



Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 05:31 PM EDT

PDB ID : 2BCC
Title : STIGMATELLIN-BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on : 1998-09-18
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

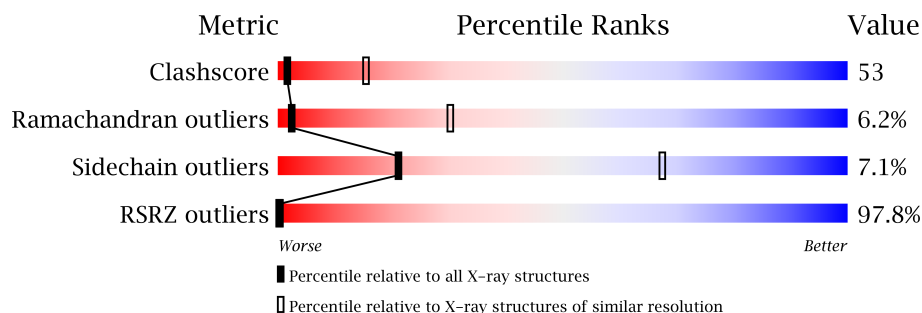
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	422	
3	C	380	
4	D	241	
5	E	196	
6	F	109	
7	G	81	
8	H	78	
9	I	33	
10	J	62	

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

Mol	Type	Chain	Res	Geometry	Electron density
11	BOG	D	242	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
12	HEM	C	381	-	X
12	HEM	C	382	-	X
12	HEM	D	243	-	X
13	FES	E	197	-	X
14	U10	C	383	-	X
15	PEE	C	384	-	X
15	PEE	E	198	-	X
16	SIG	C	385	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 15754 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			2994	1878	518	591	7			

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3002	2013	473	504	12			

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1899	1214	326	345	14			

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1512	953	266	285	8			

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			875	557	153	162	3			

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

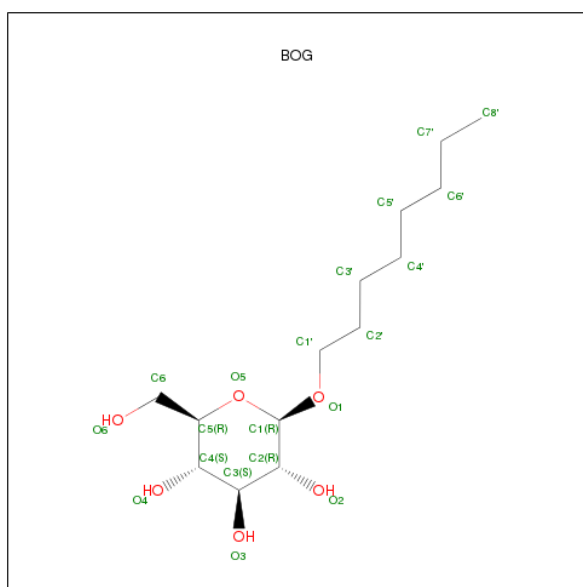
- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

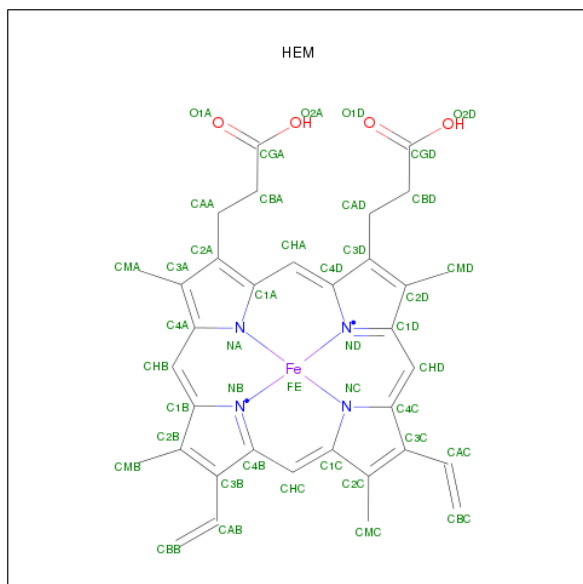
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

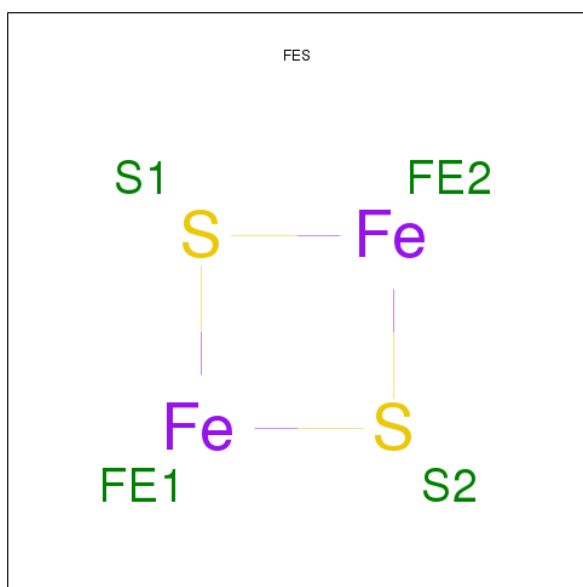
- Molecule 11 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			20	14	6		

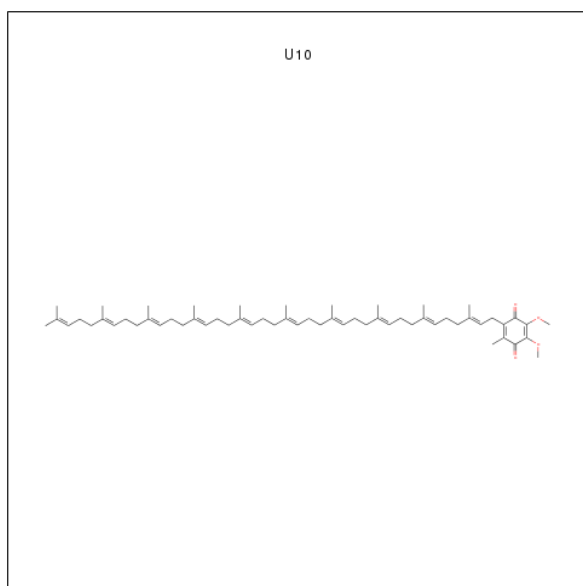
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





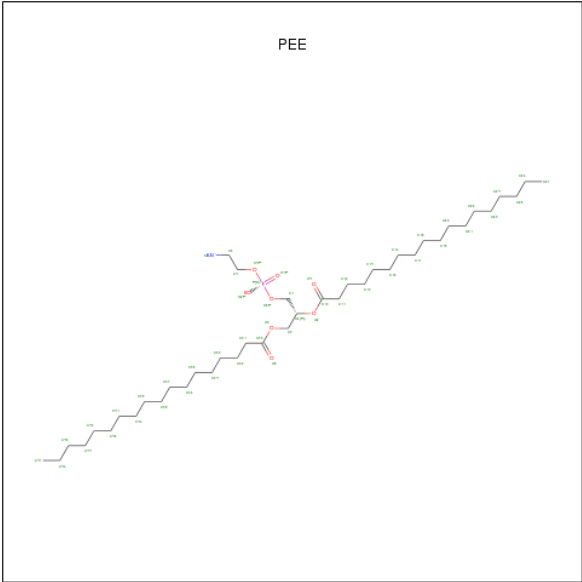
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



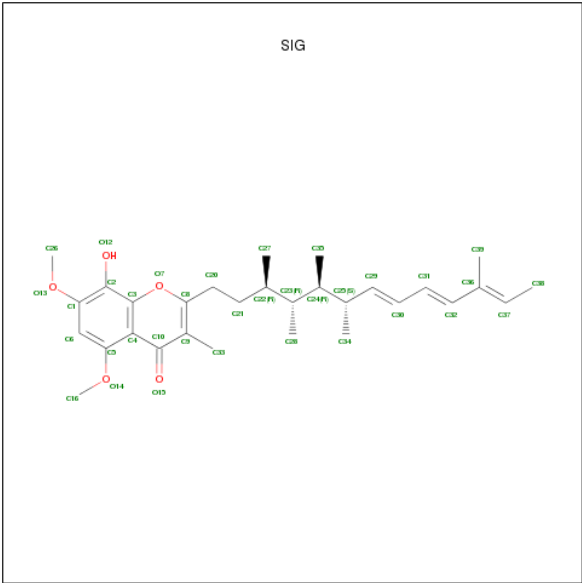
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 15 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 16 is STIGMATELLIN (three-letter code: SIG) (formula: C₃₀H₄₂O₅).

