Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:10 AM GMT

PDB ID	:	3L4D
Title	:	Crystal structure of sterol 14-alpha demethylase (CYP51) from Leishmania infantum in complex with fluconazole
Authors	:	Lepesheva, G.I.; Hargrove, T.Y.; Wawrzak, Z.; Waterman, M.R.
Deposited on	:	2009-12-19
Resolution	:	2.75 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:

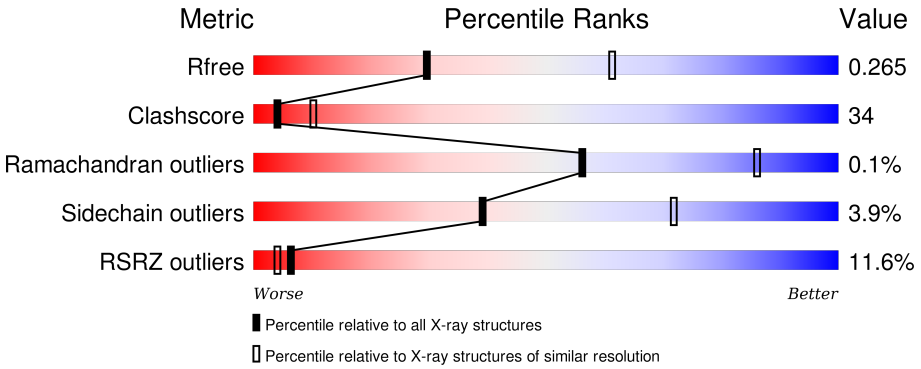
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	453	9% 56% 40%
1	B	453	10% 59% 36%
1	C	453	14% 50% 46%
1	D	453	13% 51% 44%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	N8E	C	1	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14534 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.

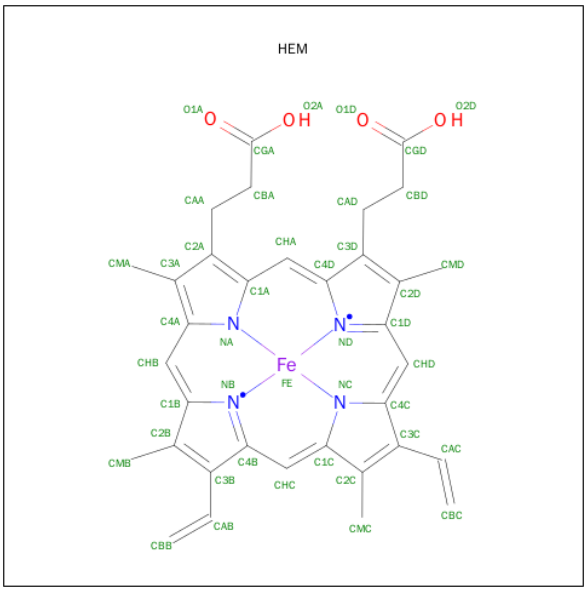
- Molecule 1 is a protein called Sterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3553	2270	619	635	29			
1	B	449	Total	C	N	O	S	0	0	0
			3562	2276	621	636	29			
1	C	447	Total	C	N	O	S	0	0	0
			3545	2266	617	633	29			
1	D	445	Total	C	N	O	S	0	0	0
			3529	2257	615	628	29			

There are 16 discrepancies between the modelled and reference sequences:

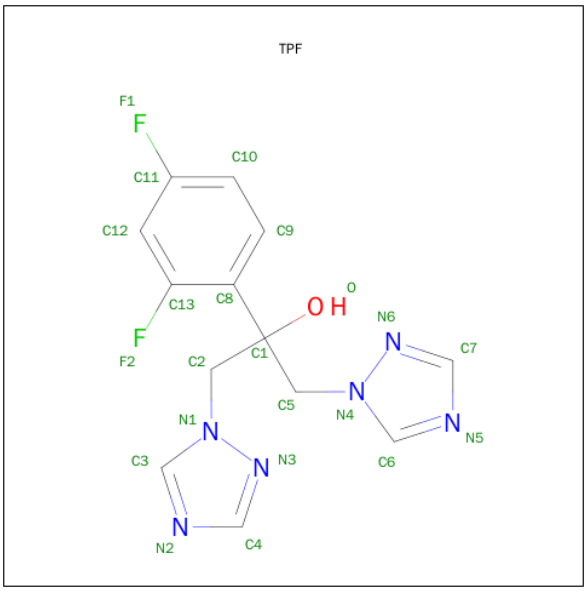
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
A	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
A	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
A	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
B	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
B	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
B	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
B	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
C	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
C	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
C	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
C	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
D	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
D	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
D	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
D	31	LEU	-	EXPRESSION TAG	UNP A2TEF2

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



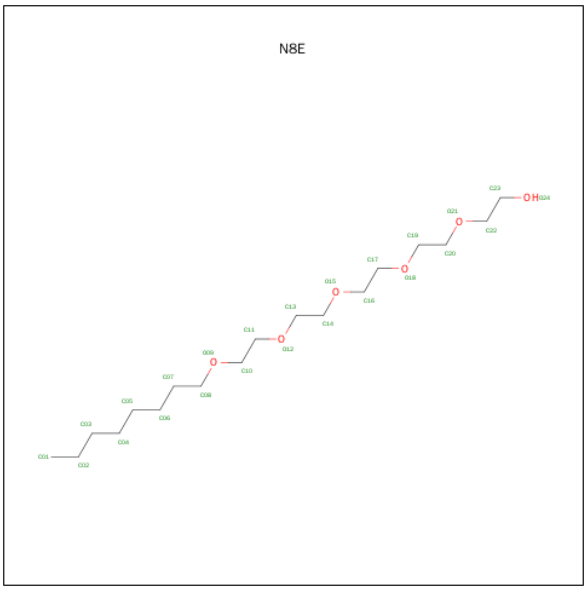
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (three-letter code: TPF) (formula: $C_{13}H_{12}F_2N_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	B	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	C	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	D	1	Total	C	F	N	O	0	0
			22	13	2	6	1		

- Molecule 4 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			24	18	6		

- Molecule 5 is water.

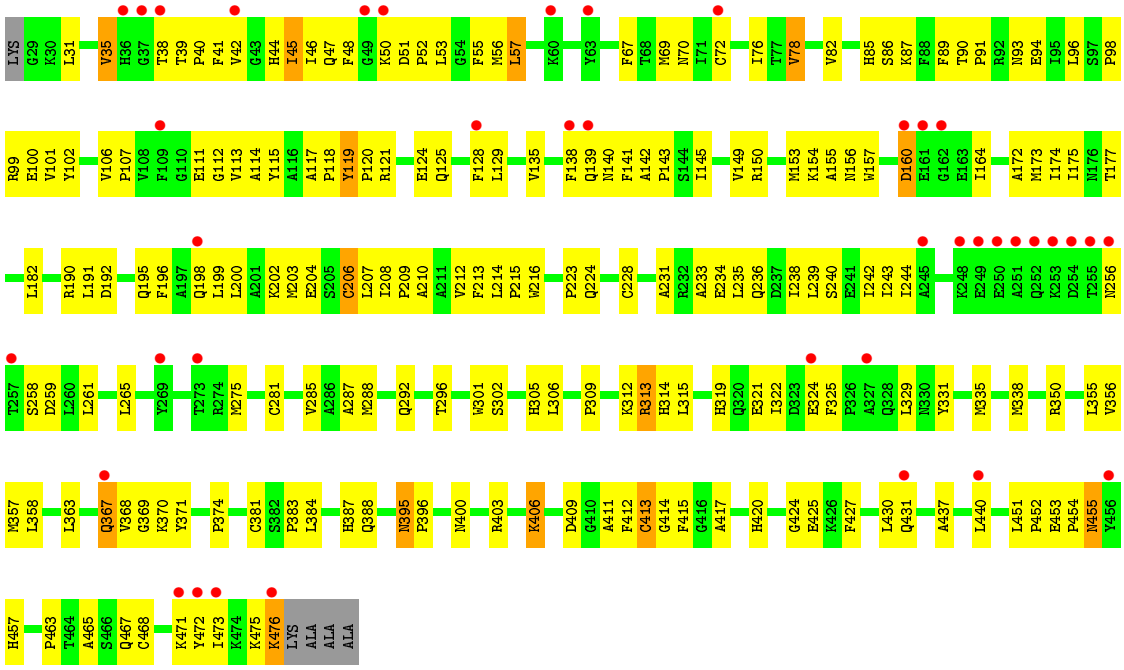
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	11	Total	O	0	0
			11	11		
5	C	16	Total	O	0	0
			16	16		
5	D	18	Total	O	0	0
			18	18		

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.

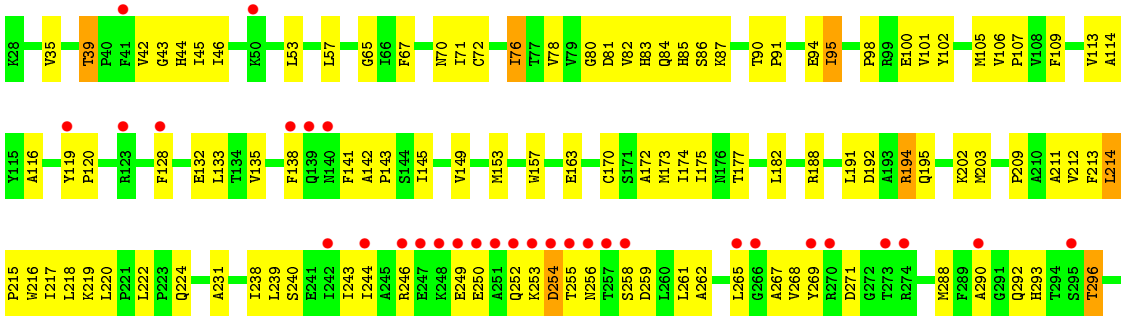
- Molecule 1: Sterol 14-alpha demethylase

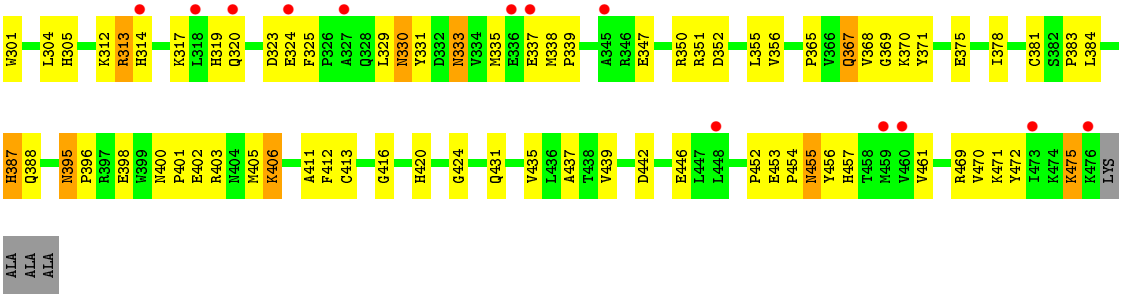
Chain A:



- Molecule 1: Sterol 14-alpha demethylase

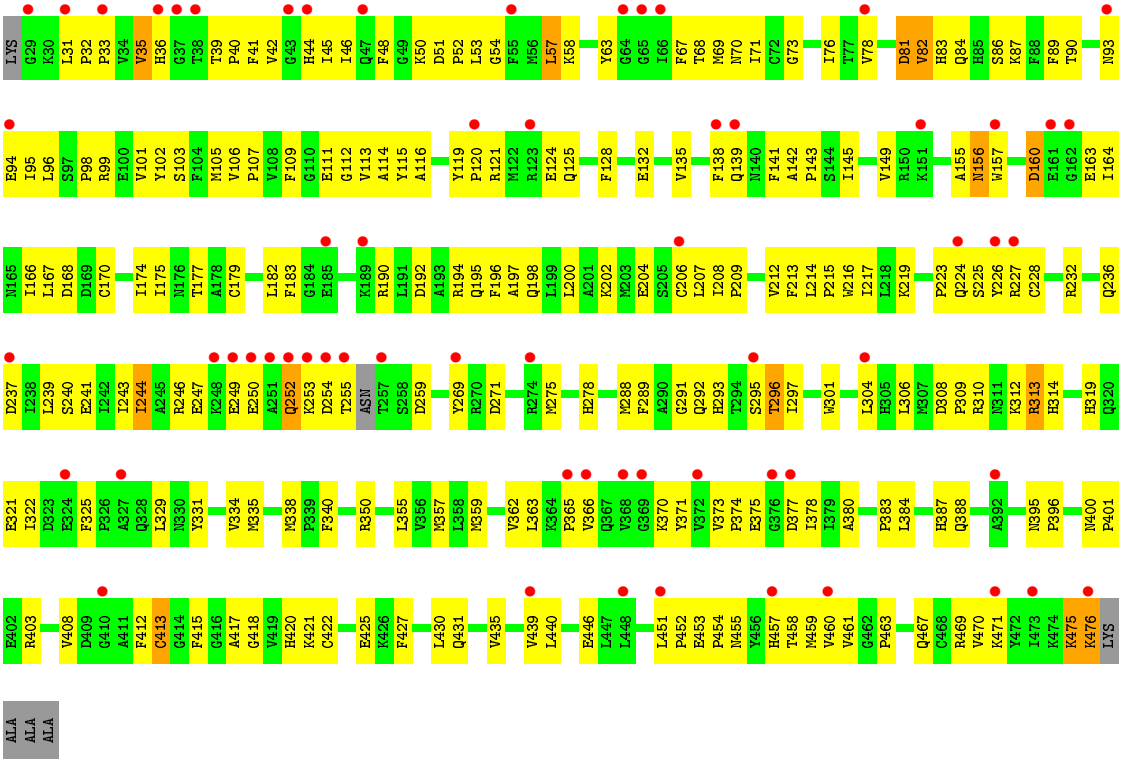
Chain B:





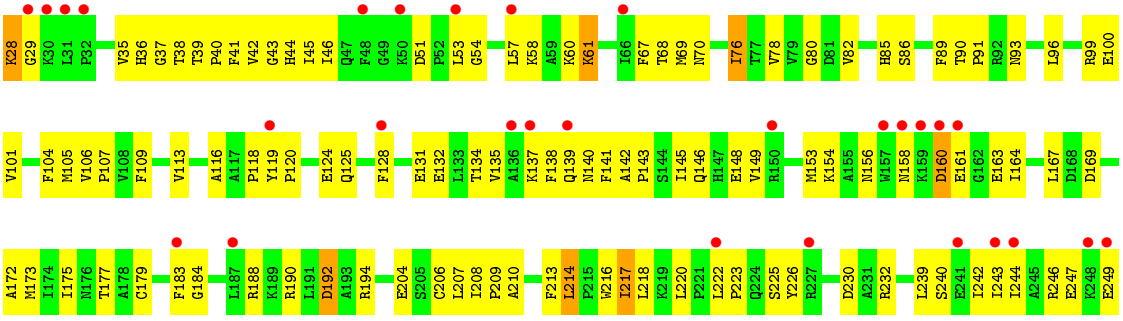
• Molecule 1: Sterol 14-alpha demethylase

