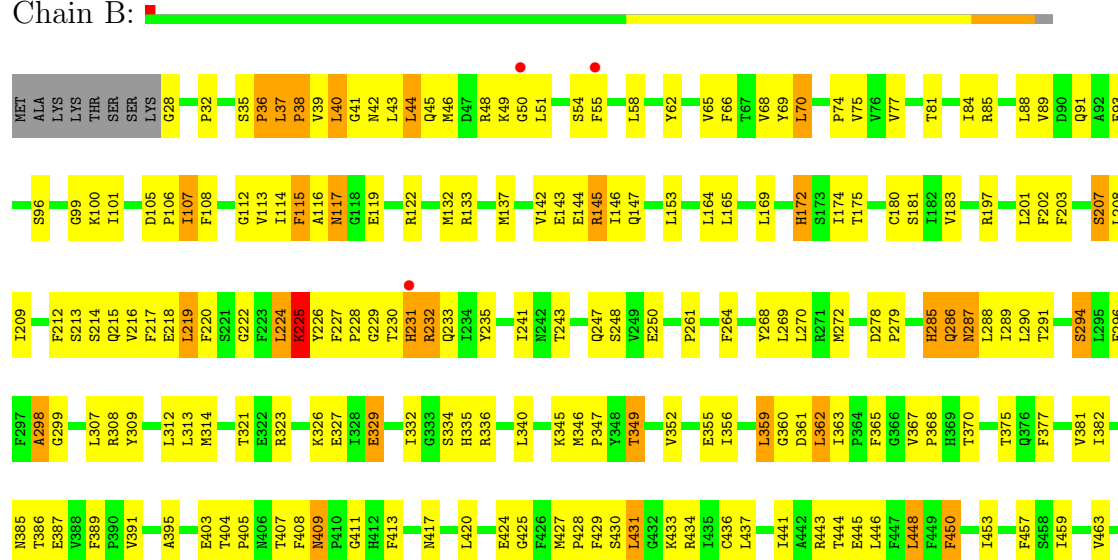
• Molecule 1: Cytochrome P450 2B4

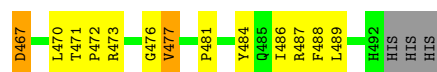
Chain A:



• Molecule 1: Cytochrome P450 2B4

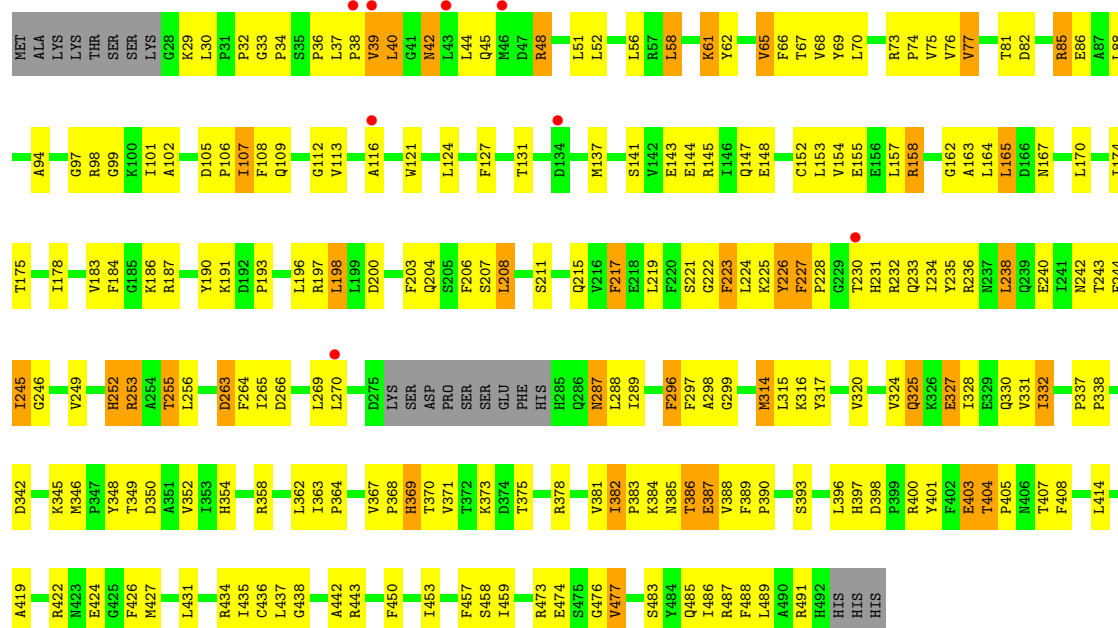
Chain B:





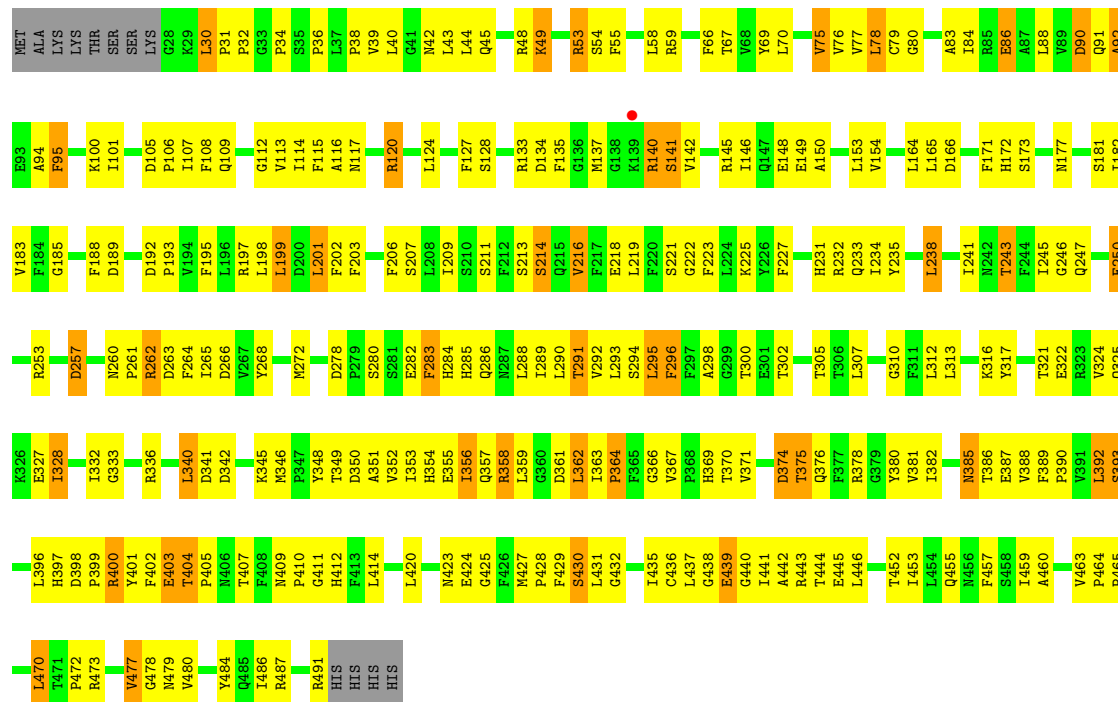
• Molecule 1: Cytochrome P450 2B4

Chain C:



• Molecule 1: Cytochrome P450 2B4

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.92Å 153.69Å 129.66Å 90.00° 122.22° 90.00°	Depositor
Resolution (Å)	53.43 – 3.00 53.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (53.43-3.00) 99.3 (53.44-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4.486)	Depositor
R, R_{free}	0.242 , 0.288 0.241 , 0.281	Depositor DCC
R_{free} test set	3234 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63927 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14499	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, TB2, SUC

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	0.31	1/3672 (0.0%)	0.56	6/4995 (0.1%)
1	B	0.35	0/3679	0.69	14/5003 (0.3%)
1	C	0.31	0/3484	0.67	5/4749 (0.1%)
1	D	0.32	0/3527	0.70	9/4814 (0.2%)
All	All	0.32	1/14362 (0.0%)	0.66	34/19561 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	LYS	CA-CB	-5.92	1.41	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	LEU	N-CA-C	-5.98	94.85	111.00
1	D	328	ILE	CB-CA-C	-5.98	99.64	111.60
1	D	378	ARG	N-CA-C	5.97	127.12	111.00
1	B	335	HIS	N-CA-C	5.95	127.07	111.00
1	C	255	THR	N-CA-CB	-5.93	99.03	110.30
1	B	48	ARG	N-CA-C	5.93	127.00	111.00
1	B	38	PRO	CA-N-CD	-5.84	103.32	111.50
1	B	231	HIS	N-CA-C	-5.84	95.24	111.00
1	B	298	ALA	CB-CA-C	-5.82	101.37	110.10
1	C	263	ASP	CB-CA-C	-5.75	98.90	110.40
1	B	48	ARG	CB-CA-C	-5.70	99.00	110.40
1	A	161	LYS	N-CA-CB	-5.68	100.37	110.60
1	D	404	THR	N-CA-C	-5.66	95.73	111.00
1	C	256	LEU	CB-CA-C	-5.65	99.46	110.20
1	A	70	LEU	CB-CA-C	-5.65	99.47	110.20
1	D	477	VAL	CB-CA-C	-5.64	100.69	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	ILE	N-CA-C	5.62	126.16	111.00
1	D	232	ARG	N-CA-CB	-5.60	100.52	110.60
1	B	48	ARG	N-CA-CB	-5.59	100.53	110.60
1	A	160	SER	CB-CA-C	5.58	120.70	110.10
1	C	403	GLU	CB-CA-C	5.54	121.49	110.40
1	B	49	LYS	CB-CA-C	-5.48	99.44	110.40
1	D	403	GLU	CB-CA-C	-5.45	99.51	110.40
1	B	334	SER	N-CA-C	5.41	125.61	111.00
1	B	40	LEU	CB-CA-C	-5.38	99.98	110.20
1	A	259	SER	CB-CA-C	5.34	120.25	110.10
1	D	233	GLN	CB-CA-C	-5.32	99.76	110.40
1	B	335	HIS	N-CA-CB	-5.30	101.06	110.60
1	D	92	ALA	CB-CA-C	-5.28	102.18	110.10
1	B	385	ASN	N-CA-C	5.19	125.01	111.00
1	B	225	LYS	N-CA-CB	-5.14	101.35	110.60
1	D	86	GLU	CB-CA-C	5.13	120.67	110.40
1	A	37	LEU	N-CA-C	-5.04	97.38	111.00
1	A	161	LYS	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3583	0	3434	226	0
1	B	3589	0	3460	209	0
1	C	3406	0	3187	300	0
1	D	3445	0	3216	382	0
2	A	43	0	30	17	0
2	B	43	0	30	14	0
2	C	43	0	30	12	0
2	D	43	0	30	25	0
3	A	13	0	15	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	15	5	0
3	C	13	0	15	6	0
3	D	13	0	15	14	0
4	A	23	0	22	6	0
4	B	23	0	22	12	0
4	C	23	0	22	5	0
4	D	23	0	22	11	0
5	A	58	0	73	5	0
5	B	68	0	84	5	0
5	D	34	0	42	3	0
All	All	14499	0	13764	1119	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

