



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:56 AM GMT

PDB ID : 3K9Y  
Title : Crystal structure of rat mitochondrial P450 24A1 S57D in complex with CYMAL-5  
Authors : Annalora, A.J.; Goodin, D.B.; Hong, W.; Zhang, Q.; Johnson, E.F.; Stout, C.D.  
Deposited on : 2009-10-16  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

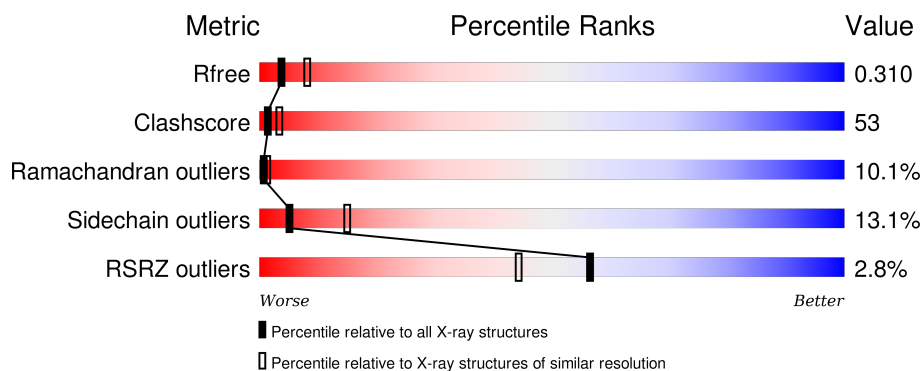
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	482	<div> <div>2%</div> <div>30% 51% 12% . .</div> </div>
1	B	482	<div> <div>3%</div> <div>30% 49% 15% . .</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CM5	A	516	X	-	-	X
3	CM5	A	517	X	-	X	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7703 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 1,25-dihydroxyvitamin D(3) 24-hydroxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3769	2415	656	677	21			
1	B	462	Total	C	N	O	S	0	0	0
			3780	2421	660	678	21			

There are 4 discrepancies between the modelled and reference sequences:

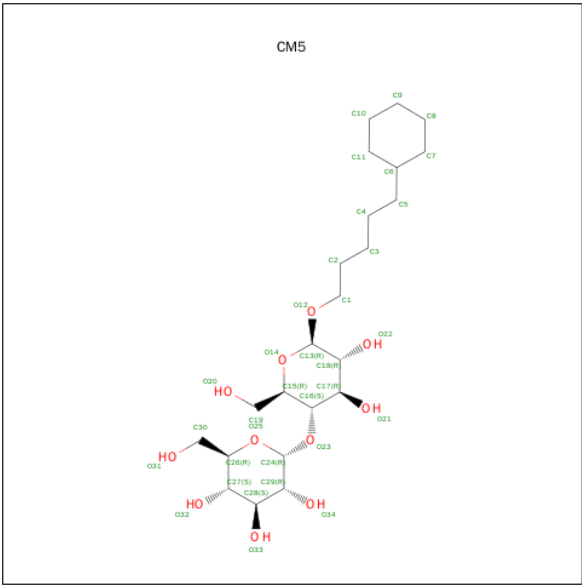
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	EXPRESSION TAG	UNP Q09128
A	57	ASP	SER	ENGINEERED	UNP Q09128
B	33	MET	-	EXPRESSION TAG	UNP Q09128
B	57	ASP	SER	ENGINEERED	UNP Q09128

- 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		

- Molecule 3 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSIDE (three-letter code: CM5) (formula: C<sub>23</sub>H<sub>42</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			34	23	11		
3	A	1	Total	C	O	0	0
			34	23	11		



R505	I441	N373	Q308	K174
E506	Q442	M374	D309	L175
L507	K443	P375	R310	D176
P508	E444	Y376	I311	K177
I509	K445	L377	S312	K178
A510	K446	K378	K313	E181
F511	I447	A379	K314	L182
P512	F450	C380	E315	V183
R514	L453	L381	L316	L183
	L453	K382	Y317	A184
	P454	E383	A318	
	P455	R386	A319	L187
	G456	L387	V320	F188
	I457	T388	T321	R189
	G458	P389	E322	M190
	K459		L323	D191
	R460	P392	Q324	E192
	M461	F393	L325	L193
	G462	T394		C194
	I463	T395	E328	
	G464	R396	E329	R197
	R465	T397	T330	G198
	R466	L398	T331	R199
	I467		A332	L200
	A468	T402	N333	E201
	E469	V403	S334	D202
	L470	L404	M335	L203
	Q471	G405	M336	L204
	L472	E406	E337	S205
	H473		I338	E206
	L474	P410	L339	L207
	A475	K411	Y340	M208
	L476	G412	N341	K209
	C477	T413	L342	W210
	W478	V414	S343	S211
	I479	L415	R344	F212
	L480	T416	N345	
	Q481	L417	A348	I215
	K482	N418	Q349	C216
	Y483	T419	R350	L217
	D484	Q420	R351	V218
	I485	V421	L352	L219
	V486	L422	L353	Y220
	A487		Q354	E221
	T488	S425	E355	K222
	D489	E426	V356	R223
	M490	D427	Q291	F224
	E491	N428	R292	G225
	P492	F429	Y293	L226
	M495	E430	L360	L227
	L496	D431	S294	Q228
	H497	S432	Q295	K229
	L498	F435	D300	E230
	G499	R436	F301	T231
	I500	P437	R367	E232
	L501	E438	A368	E233
	S504	L501	E369	E234
			D370	A235
			L371	
			Y306	
			Q307	
			R372	
				I239

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.30Å 81.30Å 108.71Å 90.00° 122.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 36.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.80) 97.2 (36.74-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.251 , 0.318 0.257 , 0.310	Depositor DCC
$R_{free}$ test set	1619 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 84.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32345 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CM5

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	0.41	0/3857	0.72	1/5216 (0.0%)
1	B	0.44	0/3868	0.72	1/5230 (0.0%)
All	All	0.42	0/7725	0.72	2/10446 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	LEU	CA-CB-CG	5.09	127.02	115.30
1	B	486	VAL	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3827	394	0
1	B	3780	0	3840	406	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	68	0	84	31	0
All	All	7703	0	7811	821	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 53.