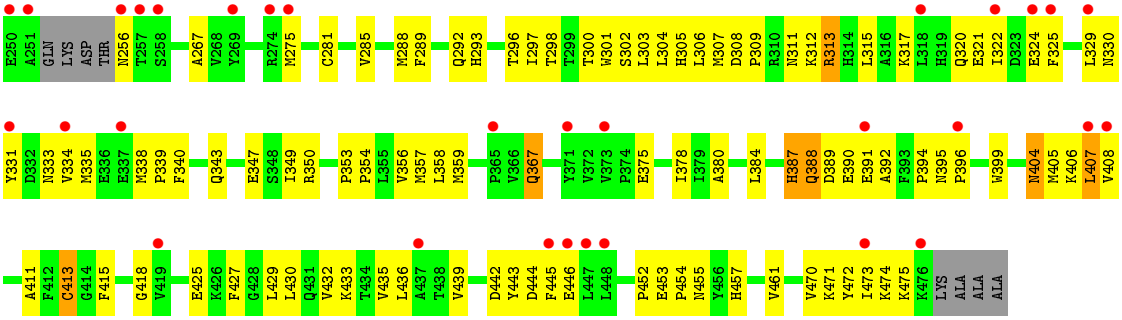
Chain C:



• Molecule 1: Sterol 14-alpha demethylase

Chain D:




E250 A251 GLN LYS ASP THR N256 T257 S258 A267 Y268 Y269 R274 M275 C281 V285 M288 F289 Q292 H293 T296 I297 T298 T299 T300 W301 S302 L303 L304 H305 L306 M307 D308 P309 R310 N311 K312 R313 H314 L315 A316 K317 L318 H319 Q320 E321 I322 D323 E324 F325 L329 N330
Y331 D332 N333 V334 M335 E336 E337 M338 P339 F340 Q343 E347 S348 I349 R350 P353 P354 L355 V356 M357 L358 M359 P365 V366 Q367 Y371 V372 V373 P374 E375 I378 I379 A380 L384 H387 Q388 D389 E390 E391 A392 F393 P394 N395 P396 W399 N404 M405 K406 L407 V408
A411 F412 C413 G414 F415 G418 V419 E425 K426 F427 G428 L429 L430 Q431 V432 K433 T434 V435 L436 A437 T438 V439 D442 Y443 D444 F445 E446 L447 L448 P452 E453 P454 N455 Y456 H457 V461 V470 K471 Y472 I473 K474 K475 K476 LYS ALA ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.89Å 118.51Å 100.96Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	48.80 – 2.75 48.80 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.80-2.75) 97.6 (48.80-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.267 0.216 , 0.265	Depositor DCC
R_{free} test set	2494 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	90.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 49210 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14534	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: N8E, TPF, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/3636	0.44	0/4917
1	B	0.27	0/3645	0.41	0/4928
1	C	0.37	1/3627 (0.0%)	0.42	0/4903
1	D	0.32	0/3611	0.39	0/4881
All	All	0.35	1/14519 (0.0%)	0.42	0/19629

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	CYS	CB-SG	-5.28	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3553	0	3579	246	0
1	B	3562	0	3592	201	0
1	C	3545	0	3572	287	0
1	D	3529	0	3559	262	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	8	0
2	D	43	0	30	8	0
3	A	22	0	12	6	0
3	B	22	0	12	6	0
3	C	22	0	12	6	0
3	D	22	0	12	4	0
4	C	24	0	38	8	0
5	A	16	0	0	0	0
5	B	11	0	0	0	0
5	C	16	0	0	1	0
5	D	18	0	0	2	0
All	All	14534	0	14508	982	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 34.