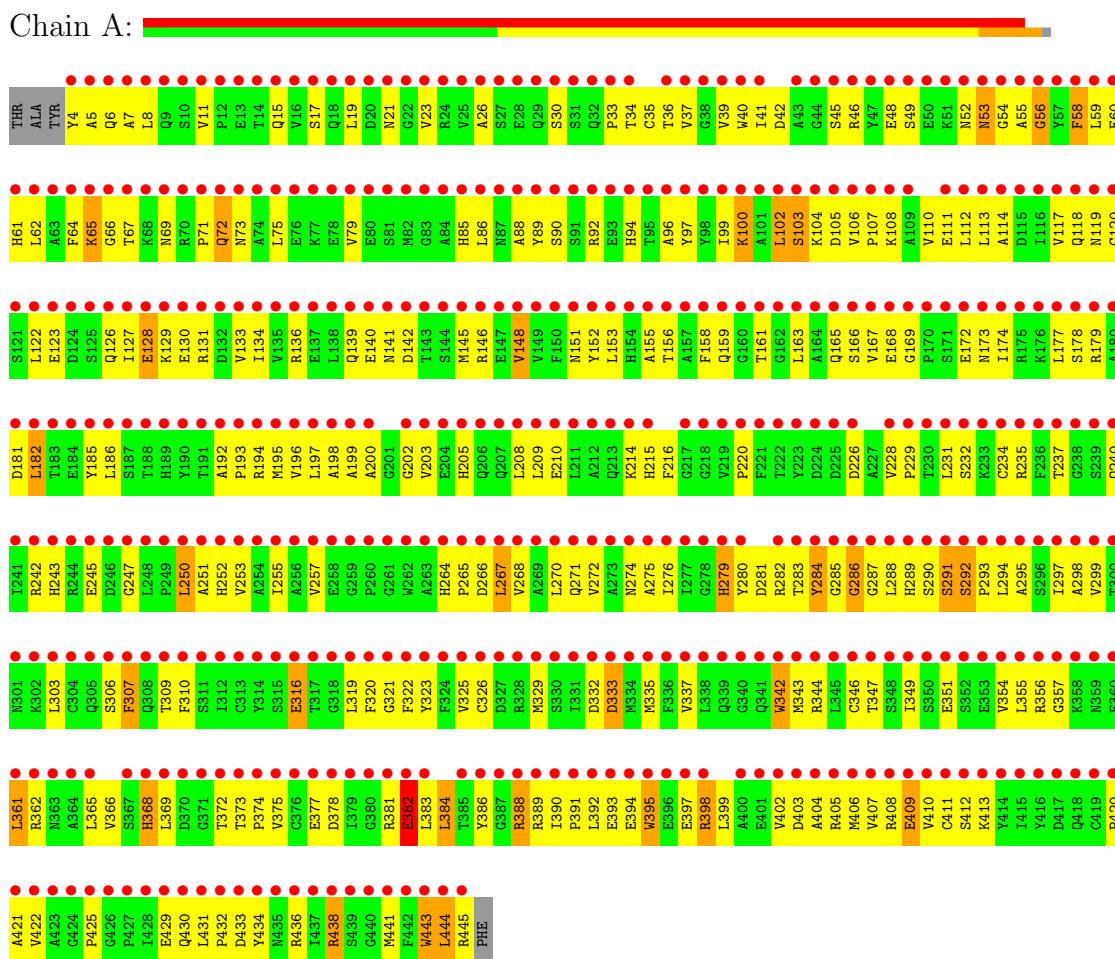


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			35	30	5		

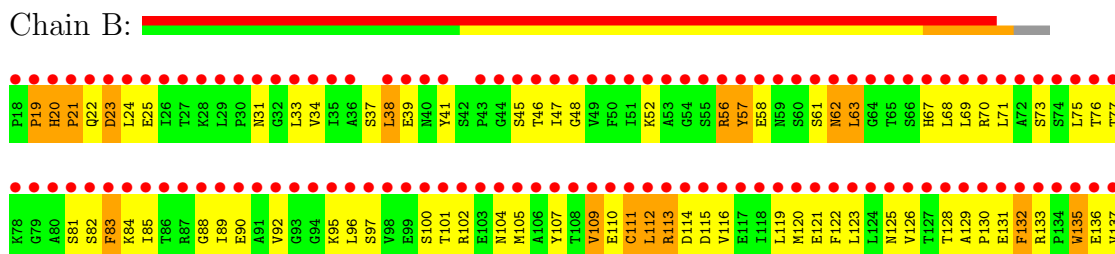
3 Residue-property plots

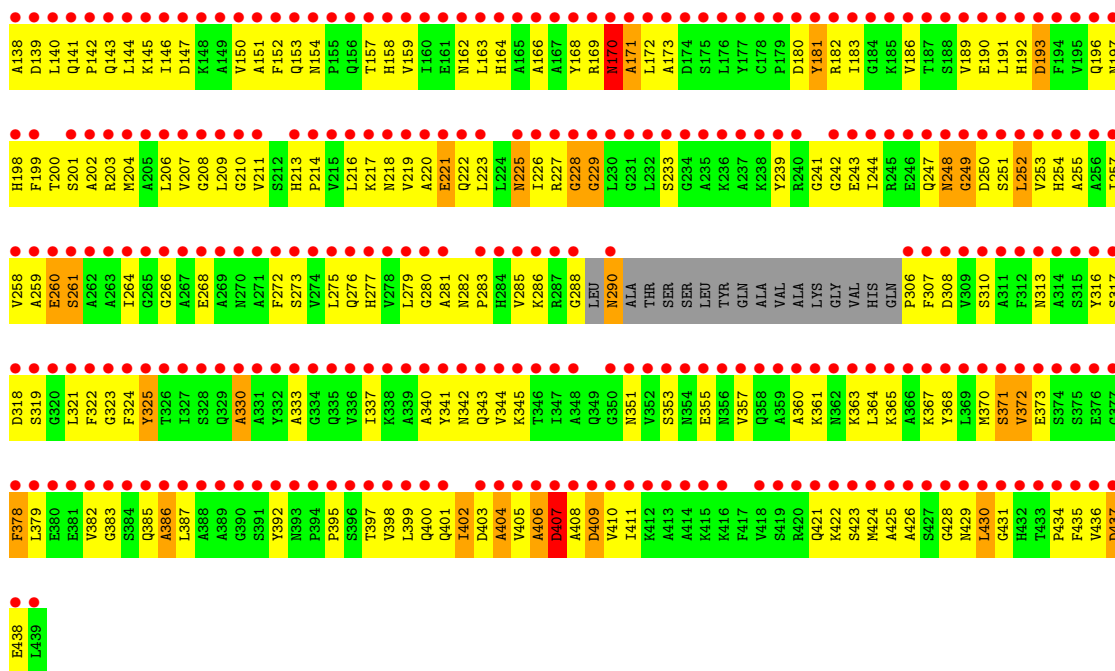
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



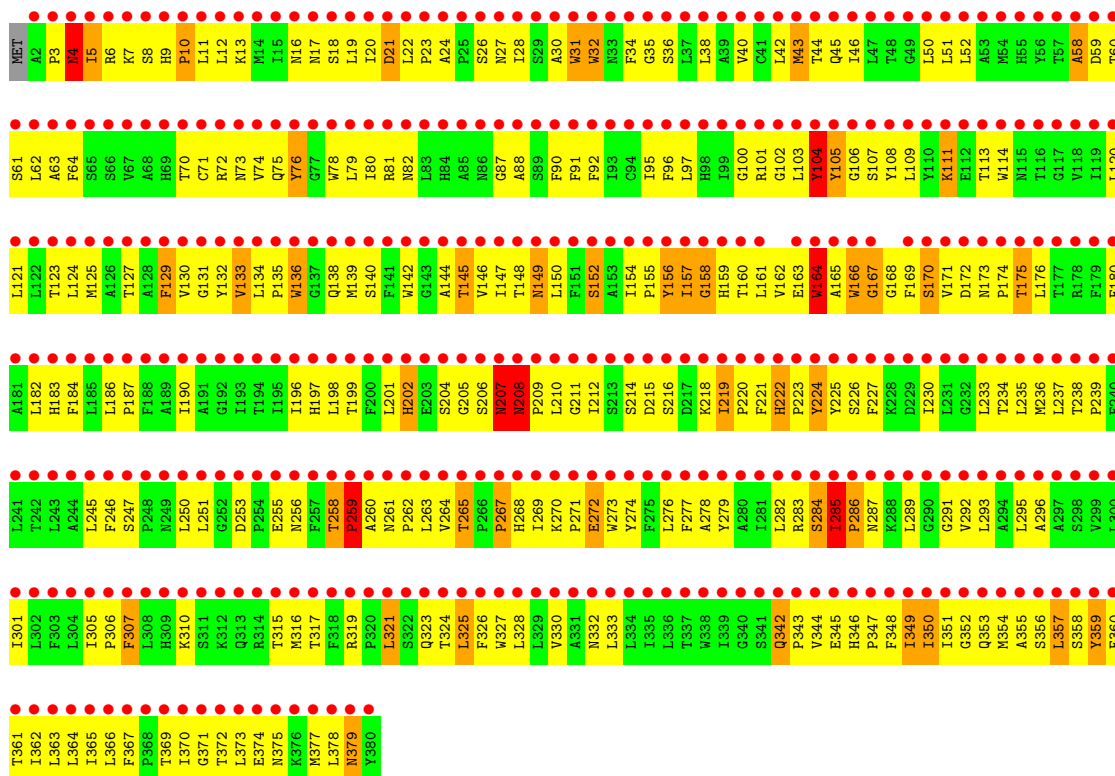
• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE





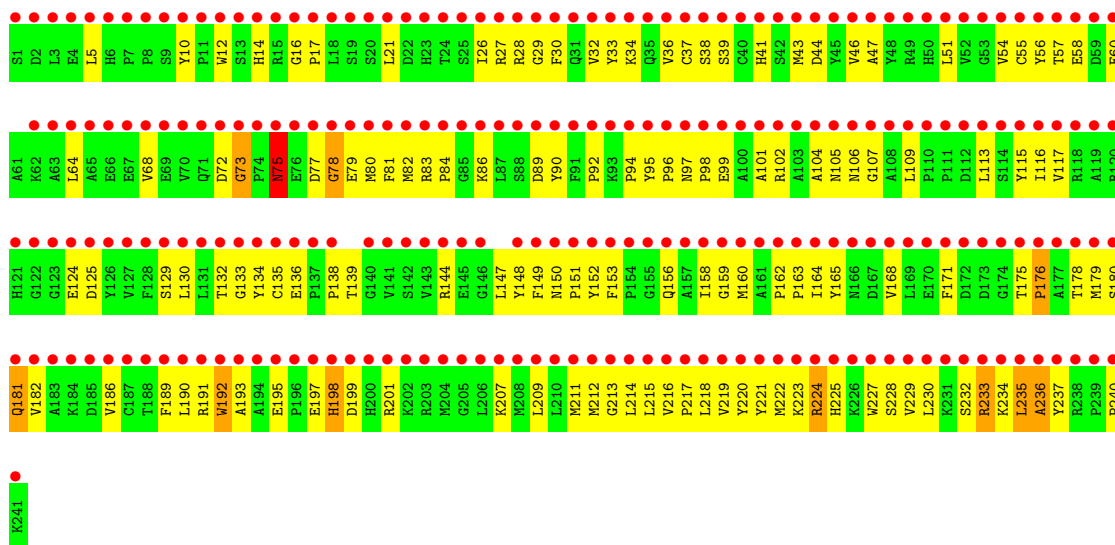
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain C:



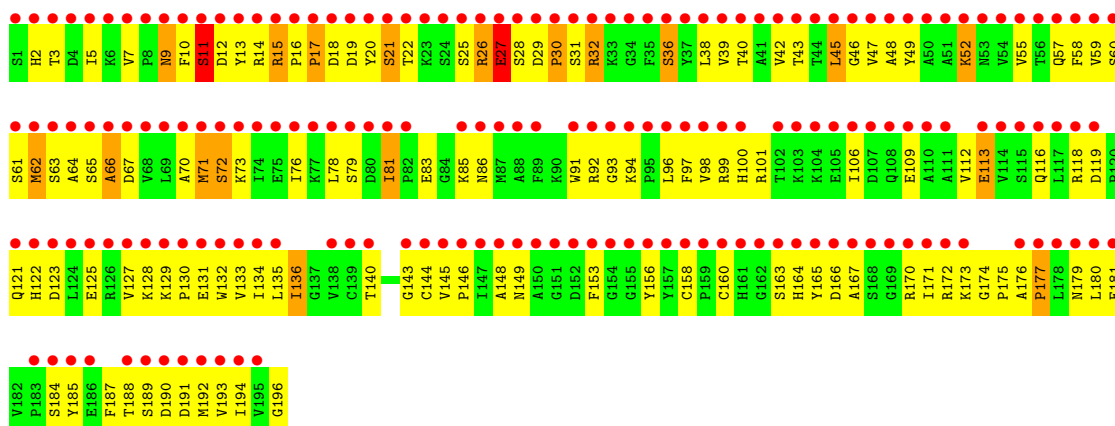
• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain D:



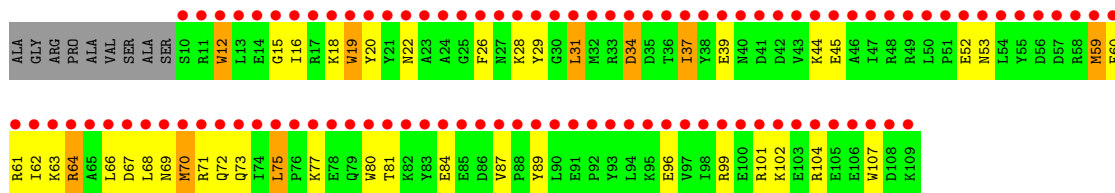
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



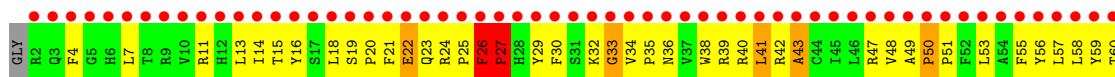
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

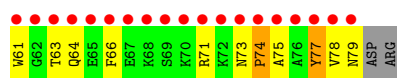
Chain F:



• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

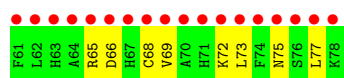
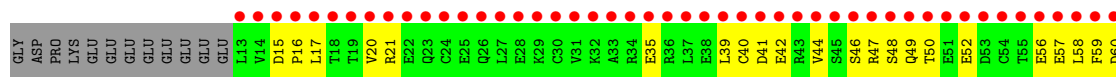
Chain G:





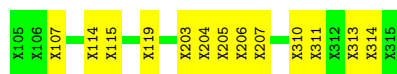
● Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain H:



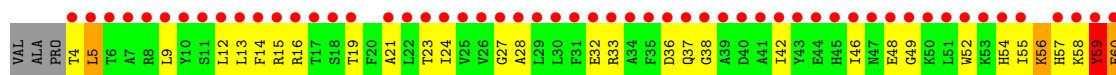
● Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I:



● Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.50 87.05 – 3.02	Depositor EDS
% Data completeness (in resolution range)	85.6 (12.00-3.50) 62.8 (87.05-3.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.01Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.284 , 0.317 0.244 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.3	EDS
Estimated twinning fraction	0.239 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 118814 reflections	Xtriage
F_o, F_c correlation	0.61	EDS
Total number of atoms	15754	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, SIG, FES, HEM, PEE, BOG

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	0.45	0/3495	0.78	1/4742 (0.0%)
2	B	0.43	0/3046	0.73	0/4132
3	C	0.52	0/3104	0.85	5/4252 (0.1%)
4	D	0.50	0/1960	0.81	1/2665 (0.0%)
5	E	0.46	0/1548	0.78	1/2095 (0.0%)
6	F	0.49	0/896	0.76	0/1206
7	G	0.53	0/648	1.17	3/882 (0.3%)
8	H	0.44	0/495	0.69	0/669
10	J	0.52	0/470	0.80	1/635 (0.2%)
All	All	0.48	0/15662	0.81	12/21278 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
10	J	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	26	PHE	C-N-CD	-18.95	78.91	120.60
7	G	26	PHE	C-N-CA	13.72	179.63	122.00
7	G	27	PRO	CA-N-CD	-7.67	100.76	111.50
10	J	61	ASN	N-CA-C	6.56	128.72	111.00
3	C	267	PRO	N-CA-C	-6.18	96.03	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	235	LEU	CA-CB-CG	5.65	128.29	115.30
3	C	265	THR	N-CA-C	-5.50	96.16	111.00
3	C	104	TYR	CA-CB-CG	-5.33	103.28	113.40
3	C	35	GLY	N-CA-C	-5.32	99.79	113.10
5	E	143	GLY	N-CA-C	5.32	126.39	113.10
3	C	285	ILE	N-CA-C	-5.21	96.94	111.00
1	A	329	MET	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	TYR	Sidechain
10	J	59	TYR	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3423	0	3286	359	0
2	B	2994	0	2906	345	0
3	C	3002	0	3036	423	0
4	D	1899	0	1822	216	0
5	E	1512	0	1483	177	0
6	F	875	0	839	70	0
7	G	626	0	591	83	0
8	H	490	0	445	57	0
9	I	159	0	46	20	0
10	J	459	0	424	53	0
11	D	20	0	28	1	0
12	C	86	0	60	19	0
12	D	43	0	30	2	0
13	E	4	0	0	1	0
14	C	29	0	33	9	0
15	C	49	0	70	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	E	49	0	70	4	0
16	C	35	0	42	12	0
All	All	15754	0	15211	1654	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 53.