All (821) 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)
3:A:517:CM5:H11	3:A:517:CM5:H15	1.29	1.10
1:A:352:LEU:HD12	1:A:480:ILE:HD13	1.37	1.06
3:A:516:CM5:H18	3:A:516:CM5:H22A	1.34	1.05
1:A:165:LYS:HD3	1:A:301:PHE:HB2	1.35	1.05
1:B:118:LEU:HB2	1:B:404:LEU:HD21	1.35	1.04
1:B:328:VAL:HG23	1:B:329:GLU:N	1.76	1.00
1:B:356:VAL:HG21	1:B:480:ILE:HG21	1.45	0.98
1:B:343:SER:HB3	1:B:485:ILE:HG22	1.45	0.98
1:A:475:ALA:O	1:A:476:LEU:HB2	1.61	0.98
1:A:70:LEU:HD13	1:A:101:LEU:HB3	1.46	0.97
3:A:517:CM5:C1	3:A:517:CM5:H15	1.94	0.96
1:B:446:LYS:HG3	1:B:447:ILE:H	1.28	0.96
1:B:328:VAL:CG2	1:B:329:GLU:H	1.79	0.95
1:B:374:MET:H	1:B:375:PRO:HD3	1.30	0.94
1:B:200:ILE:HD12	1:B:203:LEU:HD13	1.47	0.94
1:B:260:HIS:ND1	1:B:265:THR:HG21	1.83	0.94
3:A:516:CM5:H21A	3:A:517:CM5:H192	1.47	0.93
1:A:465:ARG:NH2	1:A:466:ARG:HH12	1.69	0.91
1:A:82:GLN:HE22	3:A:517:CM5:H13	1.37	0.90
1:B:505:ARG:HB3	1:B:505:ARG:NH1	1.87	0.90
1:A:368:ALA:O	1:A:369:GLU:HB2	1.70	0.89
1:B:328:VAL:CG2	1:B:329:GLU:N	2.33	0.89
3:A:516:CM5:H71	3:A:517:CM5:H72	1.52	0.89
3:A:517:CM5:H11	3:A:517:CM5:C15	2.03	0.88
3:A:517:CM5:O34	3:A:517:CM5:H16	1.70	0.88
1:A:245:MET:HB2	1:A:274:ALA:HB1	1.56	0.88
1:A:361:PRO:O	1:A:362:ASP:HB3	1.72	0.87
1:A:107:VAL:HG13	1:A:415:LEU:HD23	1.58	0.86
1:A:128:ARG:HG2	1:A:395:THR:O	1.74	0.86
1:B:263:LEU:O	1:B:263:LEU:HD12	1.75	0.86
1:B:187:LEU:HD22	1:B:478:TRP:HE3	1.39	0.86
1:B:505:ARG:HH11	1:B:505:ARG:HB3	1.38	0.85
1:B:199:ARG:CD	1:B:200:ILE:H	1.89	0.85
1:A:58:LEU:HB2	1:A:59:PRO:O	1.77	0.85
1:A:183:LEU:HD21	1:A:475:ALA:CB	2.07	0.84
1:A:58:LEU:HB2	1:A:59:PRO:C	1.98	0.84
1:A:207:LEU:HG	1:A:335:LEU:HD12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLY:H	1:B:149:ILE:HD11	1.42	0.83
1:A:146:GLY:O	1:A:148:MET:N	2.12	0.83
1:B:210:TRP:CZ3	1:B:335:LEU:HD23	2.13	0.83
1:A:247:SER:HA	3:A:516:CM5:H29	1.60	0.82
1:A:352:LEU:HD12	1:A:480:ILE:CD1	2.09	0.82
1:B:71:LEU:HG	1:B:72:GLU:H	1.42	0.82
1:B:199:ARG:HH12	1:B:203:LEU:HB2	1.43	0.82
3:A:516:CM5:H21A	3:A:517:CM5:C19	2.08	0.82
1:A:236:LEU:H	1:A:236:LEU:HD13	1.44	0.82
1:B:191:ASP:HA	1:B:194:CYS:HB2	1.60	0.81
1:A:457:ILE:HG13	1:A:458:GLY:H	1.45	0.81
1:A:238:PHE:O	1:A:242:ILE:HG12	1.79	0.81
1:B:215:ILE:HG13	1:B:219:LEU:HD22	1.61	0.81
1:B:463:ILE:HD13	1:B:463:ILE:O	1.80	0.81
1:A:398:LEU:HD21	1:A:415:LEU:HD11	1.61	0.81
1:B:446:LYS:O	1:B:447:ILE:HD13	1.82	0.80
1:B:500:ILE:N	1:B:500:ILE:HD13	1.97	0.80
1:A:514:ARG:HG3	1:A:514:ARG:HH21	1.47	0.80
1:B:145:TYR:HB2	1:B:150:LEU:CD1	2.12	0.80
1:A:183:LEU:HD21	1:A:475:ALA:HB2	1.61	0.80
1:A:280:LYS:HB3	1:A:280:LYS:NZ	1.96	0.80
1:B:64:TRP:HB3	1:B:67:LEU:HB3	1.64	0.80
1:A:293:TYR:CD1	1:A:300:ASP:HB2	2.17	0.79
1:B:71:LEU:HD23	1:B:71:LEU:H	1.48	0.79
1:A:166:LEU:HA	1:A:172:ILE:HD11	1.63	0.79
1:B:328:VAL:HG23	1:B:329:GLU:H	1.41	0.79
1:B:335:LEU:HD12	1:B:335:LEU:O	1.83	0.79
1:A:197:ARG:HH21	1:B:295:GLN:NE2	1.81	0.79
1:B:101:LEU:HD12	1:B:104:PHE:HB3	1.63	0.79
1:B:199:ARG:HH11	1:B:201:PRO:HA	1.46	0.78
1:B:182:VAL:HG22	1:B:223:ARG:NH2	1.97	0.78
1:A:164:LYS:O	1:A:164:LYS:HE3	1.83	0.78
1:B:374:MET:N	1:B:375:PRO:HD3	1.99	0.78
1:B:199:ARG:HD2	1:B:200:ILE:H	1.49	0.78
1:B:199:ARG:NH1	1:B:203:LEU:HB2	1.97	0.78
1:B:118:LEU:HB2	1:B:404:LEU:CD2	2.13	0.78
1:B:149:ILE:H	1:B:149:ILE:HD13	1.49	0.77
1:B:459:LYS:H	1:B:459:LYS:HD2	1.49	0.77
1:A:97:PHE:O	1:A:107:VAL:HG23	1.85	0.77
1:A:235:ALA:O	1:A:239:ILE:HG12	1.85	0.77
1:A:127:GLN:HE21	1:A:397:THR:HG21	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PRO:N	1:A:411:LYS:HB2	2.00	0.76
1:A:178:LYS:HD3	1:A:217:LEU:HD13	1.67	0.76
1:B:159:ARG:NH2	1:B:461:MET:O	2.17	0.76
1:A:58:LEU:HB2	1:A:59:PRO:CA	2.15	0.76
1:B:286:ILE:HD11	1:B:320:VAL:HG11	1.66	0.76
1:B:405:GLY:O	1:B:406:GLU:HB2	1.84	0.76
1:A:62:THR:HB	1:A:64:TRP:CZ2	2.20	0.76
1:B:169:PRO:O	1:B:173:MET:HG3	1.84	0.75
1:B:259:LEU:HD12	1:B:260:HIS:N	2.01	0.75
3:A:517:CM5:H91	3:A:517:CM5:C5	2.16	0.75
1:B:350:ARG:HH11	1:B:354:GLN:HB2	1.51	0.75
1:B:95:GLN:HG3	1:B:114:LEU:HD11	1.68	0.75
3:A:516:CM5:C2	3:A:517:CM5:H192	2.16	0.74
1:B:165:LYS:HG3	1:B:305:ILE:HD11	1.66	0.74
1:B:146:GLY:HA3	1:B:322:GLU:HG3	1.69	0.74
3:A:516:CM5:C18	3:A:516:CM5:H22A	2.14	0.74
1:B:453:LEU:HD22	1:B:457:ILE:HG13	1.69	0.73
3:A:516:CM5:H12	3:A:517:CM5:H24	1.71	0.73
1:A:359:VAL:C	1:A:360:LEU:HD12	2.09	0.73
1:B:95:GLN:HE21	1:B:114:LEU:HG	1.52	0.72
1:B:91:LYS:HB3	1:B:91:LYS:NZ	2.04	0.72
1:A:377:LEU:HD23	1:A:378:LYS:N	2.04	0.72
1:B:203:LEU:HD22	1:B:509:ILE:HD11	1.72	0.72
1:B:340:TYR:HB2	1:B:507:LEU:HD21	1.70	0.72
1:B:266:LYS:HD3	1:B:269:GLN:NE2	2.05	0.72
1:B:277:THR:O	1:B:280:LYS:HB3	1.89	0.72
1:A:197:ARG:HE	1:B:295:GLN:HE21	1.35	0.71
1:A:135:LYS:HG2	1:A:145:TYR:CE2	2.25	0.71
1:B:467:LEU:HG	1:B:471:GLN:HE21	1.53	0.71
1:B:140:HIS:HD1	1:B:268:TRP:HZ2	1.38	0.71
3:A:517:CM5:O34	3:A:517:CM5:C16	2.39	0.71
1:A:164:LYS:O	1:A:165:LYS:HB2	1.91	0.71
1:B:389:PRO:HG3	1:B:420:GLN:HB2	1.72	0.71
1:A:312:SER:OG	1:A:315:GLU:HG3	1.91	0.71
1:B:108:HIS:CE1	1:B:416:THR:HG21	2.26	0.71
3:A:516:CM5:C7	3:A:517:CM5:H72	2.20	0.71
1:B:149:ILE:N	1:B:149:ILE:HD13	2.06	0.71
3:A:517:CM5:H52	3:A:517:CM5:H91	1.73	0.70
3:A:517:CM5:H12	3:A:517:CM5:O22	1.90	0.70
1:A:467:LEU:O	1:A:471:GLN:HG3	1.91	0.70
1:A:420:GLN:O	1:A:422:LEU:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HG2	1:A:114:LEU:HD11	1.74	0.70
1:B:430:GLU:O	1:B:439:ARG:NH2	2.25	0.70
1:A:472:LEU:O	1:A:476:LEU:HD12	1.92	0.70
1:B:248:THR:HG21	1:B:270:ALA:O	1.92	0.69
1:B:187:LEU:HD22	1:B:478:TRP:CE3	2.26	0.69
1:A:82:GLN:NE2	3:A:517:CM5:H13	2.07	0.69
1:B:328:VAL:HG22	1:B:329:GLU:H	1.58	0.69
1:B:199:ARG:NH1	1:B:201:PRO:HA	2.08	0.69
1:B:425:SER:C	1:B:427:ASP:H	1.95	0.69
1:A:225:GLY:HA3	1:A:231:THR:CG2	2.23	0.69
1:B:355:GLU:O	1:B:359:VAL:HG23	1.92	0.69
1:A:409:LEU:CD2	1:A:415:LEU:HD21	2.22	0.69
1:A:58:LEU:CG	1:A:59:PRO:HA	2.23	0.69
1:A:165:LYS:CD	1:A:301:PHE:HB2	2.19	0.68
1:B:335:LEU:C	1:B:335:LEU:HD12	2.14	0.68
1:B:118:LEU:CB	1:B:404:LEU:HD21	2.17	0.68
1:B:146:GLY:O	1:B:150:LEU:HB2	1.93	0.68
1:A:457:ILE:CG1	1:A:458:GLY:H	2.06	0.68
1:A:340:TYR:HB2	1:A:507:LEU:HD21	1.73	0.68
1:B:479:ILE:HG22	1:B:485:ILE:HD11	1.76	0.68
1:A:505:ARG:HH11	1:A:505:ARG:HG3	1.57	0.68
1:B:403:VAL:O	1:B:404:LEU:HD12	1.94	0.68
1:B:379:ALA:HB1	1:B:440:TRP:HB2	1.76	0.68
1:B:175:LEU:HD12	1:B:218:VAL:HG22	1.74	0.68
1:B:145:TYR:HB2	1:B:150:LEU:HD12	1.74	0.67
1:B:205:SER:O	1:B:209:LYS:HG3	1.94	0.67
1:B:232:GLU:HG3	1:B:234:GLU:OE1	1.93	0.67
1:A:381:LEU:O	1:A:381:LEU:HD23	1.94	0.67
1:B:320:VAL:O	1:B:323:LEU:HB2	1.94	0.67
1:A:62:THR:HB	1:A:64:TRP:CE2	2.29	0.67
1:B:484:ASP:HB2	1:B:514:ARG:HE	1.59	0.67
1:B:101:LEU:O	1:B:101:LEU:HD12	1.93	0.67
1:A:306:TYR:HB2	1:A:316:LEU:HD11	1.76	0.67
1:A:352:LEU:O	1:A:356:VAL:HG23	1.95	0.67
1:A:95:GLN:HG2	1:A:114:LEU:CD1	2.24	0.67
1:A:74:PHE:C	1:A:76:LYS:H	1.97	0.67
1:B:495:MET:O	1:B:496:LEU:HD23	1.94	0.67
1:A:497:HIS:O	1:A:498:LEU:HD23	1.95	0.67
1:B:266:LYS:HA	1:B:269:GLN:HE21	1.59	0.67
1:A:167:MET:HA	1:A:466:ARG:HG3	1.76	0.67
1:A:393:PHE:HA	1:A:419:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PRO:O	1:B:260:HIS:HD2	1.76	0.66
1:A:232:GLU:HB3	1:A:236:LEU:CD1	2.25	0.66
1:A:418:ASN:O	1:A:421:VAL:HG12	1.96	0.66
1:A:255:THR:OG1	1:A:260:HIS:HE1	1.78	0.66
1:A:396:ARG:HH11	1:A:396:ARG:HG2	1.59	0.66
1:B:500:ILE:HD13	1:B:500:ILE:H	1.61	0.66
1:A:467:LEU:HD12	1:A:467:LEU:O	1.96	0.66
1:B:187:LEU:CD2	1:B:478:TRP:HE3	2.10	0.65
1:B:125:HIS:HA	1:B:155:TRP:CZ3	2.31	0.65
1:A:318:ALA:O	1:A:322:GLU:HG3	1.97	0.65
1:B:252:MET:CE	1:B:257:VAL:HG23	2.26	0.65
1:A:403:VAL:O	1:A:404:LEU:HD22	1.96	0.65
1:B:321:THR:O	1:B:325:LEU:HG	1.96	0.65
1:B:356:VAL:HG21	1:B:480:ILE:CG2	2.25	0.65
1:A:129:LEU:H	1:A:395:THR:CG2	2.11	0.64
1:A:514:ARG:NH2	1:A:514:ARG:HG3	2.10	0.64
1:A:69:SER:C	1:A:71:LEU:H	2.00	0.64
1:A:145:TYR:HB2	1:A:150:LEU:HD13	1.77	0.64
1:B:264:ASN:O	1:B:265:THR:O	2.15	0.64
1:B:374:MET:H	1:B:375:PRO:CD	2.07	0.64
1:B:95:GLN:HB2	1:B:111:SER:HB3	1.78	0.64
1:A:286:ILE:HD13	1:A:320:VAL:HG21	1.80	0.64
1:A:56:THR:O	1:A:56:THR:HG22	1.97	0.64
3:A:517:CM5:C9	3:A:517:CM5:C5	2.75	0.64
1:A:245:MET:HB2	1:A:274:ALA:CB	2.26	0.64
1:A:58:LEU:CB	1:A:59:PRO:CA	2.75	0.64
1:B:155:TRP:CD1	1:B:460:ARG:NH2	2.65	0.64
1:A:96:ILE:HB	1:A:114:LEU:HD11	1.80	0.64
1:A:75:TRP:O	1:A:76:LYS:HG3	1.96	0.63
1:B:161:ALA:O	1:B:305:ILE:HD12	1.98	0.63
1:A:182:VAL:HG21	1:A:214:SER:HA	1.80	0.63
1:A:145:TYR:CB	1:A:150:LEU:HD13	2.29	0.63
1:A:58:LEU:CB	1:A:59:PRO:HA	2.27	0.63
1:B:228:GLN:O	1:B:229:LYS:O	2.16	0.63
1:B:361:PRO:O	1:B:362:ASP:HB2	1.98	0.63
1:B:422:LEU:CD1	1:B:453:LEU:HD12	2.29	0.63
1:B:199:ARG:HD3	1:B:200:ILE:H	1.61	0.63
1:A:286:ILE:O	1:A:286:ILE:HG22	1.99	0.63
1:B:265:THR:HG23	1:B:268:TRP:H	1.64	0.63
1:B:343:SER:HB3	1:B:485:ILE:CG2	2.25	0.63
1:B:487:ALA:HB2	1:B:510:ALA:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:240:THR:HG23	1.99	0.62
1:B:353:LEU:HD21	1:B:514:ARG:HH22	1.64	0.62