All (982) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:PHE:C	1:D:214:LEU:HD22	1.48	1.32
1:C:252:GLN:NE2	1:C:254:ASP:HB3	1.48	1.29
1:A:209:PRO:O	1:A:212:VAL:HG23	1.35	1.25
1:D:407:LEU:O	1:D:407:LEU:HD12	1.38	1.18
1:B:292:GLN:O	1:B:296:THR:HG22	1.43	1.17
1:A:292:GLN:O	1:A:296:THR:HG23	1.48	1.14
1:D:388:GLN:HE21	1:D:388:GLN:CA	1.61	1.13
1:C:292:GLN:O	1:C:296:THR:HG23	1.50	1.12
1:D:367:GLN:HE21	1:D:367:GLN:N	1.49	1.11
1:B:330:ASN:N	1:B:333:ASN:HD21	1.47	1.10
1:D:388:GLN:HE21	1:D:388:GLN:N	1.51	1.09
1:D:334:VAL:HA	1:D:338:MET:SD	1.94	1.07
1:A:206:CYS:HB3	1:A:228:CYS:SG	1.95	1.07
1:D:288:MET:HE2	1:D:288:MET:HA	1.34	1.07
1:D:407:LEU:HD12	1:D:407:LEU:C	1.78	1.02
1:B:330:ASN:H	1:B:333:ASN:ND2	1.57	1.02
1:C:44:HIS:HD2	1:C:70:ASN:H	1.03	1.01
2:C:481:HEM:HHD	2:C:481:HEM:HBC2	1.43	1.01
1:D:45:ILE:HG23	1:D:46:ILE:HD12	1.39	1.00
1:C:239:LEU:O	1:C:243:ILE:HG13	1.60	0.99
1:D:321:GLU:OE1	1:D:340:PHE:HB3	1.62	0.99
1:A:119:TYR:CD1	1:A:120:PRO:N	2.30	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PRO:O	1:C:312:LYS:HG3	1.61	0.98
1:D:387:HIS:C	1:D:388:GLN:HE21	1.66	0.98
1:C:451:LEU:HD12	1:C:452:PRO:HD2	1.45	0.98
1:D:214:LEU:N	1:D:214:LEU:HD22	1.70	0.97
1:A:451:LEU:HD12	1:A:452:PRO:HD2	1.44	0.96
1:A:48:PHE:CD1	1:A:69:MET:HE3	1.99	0.95
1:D:446:GLU:O	1:D:470:VAL:HG13	1.66	0.95
1:B:188:ARG:HA	1:B:191:LEU:O	1.66	0.95
1:D:214:LEU:N	1:D:214:LEU:CD2	2.30	0.94
1:A:309:PRO:O	1:A:312:LYS:HG3	1.66	0.94
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.46	0.94
1:D:61:LYS:HE2	1:D:61:LYS:HA	1.49	0.94
1:D:388:GLN:HE21	1:D:388:GLN:HA	1.28	0.94
1:D:415:PHE:HE2	2:D:481:HEM:HBB2	1.33	0.94
1:B:72:CYS:SG	1:C:219:LYS:NZ	2.41	0.94
1:C:252:GLN:NE2	1:C:254:ASP:CB	2.30	0.93
1:C:252:GLN:HE21	1:C:254:ASP:HB3	1.27	0.93
1:A:120:PRO:HD2	1:A:121:ARG:H	1.34	0.93
3:B:490:TPF:F2	3:B:490:TPF:HC52	1.59	0.93
1:C:41:PHE:HB3	4:C:1:N8E:H232	1.50	0.92
1:D:312:LYS:HB2	1:D:313:ARG:NH2	1.84	0.92
1:D:334:VAL:HA	1:D:338:MET:CG	1.99	0.92
1:C:244:ILE:HD13	1:C:244:ILE:H	1.36	0.91
1:B:35:VAL:HG23	1:B:44:HIS:CE1	2.04	0.91
1:D:388:GLN:NE2	1:D:388:GLN:CA	2.31	0.91
1:D:288:MET:HA	1:D:288:MET:CE	2.00	0.91
1:D:367:GLN:HE21	1:D:367:GLN:H	1.15	0.90
1:D:388:GLN:NE2	1:D:388:GLN:HA	1.85	0.90
1:B:44:HIS:HD2	1:B:70:ASN:H	1.16	0.90
1:A:41:PHE:HD2	1:C:42:VAL:HG21	1.37	0.90
1:B:367:GLN:HE21	1:B:367:GLN:N	1.69	0.90
1:A:44:HIS:HD2	1:A:70:ASN:H	1.10	0.89
1:A:41:PHE:CD2	1:C:42:VAL:CG2	2.54	0.89
1:B:325:PHE:CE2	1:B:333:ASN:HB2	2.07	0.89
1:D:99:ARG:HH22	1:D:118:PRO:HA	1.37	0.89
1:D:214:LEU:O	1:D:217:ILE:HG23	1.72	0.89
1:D:213:PHE:C	1:D:214:LEU:CD2	2.40	0.88
1:A:138:PHE:CD1	1:A:430:LEU:HD22	2.07	0.88
1:B:455:ASN:C	1:B:455:ASN:HD22	1.76	0.88
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.53	0.88
1:A:118:PRO:C	1:A:120:PRO:HD2	1.95	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CD1	1:A:430:LEU:CD2	2.58	0.87
4:C:1:N8E:H012	4:C:1:N8E:H052	1.57	0.86
1:D:334:VAL:HA	1:D:338:MET:HG3	1.57	0.86
1:C:42:VAL:HG11	1:C:46:ILE:HD13	1.58	0.86
1:D:292:GLN:O	1:D:296:THR:HG22	1.75	0.86
1:D:387:HIS:C	1:D:388:GLN:NE2	2.30	0.85
1:C:128:PHE:HD1	1:C:275:MET:CE	1.89	0.85
1:A:119:TYR:N	1:A:120:PRO:CD	2.40	0.85
1:A:101:VAL:HG12	1:A:102:TYR:CD1	2.11	0.85
1:B:335:MET:HA	1:B:335:MET:CE	2.07	0.84
1:C:252:GLN:CD	1:C:254:ASP:H	1.80	0.84
1:C:240:SER:O	1:C:244:ILE:CD1	2.25	0.84
1:B:292:GLN:O	1:B:296:THR:CG2	2.25	0.84
1:C:453:GLU:HG3	1:C:454:PRO:HD2	1.58	0.84
1:C:135:VAL:HA	1:C:138:PHE:CD2	2.13	0.83
1:C:44:HIS:CD2	1:C:70:ASN:H	1.92	0.83
1:C:42:VAL:HG13	1:C:45:ILE:HG22	1.61	0.83
1:A:120:PRO:CD	1:A:121:ARG:H	1.92	0.82
1:C:32:PRO:HA	1:C:371:TYR:CD2	2.15	0.82
1:C:476:LYS:HB3	1:C:476:LYS:NZ	1.95	0.81
1:B:455:ASN:ND2	1:B:457:HIS:H	1.77	0.81
1:A:42:VAL:HG21	1:C:40:PRO:CB	2.09	0.81
1:A:42:VAL:CG2	1:C:40:PRO:HB2	2.09	0.81
1:A:48:PHE:HD1	1:A:69:MET:HE3	1.42	0.81
1:B:330:ASN:HD22	1:B:331:TYR:H	1.28	0.81
3:C:490:TPF:F2	3:C:490:TPF:HC52	1.70	0.81
1:D:138:PHE:HD2	1:D:430:LEU:HD22	1.45	0.81
1:D:388:GLN:NE2	1:D:388:GLN:N	2.29	0.81
1:B:101:VAL:HG12	1:B:102:TYR:CD1	2.16	0.81
1:A:48:PHE:CD1	1:A:69:MET:CE	2.64	0.80
1:B:44:HIS:CD2	1:B:70:ASN:H	1.98	0.80
1:C:128:PHE:HD1	1:C:275:MET:HE3	1.46	0.80
1:A:119:TYR:N	1:A:120:PRO:HD3	1.94	0.80
1:A:452:PRO:HA	1:A:467:GLN:OE1	1.81	0.80
1:C:200:LEU:O	1:C:204:GLU:HG3	1.80	0.80
4:C:1:N8E:H172	1:D:220:LEU:HD22	1.63	0.80
1:C:42:VAL:HG13	1:C:45:ILE:CG2	2.12	0.80
1:C:240:SER:O	1:C:244:ILE:HD11	1.80	0.80
1:A:41:PHE:HD2	1:C:42:VAL:CG2	1.92	0.80
1:C:89:PHE:CG	1:C:417:ALA:HB3	2.16	0.79
1:A:139:GLN:OE1	1:A:140:ASN:N	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HB	1:A:40:PRO:HD2	1.66	0.78
1:D:135:VAL:HA	1:D:138:PHE:CD1	2.17	0.78
1:D:214:LEU:O	1:D:217:ILE:CG2	2.31	0.78
1:C:254:ASP:O	1:C:255:THR:HB	1.82	0.78
3:D:490:TPF:HC52	3:D:490:TPF:F2	1.71	0.78
1:D:293:HIS:HA	1:D:296:THR:CG2	2.14	0.78
1:B:101:VAL:HG12	1:B:102:TYR:HD1	1.47	0.78
1:A:191:LEU:HD21	1:A:196:PHE:HD2	1.46	0.78
1:B:250:GLU:O	1:B:253:LYS:CG	2.32	0.78
1:B:182:LEU:O	1:B:259:ASP:HB2	1.84	0.78
1:A:41:PHE:CD2	1:C:42:VAL:HG21	2.16	0.77
1:A:42:VAL:CG1	1:A:45:ILE:HG23	2.15	0.77
1:B:350:ARG:O	1:B:350:ARG:HD2	1.84	0.77
1:A:119:TYR:CD1	1:A:119:TYR:C	2.58	0.77
1:D:61:LYS:CA	1:D:61:LYS:HE2	2.15	0.77
1:C:254:ASP:O	1:C:255:THR:CB	2.33	0.77
1:B:330:ASN:H	1:B:333:ASN:HD21	0.80	0.77
1:A:203:MET:O	1:A:228:CYS:SG	2.43	0.77
2:D:481:HEM:HBC2	2:D:481:HEM:HMC1	1.67	0.76
1:B:330:ASN:HB3	1:B:333:ASN:OD1	1.85	0.76
1:C:42:VAL:CG1	1:C:45:ILE:HG22	2.15	0.76
1:D:334:VAL:HG13	1:D:338:MET:SD	2.26	0.76
1:A:182:LEU:O	1:A:259:ASP:HB2	1.86	0.76
1:C:204:GLU:OE1	1:C:293:HIS:CE1	2.39	0.76
1:D:28:LYS:HD3	1:D:28:LYS:C	2.05	0.76
1:C:182:LEU:HD12	1:C:288:MET:HE1	1.68	0.76
1:A:42:VAL:HG11	1:A:46:ILE:HD13	1.68	0.76
1:B:95:ILE:N	1:B:95:ILE:HD12	2.01	0.75
1:D:350:ARG:HD2	1:D:350:ARG:O	1.85	0.75
1:D:367:GLN:NE2	1:D:367:GLN:N	2.31	0.75
1:B:367:GLN:HE21	1:B:367:GLN:H	1.34	0.75
1:D:148:GLU:HB2	1:D:177:THR:HG22	1.65	0.75
1:D:69:MET:HB2	1:D:76:ILE:HG23	1.67	0.75
1:A:155:ALA:C	1:A:156:ASN:HD22	1.89	0.75
1:C:179:CYS:O	1:C:183:PHE:HB2	1.86	0.75
1:A:199:LEU:HD13	1:A:235:LEU:HB2	1.67	0.75
3:C:490:TPF:HC6	3:C:490:TPF:O	1.87	0.74
3:A:490:TPF:O	3:A:490:TPF:HC6	1.86	0.74
1:C:292:GLN:O	1:C:296:THR:CG2	2.33	0.74
1:D:142:ALA:HB3	1:D:143:PRO:HD3	1.69	0.74
1:A:118:PRO:C	1:A:120:PRO:CD	2.55	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CE1	1:A:430:LEU:CD2	2.71	0.74
1:B:455:ASN:HD21	1:B:457:HIS:HB2	1.53	0.74
1:D:208:ILE:HG21	1:D:217:ILE:HD11	1.70	0.73
4:C:1:N8E:H013	1:D:45:ILE:CD1	2.18	0.73
1:C:95:ILE:HD12	1:C:95:ILE:N	2.02	0.73
1:A:42:VAL:HG21	1:C:40:PRO:HB2	1.68	0.73
1:A:119:TYR:HD1	1:A:120:PRO:N	1.87	0.73
1:A:471:LYS:HE2	1:A:473:ILE:HD11	1.70	0.73
1:C:308:ASP:OD2	1:C:310:ARG:NH2	2.21	0.72
3:A:490:TPF:HC52	3:A:490:TPF:F2	1.79	0.72
1:B:192:ASP:OD2	1:B:195:GLN:HG3	1.89	0.72
2:D:481:HEM:HBC2	2:D:481:HEM:CMC	2.19	0.72
1:C:135:VAL:HA	1:C:138:PHE:CE2	2.24	0.72
1:C:128:PHE:O	1:C:132:GLU:HG2	1.89	0.72
1:D:213:PHE:O	1:D:214:LEU:HD22	1.88	0.71
1:C:48:PHE:CD1	1:C:69:MET:CE	2.72	0.71
1:A:118:PRO:O	1:A:120:PRO:HD2	1.89	0.71
1:A:453:GLU:HG3	1:A:454:PRO:HD2	1.72	0.71
1:A:475:LYS:O	1:A:476:LYS:CB	2.39	0.71
1:C:475:LYS:O	1:C:476:LYS:O	2.09	0.71
1:A:350:ARG:O	1:A:350:ARG:HD2	1.91	0.71
1:A:42:VAL:HG13	1:A:45:ILE:HG23	1.71	0.71
1:C:48:PHE:CD1	1:C:69:MET:HE3	2.25	0.71
1:D:67:PHE:CZ	1:D:78:VAL:HG21	2.25	0.70
1:D:350:ARG:HA	1:D:387:HIS:CD2	2.26	0.70
1:A:206:CYS:HA	1:A:224:GLN:HB3	1.72	0.70
1:C:387:HIS:HE1	1:C:413:CYS:H	1.39	0.70
1:B:250:GLU:O	1:B:253:LYS:HG3	1.90	0.70
1:B:424:GLY:HA3	2:B:481:HEM:C3C	2.26	0.70
1:A:72:CYS:SG	1:A:214:LEU:HD11	2.31	0.70
1:A:234:GLU:OE2	1:B:469:ARG:NH1	2.24	0.70
1:A:128:PHE:HD1	1:A:275:MET:CE	2.04	0.70
1:A:206:CYS:CB	1:A:228:CYS:SG	2.77	0.70
1:B:35:VAL:CG2	1:B:44:HIS:CE1	2.74	0.70
1:C:455:ASN:ND2	1:C:457:HIS:HD2	1.90	0.70
1:A:139:GLN:C	1:A:139:GLN:OE1	2.30	0.70
1:C:455:ASN:HD21	1:C:457:HIS:HD2	1.38	0.70
1:C:246:ARG:O	1:C:250:GLU:HB2	1.92	0.70
1:C:99:ARG:HD2	1:C:115:TYR:O	1.90	0.70
1:A:451:LEU:HD12	1:A:452:PRO:CD	2.21	0.70
1:D:392:ALA:HB2	1:D:408:VAL:HG21	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LEU:O	1:B:217:ILE:HG22	1.92	0.69
1:A:292:GLN:O	1:A:296:THR:CG2	2.35	0.69
1:C:455:ASN:HD21	1:C:457:HIS:CD2	2.10	0.69
1:A:206:CYS:O	1:A:208:ILE:HG13	1.92	0.69
1:C:81:ASP:OD1	1:C:81:ASP:C	2.30	0.69
1:B:335:MET:HE3	1:B:335:MET:HA	1.73	0.69
1:B:330:ASN:ND2	1:B:331:TYR:H	1.90	0.68
3:A:490:TPF:C6	3:A:490:TPF:O	2.40	0.68
1:B:258:SER:HB3	1:B:262:ALA:HB3	1.74	0.68
1:A:235:LEU:CD2	1:A:285:VAL:HG22	2.23	0.68
1:B:455:ASN:C	1:B:455:ASN:ND2	2.46	0.68
1:A:476:LYS:HD3	1:A:476:LYS:C	2.13	0.68
1:C:190:ARG:NH2	1:C:241:GLU:OE1	2.26	0.68
1:B:317:LYS:NZ	1:B:402:GLU:OE2	2.22	0.68
1:A:82:VAL:HG22	1:A:411:ALA:HA	1.75	0.68
1:A:138:PHE:CE1	1:A:430:LEU:HD22	2.29	0.68
3:C:490:TPF:O	3:C:490:TPF:C6	2.39	0.68
1:D:138:PHE:CD2	1:D:430:LEU:HD22	2.27	0.68
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.74	0.68
1:A:190:ARG:HA	1:B:163:GLU:OE2	1.93	0.68
1:D:154:LYS:HG2	1:D:154:LYS:O	1.94	0.68
1:D:407:LEU:CD1	1:D:407:LEU:C	2.55	0.68
1:A:370:LYS:HE3	1:A:371:TYR:CZ	2.29	0.68
1:A:101:VAL:HG12	1:A:102:TYR:HD1	1.58	0.67
1:A:42:VAL:HG13	1:A:45:ILE:CG2	2.24	0.67
1:D:444:ASP:HB2	1:D:473:ILE:HB	1.75	0.67
1:D:415:PHE:CE2	2:D:481:HEM:HBB2	2.23	0.67
1:C:350:ARG:O	1:C:350:ARG:HD2	1.93	0.67
1:D:39:THR:HB	1:D:40:PRO:HD2	1.77	0.67
1:A:44:HIS:CD2	1:A:70:ASN:H	2.03	0.67
1:C:101:VAL:HG11	1:C:359:MET:HB2	1.75	0.67
1:B:455:ASN:HD22	1:B:457:HIS:H	1.43	0.66
1:D:407:LEU:O	1:D:407:LEU:CD1	2.30	0.66
1:A:40:PRO:HG3	1:C:39:THR:HB	1.78	0.66
1:C:253:LYS:HG3	1:C:253:LYS:O	1.94	0.66
1:A:424:GLY:HA3	2:A:481:HEM:C3C	2.30	0.66
1:A:76:ILE:HD11	1:A:357:MET:HE1	1.78	0.66
1:B:84:GLN:OE1	1:B:87:LYS:HE2	1.96	0.66
1:A:39:THR:CB	1:A:40:PRO:HD2	2.25	0.66
1:B:314:HIS:CE1	1:B:401:PRO:HD2	2.30	0.66
1:B:216:TRP:CZ3	1:C:216:TRP:HB3	2.30	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD11	1:B:469:ARG:CD	2.26	0.66
1:C:206:CYS:HB2	1:C:228:CYS:HB2	1.78	0.66
1:B:288:MET:HA	1:B:288:MET:HE2	1.78	0.66
1:C:41:PHE:CB	4:C:1:N8E:H232	2.23	0.66
1:B:250:GLU:O	1:B:253:LYS:HG2	1.95	0.66
1:A:138:PHE:CE1	1:A:430:LEU:HD23	2.31	0.65
1:B:119:TYR:HB2	1:B:120:PRO:HD3	1.75	0.65
1:D:154:LYS:C	5:D:482:HOH:O	2.34	0.65
1:C:400:ASN:O	1:C:403:ARG:HG2	1.96	0.65
1:C:252:GLN:OE1	1:C:253:LYS:N	2.30	0.65
1:C:42:VAL:CG1	1:C:46:ILE:HD13	2.25	0.65
1:D:28:LYS:HD3	1:D:29:GLY:N	2.12	0.65
1:B:254:ASP:OD1	1:B:254:ASP:N	2.30	0.65
1:B:453:GLU:HG3	1:B:454:PRO:HD2	1.79	0.65
1:C:155:ALA:C	1:C:156:ASN:HD22	2.01	0.64
1:A:42:VAL:HG21	1:C:40:PRO:HB3	1.77	0.64
1:A:213:PHE:C	1:A:214:LEU:HD12	2.18	0.64
1:D:387:HIS:O	1:D:388:GLN:NE2	2.30	0.64
1:C:121:ARG:O	1:C:125:GLN:HG3	1.98	0.64
1:A:39:THR:OG1	1:A:42:VAL:HB	1.98	0.64
1:D:51:ASP:OD2	1:D:54:GLY:HA3	1.96	0.64
1:C:331:TYR:CE1	1:C:335:MET:HG3	2.32	0.64
1:B:135:VAL:HA	1:B:138:PHE:CD2	2.32	0.64
1:D:442:ASP:O	1:D:475:LYS:HG2	1.98	0.64
1:C:223:PRO:HA	1:C:226:TYR:HD2	1.61	0.64
1:A:50:LYS:HD3	1:A:50:LYS:C	2.18	0.64
1:D:334:VAL:CA	1:D:338:MET:HG3	2.28	0.64
1:C:309:PRO:O	1:C:312:LYS:CG	2.40	0.63
1:B:304:LEU:HD13	1:B:452:PRO:HG2	1.79	0.63
1:D:472:TYR:O	1:D:472:TYR:CD1	2.52	0.63
1:A:415:PHE:CE2	1:A:425:GLU:HG3	2.34	0.63
1:C:475:LYS:O	1:C:476:LYS:C	2.35	0.63
1:C:206:CYS:CB	1:C:228:CYS:HB2	2.29	0.63
1:B:135:VAL:HB	1:B:331:TYR:OH	1.98	0.63
1:D:473:ILE:HD12	1:D:473:ILE:N	2.13	0.63
1:C:81:ASP:OD1	1:C:83:HIS:N	2.30	0.63
4:C:1:N8E:H013	1:D:45:ILE:HD11	1.81	0.63
1:A:42:VAL:HG23	1:C:40:PRO:HB2	1.79	0.63
3:B:490:TPF:HC6	3:B:490:TPF:O	1.99	0.63
1:C:476:LYS:HZ2	1:C:476:LYS:HB3	1.63	0.63
1:D:358:LEU:HD22	2:D:481:HEM:CGA	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ILE:HG21	1:C:366:VAL:CG1	2.29	0.63
1:A:135:VAL:HA	1:A:138:PHE:CD2	2.33	0.62
1:C:128:PHE:HD1	1:C:275:MET:HE2	1.63	0.62
1:D:395:ASN:N	1:D:396:PRO:HD3	2.14	0.62
1:C:141:PHE:O	1:C:145:ILE:HG13	1.98	0.62
1:C:145:ILE:O	1:C:149:VAL:HG23	1.98	0.62
1:B:330:ASN:HD22	1:B:331:TYR:N	1.95	0.62
1:D:223:PRO:HA	1:D:226:TYR:HD2	1.65	0.62
1:B:105:MET:CE	1:B:109:PHE:CZ	2.83	0.62
1:D:106:VAL:N	1:D:107:PRO:CD	2.62	0.62
1:A:384:LEU:O	1:A:388:GLN:HG2	1.99	0.62
1:A:288:MET:HE2	1:A:288:MET:HA	1.81	0.62
1:A:89:PHE:CG	1:A:417:ALA:HB3	2.35	0.62
1:B:105:MET:HE2	1:B:109:PHE:CZ	2.34	0.62
1:A:94:GLU:O	1:A:363:LEU:HD12	2.00	0.62
1:B:42:VAL:HB	1:B:45:ILE:CG2	2.29	0.62
1:A:82:VAL:CG2	1:A:411:ALA:HA	2.30	0.62
1:B:331:TYR:CE1	1:B:335:MET:HG3	2.35	0.62
1:A:177:THR:OG1	1:A:431:GLN:NE2	2.33	0.62
1:D:304:LEU:HD13	1:D:452:PRO:HG2	1.82	0.62
1:D:128:PHE:CD2	1:D:267:ALA:HB1	2.35	0.61
1:A:406:LYS:HD2	1:A:409:ASP:OD2	2.00	0.61
2:C:481:HEM:HBC2	2:C:481:HEM:CHD	2.21	0.61
1:D:39:THR:OG1	1:D:42:VAL:HG12	2.01	0.61
1:D:41:PHE:CD1	1:D:41:PHE:O	2.54	0.61
1:C:331:TYR:CZ	1:C:335:MET:HG3	2.35	0.61
1:C:51:ASP:OD1	1:C:54:GLY:HA3	2.00	0.61
1:B:350:ARG:C	1:B:350:ARG:HD2	2.20	0.61
1:C:31:LEU:HD22	1:C:374:PRO:HD3	1.83	0.61
1:C:128:PHE:CD1	1:C:275:MET:HE3	2.31	0.61
1:B:177:THR:OG1	1:B:431:GLN:NE2	2.33	0.61
1:C:93:ASN:HA	1:C:96:LEU:O	2.00	0.61
1:C:111:GLU:O	1:C:278:HIS:HE1	1.84	0.61
1:D:204:GLU:OE1	1:D:293:HIS:NE2	2.32	0.60
3:D:490:TPF:O	3:D:490:TPF:HC6	2.00	0.60
1:A:238:ILE:HD11	1:B:469:ARG:NE	2.15	0.60
1:A:209:PRO:O	1:A:212:VAL:CG2	2.30	0.60
1:A:355:LEU:HD11	3:A:490:TPF:N4	2.15	0.60
1:D:339:PRO:O	1:D:343:GLN:HG3	2.01	0.60
1:C:207:LEU:HD13	1:C:459:MET:SD	2.41	0.60
1:B:45:ILE:HG23	1:B:46:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PHE:CD1	1:C:275:MET:CE	2.80	0.60
1:C:252:GLN:CD	1:C:254:ASP:N	2.54	0.60
1:C:31:LEU:CD2	1:C:374:PRO:HD3	2.32	0.60
1:A:35:VAL:O	1:A:44:HIS:CE1	2.55	0.59
1:D:453:GLU:HG3	1:D:454:PRO:HD2	1.83	0.59
1:C:297:ILE:CD1	1:C:460:VAL:HG12	2.32	0.59
1:A:287:ALA:HB1	2:A:481:HEM:HBC1	1.84	0.59
1:C:306:LEU:HD13	1:C:440:LEU:HD11	1.84	0.59
1:A:42:VAL:CG1	1:A:45:ILE:CG2	2.81	0.59
1:D:288:MET:CA	1:D:288:MET:CE	2.79	0.59
1:C:452:PRO:HA	1:C:467:GLN:OE1	2.02	0.59
1:B:290:ALA:HB1	3:B:490:TPF:C7	2.33	0.59
1:D:101:VAL:HG11	1:D:359:MET:HB2	1.85	0.59
1:A:39:THR:HB	1:A:40:PRO:CD	2.32	0.59
1:B:170:CYS:O	1:B:174:ILE:HG12	2.03	0.59
1:C:422:CYS:HB2	2:C:481:HEM:NA	2.17	0.59
1:B:470:VAL:CG1	1:B:471:LYS:N	2.66	0.59
1:D:141:PHE:O	1:D:145:ILE:HG13	2.02	0.58
1:D:53:LEU:O	1:D:57:LEU:HB2	2.03	0.58