All (1654) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:166:TRP:HB2	3:C:175:THR:HB	1.22	1.17
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.22	1.17
2:B:280:GLY:H	2:B:283:PRO:HD2	1.06	1.16
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.36	1.05
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.19	1.01
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.43	0.99
2:B:337:ILE:HD11	2:B:434:PRO:HD2	1.41	0.99
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.27	0.98
10:J:57:HIS:HB2	10:J:61:ASN:C	1.84	0.98
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.45	0.97
3:C:138:GLN:NE2	3:C:261:ASN:H	1.62	0.97
4:D:158:ILE:HG22	4:D:160:MET:H	1.30	0.96
5:E:16:PRO:HG2	5:E:32:ARG:HH12	1.30	0.96
3:C:166:TRP:HB2	3:C:175:THR:CB	1.95	0.95
3:C:138:GLN:HE21	3:C:260:ALA:HA	1.32	0.95
3:C:207:ASN:O	3:C:208:ASN:HB3	1.66	0.93
3:C:327:TRP:HA	3:C:330:VAL:HG12	1.48	0.93
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.51	0.93
3:C:138:GLN:HE22	3:C:261:ASN:H	1.03	0.93
7:G:26:PHE:HD1	7:G:26:PHE:H	1.17	0.92
5:E:13:TYR:O	5:E:14:ARG:HD3	1.69	0.92
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.49	0.92
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.52	0.91
3:C:107:SER:HB3	12:C:382:HEM:HBD1	1.52	0.91
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.36	0.91
3:C:202:HIS:CE1	14:C:383:U10:O2	2.24	0.91
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.50	0.91
3:C:166:TRP:CB	3:C:175:THR:HB	2.02	0.91
3:C:238:THR:OG1	4:D:212:MET:HG3	1.70	0.90
2:B:280:GLY:N	2:B:283:PRO:HD2	1.85	0.90
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.52	0.90
2:B:69:LEU:HD12	2:B:105:MET:HE1	1.54	0.90
3:C:120:LEU:HB3	12:C:382:HEM:HBB2	1.51	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:172:ASP:H	3:C:175:THR:HG23	1.37	0.90
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.90
5:E:16:PRO:HG2	5:E:32:ARG:NH1	1.87	0.90
1:A:391:PRO:HG2	1:A:394:GLU:HB2	1.53	0.89
5:E:72:SER:O	5:E:196:GLY:HA3	1.69	0.89
1:A:152:TYR:OH	5:E:5:ILE:HD12	1.73	0.88
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.54	0.88
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.35	0.88
4:D:224:ARG:HH22	7:G:27:PRO:HG3	1.34	0.88
5:E:9:ASN:ND2	5:E:11:SER:HB3	1.89	0.88
1:A:166:SER:OG	5:E:3:THR:HG23	1.73	0.87
4:D:75:ASN:HB2	4:D:77:ASP:H	1.39	0.87
4:D:83:ARG:NH1	4:D:86:LYS:HG3	1.89	0.86
1:A:333:ASP:O	1:A:337:VAL:HG23	1.73	0.86
2:B:25:GLU:HB2	2:B:213:HIS:ND1	1.90	0.86
4:D:165:TYR:O	4:D:168:VAL:HG23	1.76	0.85
2:B:122:PHE:O	2:B:126:VAL:HG23	1.77	0.85
3:C:283:ARG:O	3:C:283:ARG:HG3	1.77	0.85
3:C:342:GLN:NE2	3:C:343:PRO:HD2	1.90	0.85
4:D:132:THR:HA	4:D:179:MET:CE	2.07	0.84
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.57	0.84
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.59	0.84
1:A:281:ASP:HB3	1:A:284:TYR:HE1	1.41	0.84
2:B:280:GLY:H	2:B:283:PRO:CD	1.87	0.83
3:C:272:GLU:N	3:C:272:GLU:OE1	2.10	0.83
5:E:122:HIS:O	5:E:125:GLU:HG2	1.76	0.83
10:J:56:LYS:O	10:J:60:GLU:HB2	1.78	0.83
3:C:142:TRP:CE3	3:C:265:THR:HG22	2.13	0.83
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.14	0.83
2:B:154:ASN:O	2:B:157:THR:HG22	1.79	0.82
2:B:258:VAL:HG13	2:B:322:PHE:H	1.44	0.82
5:E:47:VAL:HG21	15:E:198:PEE:H162	1.60	0.82
10:J:57:HIS:O	10:J:61:ASN:N	2.13	0.82
3:C:31:TRP:CZ3	15:C:384:PEE:H131	2.15	0.82
1:A:250:LEU:HD22	1:A:250:LEU:C	1.98	0.82
3:C:245:LEU:O	4:D:201:ARG:HD3	1.79	0.82
3:C:27:ASN:HB2	6:F:69:ASN:HD22	1.44	0.82
8:H:47:ARG:HD3	8:H:48:SER:H	1.41	0.82
3:C:317:THR:HG23	15:C:384:PEE:O2P	1.80	0.81
3:C:316:MET:SD	3:C:319:ARG:HG3	2.19	0.81
4:D:158:ILE:HG22	4:D:159:GLY:N	1.94	0.81
2:B:143:GLN:OE1	2:B:146:ILE:HD11	1.80	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:62:MET:HG3	5:E:63:SER:H	1.46	0.81
5:E:189:SER:OG	5:E:192:MET:HB2	1.81	0.80
1:A:33:PRO:HG2	1:A:34:THR:H	1.46	0.80
2:B:62:ASN:HD22	2:B:63:LEU:N	1.79	0.80
3:C:295:LEU:HD21	16:C:385:SIG:H273	1.63	0.80
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.17	0.80
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.17	0.80
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.46	0.79
3:C:120:LEU:CB	12:C:382:HEM:HBB2	2.11	0.79
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.46	0.79
1:A:90:SER:O	1:A:167:VAL:HG11	1.83	0.79
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.62	0.79
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.18	0.79
1:A:49:SER:H	1:A:52:ASN:HB3	1.47	0.79
2:B:248:ASN:HD22	2:B:249:GLY:N	1.81	0.79
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.11	0.79
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.65	0.78
3:C:325:LEU:HD13	3:C:367:PHE:CD1	2.18	0.78
4:D:75:ASN:N	4:D:75:ASN:HD22	1.82	0.78
1:A:444:LEU:HD12	1:A:444:LEU:H	1.48	0.78
3:C:172:ASP:H	3:C:175:THR:CG2	1.95	0.78
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.66	0.78
1:A:65:LYS:NZ	9:I:311:UNK:HA	1.99	0.77
6:F:60:PHE:HD1	7:G:13:LEU:HD22	1.48	0.77
1:A:240:GLN:HB3	1:A:422:VAL:HG12	1.67	0.77
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.14	0.77
4:D:132:THR:HA	4:D:179:MET:HE1	1.65	0.77
3:C:319:ARG:NH2	3:C:371:GLY:HA2	2.00	0.77
3:C:327:TRP:HA	3:C:330:VAL:CG1	2.14	0.77
4:D:57:THR:HB	4:D:60:GLU:HB2	1.66	0.76
1:A:142:ASP:OD1	5:E:2:HIS:HB3	1.85	0.76
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.67	0.76
5:E:29:ASP:C	5:E:31:SER:H	1.88	0.76
2:B:62:ASN:C	2:B:62:ASN:HD22	1.89	0.76
3:C:138:GLN:NE2	3:C:261:ASN:N	2.33	0.76
4:D:55:CYS:HG	4:D:56:TYR:HD1	1.33	0.76
1:A:42:ASP:HB2	1:A:384:LEU:HD21	1.66	0.76
2:B:24:LEU:H	2:B:24:LEU:HD23	1.50	0.76
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.20	0.76
4:D:164:ILE:HD11	4:D:182:VAL:HG22	1.66	0.76
6:F:68:LEU:HD21	6:F:75:LEU:HD13	1.68	0.76
2:B:146:ILE:HG13	2:B:147:ASP:N	2.01	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.67	0.75
2:B:258:VAL:HG12	2:B:259:ALA:N	2.01	0.75
1:A:237:THR:HG23	7:G:22:GLU:HG2	1.69	0.75
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.66	0.75
4:D:224:ARG:NH2	7:G:27:PRO:HG3	2.00	0.75
2:B:260:GLU:O	2:B:261:SER:HB3	1.86	0.75
1:A:85:HIS:HA	9:I:314:UNK:HG1	1.67	0.75
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.22	0.75
2:B:258:VAL:HG13	2:B:322:PHE:N	2.01	0.75
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.68	0.75
1:A:240:GLN:CB	1:A:422:VAL:HG12	2.17	0.74
2:B:341:TYR:OH	2:B:422:LYS:HE3	1.87	0.74
2:B:257:ILE:O	2:B:323:GLY:HA3	1.87	0.74
3:C:350:ILE:HD13	3:C:350:ILE:N	2.02	0.74
1:A:106:VAL:HG21	1:A:203:VAL:HG13	1.69	0.74
1:A:288:LEU:HD13	2:B:83:PHE:HA	1.70	0.74
3:C:73:ASN:O	5:E:66:ALA:HB3	1.88	0.74
7:G:29:TYR:O	7:G:30:PHE:HB2	1.88	0.74
1:A:67:THR:HB	1:A:119:ASN:O	1.86	0.74
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.23	0.73
3:C:131:GLY:HA2	3:C:134:LEU:HD13	1.69	0.73
4:D:225:HIS:HA	7:G:25:PRO:HB3	1.69	0.73
3:C:206:SER:OG	14:C:383:U10:H3M1	1.87	0.73
5:E:10:PHE:O	5:E:11:SER:O	2.05	0.73
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.18	0.73
2:B:109:VAL:HG22	2:B:119:LEU:HD11	1.68	0.73
3:C:31:TRP:O	3:C:101:ARG:HG3	1.87	0.73
3:C:172:ASP:O	3:C:175:THR:HG23	1.89	0.73
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.19	0.73
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.03	0.73
2:B:264:ILE:HG12	2:B:316:TYR:O	1.89	0.73
2:B:337:ILE:HD11	2:B:434:PRO:CD	2.19	0.73
1:A:240:GLN:NE2	1:A:242:ARG:HE	1.87	0.72
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.54	0.72
7:G:29:TYR:HD1	7:G:30:PHE:CD1	2.07	0.72
1:A:252:HIS:HB3	1:A:323:TYR:HE1	1.55	0.72
2:B:243:GLU:OE2	2:B:436:VAL:HG22	1.89	0.72
3:C:350:ILE:H	3:C:350:ILE:HD13	1.53	0.72
5:E:45:LEU:HD11	10:J:28:ALA:HA	1.71	0.72
1:A:88:ALA:HB1	1:A:96:ALA:O	1.89	0.72
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.72	0.72
3:C:145:THR:O	3:C:149:ASN:HB2	1.90	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:104:TYR:CZ	3:C:316:MET:HB2	2.24	0.72
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.72	0.72
3:C:138:GLN:NE2	3:C:260:ALA:HA	2.05	0.72
3:C:316:MET:HE3	3:C:319:ARG:HE	1.55	0.72
3:C:7:LYS:O	3:C:13:LYS:HD2	1.90	0.71
3:C:120:LEU:CG	12:C:382:HEM:HBB2	2.20	0.71
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.19	0.71
10:J:57:HIS:HA	10:J:60:GLU:C	2.09	0.71
1:A:250:LEU:N	1:A:250:LEU:HD13	2.05	0.71
1:A:35:CYS:HA	1:A:372:THR:HG21	1.72	0.71
3:C:142:TRP:CD2	3:C:265:THR:HG22	2.26	0.71
5:E:16:PRO:CG	5:E:32:ARG:HH12	2.02	0.71
7:G:78:VAL:C	7:G:79:ASN:HD22	1.93	0.71
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.72	0.71
2:B:273:SER:O	2:B:276:GLN:HB3	1.90	0.71
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.91	0.71
1:A:291:SER:HB2	1:A:356:ARG:NH2	2.05	0.71
2:B:46:THR:HG22	2:B:110:GLU:HB2	1.72	0.71
2:B:250:ASP:O	2:B:252:LEU:HD23	1.89	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.73	0.71
3:C:226:SER:O	3:C:230:ILE:HG13	1.90	0.71
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.21	0.71
5:E:71:MET:O	5:E:73:LYS:N	2.23	0.71