1:A:286:ILE:HG23	1:A:302:LEU:HD21	1.80	0.62
1:B:341:ASN:HB3	1:B:435:PHE:CE2	2.34	0.62
1:A:183:LEU:HD11	1:A:475:ALA:N	2.14	0.62
1:B:145:TYR:HB3	1:B:149:ILE:HG12	1.81	0.62
1:A:428:ASN:OD1	1:A:447:ILE:HA	1.99	0.62
1:A:58:LEU:HG	1:A:59:PRO:HA	1.80	0.62
1:A:129:LEU:HD13	1:A:395:THR:HG21	1.81	0.62
1:A:127:GLN:NE2	1:A:397:THR:HG21	2.13	0.62
1:B:222:LYS:HD3	1:B:224:PHE:CE1	2.33	0.62
1:B:505:ARG:HH11	1:B:505:ARG:CB	2.12	0.62
1:A:197:ARG:HE	1:B:295:GLN:NE2	1.98	0.62
1:A:254:VAL:HG23	1:A:255:THR:HG23	1.82	0.62
1:B:312:SER:OG	1:B:315:GLU:HG3	1.99	0.62
1:A:337:TRP:CZ2	1:A:503:PRO:HG3	2.35	0.62
1:A:323:LEU:HG	2:A:520:HEM:HBC1	1.81	0.62
1:A:457:ILE:HG13	1:A:458:GLY:N	2.15	0.62
1:B:278:ILE:HD11	1:B:321:THR:HG21	1.82	0.62
1:A:70:LEU:CD1	1:A:101:LEU:HB3	2.26	0.61
1:B:177:LYS:O	1:B:181:GLU:HG3	2.00	0.61
1:A:100:LYS:HG2	1:A:102:GLY:O	2.00	0.61
1:A:66:LEU:N	1:A:66:LEU:HD22	2.14	0.61
1:B:199:ARG:HD3	1:B:200:ILE:N	2.16	0.61
1:A:116:GLU:C	1:A:118:LEU:H	2.04	0.61
1:B:175:LEU:HD11	1:B:218:VAL:HG13	1.81	0.61
1:B:220:TYR:CD2	1:B:285:CYS:HB3	2.36	0.61
1:A:84:ASP:O	1:A:87:ALA:HB3	2.00	0.61
3:A:517:CM5:C1	3:A:517:CM5:C15	2.71	0.61
1:A:238:PHE:CE1	1:A:242:ILE:HD11	2.36	0.60
1:B:182:VAL:HG22	1:B:223:ARG:HH21	1.66	0.60
1:B:259:LEU:HD13	1:B:263:LEU:HD23	1.83	0.60
1:A:349:GLN:HE22	1:A:485:ILE:H	1.49	0.60
1:A:234:GLU:HA	1:A:237:THR:HG23	1.83	0.60
1:B:274:ALA:O	1:B:277:THR:HB	2.02	0.60
1:B:235:ALA:O	1:B:239:ILE:HG12	2.02	0.60
1:B:211:SER:OG	1:B:332:ALA:HB2	2.01	0.60
1:B:329:GLU:OE2	1:B:500:ILE:HD11	2.02	0.59
1:B:383:GLU:OE2	1:B:386:ARG:NH1	2.35	0.59
1:B:229:LYS:N	1:B:229:LYS:HD2	2.17	0.59
1:B:199:ARG:CD	1:B:200:ILE:N	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:OG1	1:B:271:HIS:HB2	2.02	0.59
1:A:232:GLU:HB3	1:A:236:LEU:HD11	1.83	0.59
1:A:223:ARG:HH21	1:A:223:ARG:HG3	1.66	0.59
1:A:141:ARG:HH21	1:A:272:THR:CG2	2.16	0.59
1:A:328:VAL:HG12	1:A:329:GLU:N	2.16	0.59
1:A:167:MET:O	1:A:168:LYS:HD3	2.03	0.59
1:A:107:VAL:HG13	1:A:415:LEU:CD2	2.32	0.59
1:B:146:GLY:HA3	1:B:322:GLU:CG	2.31	0.59
1:B:70:LEU:HD12	1:B:73:ILE:HG21	1.84	0.59
1:B:435:PHE:HE1	1:B:437:PRO:HG3	1.67	0.59
1:B:491:GLU:HG2	1:B:492:PRO:HD2	1.85	0.59
1:B:131:ILE:HG13	1:B:131:ILE:O	2.02	0.59
1:B:67:LEU:HD13	1:B:70:LEU:HB3	1.83	0.59
1:A:453:LEU:HD22	1:A:457:ILE:HB	1.84	0.59
1:A:65:PRO:O	1:A:67:LEU:N	2.29	0.59
1:A:336:MET:HG2	1:A:507:LEU:HD22	1.85	0.59
1:B:352:LEU:O	1:B:356:VAL:HG23	2.02	0.58
1:A:196:GLU:OE2	1:A:197:ARG:HG2	2.01	0.58
1:B:224:PHE:O	1:B:225:GLY:C	2.42	0.58
1:A:203:LEU:HD21	1:A:509:ILE:HD11	1.85	0.58
1:B:442:GLN:OE1	1:B:445:LYS:HD3	2.02	0.58
1:A:381:LEU:HD11	1:A:472:LEU:HB3	1.85	0.58
1:B:467:LEU:HG	1:B:471:GLN:NE2	2.17	0.58
1:B:352:LEU:CD2	1:B:377:LEU:HA	2.32	0.58
1:A:280:LYS:HB3	1:A:280:LYS:HZ3	1.68	0.58
1:A:107:VAL:CG1	1:A:415:LEU:HD23	2.32	0.58
1:B:377:LEU:O	1:B:380:CYS:HB2	2.03	0.58
1:B:259:LEU:C	1:B:259:LEU:HD12	2.24	0.58
1:A:383:GLU:OE1	1:A:439:ARG:NH1	2.36	0.58
1:B:491:GLU:CG	1:B:492:PRO:HD2	2.33	0.58
1:A:489:ASP:C	1:A:490:ASN:HD22	2.07	0.58
1:A:366:PRO:O	1:A:367:ARG:HG2	2.04	0.58
1:B:318:ALA:O	1:B:322:GLU:HG2	2.04	0.58
1:B:73:ILE:HG23	1:B:74:PHE:HD1	1.68	0.58
1:A:396:ARG:HG2	1:A:396:ARG:NH1	2.18	0.58
1:B:279:PHE:O	1:B:283:LYS:HG3	2.03	0.58
1:A:197:ARG:HG3	1:A:197:ARG:HH11	1.67	0.58
1:B:245:MET:HB3	1:B:274:ALA:HB1	1.86	0.58
1:B:368:ALA:O	1:B:369:GLU:HB2	2.01	0.58
1:A:341:ASN:O	1:A:345:ASN:ND2	2.37	0.58
1:A:183:LEU:HD21	1:A:475:ALA:CA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:TRP:CB	1:B:67:LEU:HB3	2.34	0.58
1:B:169:PRO:HA	1:B:172:ILE:HD12	1.85	0.58
1:A:375:PRO:O	1:A:441:LEU:HD21	2.03	0.58
1:B:159:ARG:HH11	1:B:163:GLN:HE22	1.50	0.58
1:A:260:HIS:HD2	1:A:265:THR:OG1	1.87	0.58
1:B:219:LEU:O	1:B:289:ARG:NH2	2.35	0.57
1:B:167:MET:O	1:B:466:ARG:NH1	2.37	0.57
1:A:382:LYS:O	1:A:384:SER:N	2.37	0.57
1:A:150:LEU:HD21	1:A:158:VAL:HG21	1.86	0.57
1:B:486:VAL:O	1:B:487:ALA:HB2	2.03	0.57
1:B:487:ALA:HB3	1:B:509:ILE:HA	1.85	0.57
1:B:244:THR:O	1:B:248:THR:HG23	2.03	0.57
1:A:300:ASP:HB3	1:A:303:CYS:HB3	1.85	0.57
1:A:475:ALA:O	1:A:476:LEU:CB	2.43	0.57
1:A:207:LEU:HG	1:A:335:LEU:CD1	2.34	0.57
3:A:516:CM5:C15	3:A:516:CM5:O22	2.53	0.57
1:A:111:SER:O	1:A:115:LEU:HD23	2.03	0.57
1:B:172:ILE:HD13	1:B:466:ARG:HB3	1.86	0.57
1:A:505:ARG:NH1	1:A:505:ARG:HG3	2.20	0.57
1:A:335:LEU:O	1:A:338:ILE:HG22	2.04	0.57
1:A:465:ARG:NH2	1:A:466:ARG:NH1	2.47	0.57
1:B:252:MET:HE3	1:B:257:VAL:HG23	1.87	0.57
1:B:193:LEU:HD23	1:B:200:ILE:HG23	1.87	0.57
1:B:487:ALA:HB2	1:B:510:ALA:H	1.70	0.56
1:A:166:LEU:CA	1:A:172:ILE:HD11	2.35	0.56
1:A:225:GLY:HA3	1:A:231:THR:HG22	1.86	0.56
1:B:495:MET:C	1:B:496:LEU:HD23	2.25	0.56
1:B:314:LYS:HB2	1:B:314:LYS:NZ	2.21	0.56
1:B:436:ARG:C	1:B:438:GLU:H	2.07	0.56
1:A:64:TRP:CZ3	1:A:72:GLU:OE2	2.59	0.56
1:A:117:ALA:O	1:A:404:LEU:HD11	2.06	0.56
1:B:128:ARG:NH1	2:B:520:HEM:O2D	2.39	0.56
1:B:338:ILE:HD13	1:B:476:LEU:HD11	1.87	0.56
1:A:245:MET:C	1:A:245:MET:SD	2.84	0.56
1:A:280:LYS:HB3	1:A:280:LYS:HZ2	1.71	0.56
1:A:63:ASN:O	1:A:64:TRP:O	2.23	0.56
1:B:366:PRO:HG2	1:B:477:CYS:HB3	1.87	0.56
1:A:370:ASP:N	1:A:370:ASP:OD2	2.39	0.56
1:B:447:ILE:O	1:B:447:ILE:HG12	2.05	0.55
1:B:473:HIS:C	1:B:475:ALA:H	2.10	0.55
1:A:377:LEU:HD23	1:A:377:LEU:C	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:O	1:A:477:CYS:HB2	2.06	0.55
1:A:95:GLN:HG3	1:A:111:SER:CB	2.37	0.55
1:B:304:ASP:HB3	1:B:308:GLN:OE1	2.05	0.55
1:A:386:ARG:HH12	1:A:432:SER:HA	1.70	0.55
1:A:183:LEU:HD21	1:A:475:ALA:HA	1.88	0.55
1:B:350:ARG:NH1	1:B:354:GLN:HB2	2.21	0.55
1:B:436:ARG:HH11	1:B:436:ARG:HG2	1.70	0.55
1:A:405:GLY:C	1:A:407:TYR:H	2.08	0.55
1:B:398:LEU:HD12	1:B:413:THR:HB	1.89	0.55
1:A:352:LEU:HD23	1:A:376:TYR:HD2	1.71	0.55
1:A:164:LYS:O	1:A:164:LYS:HG2	2.05	0.55
1:B:222:LYS:HD3	1:B:224:PHE:HE1	1.71	0.55
1:A:171:GLU:HA	1:A:171:GLU:OE1	2.06	0.55
1:A:464:GLY:O	1:A:466:ARG:N	2.40	0.55
1:A:178:LYS:HB3	1:A:217:LEU:CD1	2.37	0.55
1:A:195:ASP:OD2	1:A:196:GLU:N	2.37	0.55
1:B:419:THR:CG2	1:B:420:GLN:N	2.69	0.55
1:A:125:HIS:CG	1:A:152:GLY:HA2	2.40	0.55
1:B:224:PHE:O	1:B:226:LEU:N	2.40	0.54
1:A:233:GLU:OE1	1:A:233:GLU:N	2.39	0.54
1:B:453:LEU:HD22	1:B:457:ILE:CG1	2.38	0.54
1:B:265:THR:OG1	1:B:266:LYS:N	2.39	0.54
1:B:127:GLN:O	1:B:396:ARG:HA	2.07	0.54
1:A:220:TYR:HB3	1:A:285:CYS:HB3	1.88	0.54
1:B:80:LYS:HG2	1:B:498:LEU:CD2	2.37	0.54
1:A:371:LEU:O	1:A:378:LYS:HD2	2.08	0.54
1:A:58:LEU:HB3	1:A:98:ARG:HG3	1.89	0.54
1:A:59:PRO:O	1:A:97:PHE:HB2	2.07	0.54
1:A:293:TYR:N	1:A:293:TYR:HD2	2.05	0.54
1:A:255:THR:OG1	1:A:260:HIS:CE1	2.59	0.54
1:A:182:VAL:HG11	1:A:214:SER:HB2	1.89	0.54
1:B:373:ASN:O	1:B:374:MET:HG3	2.07	0.54
1:B:252:MET:HE2	1:B:257:VAL:HG23	1.90	0.54
1:A:83:HIS:NE2	1:A:84:ASP:OD2	2.41	0.54
1:B:253:MET:O	1:B:254:VAL:HG23	2.08	0.54
1:B:413:THR:HG22	1:B:414:VAL:N	2.23	0.54
1:A:225:GLY:HA3	1:A:231:THR:HG21	1.89	0.53
1:A:381:LEU:HD11	1:A:472:LEU:CB	2.38	0.53
1:A:403:VAL:C	1:A:404:LEU:HD22	2.28	0.53
1:B:260:HIS:HB3	1:B:268:TRP:HB2	1.91	0.53
1:A:457:ILE:CG1	1:A:458:GLY:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLU:OE2	1:A:430:GLU:HA	2.08	0.53
1:A:442:GLN:OE1	1:A:445:LYS:HB3	2.08	0.53
1:A:382:LYS:O	1:A:385:MET:N	2.39	0.53
1:A:162:PHE:O	1:A:164:LYS:N	2.41	0.53
1:B:278:ILE:HG13	1:B:279:PHE:N	2.23	0.53
1:B:413:THR:CG2	1:B:414:VAL:N	2.71	0.53
1:A:497:HIS:CD2	1:A:499:GLY:H	2.26	0.53
1:B:418:ASN:O	1:B:421:VAL:HG12	2.09	0.53
1:A:178:LYS:HB3	1:A:217:LEU:HD12	1.89	0.53
1:A:293:TYR:N	1:A:293:TYR:CD2	2.77	0.53
1:B:278:ILE:HD12	1:B:278:ILE:C	2.28	0.53
1:A:57:ASP:O	1:A:58:LEU:C	2.47	0.53
1:B:425:SER:C	1:B:427:ASP:N	2.61	0.53
1:A:386:ARG:HH21	1:A:387:LEU:HD13	1.74	0.53
1:A:74:PHE:C	1:A:76:LYS:N	2.60	0.53
1:A:352:LEU:HD21	1:A:377:LEU:HA	1.91	0.52
1:A:401:PRO:CD	1:A:411:LYS:HB2	2.39	0.52
1:A:155:TRP:CZ2	1:A:460:ARG:HG3	2.43	0.52
1:B:137:TYR:CE2	1:B:275:TRP:HB2	2.44	0.52
1:A:448:ASN:O	1:A:450:PHE:N	2.41	0.52
1:B:162:PHE:O	1:B:164:LYS:N	2.42	0.52
1:A:457:ILE:O	1:A:461:MET:HB3	2.09	0.52
1:A:393:PHE:HB3	1:A:418:ASN:HA	1.90	0.52
1:B:209:LYS:HB3	1:B:226:LEU:HD23	1.92	0.52
1:B:231:THR:O	1:B:232:GLU:C	2.46	0.52
1:B:289:ARG:HH11	1:B:300:ASP:CG	2.13	0.52
1:B:349:GLN:NE2	1:B:485:ILE:O	2.41	0.52
1:B:500:ILE:N	1:B:500:ILE:CD1	2.68	0.52
1:A:118:LEU:CD1	1:A:404:LEU:HD21	2.40	0.52
1:B:453:LEU:N	1:B:454:PRO:HD3	2.24	0.52
3:A:516:CM5:H82	3:A:517:CM5:C8	2.39	0.52
1:A:400:LYS:N	1:A:411:LYS:HD3	2.25	0.52
1:A:69:SER:C	1:A:71:LEU:N	2.63	0.52
1:B:436:ARG:C	1:B:438:GLU:N	2.61	0.52
1:A:147:LEU:HB3	2:A:520:HEM:O1D	2.09	0.52
1:B:446:LYS:HG3	1:B:447:ILE:N	2.11	0.52
1:B:425:SER:HB3	1:B:428:ASN:HB2	1.91	0.52
1:A:337:TRP:CH2	1:A:495:MET:HG2	2.45	0.52
1:A:283:LYS:HB2	1:A:284:PRO:HD3	1.92	0.52
1:B:351:ARG:HD2	1:B:376:TYR:CD1	2.45	0.52
1:B:289:ARG:HD3	1:B:302:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ARG:HG3	1:B:460:ARG:O	2.10	0.51
1:B:231:THR:O	1:B:231:THR:HG22	2.10	0.51
1:B:398:LEU:HD21	1:B:415:LEU:HD11	1.92	0.51