All (1119) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:30:LEU:HD12	1:D:31:PRO:CD	1.18	1.61
1:A:298:ALA:HB1	3:A:501:TB2:C8	1.39	1.52
1:D:30:LEU:CD1	1:D:31:PRO:HD2	1.39	1.51
1:D:298:ALA:HB2	3:D:501:TB2:C7	1.52	1.37
1:C:233:GLN:NE2	1:C:236:ARG:HD3	1.43	1.34
1:A:293:LEU:HD12	1:A:294:SER:N	1.40	1.33
1:D:402:PHE:HE2	1:D:425:GLY:HA3	1.07	1.17
1:C:238:LEU:O	1:C:238:LEU:HD12	1.46	1.16
1:D:402:PHE:CE2	1:D:425:GLY:HA3	1.81	1.15
1:D:298:ALA:CB	3:D:501:TB2:C7	2.25	1.14
1:A:298:ALA:HB1	3:A:501:TB2:H8	1.20	1.12
1:C:231:HIS:HA	1:C:234:ILE:HG21	1.28	1.11
1:C:206:PHE:CD1	1:C:208:LEU:HD11	1.86	1.11
1:D:292:VAL:O	1:D:296:PHE:HB2	1.49	1.11
1:B:38:PRO:O	1:B:39:VAL:HG12	1.50	1.11
1:D:420:LEU:HD21	4:D:604:SUC:O4	1.51	1.10
1:C:224:LEU:HD13	1:C:224:LEU:C	1.72	1.10
1:C:32:PRO:HB2	1:C:62:TYR:HD1	1.12	1.09
1:A:298:ALA:CB	3:A:501:TB2:C8	2.31	1.08
1:C:231:HIS:HA	1:C:234:ILE:CG2	1.84	1.07
1:C:208:LEU:HD12	1:C:208:LEU:N	1.71	1.06
1:A:224:LEU:O	1:A:224:LEU:HD13	1.54	1.05
1:D:295:LEU:HD13	2:D:500:HEM:CBC	1.87	1.04
1:A:298:ALA:CB	3:A:501:TB2:H8	1.89	1.03
4:D:604:SUC:O5	4:D:604:SUC:H1'2	1.57	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:58:LEU:HD11	1:C:66:PHE:CZ	1.93	1.03
1:C:224:LEU:HD13	1:C:224:LEU:O	1.59	1.02
1:A:298:ALA:HB1	3:A:501:TB2:C7	1.88	1.02
1:C:208:LEU:HD23	1:C:232:ARG:HG3	1.39	1.02
1:C:231:HIS:CA	1:C:234:ILE:HG22	1.90	1.01
1:B:225:LYS:HD2	1:B:225:LYS:H	1.24	1.01
1:B:232:ARG:HG3	1:B:233:GLN:N	1.71	1.00
1:B:287:ASN:OD1	1:B:287:ASN:O	1.79	1.00
1:D:30:LEU:HD12	1:D:31:PRO:HD3	1.42	1.00
1:C:36:PRO:HB3	1:C:69:TYR:HB2	1.44	0.99
1:A:308:ARG:NH2	1:A:483:SER:HA	1.77	0.98
1:C:231:HIS:CA	1:C:234:ILE:CG2	2.41	0.98
1:D:245:ILE:HG21	1:D:288:LEU:HD13	1.43	0.98
4:B:602:SUC:O5	4:B:602:SUC:H4'	1.64	0.98
4:B:602:SUC:C1	4:B:602:SUC:H4'	1.94	0.97
1:B:209:ILE:HG22	1:C:207:SER:HA	1.45	0.97
1:A:208:LEU:O	1:D:207:SER:HA	1.65	0.97
1:B:38:PRO:O	1:B:39:VAL:CG1	2.13	0.97
1:D:298:ALA:CB	3:D:501:TB2:C8	2.44	0.96
1:A:491:ARG:O	1:A:492:HIS:HB2	1.66	0.95
1:D:30:LEU:CD1	1:D:31:PRO:CD	2.14	0.95
1:C:206:PHE:CE1	1:C:208:LEU:HD11	1.99	0.95
1:A:293:LEU:HD12	1:A:294:SER:H	1.13	0.95
1:A:293:LEU:CD1	1:A:294:SER:N	2.30	0.94
1:D:358:ARG:NH1	1:D:402:PHE:CD1	2.35	0.94
1:A:290:LEU:HA	1:A:293:LEU:HG	1.47	0.94
1:D:296:PHE:CE1	1:D:300:THR:HG21	2.03	0.94
1:C:58:LEU:HD11	1:C:66:PHE:CE2	2.03	0.94
1:B:367:VAL:HG13	1:C:221:SER:HB2	1.50	0.94
1:B:227:PHE:HD2	1:B:229:GLY:H	1.15	0.93
1:C:32:PRO:HB2	1:C:62:TYR:CD1	2.02	0.93
1:D:42:ASN:HB2	1:D:45:GLN:HE21	1.34	0.93
4:B:602:SUC:C4'	4:B:602:SUC:C1	2.47	0.92
1:C:208:LEU:CD1	1:C:208:LEU:N	2.30	0.92
1:A:101:ILE:HG21	1:D:219:LEU:O	1.67	0.92
1:B:299:GLY:HA2	2:B:500:HEM:C1C	2.04	0.92
1:A:206:PHE:CG	1:A:233:GLN:HG2	2.05	0.92
4:D:604:SUC:H3	4:D:604:SUC:O1'	1.69	0.92
4:B:602:SUC:C4'	4:B:602:SUC:H1	1.99	0.92
1:B:352:VAL:HG23	1:B:408:PHE:HZ	1.34	0.91
1:D:203:PHE:HZ	1:D:300:THR:OG1	1.51	0.91
1:D:288:LEU:HD12	1:D:289:ILE:N	1.84	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:37:LEU:HD22	1:C:42:ASN:HA	1.51	0.91
1:A:278:ASP:OD1	1:A:279:PRO:HD2	1.69	0.91
1:C:61:LYS:HG3	1:C:62:TYR:CD2	2.06	0.90
1:C:233:GLN:HE21	1:C:236:ARG:HD3	1.12	0.90
1:C:32:PRO:CB	1:C:62:TYR:HD1	1.85	0.90
1:C:61:LYS:HG3	1:C:62:TYR:HD2	1.35	0.90
1:D:280:SER:O	1:D:283:PHE:HB3	1.71	0.90
1:B:229:GLY:O	1:B:230:THR:HG22	1.72	0.90
2:A:500:HEM:HBC2	2:A:500:HEM:HHD	1.52	0.89
1:A:295:LEU:HG	2:A:500:HEM:HBC1	1.54	0.89
1:D:460:ALA:HB3	1:D:487:ARG:HB2	1.54	0.89
4:B:602:SUC:H1	4:B:602:SUC:H4'	1.54	0.89
1:D:436:CYS:SG	2:D:500:HEM:C4A	2.66	0.88
1:D:296:PHE:CD1	1:D:300:THR:HG21	2.08	0.88
1:A:208:LEU:O	1:D:207:SER:CB	2.21	0.88
1:A:358:ARG:HA	1:A:396:LEU:HD12	1.56	0.88
1:A:208:LEU:O	1:D:207:SER:CA	2.22	0.88
1:B:93:GLU:OE1	1:B:433:LYS:HE3	1.72	0.88
1:A:221:SER:HB3	1:D:367:VAL:HG22	1.55	0.88
1:C:97:GLY:H	1:C:434:ARG:HH21	1.22	0.88
1:C:207:SER:C	1:C:208:LEU:HD12	1.93	0.87
1:D:355:GLU:O	1:D:359:LEU:HD23	1.75	0.87
1:A:224:LEU:C	1:A:224:LEU:HD13	1.93	0.87
2:C:500:HEM:HBC2	2:C:500:HEM:HHD	1.56	0.87
1:D:223:PHE:HB3	1:D:227:PHE:HE1	1.39	0.86
1:A:218:GLU:O	1:A:222:GLY:HA3	1.73	0.86
1:D:298:ALA:HB2	3:D:501:TB2:H7	1.54	0.86
1:C:224:LEU:CD1	1:C:224:LEU:C	2.41	0.86
1:C:231:HIS:C	1:C:234:ILE:HG22	1.94	0.86
1:D:203:PHE:CZ	1:D:300:THR:OG1	2.24	0.86
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.56	0.86
1:A:219:LEU:HD13	1:A:219:LEU:C	1.96	0.85
1:D:290:LEU:H	1:D:290:LEU:HD12	1.42	0.85
2:D:500:HEM:HMB1	2:D:500:HEM:HBB2	1.59	0.85
1:C:66:PHE:CZ	1:C:77:VAL:HG21	2.11	0.84
1:C:228:PRO:O	1:C:231:HIS:CD2	2.30	0.84
1:A:477:VAL:HG13	1:A:477:VAL:O	1.77	0.84
1:D:286:GLN:O	1:D:290:LEU:CD1	2.25	0.84
1:C:263:ASP:OD1	1:C:265:ILE:HG12	1.77	0.84
1:A:298:ALA:CB	3:A:501:TB2:C7	2.55	0.84
1:D:302:THR:HG21	2:D:500:HEM:C3B	2.13	0.84
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:446:LEU:O	1:B:450:PHE:HB2	1.78	0.84
1:B:228:PRO:HB2	1:B:231:HIS:CB	2.07	0.84
1:D:53:ARG:HG3	1:D:53:ARG:HH11	1.43	0.84
1:D:88:LEU:HG	1:D:432:GLY:O	1.78	0.83
1:B:38:PRO:C	1:B:39:VAL:HG12	1.99	0.83
1:D:302:THR:HG21	2:D:500:HEM:C2B	2.14	0.83
2:C:500:HEM:HBB2	2:C:500:HEM:HHC	1.61	0.83
1:C:208:LEU:HD23	1:C:232:ARG:CG	2.08	0.83
1:B:477:VAL:HG22	1:B:477:VAL:O	1.80	0.82
1:B:287:ASN:C	1:B:287:ASN:OD1	2.17	0.82
4:B:602:SUC:O3'	4:B:602:SUC:H5	1.79	0.82
1:A:218:GLU:HA	1:A:222:GLY:HA3	1.62	0.82
1:C:203:PHE:CZ	1:C:296:PHE:HE1	1.98	0.82
1:B:209:ILE:HG22	1:C:207:SER:CA	2.10	0.81
1:C:208:LEU:CD2	1:C:232:ARG:HG3	2.10	0.81
1:B:287:ASN:HA	1:B:290:LEU:HD13	1.62	0.81
1:C:249:VAL:O	1:C:253:ARG:HB3	1.80	0.81
1:C:238:LEU:C	1:C:238:LEU:HD12	2.00	0.81
1:D:431:LEU:O	1:D:435:ILE:HG12	1.81	0.80
4:B:602:SUC:C4'	4:B:602:SUC:O5	2.30	0.80
1:D:392:LEU:HD12	1:D:392:LEU:H	1.46	0.80
1:D:358:ARG:HH12	1:D:402:PHE:HB3	1.42	0.80
1:D:292:VAL:O	1:D:296:PHE:CB	2.30	0.80
1:C:37:LEU:HD13	1:C:42:ASN:HB3	1.63	0.80
1:C:233:GLN:HE21	1:C:236:ARG:CD	1.93	0.80
1:A:290:LEU:HD12	1:A:291:THR:N	1.97	0.80
1:D:78:LEU:HD21	1:D:390:PRO:HA	1.64	0.80
1:A:292:VAL:O	1:A:296:PHE:CB	2.30	0.79
1:A:218:GLU:O	1:A:222:GLY:CA	2.30	0.79
4:D:604:SUC:C2	4:D:604:SUC:O1'	2.30	0.79
4:A:601:SUC:H1'1	4:A:601:SUC:O5	1.81	0.79
4:D:604:SUC:C3	4:D:604:SUC:O1'	2.30	0.79
1:A:39:VAL:O	1:D:106:PRO:HG3	1.83	0.79
1:A:278:ASP:OD1	1:A:279:PRO:CD	2.31	0.78
1:B:46:MET:CB	1:B:50:GLY:HA3	2.13	0.78
1:B:208:LEU:O	1:C:208:LEU:HD13	1.83	0.78
2:D:500:HEM:HHD	2:D:500:HEM:HBC2	1.66	0.78
4:A:601:SUC:C1'	4:A:601:SUC:O5	2.30	0.78
1:D:342:ASP:HA	1:D:345:LYS:HE2	1.66	0.78
1:B:225:LYS:HD2	1:B:225:LYS:N	1.99	0.77
1:D:77:VAL:HG12	1:D:389:PHE:HB2	1.66	0.77
1:C:121:TRP:CZ3	1:C:124:LEU:HD12	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:403:GLU:HG2	1:D:404:THR:HG23	1.66	0.77
1:D:298:ALA:HA	3:D:501:TB2:H8	1.66	0.77
1:A:218:GLU:CA	1:A:222:GLY:HA3	2.15	0.76
1:B:36:PRO:HB3	1:B:69:TYR:HB2	1.67	0.76
1:D:30:LEU:HD11	1:D:31:PRO:HD2	1.62	0.76
1:A:308:ARG:NH1	1:A:481:PRO:HG2	2.01	0.76
1:D:150:ALA:HB1	1:D:452:THR:HG21	1.67	0.76
1:D:298:ALA:HA	3:D:501:TB2:C8	2.16	0.75
1:C:476:GLY:O	1:C:477:VAL:HG12	1.86	0.75
1:D:245:ILE:CG2	1:D:288:LEU:HD13	2.15	0.75
1:D:430:SER:HB2	2:D:500:HEM:HAA1	1.68	0.75
1:C:371:VAL:HG11	1:C:382:ILE:HG21	1.66	0.75
1:B:225:LYS:HE2	1:C:102:ALA:H	1.51	0.75
1:A:292:VAL:O	1:A:296:PHE:HB2	1.86	0.75
1:A:44:LEU:O	1:A:45:GLN:CB	2.35	0.75
1:C:61:LYS:HZ3	1:C:62:TYR:HE2	1.32	0.74
1:D:291:THR:O	1:D:295:LEU:HB3	1.87	0.74
1:A:473:ARG:NH1	1:A:482:PRO:HA	2.01	0.74
1:A:289:ILE:O	1:A:292:VAL:CG1	2.35	0.74
1:D:245:ILE:CD1	1:D:292:VAL:HG21	2.16	0.74
1:C:98:ARG:HE	1:C:99:GLY:H	1.32	0.74
1:C:358:ARG:HA	1:C:396:LEU:HD12	1.70	0.74
1:D:105:ASP:O	1:D:109:GLN:CB	2.35	0.74
2:B:500:HEM:HMC1	2:B:500:HEM:HBC2	1.69	0.74
1:D:78:LEU:CD2	1:D:390:PRO:HA	2.18	0.74
1:D:117:ASN:N	1:D:120:ARG:NH2	2.35	0.74
1:A:363:ILE:HG22	1:A:366:GLY:HA2	1.68	0.74
1:C:206:PHE:HD1	1:C:208:LEU:HD11	1.44	0.73
1:C:225:LYS:HG3	1:C:226:TYR:CE2	2.23	0.73
1:C:231:HIS:O	1:C:234:ILE:HG22	1.87	0.73
1:D:94:ALA:C	1:D:95:PHE:HD2	1.92	0.73
1:A:308:ARG:HH21	1:A:483:SER:HA	1.48	0.73
1:C:255:THR:O	1:C:255:THR:HG22	1.88	0.73
1:D:430:SER:HB3	1:D:435:ILE:HD13	1.70	0.73
1:A:219:LEU:HD13	1:A:219:LEU:O	1.88	0.73
1:D:402:PHE:CE2	1:D:425:GLY:CA	2.67	0.73
1:D:117:ASN:H	1:D:120:ARG:NH2	1.86	0.73
1:D:439:GLU:O	1:D:443:ARG:HG3	1.87	0.73
1:A:434:ARG:HA	1:A:434:ARG:HE	1.53	0.73
1:D:436:CYS:SG	2:D:500:HEM:C1A	2.78	0.73
1:D:36:PRO:HA	1:D:42:ASN:HB3	1.69	0.73
1:C:167:ASN:HD22	1:C:486:ILE:HG21	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:299:GLY:HA3	2:B:500:HEM:C2C	2.24	0.72
1:C:98:ARG:NE	1:C:99:GLY:H	1.86	0.72
1:A:288:LEU:HD13	5:A:605:CM5:H81	1.70	0.72
1:D:223:PHE:O	1:D:227:PHE:HD1	1.72	0.72
1:D:288:LEU:O	1:D:292:VAL:HG22	1.88	0.72
1:A:224:LEU:CD1	1:A:224:LEU:C	2.58	0.72
1:B:85:ARG:NE	1:B:424:GLU:HG3	2.05	0.72
1:B:299:GLY:CA	2:B:500:HEM:C2C	2.73	0.72
1:D:243:THR:O	1:D:247:GLN:HG2	1.88	0.72
1:C:223:PHE:O	1:C:227:PHE:HE2	1.72	0.72
1:B:232:ARG:CG	1:B:233:GLN:N	2.52	0.72
1:D:285:HIS:O	1:D:288:LEU:HG	1.89	0.72
1:D:91:GLN:HG3	1:D:94:ALA:HB3	1.72	0.72
1:D:305:THR:HG22	1:D:362:LEU:HD21	1.70	0.72
1:A:289:ILE:O	1:A:292:VAL:HG13	1.90	0.71
1:D:59:ARG:HA	1:D:66:PHE:HE1	1.54	0.71
1:D:298:ALA:CA	3:D:501:TB2:C8	2.68	0.71
1:D:164:LEU:HB3	1:D:487:ARG:HG2	1.72	0.71
1:B:230:THR:O	1:B:230:THR:HG23	1.90	0.71
1:D:84:ILE:HD12	1:D:84:ILE:H	1.55	0.71
1:A:290:LEU:HA	1:A:293:LEU:CG	2.18	0.71
4:B:602:SUC:C5	4:B:602:SUC:O3'	2.38	0.71
1:B:314:MET:HE1	1:B:450:PHE:CZ	2.25	0.71
1:C:296:PHE:C	1:C:296:PHE:CD1	2.63	0.71
1:D:401:TYR:C	1:D:402:PHE:CD2	2.65	0.71
1:B:146:ILE:HD12	1:B:445:GLU:HG2	1.72	0.71
1:C:231:HIS:CB	1:C:234:ILE:HG22	2.21	0.70
4:B:602:SUC:H1	4:B:602:SUC:C5'	2.21	0.70
1:D:201:LEU:HB3	1:D:241:ILE:HD11	1.74	0.70
1:C:66:PHE:CZ	1:C:77:VAL:CG2	2.74	0.70
1:D:42:ASN:O	1:D:45:GLN:HG3	1.91	0.70
1:C:58:LEU:HD11	1:C:66:PHE:CE1	2.27	0.70
1:A:100:LYS:O	1:D:225:LYS:HD3	1.91	0.70
1:D:282:GLU:OE1	1:D:282:GLU:C	2.30	0.70
2:D:500:HEM:HBC2	2:D:500:HEM:CHD	2.21	0.70
1:A:160:SER:O	1:A:161:LYS:CB	2.40	0.70
1:C:206:PHE:HE1	1:C:208:LEU:HD21	1.57	0.69
1:C:98:ARG:HA	1:C:98:ARG:HE	1.56	0.69
1:A:206:PHE:CD2	1:A:233:GLN:HG2	2.27	0.69
1:A:282:GLU:C	1:A:282:GLU:OE1	2.30	0.69
1:A:299:GLY:HA3	2:A:500:HEM:C2C	2.27	0.69
1:D:358:ARG:NH1	1:D:402:PHE:HD1	1.88	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:113:VAL:HA	1:D:116:ALA:CB	2.22	0.69
1:D:298:ALA:HB2	3:D:501:TB2:C6	2.22	0.69
1:C:371:VAL:HG21	1:C:382:ILE:CG2	2.23	0.69
1:D:182:ILE:HG21	5:D:610:CM5:H111	1.76	0.68
1:D:305:THR:CG2	1:D:362:LEU:HD21	2.24	0.68
1:D:100:LYS:HD2	1:D:101:ILE:H	1.58	0.68
1:A:162:GLY:O	1:A:487:ARG:NH1	2.27	0.68
1:C:225:LYS:HG3	1:C:226:TYR:CD2	2.29	0.68
1:A:278:ASP:OD1	1:A:279:PRO:N	2.27	0.68
1:A:218:GLU:HA	1:A:222:GLY:CA	2.23	0.68
1:D:245:ILE:HD13	1:D:292:VAL:HG21	1.76	0.67
1:C:29:LYS:C	1:C:30:LEU:HD12	2.14	0.67
1:D:470:LEU:O	1:D:472:PRO:HD3	1.93	0.67
1:A:299:GLY:HA3	2:A:500:HEM:C3C	2.30	0.67
4:D:604:SUC:H3	4:D:604:SUC:C1'	2.25	0.67
1:C:30:LEU:N	1:C:30:LEU:HD12	2.10	0.67
1:D:358:ARG:HA	1:D:396:LEU:HD13	1.75	0.67
1:A:456:ASN:O	1:A:491:ARG:HG2	1.95	0.67
1:C:287:ASN:HD22	1:C:287:ASN:C	1.98	0.67
1:D:437:LEU:O	1:D:437:LEU:HD23	1.93	0.67
1:D:140:ARG:HH22	1:D:148:GLU:CB	2.08	0.67
1:B:142:VAL:O	1:B:146:ILE:HG12	1.95	0.66
1:B:286:GLN:O	1:B:289:ILE:HG22	1.95	0.66
1:B:43:LEU:HD23	1:B:44:LEU:N	2.10	0.66
1:D:116:ALA:N	1:D:120:ARG:HH22	1.93	0.66
1:C:143:GLU:O	1:C:147:GLN:HG3	1.96	0.66
1:D:153:LEU:HD21	1:D:453:ILE:HD11	1.78	0.66
1:C:231:HIS:HB3	1:C:234:ILE:HG22	1.77	0.66
1:B:352:VAL:HG23	1:B:408:PHE:CZ	2.25	0.66
1:A:476:GLY:O	1:A:477:VAL:HG12	1.96	0.66
1:D:30:LEU:HD12	1:D:31:PRO:HD2	0.66	0.66
1:D:402:PHE:HZ	1:D:425:GLY:C	1.99	0.66
1:C:228:PRO:O	1:C:231:HIS:HD2	1.79	0.66
1:B:42:ASN:OD1	1:B:43:LEU:N	2.28	0.66
1:A:41:GLY:HA3	1:A:44:LEU:HB2	1.75	0.66
1:A:290:LEU:CA	1:A:293:LEU:HG	2.25	0.66
1:D:296:PHE:O	1:D:300:THR:HG23	1.96	0.66
1:D:342:ASP:O	1:D:346:MET:HB2	1.96	0.66
1:B:278:ASP:OD2	1:B:279:PRO:N	2.29	0.66
1:D:59:ARG:HA	1:D:66:PHE:CE1	2.31	0.65
1:C:58:LEU:C	1:C:58:LEU:HD12	2.17	0.65
1:D:214:SER:O	1:D:218:GLU:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:TYR:HD1	1:A:111:TYR:N	1.93	0.65
1:C:206:PHE:CD1	1:C:208:LEU:CD1	2.73	0.65
1:C:223:PHE:O	1:C:227:PHE:CE2	2.49	0.65
1:C:203:PHE:CZ	1:C:296:PHE:CE1	2.82	0.65