1:D:321:GLU:OE1	1:D:340:PHE:CB	2.47	0.58
1:A:120:PRO:CD	1:A:121:ARG:N	2.59	0.58
1:A:128:PHE:HD1	1:A:275:MET:HE3	1.66	0.58
1:A:145:ILE:O	1:A:149:VAL:HG23	2.04	0.58
1:C:142:ALA:HB3	1:C:143:PRO:CD	2.27	0.58
1:D:334:VAL:CA	1:D:338:MET:SD	2.81	0.58
1:B:333:ASN:O	1:B:338:MET:HG3	2.04	0.58
1:D:313:ARG:H	1:D:313:ARG:NE	2.02	0.58
1:B:350:ARG:HA	1:B:387:HIS:CD2	2.39	0.58
1:C:291:GLY:O	1:C:295:SER:HB2	2.04	0.58
1:A:40:PRO:HG3	1:C:39:THR:CB	2.34	0.58
1:C:82:VAL:O	1:C:82:VAL:HG13	2.02	0.58
3:B:490:TPF:C6	3:B:490:TPF:O	2.51	0.58
1:A:475:LYS:O	1:A:476:LYS:HB3	2.04	0.58
1:D:392:ALA:HB2	1:D:408:VAL:CG2	2.33	0.58
1:D:300:THR:O	1:D:304:LEU:HG	2.03	0.57
1:C:51:ASP:OD2	1:C:52:PRO:HD2	2.03	0.57
1:D:149:VAL:O	1:D:153:MET:HG3	2.04	0.57
1:C:254:ASP:O	1:C:255:THR:HG22	2.03	0.57
1:B:335:MET:HA	1:B:335:MET:HE2	1.86	0.57
1:B:95:ILE:N	1:B:95:ILE:CD1	2.65	0.57
1:C:112:GLY:HA2	1:C:116:ALA:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HG3	1:A:420:HIS:CE1	2.39	0.57
1:D:214:LEU:HB3	1:D:217:ILE:HG22	1.85	0.57
1:A:111:GLU:CD	1:D:40:PRO:O	2.43	0.57
1:B:214:LEU:O	1:B:217:ILE:CG2	2.52	0.57
1:C:387:HIS:CE1	1:C:413:CYS:H	2.21	0.57
1:D:137:LYS:C	1:D:139:GLN:OE1	2.43	0.57
1:D:330:ASN:OD1	1:D:330:ASN:C	2.43	0.57
1:C:422:CYS:HB2	2:C:481:HEM:C4A	2.40	0.57
1:C:325:PHE:HB3	1:C:329:LEU:HD21	1.86	0.57
1:B:76:ILE:HA	1:B:378:ILE:O	2.04	0.57
1:A:86:SER:O	1:A:90:THR:HB	2.02	0.57
3:D:490:TPF:C6	3:D:490:TPF:O	2.53	0.57
1:D:93:ASN:HA	1:D:96:LEU:O	2.05	0.57
1:B:347:GLU:OE1	1:B:403:ARG:HD2	2.05	0.57
1:C:240:SER:O	1:C:244:ILE:HD13	2.02	0.57
1:C:370:LYS:HE2	1:C:371:TYR:CZ	2.40	0.57
1:A:338:MET:HE1	1:A:437:ALA:HB2	1.85	0.57
1:C:32:PRO:HA	1:C:371:TYR:CE2	2.40	0.57
1:B:182:LEU:CD1	1:B:288:MET:HE3	2.35	0.57
1:A:173:MET:O	1:A:177:THR:HG23	2.05	0.57
1:C:254:ASP:C	1:C:255:THR:HG22	2.25	0.56
1:C:244:ILE:HD13	1:C:244:ILE:N	2.15	0.56
1:C:95:ILE:HD12	1:C:95:ILE:H	1.70	0.56
1:A:350:ARG:HA	1:A:387:HIS:CD2	2.40	0.56
1:B:330:ASN:ND2	1:B:331:TYR:N	2.52	0.56
1:C:314:HIS:CE1	1:C:401:PRO:HD2	2.40	0.56
1:C:33:PRO:HD3	1:C:371:TYR:CE2	2.40	0.56
1:D:347:GLU:HA	1:D:405:MET:HE1	1.85	0.56
1:A:45:ILE:HG12	1:A:46:ILE:N	2.17	0.56
1:C:288:MET:CE	1:C:288:MET:HA	2.35	0.56
1:D:36:HIS:CD2	1:D:37:GLY:H	2.23	0.56
1:D:45:ILE:CG2	1:D:46:ILE:HD12	2.26	0.56
1:B:71:ILE:HG21	1:B:213:PHE:CD1	2.41	0.56
1:D:239:LEU:O	1:D:243:ILE:HG13	2.05	0.56
1:C:252:GLN:OE1	1:C:254:ASP:N	2.30	0.56
1:C:254:ASP:O	1:C:255:THR:CG2	2.53	0.56
1:B:182:LEU:HD13	1:B:288:MET:HE3	1.86	0.56
1:C:82:VAL:HG11	1:C:408:VAL:HG11	1.88	0.56
1:D:104:PHE:HA	1:D:218:LEU:HD11	1.86	0.56
1:C:446:GLU:O	1:C:470:VAL:HG13	2.04	0.56
1:A:42:VAL:CG1	1:A:46:ILE:HD13	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:CD	1:D:100:GLU:H	2.09	0.56
1:C:45:ILE:HG23	1:C:46:ILE:N	2.20	0.56
1:A:76:ILE:HG23	1:A:76:ILE:O	2.06	0.56
1:A:281:CYS:O	1:A:285:VAL:HG23	2.04	0.56
1:D:35:VAL:HG12	1:D:68:THR:O	2.06	0.56
1:D:350:ARG:HD2	1:D:350:ARG:C	2.25	0.56
1:A:120:PRO:O	1:A:124:GLU:HG3	2.06	0.56
1:A:139:GLN:C	1:A:139:GLN:CD	2.65	0.56
1:B:42:VAL:HB	1:B:45:ILE:HG22	1.88	0.56
1:B:106:VAL:N	1:B:107:PRO:CD	2.69	0.56
1:A:206:CYS:O	1:A:207:LEU:C	2.44	0.56
1:A:350:ARG:O	1:A:387:HIS:HB3	2.06	0.56
1:C:195:GLN:NE2	1:D:163:GLU:O	2.37	0.56
1:D:387:HIS:HE1	1:D:413:CYS:H	1.52	0.55
1:D:61:LYS:CA	1:D:61:LYS:CE	2.82	0.55
1:A:101:VAL:CG1	1:A:102:TYR:CD1	2.87	0.55
1:C:101:VAL:HG13	1:C:359:MET:HE3	1.86	0.55
1:D:293:HIS:O	1:D:296:THR:HG23	2.06	0.55
1:D:134:THR:C	1:D:138:PHE:HE1	2.09	0.55
1:D:169:ASP:O	1:D:173:MET:HG3	2.06	0.55
1:C:82:VAL:HG12	1:C:83:HIS:N	2.21	0.55
1:B:356:VAL:HG21	1:B:461:VAL:HG21	1.87	0.55
1:B:252:GLN:HA	1:B:252:GLN:OE1	2.07	0.55
1:D:281:CYS:O	1:D:285:VAL:HG23	2.06	0.55
1:C:395:ASN:N	1:C:396:PRO:HD3	2.21	0.55
1:B:240:SER:O	1:B:244:ILE:HG12	2.07	0.55
1:C:384:LEU:O	1:C:388:GLN:HG2	2.06	0.55
1:D:44:HIS:HD2	1:D:70:ASN:H	1.54	0.55
1:B:325:PHE:CE2	1:B:333:ASN:CB	2.85	0.55
2:C:481:HEM:HAD1	3:C:490:TPF:H10	1.88	0.55
1:A:120:PRO:HD2	1:A:121:ARG:N	2.13	0.55
1:B:213:PHE:O	1:B:214:LEU:HD12	2.07	0.55
1:C:67:PHE:CZ	1:C:78:VAL:HG21	2.42	0.55
1:D:190:ARG:O	1:D:190:ARG:HD2	2.05	0.55
1:C:243:ILE:O	1:C:246:ARG:HB2	2.06	0.55
1:A:472:TYR:C	1:A:473:ILE:HD12	2.27	0.55
1:C:206:CYS:SG	1:C:225:SER:HA	2.47	0.55
1:C:415:PHE:CE2	1:C:425:GLU:HG3	2.42	0.55
1:C:175:ILE:HG12	1:C:197:ALA:HB2	1.88	0.55
1:D:204:GLU:OE1	1:D:289:PHE:CD1	2.59	0.55
1:C:476:LYS:HZ3	1:C:476:LYS:HB3	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PHE:CZ	1:B:78:VAL:HG21	2.41	0.55
1:B:355:LEU:HD11	3:B:490:TPF:N4	2.21	0.55
1:D:138:PHE:HE2	1:D:427:PHE:HA	1.72	0.55
1:A:358:LEU:HD22	2:A:481:HEM:HBA2	1.89	0.55
1:C:252:GLN:NE2	1:C:254:ASP:CA	2.69	0.55
1:C:355:LEU:HD11	3:C:490:TPF:N4	2.21	0.54
1:C:48:PHE:CD1	1:C:69:MET:HE1	2.41	0.54
1:D:443:TYR:OH	1:D:474:LYS:NZ	2.40	0.54
1:B:138:PHE:CD1	1:B:141:PHE:CD2	2.95	0.54
1:C:475:LYS:HA	1:C:475:LYS:HE3	1.89	0.54
1:C:206:CYS:O	1:C:208:ILE:HG13	2.07	0.54
1:C:106:VAL:N	1:C:107:PRO:CD	2.69	0.54
1:D:455:ASN:ND2	1:D:457:HIS:H	2.04	0.54
1:D:45:ILE:HG23	1:D:46:ILE:CD1	2.25	0.54
1:D:135:VAL:CA	1:D:138:PHE:CD1	2.89	0.54
4:C:1:N8E:C01	4:C:1:N8E:H052	2.35	0.54
1:C:51:ASP:CG	1:C:54:GLY:H	2.10	0.54
1:D:146:GLN:HE22	1:D:329:LEU:HG	1.73	0.54
1:D:42:VAL:HG22	1:D:45:ILE:CG2	2.38	0.54
1:C:196:PHE:CZ	1:C:288:MET:HG3	2.43	0.54
1:D:303:LEU:O	1:D:307:MET:HG2	2.07	0.54
1:D:82:VAL:HG21	1:D:411:ALA:HB1	1.89	0.54
1:C:95:ILE:CG2	1:C:366:VAL:CG1	2.85	0.54
1:D:331:TYR:CE1	1:D:335:MET:HG3	2.42	0.54
1:C:420:HIS:HA	2:C:481:HEM:O2D	2.08	0.54
1:A:41:PHE:CD2	1:C:42:VAL:HG22	2.42	0.54
1:D:160:ASP:N	1:D:160:ASP:OD2	2.40	0.54
1:D:38:THR:HB	1:D:44:HIS:NE2	2.23	0.54
1:A:139:GLN:OE1	1:A:140:ASN:CB	2.56	0.54
1:A:465:ALA:O	1:A:468:CYS:HB2	2.07	0.54
1:C:109:PHE:O	1:C:232:ARG:NH2	2.40	0.54
1:D:213:PHE:HB2	1:D:214:LEU:CD2	2.38	0.53
1:B:470:VAL:HG12	1:B:471:LYS:N	2.22	0.53
1:A:331:TYR:CE1	1:A:335:MET:HG3	2.43	0.53
1:D:135:VAL:HA	1:D:138:PHE:CE1	2.43	0.53
1:A:149:VAL:O	1:A:153:MET:HG3	2.08	0.53
1:C:35:VAL:HG12	1:C:68:THR:O	2.08	0.53
1:D:293:HIS:HA	1:D:296:THR:HG22	1.88	0.53
1:B:387:HIS:HE1	1:B:413:CYS:H	1.55	0.53
1:D:240:SER:O	1:D:244:ILE:HG13	2.07	0.53
1:B:395:ASN:OD1	1:B:398:GLU:OE1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:PRO:O	1:B:212:VAL:HG23	2.09	0.53
1:C:223:PRO:HA	1:C:226:TYR:CD2	2.43	0.53
1:A:39:THR:CB	1:A:40:PRO:CD	2.86	0.53
1:A:302:SER:O	1:A:306:LEU:HG	2.07	0.53
1:A:322:ILE:HA	1:A:325:PHE:HD1	1.72	0.53
1:B:330:ASN:O	1:B:333:ASN:ND2	2.41	0.53
1:D:472:TYR:C	1:D:472:TYR:CD1	2.82	0.53
1:A:288:MET:CA	1:A:288:MET:HE2	2.38	0.53
1:B:319:HIS:O	1:B:323:ASP:CG	2.46	0.53
1:A:101:VAL:O	1:A:101:VAL:HG13	2.09	0.53
1:C:69:MET:HB2	1:C:76:ILE:HG23	1.89	0.53
1:D:243:ILE:O	1:D:247:GLU:HG3	2.09	0.53
1:A:387:HIS:HE1	1:A:413:CYS:H	1.56	0.53
1:D:312:LYS:H	1:D:313:ARG:HH21	1.57	0.53
1:C:325:PHE:HB3	1:C:329:LEU:CD2	2.39	0.53
1:B:87:LYS:HD3	1:B:368:VAL:HA	1.91	0.53
1:A:55:PHE:CE2	1:A:69:MET:HE3	2.44	0.52
1:A:138:PHE:CE1	1:A:427:PHE:HD1	2.27	0.52
1:D:173:MET:O	1:D:177:THR:HG23	2.09	0.52
1:C:350:ARG:C	1:C:350:ARG:HD2	2.29	0.52
1:C:244:ILE:CD1	1:C:244:ILE:H	2.04	0.52
1:C:383:PRO:O	1:C:387:HIS:CG	2.62	0.52
1:B:216:TRP:CG	1:C:215:PRO:HG2	2.45	0.52
1:A:239:LEU:O	1:A:243:ILE:HG13	2.09	0.52
1:D:128:PHE:CE2	1:D:267:ALA:HB1	2.44	0.52
1:A:321:GLU:OE2	1:A:338:MET:HA	2.08	0.52
1:C:50:LYS:HD3	1:C:50:LYS:C	2.30	0.52
1:D:350:ARG:O	1:D:387:HIS:CD2	2.62	0.52
1:B:331:TYR:O	1:B:335:MET:HG2	2.10	0.52
1:C:48:PHE:HD1	1:C:69:MET:HE3	1.72	0.52
1:B:400:ASN:O	1:B:403:ARG:HG2	2.10	0.52
1:C:301:TRP:NE1	1:C:463:PRO:HD3	2.24	0.52
1:A:31:LEU:HD22	1:A:374:PRO:HD3	1.91	0.52
1:C:119:TYR:N	1:C:120:PRO:HD2	2.24	0.52
1:B:65:GLY:O	1:B:80:GLY:N	2.42	0.52
1:C:101:VAL:O	1:C:101:VAL:HG12	2.10	0.52
1:A:322:ILE:HA	1:A:325:PHE:CD1	2.45	0.52
1:A:224:GLN:HE22	1:B:224:GLN:HG2	1.74	0.52
1:A:309:PRO:O	1:A:312:LYS:CG	2.49	0.52
2:D:481:HEM:HMC1	2:D:481:HEM:CBC	2.37	0.52
1:A:156:ASN:HD22	1:A:156:ASN:N	2.03	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:O	1:B:175:ILE:HG22	2.09	0.52
1:A:200:LEU:O	1:A:204:GLU:HG2	2.10	0.52
1:D:43:GLY:HA3	1:D:70:ASN:O	2.10	0.52
1:B:213:PHE:C	1:B:214:LEU:HD12	2.31	0.52
1:C:297:ILE:HD12	1:C:460:VAL:HG12	1.92	0.52
1:D:308:ASP:OD1	1:D:309:PRO:HD2	2.09	0.52
1:D:125:GLN:HA	1:D:128:PHE:CD1	2.46	0.51
1:B:53:LEU:HD13	1:B:384:LEU:HG	1.91	0.51
1:B:82:VAL:HG22	1:B:411:ALA:HA	1.90	0.51
1:C:39:THR:OG1	1:C:42:VAL:HB	2.10	0.51
1:A:415:PHE:CD2	1:A:425:GLU:HG3	2.45	0.51
1:A:224:GLN:NE2	1:B:224:GLN:HG2	2.24	0.51
1:D:38:THR:HB	1:D:44:HIS:CE1	2.46	0.51
1:D:298:THR:HG21	1:D:349:ILE:HD11	1.92	0.51
1:B:135:VAL:HA	1:B:138:PHE:CE2	2.46	0.51
1:B:424:GLY:HA3	2:B:481:HEM:C2C	2.45	0.51
1:D:322:ILE:HA	1:D:325:PHE:HD1	1.75	0.51
1:A:451:LEU:CD1	1:A:452:PRO:HD2	2.30	0.51
1:C:435:VAL:O	1:C:439:VAL:HG23	2.10	0.51
1:D:297:ILE:HD13	1:D:461:VAL:O	2.11	0.51
1:B:128:PHE:CD2	1:B:267:ALA:HB1	2.45	0.51
1:D:470:VAL:HG12	1:D:471:LYS:N	2.26	0.51
1:D:334:VAL:HG12	1:D:433:LYS:HE2	1.92	0.51
1:C:69:MET:HE2	1:C:71:ILE:HD11	1.93	0.51
1:D:158:ASN:HB3	5:D:482:HOH:O	2.10	0.51
1:A:101:VAL:CG1	1:A:102:TYR:HD1	2.24	0.51
1:B:149:VAL:O	1:B:153:MET:HG3	2.11	0.50
1:B:333:ASN:HA	1:B:337:GLU:HB2	1.93	0.50
1:B:192:ASP:OD1	1:B:194:ARG:HB2	2.09	0.50
1:A:150:ARG:HA	1:A:153:MET:HE2	1.93	0.50
1:B:405:MET:HE3	1:B:412:PHE:CD1	2.46	0.50
3:C:490:TPF:F2	3:C:490:TPF:C5	2.46	0.50
4:C:1:N8E:H013	1:D:45:ILE:HD13	1.90	0.50
1:B:367:GLN:NE2	1:B:367:GLN:N	2.49	0.50
1:A:350:ARG:C	1:A:350:ARG:HD2	2.32	0.50
1:B:312:LYS:HB2	1:B:313:ARG:NH2	2.26	0.50
1:A:288:MET:CE	1:A:288:MET:HA	2.41	0.50
1:A:455:ASN:HD22	1:A:455:ASN:C	2.15	0.50
1:B:288:MET:CA	1:B:288:MET:HE2	2.42	0.50
1:B:39:THR:OG1	1:B:43:GLY:O	2.28	0.50
1:B:331:TYR:CE1	1:B:335:MET:CG	2.95	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASP:O	1:B:256:ASN:OD1	2.30	0.50
1:D:82:VAL:CG2	1:D:411:ALA:HA	2.42	0.50
1:B:406:LYS:O	1:B:406:LYS:CG	2.60	0.50
1:A:93:ASN:HA	1:A:96:LEU:O	2.11	0.50
1:D:406:LYS:O	1:D:407:LEU:C	2.48	0.50
1:C:313:ARG:H	1:C:313:ARG:NE	2.10	0.50
1:D:139:GLN:O	1:D:140:ASN:CG	2.49	0.50
1:D:305:HIS:C	1:D:311:ASN:HD22	2.15	0.50
1:A:154:LYS:O	1:A:154:LYS:CG	2.60	0.50
1:D:293:HIS:HA	1:D:296:THR:HG21	1.94	0.50
1:C:54:GLY:O	1:C:58:LYS:HG3	2.11	0.50
1:B:173:MET:O	1:B:177:THR:HG23	2.11	0.50
1:C:86:SER:O	1:C:90:THR:HB	2.12	0.50
1:A:119:TYR:CD1	1:A:120:PRO:CA	2.95	0.50
1:A:142:ALA:HB3	1:A:143:PRO:CD	2.36	0.50
1:D:246:ARG:HA	1:D:249:GLU:HG2	1.94	0.50
1:D:192:ASP:C	1:D:192:ASP:OD1	2.50	0.50
1:A:99:ARG:HG3	1:A:115:TYR:O	2.12	0.50
1:C:156:ASN:HD22	1:C:156:ASN:N	2.06	0.50
1:C:156:ASN:O	1:C:157:TRP:HD1	1.94	0.50
1:A:39:THR:CB	1:C:40:PRO:HG2	2.42	0.49
1:D:167:LEU:HD13	1:D:300:THR:HG21	1.94	0.49
1:D:139:GLN:O	1:D:140:ASN:OD1	2.30	0.49
1:B:90:THR:HB	1:B:91:PRO:HD3	1.94	0.49
1:A:53:LEU:HG	1:A:57:LEU:HD22	1.94	0.49
1:C:254:ASP:OD2	1:C:254:ASP:O	2.30	0.49
1:D:404:ASN:HD22	1:D:405:MET:H	1.60	0.49
1:A:174:ILE:CB	1:A:296:THR:HG22	2.41	0.49
1:A:135:VAL:HB	1:A:331:TYR:OH	2.12	0.49
1:B:202:LYS:HB3	1:B:231:ALA:HB2	1.93	0.49
1:A:206:CYS:O	1:A:208:ILE:CG1	2.60	0.49
1:C:237:ASP:O	1:C:241:GLU:HG3	2.13	0.49
1:A:82:VAL:HG23	1:A:85:HIS:CE1	2.47	0.49
1:C:470:VAL:HG12	1:C:471:LYS:N	2.27	0.49
1:A:306:LEU:HD13	1:A:440:LEU:HD11	1.95	0.49
1:A:235:LEU:CD2	1:A:285:VAL:CG2	2.90	0.49
1:A:39:THR:OG1	1:C:40:PRO:HG2	2.11	0.49
1:D:140:ASN:O	1:D:140:ASN:OD1	2.30	0.49
1:B:370:LYS:HE3	1:B:371:TYR:CZ	2.47	0.49
3:B:490:TPF:F2	3:B:490:TPF:C5	2.40	0.49
1:A:50:LYS:HD3	1:A:50:LYS:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD1	1:A:195:GLN:HG2	2.12	0.49
1:D:139:GLN:CD	1:D:139:GLN:H	2.13	0.49
1:C:209:PRO:O	1:C:212:VAL:HG23	2.12	0.49
1:C:271:ASP:OD1	1:C:271:ASP:C	2.49	0.49
1:A:42:VAL:CG2	1:C:40:PRO:CB	2.78	0.49
1:B:416:GLY:N	2:B:481:HEM:HMA3	2.27	0.49
1:C:246:ARG:HA	1:C:249:GLU:HG2	1.95	0.49
1:A:121:ARG:O	1:A:125:GLN:HG3	2.13	0.49
1:C:168:ASP:CG	1:D:194:ARG:NH2	2.66	0.49
2:C:481:HEM:HHD	2:C:481:HEM:CBC	2.30	0.48
1:A:42:VAL:O	1:A:45:ILE:HG22	2.13	0.48
1:D:220:LEU:HB2	1:D:222:LEU:CD1	2.42	0.48
1:A:135:VAL:HA	1:A:138:PHE:CE2	2.47	0.48
1:B:455:ASN:HD22	1:B:456:TYR:N	2.11	0.48
1:A:455:ASN:ND2	1:A:455:ASN:C	2.66	0.48
1:C:182:LEU:CD1	1:C:288:MET:HE1	2.41	0.48
1:A:53:LEU:CD1	1:A:57:LEU:HD22	2.43	0.48
1:D:184:GLY:O	1:D:188:ARG:HG3	2.13	0.48
1:B:84:GLN:NE2	1:B:369:GLY:HA2	2.29	0.48
1:B:105:MET:CE	1:B:109:PHE:HZ	2.26	0.48
1:D:125:GLN:HA	1:D:128:PHE:HD1	1.78	0.48
1:D:214:LEU:CB	1:D:217:ILE:HG22	2.42	0.48
1:C:95:ILE:HG21	1:C:366:VAL:HG12	1.96	0.48
1:D:106:VAL:N	1:D:107:PRO:HD2	2.29	0.48
1:D:145:ILE:O	1:D:149:VAL:HG23	2.13	0.48
1:A:157:TRP:NE1	1:A:164:ILE:HD13	2.28	0.48
1:D:214:LEU:HB2	1:D:217:ILE:CG2	2.43	0.48
1:B:325:PHE:HB3	1:B:329:LEU:CD2	2.43	0.48
1:C:81:ASP:OD2	1:C:84:GLN:HG2	2.13	0.48
1:C:168:ASP:CG	1:D:194:ARG:HH21	2.17	0.48
1:C:200:LEU:HB3	1:C:204:GLU:OE2	2.13	0.48
1:D:82:VAL:HG22	1:D:411:ALA:HA	1.95	0.48
1:C:252:GLN:NE2	1:C:254:ASP:H	2.11	0.48
1:D:350:ARG:C	1:D:350:ARG:CD	2.81	0.48
1:C:422:CYS:HA	2:C:481:HEM:CHA	2.44	0.48
1:C:289:PHE:CD2	1:C:289:PHE:C	2.87	0.48
1:B:338:MET:HE3	1:B:437:ALA:HB2	1.94	0.48
1:D:293:HIS:CA	1:D:296:THR:HG22	2.44	0.48
1:B:216:TRP:CB	1:C:215:PRO:HG2	2.43	0.48
1:A:94:GLU:O	1:A:363:LEU:HB2	2.14	0.48
1:A:202:LYS:HB3	1:A:231:ALA:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:CYS:O	1:B:383:PRO:HD3	2.12	0.48
1:D:404:ASN:HD22	1:D:405:MET:N	2.12	0.48
1:A:42:VAL:CG2	1:C:41:PHE:HD2	2.27	0.48
1:D:220:LEU:HB2	1:D:222:LEU:HD13	1.96	0.48
1:A:331:TYR:O	1:A:335:MET:HG2	2.14	0.48
1:C:319:HIS:HA	1:C:322:ILE:HG12	1.95	0.48
1:B:261:LEU:O	1:B:265:LEU:HG	2.13	0.48
1:A:106:VAL:N	1:A:107:PRO:CD	2.76	0.48
3:A:490:TPF:C5	3:A:490:TPF:F2	2.50	0.48
1:D:146:GLN:NE2	1:D:329:LEU:HG	2.29	0.48
1:B:138:PHE:HD1	1:B:141:PHE:CD2	2.31	0.47
1:D:204:GLU:OE1	1:D:289:PHE:CE1	2.67	0.47
1:D:134:THR:C	1:D:138:PHE:CE1	2.87	0.47
1:B:213:PHE:C	1:B:215:PRO:HD3	2.35	0.47
1:B:203:MET:HG3	1:B:231:ALA:HB3	1.95	0.47
1:C:202:LYS:NZ	1:C:202:LYS:HB3	2.29	0.47
1:A:128:PHE:HD1	1:A:275:MET:HE1	1.75	0.47
1:A:240:SER:O	1:A:244:ILE:HG13	2.14	0.47
1:A:324:GLU:O	1:A:324:GLU:HG3	2.15	0.47
1:B:94:GLU:N	1:B:94:GLU:OE1	2.42	0.47
1:B:258:SER:HB3	1:B:262:ALA:CB	2.42	0.47
1:C:297:ILE:HD13	1:C:461:VAL:O	2.14	0.47
1:C:106:VAL:HG22	1:C:116:ALA:HB2	1.95	0.47
1:A:455:ASN:ND2	1:A:457:HIS:H	2.13	0.47