1:A:409:LEU:HD12	1:A:409:LEU:N	2.25	0.51
1:B:59:PRO:HB2	1:B:93:TYR:HB3	1.92	0.51
1:A:443:LYS:NZ	1:A:443:LYS:HB2	2.24	0.51
1:B:417:LEU:O	1:B:419:THR:N	2.43	0.51
1:A:347:GLN:O	1:A:350:ARG:HB2	2.10	0.51
1:B:215:ILE:HG21	1:B:328:VAL:HG12	1.93	0.51
1:A:197:ARG:HH21	1:B:295:GLN:CD	2.14	0.51
1:B:496:LEU:HD11	1:B:504:SER:HA	1.92	0.51
1:A:68:GLY:HA3	1:A:100:LYS:O	2.11	0.51
1:A:438:GLU:O	1:A:441:LEU:N	2.38	0.51
1:A:159:ARG:O	1:A:163:GLN:HB3	2.10	0.51
1:B:203:LEU:CD2	1:B:509:ILE:HD11	2.39	0.51
1:A:130:GLU:HG3	1:A:135:LYS:HZ2	1.75	0.51
1:B:215:ILE:HG23	1:B:216:CYS:N	2.26	0.51
1:A:448:ASN:ND2	1:A:450:PHE:HB2	2.26	0.51
1:B:484:ASP:HB2	1:B:514:ARG:NE	2.23	0.51
1:B:331:THR:O	1:B:334:SER:N	2.44	0.51
1:B:466:ARG:O	1:B:467:LEU:C	2.49	0.51
1:B:112:PRO:HB3	1:B:450:PHE:O	2.11	0.51
1:B:306:TYR:HD2	1:B:316:LEU:HD11	1.75	0.51
1:B:289:ARG:NH1	1:B:300:ASP:OD1	2.38	0.51
1:A:61:PRO:O	1:A:62:THR:C	2.49	0.51
1:B:457:ILE:HD12	1:B:457:ILE:N	2.24	0.51
1:A:233:GLU:C	1:A:235:ALA:N	2.65	0.51
1:A:349:GLN:NE2	1:A:485:ILE:H	2.08	0.51
1:A:283:LYS:HG2	1:A:317:TYR:CD1	2.46	0.51
3:A:516:CM5:C2	3:A:516:CM5:H18	2.22	0.50
1:A:83:HIS:CD2	1:A:84:ASP:N	2.79	0.50
1:A:329:GLU:HG2	1:A:500:ILE:HD11	1.91	0.50
1:B:410:PRO:HG2	1:B:413:THR:OG1	2.11	0.50
1:A:402:THR:O	1:A:409:LEU:N	2.39	0.50
1:B:115:LEU:HD21	1:B:417:LEU:HB3	1.93	0.50
1:B:212:PHE:CE2	1:B:226:LEU:HD13	2.47	0.50
1:B:335:LEU:HD12	1:B:339:LEU:HG	1.94	0.50
1:A:112:PRO:HB3	1:A:448:ASN:HD21	1.76	0.50
1:A:122:GLU:OE1	1:A:458:GLY:HA2	2.11	0.50
1:A:197:ARG:NH2	1:B:295:GLN:NE2	2.57	0.50
1:A:495:MET:O	1:A:496:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:O	1:B:291:GLN:HB3	2.11	0.50
1:B:338:ILE:HD12	1:B:381:LEU:HA	1.92	0.50
1:A:74:PHE:O	1:A:76:LYS:N	2.34	0.50
1:A:460:ARG:HG2	2:A:520:HEM:O2D	2.12	0.50
1:A:352:LEU:HD23	1:A:376:TYR:CD2	2.46	0.50
1:B:146:GLY:HA3	1:B:322:GLU:CD	2.32	0.50
1:B:483:TYR:CD2	1:B:511:PHE:HB3	2.46	0.50
1:B:159:ARG:O	1:B:163:GLN:HB2	2.12	0.50
1:A:216:CYS:HB3	1:A:224:PHE:CE1	2.47	0.50
3:A:517:CM5:C1	3:A:517:CM5:O22	2.59	0.50
1:A:301:PHE:O	1:A:305:ILE:HG13	2.11	0.50
1:B:374:MET:N	1:B:375:PRO:CD	2.68	0.50
1:A:128:ARG:HB3	1:A:395:THR:HG22	1.93	0.50
1:B:145:TYR:CB	1:B:150:LEU:CD1	2.88	0.50
1:A:450:PHE:HE1	1:A:457:ILE:HD11	1.76	0.50
1:B:292:ARG:O	1:B:294:SER:N	2.44	0.50
1:B:200:ILE:HG21	1:B:206:GLU:HG3	1.93	0.49
1:B:487:ALA:CB	1:B:510:ALA:N	2.75	0.49
1:A:398:LEU:HD22	1:A:402:THR:HG21	1.94	0.49
1:A:129:LEU:H	1:A:395:THR:HG21	1.77	0.49
1:B:101:LEU:HD11	1:B:104:PHE:CD1	2.47	0.49
1:B:137:TYR:C	1:B:137:TYR:CD1	2.85	0.49
1:B:233:GLU:CD	1:B:233:GLU:N	2.65	0.49
1:B:259:LEU:O	1:B:263:LEU:HB3	2.13	0.49
1:A:398:LEU:HD21	1:A:415:LEU:CD1	2.39	0.49
1:B:73:ILE:O	1:B:78:GLY:N	2.44	0.49
1:A:72:GLU:O	1:A:74:PHE:N	2.45	0.49
1:B:229:LYS:C	1:B:230:GLU:HG3	2.32	0.49
1:A:316:LEU:O	1:A:320:VAL:HG23	2.11	0.49
1:B:378:LYS:O	1:B:380:CYS:N	2.45	0.49
1:B:158:VAL:O	1:B:161:ALA:N	2.43	0.49
1:A:486:VAL:HG13	1:A:510:ALA:HB3	1.93	0.49
1:B:497:HIS:C	1:B:498:LEU:HD23	2.32	0.49
1:B:128:ARG:HA	1:B:395:THR:O	2.13	0.49
1:B:367:ARG:O	1:B:369:GLU:N	2.46	0.49
1:B:197:ARG:HH11	1:B:197:ARG:HG2	1.78	0.49
1:A:140:HIS:CD2	1:A:261:LYS:HE3	2.48	0.49
1:B:485:ILE:HD12	1:B:485:ILE:N	2.28	0.49
1:A:274:ALA:O	1:A:278:ILE:HG13	2.13	0.49
1:A:58:LEU:HB3	1:A:98:ARG:CG	2.43	0.49
1:A:95:GLN:HG3	1:A:111:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.13	0.49
1:B:386:ARG:HG2	1:B:386:ARG:O	2.12	0.49
1:B:456:GLY:HA3	2:B:520:HEM:HBA1	1.95	0.49
1:B:507:LEU:HD12	1:B:508:PRO:HD2	1.95	0.49
1:A:335:LEU:O	1:A:339:LEU:HG	2.13	0.48
1:A:386:ARG:NH2	1:A:387:LEU:HD13	2.28	0.48
1:B:269:GLN:C	1:B:271:HIS:H	2.15	0.48
1:A:95:GLN:HG3	1:A:111:SER:OG	2.13	0.48
1:A:359:VAL:HG12	1:A:360:LEU:HD12	1.95	0.48
1:B:91:LYS:HZ3	1:B:91:LYS:HB3	1.76	0.48
1:B:91:LYS:CB	1:B:91:LYS:NZ	2.75	0.48
1:A:484:ASP:C	1:A:485:ILE:HD12	2.33	0.48
1:B:55:VAL:O	1:B:57:ASP:N	2.46	0.48
1:A:455:PHE:CE1	1:A:465:ARG:HA	2.48	0.48
1:B:341:ASN:HB3	1:B:435:PHE:HE2	1.77	0.48
1:B:378:LYS:C	1:B:380:CYS:N	2.66	0.48
1:B:184:ALA:O	1:B:187:LEU:N	2.47	0.48
1:B:345:ASN:O	1:B:348:ALA:HB3	2.14	0.48
1:A:338:ILE:HG23	1:A:339:LEU:N	2.28	0.48
1:A:292:ARG:C	1:A:293:TYR:HD2	2.16	0.48
1:B:162:PHE:O	1:B:163:GLN:C	2.52	0.48
1:B:396:ARG:HG2	1:B:396:ARG:HH11	1.78	0.48
1:A:283:LYS:HG2	1:A:317:TYR:CE1	2.48	0.48
1:B:116:GLU:HB2	1:B:450:PHE:CD2	2.48	0.48
1:A:63:ASN:O	1:A:64:TRP:C	2.51	0.48
1:A:258:GLU:H	1:A:258:GLU:CD	2.17	0.48
1:A:379:ALA:HA	1:A:382:LYS:HG3	1.95	0.48
1:A:70:LEU:HD11	3:A:517:CM5:H111	1.96	0.47
1:A:164:LYS:O	1:A:164:LYS:CG	2.61	0.47
1:B:308:GLN:C	1:B:310:HIS:H	2.18	0.47
1:A:73:ILE:HD11	1:A:99:MET:HE1	1.96	0.47
1:A:181:GLU:O	1:A:184:ALA:HB3	2.14	0.47
1:B:178:LYS:HE2	1:B:217:LEU:HD13	1.95	0.47
1:A:436:ARG:O	1:A:438:GLU:N	2.47	0.47
1:B:374:MET:CE	1:B:377:LEU:HD22	2.45	0.47
1:A:277:THR:HG22	1:A:278:ILE:N	2.29	0.47
1:A:69:SER:O	1:A:71:LEU:N	2.47	0.47
1:A:329:GLU:OE2	1:A:500:ILE:HD11	2.14	0.47
1:A:191:ASP:OD1	1:A:192:GLU:N	2.47	0.47
1:B:338:ILE:CD1	1:B:476:LEU:HD11	2.44	0.47
1:B:187:LEU:O	1:B:190:MET:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LYS:NZ	1:B:267:VAL:HG11	2.29	0.47
1:A:172:ILE:HG22	1:A:470:LEU:HD22	1.97	0.47
1:B:229:LYS:O	1:B:230:GLU:CB	2.63	0.47
1:A:236:LEU:H	1:A:236:LEU:CD1	2.21	0.47
1:A:485:ILE:N	1:A:485:ILE:HD12	2.30	0.47
1:A:203:LEU:CD2	1:A:509:ILE:HD11	2.44	0.47
1:A:378:LYS:O	1:A:382:LYS:HG3	2.14	0.47
1:A:183:LEU:HD11	1:A:475:ALA:H	1.80	0.47
1:B:472:LEU:HD11	2:B:520:HEM:HBB1	1.97	0.47
1:A:497:HIS:HD2	1:A:499:GLY:H	1.61	0.47
1:B:108:HIS:HA	1:B:416:THR:HG23	1.96	0.47
1:B:442:GLN:CD	1:B:445:LYS:HD3	2.35	0.47
1:B:473:HIS:C	1:B:475:ALA:N	2.67	0.47
1:B:115:LEU:CD1	1:B:422:LEU:HD11	2.45	0.47
1:B:97:PHE:CD1	1:B:97:PHE:C	2.87	0.47
1:B:71:LEU:CG	1:B:72:GLU:H	2.16	0.47
3:A:517:CM5:H192	3:A:517:CM5:H24	1.97	0.46
1:A:312:SER:HG	1:A:315:GLU:HG3	1.79	0.46
1:A:338:ILE:HA	1:A:384:SER:OG	2.15	0.46
1:A:338:ILE:HD13	1:A:384:SER:HB2	1.98	0.46
1:B:360:LEU:CD1	1:B:366:PRO:HG3	2.46	0.46
1:A:64:TRP:HZ3	1:A:72:GLU:OE2	1.98	0.46
1:B:514:ARG:HD2	1:B:514:ARG:C	2.35	0.46
1:B:129:LEU:H	1:B:395:THR:CG2	2.28	0.46
1:B:417:LEU:HD23	1:B:417:LEU:N	2.30	0.46
1:A:388:THR:HB	1:A:495:MET:HE3	1.97	0.46
1:B:369:GLU:C	1:B:371:LEU:H	2.17	0.46
1:A:455:PHE:CD1	1:A:465:ARG:HG3	2.51	0.46
1:A:465:ARG:CZ	1:A:466:ARG:HH12	2.28	0.46
1:A:155:TRP:O	1:A:157:ARG:N	2.48	0.46
1:A:431:ASP:HB3	1:A:434:LYS:HG3	1.97	0.46
1:A:356:VAL:O	1:A:360:LEU:HB2	2.15	0.46
1:B:149:ILE:CD1	1:B:149:ILE:N	2.77	0.46
1:B:283:LYS:HB2	1:B:284:PRO:HD3	1.98	0.46
1:A:430:GLU:HA	1:A:430:GLU:OE1	2.15	0.46
1:B:265:THR:O	1:B:269:GLN:NE2	2.48	0.46
1:B:204:TYR:OH	1:B:333:ASN:HB2	2.16	0.46
1:B:286:ILE:HD12	1:B:320:VAL:HG21	1.98	0.46
1:B:314:LYS:HA	1:B:317:TYR:CD1	2.51	0.46
1:A:187:LEU:N	1:A:187:LEU:HD12	2.31	0.46
1:B:125:HIS:HD2	1:B:156:GLN:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:O	1:A:337:TRP:HD1	1.98	0.46
1:B:116:GLU:HB2	1:B:450:PHE:CE2	2.51	0.46
1:B:482:LYS:HG2	1:B:483:TYR:CD1	2.51	0.46
1:A:335:LEU:O	1:A:338:ILE:CG2	2.63	0.46
1:B:269:GLN:C	1:B:271:HIS:N	2.69	0.46
1:A:204:TYR:HD1	1:A:336:MET:SD	2.39	0.46
1:A:352:LEU:CD1	1:A:480:ILE:HD13	2.27	0.46
1:B:272:THR:O	1:B:276:ASP:HB2	2.16	0.46
1:B:352:LEU:HD23	1:B:377:LEU:HA	1.98	0.45
1:B:436:ARG:O	1:B:439:ARG:HG2	2.15	0.45
1:A:488:THR:HG22	1:A:510:ALA:HB2	1.98	0.45
1:A:116:GLU:OE1	1:A:120:ARG:NH1	2.47	0.45
1:B:251:LYS:C	1:B:253:MET:H	2.18	0.45
3:A:516:CM5:H15	3:A:516:CM5:O22	2.15	0.45
1:B:121:THR:O	1:B:121:THR:HG23	2.15	0.45
1:B:351:ARG:HG2	1:B:351:ARG:O	2.15	0.45
1:B:146:GLY:H	1:B:149:ILE:CD1	2.22	0.45
1:A:74:PHE:CD1	1:A:78:GLY:HA2	2.51	0.45
1:B:279:PHE:O	1:B:283:LYS:HE3	2.16	0.45
1:A:66:LEU:CD2	1:A:66:LEU:N	2.78	0.45
1:A:365:THR:HG23	1:A:478:TRP:CZ2	2.51	0.45
1:B:344:ARG:HH12	1:B:490:ASN:HA	1.81	0.45
1:A:321:THR:O	1:A:325:LEU:HG	2.16	0.45
3:A:516:CM5:H24	3:A:516:CM5:O20	2.16	0.45
1:B:65:PRO:C	1:B:67:LEU:H	2.18	0.45
1:A:203:LEU:O	1:A:206:GLU:HB2	2.16	0.45
1:B:466:ARG:HG3	1:B:466:ARG:HH11	1.81	0.45
1:A:272:THR:HG22	1:A:276:ASP:OD1	2.17	0.45
1:B:220:TYR:CD2	1:B:285:CYS:CB	2.99	0.45
1:B:410:PRO:O	1:B:411:LYS:C	2.55	0.45
1:B:251:LYS:NZ	1:B:267:VAL:CG1	2.79	0.45
1:B:178:LYS:HB3	1:B:217:LEU:HD13	1.98	0.45
1:A:187:LEU:O	1:A:190:MET:HB2	2.17	0.45
1:A:336:MET:CG	1:A:507:LEU:HD22	2.47	0.45
1:B:383:GLU:O	1:B:387:LEU:HD23	2.17	0.45
1:B:262:ARG:C	1:B:264:ASN:H	2.19	0.45
1:B:466:ARG:O	1:B:469:GLU:N	2.50	0.45
1:B:436:ARG:O	1:B:438:GLU:N	2.50	0.45
1:A:438:GLU:O	1:A:440:TRP:N	2.50	0.45
1:A:277:THR:O	1:A:280:LYS:N	2.46	0.45
1:A:386:ARG:NH2	1:A:432:SER:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:PHE:HB3	1:A:283:LYS:HZ3	1.82	0.45
1:B:138:ARG:O	1:B:142:ASN:N	2.50	0.45
1:A:180:ASN:OD1	1:A:474:LEU:HD13	2.17	0.44
1:A:129:LEU:HD11	1:A:414:VAL:CG1	2.47	0.44
1:A:146:GLY:C	1:A:148:MET:H	2.21	0.44
1:A:236:LEU:N	1:A:236:LEU:HD13	2.24	0.44
1:B:129:LEU:H	1:B:395:THR:HG23	1.82	0.44