1:A:473:ARG:HH11	1:A:482:PRO:HA	1.61	0.65
1:B:153:LEU:HD21	1:B:453:ILE:HD11	1.79	0.65
1:C:219:LEU:HA	1:C:224:LEU:HB2	1.79	0.65
1:C:298:ALA:O	3:C:501:TB2:C1	2.44	0.65
1:A:235:TYR:CE1	1:D:44:LEU:HB3	2.31	0.65
1:D:374:ASP:HA	1:D:382:ILE:O	1.97	0.65
1:D:366:GLY:HA3	1:D:392:LEU:HD11	1.78	0.65
1:D:457:PHE:O	1:D:491:ARG:HD2	1.97	0.65
1:D:358:ARG:NH1	1:D:402:PHE:HB3	2.12	0.65
1:D:358:ARG:HH12	1:D:402:PHE:CB	2.10	0.65
1:A:218:GLU:C	1:A:222:GLY:HA3	2.18	0.65
1:D:222:GLY:O	1:D:225:LYS:HE2	1.97	0.65
1:A:219:LEU:C	1:A:219:LEU:CD1	2.65	0.65
1:A:253:ARG:NH1	1:A:276:LYS:NZ	2.45	0.65
1:B:219:LEU:HD12	1:B:219:LEU:O	1.95	0.65
1:C:371:VAL:HG21	1:C:383:PRO:O	1.96	0.65
1:A:293:LEU:C	1:A:293:LEU:HD12	2.14	0.64
1:C:65:VAL:HG21	1:C:378:ARG:HD2	1.79	0.64
1:D:305:THR:CB	1:D:362:LEU:HD11	2.26	0.64
1:D:398:ASP:OD1	1:D:400:ARG:N	2.30	0.64
4:B:602:SUC:C3'	4:B:602:SUC:O5	2.46	0.64
1:A:70:LEU:O	1:A:73:ARG:HG2	1.97	0.64
1:B:476:GLY:O	1:B:477:VAL:CG1	2.45	0.64
1:C:29:LYS:HA	1:C:381:VAL:HG12	1.79	0.64
3:B:501:TB2:H4	1:C:217:PHE:HB2	1.79	0.64
1:A:153:LEU:HD21	1:A:453:ILE:HD11	1.79	0.64
1:D:30:LEU:HD12	1:D:31:PRO:N	2.08	0.64
1:D:366:GLY:CA	1:D:392:LEU:HD11	2.26	0.64
1:A:218:GLU:O	1:A:222:GLY:N	2.31	0.64
1:C:94:ALA:HB1	1:C:375:THR:HG21	1.80	0.64
1:B:65:VAL:HG21	1:B:377:PHE:HE2	1.63	0.64
1:D:31:PRO:HA	1:D:380:TYR:CD2	2.32	0.64
1:D:295:LEU:CD1	2:D:500:HEM:CBC	2.71	0.64
1:D:298:ALA:HB1	3:D:501:TB2:C8	2.27	0.64
1:C:231:HIS:O	1:C:234:ILE:CG2	2.46	0.64
1:C:381:VAL:O	1:C:381:VAL:HG13	1.98	0.64
1:D:295:LEU:CD1	2:D:500:HEM:CAC	2.76	0.64
1:C:48:ARG:HH21	1:C:51:LEU:HD11	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:352:VAL:O	1:B:356:ILE:HG13	1.98	0.64
1:C:98:ARG:HE	1:C:99:GLY:N	1.96	0.64
1:C:164:LEU:HD12	1:C:164:LEU:H	1.63	0.64
1:A:290:LEU:O	1:A:293:LEU:HD12	1.97	0.63
1:A:164:LEU:HG	1:A:487:ARG:NH2	2.12	0.63
1:A:135:PHE:O	1:A:137:MET:N	2.31	0.63
1:B:88:LEU:HB2	1:B:431:LEU:CD1	2.28	0.63
1:C:206:PHE:HD1	1:C:208:LEU:CD1	2.10	0.63
1:A:292:VAL:O	1:A:296:PHE:N	2.29	0.63
1:C:42:ASN:OD1	1:C:42:ASN:N	2.30	0.63
1:C:226:TYR:CD2	1:C:226:TYR:N	2.65	0.63
1:D:78:LEU:H	1:D:78:LEU:HD22	1.64	0.63
1:A:316:LYS:O	1:A:318:PRO:HD3	1.98	0.63
1:D:316:LYS:O	1:D:465:PRO:HB3	1.99	0.63
1:B:36:PRO:HB3	1:B:69:TYR:CB	2.27	0.63
1:D:113:VAL:HA	1:D:116:ALA:HB3	1.77	0.63
1:A:296:PHE:CD1	1:A:296:PHE:C	2.72	0.63
1:D:402:PHE:CZ	1:D:425:GLY:C	2.72	0.63
1:C:226:TYR:N	1:C:226:TYR:HD2	1.95	0.63
1:A:264:PHE:HB3	5:A:605:CM5:H102	1.81	0.63
1:B:298:ALA:O	3:B:501:TB2:C1	2.46	0.63
1:C:52:LEU:O	1:C:56:LEU:HG	1.98	0.63
1:C:298:ALA:CB	3:C:501:TB2:C4	2.77	0.63
1:C:231:HIS:CB	1:C:234:ILE:CG2	2.77	0.63
3:D:501:TB2:C4	3:D:501:TB2:O1	2.47	0.63
1:C:208:LEU:CG	1:C:232:ARG:HG3	2.28	0.63
1:C:232:ARG:O	1:C:233:GLN:CB	2.45	0.63
1:C:232:ARG:O	1:C:233:GLN:HB3	1.99	0.63
1:D:398:ASP:OD1	1:D:398:ASP:C	2.37	0.63
1:C:299:GLY:HA3	2:C:500:HEM:C2C	2.34	0.63
1:B:476:GLY:O	1:B:477:VAL:HG13	1.99	0.63
1:B:202:PHE:CE1	1:B:241:ILE:HD13	2.34	0.63
1:A:291:THR:O	1:A:295:LEU:HB2	1.98	0.62
1:D:302:THR:HG22	2:D:500:HEM:CBB	2.29	0.62
1:B:429:PHE:O	1:B:430:SER:HB3	1.97	0.62
1:C:231:HIS:O	1:C:234:ILE:CB	2.47	0.62
1:D:286:GLN:O	1:D:290:LEU:HD12	1.96	0.62
1:B:269:LEU:HD23	1:B:272:MET:SD	2.39	0.62
1:C:320:VAL:O	1:C:324:VAL:HG23	2.00	0.62
1:D:402:PHE:HE2	1:D:425:GLY:CA	1.97	0.62
1:C:127:PHE:O	1:C:131:THR:HG22	2.00	0.62
1:B:403:GLU:O	1:B:405:PRO:HD3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:HIS:HD1	1:B:285:HIS:C	2.03	0.62
1:A:362:LEU:HD12	1:A:362:LEU:N	2.15	0.62
1:D:295:LEU:HD13	2:D:500:HEM:CAC	2.29	0.62
1:C:101:ILE:O	1:C:101:ILE:HG13	1.99	0.62
1:D:327:GLU:OE1	1:D:348:TYR:HB3	1.99	0.62
1:D:402:PHE:CZ	1:D:425:GLY:O	2.53	0.61
1:C:358:ARG:HG3	1:C:396:LEU:HD12	1.82	0.61
1:A:69:TYR:O	1:A:70:LEU:HD23	2.01	0.61
1:D:375:THR:O	1:D:381:VAL:HA	2.00	0.61
1:D:223:PHE:O	1:D:227:PHE:CD1	2.51	0.61
1:D:145:ARG:NH1	1:D:182:ILE:HA	2.15	0.61
1:D:470:LEU:H	1:D:470:LEU:HD13	1.65	0.61
1:C:82:ASP:O	1:C:86:GLU:HG3	2.01	0.61
1:A:308:ARG:HH22	1:A:483:SER:HA	1.60	0.61
1:C:266:ASP:O	1:C:270:LEU:HD23	2.00	0.61
1:C:154:VAL:HG13	1:C:457:PHE:CE2	2.36	0.61
1:B:332:ILE:HG23	1:B:336:ARG:HE	1.64	0.61
1:B:164:LEU:HG	1:B:487:ARG:CZ	2.31	0.61
1:D:173:SER:HB3	1:D:195:PHE:HE2	1.66	0.61
1:B:370:THR:HG22	1:B:387:GLU:HG2	1.82	0.61
1:D:325:GLN:O	1:D:328:ILE:HB	2.01	0.61
2:B:500:HEM:CMC	2:B:500:HEM:HBC2	2.31	0.60
1:D:283:PHE:CD1	1:D:283:PHE:C	2.73	0.60
1:A:290:LEU:O	1:A:293:LEU:CD1	2.49	0.60
2:D:500:HEM:CMB	2:D:500:HEM:HBB2	2.29	0.60
1:B:35:SER:O	1:B:42:ASN:HB2	2.01	0.60
1:B:268:TYR:CE2	5:B:606:CM5:H31A	2.36	0.60
1:B:84:ILE:HD11	1:B:391:VAL:O	1.99	0.60
1:B:477:VAL:CG2	1:B:477:VAL:O	2.49	0.60
1:D:398:ASP:OD1	1:D:399:PRO:N	2.34	0.60
1:B:346:MET:HB3	1:B:349:THR:OG1	2.02	0.60
1:D:223:PHE:HB3	1:D:227:PHE:CE1	2.29	0.60
1:A:235:TYR:HE1	1:D:44:LEU:HB3	1.67	0.60
1:C:183:VAL:HA	1:C:264:PHE:CB	2.32	0.60
1:D:32:PRO:HD3	1:D:380:TYR:CE2	2.37	0.60
1:D:296:PHE:CD1	1:D:300:THR:CG2	2.84	0.60
1:C:265:ILE:HG13	1:C:266:ASP:N	2.16	0.60
1:D:154:VAL:HG13	1:D:457:PHE:HE2	1.67	0.60
1:D:140:ARG:HH22	1:D:148:GLU:HG3	1.67	0.60
2:A:500:HEM:HBC2	2:A:500:HEM:CHD	2.26	0.60
1:D:78:LEU:HD11	1:D:388:VAL:CG1	2.32	0.60
1:B:164:LEU:HG	1:B:487:ARG:NE	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:ARG:O	1:B:201:LEU:HD12	2.01	0.60
1:B:214:SER:O	1:B:218:GLU:HG3	2.01	0.60
1:C:231:HIS:HB3	1:C:234:ILE:CG2	2.31	0.60
1:C:287:ASN:HD22	1:C:288:LEU:N	2.00	0.60
1:D:101:ILE:HD11	1:D:112:GLY:O	2.02	0.60
1:D:295:LEU:HD13	2:D:500:HEM:HBC1	1.77	0.59
1:A:39:VAL:HG13	1:D:106:PRO:CB	2.32	0.59
1:C:76:VAL:O	1:C:388:VAL:HA	2.02	0.59
1:C:231:HIS:O	1:C:234:ILE:HB	2.02	0.59
1:A:226:TYR:CD2	1:A:226:TYR:N	2.70	0.59
1:A:206:PHE:CD1	1:A:233:GLN:HG2	2.37	0.59
1:C:98:ARG:CA	1:C:98:ARG:HE	2.16	0.59
1:C:155:GLU:O	1:C:158:ARG:HG2	2.02	0.59
1:D:442:ALA:O	1:D:446:LEU:HG	2.02	0.59
1:B:212:PHE:O	1:B:216:VAL:HG23	2.02	0.59
1:D:188:PHE:HB3	1:D:195:PHE:HB2	1.84	0.59
1:C:167:ASN:ND2	1:C:486:ILE:HG21	2.17	0.59
1:B:224:LEU:O	1:B:224:LEU:HD12	2.02	0.59
1:D:48:ARG:C	1:D:49:LYS:HG3	2.23	0.59
1:C:154:VAL:HG13	1:C:457:PHE:HE2	1.67	0.59
1:B:107:ILE:HG13	1:B:108:PHE:N	2.17	0.59
1:B:225:LYS:CD	1:B:225:LYS:H	2.06	0.59
1:D:115:PHE:C	1:D:120:ARG:NH2	2.56	0.59
1:B:332:ILE:HG12	1:B:336:ARG:HH21	1.68	0.59
1:A:308:ARG:HH11	1:A:481:PRO:HG2	1.67	0.59
1:B:227:PHE:HD2	1:B:229:GLY:N	1.93	0.59
1:D:53:ARG:CG	1:D:53:ARG:HH11	2.15	0.59
1:C:200:ASP:O	1:C:204:GLN:HB3	2.02	0.59
1:B:299:GLY:HA2	2:B:500:HEM:C2C	2.37	0.58
1:B:314:MET:HE1	1:B:450:PHE:CE1	2.37	0.58
1:A:68:VAL:HG12	1:A:75:VAL:HG22	1.85	0.58
1:B:349:THR:HA	1:B:352:VAL:HG12	1.84	0.58
1:C:94:ALA:HB1	1:C:375:THR:CG2	2.33	0.58
1:D:298:ALA:CB	3:D:501:TB2:C6	2.81	0.58
1:A:434:ARG:HA	1:A:434:ARG:NE	2.18	0.58
1:D:429:PHE:O	1:D:430:SER:CB	2.52	0.58
1:C:370:THR:HA	1:C:386:THR:O	2.03	0.58
1:B:314:MET:HE1	1:B:450:PHE:HZ	1.69	0.58
1:D:127:PHE:HD1	1:D:128:SER:N	2.01	0.58
1:B:313:LEU:HD21	1:B:408:PHE:CD1	2.38	0.58
1:D:321:THR:O	1:D:324:VAL:HG22	2.03	0.58
1:B:113:VAL:O	1:B:113:VAL:HG22	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:109:GLN:O	1:C:113:VAL:HG23	2.03	0.58
1:B:314:MET:CE	1:B:450:PHE:CZ	2.86	0.58
1:D:116:ALA:N	1:D:120:ARG:NH2	2.51	0.58
1:B:113:VAL:HG22	1:B:116:ALA:HB2	1.86	0.58
1:B:209:ILE:HG22	1:C:207:SER:CB	2.33	0.58
1:D:358:ARG:HG3	1:D:396:LEU:HB3	1.85	0.58
1:D:398:ASP:OD1	1:D:400:ARG:HG2	2.02	0.58
1:C:222:GLY:O	1:C:225:LYS:HE2	2.03	0.58
1:D:76:VAL:O	1:D:388:VAL:HA	2.04	0.58
1:C:34:PRO:HD3	1:C:62:TYR:CE2	2.39	0.58
1:C:296:PHE:HD1	1:C:296:PHE:C	2.07	0.58
1:D:305:THR:HB	1:D:362:LEU:HD11	1.84	0.58
1:A:111:TYR:N	1:A:111:TYR:CD1	2.66	0.58
1:D:361:ASP:OD2	1:D:393:SER:HB3	2.04	0.58
1:C:245:ILE:HG23	1:C:246:GLY:N	2.19	0.58
1:B:101:ILE:HG13	1:B:101:ILE:O	2.02	0.58
1:D:398:ASP:OD2	1:D:400:ARG:HG3	2.04	0.57
1:D:245:ILE:HG22	1:D:245:ILE:O	2.03	0.57
1:D:353:ILE:HG22	1:D:354:HIS:N	2.19	0.57
1:D:164:LEU:HB3	1:D:487:ARG:CG	2.33	0.57
1:D:473:ARG:O	1:D:479:ASN:HA	2.05	0.57
1:B:457:PHE:CD1	1:B:488:PHE:HB3	2.39	0.57
1:B:43:LEU:HD23	1:B:43:LEU:C	2.25	0.57
1:D:280:SER:O	1:D:283:PHE:CB	2.49	0.57
1:B:308:ARG:HG2	1:B:484:TYR:CE1	2.38	0.57
1:D:358:ARG:NH1	1:D:402:PHE:CG	2.72	0.57
1:D:95:PHE:N	1:D:95:PHE:CD2	2.72	0.57
1:D:48:ARG:O	1:D:49:LYS:HG3	2.05	0.57
1:C:245:ILE:HG21	1:C:289:ILE:CB	2.35	0.57
1:C:240:GLU:O	1:C:243:THR:HB	2.05	0.57
1:B:463:VAL:HG13	1:B:467:ASP:HB3	1.86	0.57
1:D:164:LEU:HD22	1:D:487:ARG:CZ	2.34	0.57
1:D:145:ARG:HH12	1:D:182:ILE:HA	1.68	0.57
1:C:435:ILE:HG12	1:C:436:CYS:N	2.19	0.57
1:A:289:ILE:O	1:A:292:VAL:HG12	2.04	0.57
1:D:295:LEU:O	1:D:295:LEU:HD12	2.05	0.57
2:C:500:HEM:HBC2	2:C:500:HEM:CHD	2.31	0.57
1:B:112:GLY:O	1:B:113:VAL:HG12	2.05	0.57
1:C:98:ARG:NE	1:C:98:ARG:HA	2.20	0.57
1:D:472:PRO:HB2	1:D:479:ASN:HB2	1.86	0.57
1:C:37:LEU:HD13	1:C:42:ASN:CB	2.34	0.57
1:D:95:PHE:N	1:D:95:PHE:HD2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:ARG:HG3	1:A:49:LYS:N	2.20	0.57
1:C:299:GLY:HA2	2:C:500:HEM:C1C	2.40	0.56
1:D:221:SER:HG	1:D:223:PHE:HD2	1.53	0.56
1:D:86:GLU:O	1:D:90:ASP:OD2	2.23	0.56
1:C:227:PHE:N	1:C:228:PRO:HD3	2.20	0.56
1:B:429:PHE:HB3	1:B:436:CYS:HB3	1.87	0.56
1:A:157:LEU:HB3	1:A:457:PHE:CZ	2.40	0.56
1:D:117:ASN:H	1:D:120:ARG:HH22	1.54	0.56
1:A:226:TYR:HD2	1:A:226:TYR:N	2.02	0.56
1:C:327:GLU:OE1	1:C:346:MET:HB3	2.05	0.56
4:A:601:SUC:O1'	4:A:601:SUC:H1	2.04	0.56
1:D:127:PHE:CD1	1:D:128:SER:N	2.73	0.56
1:D:146:ILE:HD13	1:D:445:GLU:HG2	1.86	0.56
1:C:231:HIS:O	1:C:234:ILE:N	2.35	0.56
1:B:43:LEU:HD23	1:B:45:GLN:H	1.71	0.56
1:B:243:THR:O	1:B:247:GLN:HG3	2.06	0.56
1:A:253:ARG:NH1	1:A:276:LYS:HZ1	2.04	0.56
1:A:206:PHE:CD1	1:A:206:PHE:O	2.58	0.56
1:C:296:PHE:O	1:C:296:PHE:CD1	2.59	0.56
1:C:298:ALA:HB2	3:C:501:TB2:C4	2.36	0.56
1:C:342:ASP:O	1:C:346:MET:HG3	2.06	0.56
1:B:137:MET:HE1	1:B:264:PHE:CD2	2.41	0.56
1:B:226:TYR:CD1	1:C:70:LEU:HD13	2.40	0.56
1:B:314:MET:CE	1:B:450:PHE:HZ	2.19	0.56
1:A:286:GLN:HA	1:A:289:ILE:HG22	1.86	0.56
1:C:233:GLN:NE2	1:C:236:ARG:CD	2.40	0.56
1:C:58:LEU:HA	1:C:61:LYS:CD	2.36	0.56
1:A:362:LEU:CD1	1:A:362:LEU:N	2.69	0.56
1:C:154:VAL:O	1:C:158:ARG:HG2	2.05	0.56
1:B:113:VAL:HG13	1:B:113:VAL:O	2.05	0.56
1:C:68:VAL:HG13	1:C:75:VAL:HG13	1.88	0.56
1:D:358:ARG:NH1	1:D:402:PHE:CB	2.69	0.55
1:D:288:LEU:HD12	1:D:289:ILE:H	1.71	0.55
1:B:299:GLY:HA3	2:B:500:HEM:C3C	2.41	0.55
1:D:183:VAL:O	1:D:265:ILE:HG12	2.06	0.55
1:C:81:THR:O	1:C:85:ARG:HB2	2.07	0.55
1:A:192:ASP:OD1	1:A:194:VAL:HG23	2.04	0.55
1:B:229:GLY:O	1:B:230:THR:CG2	2.51	0.55
1:D:402:PHE:CZ	1:D:425:GLY:HA3	2.38	0.55
1:B:299:GLY:CA	2:B:500:HEM:C1C	2.85	0.55
1:C:371:VAL:CG2	1:C:383:PRO:O	2.54	0.55
1:D:257:ASP:HB3	1:D:260:ASN:OD1	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:54:SER:O	1:D:58:LEU:HB2	2.06	0.55
1:B:38:PRO:C	1:B:39:VAL:CG1	2.68	0.55
1:A:473:ARG:HG2	1:A:480:VAL:HG13	1.87	0.55
1:D:257:ASP:HB3	1:D:260:ASN:H	1.71	0.55
1:C:224:LEU:HD13	1:C:225:LYS:N	2.21	0.55
1:D:80:GLY:O	1:D:84:ILE:HD12	2.06	0.55
1:C:48:ARG:HE	1:C:51:LEU:HD21	1.72	0.55
1:D:420:LEU:HD21	4:D:604:SUC:C4	2.34	0.55
1:A:226:TYR:HD1	1:D:70:LEU:HD13	1.71	0.55
1:A:303:THR:OG1	2:A:500:HEM:CBB	2.55	0.55
1:B:35:SER:O	1:B:42:ASN:CB	2.55	0.55
1:B:105:ASP:OD2	1:B:107:ILE:HG23	2.07	0.55
1:C:224:LEU:CD1	1:C:225:LYS:N	2.71	0.54
1:D:302:THR:CG2	2:D:500:HEM:CAB	2.84	0.54
1:B:36:PRO:HA	1:B:42:ASN:HB3	1.89	0.54
1:A:474:GLU:OE1	1:A:474:GLU:HA	2.06	0.54
1:A:288:LEU:HD12	1:A:288:LEU:C	2.27	0.54
1:C:58:LEU:HD11	1:C:66:PHE:CD2	2.42	0.54
1:A:208:LEU:O	1:D:207:SER:HB2	2.07	0.54
1:A:291:THR:HG21	5:A:605:CM5:H72	1.88	0.54
1:B:225:LYS:CD	1:B:225:LYS:N	2.70	0.54
1:D:154:VAL:HG13	1:D:457:PHE:CE2	2.43	0.54
5:D:610:CM5:O22	5:D:610:CM5:H11	2.08	0.54
1:C:144:GLU:OE1	1:C:144:GLU:N	2.37	0.54
1:A:51:LEU:HD12	1:A:51:LEU:O	2.08	0.54
1:A:150:ALA:O	1:A:154:VAL:HG23	2.08	0.54
1:C:234:ILE:HG23	1:C:235:TYR:N	2.21	0.54
1:C:265:ILE:CG1	1:C:266:ASP:N	2.71	0.54
1:B:207:SER:HA	1:C:208:LEU:O	2.07	0.54
1:B:69:TYR:CE1	1:B:74:PRO:HB3	2.43	0.54
1:D:140:ARG:HG3	1:D:145:ARG:HE	1.73	0.54
1:B:183:VAL:HA	1:B:264:PHE:HB2	1.88	0.54
1:D:397:HIS:HA	1:D:405:PRO:CB	2.38	0.54
1:C:61:LYS:NZ	1:C:62:TYR:HE2	2.03	0.54
4:A:601:SUC:O1'	4:A:601:SUC:C1	2.52	0.54
1:B:367:VAL:HG13	1:C:221:SER:CB	2.32	0.54
1:D:328:ILE:HA	1:D:346:MET:HE3	1.91	0.54