1:D:432:VAL:O	1:D:436:LEU:HG	2.15	0.47
1:A:113:VAL:O	1:A:114:ALA:C	2.50	0.47
1:D:356:VAL:HG12	1:D:357:MET:HG2	1.96	0.47
1:C:106:VAL:HB	1:C:107:PRO:HD3	1.96	0.47
1:C:78:VAL:HA	1:C:380:ALA:O	2.15	0.47
1:C:288:MET:HE2	1:C:288:MET:HA	1.97	0.47
1:A:475:LYS:O	1:A:476:LYS:HB2	2.15	0.47
1:D:317:LYS:O	1:D:320:GLN:HB2	2.15	0.47
1:B:325:PHE:HE2	1:B:333:ASN:CB	2.26	0.47
1:C:42:VAL:CG1	1:C:45:ILE:CG2	2.84	0.47
1:C:128:PHE:CD1	1:C:275:MET:HE2	2.45	0.47
1:A:313:ARG:HG2	1:A:314:HIS:N	2.30	0.47
1:D:172:ALA:O	1:D:175:ILE:HG22	2.14	0.47
1:C:253:LYS:O	1:C:253:LYS:CG	2.63	0.47
1:B:141:PHE:O	1:B:145:ILE:HG13	2.15	0.47
1:A:135:VAL:HA	1:A:138:PHE:HD2	1.76	0.47
1:B:288:MET:HA	1:B:288:MET:CE	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:O	1:B:45:ILE:HG22	2.15	0.47
1:D:222:LEU:O	1:D:226:TYR:CD2	2.68	0.47
1:B:182:LEU:HD12	1:B:288:MET:CE	2.45	0.47
1:C:95:ILE:CD1	1:C:95:ILE:N	2.73	0.47
1:A:356:VAL:HG22	1:A:384:LEU:HD22	1.96	0.47
1:C:195:GLN:HE22	1:D:164:ILE:HA	1.80	0.47
1:B:395:ASN:N	1:B:396:PRO:HD3	2.29	0.47
1:B:128:PHE:O	1:B:132:GLU:HG2	2.15	0.47
1:D:350:ARG:O	1:D:387:HIS:HD2	1.98	0.47
1:D:367:GLN:NE2	1:D:367:GLN:H	1.98	0.47
1:B:317:LYS:HA	1:B:320:GLN:HE21	1.79	0.47
1:D:36:HIS:CD2	1:D:37:GLY:N	2.83	0.47
1:D:119:TYR:N	1:D:120:PRO:HD2	2.31	0.47
1:C:101:VAL:HG11	1:C:359:MET:CB	2.44	0.46
1:B:53:LEU:HD11	1:B:388:GLN:HG3	1.98	0.46
1:B:98:PRO:HG3	1:B:420:HIS:CE1	2.50	0.46
1:C:36:HIS:HD2	1:C:63:TYR:OH	1.97	0.46
1:D:333:ASN:O	1:D:338:MET:CG	2.63	0.46
1:B:191:LEU:HD13	1:B:238:ILE:HD13	1.96	0.46
1:B:217:ILE:HG23	1:B:218:LEU:N	2.29	0.46
1:C:206:CYS:HA	1:C:224:GLN:HB3	1.98	0.46
1:D:324:GLU:O	1:D:324:GLU:HG3	2.15	0.46
1:B:113:VAL:CG1	1:B:114:ALA:N	2.75	0.46
1:C:44:HIS:HD2	1:C:70:ASN:N	1.89	0.46
1:A:356:VAL:CG2	1:A:384:LEU:HD22	2.45	0.46
1:A:195:GLN:O	1:A:198:GLN:HB2	2.15	0.46
1:B:435:VAL:O	1:B:439:VAL:HG23	2.15	0.46
1:D:89:PHE:O	1:D:418:GLY:HA3	2.16	0.46
1:D:435:VAL:O	1:D:439:VAL:HG23	2.15	0.46
1:A:87:LYS:HD3	1:A:367:GLN:O	2.15	0.46
1:A:370:LYS:HE3	1:A:371:TYR:OH	2.15	0.46
1:D:210:ALA:O	1:D:214:LEU:HD23	2.16	0.46
1:C:204:GLU:OE1	1:C:293:HIS:NE2	2.48	0.46
1:C:101:VAL:CG1	1:C:359:MET:HE3	2.45	0.46
1:C:213:PHE:C	1:C:214:LEU:HD12	2.35	0.46
1:A:40:PRO:CG	1:C:39:THR:HB	2.45	0.46
1:C:50:LYS:O	1:C:50:LYS:HD3	2.16	0.46
1:A:78:VAL:CG2	1:A:78:VAL:O	2.63	0.46
1:B:472:TYR:C	1:B:472:TYR:CD1	2.89	0.46
1:B:239:LEU:O	1:B:243:ILE:HG13	2.16	0.46
1:A:98:PRO:HG3	1:A:420:HIS:NE2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:VAL:HG22	1:B:116:ALA:HB2	1.98	0.46
1:A:315:LEU:HD11	1:A:319:HIS:CE1	2.51	0.46
1:C:84:GLN:OE1	1:C:87:LYS:HG3	2.16	0.46
1:C:470:VAL:CG1	1:C:471:LYS:N	2.79	0.46
1:B:133:LEU:HD13	2:B:481:HEM:HAC	1.98	0.45
1:A:174:ILE:HB	1:A:296:THR:HG22	1.99	0.45
1:C:204:GLU:OE1	1:C:293:HIS:HE1	1.97	0.45
1:A:128:PHE:CD1	1:A:275:MET:HE3	2.48	0.45
1:C:103:SER:O	1:C:106:VAL:HG23	2.15	0.45
1:B:246:ARG:HA	1:B:249:GLU:HG2	1.98	0.45
1:A:112:GLY:O	1:A:117:ALA:HB2	2.16	0.45
1:B:335:MET:CA	1:B:335:MET:CE	2.90	0.45
1:D:161:GLU:HB2	1:D:471:LYS:HE3	1.99	0.45
1:D:293:HIS:CA	1:D:296:THR:CG2	2.92	0.45
1:C:170:CYS:O	1:C:174:ILE:HG12	2.17	0.45
1:C:69:MET:CE	1:C:71:ILE:HD11	2.46	0.45
1:D:138:PHE:CE2	1:D:427:PHE:HA	2.52	0.45
1:C:455:ASN:ND2	1:C:457:HIS:CD2	2.75	0.45
1:B:119:TYR:N	1:B:120:PRO:CD	2.79	0.45
1:C:322:ILE:HA	1:C:325:PHE:HD1	1.82	0.45
1:C:321:GLU:OE2	1:C:338:MET:HA	2.17	0.45
1:D:39:THR:OG1	1:D:43:GLY:N	2.50	0.45
1:B:215:PRO:C	1:B:217:ILE:N	2.69	0.45
1:C:84:GLN:OE1	1:C:87:LYS:HE3	2.17	0.45
1:C:224:GLN:N	1:C:224:GLN:OE1	2.41	0.45
1:D:470:VAL:CG1	1:D:471:LYS:N	2.79	0.45
1:B:211:ALA:HA	1:B:217:ILE:HG21	1.98	0.45
1:C:101:VAL:O	1:C:101:VAL:CG1	2.65	0.45
1:C:236:GLN:HE22	1:C:278:HIS:HA	1.82	0.45
1:A:368:VAL:O	1:A:369:GLY:C	2.55	0.45
1:C:53:LEU:CD1	1:C:57:LEU:HD13	2.47	0.45
1:D:39:THR:OG1	1:D:42:VAL:CG1	2.64	0.45
1:D:46:ILE:HD12	1:D:46:ILE:N	2.32	0.45
1:B:188:ARG:CA	1:B:191:LEU:O	2.52	0.45
1:D:76:ILE:HA	1:D:378:ILE:O	2.17	0.45
1:B:87:LYS:CD	1:B:368:VAL:HA	2.47	0.45
1:B:216:TRP:HB3	1:C:215:PRO:HG2	1.99	0.45
1:A:301:TRP:O	1:A:305:HIS:CD2	2.70	0.45
1:A:325:PHE:HB3	1:A:329:LEU:HD21	1.98	0.45
1:C:95:ILE:CG2	1:C:366:VAL:HG13	2.46	0.44
1:C:141:PHE:HB2	5:C:484:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:MET:HE1	1:A:285:VAL:HG13	1.98	0.44
1:D:470:VAL:HG12	1:D:471:LYS:O	2.17	0.44
1:A:129:LEU:HD21	1:A:287:ALA:HB2	1.99	0.44
1:B:45:ILE:HG23	1:B:46:ILE:N	2.33	0.44
1:D:324:GLU:HA	1:D:324:GLU:OE1	2.16	0.44
1:D:429:LEU:O	1:D:433:LYS:HD3	2.18	0.44
1:B:182:LEU:CD1	1:B:288:MET:CE	2.95	0.44
1:C:82:VAL:CG1	1:C:408:VAL:HG11	2.48	0.44
1:B:384:LEU:O	1:B:388:GLN:HG2	2.16	0.44
1:A:301:TRP:NE1	1:A:463:PRO:HD3	2.33	0.44
1:D:389:ASP:O	1:D:391:GLU:N	2.51	0.44
1:C:377:ASP:OD1	1:C:378:ILE:N	2.51	0.44
1:D:305:HIS:HB3	1:D:399:TRP:CE3	2.53	0.44
1:C:163:GLU:OE2	1:C:469:ARG:NH2	2.51	0.44
1:A:42:VAL:HG12	1:A:45:ILE:HG23	1.97	0.44
1:D:120:PRO:O	1:D:124:GLU:HG3	2.18	0.44
1:C:321:GLU:OE1	1:C:340:PHE:HB3	2.17	0.44
1:C:98:PRO:HG3	1:C:420:HIS:CE1	2.52	0.44
1:C:312:LYS:H	1:C:313:ARG:HH21	1.64	0.44
1:C:453:GLU:CG	1:C:454:PRO:HD2	2.36	0.44
1:A:191:LEU:HD21	1:A:196:PHE:CD2	2.37	0.44
1:B:350:ARG:O	1:B:387:HIS:CD2	2.70	0.44
1:B:254:ASP:O	1:B:255:THR:C	2.56	0.44
1:C:94:GLU:O	1:C:363:LEU:HB2	2.18	0.44
1:D:214:LEU:CB	1:D:217:ILE:CG2	2.95	0.44
1:C:383:PRO:O	1:C:387:HIS:CD2	2.70	0.44
1:C:103:SER:O	1:C:105:MET:N	2.51	0.44
1:A:256:ASN:N	1:A:256:ASN:OD1	2.50	0.44
1:B:81:ASP:OD1	1:B:83:HIS:HB2	2.17	0.44
1:C:313:ARG:HG2	1:C:314:HIS:N	2.32	0.44
1:D:82:VAL:HG21	1:D:411:ALA:CB	2.48	0.44
1:A:51:ASP:C	1:A:51:ASP:OD1	2.56	0.44
1:A:210:ALA:C	1:A:212:VAL:N	2.71	0.44
1:A:39:THR:HG1	1:A:42:VAL:HB	1.81	0.44
1:C:247:GLU:O	1:C:250:GLU:HB3	2.17	0.44
1:D:90:THR:N	1:D:91:PRO:CD	2.81	0.44
1:D:242:ILE:HA	1:D:242:ILE:HD13	1.92	0.44
1:D:78:VAL:HA	1:D:380:ALA:O	2.18	0.43
1:A:238:ILE:O	1:A:242:ILE:HG12	2.17	0.43
1:C:194:ARG:CD	1:D:156:ASN:OD1	2.66	0.43
1:A:216:TRP:HB3	1:D:216:TRP:CH2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:HD1	1:A:430:LEU:CD2	2.24	0.43
1:B:350:ARG:C	1:B:350:ARG:CD	2.85	0.43
1:A:213:PHE:C	1:A:215:PRO:HD3	2.39	0.43
1:B:42:VAL:HB	1:B:45:ILE:HG21	1.99	0.43
1:D:307:MET:CE	1:D:445:PHE:HB3	2.48	0.43
1:A:113:VAL:HG12	1:A:114:ALA:N	2.33	0.43
1:B:351:ARG:NH1	1:B:352:ASP:OD1	2.49	0.43
1:D:256:ASN:N	1:D:256:ASN:OD1	2.51	0.43
1:D:42:VAL:HG22	1:D:45:ILE:HG22	2.00	0.43
1:B:215:PRO:O	1:B:217:ILE:N	2.51	0.43
1:C:224:GLN:O	1:C:227:ARG:HB2	2.18	0.43
1:D:353:PRO:HA	1:D:354:PRO:HD3	1.91	0.43
1:D:306:LEU:O	1:D:315:LEU:HD22	2.18	0.43
1:C:113:VAL:O	1:C:114:ALA:C	2.54	0.43
1:A:45:ILE:O	1:A:46:ILE:C	2.57	0.43
1:C:142:ALA:CB	1:C:143:PRO:CD	2.94	0.43
1:A:414:GLY:O	2:A:481:HEM:HMA1	2.18	0.43
1:D:109:PHE:O	1:D:232:ARG:NH2	2.50	0.43
1:A:55:PHE:CE2	1:A:69:MET:CE	3.01	0.43
1:A:350:ARG:CD	1:A:350:ARG:C	2.87	0.43
1:D:390:GLU:O	1:D:394:PRO:HG3	2.18	0.43
1:B:301:TRP:O	1:B:305:HIS:CD2	2.71	0.43
1:D:358:LEU:HD22	2:D:481:HEM:HBA2	1.99	0.43
1:D:301:TRP:O	1:D:304:LEU:N	2.52	0.43
1:C:51:ASP:OD1	1:C:54:GLY:CA	2.66	0.43
1:D:453:GLU:CG	1:D:454:PRO:HD2	2.48	0.43
1:B:375:GLU:OE2	1:C:119:TYR:CE2	2.71	0.43
1:C:214:LEU:O	1:C:217:ILE:HG13	2.19	0.43
1:C:365:PRO:HA	1:C:373:VAL:O	2.19	0.43
1:C:304:LEU:HB3	1:C:451:LEU:HD11	2.01	0.43
1:A:424:GLY:HA3	2:A:481:HEM:C2C	2.53	0.43
1:D:139:GLN:N	1:D:139:GLN:OE1	2.30	0.43
1:A:154:LYS:HG2	1:A:154:LYS:O	2.18	0.43
1:D:353:PRO:CG	1:D:384:LEU:HA	2.49	0.43
1:A:67:PHE:CZ	1:A:78:VAL:HG21	2.53	0.43
1:A:40:PRO:HG3	1:C:39:THR:CG2	2.49	0.43
1:D:292:GLN:O	1:D:296:THR:CG2	2.59	0.43
1:C:475:LYS:CA	1:C:475:LYS:HE3	2.49	0.43
1:C:177:THR:OG1	1:C:431:GLN:NE2	2.52	0.43
1:D:54:GLY:O	1:D:58:LYS:HG3	2.19	0.43
1:C:325:PHE:CB	1:C:329:LEU:HD21	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:VAL:CG1	1:D:338:MET:SD	3.04	0.43
1:A:223:PRO:HG2	1:A:224:GLN:OE1	2.19	0.43
1:A:69:MET:HB3	1:A:69:MET:HE2	1.90	0.43
1:A:101:VAL:C	1:A:102:TYR:HD1	2.22	0.43
1:C:182:LEU:O	1:C:259:ASP:HB2	2.19	0.43
1:B:86:SER:O	1:B:90:THR:HB	2.19	0.43
1:D:353:PRO:HG3	1:D:384:LEU:HA	2.00	0.43
1:C:362:VAL:HG12	1:C:375:GLU:HA	2.00	0.43
1:B:325:PHE:HB3	1:B:329:LEU:HD21	2.01	0.42
1:B:453:GLU:CG	1:B:454:PRO:HD2	2.46	0.42
1:C:350:ARG:C	1:C:350:ARG:CD	2.88	0.42
1:A:476:LYS:O	1:A:476:LYS:HD3	2.19	0.42
1:A:50:LYS:CD	1:A:50:LYS:C	2.88	0.42
1:B:105:MET:HE1	1:B:109:PHE:HZ	1.84	0.42
1:D:389:ASP:O	1:D:390:GLU:C	2.57	0.42
1:D:60:LYS:HE3	1:D:80:GLY:O	2.19	0.42
1:D:42:VAL:HG22	1:D:45:ILE:HG21	2.01	0.42
1:B:101:VAL:HG12	1:B:102:TYR:CE1	2.51	0.42
2:A:481:HEM:NC	3:A:490:TPF:HC7	2.35	0.42
1:B:213:PHE:C	1:B:214:LEU:CD1	2.88	0.42
1:B:304:LEU:CD1	1:B:452:PRO:HG2	2.47	0.42
1:D:38:THR:HA	1:D:44:HIS:CE1	2.55	0.42
1:B:217:ILE:CG2	1:B:218:LEU:N	2.83	0.42
1:C:101:VAL:C	1:C:102:TYR:HD1	2.23	0.42
1:B:446:GLU:O	1:B:470:VAL:HG13	2.20	0.42
1:C:103:SER:C	1:C:105:MET:H	2.22	0.42
1:C:105:MET:C	1:C:107:PRO:HD2	2.39	0.42
1:D:179:CYS:HG	1:D:183:PHE:HE1	1.67	0.42
1:A:412:PHE:C	1:A:412:PHE:CD2	2.92	0.42
1:B:271:ASP:OD1	1:B:271:ASP:C	2.57	0.42
1:C:252:GLN:NE2	1:C:254:ASP:N	2.67	0.42
1:B:335:MET:HE3	1:B:335:MET:CA	2.43	0.42
3:D:490:TPF:C5	3:D:490:TPF:F2	2.48	0.42
1:C:103:SER:C	1:C:105:MET:N	2.72	0.42
1:C:194:ARG:HD2	1:D:156:ASN:OD1	2.20	0.42
1:B:220:LEU:O	1:B:222:LEU:N	2.52	0.42
1:C:190:ARG:HH22	1:C:241:GLU:CD	2.22	0.42
1:B:142:ALA:N	1:B:143:PRO:CD	2.82	0.42
1:D:82:VAL:HA	1:D:85:HIS:CD2	2.54	0.42
1:B:65:GLY:O	1:B:80:GLY:CA	2.67	0.42
1:B:330:ASN:N	1:B:333:ASN:ND2	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:HE1	1:A:430:LEU:HD23	1.81	0.42
1:A:415:PHE:CZ	1:A:425:GLU:HG3	2.54	0.42
1:D:325:PHE:HB3	1:D:329:LEU:HD21	2.02	0.42
1:B:442:ASP:O	1:B:475:LYS:HB2	2.20	0.42
1:C:160:ASP:N	1:C:160:ASP:OD2	2.53	0.42
1:B:293:HIS:O	1:B:296:THR:HG23	2.20	0.42
1:D:67:PHE:CZ	1:D:78:VAL:CG2	3.00	0.42
1:D:128:PHE:O	1:D:132:GLU:HG2	2.19	0.42
1:C:120:PRO:O	1:C:124:GLU:HG3	2.20	0.42
1:D:356:VAL:HG13	1:D:384:LEU:CD2	2.49	0.42
1:C:166:ILE:HG23	1:C:167:LEU:N	2.35	0.42
1:A:160:ASP:N	1:A:160:ASP:OD2	2.52	0.42
1:A:233:ALA:O	1:A:236:GLN:HB3	2.20	0.42
1:D:61:LYS:HB3	1:D:61:LYS:NZ	2.35	0.42
1:B:254:ASP:O	1:B:256:ASN:CG	2.58	0.42
1:D:301:TRP:O	1:D:302:SER:C	2.58	0.42
1:D:82:VAL:CG2	1:D:411:ALA:CB	2.98	0.42
1:C:124:GLU:OE2	1:C:269:TYR:HD2	2.03	0.42
1:D:86:SER:O	1:D:90:THR:HB	2.20	0.42
1:B:268:VAL:HG12	1:B:269:TYR:O	2.20	0.42
1:D:293:HIS:O	1:D:296:THR:CG2	2.67	0.41
1:C:196:PHE:C	1:C:198:GLN:N	2.74	0.41
1:B:82:VAL:HA	1:B:85:HIS:CD2	2.54	0.41
1:C:334:VAL:HA	1:C:338:MET:SD	2.60	0.41
1:D:90:THR:HB	1:D:91:PRO:HD3	2.01	0.41
1:B:100:GLU:CD	1:B:100:GLU:H	2.22	0.41
1:B:324:GLU:OE1	1:B:324:GLU:HA	2.19	0.41
1:D:358:LEU:HD22	2:D:481:HEM:CBA	2.50	0.41
1:C:387:HIS:CE1	1:C:412:PHE:HA	2.55	0.41
1:D:206:CYS:SG	1:D:225:SER:HA	2.60	0.41
1:C:452:PRO:CA	1:C:467:GLN:OE1	2.67	0.41
1:C:89:PHE:CD2	1:C:417:ALA:HB3	2.55	0.41
1:D:101:VAL:HG11	1:D:359:MET:CB	2.50	0.41
1:D:113:VAL:H	1:D:116:ALA:HB3	1.85	0.41
1:A:46:ILE:HG22	1:A:47:GLN:N	2.35	0.41
1:A:120:PRO:CG	1:A:121:ARG:H	2.33	0.41
1:A:288:MET:HE2	1:A:288:MET:N	2.35	0.41
1:C:67:PHE:CE2	1:C:78:VAL:CG2	3.03	0.41
1:D:331:TYR:CZ	1:D:335:MET:HG3	2.55	0.41
1:D:415:PHE:CE2	1:D:425:GLU:HG3	2.55	0.41
1:D:312:LYS:N	1:D:313:ARG:HH21	2.17	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:O	1:A:265:LEU:HG	2.20	0.41
1:A:172:ALA:O	1:A:175:ILE:HG22	2.21	0.41
1:A:400:ASN:O	1:A:403:ARG:HG2	2.20	0.41
1:D:217:ILE:HG21	1:D:217:ILE:HD13	1.78	0.41
1:C:246:ARG:O	1:C:250:GLU:N	2.54	0.41
1:A:142:ALA:CB	1:A:143:PRO:HD3	2.36	0.41
1:A:128:PHE:CD1	1:A:275:MET:CE	2.94	0.41
1:C:457:HIS:CE1	1:D:230:ASP:OD2	2.73	0.41
1:C:202:LYS:HZ3	1:C:202:LYS:HB3	1.86	0.41
1:B:157:TRP:HB3	1:B:472:TYR:CZ	2.56	0.41
1:C:418:GLY:O	1:C:421:LYS:HG2	2.21	0.41
1:B:145:ILE:O	1:B:149:VAL:HG23	2.21	0.41
1:C:113:VAL:CG1	1:C:114:ALA:N	2.84	0.41
1:D:375:GLU:OE1	1:D:375:GLU:N	2.37	0.41
1:D:350:ARG:HA	1:D:387:HIS:HD2	1.80	0.41
1:D:334:VAL:HG22	1:D:338:MET:SD	2.61	0.41
1:C:308:ASP:OD1	1:C:309:PRO:N	2.54	0.41
1:A:48:PHE:CD1	1:A:69:MET:HE1	2.52	0.41
1:C:240:SER:C	1:C:244:ILE:HD11	2.41	0.41
1:A:139:GLN:OE1	1:A:140:ASN:CG	2.59	0.41
1:B:95:ILE:H	1:B:95:ILE:CD1	2.34	0.41
1:D:473:ILE:CD1	1:D:473:ILE:N	2.83	0.41
1:D:125:GLN:HG2	1:D:275:MET:HE3	2.02	0.41
1:D:207:LEU:O	1:D:209:PRO:HD3	2.21	0.41
1:A:52:PRO:O	1:A:56:MET:HG3	2.21	0.41
1:C:192:ASP:C	1:C:192:ASP:OD1	2.59	0.41
1:A:235:LEU:HD21	1:A:285:VAL:HG22	2.00	0.41
1:C:156:ASN:C	1:C:157:TRP:CD1	2.94	0.41
1:D:105:MET:C	1:D:107:PRO:HD2	2.41	0.41
1:B:45:ILE:HG23	1:B:46:ILE:CD1	2.50	0.41
1:C:415:PHE:CZ	1:C:425:GLU:HG3	2.56	0.41
1:C:175:ILE:HD12	1:C:175:ILE:HA	1.92	0.41
1:A:395:ASN:N	1:A:396:PRO:HD3	2.36	0.41
1:A:100:GLU:H	1:A:100:GLU:CD	2.24	0.41
1:A:174:ILE:HG13	1:A:296:THR:HG22	2.03	0.40
1:D:333:ASN:O	1:D:338:MET:HG2	2.20	0.40
1:A:40:PRO:HG2	1:A:41:PHE:H	1.86	0.40
1:A:138:PHE:CD1	1:A:141:PHE:CD2	3.10	0.40
1:D:298:THR:HG23	1:D:349:ILE:HG13	2.03	0.40
1:C:76:ILE:HA	1:C:378:ILE:O	2.21	0.40
1:C:139:GLN:OE1	1:C:139:GLN:HA	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:GLU:HG3	1:C:454:PRO:CD	2.42	0.40
1:B:356:VAL:CG2	1:B:461:VAL:HG21	2.49	0.40
1:C:113:VAL:HG12	1:C:114:ALA:N	2.35	0.40
1:D:214:LEU:HB2	1:D:217:ILE:HG21	2.04	0.40
1:D:404:ASN:OD1	1:D:406:LYS:HG2	2.21	0.40
1:D:69:MET:HE2	1:D:69:MET:HB3	1.98	0.40
1:A:453:GLU:CG	1:A:454:PRO:HD2	2.48	0.40
1:A:90:THR:N	1:A:91:PRO:CD	2.85	0.40
1:B:219:LYS:HE2	1:C:73:GLY:O	2.21	0.40
1:C:45:ILE:HG23	1:C:46:ILE:CD1	2.52	0.40
1:C:76:ILE:HD11	1:C:357:MET:HE1	2.03	0.40
1:B:214:LEU:CD1	1:B:214:LEU:N	2.84	0.40
1:C:157:TRP:NE1	1:C:164:ILE:HD13	2.37	0.40
1:D:131:GLU:O	1:D:137:LYS:HE3	2.22	0.40
1:B:365:PRO:HD3	1:B:375:GLU:OE1	2.22	0.40
1:C:427:PHE:O	1:C:430:LEU:HB3	2.22	0.40
1:A:381:CYS:O	1:A:383:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	446/453 (98%)	428 (96%)	18 (4%)	0	100 100
1	B	447/453 (99%)	422 (94%)	24 (5%)	1 (0%)	52 83
1	C	443/453 (98%)	419 (95%)	24 (5%)	0	100 100
1	D	441/453 (97%)	420 (95%)	21 (5%)	0	100 100
All	All	1777/1812 (98%)	1689 (95%)	87 (5%)	1 (0%)	56 86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/388 (100%)	370 (96%)	16 (4%)	37	69
1	B	387/388 (100%)	370 (96%)	17 (4%)	35	67
1	C	385/388 (99%)	372 (97%)	13 (3%)	44	76
1	D	383/388 (99%)	369 (96%)	14 (4%)	41	74
All	All	1541/1552 (99%)	1481 (96%)	60 (4%)	39	72