1:B:91:LYS:HZ2	1:B:91:LYS:HB3	1.79	0.44
1:B:90:HIS:CE1	1:B:110:GLY:HA3	2.52	0.44
1:A:162:PHE:O	1:A:163:GLN:C	2.55	0.44
1:B:374:MET:HE1	1:B:377:LEU:HD22	1.99	0.44
1:B:192:GLU:CB	1:B:193:LEU:HD13	2.47	0.44
1:A:455:PHE:CG	1:A:465:ARG:HG3	2.52	0.44
1:A:62:THR:O	1:A:64:TRP:CE3	2.70	0.44
1:B:369:GLU:C	1:B:371:LEU:N	2.70	0.44
1:A:407:TYR:CD1	1:A:407:TYR:N	2.85	0.44
1:A:276:ASP:O	1:A:280:LYS:HG3	2.16	0.44
1:A:132:LYS:HB3	1:A:132:LYS:NZ	2.32	0.44
3:A:516:CM5:H82	3:A:517:CM5:H81	2.00	0.44
1:A:366:PRO:HG2	1:A:477:CYS:HB3	2.00	0.44
1:A:509:ILE:O	1:A:509:ILE:HG13	2.17	0.44
1:A:391:VAL:HA	1:A:392:PRO:HD3	1.82	0.44
1:B:426:GLU:HG2	1:B:432:SER:OG	2.17	0.44
1:A:164:LYS:O	1:A:164:LYS:CE	2.60	0.44
1:A:114:LEU:HA	1:A:117:ALA:HB3	1.99	0.44
1:A:155:TRP:CE3	1:A:156:GLN:N	2.85	0.44
1:B:251:LYS:O	1:B:253:MET:N	2.47	0.44
1:A:162:PHE:C	1:A:164:LYS:N	2.69	0.44
1:A:163:GLN:HA	1:A:463:ILE:HD11	2.00	0.44
1:A:463:ILE:HG12	1:A:463:ILE:O	2.18	0.44
1:B:189:ARG:HE	1:B:227:LEU:C	2.21	0.44
1:A:197:ARG:HG3	1:A:197:ARG:NH1	2.30	0.44
1:B:100:LYS:CB	1:B:100:LYS:NZ	2.80	0.44
1:A:158:VAL:O	1:A:159:ARG:C	2.56	0.44
1:B:70:LEU:HD12	1:B:73:ILE:CG2	2.48	0.44
1:A:64:TRP:HA	1:A:65:PRO:HD3	1.82	0.44
1:A:69:SER:HB2	1:A:99:MET:HE2	1.99	0.44
1:B:215:ILE:CG1	1:B:219:LEU:HD22	2.40	0.44
1:B:410:PRO:HG2	1:B:413:THR:HG1	1.83	0.44
1:B:89:TYR:HB3	1:B:97:PHE:CE2	2.53	0.44
1:A:355:GLU:OE2	1:A:374:MET:CA	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:O	1:B:121:THR:O	2.36	0.43
1:B:343:SER:OG	1:B:509:ILE:HG22	2.18	0.43
1:A:195:ASP:CG	1:A:196:GLU:H	2.20	0.43
1:A:159:ARG:O	1:A:160:SER:C	2.57	0.43
1:B:159:ARG:NH1	1:B:163:GLN:HE22	2.16	0.43
1:B:396:ARG:HH22	2:B:520:HEM:CGA	2.30	0.43
1:B:229:LYS:O	1:B:230:GLU:CG	2.66	0.43
1:B:64:TRP:CE2	1:B:71:LEU:HD13	2.54	0.43
1:B:68:GLY:C	1:B:70:LEU:H	2.22	0.43
1:B:396:ARG:NH1	1:B:396:ARG:HG2	2.34	0.43
1:B:436:ARG:NH1	1:B:436:ARG:HG2	2.33	0.43
1:A:333:ASN:O	1:A:337:TRP:CD1	2.71	0.43
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.91	0.43
1:A:382:LYS:O	1:A:383:GLU:C	2.56	0.43
1:A:383:GLU:HB2	1:A:440:TRP:HE1	1.83	0.43
1:B:338:ILE:HG12	1:B:342:LEU:HD22	1.99	0.43
1:B:262:ARG:C	1:B:264:ASN:N	2.71	0.43
1:A:466:ARG:O	1:A:468:ALA:N	2.51	0.43
1:A:491:GLU:HA	1:A:492:PRO:HD3	1.94	0.43
1:B:229:LYS:N	1:B:229:LYS:CD	2.81	0.43
1:A:333:ASN:ND2	1:A:502:VAL:HG12	2.32	0.43
1:A:424:SER:O	1:A:426:GLU:N	2.52	0.43
1:B:443:LYS:O	1:B:443:LYS:HG3	2.18	0.43
1:A:352:LEU:CD2	1:A:376:TYR:HD2	2.31	0.43
1:B:376:TYR:O	1:B:380:CYS:HB2	2.18	0.43
1:A:58:LEU:HD23	1:A:58:LEU:N	2.34	0.43
1:B:187:LEU:HA	1:B:187:LEU:HD12	1.83	0.43
1:B:476:LEU:O	1:B:477:CYS:C	2.57	0.43
1:A:245:MET:O	1:A:245:MET:SD	2.77	0.43
1:A:409:LEU:HA	1:A:410:PRO:HD3	1.63	0.43
1:B:227:LEU:O	1:B:228:GLN:C	2.56	0.43
1:B:229:LYS:C	1:B:231:THR:H	2.21	0.43
1:A:202:ASP:HB3	1:A:205:SER:HB3	2.00	0.43
1:B:377:LEU:CD1	1:B:476:LEU:HD12	2.49	0.43
1:A:57:ASP:O	1:A:59:PRO:N	2.52	0.43
1:A:116:GLU:OE1	1:A:120:ARG:NE	2.51	0.43
1:B:122:GLU:O	1:B:123:SER:O	2.37	0.43
1:B:352:LEU:HD21	1:B:377:LEU:HA	2.01	0.43
1:B:447:ILE:CG1	1:B:447:ILE:O	2.66	0.43
1:A:465:ARG:NH1	1:A:465:ARG:HG2	2.33	0.43
1:B:125:HIS:HA	1:B:155:TRP:HZ3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD21	1:B:405:GLY:HA2	2.00	0.43
1:B:507:LEU:HA	1:B:507:LEU:HD12	1.83	0.43
1:A:233:GLU:O	1:A:236:LEU:HD13	2.19	0.43
1:B:304:ASP:O	1:B:305:ILE:C	2.57	0.43
1:A:76:LYS:HD3	1:A:85:THR:HG22	1.99	0.43
1:A:491:GLU:OE2	1:B:313:LYS:HG3	2.18	0.43
1:A:207:LEU:HA	1:A:207:LEU:HD12	1.77	0.43
1:B:72:GLU:O	1:B:74:PHE:N	2.52	0.43
1:A:202:ASP:O	1:A:206:GLU:HG2	2.19	0.43
1:A:405:GLY:C	1:A:407:TYR:N	2.72	0.43
1:B:426:GLU:OE1	1:B:431:ASP:HA	2.19	0.43
1:A:355:GLU:OE2	1:A:374:MET:HA	2.18	0.43
1:A:145:TYR:HB2	1:A:150:LEU:CD1	2.46	0.42
1:A:401:PRO:HD3	1:A:411:LYS:HB2	2.00	0.42
1:B:467:LEU:CG	1:B:471:GLN:HE21	2.27	0.42
1:B:419:THR:HG22	1:B:420:GLN:N	2.34	0.42
1:B:456:GLY:C	1:B:457:ILE:HD12	2.39	0.42
1:A:286:ILE:CD1	1:A:320:VAL:HG21	2.49	0.42
1:A:465:ARG:HH21	1:A:466:ARG:HH12	1.58	0.42
1:B:126:PRO:HG2	1:B:460:ARG:CB	2.49	0.42
1:B:245:MET:O	1:B:249:PHE:HB3	2.19	0.42
1:A:420:GLN:O	1:A:421:VAL:C	2.57	0.42
1:B:291:GLN:HB2	1:B:291:GLN:HE21	1.58	0.42
1:A:86:LEU:HD22	1:A:108:HIS:CD2	2.53	0.42
1:A:212:PHE:O	1:A:215:ILE:HG22	2.19	0.42
1:B:193:LEU:H	1:B:193:LEU:HD22	1.85	0.42
1:B:487:ALA:CB	1:B:509:ILE:HA	2.49	0.42
1:B:229:LYS:O	1:B:230:GLU:HG3	2.18	0.42
1:B:331:THR:O	1:B:332:ALA:C	2.56	0.42
1:B:480:ILE:CG2	1:B:481:GLN:N	2.83	0.42
1:B:343:SER:CB	1:B:485:ILE:HG22	2.33	0.42
1:B:455:PHE:CG	1:B:465:ARG:HG3	2.54	0.42
1:A:178:LYS:HD3	1:A:217:LEU:CD1	2.45	0.42
1:A:125:HIS:ND1	1:A:152:GLY:HA2	2.34	0.42
1:A:338:ILE:HG23	1:A:339:LEU:H	1.85	0.42
1:A:176:ASP:OD2	1:A:368:ALA:HB3	2.19	0.42
1:A:491:GLU:O	1:A:505:ARG:NH2	2.53	0.42
1:B:383:GLU:OE1	1:B:440:TRP:NE1	2.45	0.42
1:A:292:ARG:HE	1:A:293:TYR:HE2	1.68	0.42
1:A:223:ARG:NH2	1:A:223:ARG:HG3	2.33	0.42
1:A:438:GLU:CD	1:A:438:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ILE:O	1:B:509:ILE:HD12	2.20	0.42
1:A:116:GLU:O	1:A:118:LEU:N	2.49	0.42
1:A:67:LEU:N	1:A:67:LEU:HD22	2.35	0.42
1:B:178:LYS:NZ	1:B:221:GLU:HG2	2.35	0.42
1:A:173:MET:O	1:A:176:ASP:HB2	2.19	0.42
1:A:72:GLU:C	1:A:74:PHE:N	2.73	0.42
1:A:100:LYS:HA	1:A:104:PHE:O	2.19	0.42
1:A:183:LEU:CD1	1:A:474:LEU:HB3	2.50	0.41
1:A:72:GLU:O	1:A:73:ILE:C	2.58	0.41
1:A:187:LEU:CD2	1:A:478:TRP:HB3	2.49	0.41
1:B:374:MET:HB3	1:B:377:LEU:HB3	2.01	0.41
1:B:487:ALA:HB1	1:B:488:THR:H	1.68	0.41
1:A:240:THR:O	1:A:241:ALA:C	2.58	0.41
1:A:289:ARG:HE	1:A:300:ASP:CG	2.22	0.41
1:B:435:PHE:CE1	1:B:437:PRO:HG3	2.52	0.41
1:A:201:PRO:O	1:A:202:ASP:HB2	2.20	0.41
1:A:187:LEU:O	1:A:190:MET:N	2.53	0.41
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.89	0.41
1:A:175:LEU:HA	1:A:175:LEU:HD13	1.76	0.41
1:A:309:ASP:O	1:A:310:HIS:O	2.37	0.41
1:B:193:LEU:O	1:B:200:ILE:HA	2.19	0.41
1:A:245:MET:HA	1:A:248:THR:CG2	2.50	0.41
1:A:58:LEU:HD23	1:A:58:LEU:H	1.85	0.41
1:B:128:ARG:HH12	2:B:520:HEM:HAD2	1.84	0.41
1:B:278:ILE:HD11	1:B:321:THR:CG2	2.49	0.41
1:B:131:ILE:HD12	1:B:134:TRP:CD2	2.55	0.41
1:A:189:ARG:NH1	1:A:206:GLU:OE2	2.53	0.41
1:A:130:GLU:OE2	1:A:135:LYS:NZ	2.50	0.41
1:B:199:ARG:CZ	1:B:203:LEU:HB2	2.51	0.41
1:B:509:ILE:C	1:B:509:ILE:HD12	2.40	0.41
1:B:155:TRP:CG	1:B:460:ARG:NH2	2.88	0.41
1:B:175:LEU:CD1	1:B:218:VAL:HG13	2.49	0.41
1:B:197:ARG:HG2	1:B:197:ARG:NH1	2.35	0.41
1:B:489:ASP:O	1:B:490:ASN:OD1	2.37	0.41
1:A:132:LYS:N	1:A:133:PRO:CD	2.83	0.41
1:A:464:GLY:O	1:A:465:ARG:C	2.58	0.41
1:B:435:PHE:CD1	1:B:437:PRO:HD3	2.55	0.41
1:B:392:PRO:O	1:B:393:PHE:HB3	2.20	0.41
1:B:377:LEU:HD12	1:B:476:LEU:HD12	2.02	0.41
1:A:140:HIS:CD2	1:A:268:TRP:HZ2	2.38	0.41
1:B:335:LEU:O	1:B:338:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:HD23	1:B:155:TRP:HA	2.01	0.41
1:A:146:GLY:C	1:A:148:MET:N	2.73	0.41
1:A:424:SER:HA	1:A:432:SER:HB2	2.03	0.41
1:B:292:ARG:NH2	1:B:293:TYR:OH	2.54	0.41
1:B:72:GLU:C	1:B:74:PHE:N	2.72	0.41
1:B:91:LYS:CB	1:B:91:LYS:HZ2	2.34	0.41
1:A:396:ARG:HD3	1:A:396:ARG:HA	1.90	0.41
1:B:392:PRO:HD3	1:B:501:LEU:HG	2.03	0.41
1:B:373:ASN:O	1:B:374:MET:CB	2.69	0.41
1:B:150:LEU:HB3	1:B:155:TRP:HB2	2.03	0.41
1:A:232:GLU:HB3	1:A:233:GLU:H	1.38	0.41
1:A:453:LEU:CD2	1:A:457:ILE:HB	2.51	0.41
1:A:217:LEU:O	1:A:221:GLU:HA	2.21	0.41
1:A:221:GLU:HG3	1:A:289:ARG:NH2	2.36	0.41
1:A:127:GLN:HG3	1:A:397:THR:HB	2.02	0.41
1:B:159:ARG:HH11	1:B:163:GLN:NE2	2.16	0.41
1:B:301:PHE:O	1:B:305:ILE:HG12	2.21	0.41
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.89	0.41
1:B:378:LYS:C	1:B:380:CYS:H	2.23	0.41
1:B:378:LYS:O	1:B:379:ALA:C	2.60	0.41
1:A:180:ASN:HA	1:A:183:LEU:HB2	2.03	0.41
1:A:233:GLU:C	1:A:235:ALA:H	2.22	0.41
1:A:424:SER:HA	1:A:432:SER:CB	2.51	0.41
1:A:139:ASP:OD1	1:A:145:TYR:OH	2.34	0.40
1:A:145:TYR:HB3	1:A:150:LEU:HD13	2.02	0.40
3:A:516:CM5:C2	3:A:516:CM5:C18	2.88	0.40
1:B:67:LEU:O	1:B:67:LEU:HD13	2.21	0.40
1:A:111:SER:HA	1:A:112:PRO:HD3	1.90	0.40
1:A:292:ARG:HG2	1:A:293:TYR:CE2	2.57	0.40
1:B:129:LEU:HB2	1:B:395:THR:HG21	2.03	0.40
1:B:328:VAL:O	1:B:329:GLU:C	2.60	0.40
1:B:193:LEU:N	1:B:193:LEU:HD13	2.36	0.40
1:B:389:PRO:HG3	1:B:420:GLN:CB	2.47	0.40
1:A:474:LEU:O	1:A:475:ALA:C	2.57	0.40
1:B:69:SER:C	1:B:71:LEU:HD23	2.42	0.40
1:B:182:VAL:HA	1:B:223:ARG:HH22	1.86	0.40
1:B:158:VAL:O	1:B:159:ARG:C	2.60	0.40
1:B:212:PHE:CD2	1:B:226:LEU:HD13	2.57	0.40
1:B:497:HIS:O	1:B:498:LEU:HD23	2.21	0.40
1:B:250:GLY:O	1:B:253:MET:HB2	2.22	0.40
1:A:360:LEU:N	1:A:360:LEU:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.85	0.40
1:A:443:LYS:HB2	1:A:443:LYS:HZ3	1.85	0.40
1:B:217:LEU:O	1:B:221:GLU:HA	2.22	0.40
1:B:204:TYR:HD1	1:B:336:MET:SD	2.44	0.40
1:A:222:LYS:HE3	1:A:222:LYS:HB2	1.96	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	459/482 (95%)	341 (74%)	66 (14%)	52 (11%)	0	1
1	B	460/482 (95%)	340 (74%)	79 (17%)	41 (9%)	1	2
All	All	919/964 (95%)	681 (74%)	145 (16%)	93 (10%)	1	1