1:D:171:PHE:CD2	1:D:307:LEU:HB3	2.43	0.54
1:B:38:PRO:O	1:B:39:VAL:HG13	2.07	0.53
1:B:231:HIS:O	1:B:235:TYR:CB	2.56	0.53
1:D:397:HIS:CD2	1:D:405:PRO:HB2	2.43	0.53
1:C:40:LEU:H	1:C:40:LEU:HD22	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:SER:HB3	1:D:367:VAL:CG2	2.35	0.53
1:D:75:VAL:HG23	1:D:387:GLU:HB2	1.90	0.53
1:B:146:ILE:CD1	1:B:445:GLU:HG2	2.38	0.53
1:C:424:GLU:OE1	1:C:424:GLU:HA	2.08	0.53
1:C:33:GLY:HA3	1:C:67:THR:O	2.07	0.53
1:D:150:ALA:O	1:D:154:VAL:HG23	2.08	0.53
1:A:290:LEU:HD12	1:A:291:THR:H	1.71	0.53
1:C:36:PRO:HA	1:C:42:ASN:HD21	1.74	0.53
1:D:36:PRO:HG3	1:D:69:TYR:CD2	2.44	0.53
1:D:39:VAL:HG12	1:D:40:LEU:HD22	1.91	0.53
4:A:601:SUC:C5	4:A:601:SUC:H1'1	2.39	0.53
1:D:324:VAL:HG12	1:D:348:TYR:HE2	1.73	0.53
1:D:231:HIS:HA	1:D:234:ILE:HB	1.89	0.53
1:A:296:PHE:O	1:A:300:THR:HB	2.09	0.53
1:A:358:ARG:NH2	1:A:359:LEU:HD21	2.24	0.53
1:D:53:ARG:HG3	1:D:53:ARG:NH1	2.20	0.53
1:B:268:TYR:O	1:B:272:MET:HG3	2.09	0.53
1:B:349:THR:O	1:B:352:VAL:HG12	2.08	0.53
1:D:173:SER:HB3	1:D:195:PHE:CE2	2.44	0.53
1:B:308:ARG:HG2	1:B:484:TYR:HE1	1.74	0.53
1:B:43:LEU:HD23	1:B:45:GLN:N	2.23	0.53
1:A:293:LEU:HD12	1:A:294:SER:CA	2.35	0.52
1:C:434:ARG:NH1	1:C:434:ARG:HA	2.24	0.52
1:D:376:GLN:HA	1:D:380:TYR:O	2.09	0.52
1:D:140:ARG:HH22	1:D:148:GLU:HB2	1.74	0.52
1:D:88:LEU:O	1:D:88:LEU:HD12	2.09	0.52
1:D:113:VAL:HA	1:D:116:ALA:HB2	1.91	0.52
1:D:473:ARG:N	1:D:480:VAL:O	2.37	0.52
1:D:349:THR:HG22	1:D:353:ILE:HD13	1.92	0.52
1:C:153:LEU:O	1:C:157:LEU:HB2	2.09	0.52
1:B:290:LEU:O	1:B:294:SER:HB2	2.09	0.52
1:A:269:LEU:HD23	1:A:272:MET:CE	2.40	0.52
1:D:140:ARG:HH22	1:D:148:GLU:CG	2.21	0.52
1:B:326:LYS:HA	1:B:329:GLU:HB2	1.91	0.52
1:D:32:PRO:O	1:D:66:PHE:HB2	2.10	0.52
1:C:58:LEU:O	1:C:61:LYS:HG2	2.10	0.52
1:D:470:LEU:N	1:D:470:LEU:HD13	2.24	0.52
4:C:603:SUC:H1'2	4:C:603:SUC:O5	2.08	0.52
1:C:107:ILE:HG13	1:C:108:PHE:H	1.75	0.52
1:B:441:ILE:O	1:B:445:GLU:HG3	2.10	0.52
1:A:487:ARG:HG2	1:A:489:LEU:CD1	2.40	0.52
1:C:30:LEU:N	1:C:30:LEU:CD1	2.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:402:PHE:CZ	1:D:425:GLY:CA	2.93	0.52
1:C:226:TYR:C	1:C:228:PRO:HD3	2.31	0.52
1:D:292:VAL:HG23	1:D:293:LEU:N	2.25	0.52
1:D:429:PHE:O	1:D:430:SER:HB3	2.10	0.52
1:C:124:LEU:C	1:C:124:LEU:HD13	2.30	0.52
1:D:397:HIS:HA	1:D:405:PRO:HB3	1.91	0.52
1:D:374:ASP:OD2	1:D:381:VAL:HG22	2.10	0.51
1:D:356:ILE:HG22	1:D:357:GLN:N	2.25	0.51
1:A:235:TYR:HE1	1:D:44:LEU:HD13	1.75	0.51
1:B:226:TYR:OH	1:C:387:GLU:OE1	2.28	0.51
1:D:427:MET:N	1:D:428:PRO:CD	2.72	0.51
1:C:58:LEU:O	1:C:58:LEU:HD12	2.10	0.51
1:B:340:LEU:HD13	1:B:444:THR:HG23	1.93	0.51
1:D:285:HIS:O	1:D:285:HIS:HD2	1.93	0.51
1:C:32:PRO:CB	1:C:62:TYR:CD1	2.77	0.51
1:A:88:LEU:O	1:A:92:ALA:HA	2.11	0.51
1:D:477:VAL:O	1:D:477:VAL:HG23	2.10	0.51
1:A:473:ARG:O	1:A:473:ARG:HG2	2.11	0.51
1:A:387:GLU:OE1	1:D:225:LYS:NZ	2.44	0.51
1:D:353:ILE:O	1:D:356:ILE:HB	2.09	0.51
1:D:257:ASP:CB	1:D:260:ASN:OD1	2.58	0.51
1:B:345:LYS:C	1:B:347:PRO:HD3	2.31	0.51
1:D:268:TYR:CE1	1:D:284:HIS:ND1	2.78	0.51
1:C:225:LYS:HE3	1:C:226:TYR:HE2	1.75	0.51
1:A:441:ILE:O	1:A:441:ILE:HD13	2.11	0.51
1:D:135:PHE:CE1	1:D:261:PRO:HG2	2.45	0.51
1:A:298:ALA:CB	3:A:501:TB2:H7	2.36	0.51
1:D:398:ASP:OD1	1:D:400:ARG:CG	2.59	0.51
1:A:400:ARG:NH1	1:A:400:ARG:HB3	2.25	0.51
1:C:426:PHE:O	1:C:426:PHE:CD2	2.63	0.51
1:B:314:MET:HG3	1:B:321:THR:OG1	2.10	0.51
1:D:439:GLU:HG3	1:D:440:GLY:N	2.26	0.51
1:D:305:THR:HG21	1:D:362:LEU:HD11	1.91	0.51
1:A:217:PHE:O	1:A:217:PHE:CD1	2.64	0.51
1:B:459:ILE:CG2	1:B:486:ILE:HD11	2.40	0.51
1:C:364:PRO:HA	1:C:393:SER:HB2	1.93	0.51
1:A:312:LEU:HD13	1:A:484:TYR:CD1	2.46	0.51
1:A:288:LEU:HD13	5:A:605:CM5:C8	2.38	0.50
1:A:367:VAL:HG21	2:A:500:HEM:HAA2	1.91	0.50
1:B:232:ARG:HG3	1:B:233:GLN:H	1.68	0.50
1:D:100:LYS:HE2	1:D:116:ALA:HB1	1.93	0.50
1:A:114:ILE:O	1:A:120:ARG:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:VAL:O	1:B:220:PHE:HD2	1.93	0.50
1:A:217:PHE:C	1:A:217:PHE:CD1	2.82	0.50
1:B:213:SER:HB3	1:C:297:PHE:CB	2.41	0.50
1:A:128:SER:O	1:A:132:MET:HB2	2.11	0.50
1:D:399:PRO:O	1:D:402:PHE:O	2.30	0.50
1:B:404:THR:HB	1:B:407:THR:HB	1.92	0.50
1:D:203:PHE:HZ	1:D:300:THR:HG1	0.69	0.50
1:A:208:LEU:O	1:D:207:SER:HB3	2.09	0.50
1:C:354:HIS:NE2	4:C:603:SUC:H3	2.27	0.50
1:C:314:MET:SD	1:C:450:PHE:HZ	2.35	0.50
1:B:219:LEU:O	1:C:101:ILE:HG21	2.12	0.50
1:B:105:ASP:CG	1:B:106:PRO:HD2	2.32	0.50
1:A:429:PHE:CE1	1:A:439:GLU:HA	2.47	0.50
4:B:602:SUC:O3'	4:B:602:SUC:O5	2.30	0.50
1:D:369:HIS:O	1:D:388:VAL:N	2.45	0.50
1:D:137:MET:HB3	1:D:140:ARG:O	2.12	0.50
1:C:435:ILE:HG12	1:C:436:CYS:H	1.76	0.50
1:B:443:ARG:NH2	4:B:602:SUC:H3'	2.27	0.50
1:D:78:LEU:HD22	1:D:389:PHE:O	2.12	0.50
1:C:320:VAL:HG21	1:C:408:PHE:HE2	1.76	0.50
1:D:310:GLY:HA3	1:D:356:ILE:HD13	1.94	0.50
1:A:310:GLY:O	1:A:314:MET:HG2	2.12	0.50
1:A:298:ALA:O	1:A:302:THR:OG1	2.30	0.49
1:D:296:PHE:HE1	1:D:300:THR:HG21	1.66	0.49
1:A:287:ASN:OD1	1:A:287:ASN:C	2.50	0.49
1:A:115:PHE:HE2	1:A:290:LEU:CD1	2.24	0.49
1:A:299:GLY:CA	2:A:500:HEM:C1C	2.95	0.49
1:B:227:PHE:CD2	1:B:228:PRO:HD2	2.47	0.49
1:C:298:ALA:HB1	3:C:501:TB2:C4	2.42	0.49
1:C:197:ARG:HD3	1:C:240:GLU:OE2	2.13	0.49
1:C:350:ASP:OD2	4:C:603:SUC:O6	2.25	0.49
1:A:217:PHE:HD2	1:D:477:VAL:HG11	1.78	0.49
1:D:189:ASP:HB3	1:D:192:ASP:HB2	1.93	0.49
1:A:299:GLY:HA2	2:A:500:HEM:C1C	2.47	0.49
1:D:282:GLU:OE1	1:D:282:GLU:O	2.30	0.49
1:A:253:ARG:NH1	1:A:276:LYS:HZ3	2.10	0.49
1:C:363:ILE:N	1:C:363:ILE:HD12	2.28	0.49
1:C:299:GLY:CA	2:C:500:HEM:C2C	2.95	0.49
1:B:298:ALA:HB2	3:B:501:TB2:C5	2.43	0.49
1:C:211:SER:O	1:C:215:GLN:HG3	2.12	0.49
1:B:355:GLU:OE1	1:B:413:PHE:HE2	1.95	0.49
1:A:174:ILE:HG13	1:A:175:THR:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:305:THR:CG2	1:D:362:LEU:HD11	2.42	0.49
4:D:604:SUC:H3	4:D:604:SUC:H1'2	1.95	0.49
1:D:283:PHE:O	1:D:283:PHE:HD1	1.95	0.49
1:C:88:LEU:HD21	1:C:369:HIS:CD2	2.47	0.49
1:C:381:VAL:O	1:C:381:VAL:CG1	2.60	0.49
1:A:107:ILE:HD12	1:A:108:PHE:N	2.27	0.49
2:D:500:HEM:HHD	2:D:500:HEM:CBC	2.39	0.49
1:B:227:PHE:HE2	1:B:230:THR:H	1.61	0.49
1:C:315:LEU:HD11	1:C:486:ILE:HD12	1.94	0.49
1:D:165:LEU:HG	1:D:166:ASP:N	2.28	0.49
1:D:172:HIS:CE1	1:D:203:PHE:HB3	2.47	0.49
1:B:313:LEU:HD21	1:B:408:PHE:CE1	2.47	0.49
1:A:293:LEU:C	1:A:293:LEU:CD1	2.75	0.49
1:A:303:THR:OG1	2:A:500:HEM:HBB2	2.13	0.49
1:A:101:ILE:CG2	1:D:219:LEU:O	2.50	0.48
1:C:434:ARG:HG3	2:C:500:HEM:O1A	2.13	0.48
1:C:245:ILE:HG13	1:C:289:ILE:HA	1.95	0.48
1:C:225:LYS:HG3	1:C:226:TYR:HE2	1.72	0.48
1:B:363:ILE:HD12	2:B:500:HEM:HHB	1.95	0.48
1:A:387:GLU:CD	1:D:225:LYS:HZ1	2.17	0.48
1:D:479:ASN:OD1	1:D:479:ASN:O	2.31	0.48
1:C:141:SER:O	1:C:145:ARG:HG3	2.13	0.48
1:C:316:LYS:HG2	1:C:317:TYR:CE2	2.48	0.48
1:A:34:PRO:HG3	1:A:58:LEU:HD22	1.95	0.48
1:A:293:LEU:HA	1:A:296:PHE:HB3	1.93	0.48
1:A:299:GLY:CA	2:A:500:HEM:C2C	2.95	0.48
1:D:302:THR:CG2	2:D:500:HEM:CBB	2.91	0.48
1:A:41:GLY:CA	1:A:44:LEU:HD13	2.43	0.48
1:C:217:PHE:C	1:C:217:PHE:CD1	2.86	0.48
1:B:463:VAL:CG1	1:B:467:ASP:HB3	2.43	0.48
1:C:107:ILE:HG13	1:C:108:PHE:N	2.29	0.48
1:C:362:LEU:C	1:C:364:PRO:HD3	2.34	0.48
1:D:302:THR:CG2	2:D:500:HEM:C3B	2.92	0.48
1:B:219:LEU:HD12	1:B:219:LEU:C	2.32	0.48
1:A:363:ILE:CG2	1:A:366:GLY:HA2	2.41	0.48
1:A:65:VAL:HG21	1:A:377:PHE:HE2	1.78	0.48
1:C:384:LYS:O	1:C:385:ASN:HB2	2.13	0.48
1:C:112:GLY:O	1:C:116:ALA:HB2	2.13	0.48
1:C:208:LEU:H	1:C:208:LEU:CD1	2.20	0.48
1:A:127:PHE:CE1	5:A:605:CM5:H111	2.48	0.48
1:D:285:HIS:HA	1:D:288:LEU:CD2	2.43	0.48
1:D:438:GLY:HA3	2:D:500:HEM:C2C	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:321:THR:HG21	1:D:459:ILE:HD11	1.95	0.48
1:D:43:LEU:CB	1:D:70:LEU:HD23	2.44	0.48
1:D:234:ILE:HG22	1:D:235:TYR:N	2.27	0.48
1:A:426:PHE:CZ	1:A:428:PRO:HG2	2.49	0.48
1:D:366:GLY:N	1:D:392:LEU:CD1	2.76	0.48
4:A:601:SUC:O1'	4:A:601:SUC:O5	2.30	0.48
1:C:288:LEU:HD13	1:C:288:LEU:C	2.34	0.48
1:A:362:LEU:CD1	1:A:362:LEU:H	2.25	0.48
1:A:298:ALA:O	3:A:501:TB2:C1	2.62	0.48
1:C:174:ILE:HG13	1:C:175:THR:N	2.29	0.48
1:D:427:MET:N	1:D:428:PRO:HD3	2.29	0.48
1:D:115:PHE:C	1:D:120:ARG:HH21	2.17	0.48
1:D:145:ARG:HD3	1:D:181:SER:OG	2.14	0.48
1:B:132:MET:HE3	5:B:607:CM5:H72	1.95	0.48
1:B:427:MET:N	1:B:428:PRO:HD3	2.29	0.48
1:B:114:ILE:HG23	1:B:115:PHE:N	2.29	0.48
1:A:93:GLU:HG2	1:A:433:LYS:NZ	2.28	0.48
1:A:245:ILE:HD13	1:A:289:ILE:HA	1.95	0.48
1:A:360:GLY:C	1:A:362:LEU:HD12	2.34	0.48
1:C:157:LEU:HD11	1:C:488:PHE:CD2	2.49	0.48
1:C:404:THR:HB	1:C:407:THR:HB	1.96	0.48
1:B:309:TYR:CZ	1:B:360:GLY:HA2	2.49	0.48
1:D:197:ARG:NH1	1:D:201:LEU:HD13	2.29	0.48
1:C:328:ILE:HA	1:C:346:MET:HE1	1.96	0.48
1:B:32:PRO:O	1:B:66:PHE:HB2	2.14	0.48
1:B:51:LEU:HD11	1:B:365:PHE:CZ	2.48	0.48
1:C:230:THR:OG1	1:C:230:THR:O	2.30	0.48
4:D:604:SUC:H3	4:D:604:SUC:HO1'	1.77	0.47
1:D:350:ASP:OD2	4:D:604:SUC:O4	2.32	0.47
1:A:487:ARG:HG2	1:A:489:LEU:HD11	1.96	0.47
1:B:309:TYR:HB2	1:B:481:PRO:HG3	1.96	0.47
1:B:180:CYS:HG	1:B:296:PHE:HZ	1.62	0.47
1:A:403:GLU:O	1:A:405:PRO:HD3	2.13	0.47
4:D:604:SUC:O1'	4:D:604:SUC:O2	2.33	0.47
1:D:375:THR:HG22	1:D:376:GLN:H	1.79	0.47
1:D:396:LEU:HD21	1:D:428:PRO:HD3	1.95	0.47
1:B:313:LEU:HD12	1:B:470:LEU:HD13	1.95	0.47
1:A:276:LYS:O	1:A:277:SER:CB	2.60	0.47
1:A:382:ILE:HG22	1:A:386:THR:HB	1.97	0.47
1:C:442:ALA:HB1	2:C:500:HEM:CBB	2.45	0.47
1:D:53:ARG:NH1	1:D:53:ARG:CG	2.76	0.47
1:C:242:ASN:HA	1:C:245:ILE:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:312:LEU:HB2	1:B:484:TYR:CE1	2.50	0.47
1:D:430:SER:HB2	2:D:500:HEM:HMA2	1.96	0.47
1:D:76:VAL:HG12	1:D:387:GLU:O	2.14	0.47
1:B:43:LEU:CD2	1:B:43:LEU:C	2.83	0.47
1:B:51:LEU:C	1:B:51:LEU:HD23	2.34	0.47
1:B:261:PRO:HG3	1:B:270:LEU:HD11	1.97	0.47
1:C:331:VAL:HG13	1:C:345:LYS:HE2	1.95	0.47
1:C:208:LEU:HB3	1:C:232:ARG:HG3	1.96	0.47
1:A:39:VAL:HG13	1:D:106:PRO:HB3	1.97	0.47
1:D:328:ILE:HD13	1:D:455:GLN:HB2	1.97	0.47
1:B:37:LEU:O	1:B:41:GLY:O	2.31	0.47
1:B:42:ASN:CG	1:B:43:LEU:N	2.68	0.47
1:A:282:GLU:OE1	1:A:283:PHE:N	2.48	0.47
1:D:141:SER:OG	1:D:142:VAL:N	2.47	0.47
1:C:48:ARG:HD3	1:C:474:GLU:CD	2.35	0.47
1:C:48:ARG:NH1	1:C:48:ARG:HB3	2.30	0.47
1:C:154:VAL:O	1:C:158:ARG:HD2	2.14	0.47
1:D:173:SER:HA	1:D:199:LEU:HD11	1.97	0.47
1:D:268:TYR:HE1	1:D:284:HIS:ND1	2.12	0.47
1:D:246:GLY:O	1:D:250:GLU:HB2	2.14	0.47
1:D:262:ARG:HG2	1:D:266:ASP:OD2	2.14	0.47
1:A:320:VAL:O	1:A:324:VAL:HG23	2.15	0.47
1:B:54:SER:OG	1:B:55:PHE:N	2.48	0.47
1:A:441:ILE:O	1:A:445:GLU:HG3	2.15	0.47
1:A:234:ILE:HG22	1:A:235:TYR:N	2.30	0.47
1:A:69:TYR:CE2	1:A:74:PRO:HB3	2.50	0.47
1:C:137:MET:CB	1:C:145:ARG:HH21	2.27	0.47
1:A:30:LEU:HD21	1:A:383:PRO:HD3	1.97	0.47
1:D:298:ALA:HB1	3:D:501:TB2:C7	2.32	0.47
1:D:42:ASN:HA	1:D:45:GLN:HG3	1.97	0.47
1:C:39:VAL:CG1	1:C:40:LEU:N	2.78	0.47
1:D:268:TYR:O	1:D:272:MET:HG2	2.15	0.47
1:C:36:PRO:HB3	1:C:69:TYR:CB	2.30	0.46
1:D:328:ILE:O	1:D:332:ILE:N	2.40	0.46
1:B:448:LEU:HA	1:B:448:LEU:HD12	1.72	0.46
3:D:501:TB2:H4	3:D:501:TB2:O1	2.13	0.46
1:A:364:PRO:HA	1:A:393:SER:HB2	1.96	0.46
1:D:402:PHE:N	1:D:402:PHE:CD2	2.83	0.46
1:D:302:THR:HG21	2:D:500:HEM:CAB	2.45	0.46
1:B:429:PHE:O	1:B:430:SER:CB	2.63	0.46
1:A:40:LEU:C	1:A:40:LEU:HD23	2.36	0.46
1:B:291:THR:HG21	5:B:606:CM5:H72	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:127:PHE:CD1	1:D:127:PHE:C	2.88	0.46
1:D:288:LEU:HD12	1:D:289:ILE:CG1	2.46	0.46
1:D:124:LEU:HD22	1:D:291:THR:HG23	1.98	0.46
1:C:245:ILE:HG23	1:C:246:GLY:H	1.80	0.46
1:D:165:LEU:HG	1:D:166:ASP:H	1.80	0.46
1:B:28:GLY:O	1:B:381:VAL:HB	2.14	0.46
1:B:225:LYS:HD3	1:C:101:ILE:HA	1.98	0.46
1:B:368:PRO:HD2	1:C:221:SER:O	2.16	0.46
1:D:53:ARG:HD3	1:D:53:ARG:O	2.16	0.46
1:D:88:LEU:HD12	1:D:92:ALA:HA	1.97	0.46
1:D:140:ARG:HD2	1:D:140:ARG:HA	1.46	0.46
1:C:39:VAL:HG13	1:C:40:LEU:N	2.30	0.46
1:B:471:THR:HG22	1:B:472:PRO:HD2	1.98	0.46
1:C:44:LEU:HD23	1:C:44:LEU:C	2.36	0.46
1:D:386:THR:HG22	1:D:387:GLU:H	1.80	0.46
1:C:373:LYS:O	1:C:375:THR:HG23	2.16	0.46
1:B:137:MET:HE1	1:B:264:PHE:CE2	2.50	0.46
1:D:278:ASP:OD1	1:D:278:ASP:C	2.54	0.46
1:A:115:PHE:CE2	1:A:290:LEU:CD1	2.98	0.46
1:D:280:SER:O	1:D:283:PHE:N	2.49	0.46
1:C:255:THR:O	1:C:255:THR:CG2	2.60	0.46
1:D:141:SER:O	1:D:145:ARG:HG3	2.15	0.46
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.74	0.46
1:C:369:HIS:CE1	2:C:500:HEM:O2A	2.68	0.46
1:D:370:THR:HG22	1:D:387:GLU:HA	1.98	0.46
1:C:383:PRO:HD2	1:C:386:THR:OG1	2.15	0.46