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	38	THR
1	A	45	ILE
1	A	57	LEU
1	A	78	VAL
1	A	119	TYR
1	A	160	ASP
1	A	206	CYS
1	A	258	SER
1	A	313	ARG
1	A	367	GLN
1	A	395	ASN
1	A	406	LYS
1	A	413	CYS
1	A	455	ASN
1	A	476	LYS
1	B	39	THR
1	B	57	LEU
1	B	76	ILE
1	B	95	ILE
1	B	194	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	214	LEU
1	B	254	ASP
1	B	296	THR
1	B	313	ARG
1	B	330	ASN
1	B	333	ASN
1	B	367	GLN
1	B	387	HIS
1	B	395	ASN
1	B	406	LYS
1	B	455	ASN
1	B	475	LYS
1	C	35	VAL
1	C	57	LEU
1	C	81	ASP
1	C	82	VAL
1	C	156	ASN
1	C	160	ASP
1	C	244	ILE
1	C	252	GLN
1	C	296	THR
1	C	313	ARG
1	C	458	THR
1	C	475	LYS
1	C	476	LYS
1	D	28	LYS
1	D	61	LYS
1	D	76	ILE
1	D	160	ASP
1	D	192	ASP
1	D	214	LEU
1	D	217	ILE
1	D	313	ARG
1	D	367	GLN
1	D	387	HIS
1	D	388	GLN
1	D	404	ASN
1	D	407	LEU
1	D	413	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	44	HIS
1	A	156	ASN
1	A	198	GLN
1	A	278	HIS
1	A	320	GLN
1	A	367	GLN
1	A	387	HIS
1	A	395	ASN
1	A	431	GLN
1	A	455	ASN
1	B	44	HIS
1	B	139	GLN
1	B	278	HIS
1	B	305	HIS
1	B	314	HIS
1	B	320	GLN
1	B	328	GLN
1	B	330	ASN
1	B	333	ASN
1	B	367	GLN
1	B	387	HIS
1	B	431	GLN
1	B	455	ASN
1	C	36	HIS
1	C	44	HIS
1	C	156	ASN
1	C	278	HIS
1	C	293	HIS
1	C	314	HIS
1	C	320	GLN
1	C	387	HIS
1	C	431	GLN
1	C	455	ASN
1	C	457	HIS
1	D	36	HIS
1	D	44	HIS
1	D	198	GLN
1	D	256	ASN
1	D	278	HIS
1	D	320	GLN
1	D	328	GLN
1	D	333	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	367	GLN
1	D	387	HIS
1	D	388	GLN
1	D	431	GLN
1	D	455	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	481	1,3	30,50,50	2.18	7 (23%)	24,82,82	2.36	10 (41%)
3	TPF	A	490	2	16,24,24	4.58	5 (31%)	22,34,34	3.73	9 (40%)
2	HEM	B	481	1,3	30,50,50	2.20	8 (26%)	24,82,82	2.36	10 (41%)
3	TPF	B	490	2	16,24,24	4.56	5 (31%)	22,34,34	3.85	8 (36%)
4	N8E	C	1	-	23,23,23	0.43	0	22,22,22	0.41	0
2	HEM	C	481	1,3	30,50,50	2.14	6 (20%)	24,82,82	2.31	12 (50%)
3	TPF	C	490	2	16,24,24	4.53	5 (31%)	22,34,34	3.88	8 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	D	481	1,3	30,50,50	2.17	6 (20%)	24,82,82	2.30	9 (37%)
3	TPF	D	490	2	16,24,24	4.51	5 (31%)	22,34,34	3.84	9 (40%)