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	64	TRP
1	A	66	LEU
1	A	92	LYS
1	A	147	LEU
1	A	165	LYS
1	A	176	ASP
1	A	310	HIS
1	A	328	VAL
1	A	369	GLU
1	A	382	LYS
1	A	383	GLU
1	A	421	VAL

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Mol	Chain	Res	Type
1	A	425	SER
1	A	427	ASP
1	A	465	ARG
1	B	55	VAL
1	B	123	SER
1	B	163	GLN
1	B	184	ALA
1	B	201	PRO
1	B	225	GLY
1	B	229	LYS
1	B	254	VAL
1	B	265	THR
1	B	369	GLU
1	B	374	MET
1	B	406	GLU
1	A	156	GLN
1	A	163	GLN
1	A	196	GLU
1	A	229	LYS
1	A	309	ASP
1	A	410	PRO
1	A	411	LYS
1	A	439	ARG
1	A	445	LYS
1	A	466	ARG
1	A	467	LEU
1	A	476	LEU
1	B	56	THR
1	B	124	ALA
1	B	232	GLU
1	B	235	ALA
1	B	252	MET
1	B	293	TYR
1	B	328	VAL
1	B	386	ARG
1	B	432	SER
1	B	442	GLN
1	B	446	LYS
1	B	466	ARG
1	A	76	LYS
1	A	95	GLN
1	A	117	ALA