1:D:245:ILE:O	1:D:245:ILE:CG2	2.64	0.46
1:D:140:ARG:HG3	1:D:145:ARG:NE	2.30	0.46
1:C:324:VAL:HG13	1:C:349:THR:OG1	2.16	0.46
1:B:362:LEU:CD1	1:B:362:LEU:N	2.79	0.46
1:B:119:GLU:HA	1:B:122:ARG:CZ	2.45	0.46
1:A:212:PHE:HE2	1:D:238:LEU:HB2	1.80	0.46
1:A:209:ILE:HA	1:D:206:PHE:O	2.16	0.46
1:B:39:VAL:HG13	1:B:40:LEU:H	1.82	0.45
1:C:203:PHE:HZ	1:C:296:PHE:CE1	2.32	0.45
1:D:423:ASN:OD1	1:D:424:GLU:N	2.49	0.45
1:D:283:PHE:C	1:D:283:PHE:HD1	2.18	0.45
1:D:67:THR:HG23	1:D:75:VAL:O	2.16	0.45
1:B:100:LYS:NZ	1:B:116:ALA:HB1	2.31	0.45
1:B:137:MET:CE	1:B:264:PHE:CD2	3.00	0.45
1:B:226:TYR:HD1	1:C:70:LEU:HD13	1.81	0.45
1:C:141:SER:HB3	1:C:144:GLU:OE1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:LEU:HD23	1:A:272:MET:HE3	1.98	0.45
1:C:362:LEU:C	1:C:363:ILE:HD12	2.37	0.45
1:A:284:HIS:O	1:A:287:ASN:HB3	2.16	0.45
1:A:427:MET:N	1:A:428:PRO:HD3	2.31	0.45
1:C:227:PHE:N	1:C:227:PHE:CD2	2.83	0.45
1:D:370:THR:HG22	1:D:387:GLU:HG2	1.97	0.45
1:B:225:LYS:HE2	1:C:102:ALA:N	2.25	0.45
1:A:40:LEU:O	1:A:40:LEU:HD23	2.17	0.45
1:B:99:GLY:HA2	1:B:370:THR:HG23	1.97	0.45
1:B:361:ASP:CG	1:B:361:ASP:O	2.55	0.45
1:B:68:VAL:HG12	1:B:70:LEU:HD13	1.98	0.45
1:D:371:VAL:HG23	1:D:385:ASN:H	1.82	0.45
1:D:410:PRO:O	1:D:412:HIS:N	2.50	0.45
1:D:140:ARG:NH2	1:D:148:GLU:HG3	2.32	0.45
1:B:269:LEU:HA	1:B:272:MET:SD	2.57	0.45
1:D:32:PRO:O	1:D:66:PHE:CB	2.64	0.45
1:C:208:LEU:HG	1:C:232:ARG:HB3	1.98	0.45
1:D:409:ASN:HB2	1:D:412:HIS:CE1	2.52	0.45
1:D:183:VAL:HA	1:D:264:PHE:HB2	1.98	0.45
1:A:214:SER:OG	1:D:477:VAL:HG13	2.16	0.45
1:A:477:VAL:HG23	1:D:227:PHE:HZ	1.82	0.45
1:D:78:LEU:N	1:D:78:LEU:HD22	2.26	0.45
1:A:93:GLU:HG2	1:A:433:LYS:HZ3	1.81	0.45
1:D:302:THR:HG21	2:D:500:HEM:CMB	2.47	0.45
1:C:245:ILE:HD13	1:C:245:ILE:C	2.37	0.45
4:C:603:SUC:HO1'	4:C:603:SUC:C4'	2.30	0.45
1:C:152:CYS:SG	1:C:187:ARG:NH2	2.90	0.45
1:C:330:GLN:O	1:C:330:GLN:HG2	2.17	0.45
1:B:359:LEU:HD13	1:B:359:LEU:HA	1.84	0.45
1:D:414:LEU:HD12	1:D:414:LEU:N	2.32	0.45
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.16	0.45
1:D:177:ASN:O	1:D:181:SER:N	2.46	0.45
1:D:264:PHE:CE1	5:D:610:CM5:H112	2.52	0.45
1:C:252:HIS:HB3	1:C:265:ILE:CD1	2.47	0.44
1:C:298:ALA:HB2	3:C:501:TB2:C5	2.47	0.44
1:D:213:SER:O	1:D:216:VAL:HG13	2.17	0.44
1:C:348:TYR:O	1:C:352:VAL:HG23	2.17	0.44
1:D:302:THR:HG22	2:D:500:HEM:CAB	2.46	0.44
1:D:409:ASN:HA	1:D:410:PRO:HD3	1.81	0.44
1:D:108:PHE:O	1:D:112:GLY:HA3	2.18	0.44
1:D:31:PRO:HA	1:D:32:PRO:HD3	1.67	0.44
1:C:358:ARG:CG	1:C:396:LEU:HD12	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:603:SUC:H1	4:C:603:SUC:H1'1	1.27	0.44
1:A:430:SER:O	1:A:431:LEU:HD23	2.17	0.44
1:D:364:PRO:CD	1:D:478:GLY:HA2	2.47	0.44
1:A:288:LEU:O	1:A:292:VAL:HG12	2.18	0.44
1:C:167:ASN:HD22	1:C:486:ILE:CG2	2.28	0.44
1:D:313:LEU:HD13	1:D:356:ILE:HG12	1.98	0.44
1:C:153:LEU:HD21	1:C:453:ILE:HD11	1.99	0.44
1:B:81:THR:HG23	1:B:425:GLY:HA2	1.99	0.44
1:D:268:TYR:OH	1:D:284:HIS:CE1	2.71	0.44
1:B:145:ARG:HD3	1:B:181:SER:OG	2.17	0.44
1:C:397:HIS:O	1:C:405:PRO:HB3	2.17	0.44
1:A:292:VAL:HG13	1:A:293:LEU:N	2.33	0.44
1:B:225:LYS:NZ	1:C:101:ILE:HB	2.32	0.44
1:A:106:PRO:HG2	1:A:235:TYR:OH	2.18	0.44
1:C:314:MET:SD	1:C:450:PHE:CZ	3.11	0.44
1:B:382:ILE:HG22	1:B:386:THR:HB	1.99	0.44
1:A:367:VAL:CG2	2:A:500:HEM:HAA2	2.48	0.44
1:B:69:TYR:CD1	1:B:74:PRO:HB3	2.52	0.44
1:C:477:VAL:HG13	1:C:477:VAL:O	2.18	0.44
1:B:382:ILE:CG2	1:B:386:THR:HB	2.46	0.44
1:D:133:ARG:HG3	1:D:134:ASP:N	2.33	0.44
1:C:186:LYS:HE3	1:C:186:LYS:HB2	1.76	0.44
1:D:381:VAL:C	1:D:382:ILE:HD12	2.38	0.44
1:A:371:VAL:HG22	1:A:373:LYS:O	2.18	0.44
1:B:409:ASN:ND2	1:B:411:GLY:H	2.15	0.44
1:C:382:ILE:HA	1:C:382:ILE:HD12	1.72	0.44
1:B:88:LEU:HB2	1:B:431:LEU:HD12	1.99	0.44
1:D:441:ILE:O	1:D:445:GLU:HG3	2.18	0.44
1:C:174:ILE:O	1:C:178:ILE:HD13	2.17	0.44
1:A:109:GLN:O	1:A:113:VAL:HG23	2.17	0.44
1:C:325:GLN:HG2	1:C:491:ARG:NH2	2.33	0.44
1:A:292:VAL:O	1:A:296:PHE:HB3	2.12	0.43
1:C:434:ARG:HG3	2:C:500:HEM:CGA	2.48	0.43
1:D:80:GLY:O	1:D:83:ALA:HB3	2.17	0.43
1:A:48:ARG:CG	1:A:49:LYS:N	2.81	0.43
1:A:98:ARG:HD3	1:A:99:GLY:H	1.83	0.43
1:B:225:LYS:HZ2	1:C:101:ILE:HB	1.83	0.43
1:D:117:ASN:CB	1:D:120:ARG:CZ	2.96	0.43
1:C:51:LEU:HD12	1:C:52:LEU:N	2.32	0.43
1:A:150:ALA:HB1	1:A:452:THR:HG21	1.99	0.43
1:D:332:ILE:HG22	1:D:333:GLY:O	2.17	0.43
1:B:36:PRO:C	1:B:37:LEU:O	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:288:LEU:HD12	1:D:289:ILE:HG13	2.00	0.43
1:C:98:ARG:NE	1:C:98:ARG:CA	2.81	0.43
1:C:287:ASN:ND2	1:C:287:ASN:C	2.69	0.43
1:A:212:PHE:CD1	1:A:212:PHE:C	2.92	0.43
1:A:183:VAL:HA	1:A:264:PHE:HB2	1.99	0.43
1:A:175:THR:HB	1:A:300:THR:HG23	2.01	0.43
1:D:396:LEU:HD21	1:D:427:MET:H	1.83	0.43
1:D:431:LEU:O	1:D:435:ILE:CG1	2.58	0.43
1:B:436:CYS:HB2	2:B:500:HEM:NA	2.32	0.43
1:D:34:PRO:HB2	1:D:42:ASN:ND2	2.34	0.43
1:B:202:PHE:CZ	1:B:241:ILE:HD13	2.54	0.43
1:D:312:LEU:HB2	1:D:484:TYR:CE1	2.54	0.43
1:B:367:VAL:CG2	2:B:500:HEM:HAA2	2.49	0.43
1:A:107:ILE:HG23	1:A:235:TYR:OH	2.17	0.43
1:C:191:LYS:O	1:C:193:PRO:HD3	2.18	0.43
1:A:37:LEU:N	1:A:42:ASN:OD1	2.50	0.43
1:B:217:PHE:O	1:B:219:LEU:N	2.52	0.43
1:D:197:ARG:HE	1:D:197:ARG:HA	1.83	0.43
1:B:309:TYR:HB2	1:B:481:PRO:CG	2.48	0.43
1:D:340:LEU:HD23	1:D:444:THR:HG23	2.00	0.43
1:B:117:ASN:OD1	1:B:117:ASN:C	2.57	0.43
1:D:149:GLU:OE1	1:D:149:GLU:HA	2.19	0.43
1:C:438:GLY:HA3	2:C:500:HEM:C3C	2.54	0.43
1:B:36:PRO:HA	1:B:42:ASN:CB	2.49	0.43
1:B:226:TYR:OH	1:C:387:GLU:CD	2.57	0.43
1:C:363:ILE:HG22	1:C:363:ILE:O	2.19	0.43
1:A:308:ARG:HH22	1:A:483:SER:CA	2.30	0.43
1:B:93:GLU:HA	1:B:96:SER:HB3	2.00	0.43
1:C:367:VAL:HG21	2:C:500:HEM:HAA2	2.01	0.43
1:D:332:ILE:HG12	1:D:336:ARG:NH2	2.33	0.43
1:B:144:GLU:HA	1:B:147:GLN:HE21	1.82	0.43
1:C:208:LEU:CB	1:C:232:ARG:HG3	2.48	0.43
1:C:105:ASP:HB3	1:C:106:PRO:HD2	2.00	0.43
1:A:213:SER:HB2	1:D:202:PHE:O	2.19	0.43
1:C:269:LEU:HD12	1:C:269:LEU:N	2.34	0.43
1:C:434:ARG:HH11	1:C:434:ARG:HA	1.83	0.42
1:C:371:VAL:HG21	1:C:382:ILE:HG22	1.98	0.42
1:D:197:ARG:HA	1:D:197:ARG:NE	2.34	0.42
1:B:89:VAL:HG23	1:B:431:LEU:HD13	2.01	0.42
1:C:225:LYS:CE	1:C:226:TYR:HE2	2.32	0.42
1:C:227:PHE:N	1:C:228:PRO:CD	2.83	0.42
1:C:98:ARG:HG3	1:C:99:GLY:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:106:PRO:HG2	1:C:107:ILE:H	1.84	0.42
1:C:190:TYR:O	1:C:191:LYS:HD3	2.18	0.42
1:A:435:ILE:HG12	1:A:436:CYS:N	2.34	0.42
1:A:274:LYS:HG3	1:A:275:ASP:N	2.34	0.42
1:C:206:PHE:HE1	1:C:208:LEU:HD11	1.73	0.42
1:C:298:ALA:O	3:C:501:TB2:O1	2.37	0.42
1:B:132:MET:HE3	5:B:607:CM5:C7	2.49	0.42
1:B:307:LEU:HA	1:B:307:LEU:HD23	1.85	0.42
1:A:437:LEU:O	1:A:437:LEU:HD22	2.19	0.42
1:C:69:TYR:CE2	1:C:74:PRO:HB3	2.54	0.42
1:C:263:ASP:C	1:C:263:ASP:OD1	2.58	0.42
1:D:268:TYR:HH	1:D:284:HIS:CE1	2.37	0.42
1:B:62:TYR:CD2	1:B:62:TYR:N	2.88	0.42
1:A:315:LEU:HD11	1:A:486:ILE:HG13	2.00	0.42
1:D:296:PHE:HD1	1:D:300:THR:HG21	1.76	0.42
2:D:500:HEM:HMB1	2:D:500:HEM:CBB	2.42	0.42
1:B:289:ILE:HG23	1:B:290:LEU:HD12	2.02	0.42
1:C:51:LEU:C	1:C:51:LEU:HD12	2.39	0.42
1:A:316:LYS:HD3	1:A:470:LEU:HD11	2.01	0.42
1:A:382:ILE:HA	1:A:383:PRO:HD3	1.86	0.42
1:D:351:ALA:HB1	1:D:414:LEU:HD11	2.01	0.42
1:D:185:GLY:HA2	1:D:263:ASP:HB3	2.01	0.42
1:B:77:VAL:HG22	1:B:389:PHE:HB2	2.01	0.42
2:A:500:HEM:CBD	2:A:500:HEM:HHA	2.49	0.42
1:D:164:LEU:HA	1:D:486:ILE:O	2.20	0.42
1:D:120:ARG:HB2	1:D:120:ARG:HE	1.17	0.42
1:C:388:VAL:O	1:C:390:PRO:HD3	2.19	0.42
1:D:313:LEU:O	1:D:313:LEU:HD23	2.19	0.42
1:A:192:ASP:HA	1:A:193:PRO:HD3	1.93	0.42
1:C:398:ASP:OD1	1:C:400:ARG:CG	2.67	0.42
1:D:285:HIS:CD2	1:D:288:LEU:HD11	2.55	0.42
1:B:143:GLU:O	1:B:147:GLN:HG2	2.19	0.42
1:A:98:ARG:HH22	2:A:500:HEM:HBD1	1.84	0.42
1:D:397:HIS:O	1:D:405:PRO:HG2	2.20	0.42
1:C:105:ASP:HB3	1:C:107:ILE:HG12	2.02	0.42
1:A:371:VAL:HG11	1:A:382:ILE:HG22	2.02	0.42
1:A:295:LEU:HG	2:A:500:HEM:CBC	2.38	0.42
2:A:500:HEM:HBD1	2:A:500:HEM:HHA	2.02	0.42
3:B:501:TB2:C8	3:B:501:TB2:O1	2.64	0.42
1:A:205:SER:HA	1:D:211:SER:HB3	2.02	0.42
1:B:430:SER:HB2	2:B:500:HEM:HBA1	2.01	0.42
1:C:184:PHE:O	1:C:263:ASP:OD2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:78:LEU:O	1:D:78:LEU:HD23	2.20	0.42
1:B:226:TYR:CD2	1:B:226:TYR:N	2.88	0.42
1:D:135:PHE:CD1	1:D:261:PRO:HG2	2.55	0.42
1:C:427:MET:HB2	1:C:431:LEU:HD11	2.02	0.42
1:C:163:ALA:O	1:C:165:LEU:HD23	2.20	0.42
1:D:380:TYR:N	1:D:380:TYR:CD1	2.87	0.41
1:C:66:PHE:CE2	1:C:77:VAL:CG2	3.03	0.41
1:D:332:ILE:HG12	1:D:336:ARG:HH22	1.85	0.41
1:D:313:LEU:HD13	1:D:356:ILE:CG1	2.50	0.41
1:C:38:PRO:O	1:C:40:LEU:HD22	2.20	0.41
1:A:323:ARG:CZ	1:B:133:ARG:HG3	2.50	0.41
1:B:133:ARG:HB2	5:B:607:CM5:O20	2.20	0.41
1:B:174:ILE:HG13	1:B:175:THR:N	2.35	0.41
1:C:208:LEU:CD2	1:C:232:ARG:CB	2.99	0.41
1:C:208:LEU:HG	1:C:232:ARG:CB	2.51	0.41
1:A:288:LEU:HD12	1:A:288:LEU:O	2.21	0.41
1:C:33:GLY:N	1:C:62:TYR:CD1	2.88	0.41
1:D:386:THR:HG22	1:D:387:GLU:N	2.35	0.41
1:A:48:ARG:HG2	1:A:474:GLU:CG	2.50	0.41
1:C:398:ASP:OD1	1:C:400:ARG:HG2	2.19	0.41
1:B:91:GLN:NE2	1:B:375:THR:HG23	2.35	0.41
1:A:313:LEU:HD13	1:A:408:PHE:CD1	2.55	0.41
1:D:91:GLN:HE21	1:D:94:ALA:HB2	1.85	0.41
1:B:285:HIS:C	1:B:285:HIS:ND1	2.63	0.41
1:B:75:VAL:HG23	1:B:75:VAL:O	2.20	0.41
1:D:285:HIS:O	1:D:285:HIS:CD2	2.72	0.41
1:D:288:LEU:CD1	1:D:289:ILE:HG13	2.50	0.41
1:B:39:VAL:HG13	1:B:40:LEU:N	2.35	0.41
1:D:403:GLU:H	1:D:412:HIS:CD2	2.38	0.41
1:D:201:LEU:HD12	1:D:201:LEU:HA	1.80	0.41
1:D:464:PRO:HA	1:D:465:PRO:HD3	1.90	0.41
1:A:68:VAL:CG1	1:A:75:VAL:HG22	2.48	0.41
1:D:349:THR:O	1:D:352:VAL:HG12	2.20	0.41
1:B:137:MET:CE	1:B:264:PHE:HD2	2.33	0.41
1:D:401:TYR:O	1:D:402:PHE:CD2	2.74	0.41
1:D:164:LEU:HD23	1:D:164:LEU:N	2.35	0.41
1:C:243:THR:HG22	1:C:244:PHE:N	2.35	0.41
1:A:48:ARG:C	1:A:48:ARG:HD2	2.40	0.41
1:C:73:ARG:HA	1:C:74:PRO:HD3	1.83	0.41
1:C:383:PRO:HG2	1:C:386:THR:HG21	2.02	0.41
1:A:212:PHE:CE2	1:D:238:LEU:HD12	2.56	0.41
1:D:358:ARG:HD2	1:D:402:PHE:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:288:LEU:HD12	1:D:289:ILE:CA	2.51	0.41
1:D:410:PRO:C	1:D:412:HIS:H	2.24	0.41
1:A:296:PHE:CD1	1:A:296:PHE:O	2.74	0.41
1:B:84:ILE:HD12	1:B:395:ALA:HB2	2.03	0.41
1:C:401:TYR:CE2	1:C:424:GLU:HB2	2.55	0.41
1:D:192:ASP:OD1	1:D:193:PRO:HD2	2.21	0.41
1:A:141:SER:O	1:A:145:ARG:HG3	2.21	0.41
1:C:234:ILE:CG2	1:C:235:TYR:N	2.84	0.41
1:A:41:GLY:HA3	1:A:44:LEU:HD22	2.03	0.41
1:C:332:ILE:HD11	1:C:342:ASP:HB3	2.02	0.41
1:D:38:PRO:O	1:D:39:VAL:HB	2.21	0.41
1:C:414:LEU:HA	1:C:419:ALA:O	2.21	0.41
1:D:59:ARG:CA	1:D:66:PHE:HE1	2.30	0.41
1:D:294:SER:O	1:D:295:LEU:C	2.58	0.41
1:B:222:GLY:HA2	1:C:101:ILE:HG22	2.01	0.41
1:B:232:ARG:CG	1:B:233:GLN:H	2.29	0.41
1:C:337:PRO:HA	1:C:338:PRO:HD3	1.94	0.41
1:B:172:HIS:CD2	1:B:203:PHE:CD2	3.09	0.41
1:C:368:PRO:HG3	1:C:389:PHE:CE2	2.56	0.41
1:D:289:ILE:O	1:D:293:LEU:N	2.43	0.40
1:D:114:ILE:O	1:D:120:ARG:CZ	2.69	0.40
3:B:501:TB2:H7	3:B:501:TB2:H12B	1.89	0.40
1:C:314:MET:HB3	1:C:459:ILE:HD11	2.03	0.40
1:C:404:THR:H	1:C:404:THR:HG1	1.56	0.40
1:A:398:ASP:HA	1:A:399:PRO:HD3	1.85	0.40
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.90	0.40
1:D:55:PHE:HE1	1:D:77:VAL:HG11	1.87	0.40
1:C:245:ILE:CG2	1:C:246:GLY:N	2.84	0.40
1:A:34:PRO:HG3	1:A:58:LEU:CD2	2.51	0.40
1:D:363:ILE:HA	1:D:364:PRO:HD3	1.76	0.40
2:B:500:HEM:CBD	2:B:500:HEM:HHA	2.50	0.40
1:A:477:VAL:CG2	1:D:227:PHE:HZ	2.34	0.40
1:D:108:PHE:O	1:D:112:GLY:N	2.53	0.40
1:D:397:HIS:CD2	1:D:405:PRO:O	2.74	0.40
1:D:363:ILE:HD11	3:D:501:TB2:H4	2.04	0.40
1:C:263:ASP:OD1	1:C:263:ASP:N	2.54	0.40
1:C:383:PRO:HB2	1:C:386:THR:OG1	2.21	0.40
1:D:295:LEU:HD12	1:D:295:LEU:C	2.42	0.40
1:A:40:LEU:O	1:A:44:LEU:HD22	2.21	0.40
1:D:371:VAL:HG23	1:D:385:ASN:N	2.36	0.40
1:D:312:LEU:HD22	1:D:484:TYR:CD1	2.57	0.40
1:C:398:ASP:OD1	1:C:398:ASP:C	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:ASP:HB3	1:A:420:LEU:HD13	2.03	0.40
1:C:162:GLY:O	1:C:487:ARG:HB3	2.22	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	463/476 (97%)	440 (95%)	18 (4%)	5 (1%)	21	67
1	B	463/476 (97%)	426 (92%)	36 (8%)	1 (0%)	56	92
1	C	452/476 (95%)	423 (94%)	27 (6%)	2 (0%)	43	87
1	D	462/476 (97%)	415 (90%)	43 (9%)	4 (1%)	25	73
All	All	1840/1904 (97%)	1704 (93%)	124 (7%)	12 (1%)	30	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	45	GLN
1	D	430	SER
1	A	136	GLY
1	B	36	PRO
1	C	45	GLN
1	D	341	ASP
1	D	364	PRO
1	D	411	GLY
1	A	477	VAL
1	A	106	PRO
1	C	477	VAL