1:A:349:ILE:HG22	1:A:408:ARG:CG	2.21	0.70
1:A:286:GLY:C	1:A:288:LEU:H	1.93	0.70
2:B:169:ARG:O	2:B:170:ASN:HB3	1.90	0.70
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.72	0.70
3:C:378:LEU:O	3:C:379:ASN:HB2	1.91	0.70
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.73	0.70
3:C:354:MET:CE	3:C:354:MET:HA	2.22	0.70
6:F:31:LEU:H	6:F:31:LEU:HD23	1.57	0.70
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.72	0.70
3:C:327:TRP:CE3	3:C:330:VAL:HG11	2.26	0.70
1:A:102:LEU:C	1:A:104:LYS:H	1.94	0.70
3:C:101:ARG:C	3:C:101:ARG:HD2	2.12	0.70
3:C:12:LEU:HD23	3:C:12:LEU:O	1.91	0.70
1:A:45:SER:HA	1:A:48:GLU:HG3	1.72	0.69
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.23	0.69
3:C:261:ASN:HD21	3:C:264:VAL:CG2	2.02	0.69
5:E:140:THR:OG1	5:E:177:PRO:HD2	1.90	0.69
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.22	0.69
5:E:62:MET:HG3	5:E:63:SER:N	2.06	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:286:LYS:CB	2:B:343:GLN:HG3	2.23	0.69
3:C:319:ARG:CZ	3:C:374:GLU:HB2	2.22	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.74	0.69
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.75	0.69
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.27	0.69
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.74	0.69
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.75	0.69
3:C:13:LYS:O	3:C:17:ASN:HB2	1.93	0.69
3:C:120:LEU:HG	12:C:382:HEM:HBB2	1.75	0.68
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.07	0.68
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.73	0.68
3:C:27:ASN:HB2	6:F:69:ASN:ND2	2.07	0.68
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.57	0.68
1:A:102:LEU:H	1:A:102:LEU:HD12	1.58	0.68
4:D:28:ARG:HD2	4:D:171:PHE:CE2	2.28	0.68
1:A:102:LEU:N	1:A:102:LEU:HD12	2.08	0.68
10:J:54:HIS:O	10:J:57:HIS:CD2	2.47	0.68
1:A:4:TYR:O	1:A:7:ALA:N	2.26	0.68
1:A:388:ARG:H	1:A:388:ARG:HD3	1.58	0.68
3:C:377:MET:HE1	6:F:20:TYR:HB2	1.75	0.68
5:E:29:ASP:O	5:E:32:ARG:N	2.26	0.68
1:A:65:LYS:HZ2	9:I:311:UNK:HA	1.59	0.68
2:B:81:SER:O	2:B:85:ILE:HG22	1.94	0.68
3:C:27:ASN:ND2	3:C:208:ASN:OD1	2.23	0.68
4:D:102:ARG:NH1	4:D:109:LEU:HB2	2.08	0.68
1:A:153:LEU:C	1:A:153:LEU:HD23	2.13	0.68
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.29	0.68
3:C:120:LEU:HB3	12:C:382:HEM:CBB	2.22	0.68
8:H:73:LEU:O	8:H:73:LEU:HD23	1.94	0.68
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.75	0.67
5:E:52:LYS:HD3	5:E:52:LYS:C	2.14	0.67
2:B:19:PRO:C	2:B:21:PRO:HD3	2.14	0.67
3:C:142:TRP:CZ3	3:C:265:THR:HG22	2.29	0.67
1:A:19:LEU:C	1:A:21:ASN:H	1.97	0.67
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.59	0.67
1:A:156:THR:HA	5:E:7:VAL:HG21	1.75	0.67
3:C:348:PHE:O	3:C:350:ILE:N	2.28	0.67
6:F:16:ILE:O	6:F:19:TRP:HB3	1.94	0.67
1:A:36:THR:HG22	1:A:100:LYS:CB	2.14	0.67
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.29	0.67
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.75	0.67
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.30	0.67
5:E:160:CYS:HB2	13:E:197:FES:S2	2.35	0.67
1:A:438:ARG:HD3	1:A:438:ARG:O	1.96	0.66
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.30	0.66
6:F:59:MET:HA	6:F:59:MET:CE	2.25	0.66
8:H:35:GLU:O	8:H:39:LEU:HD13	1.95	0.66
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.59	0.66
3:C:245:LEU:O	4:D:201:ARG:CD	2.44	0.66
3:C:350:ILE:CD1	3:C:350:ILE:H	2.08	0.66
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.29	0.66
2:B:370:MET:O	2:B:373:GLU:HG3	1.96	0.66
4:D:132:THR:HA	4:D:179:MET:HE2	1.78	0.66
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.78	0.66
5:E:43:THR:O	5:E:47:VAL:HG23	1.94	0.66
8:H:69:VAL:O	8:H:73:LEU:HB2	1.95	0.66
2:B:96:LEU:HD23	2:B:97:SER:N	2.10	0.66
3:C:123:THR:O	3:C:127:THR:HG23	1.96	0.66
3:C:131:GLY:CA	3:C:134:LEU:HD13	2.25	0.66
1:A:243:HIS:O	1:A:425:PRO:HA	1.96	0.66
1:A:433:ASP:OD1	1:A:436:ARG:HG2	1.96	0.66
3:C:133:VAL:CG1	3:C:144:ALA:HB2	2.24	0.66
14:C:383:U10:C8	14:C:383:U10:H1M1	2.26	0.66
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.77	0.66
3:C:146:VAL:HG23	3:C:147:ILE:N	2.10	0.66
5:E:93:GLY:O	5:E:94:LYS:HE3	1.96	0.66
10:J:13:LEU:HD12	10:J:13:LEU:N	2.11	0.66
3:C:222:HIS:HB3	3:C:223:PRO:HD2	1.78	0.65
4:D:180:SER:HB3	8:H:15:ASP:OD1	1.96	0.65
1:A:291:SER:O	1:A:292:SER:C	2.34	0.65
1:A:297:ILE:CG2	1:A:337:VAL:HG11	2.25	0.65
4:D:75:ASN:ND2	4:D:79:GLU:O	2.27	0.65
10:J:59:TYR:O	10:J:60:GLU:HG3	1.96	0.65
1:A:94:HIS:NE2	1:A:381:ARG:HG2	2.11	0.65
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.31	0.65
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.09	0.65
1:A:252:HIS:HD1	1:A:325:VAL:HG22	1.61	0.65
2:B:379:LEU:HD13	2:B:379:LEU:O	1.96	0.65
3:C:131:GLY:O	3:C:134:LEU:HB2	1.96	0.65
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.31	0.65
10:J:55:ILE:O	10:J:57:HIS:N	2.29	0.65
2:B:61:SER:O	2:B:62:ASN:ND2	2.29	0.65
3:C:9:HIS:HB3	3:C:12:LEU:HB3	1.77	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:106:VAL:O	1:A:110:VAL:HG23	1.97	0.65
3:C:282:LEU:HD13	3:C:282:LEU:O	1.95	0.65
3:C:43:MET:CE	3:C:43:MET:HA	2.27	0.65
5:E:16:PRO:O	5:E:18:ASP:N	2.25	0.65
5:E:26:ARG:O	5:E:27:GLU:HG3	1.96	0.65
1:A:159:GLN:HE21	5:E:7:VAL:HG11	1.62	0.65
2:B:137:VAL:HG23	2:B:138:ALA:N	2.11	0.65
3:C:43:MET:HE2	3:C:43:MET:HA	1.78	0.65
2:B:272:PHE:O	2:B:276:GLN:N	2.29	0.65
14:C:383:U10:H8	14:C:383:U10:H1M1	1.78	0.65
3:C:377:MET:CE	6:F:20:TYR:HB2	2.26	0.65
1:A:403:ASP:OD2	1:A:405:ARG:HB3	1.97	0.65
2:B:101:THR:HG22	2:B:102:ARG:N	2.12	0.65
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.65
4:D:186:VAL:O	4:D:189:PHE:HB3	1.96	0.65
10:J:42:ILE:O	10:J:46:ILE:HG13	1.97	0.65
1:A:103:SER:C	1:A:105:ASP:H	1.97	0.65
4:D:43:MET:CE	4:D:46:VAL:HG21	2.26	0.65
5:E:36:SER:HG	7:G:21:PHE:HE1	1.43	0.65
2:B:385:GLN:O	2:B:387:LEU:N	2.30	0.64
3:C:233:LEU:CD1	3:C:237:LEU:HD22	2.27	0.64
2:B:62:ASN:C	2:B:62:ASN:ND2	2.48	0.64
3:C:235:LEU:O	3:C:239:PRO:HD3	1.98	0.64
1:A:100:LYS:HE3	2:B:370:MET:CE	2.27	0.64
1:A:293:PRO:O	1:A:297:ILE:N	2.26	0.64
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.79	0.64
1:A:161:THR:HG21	1:A:235:ARG:H	1.61	0.64
2:B:128:THR:C	2:B:130:PRO:HD3	2.17	0.64
3:C:349:ILE:HG22	3:C:350:ILE:HD13	1.79	0.64
4:D:44:ASP:O	4:D:90:TYR:HD2	1.80	0.64
1:A:291:SER:O	1:A:293:PRO:N	2.31	0.64
4:D:182:VAL:O	4:D:186:VAL:HG23	1.96	0.64
4:D:75:ASN:ND2	4:D:75:ASN:N	2.42	0.64
1:A:389:ARG:HD2	1:A:390:ILE:H	1.63	0.64
2:B:76:THR:CG2	2:B:82:SER:H	2.11	0.64
3:C:36:SER:O	3:C:40:VAL:HG23	1.97	0.64
3:C:347:PRO:HG3	7:G:66:PHE:CD1	2.32	0.64
2:B:33:LEU:HD21	2:B:223:LEU:HD23	1.80	0.64
3:C:130:VAL:HG12	3:C:183:HIS:HB2	1.79	0.64
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.79	0.64
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.32	0.64
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.13	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.27	0.64
2:B:166:ALA:HB1	2:B:242:GLY:C	2.18	0.64
3:C:20:ILE:O	3:C:21:ASP:HB2	1.97	0.64
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.11	0.64
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.62	0.64
4:D:178:THR:O	4:D:182:VAL:HG12	1.98	0.64
4:D:75:ASN:H	4:D:75:ASN:ND2	1.96	0.64
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.80	0.64
2:B:258:VAL:HG12	2:B:259:ALA:H	1.63	0.64
3:C:222:HIS:O	3:C:223:PRO:C	2.34	0.64
5:E:29:ASP:O	5:E:31:SER:N	2.30	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.98	0.64
3:C:282:LEU:HD23	3:C:295:LEU:HB2	1.80	0.64
5:E:16:PRO:HD3	7:G:22:GLU:O	1.98	0.64
4:D:218:LEU:O	4:D:222:MET:HG3	1.98	0.63
1:A:146:ARG:HH21	9:I:206:UNK:CB	2.12	0.63
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.33	0.63
5:E:113:GLU:OE2	5:E:116:GLN:HG3	1.98	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.62	0.63
3:C:316:MET:HE3	3:C:319:ARG:NE	2.12	0.63
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.33	0.63
3:C:238:THR:OG1	4:D:212:MET:CG	2.44	0.63
1:A:382:GLU:OE2	1:A:390:ILE:HB	1.98	0.63
1:A:436:ARG:HD3	3:C:223:PRO:HD3	1.80	0.63
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.28	0.63
1:A:102:LEU:O	1:A:104:LYS:N	2.31	0.63
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.63	0.63
3:C:113:THR:HG21	3:C:201:LEU:HA	1.81	0.63
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.33	0.63
5:E:5:ILE:HD13	7:G:14:ILE:CD1	2.29	0.63
7:G:60:THR:HG22	7:G:64:GLN:NE2	2.03	0.63
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.34	0.63
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.63
1:A:245:GLU:HG2	1:A:247:GLY:H	1.64	0.63
2:B:258:VAL:CG1	2:B:322:PHE:H	2.10	0.63
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.13	0.63
1:A:235:ARG:HD3	5:E:21:SER:H	1.64	0.63
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.80	0.62
3:C:253:ASP:OD1	3:C:255:GLU:N	2.31	0.62
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.34	0.62
10:J:59:TYR:CD1	10:J:59:TYR:N	2.67	0.62
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.35	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:5:ILE:HD13	7:G:14:ILE:HD13	1.82	0.62