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Mol	Chain	Res	Type
1	A	159	ARG
1	A	299	ALA
1	A	442	GLN
1	A	474	LEU
1	B	140	HIS
1	B	164	LYS
1	B	200	ILE
1	B	309	ASP
1	B	368	ALA
1	B	425	SER
1	B	445	LYS
1	B	490	ASN
1	A	70	LEU
1	A	73	ILE
1	A	93	TYR
1	A	184	ALA
1	A	256	PRO
1	A	362	ASP
1	A	420	GLN
1	A	449	PRO
1	B	379	ALA
1	B	439	ARG
1	B	477	CYS
1	A	75	TRP
1	A	447	ILE
1	A	481	GLN
1	A	492	PRO
1	B	136	ALA
1	B	292	ARG
1	B	362	ASP
1	B	447	ILE
1	A	426	GLU
1	B	73	ILE
1	A	437	PRO
1	B	513	PRO
1	A	55	VAL
1	A	400	LYS
1	A	457	ILE



### 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	415/433 (96%)	369 (89%)	46 (11%)	8	23
1	B	416/433 (96%)	353 (85%)	63 (15%)	3	10
All	All	831/866 (96%)	722 (87%)	109 (13%)	5	15

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	75	TRP
1	A	98	ARG
1	A	109	LEU
1	A	150	LEU
1	A	164	LYS
1	A	169	PRO
1	A	175	LEU
1	A	196	GLU
1	A	207	LEU
1	A	208	ASN
1	A	217	LEU
1	A	233	GLU
1	A	236	LEU
1	A	237	THR
1	A	248	THR
1	A	276	ASP
1	A	293	TYR
1	A	304	ASP
1	A	309	ASP
1	A	330	THR
1	A	335	LEU
1	A	342	LEU
1	A	343	SER
1	A	350	ARG
1	A	352	LEU
1	A	353	LEU