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	375/421 (89%)	338 (90%)	37 (10%)	11	40
1	B	377/421 (90%)	336 (89%)	41 (11%)	9	35
1	C	343/421 (82%)	299 (87%)	44 (13%)	6	27
1	D	345/421 (82%)	301 (87%)	44 (13%)	6	27
All	All	1440/1684 (86%)	1274 (88%)	166 (12%)	8	32

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	39	VAL
1	A	42	ASN
1	A	47	ASP
1	A	48	ARG
1	A	51	LEU
1	A	59	ARG
1	A	101	ILE
1	A	105	ASP
1	A	111	TYR
1	A	137	MET
1	A	144	GLU
1	A	165	LEU
1	A	170	LEU
1	A	198	LEU
1	A	200	ASP
1	A	217	PHE
1	A	224	LEU
1	A	226	TYR
1	A	230	THR
1	A	240	GLU
1	A	287	ASN
1	A	288	LEU
1	A	289	ILE
1	A	293	LEU
1	A	343	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	370	THR
1	A	400	ARG
1	A	420	LEU
1	A	422	ARG
1	A	434	ARG
1	A	441	ILE
1	A	473	ARG
1	A	477	VAL
1	A	486	ILE
1	A	489	LEU
1	A	491	ARG
1	B	44	LEU
1	B	58	LEU
1	B	70	LEU
1	B	107	ILE
1	B	115	PHE
1	B	117	ASN
1	B	145	ARG
1	B	165	LEU
1	B	169	LEU
1	B	172	HIS
1	B	207	SER
1	B	215	GLN
1	B	219	LEU
1	B	224	LEU
1	B	225	LYS
1	B	232	ARG
1	B	248	SER
1	B	250	GLU
1	B	285	HIS
1	B	286	GLN
1	B	287	ASN
1	B	288	LEU
1	B	294	SER
1	B	323	ARG
1	B	327	GLU
1	B	329	GLU
1	B	349	THR
1	B	359	LEU
1	B	362	LEU
1	B	409	ASN
1	B	417	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	420	LEU
1	B	431	LEU
1	B	434	ARG
1	B	437	LEU
1	B	448	LEU
1	B	450	PHE
1	B	467	ASP
1	B	473	ARG
1	B	477	VAL
1	B	489	LEU
1	C	39	VAL
1	C	40	LEU
1	C	42	ASN
1	C	48	ARG
1	C	58	LEU
1	C	61	LYS
1	C	65	VAL
1	C	77	VAL
1	C	85	ARG
1	C	148	GLU
1	C	158	ARG
1	C	165	LEU
1	C	170	LEU
1	C	196	LEU
1	C	198	LEU
1	C	208	LEU
1	C	217	PHE
1	C	223	PHE
1	C	226	TYR
1	C	227	PHE
1	C	238	LEU
1	C	245	ILE
1	C	252	HIS
1	C	253	ARG
1	C	287	ASN
1	C	296	PHE
1	C	314	MET
1	C	325	GLN
1	C	327	GLU
1	C	332	ILE
1	C	369	HIS
1	C	382	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	386	THR
1	C	387	GLU
1	C	403	GLU
1	C	404	THR
1	C	422	ARG
1	C	437	LEU
1	C	443	ARG
1	C	458	SER
1	C	473	ARG
1	C	483	SER
1	C	485	GLN
1	C	489	LEU
1	D	30	LEU
1	D	49	LYS
1	D	53	ARG
1	D	75	VAL
1	D	78	LEU
1	D	79	CYS
1	D	90	ASP
1	D	95	PHE
1	D	107	ILE
1	D	120	ARG
1	D	140	ARG
1	D	141	SER
1	D	198	LEU
1	D	199	LEU
1	D	201	LEU
1	D	209	ILE
1	D	214	SER
1	D	216	VAL
1	D	238	LEU
1	D	243	THR
1	D	250	GLU
1	D	253	ARG
1	D	257	ASP
1	D	262	ARG
1	D	283	PHE
1	D	291	THR
1	D	295	LEU
1	D	296	PHE
1	D	317	TYR
1	D	322	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	340	LEU
1	D	356	ILE
1	D	358	ARG
1	D	362	LEU
1	D	374	ASP
1	D	375	THR
1	D	385	ASN
1	D	392	LEU
1	D	393	SER
1	D	400	ARG
1	D	407	THR
1	D	439	GLU
1	D	463	VAL
1	D	470	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	B	215	GLN
1	B	233	GLN
1	B	385	ASN
1	B	409	ASN
1	C	215	GLN
1	C	231	HIS
1	C	287	ASN
1	D	42	ASN
1	D	45	GLN
1	D	91	GLN
1	D	237	ASN
1	D	242	ASN
1	D	285	HIS
1	D	479	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