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	481	1,3	-	0/10/54/54	0/0/8/8
3	TPF	A	490	2	-	0/16/16/16	0/3/3/3
2	HEM	B	481	1,3	-	0/10/54/54	0/0/8/8
3	TPF	B	490	2	-	0/16/16/16	0/3/3/3
4	N8E	C	1	-	-	0/21/21/21	0/0/0/0
2	HEM	C	481	1,3	-	0/10/54/54	0/0/8/8
3	TPF	C	490	2	-	0/16/16/16	0/3/3/3
2	HEM	D	481	1,3	-	0/10/54/54	0/0/8/8
3	TPF	D	490	2	-	0/16/16/16	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	481	HEM	C3B-C4B	-7.71	1.45	1.51
2	B	481	HEM	C3B-C4B	-7.56	1.45	1.51
2	D	481	HEM	C3B-C4B	-7.50	1.45	1.51
2	C	481	HEM	C3B-C4B	-7.07	1.45	1.51
2	D	481	HEM	C3D-C4D	-5.02	1.45	1.51
2	B	481	HEM	C3D-C4D	-4.90	1.45	1.51
2	C	481	HEM	C3D-C4D	-4.90	1.45	1.51
2	A	481	HEM	C3D-C4D	-4.36	1.46	1.51
2	A	481	HEM	C2C-C1C	-3.86	1.45	1.52
2	D	481	HEM	C2C-C1C	-3.83	1.45	1.52
2	B	481	HEM	C2C-C1C	-3.74	1.45	1.52
2	C	481	HEM	C2C-C1C	-3.52	1.45	1.52
3	D	490	TPF	C1-C8	-2.89	1.50	1.53
3	B	490	TPF	C1-C8	-2.73	1.50	1.53
3	A	490	TPF	C1-C8	-2.58	1.50	1.53
3	C	490	TPF	C1-C8	-2.30	1.50	1.53
2	D	481	HEM	C2D-C1D	-2.13	1.44	1.51
2	B	481	HEM	C2D-C1D	-2.11	1.44	1.51
2	C	481	HEM	C2D-C1D	-2.06	1.45	1.51
2	D	481	HEM	C1C-NC	2.07	1.38	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	481	HEM	FE-NC	2.07	2.04	1.95
2	B	481	HEM	C1C-NC	2.10	1.38	1.36
2	C	481	HEM	C4C-NC	2.12	1.38	1.36
2	A	481	HEM	FE-NC	2.13	2.04	1.95
2	A	481	HEM	C4C-NC	2.15	1.38	1.36
2	A	481	HEM	C1C-NC	2.18	1.38	1.36
2	B	481	HEM	FE-ND	2.22	2.09	1.97
2	B	481	HEM	C4C-NC	2.28	1.38	1.36
2	A	481	HEM	FE-ND	2.49	2.10	1.97
2	B	481	HEM	FE-NC	2.60	2.06	1.95
2	C	481	HEM	FE-NC	2.84	2.07	1.95
3	A	490	TPF	N6-N4	3.93	1.41	1.35
3	D	490	TPF	N6-N4	4.03	1.41	1.35
3	C	490	TPF	N6-N4	4.11	1.41	1.35
3	D	490	TPF	N3-N1	4.12	1.41	1.35
3	B	490	TPF	N3-N1	4.13	1.41	1.35
3	B	490	TPF	N6-N4	4.13	1.41	1.35
3	C	490	TPF	N3-N1	4.23	1.41	1.35
3	A	490	TPF	N3-N1	4.27	1.41	1.35
3	B	490	TPF	C3-N1	11.25	1.45	1.33
3	D	490	TPF	C3-N1	11.34	1.45	1.33
3	A	490	TPF	C3-N1	11.38	1.45	1.33
3	C	490	TPF	C3-N1	11.48	1.45	1.33
3	D	490	TPF	C6-N4	12.24	1.46	1.33
3	C	490	TPF	C6-N4	12.26	1.46	1.33
3	B	490	TPF	C6-N4	12.57	1.46	1.33
3	A	490	TPF	C6-N4	12.61	1.46	1.33