5:E:62:MET:O	5:E:64:ALA:O	2.17	0.62
1:A:444:LEU:O	1:A:445:ARG:O	2.17	0.62
3:C:16:ASN:OD1	3:C:16:ASN:O	2.16	0.62
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.35	0.62
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.64	0.62
3:C:325:LEU:HD13	3:C:367:PHE:HD1	1.65	0.62
4:D:95:TYR:HE2	4:D:104:ALA:HB3	1.63	0.62
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.97	0.62
7:G:71:ARG:NE	8:H:56:GLU:OE2	2.32	0.62
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.28	0.62
3:C:52:LEU:HD13	3:C:80:ILE:CG2	2.25	0.62
1:A:295:ALA:O	1:A:298:ALA:HB3	2.00	0.62
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.81	0.62
7:G:29:TYR:HA	7:G:33:GLY:HA3	1.80	0.62
10:J:57:HIS:HB2	10:J:61:ASN:O	1.99	0.62
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.48	0.61
1:A:15:GLN:O	1:A:26:ALA:HA	2.01	0.61
1:A:399:LEU:C	1:A:399:LEU:HD12	2.19	0.61
1:A:86:LEU:HD13	1:A:99:ILE:HG13	1.82	0.61
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.30	0.61
4:D:158:ILE:CG2	4:D:159:GLY:N	2.63	0.61
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.35	0.61
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.82	0.61
1:A:85:HIS:O	1:A:99:ILE:HA	2.00	0.61
6:F:60:PHE:CD1	7:G:13:LEU:HD22	2.33	0.61
1:A:267:LEU:O	1:A:271:GLN:HB2	2.01	0.61
4:D:144:ARG:HG3	4:D:147:LEU:HD23	1.83	0.61
1:A:307:PHE:C	1:A:307:PHE:CD1	2.73	0.61
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.64	0.61
2:B:19:PRO:C	2:B:21:PRO:CD	2.69	0.61
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.00	0.61
3:C:71:CYS:SG	3:C:81:ARG:HD3	2.40	0.61
3:C:362:ILE:HA	3:C:366:LEU:HD23	1.82	0.61
1:A:106:VAL:N	1:A:107:PRO:HD2	2.16	0.61
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.36	0.61
10:J:57:HIS:HB2	10:J:61:ASN:CA	2.30	0.61
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.65	0.61
7:G:57:LEU:H	7:G:57:LEU:HD22	1.65	0.61
7:G:77:TYR:CE1	8:H:52:GLU:HB2	2.35	0.61
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.65	0.60
3:C:201:LEU:O	3:C:204:SER:O	2.19	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:47:ARG:HD3	8:H:48:SER:N	2.15	0.60
3:C:344:VAL:O	3:C:344:VAL:HG23	2.00	0.60
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.29	0.60
4:D:21:LEU:HD13	4:D:26:ILE:CD1	2.30	0.60
1:A:235:ARG:HB2	5:E:21:SER:HA	1.84	0.60
1:A:255:ILE:HA	1:A:421:ALA:O	2.02	0.60
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.31	0.60
3:C:301:ILE:CD1	3:C:364:LEU:HD11	2.31	0.60
3:C:319:ARG:HH22	3:C:371:GLY:HA2	1.64	0.60
10:J:13:LEU:HA	10:J:19:THR:CG2	2.31	0.60
2:B:100:SER:OG	2:B:105:MET:HG2	2.01	0.60
2:B:399:LEU:CA	2:B:402:ILE:HG22	2.32	0.60
1:A:436:ARG:HD3	3:C:223:PRO:CD	2.31	0.60
3:C:222:HIS:HB3	3:C:223:PRO:CD	2.31	0.60
4:D:117:VAL:HG12	4:D:191:ARG:NH2	2.16	0.60
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.47	0.60
2:B:426:ALA:HB1	2:B:430:LEU:HD21	1.83	0.60
3:C:319:ARG:NH1	3:C:374:GLU:HB2	2.16	0.60
5:E:148:ALA:O	5:E:149:ASN:HB2	2.02	0.60
5:E:163:SER:OG	5:E:175:PRO:HD2	2.00	0.60
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.69	0.60
3:C:3:PRO:HG2	3:C:4:ASN:H	1.67	0.60
8:H:73:LEU:HD23	8:H:73:LEU:C	2.22	0.60
3:C:147:ILE:O	3:C:150:LEU:HB3	2.01	0.60
3:C:307:PHE:N	3:C:307:PHE:CD1	2.69	0.60
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.35	0.60
2:B:137:VAL:CG2	2:B:138:ALA:N	2.65	0.60
2:B:170:ASN:ND2	2:B:170:ASN:C	2.55	0.60
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.37	0.60
4:D:78:GLY:O	4:D:79:GLU:HG3	2.02	0.60
1:A:64:PHE:CE1	1:A:86:LEU:HG	2.37	0.59
2:B:128:THR:HG21	2:B:223:LEU:HD12	1.84	0.59
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.16	0.59
5:E:106:ILE:HG12	5:E:130:PRO:O	2.02	0.59
1:A:145:MET:CB	1:A:252:HIS:CD2	2.84	0.59
1:A:286:GLY:C	1:A:288:LEU:N	2.56	0.59
1:A:40:TRP:HZ3	1:A:89:TYR:HH	1.50	0.59
2:B:101:THR:HB	2:B:104:ASN:OD1	2.02	0.59
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.31	0.59
5:E:184:SER:O	5:E:196:GLY:N	2.29	0.59
1:A:46:ARG:HD2	1:A:163:LEU:HD21	1.83	0.59
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:150:VAL:O	2:B:153:GLN:HG3	2.02	0.59
2:B:368:TYR:O	2:B:372:VAL:HG23	2.00	0.59
2:B:58:GLU:HB3	2:B:62:ASN:HD21	1.67	0.59
4:D:32:VAL:O	4:D:36:VAL:HG13	2.02	0.59
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.67	0.59
3:C:107:SER:CB	12:C:382:HEM:HBD1	2.31	0.59
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.82	0.59
3:C:230:ILE:HG21	15:E:198:PEE:H172	1.84	0.59
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.65	0.59
3:C:149:ASN:O	3:C:152:SER:HB3	2.03	0.59
3:C:289:LEU:HG	3:C:293:LEU:CD2	2.33	0.59
5:E:81:ILE:HD13	5:E:98:VAL:HG12	1.84	0.59
1:A:378:ASP:O	1:A:382:GLU:HB2	2.02	0.59
3:C:289:LEU:HG	3:C:293:LEU:HD23	1.83	0.59
4:D:158:ILE:HG22	4:D:159:GLY:H	1.67	0.59
4:D:164:ILE:HD11	4:D:182:VAL:CG2	2.32	0.59
4:D:211:MET:HG3	11:D:242:BOG:H5'1	1.85	0.59
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.38	0.59
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.03	0.59
1:A:443:TRP:C	1:A:445:ARG:H	2.06	0.59
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.85	0.59
2:B:255:ALA:O	2:B:325:TYR:HA	2.02	0.59
1:A:288:LEU:HD13	2:B:83:PHE:CA	2.32	0.59
3:C:238:THR:CG2	4:D:212:MET:HG3	2.32	0.59
5:E:9:ASN:ND2	5:E:11:SER:H	2.01	0.59
5:E:45:LEU:O	5:E:48:ALA:HB3	2.03	0.59
2:B:217:LYS:C	2:B:219:VAL:H	2.07	0.58
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.84	0.58
3:C:27:ASN:HD22	6:F:69:ASN:HD22	1.50	0.58
1:A:85:HIS:CA	9:I:314:UNK:HG1	2.33	0.58
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.33	0.58
3:C:271:PRO:HB3	16:C:385:SIG:C2	2.33	0.58
3:C:321:LEU:HD12	3:C:374:GLU:HG2	1.85	0.58
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.38	0.58
4:D:134:TYR:O	4:D:135:CYS:HB3	2.03	0.58
5:E:11:SER:OG	5:E:12:ASP:N	2.36	0.58
4:D:230:LEU:HB3	6:F:70:MET:CE	2.34	0.58
2:B:101:THR:HG22	2:B:102:ARG:H	1.68	0.58
3:C:283:ARG:O	3:C:284:SER:HB3	2.03	0.58
4:D:224:ARG:NH1	7:G:25:PRO:O	2.36	0.58
6:F:61:ARG:HG3	6:F:61:ARG:HH11	1.68	0.58
1:A:290:SER:O	1:A:291:SER:C	2.42	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.68	0.58
2:B:113:ARG:HG3	2:B:114:ASP:N	2.19	0.58
2:B:248:ASN:HD22	2:B:248:ASN:C	2.04	0.58
1:A:146:ARG:NH2	9:I:206:UNK:CB	2.67	0.58
1:A:153:LEU:CD2	1:A:319:LEU:HD13	2.33	0.58
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.58
1:A:391:PRO:CG	1:A:394:GLU:HB2	2.29	0.58
2:B:397:THR:HA	2:B:400:GLN:HB3	1.86	0.58
3:C:6:ARG:HA	3:C:12:LEU:HD22	1.85	0.58
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.37	0.58
1:A:272:VAL:O	1:A:275:ALA:HB3	2.03	0.58
1:A:351:GLU:O	1:A:354:VAL:HG22	2.03	0.58
1:A:250:LEU:N	1:A:250:LEU:CD1	2.66	0.58
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.33	0.58
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.84	0.58
6:F:18:LYS:O	6:F:22:ASN:ND2	2.37	0.58
1:A:85:HIS:CB	9:I:314:UNK:HG1	2.33	0.58
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.16	0.58
3:C:61:SER:C	3:C:62:LEU:HD22	2.23	0.58
3:C:18:SER:C	3:C:19:LEU:HD12	2.24	0.57
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.03	0.57
2:B:193:ASP:O	2:B:197:ASN:ND2	2.37	0.57
2:B:280:GLY:C	2:B:282:ASN:N	2.56	0.57
3:C:104:TYR:O	3:C:105:TYR:CD2	2.57	0.57
4:D:233:ARG:O	6:F:71:ARG:NH2	2.37	0.57
2:B:228:GLY:O	2:B:229:GLY:C	2.42	0.57
2:B:285:VAL:HG12	2:B:285:VAL:O	2.03	0.57
2:B:243:GLU:CD	2:B:436:VAL:HG22	2.24	0.57
3:C:307:PHE:N	3:C:307:PHE:HD1	2.02	0.57
3:C:346:HIS:N	3:C:347:PRO:HD2	2.19	0.57
3:C:3:PRO:O	3:C:5:ILE:HG13	2.04	0.57
2:B:400:GLN:O	2:B:404:ALA:HB2	2.05	0.57
3:C:92:PHE:CZ	3:C:124:LEU:HD13	2.39	0.57
3:C:323:GLN:HE21	7:G:47:ARG:HD3	1.69	0.57
1:A:351:GLU:HA	1:A:351:GLU:OE1	2.04	0.57
1:A:45:SER:HA	1:A:48:GLU:CG	2.35	0.57
1:A:75:LEU:O	1:A:79:VAL:HG23	2.05	0.57
2:B:402:ILE:HD13	2:B:402:ILE:O	2.04	0.57
3:C:370:ILE:O	3:C:374:GLU:HG3	2.04	0.57
5:E:85:LYS:HG2	5:E:86:ASN:N	2.19	0.57
6:F:101:ARG:HA	6:F:104:ARG:HE	1.69	0.57
3:C:373:LEU:HD23	3:C:373:LEU:C	2.24	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:250:LEU:C	1:A:250:LEU:CD2	2.71	0.57
2:B:199:PHE:HA	2:B:204:MET:HE2	1.87	0.57
3:C:325:LEU:HD21	3:C:362:ILE:HG23	1.87	0.57
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.86	0.57
4:D:233:ARG:HB3	6:F:71:ARG:HH21	1.70	0.57
10:J:21:ALA:O	10:J:24:ILE:N	2.37	0.57
3:C:206:SER:OG	14:C:383:U10:C3M	2.53	0.57
2:B:258:VAL:CG1	2:B:259:ALA:N	2.68	0.57
4:D:212:MET:O	4:D:216:VAL:HG22	2.04	0.57
4:D:28:ARG:HD2	4:D:171:PHE:CD2	2.40	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.35	0.57
5:E:9:ASN:HD21	5:E:11:SER:CB	2.18	0.57
1:A:250:LEU:HD13	1:A:250:LEU:H	1.67	0.57
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.68	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.57
6:F:31:LEU:N	6:F:31:LEU:HD23	2.18	0.57
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.19	0.56
3:C:28:ILE:HG23	3:C:32:TRP:HB2	1.87	0.56
10:J:13:LEU:CD1	10:J:13:LEU:N	2.68	0.56