17 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	49,50,50	2.30	14 (28%)	46,82,82	2.07	7 (15%)
3	TB2	A	501	1	13,13,13	0.56	0	18,18,18	0.82	0
4	SUC	A	601	-	24,24,24	1.06	2 (8%)	36,36,36	1.77	12 (33%)
5	CM5	A	605	-	24,25,36	0.43	0	31,32,49	0.88	1 (3%)
5	CM5	A	608	-	36,36,36	0.43	0	49,49,49	1.21	4 (8%)
2	HEM	B	500	1	49,50,50	2.26	14 (28%)	46,82,82	2.06	6 (13%)
3	TB2	B	501	1	13,13,13	0.56	0	18,18,18	0.76	0
4	SUC	B	602	-	24,24,24	1.02	0	36,36,36	1.81	13 (36%)
5	CM5	B	606	-	36,36,36	0.40	0	49,49,49	1.02	3 (6%)
5	CM5	B	607	-	36,36,36	0.40	0	49,49,49	0.82	1 (2%)
2	HEM	C	500	1	49,50,50	2.24	13 (26%)	46,82,82	2.06	5 (10%)
3	TB2	C	501	1	13,13,13	0.57	0	18,18,18	0.86	0
4	SUC	C	603	-	24,24,24	1.06	2 (8%)	36,36,36	2.01	11 (30%)
2	HEM	D	500	1	49,50,50	2.24	13 (26%)	46,82,82	1.93	7 (15%)
3	TB2	D	501	1	13,13,13	0.63	0	18,18,18	1.29	1 (5%)
4	SUC	D	604	-	24,24,24	1.04	1 (4%)	36,36,36	1.87	13 (36%)
5	CM5	D	610	-	36,36,36	0.39	0	49,49,49	0.77	1 (2%)