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Mol	Chain	Res	Type
1	A	362	ASP
1	A	369	GLU
1	A	370	ASP
1	A	380	CYS
1	A	386	ARG
1	A	390	SER
1	A	393	PHE
1	A	397	THR
1	A	407	TYR
1	A	419	THR
1	A	428	ASN
1	A	442	GLN
1	A	443	LYS
1	A	445	LYS
1	A	474	LEU
1	A	477	CYS
1	A	481	GLN
1	A	492	PRO
1	A	500	ILE
1	B	55	VAL
1	B	56	THR
1	B	64	TRP
1	B	71	LEU
1	B	101	LEU
1	B	113	SER
1	B	120	ARG
1	B	127	GLN
1	B	128	ARG
1	B	141	ARG
1	B	149	ILE
1	B	150	LEU
1	B	159	ARG
1	B	193	LEU
1	B	199	ARG
1	B	201	PRO
1	B	207	LEU
1	B	217	LEU
1	B	219	LEU
1	B	226	LEU
1	B	229	LYS
1	B	232	GLU
1	B	233	GLU

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Mol	Chain	Res	Type
1	B	245	MET
1	B	248	THR
1	B	249	PHE
1	B	259	LEU
1	B	263	LEU
1	B	264	ASN
1	B	276	ASP
1	B	278	ILE
1	B	280	LYS
1	B	291	GLN
1	B	301	PHE
1	B	310	HIS
1	B	323	LEU
1	B	328	VAL
1	B	335	LEU
1	B	342	LEU
1	B	350	ARG
1	B	362	ASP
1	B	369	GLU
1	B	380	CYS
1	B	386	ARG
1	B	402	THR
1	B	403	VAL
1	B	417	LEU
1	B	419	THR
1	B	420	GLN
1	B	426	GLU
1	B	430	GLU
1	B	435	PHE
1	B	445	LYS
1	B	447	ILE
1	B	453	LEU
1	B	459	LYS
1	B	463	ILE
1	B	488	THR
1	B	497	HIS
1	B	500	ILE
1	B	505	ARG
1	B	506	GLU
1	B	508	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	82	GLN
1	A	95	GLN
1	A	127	GLN
1	A	140	HIS
1	A	208	ASN
1	A	260	HIS
1	A	269	GLN
1	A	288	ASN
1	A	341	ASN
1	A	347	GLN
1	A	349	GLN
1	A	354	GLN
1	A	490	ASN
1	A	497	HIS
1	B	90	HIS
1	B	95	GLN
1	B	125	HIS
1	B	127	GLN
1	B	269	GLN
1	B	291	GLN
1	B	295	GLN
1	B	428	ASN
1	B	452	HIS
1	B	471	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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
3	CM5	A	516	-	36,36,36	0.56	1 (2%)	49,49,49	2.40	15 (30%)
3	CM5	A	517	-	36,36,36	0.56	1 (2%)	49,49,49	1.09	4 (8%)
2	HEM	A	520	1	30,50,50	3.64	12 (40%)	24,82,82	2.70	10 (41%)
2	HEM	B	520	1	30,50,50	3.63	12 (40%)	24,82,82	2.58	9 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CM5	A	516	-	5/5/11/11	0/17/65/65	0/3/3/3
3	CM5	A	517	-	5/5/11/11	0/17/65/65	0/3/3/3
2	HEM	A	520	1	-	0/10/54/54	0/0/8/8
2	HEM	B	520	1	-	0/10/54/54	0/0/8/8

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	520	HEM	C3B-C4B	-9.85	1.43	1.51
2	B	520	HEM	C3B-C4B	-9.74	1.43	1.51
2	B	520	HEM	C3C-CAC	-8.26	1.35	1.51
2	B	520	HEM	C3D-C4D	-7.96	1.41	1.51
2	A	520	HEM	C3D-C4D	-7.82	1.41	1.51
2	A	520	HEM	C2C-C1C	-7.53	1.38	1.52
2	A	520	HEM	C3C-CAC	-7.46	1.37	1.51
2	B	520	HEM	C2C-C1C	-6.78	1.39	1.52
2	B	520	HEM	C2D-C3D	-6.13	1.36	1.54
2	A	520	HEM	C2D-C3D	-5.84	1.37	1.54
2	B	520	HEM	C3B-CAB	-4.23	1.43	1.51
2	A	520	HEM	C2B-C1B	-3.81	1.39	1.51
2	A	520	HEM	C2D-C1D	-3.73	1.39	1.51
2	B	520	HEM	C2D-C1D	-3.67	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	520	HEM	C3B-CAB	-3.52	1.44	1.51
2	B	520	HEM	C2B-C1B	-2.89	1.42	1.51
2	B	520	HEM	C1C-NC	-2.52	1.32	1.36
2	A	520	HEM	FE-NC	2.10	2.04	1.95
2	B	520	HEM	CBC-CAC	2.19	1.42	1.29
3	A	516	CM5	O12-C13	2.24	1.44	1.40
3	A	517	CM5	O12-C13	2.25	1.44	1.40
2	A	520	HEM	CBC-CAC	2.28	1.42	1.29
2	B	520	HEM	FE-NC	2.40	2.05	1.95
2	A	520	HEM	CMA-C3A	3.01	1.57	1.51
2	B	520	HEM	CBB-CAB	3.46	1.49	1.29
2	A	520	HEM	CBB-CAB	3.57	1.49	1.29

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	516	CM5	C24-O23-C16	-9.00	94.50	118.01
3	A	516	CM5	C13-C18-C17	-5.09	99.94	109.97
3	A	516	CM5	C28-C27-C26	-4.27	102.76	110.20
3	A	516	CM5	C3-C4-C5	-2.79	103.74	113.66
3	A	516	CM5	C5-C6-C11	-2.68	106.43	112.10
3	A	517	CM5	C24-O23-C16	-2.65	111.08	118.01
3	A	517	CM5	C13-O14-C15	-2.20	109.47	113.75
3	A	517	CM5	C30-C26-C27	-2.09	107.87	113.02
2	A	520	HEM	C2D-C3D-C4D	2.05	104.98	101.50
2	A	520	HEM	CBA-CAA-C2A	2.07	116.24	112.53
3	A	516	CM5	C1-O12-C13	2.13	117.67	113.94
3	A	516	CM5	O21-C17-C18	2.20	115.28	110.34
2	B	520	HEM	C1D-CHD-C4C	2.20	129.50	125.82
2	B	520	HEM	CMD-C2D-C3D	2.40	124.94	114.35
3	A	516	CM5	C29-C28-C27	2.40	115.28	110.79
2	A	520	HEM	CMD-C2D-C3D	2.56	125.67	114.35
2	A	520	HEM	C4B-CHC-C1C	2.57	130.12	125.82
3	A	516	CM5	O12-C13-C18	2.68	111.42	108.04
3	A	516	CM5	O23-C24-C29	2.84	115.02	108.10
2	B	520	HEM	C4B-CHC-C1C	2.91	130.68	125.82
3	A	516	CM5	O14-C13-O12	3.37	118.17	110.05
3	A	516	CM5	O25-C26-C30	3.47	115.12	106.36
3	A	516	CM5	C17-C16-C15	3.50	118.74	110.84
3	A	517	CM5	O12-C13-C18	3.57	112.54	108.04
2	A	520	HEM	C3B-CAB-CBB	4.01	130.61	124.46
2	B	520	HEM	C3B-CAB-CBB	4.01	130.61	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	516	CM5	O23-C16-C15	4.02	119.89	109.32
2	B	520	HEM	CAD-C3D-C2D	4.15	125.15	113.22
2	A	520	HEM	C3C-CAC-CBC	4.18	130.87	124.46
2	A	520	HEM	CAD-C3D-C4D	4.26	127.50	112.47
2	B	520	HEM	CMC-C2C-C3C	4.40	127.51	116.53
2	B	520	HEM	C3C-CAC-CBC	4.60	131.51	124.46
2	A	520	HEM	CMC-C2C-C3C	4.63	128.08	116.53
2	A	520	HEM	CAD-C3D-C2D	4.97	127.52	113.22
3	A	516	CM5	O25-C24-C29	5.02	120.58	110.28
2	B	520	HEM	CAD-C3D-C4D	5.09	130.41	112.47
2	B	520	HEM	CMB-C2B-C3B	5.17	129.44	116.53
2	A	520	HEM	CMB-C2B-C3B	6.17	131.92	116.53

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	517	CM5	C15
3	A	517	CM5	C18
3	A	517	CM5	C16
3	A	517	CM5	C29
3	A	517	CM5	C24
3	A	516	CM5	C15
3	A	516	CM5	C18
3	A	516	CM5	C16
3	A	516	CM5	C29
3	A	516	CM5	C24

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	516	CM5	16	0
3	A	517	CM5	23	0
2	A	520	HEM	3	0
2	B	520	HEM	5	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	461/482 (95%)	0.06	11 (2%)	62 50	29, 73, 117, 182	0
1	B	462/482 (95%)	0.12	15 (3%)	51 39	28, 74, 120, 184	0
All	All	923/964 (95%)	0.09	26 (2%)	56 44	28, 74, 119, 184	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	5.3
1	A	447	ILE	5.2
1	A	230	GLU	3.8
1	B	75	TRP	3.7
1	A	231	THR	3.3
1	A	75	TRP	3.1
1	B	123	SER	3.1
1	B	231	THR	3.1
1	B	362	ASP	2.9
1	A	226	LEU	2.9
1	B	262	ARG	2.9
1	B	257	VAL	2.8
1	B	263	LEU	2.6
1	A	442	GLN	2.5
1	B	370	ASP	2.4
1	B	259	LEU	2.4
1	B	291	GLN	2.4
1	A	446	LYS	2.2
1	B	256	PRO	2.2
1	B	132	LYS	2.2
1	B	427	ASP	2.2
1	B	258	GLU	2.1
1	B	261	LYS	2.1
1	A	428	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	430	GLU	2.1
1	A	57	ASP	2.1

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CM5	A	516	34/34	0.74	0.32	3.02	78,92,101,102	0
3	CM5	A	517	34/34	0.75	0.32	2.94	78,89,96,100	0
2	HEM	B	520	43/43	0.96	0.21	-0.54	26,32,39,72	0
2	HEM	A	520	43/43	0.96	0.20	-0.98	25,37,50,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.