1:A:343:MET:O	1:A:347:THR:HG22	2.05	0.56
2:B:213:HIS:N	2:B:214:PRO:HD2	2.20	0.56
5:E:45:LEU:CD1	10:J:28:ALA:HA	2.34	0.56
1:A:152:TYR:CZ	5:E:5:ILE:HD12	2.38	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.86	0.56
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.31	0.56
2:B:202:ALA:HB3	2:B:229:GLY:HA2	1.85	0.56
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.40	0.56
2:B:405:VAL:HG12	2:B:406:ALA:N	2.19	0.56
2:B:76:THR:HG22	2:B:82:SER:N	2.13	0.56
3:C:342:GLN:HB3	3:C:348:PHE:CE2	2.41	0.56
3:C:358:SER:O	3:C:362:ILE:HG13	2.05	0.56
1:A:59:LEU:HD11	1:A:186:LEU:HD11	1.87	0.56
1:A:270:LEU:HG	1:A:320:PHE:CE2	2.40	0.56
3:C:101:ARG:C	3:C:101:ARG:CD	2.74	0.56
3:C:182:LEU:HD22	16:C:385:SIG:H381	1.87	0.56
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.87	0.56
3:C:366:LEU:H	3:C:366:LEU:HD22	1.70	0.56
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.04	0.56
1:A:250:LEU:HB2	1:A:326:CYS:O	2.06	0.56
3:C:105:TYR:CD1	3:C:209:PRO:HA	2.40	0.56
3:C:22:LEU:HD21	14:C:383:U10:H3M2	1.86	0.56
4:D:178:THR:OG1	4:D:181:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:79:GLU:O	4:D:80:MET:C	2.44	0.56
3:C:223:PRO:O	3:C:227:PHE:HD2	1.87	0.56
5:E:26:ARG:O	5:E:28:SER:N	2.31	0.56
5:E:32:ARG:HD3	5:E:32:ARG:C	2.26	0.56
9:I:310:UNK:O	9:I:311:UNK:C	2.53	0.56
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.36	0.56
2:B:111:CYS:O	2:B:112:LEU:HB3	2.06	0.56
2:B:143:GLN:OE1	2:B:146:ILE:CD1	2.53	0.56
2:B:169:ARG:O	2:B:170:ASN:CB	2.53	0.56
2:B:96:LEU:C	2:B:96:LEU:HD23	2.25	0.56
4:D:43:MET:HE2	4:D:46:VAL:CG2	2.35	0.56
5:E:94:LYS:HE2	5:E:94:LYS:HA	1.87	0.56
1:A:293:PRO:O	1:A:294:LEU:C	2.44	0.56
3:C:319:ARG:NH2	3:C:374:GLU:OE2	2.38	0.56
4:D:153:PHE:CD2	4:D:158:ILE:HG12	2.41	0.56
1:A:159:GLN:OE1	5:E:15:ARG:NH2	2.35	0.56
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.41	0.56
3:C:133:VAL:HG11	3:C:144:ALA:HB2	1.87	0.56
3:C:293:LEU:O	3:C:296:ALA:HB3	2.06	0.56
4:D:215:LEU:O	4:D:219:VAL:HG22	2.05	0.56
4:D:97:ASN:OD1	4:D:99:GLU:HG2	2.06	0.56
5:E:85:LYS:HG2	5:E:86:ASN:H	1.71	0.56
10:J:57:HIS:CE1	10:J:62:LYS:C	2.79	0.56
1:A:103:SER:C	1:A:105:ASP:N	2.59	0.56
1:A:145:MET:HB3	1:A:252:HIS:HD2	1.71	0.56
3:C:219:ILE:HD13	4:D:230:LEU:HD11	1.88	0.56
6:F:28:LYS:O	6:F:75:LEU:HB2	2.06	0.56
1:A:108:LYS:HA	1:A:108:LYS:HE3	1.88	0.56
2:B:113:ARG:O	2:B:116:VAL:HG23	2.06	0.56
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.25	0.56
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.87	0.56
2:B:397:THR:O	2:B:401:GLN:HG2	2.05	0.56
1:A:346:CYS:HB3	1:A:411:CYS:CB	2.36	0.55
2:B:150:VAL:HG23	2:B:151:ALA:N	2.21	0.55
3:C:261:ASN:ND2	3:C:264:VAL:CG2	2.67	0.55
3:C:104:TYR:CZ	3:C:316:MET:CB	2.88	0.55
4:D:55:CYS:SG	4:D:56:TYR:HD1	2.29	0.55
5:E:171:ILE:HD12	5:E:172:ARG:H	1.71	0.55
10:J:13:LEU:HA	10:J:19:THR:HG21	1.87	0.55
10:J:55:ILE:C	10:J:57:HIS:H	2.09	0.55
1:A:100:LYS:HE3	2:B:370:MET:HE2	1.88	0.55
1:A:145:MET:HA	1:A:148:VAL:CG1	2.35	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:409:ASP:O	2:B:411:ILE:N	2.40	0.55
3:C:233:LEU:O	3:C:237:LEU:HB2	2.05	0.55
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.86	0.55
3:C:4:ASN:O	3:C:5:ILE:HB	2.05	0.55
4:D:192:TRP:CD1	4:D:193:ALA:N	2.75	0.55
1:A:391:PRO:O	1:A:394:GLU:N	2.38	0.55
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.42	0.55
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.37	0.55
5:E:65:SER:C	5:E:67:ASP:H	2.10	0.55
9:I:313:UNK:CB	9:I:314:UNK:CD	2.84	0.55
2:B:399:LEU:HA	2:B:402:ILE:CG2	2.32	0.55
3:C:283:ARG:O	3:C:283:ARG:CG	2.51	0.55
6:F:12:TRP:HB3	6:F:15:GLY:H	1.71	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD11	1.88	0.55
3:C:345:GLU:HB3	3:C:347:PRO:HD2	1.86	0.55
3:C:75:GLN:O	3:C:76:TYR:HB2	2.07	0.55
4:D:218:LEU:CD1	5:E:42:VAL:HG12	2.37	0.55
3:C:173:ASN:N	3:C:174:PRO:HD2	2.22	0.55
4:D:75:ASN:H	4:D:79:GLU:H	1.53	0.55
7:G:42:ARG:O	7:G:43:ALA:HB2	2.07	0.55
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.22	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.87	0.55
3:C:92:PHE:O	3:C:95:ILE:HG22	2.06	0.55
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.34	0.55
1:A:266:ASP:O	1:A:268:VAL:N	2.40	0.55
4:D:230:LEU:HB3	6:F:70:MET:HE1	1.88	0.55
3:C:323:GLN:NE2	7:G:47:ARG:HD3	2.22	0.55
10:J:14:PHE:CD1	10:J:14:PHE:N	2.71	0.55
8:H:57:GLU:CD	8:H:57:GLU:H	2.11	0.55
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.07	0.55
1:A:250:LEU:HD22	1:A:251:ALA:N	2.21	0.55
1:A:297:ILE:HG21	1:A:337:VAL:CG1	2.32	0.55
4:D:164:ILE:CD1	4:D:182:VAL:HG13	2.37	0.55
1:A:158:PHE:CE2	1:A:319:LEU:HD21	2.42	0.54
1:A:365:LEU:HD21	1:A:395:TRP:CD1	2.42	0.54
3:C:295:LEU:CD2	16:C:385:SIG:H273	2.35	0.54
1:A:344:ARG:HA	1:A:347:THR:HG22	1.89	0.54
2:B:25:GLU:CB	2:B:213:HIS:ND1	2.67	0.54
2:B:24:LEU:CD2	2:B:24:LEU:H	2.19	0.54
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.54
3:C:130:VAL:HA	3:C:133:VAL:HG23	1.90	0.54
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:230:ILE:CG2	15:E:198:PEE:H172	2.37	0.54
2:B:129:ALA:N	2:B:130:PRO:HD3	2.23	0.54
2:B:260:GLU:O	2:B:261:SER:CB	2.56	0.54
2:B:370:MET:O	2:B:372:VAL:N	2.38	0.54
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.37	0.54
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.25	0.54
4:D:144:ARG:CZ	4:D:147:LEU:HD21	2.37	0.54
4:D:218:LEU:HD11	5:E:42:VAL:CG1	2.37	0.54
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.89	0.54
5:E:26:ARG:C	5:E:28:SER:H	2.10	0.54
8:H:73:LEU:CD2	8:H:77:LEU:HD11	2.38	0.54
1:A:373:THR:HB	1:A:374:PRO:CD	2.38	0.54
3:C:130:VAL:HG12	3:C:131:GLY:N	2.23	0.54
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.89	0.54
3:C:166:TRP:CA	3:C:175:THR:HB	2.37	0.54
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.42	0.54
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.90	0.54
5:E:96:LEU:HD12	5:E:135:LEU:O	2.08	0.54
5:E:32:ARG:HH11	5:E:32:ARG:HG3	1.72	0.54
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.54
10:J:57:HIS:CA	10:J:60:GLU:C	2.74	0.54
2:B:281:ALA:O	2:B:285:VAL:HB	2.07	0.54
3:C:270:LYS:HG3	3:C:270:LYS:O	2.06	0.54
1:A:445:ARG:NH1	10:J:16:ARG:HG2	2.23	0.54
2:B:52:LYS:HB2	2:B:203:ARG:HB2	1.90	0.54
5:E:190:ASP:N	5:E:190:ASP:OD1	2.40	0.54
2:B:170:ASN:C	2:B:170:ASN:HD22	2.11	0.54
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.89	0.54
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.89	0.54
3:C:369:THR:C	3:C:371:GLY:N	2.60	0.54
1:A:41:ILE:HG23	1:A:195:MET:HG2	1.90	0.53
1:A:49:SER:HB2	1:A:52:ASN:HB3	1.89	0.53
2:B:20:HIS:N	2:B:21:PRO:CD	2.71	0.53
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.42	0.53
2:B:171:ALA:O	2:B:172:LEU:HB3	2.09	0.53
3:C:332:ASN:HD21	3:C:359:TYR:HA	1.72	0.53
5:E:29:ASP:C	5:E:31:SER:N	2.60	0.53
10:J:55:ILE:C	10:J:57:HIS:N	2.62	0.53
1:A:65:LYS:HD2	1:A:65:LYS:N	2.23	0.53
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.23	0.53
7:G:25:PRO:O	7:G:26:PHE:C	2.47	0.53
7:G:53:LEU:O	7:G:56:TYR:HB3	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:LEU:O	1:A:298:ALA:N	2.38	0.53
2:B:24:LEU:N	2:B:24:LEU:HD23	2.22	0.53
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.41	0.53
7:G:77:TYR:CZ	8:H:52:GLU:HB2	2.44	0.53
10:J:12:LEU:O	10:J:19:THR:HG21	2.09	0.53
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.42	0.53
1:A:102:LEU:C	1:A:104:LYS:N	2.62	0.53
4:D:47:ALA:HB1	4:D:89:ASP:O	2.08	0.53
5:E:20:TYR:O	5:E:21:SER:O	2.27	0.53
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.39	0.53
1:A:290:SER:N	2:B:90:GLU:OE1	2.40	0.53
2:B:198:HIS:HD2	2:B:203:ARG:HH22	1.57	0.53
3:C:113:THR:HG22	3:C:201:LEU:N	2.24	0.53
3:C:142:TRP:HA	3:C:145:THR:OG1	2.08	0.53
5:E:52:LYS:O	5:E:52:LYS:HD3	2.08	0.53
1:A:19:LEU:C	1:A:21:ASN:N	2.61	0.53
1:A:410:VAL:O	1:A:413:LYS:HB3	2.09	0.53
2:B:166:ALA:HB1	2:B:242:GLY:CA	2.38	0.53
2:B:333:ALA:O	2:B:337:ILE:HG12	2.09	0.53
3:C:81:ARG:NH1	12:C:381:HEM:O2D	2.42	0.53
8:H:40:CYS:O	8:H:44:VAL:HG23	2.09	0.53
4:D:27:ARG:NH2	10:J:59:TYR:CE2	2.77	0.53
1:A:145:MET:CB	1:A:252:HIS:NE2	2.72	0.53
1:A:264:HIS:CD2	1:A:266:ASP:HB2	2.44	0.53
1:A:391:PRO:HG2	1:A:394:GLU:CB	2.34	0.53
2:B:372:VAL:O	2:B:372:VAL:HG12	2.09	0.53
3:C:146:VAL:HG23	3:C:147:ILE:H	1.72	0.53
4:D:27:ARG:NH2	10:J:59:TYR:HE2	2.07	0.53
1:A:362:ARG:HG3	1:A:399:LEU:HD11	1.91	0.53
2:B:202:ALA:CB	2:B:229:GLY:HA2	2.39	0.53
3:C:283:ARG:O	3:C:284:SER:CB	2.57	0.53
1:A:444:LEU:H	1:A:444:LEU:CD1	2.21	0.52
2:B:141:GLN:N	2:B:142:PRO:HD2	2.25	0.52
2:B:242:GLY:O	2:B:423:SER:HA	2.08	0.52
3:C:3:PRO:HG2	3:C:4:ASN:N	2.24	0.52
4:D:224:ARG:HB3	4:D:224:ARG:HH11	1.74	0.52
7:G:26:PHE:HD1	7:G:26:PHE:N	1.96	0.52
1:A:104:LYS:O	1:A:104:LYS:HG2	2.10	0.52
1:A:120:CYS:O	1:A:122:LEU:HG	2.09	0.52
1:A:159:GLN:OE1	1:A:237:THR:HG21	2.09	0.52
1:A:287:GLY:HA2	1:A:299:VAL:HG11	1.92	0.52
1:A:252:HIS:ND1	1:A:325:VAL:HG22	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:361:LYS:NZ	2:B:403:ASP:O	2.42	0.52
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.91	0.52