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	-	0/14/114/114	0/0/8/8
3	TB2	A	501	1	-	0/9/9/9	0/1/1/1
4	SUC	A	601	-	-	0/12/51/51	0/2/2/2
5	CM5	A	605	-	-	0/13/41/65	0/2/2/3
5	CM5	A	608	-	-	0/17/65/65	0/3/3/3
2	HEM	B	500	1	-	0/14/114/114	0/0/8/8
3	TB2	B	501	1	-	0/9/9/9	0/1/1/1
4	SUC	B	602	-	-	0/12/51/51	0/2/2/2
5	CM5	B	606	-	-	0/17/65/65	0/3/3/3
5	CM5	B	607	-	-	0/17/65/65	0/3/3/3
2	HEM	C	500	1	-	0/14/114/114	0/0/8/8
3	TB2	C	501	1	-	0/9/9/9	0/1/1/1
4	SUC	C	603	-	-	0/12/51/51	0/2/2/2
2	HEM	D	500	1	-	0/14/114/114	0/0/8/8
3	TB2	D	501	1	-	0/9/9/9	0/1/1/1
4	SUC	D	604	-	-	0/12/51/51	0/2/2/2
5	CM5	D	610	-	-	0/17/65/65	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C3D-C2D	5.87	1.54	1.43
2	A	500	HEM	C3C-C2C	-5.83	1.33	1.43
2	C	500	HEM	C3B-C2B	-5.78	1.33	1.43
2	D	500	HEM	C3D-C2D	5.74	1.53	1.43
2	A	500	HEM	C3B-C2B	-5.74	1.33	1.43
2	B	500	HEM	C3B-C2B	-5.72	1.33	1.43
2	D	500	HEM	C3C-C2C	-5.69	1.33	1.43
2	C	500	HEM	C3C-C2C	-5.63	1.33	1.43
2	B	500	HEM	C3D-C2D	5.62	1.53	1.43
2	A	500	HEM	C3D-C2D	5.58	1.53	1.43
2	D	500	HEM	C3B-C2B	-5.51	1.34	1.43
2	B	500	HEM	C3C-C2C	-5.31	1.34	1.43
2	D	500	HEM	C3B-CAB	4.70	1.55	1.40
2	B	500	HEM	C3B-CAB	4.64	1.55	1.40
2	C	500	HEM	C3C-CAC	4.64	1.55	1.40
2	B	500	HEM	C3C-CAC	4.63	1.55	1.40
2	A	500	HEM	C3B-CAB	4.63	1.55	1.40
2	C	500	HEM	C3B-CAB	4.59	1.54	1.40
2	D	500	HEM	C3C-CAC	4.56	1.54	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-CAC	4.54	1.54	1.40
2	B	500	HEM	C4A-C3A	4.13	1.45	1.40
2	B	500	HEM	C3D-C4D	4.11	1.45	1.44
2	A	500	HEM	C4A-C3A	4.03	1.45	1.40
2	D	500	HEM	C4A-C3A	3.99	1.45	1.40
2	C	500	HEM	C4A-C3A	3.95	1.45	1.40
2	A	500	HEM	C3D-C4D	3.81	1.45	1.44
2	D	500	HEM	C2B-C1B	3.28	1.45	1.44
2	C	500	HEM	FE-NA	3.24	2.06	1.92
2	A	500	HEM	FE-ND	3.23	2.09	1.97
2	A	500	HEM	FE-NB	3.15	2.09	1.97
2	D	500	HEM	FE-NA	3.13	2.05	1.92
2	A	500	HEM	FE-NA	3.11	2.05	1.92
2	C	500	HEM	C2D-C1D	3.09	1.45	1.44
2	B	500	HEM	FE-ND	3.07	2.09	1.97
2	C	500	HEM	FE-ND	3.01	2.08	1.97
2	D	500	HEM	FE-ND	3.00	2.08	1.97
2	B	500	HEM	FE-NA	2.76	2.04	1.92
2	C	500	HEM	FE-NB	2.56	2.07	1.97
2	D	500	HEM	FE-NB	2.53	2.07	1.97
2	B	500	HEM	C2B-C1B	2.52	1.45	1.44
2	B	500	HEM	CMC-C2C	2.49	1.55	1.47
2	B	500	HEM	FE-NB	2.45	2.06	1.97
2	D	500	HEM	CMD-C2D	2.45	1.55	1.47
2	A	500	HEM	CMD-C2D	2.41	1.54	1.47
2	B	500	HEM	CMD-C2D	2.40	1.54	1.47
2	C	500	HEM	CMC-C2C	2.41	1.54	1.47
2	D	500	HEM	CMC-C2C	2.38	1.54	1.47
2	A	500	HEM	CMC-C2C	2.38	1.54	1.47
2	C	500	HEM	CMB-C2B	2.38	1.54	1.47
2	C	500	HEM	CMD-C2D	2.37	1.54	1.47
2	D	500	HEM	CMB-C2B	2.37	1.54	1.47
2	B	500	HEM	CMB-C2B	2.36	1.54	1.47
2	A	500	HEM	CMB-C2B	2.33	1.54	1.47
2	A	500	HEM	C2D-C1D	2.28	1.45	1.44
4	C	603	SUC	O3'-C3'	-2.16	1.38	1.42
4	A	601	SUC	O3'-C3'	-2.13	1.38	1.42
4	D	604	SUC	O3'-C3'	-2.06	1.38	1.42
4	A	601	SUC	O4'-C4'	-2.03	1.38	1.43
4	C	603	SUC	O4-C4	-2.01	1.38	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C3B-C4B-NB	-9.01	107.55	114.00
2	B	500	HEM	C3B-C4B-NB	-8.98	107.57	114.00
2	A	500	HEM	C3B-C4B-NB	-8.68	107.79	114.00
2	D	500	HEM	C3B-C4B-NB	-7.76	108.44	114.00
2	A	500	HEM	C4D-ND-C1D	6.32	111.63	105.16
2	C	500	HEM	C4D-ND-C1D	6.31	111.61	105.16
2	B	500	HEM	C4D-ND-C1D	6.15	111.45	105.16
2	D	500	HEM	C4D-ND-C1D	6.00	111.30	105.16
3	D	501	TB2	O1-C1-C2	-4.28	104.91	125.07
4	C	603	SUC	O5-C5-C6	4.26	116.81	106.34
4	B	602	SUC	O5-C5-C6	4.05	116.28	106.34
5	A	608	CM5	O25-C26-C27	4.00	117.17	109.76
4	C	603	SUC	C2'-O1-C1	-3.93	107.29	117.50
4	D	604	SUC	O5-C5-C6	3.91	115.94	106.34
5	A	608	CM5	C24-O25-C26	3.88	121.27	113.73
4	A	601	SUC	O5-C5-C6	3.73	115.52	106.34
2	A	500	HEM	C2D-C1D-ND	-3.62	108.66	112.93
2	C	500	HEM	C2D-C1D-ND	-3.59	108.70	112.93
4	C	603	SUC	O3-C3-C2	3.28	117.72	110.35
2	B	500	HEM	C2D-C1D-ND	-3.28	109.06	112.93
2	A	500	HEM	CAD-C3D-C4D	3.22	130.32	124.53
4	D	604	SUC	C2'-O1-C1	-3.18	109.24	117.50
2	D	500	HEM	C2D-C1D-ND	-3.14	109.22	112.93
4	C	603	SUC	O4-C4-C5	3.13	117.54	109.28
4	C	603	SUC	O2-C2-C1	3.08	116.76	110.04
5	B	606	CM5	C18-C17-C16	3.05	116.24	109.61
4	D	604	SUC	O2-C2-C1	3.02	116.64	110.04
4	C	603	SUC	O2'-C2'-C1'	3.00	116.21	108.08
4	D	604	SUC	O2'-C2'-C1'	3.00	116.20	108.08
4	C	603	SUC	O2'-C5'-C6'	2.99	117.75	108.65
4	A	601	SUC	O3-C3-C2	2.97	117.01	110.35
2	B	500	HEM	CAD-C3D-C4D	2.93	129.80	124.53
2	B	500	HEM	C1B-NB-C4B	2.93	108.16	105.16
4	B	602	SUC	O2-C2-C1	2.88	116.31	110.04
4	C	603	SUC	O4-C4-C3	2.81	116.66	110.35
4	C	603	SUC	O2-C2-C3	2.80	116.64	110.35
4	B	602	SUC	O4-C4-C5	2.78	116.62	109.28
4	D	604	SUC	O4-C4-C3	2.74	116.50	110.35
2	C	500	HEM	C1B-NB-C4B	2.74	107.97	105.16
4	A	601	SUC	O2'-C5'-C6'	2.74	116.99	108.65
4	A	601	SUC	O4-C4-C5	2.73	116.49	109.28
4	D	604	SUC	O3-C3-C4	2.72	116.46	110.35
4	B	602	SUC	O3-C3-C2	2.71	116.43	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	SUC	O2-C2-C3	2.71	116.42	110.35
4	C	603	SUC	O3-C3-C4	2.70	116.40	110.35
2	C	500	HEM	C4C-NC-C1C	2.69	108.33	105.53
4	B	602	SUC	O2'-C5'-C6'	2.69	116.83	108.65
4	D	604	SUC	O2'-C5'-C6'	2.68	116.82	108.65
4	D	604	SUC	O4-C4-C5	2.67	116.33	109.28
4	A	601	SUC	O4-C4-C3	2.67	116.34	110.35
4	A	601	SUC	O3-C3-C4	2.67	116.33	110.35
2	A	500	HEM	C1B-NB-C4B	2.66	107.88	105.16
4	A	601	SUC	O2-C2-C1	2.66	115.84	110.04
4	B	602	SUC	O4-C4-C3	2.64	116.28	110.35
4	A	601	SUC	O2-C2-C3	2.61	116.20	110.35
2	A	500	HEM	C4C-NC-C1C	2.60	108.23	105.53
4	B	602	SUC	O3-C3-C4	2.59	116.17	110.35
4	C	603	SUC	O1-C1-C2	2.59	116.65	108.24
5	A	605	CM5	C13-C18-C17	2.56	114.97	110.00
4	D	604	SUC	O1-C1-C2	2.56	116.56	108.24
2	D	500	HEM	CBD-CAD-C3D	-2.52	108.86	114.37
4	D	604	SUC	O2-C2-C3	2.51	115.99	110.35
4	A	601	SUC	O2'-C2'-C1'	2.44	114.69	108.08
4	D	604	SUC	O3-C3-C2	2.42	115.79	110.35
4	A	601	SUC	O5-C1-O1	2.39	117.88	109.95
2	A	500	HEM	CMA-C3A-C4A	-2.37	124.98	128.62
2	D	500	HEM	C1B-NB-C4B	2.33	107.55	105.16
4	B	602	SUC	O5-C1-O1	2.32	117.62	109.95
2	B	500	HEM	C4C-NC-C1C	2.28	107.91	105.53
4	A	601	SUC	O1-C1-C2	2.24	115.53	108.24
4	D	604	SUC	O4'-C4'-C5'	2.24	117.68	111.08
4	B	602	SUC	O1-C1-C2	2.23	115.50	108.24
4	B	602	SUC	O4'-C4'-C5'	2.23	117.64	111.08
5	B	606	CM5	C13-C18-C17	2.21	114.30	110.00
5	D	610	CM5	O14-C15-C16	2.18	114.24	109.70
2	D	500	HEM	C4C-NC-C1C	2.15	107.77	105.53
4	B	602	SUC	O2'-C2'-C1'	2.15	113.90	108.08
5	A	608	CM5	C28-C27-C26	2.13	114.00	110.20
4	D	604	SUC	O5-C1-O1	2.11	116.94	109.95
2	D	500	HEM	CHD-C4C-NC	2.10	126.56	124.73
5	B	607	CM5	C1-O12-C13	-2.09	110.20	113.96
5	B	606	CM5	C13-O14-C15	-2.08	109.67	113.73
4	A	601	SUC	O4'-C4'-C5'	2.04	117.09	111.08
4	B	602	SUC	C2'-O1-C1	-2.03	112.22	117.50
5	A	608	CM5	C24-O23-C16	-2.00	112.89	117.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	465/476 (97%)	-0.18	2 (0%)	90 41	49, 79, 130, 196	2 (0%)
1	B	465/476 (97%)	-0.12	3 (0%)	86 32	54, 88, 160, 184	2 (0%)
1	C	456/476 (95%)	0.01	8 (1%)	65 14	56, 97, 181, 211	1 (0%)
1	D	464/476 (97%)	-0.01	1 (0%)	93 54	60, 127, 166, 206	0
All	All	1850/1904 (97%)	-0.07	14 (0%)	81 26	49, 95, 166, 211	5 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	GLY	5.6
1	C	43	LEU	4.1
1	A	38	PRO	3.7
1	C	39	VAL	3.4
1	A	39	VAL	3.4
1	D	139	LYS	3.0
1	C	270	LEU	2.6
1	B	231	HIS	2.5
1	C	38	PRO	2.4
1	C	116	ALA	2.2
1	C	134	ASP	2.2
1	C	46	MET	2.1
1	B	55	PHE	2.0
1	C	230	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CM5	A	608	34/34	0.39	2.69	61,125,148,155	0
5	CM5	A	605	24/34	0.39	2.26	65,96,109,115	0
5	CM5	D	610	34/34	0.35	2.03	89,144,167,172	0
3	TB2	D	501	13/13	0.41	1.45	98,106,114,116	0
2	HEM	B	500	43/43	0.28	1.27	46,60,72,85	0
5	CM5	B	607	34/34	0.29	1.24	59,122,134,136	0
4	SUC	C	603	23/23	0.22	1.10	82,101,110,120	0
3	TB2	B	501	13/13	0.31	1.00	53,65,74,76	0
2	HEM	A	500	43/43	0.27	0.70	40,54,64,71	0
3	TB2	A	501	13/13	0.28	0.67	50,61,66,68	0
2	HEM	D	500	43/43	0.29	0.38	94,103,118,127	0
3	TB2	C	501	13/13	0.32	0.36	71,79,85,88	0
5	CM5	B	606	34/34	0.26	0.21	68,114,133,137	0
2	HEM	C	500	43/43	0.27	0.16	66,83,95,108	0
4	SUC	D	604	23/23	0.16	-0.91	140,147,153,155	0
4	SUC	B	602	23/23	0.14	-1.22	78,89,98,100	0
4	SUC	A	601	23/23	0.17	-1.47	54,81,93,98	0

6.5 Other polymers ⓘ

There are no such residues in this entry.