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	490	TPF	C1-C8-C13	-5.40	118.70	122.92
3	D	490	TPF	C1-C8-C13	-5.37	118.73	122.92
3	A	490	TPF	C12-C13-C8	-5.16	120.22	124.21
3	D	490	TPF	C12-C13-C8	-5.14	120.24	124.21
3	B	490	TPF	C12-C13-C8	-5.05	120.31	124.21
3	C	490	TPF	C12-C13-C8	-4.82	120.48	124.21
3	C	490	TPF	C1-C8-C13	-4.76	119.21	122.92
2	A	481	HEM	C3C-CAC-CBC	-3.92	118.44	124.46
3	A	490	TPF	C1-C8-C13	-3.81	119.94	122.92
2	A	481	HEM	C3B-CAB-CBB	-3.41	119.22	124.46
2	B	481	HEM	C3C-CAC-CBC	-3.30	119.39	124.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	481	HEM	C3B-CAB-CBB	-2.99	119.87	124.46
2	D	481	HEM	C3C-CAC-CBC	-2.96	119.92	124.46
2	C	481	HEM	C3B-CAB-CBB	-2.94	119.94	124.46
2	D	481	HEM	C3B-CAB-CBB	-2.86	120.07	124.46
2	C	481	HEM	C3C-CAC-CBC	-2.66	120.38	124.46
3	C	490	TPF	C10-C11-C12	-2.62	119.97	123.35
3	B	490	TPF	C6-N4-N6	-2.59	105.34	108.84
2	A	481	HEM	CBA-CAA-C2A	-2.56	107.94	112.53
3	B	490	TPF	C10-C11-C12	-2.52	120.09	123.35
2	B	481	HEM	CBA-CAA-C2A	-2.52	108.02	112.53
3	D	490	TPF	C10-C11-C12	-2.48	120.15	123.35
3	A	490	TPF	C10-C11-C12	-2.47	120.16	123.35
2	D	481	HEM	CBA-CAA-C2A	-2.45	108.14	112.53
3	D	490	TPF	C6-N4-N6	-2.44	105.55	108.84
2	C	481	HEM	CBA-CAA-C2A	-2.32	108.37	112.53
3	A	490	TPF	C5-C1-C8	-2.17	105.17	110.78
3	D	490	TPF	C5-C1-C8	-2.16	105.22	110.78
2	C	481	HEM	C3B-C4B-NB	-2.10	107.61	111.63
3	A	490	TPF	C6-N4-N6	-2.10	106.00	108.84
3	C	490	TPF	C5-C1-C8	-2.02	105.56	110.78
2	B	481	HEM	C3B-C4B-CHC	2.14	126.17	123.16
2	C	481	HEM	C2C-C1C-CHC	2.14	126.94	123.68
2	A	481	HEM	C2D-C3D-C4D	2.16	105.16	101.50
2	A	481	HEM	C3B-C4B-CHC	2.21	126.28	123.16
2	B	481	HEM	C2D-C3D-C4D	2.31	105.42	101.50
2	C	481	HEM	C3B-C4B-CHC	2.34	126.46	123.16
2	D	481	HEM	C2D-C3D-C4D	2.41	105.58	101.50
2	C	481	HEM	C2D-C3D-C4D	2.52	105.77	101.50
2	A	481	HEM	CMD-C2D-C3D	2.77	126.61	114.35
2	C	481	HEM	CMD-C2D-C3D	2.82	126.84	114.35
3	A	490	TPF	C13-C12-C11	2.83	119.58	116.63
3	D	490	TPF	C13-C12-C11	2.85	119.61	116.63
3	B	490	TPF	C13-C12-C11	2.86	119.62	116.63
2	B	481	HEM	CMD-C2D-C3D	2.87	127.06	114.35
2	D	481	HEM	CMD-C2D-C3D	3.00	127.61	114.35
3	C	490	TPF	C13-C12-C11	3.01	119.78	116.63
2	A	481	HEM	CMB-C2B-C3B	3.47	125.20	116.53
2	D	481	HEM	CMB-C2B-C3B	3.68	125.72	116.53
2	C	481	HEM	CMC-C2C-C3C	3.70	125.77	116.53
2	B	481	HEM	CMC-C2C-C3C	3.70	125.77	116.53
2	C	481	HEM	CMB-C2B-C3B	3.71	125.80	116.53
3	C	490	TPF	C9-C8-C13	3.73	119.84	116.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	481	HEM	CMC-C2C-C3C	3.75	125.90	116.53
2	D	481	HEM	CMC-C2C-C3C	3.83	126.09	116.53
2	B	481	HEM	CMB-C2B-C3B	3.85	126.15	116.53
3	A	490	TPF	C9-C8-C13	4.08	120.20	116.01
2	D	481	HEM	CAD-C3D-C4D	4.15	127.12	112.47
3	B	490	TPF	C9-C8-C13	4.18	120.31	116.01
3	D	490	TPF	C9-C8-C13	4.24	120.37	116.01
2	B	481	HEM	CAD-C3D-C4D	4.32	127.71	112.47
2	C	481	HEM	CAD-C3D-C4D	4.36	127.85	112.47
2	A	481	HEM	CAD-C3D-C2D	4.52	126.22	113.22
2	A	481	HEM	CAD-C3D-C4D	4.58	128.61	112.47
2	C	481	HEM	CAD-C3D-C2D	4.58	126.38	113.22
2	B	481	HEM	CAD-C3D-C2D	4.75	126.86	113.22
2	D	481	HEM	CAD-C3D-C2D	4.90	127.30	113.22
3	B	490	TPF	C6-N5-C7	8.37	107.82	102.25
3	A	490	TPF	C6-N5-C7	8.52	107.92	102.25
3	D	490	TPF	C6-N5-C7	8.88	108.16	102.25
3	C	490	TPF	C6-N5-C7	9.69	108.70	102.25
3	D	490	TPF	C3-N2-C4	11.63	109.99	102.25
3	A	490	TPF	C3-N2-C4	11.66	110.01	102.25
3	C	490	TPF	C3-N2-C4	11.90	110.17	102.25
3	B	490	TPF	C3-N2-C4	11.94	110.19	102.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	481	HEM	6	0
3	A	490	TPF	6	0
2	B	481	HEM	4	0
3	B	490	TPF	6	0
4	C	1	N8E	8	0
2	C	481	HEM	8	0
3	C	490	TPF	6	0
2	D	481	HEM	8	0
3	D	490	TPF	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	448/453 (98%)	0.61	40 (8%) 12 8	37, 55, 77, 97	0
1	B	449/453 (99%)	0.68	44 (9%) 10 6	33, 57, 75, 97	0
1	C	447/453 (98%)	0.85	63 (14%) 4 2	33, 57, 76, 88	0
1	D	445/453 (98%)	0.95	60 (13%) 4 3	22, 54, 75, 98	0
All	All	1789/1812 (98%)	0.77	207 (11%) 6 4	22, 56, 76, 98	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	ALA	11.8
1	B	274	ARG	7.8
1	D	257	THR	7.5
1	D	250	GLU	7.4
1	C	29	GLY	7.0
1	D	158	ASN	6.9
1	D	256	ASN	6.8
1	D	331	TYR	6.8
1	D	447	LEU	6.8
1	B	140	ASN	6.3
1	D	248	LYS	6.3
1	C	255	THR	6.2
1	B	257	THR	6.1
1	C	139	GLN	6.0
1	C	31	LEU	6.0
1	B	255	THR	5.9
1	A	255	THR	5.6
1	C	161	GLU	5.5
1	A	254	ASP	5.3
1	B	248	LYS	5.2
1	B	139	GLN	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	274	ARG	5.1
1	A	138	PHE	5.0
1	A	257	THR	5.0
1	D	159	LYS	4.9
1	A	139	GLN	4.9
1	C	254	ASP	4.9
1	D	258	SER	4.9
1	B	244	ILE	4.7
1	B	254	ASP	4.7
1	D	437	ALA	4.7
1	B	249	GLU	4.6
1	D	139	GLN	4.5
1	D	244	ILE	4.4
1	C	366	VAL	4.3
1	C	368	VAL	4.2
1	A	161	GLU	4.2
1	A	252	GLN	4.2
1	C	252	GLN	4.2
1	D	137	LYS	4.1
1	D	136	ALA	4.1
1	B	128	PHE	4.1
1	C	251	ALA	4.0
1	B	50	LYS	4.0
1	B	265	LEU	4.0
1	A	37	GLY	3.8
1	A	38	THR	3.7
1	B	251	ALA	3.7
1	C	257	THR	3.7
1	B	253	LYS	3.6
1	D	66	ILE	3.6
1	D	50	LYS	3.6
1	C	36	HIS	3.6
1	A	472	TYR	3.6
1	C	410	GLY	3.6
1	B	327	ALA	3.6
1	B	320	GLN	3.6
1	C	37	GLY	3.5
1	A	251	ALA	3.5
1	B	250	GLU	3.5
1	A	269	TYR	3.4
1	D	334	VAL	3.4
1	C	38	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	248	LYS	3.4
1	C	66	ILE	3.4
1	D	187	LEU	3.3
1	D	157	TRP	3.3
1	D	161	GLU	3.3
1	A	440	LEU	3.3
1	D	446	GLU	3.2
1	B	448	LEU	3.2
1	D	160	ASP	3.2
1	D	337	GLU	3.2
1	C	253	LYS	3.2
1	A	42	VAL	3.1
1	A	250	GLU	3.1
1	B	138	PHE	3.1
1	B	266	GLY	3.1
1	A	72	CYS	3.1
1	A	327	ALA	3.1
1	C	327	ALA	3.1
1	D	476	LYS	3.0
1	A	273	THR	3.0
1	C	304	LEU	3.0
1	C	120	PRO	3.0
1	D	31	LEU	3.0
1	D	32	PRO	3.0
1	A	324	GLU	3.0
1	B	258	SER	3.0
1	C	249	GLU	3.0
1	C	94	GLU	2.9
1	A	128	PHE	2.9
1	B	476	LYS	2.9
1	C	43	GLY	2.9
1	D	29	GLY	2.9
1	C	448	LEU	2.9
1	D	183	PHE	2.9
1	B	119	TYR	2.8
1	D	53	LEU	2.8
1	D	371	TYR	2.8
1	A	456	TYR	2.8
1	A	198	GLN	2.8
1	A	253	LYS	2.8
1	A	36	HIS	2.7
1	B	318	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	206	CYS	2.7
1	C	224	GLN	2.7
1	D	57	LEU	2.7
1	D	365	PRO	2.7
1	A	473	ILE	2.7
1	C	237	ASP	2.7
1	D	325	PHE	2.7
1	D	448	LEU	2.7
1	C	457	HIS	2.7
1	A	63	TYR	2.7
1	D	241	GLU	2.7
1	C	451	LEU	2.6
1	D	407	LEU	2.6
1	C	324	GLU	2.6
1	A	367	GLN	2.6
1	B	242	ILE	2.6
1	B	324	GLU	2.6
1	C	65	GLY	2.6
1	C	189	LYS	2.6
1	B	252	GLN	2.6
1	A	49	GLY	2.5
1	C	93	ASN	2.5
1	B	247	GLU	2.5
1	B	337	GLU	2.5
1	D	318	LEU	2.5
1	D	269	TYR	2.5
1	C	55	PHE	2.5
1	C	365	PRO	2.5
1	B	256	ASN	2.5
1	C	78	VAL	2.5
1	D	249	GLU	2.5
1	D	473	ILE	2.5
1	B	473	ILE	2.5
1	C	460	VAL	2.5
1	C	162	GLY	2.5
1	D	408	VAL	2.5
1	B	273	THR	2.4
1	C	157	TRP	2.4
1	B	270	ARG	2.4
1	D	396	PRO	2.4
1	C	227	ARG	2.4
1	C	138	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	376	GLY	2.4
1	C	44	HIS	2.4
1	B	269	TYR	2.3
1	A	248	LYS	2.3
1	A	60	LYS	2.3
1	D	150	ARG	2.3
1	A	245	ALA	2.3
1	D	373	VAL	2.3
1	C	185	GLU	2.3
1	C	226	TYR	2.3
1	B	290	ALA	2.3
1	B	460	VAL	2.3
1	A	162	GLY	2.3
1	C	471	LYS	2.3
1	C	369	GLY	2.2
1	A	476	LYS	2.2
1	D	322	ILE	2.2
1	C	33	PRO	2.2
1	D	128	PHE	2.2
1	A	109	PHE	2.2
1	C	372	VAL	2.2
1	C	476	LYS	2.2
1	A	249	GLU	2.2
1	A	50	LYS	2.2
1	D	227	ARG	2.2
1	B	41	PHE	2.2
1	C	47	GLN	2.2
1	C	250	GLU	2.2
1	C	269	TYR	2.2
1	B	246	ARG	2.2
1	D	445	PHE	2.1
1	A	471	LYS	2.1
1	C	473	ILE	2.1
1	C	274	ARG	2.1
1	B	336	GLU	2.1
1	C	439	VAL	2.1
1	D	275	MET	2.1
1	A	256	ASN	2.1
1	C	377	ASP	2.1
1	B	345	ALA	2.1
1	D	243	ILE	2.1
1	D	119	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	123	ARG	2.1
1	D	222	LEU	2.1
1	C	64	GLY	2.1
1	D	329	LEU	2.1
1	D	30	LYS	2.1
1	C	123	ARG	2.0
1	D	324	GLU	2.0
1	B	314	HIS	2.0
1	C	151	LYS	2.0
1	D	391	GLU	2.0
1	A	431	GLN	2.0
1	B	295	SER	2.0
1	C	295	SER	2.0
1	A	160	ASP	2.0
1	D	48	PHE	2.0
1	B	459	MET	2.0
1	C	392	ALA	2.0
1	D	419	VAL	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
4	N8E	C	1	24/24	0.83	0.42	4.34	59,70,75,76	0
2	HEM	A	481	43/43	0.94	0.27	1.23	26,51,58,63	0
2	HEM	D	481	43/43	0.99	0.26	0.65	51,59,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	HEM	B	481	43/43	0.98	0.27	0.57	38,56,61,66	0
2	HEM	C	481	43/43	0.97	0.25	0.54	42,53,68,85	0
3	TPF	D	490	22/22	0.94	0.24	-0.13	53,56,68,69	0
3	TPF	A	490	22/22	0.95	0.21	-0.45	29,56,73,75	0
3	TPF	C	490	22/22	0.96	0.17	-1.45	32,52,63,66	0
3	TPF	B	490	22/22	0.96	0.19	-1.72	30,62,76,77	0

6.5 Other polymers

There are no such residues in this entry.