5:E:21:SER:O	5:E:22:THR:HB	2.09	0.52
2:B:21:PRO:O	2:B:21:PRO:HG2	2.09	0.52
2:B:24:LEU:O	2:B:24:LEU:HG	2.09	0.52
3:C:105:TYR:HA	3:C:315:THR:HA	1.91	0.52
3:C:155:PRO:O	3:C:156:TYR:HB2	2.10	0.52
3:C:271:PRO:HB3	16:C:385:SIG:C3	2.39	0.52
3:C:325:LEU:HD12	3:C:370:ILE:HG13	1.90	0.52
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.49	0.52
7:G:32:LYS:C	7:G:35:PRO:HD2	2.29	0.52
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.16	0.52
1:A:4:TYR:CG	2:B:113:ARG:HB3	2.44	0.52
3:C:277:PHE:CG	3:C:278:ALA:N	2.76	0.52
5:E:28:SER:O	5:E:31:SER:HB3	2.08	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.45	0.52
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.45	0.52
2:B:219:VAL:C	2:B:221:GLU:H	2.13	0.52
3:C:101:ARG:HE	3:C:102:GLY:CA	2.22	0.52
3:C:105:TYR:CE1	3:C:209:PRO:HA	2.44	0.52
3:C:43:MET:O	3:C:44:THR:C	2.48	0.52
10:J:57:HIS:C	10:J:60:GLU:H	2.13	0.52
2:B:250:ASP:C	2:B:252:LEU:H	2.13	0.52
2:B:330:ALA:O	2:B:333:ALA:HB2	2.08	0.52
3:C:107:SER:HB3	12:C:382:HEM:CBD	2.32	0.52
3:C:351:ILE:HG23	7:G:58:LEU:HD21	1.90	0.52
1:A:173:ASN:O	1:A:177:LEU:HG	2.09	0.52
2:B:111:CYS:SG	2:B:116:VAL:HA	2.50	0.52
2:B:406:ALA:O	2:B:408:ALA:N	2.43	0.52
2:B:57:TYR:CD1	2:B:57:TYR:N	2.78	0.52
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.44	0.52
3:C:28:ILE:HB	3:C:225:TYR:OH	2.10	0.52
3:C:31:TRP:CZ3	15:C:384:PEE:C13	2.89	0.52
4:D:29:GLY:HA2	4:D:32:VAL:HG12	1.92	0.52
5:E:123:ASP:O	5:E:127:VAL:HG22	2.09	0.52
2:B:258:VAL:CG1	2:B:259:ALA:H	2.22	0.52
2:B:385:GLN:CD	2:B:392:TYR:HA	2.29	0.52
2:B:405:VAL:CG1	2:B:409:ASP:OD1	2.57	0.52
3:C:169:PHE:O	3:C:170:SER:HB3	2.09	0.52
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.44	0.52
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.87	0.52
1:A:45:SER:HA	1:A:48:GLU:CD	2.29	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.35	0.52
2:B:137:VAL:C	2:B:139:ASP:N	2.63	0.52
2:B:227:ARG:O	2:B:229:GLY:N	2.43	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG11	1.92	0.52
3:C:222:HIS:CB	3:C:223:PRO:CD	2.86	0.52
6:F:26:PHE:O	6:F:31:LEU:HD23	2.10	0.52
1:A:146:ARG:NH2	9:I:206:UNK:HA	2.24	0.52
1:A:72:GLN:O	1:A:73:ASN:C	2.47	0.52
2:B:146:ILE:HG13	2:B:147:ASP:H	1.72	0.52
2:B:290:ASN:CB	2:B:306:PRO:HD2	2.39	0.52
3:C:222:HIS:CG	3:C:223:PRO:N	2.77	0.52
3:C:342:GLN:HB3	3:C:348:PHE:CD2	2.44	0.52
4:D:217:PRO:HG2	4:D:218:LEU:H	1.75	0.52
7:G:56:TYR:O	7:G:59:TYR:HB3	2.10	0.52
7:G:73:ASN:O	7:G:75:ALA:N	2.43	0.52
2:B:248:ASN:ND2	2:B:248:ASN:C	2.63	0.51
4:D:95:TYR:CE2	4:D:104:ALA:HB3	2.44	0.51
4:D:139:THR:HG23	8:H:41:ASP:OD1	2.10	0.51
5:E:136:ILE:O	5:E:136:ILE:HG22	2.10	0.51
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.75	0.51
1:A:257:VAL:HG22	1:A:320:PHE:O	2.11	0.51
1:A:276:ILE:HD11	1:A:349:ILE:HD11	1.90	0.51
1:A:409:GLU:HA	1:A:409:GLU:OE1	2.09	0.51
2:B:310:SER:O	2:B:324:PHE:HB2	2.10	0.51
9:I:203:UNK:O	9:I:204:UNK:C	2.58	0.51
2:B:385:GLN:NE2	2:B:392:TYR:HA	2.25	0.51
3:C:95:ILE:HG23	3:C:96:PHE:N	2.25	0.51
4:D:117:VAL:CG1	4:D:191:ARG:HH21	2.22	0.51
5:E:171:ILE:HD12	5:E:172:ARG:N	2.25	0.51
8:H:50:THR:HG22	8:H:52:GLU:H	1.75	0.51
10:J:57:HIS:C	10:J:59:TYR:H	2.13	0.51
2:B:89:ILE:HD11	2:B:96:LEU:HD12	1.91	0.51
3:C:282:LEU:C	3:C:282:LEU:HD13	2.29	0.51
3:C:372:THR:HA	3:C:375:ASN:HD22	1.74	0.51
5:E:60:SER:C	5:E:62:MET:H	2.14	0.51
8:H:42:GLU:O	8:H:46:SER:HB3	2.11	0.51
1:A:136:ARG:O	1:A:139:GLN:N	2.43	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
3:C:131:GLY:N	3:C:134:LEU:HD13	2.26	0.51
4:D:57:THR:HB	4:D:60:GLU:CB	2.40	0.51
5:E:21:SER:OG	5:E:22:THR:N	2.42	0.51
6:F:84:GLU:CD	6:F:84:GLU:H	2.14	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.93	0.51
1:A:127:ILE:O	1:A:129:LYS:N	2.44	0.51
1:A:389:ARG:HD2	1:A:390:ILE:N	2.25	0.51
2:B:147:ASP:O	2:B:150:VAL:HG22	2.09	0.51
2:B:61:SER:C	2:B:63:LEU:H	2.13	0.51
3:C:261:ASN:ND2	3:C:264:VAL:HB	2.25	0.51
3:C:327:TRP:HE3	3:C:330:VAL:HG11	1.75	0.51
5:E:62:MET:CG	5:E:63:SER:H	2.22	0.51
1:A:106:VAL:HB	1:A:107:PRO:CD	2.41	0.51
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.74	0.51
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.40	0.51
6:F:59:MET:HE3	6:F:59:MET:HA	1.92	0.51
1:A:153:LEU:HD22	1:A:319:LEU:HD13	1.92	0.51
2:B:198:HIS:HD2	2:B:203:ARG:NH2	2.08	0.51
2:B:365:LYS:HE2	2:B:403:ASP:OD1	2.11	0.51
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.51
5:E:10:PHE:CD2	7:G:18:LEU:HD21	2.45	0.51
3:C:166:TRP:C	3:C:166:TRP:CD1	2.84	0.51
5:E:32:ARG:HD3	5:E:32:ARG:O	2.11	0.51
7:G:57:LEU:N	7:G:57:LEU:HD22	2.24	0.51
1:A:266:ASP:C	1:A:268:VAL:N	2.63	0.51
1:A:120:CYS:HB3	1:A:122:LEU:CD2	2.42	0.50
1:A:354:VAL:HG23	1:A:355:LEU:N	2.26	0.50
1:A:434:TYR:O	1:A:438:ARG:HB2	2.11	0.50
1:A:438:ARG:HD3	1:A:438:ARG:C	2.32	0.50
1:A:7:ALA:O	1:A:11:VAL:HG23	2.11	0.50
2:B:217:LYS:O	2:B:219:VAL:N	2.44	0.50
16:C:385:SIG:H353	16:C:385:SIG:H201	1.93	0.50
4:D:116:ILE:HG23	4:D:117:VAL:N	2.26	0.50
5:E:129:LYS:HB2	5:E:187:PHE:CZ	2.47	0.50
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.92	0.50
1:A:365:LEU:HD21	1:A:395:TRP:CB	2.41	0.50
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.42	0.50
3:C:362:ILE:N	3:C:366:LEU:HD23	2.26	0.50
4:D:46:VAL:HG12	4:D:47:ALA:N	2.25	0.50
8:H:17:LEU:HD21	8:H:21:ARG:CZ	2.41	0.50
8:H:17:LEU:O	8:H:21:ARG:HG3	2.11	0.50
1:A:26:ALA:O	1:A:198:ALA:HA	2.10	0.50
4:D:213:GLY:O	4:D:217:PRO:HG3	2.10	0.50
1:A:228:VAL:HG13	1:A:228:VAL:O	2.10	0.50
1:A:36:THR:HG21	1:A:373:THR:OG1	2.12	0.50
3:C:32:TRP:HZ2	3:C:207:ASN:HB3	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:215:LEU:HD11	5:E:47:VAL:CG2	2.42	0.50
4:D:26:ILE:HD13	4:D:192:TRP:HB3	1.93	0.50
5:E:128:LYS:HB2	5:E:187:PHE:HE2	1.75	0.50
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.50
5:E:57:GLN:C	5:E:59:VAL:H	2.14	0.50
1:A:114:ALA:HA	1:A:216:PHE:CE1	2.47	0.50
1:A:33:PRO:O	1:A:103:SER:OG	2.28	0.50
3:C:219:ILE:HB	3:C:224:TYR:CD2	2.46	0.50
4:D:147:LEU:C	4:D:148:TYR:CD1	2.85	0.50
5:E:122:HIS:H	5:E:125:GLU:CD	2.15	0.50
10:J:57:HIS:HA	10:J:60:GLU:CA	2.41	0.50
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.76	0.50
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.50
2:B:82:SER:O	2:B:85:ILE:CG2	2.60	0.50
3:C:187:PRO:HG2	12:C:381:HEM:HMC3	1.94	0.50
4:D:117:VAL:CG1	4:D:191:ARG:NH2	2.75	0.50
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.26	0.50
5:E:62:MET:O	5:E:63:SER:C	2.49	0.50
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.42	0.50
3:C:167:GLY:HA2	3:C:174:PRO:HB2	1.94	0.50
3:C:269:ILE:HG22	16:C:385:SIG:H263	1.94	0.50
5:E:148:ALA:HA	5:E:156:TYR:CD1	2.47	0.50
1:A:366:VAL:C	1:A:368:HIS:H	2.14	0.50
3:C:347:PRO:HG3	7:G:66:PHE:HD1	1.76	0.50
4:D:195:GLU:O	4:D:195:GLU:HG3	2.11	0.50
1:A:4:TYR:C	1:A:6:GLN:N	2.61	0.50
1:A:85:HIS:HA	9:I:314:UNK:CG	2.37	0.50
2:B:171:ALA:O	2:B:172:LEU:CB	2.60	0.50
2:B:406:ALA:O	2:B:407:ASP:C	2.50	0.50
3:C:133:VAL:HG13	3:C:144:ALA:HB2	1.92	0.50
3:C:167:GLY:H	3:C:175:THR:CB	2.24	0.50
3:C:234:THR:HG22	15:E:198:PEE:H201	1.94	0.50
4:D:41:HIS:HB3	4:D:113:LEU:HD13	1.93	0.50
4:D:54:VAL:HG13	4:D:55:CYS:N	2.27	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.93	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.49
2:B:209:LEU:O	2:B:211:VAL:HG13	2.12	0.49
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.93	0.49
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.46	0.49
4:D:216:VAL:N	4:D:217:PRO:HD2	2.27	0.49
10:J:4:THR:O	10:J:5:LEU:C	2.49	0.49
1:A:46:ARG:NH2	1:A:232:SER:O	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:ASN:HB3	2:B:201:SER:CB	2.41	0.49
1:A:100:LYS:HG3	2:B:370:MET:HE1	1.94	0.49
5:E:14:ARG:O	7:G:24:ARG:HG2	2.12	0.49
3:C:166:TRP:O	3:C:167:GLY:C	2.51	0.49
7:G:78:VAL:C	7:G:79:ASN:ND2	2.62	0.49
1:A:92:ARG:NH1	1:A:165:GLN:O	2.45	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.48	0.49
2:B:316:TYR:HB2	2:B:319:SER:O	2.13	0.49
3:C:131:GLY:H	3:C:134:LEU:HD13	1.78	0.49
3:C:45:GLN:CB	12:C:381:HEM:HAB	2.43	0.49
1:A:245:GLU:CG	7:G:11:ARG:HG2	2.35	0.49
8:H:15:ASP:O	8:H:17:LEU:N	2.45	0.49
1:A:92:ARG:HH12	1:A:166:SER:HA	1.77	0.49
1:A:365:LEU:HD13	1:A:392:LEU:HD22	1.93	0.49
1:A:443:TRP:C	1:A:445:ARG:N	2.64	0.49
2:B:150:VAL:CG2	2:B:151:ALA:N	2.75	0.49
2:B:24:LEU:HD21	2:B:392:TYR:CD2	2.47	0.49
3:C:101:ARG:NH1	12:C:382:HEM:O2A	2.32	0.49
5:E:97:PHE:O	5:E:134:ILE:HG23	2.13	0.49
5:E:65:SER:O	5:E:67:ASP:N	2.45	0.49
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.47	0.49
1:A:298:ALA:HA	1:A:303:LEU:HD12	1.95	0.49
1:A:86:LEU:HB2	1:A:99:ILE:HG12	1.94	0.49
3:C:101:ARG:HE	3:C:102:GLY:N	2.09	0.49
3:C:362:ILE:CA	3:C:366:LEU:HD23	2.42	0.49
3:C:31:TRP:CE3	15:C:384:PEE:H111	2.47	0.49
5:E:25:SER:O	5:E:28:SER:HB3	2.13	0.49
8:H:17:LEU:HD13	8:H:73:LEU:CD1	2.43	0.49
1:A:34:THR:HA	1:A:102:LEU:HA	1.94	0.49
3:C:327:TRP:CA	3:C:330:VAL:HG12	2.32	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
2:B:146:ILE:O	2:B:147:ASP:C	2.50	0.49
2:B:318:ASP:O	2:B:319:SER:HB2	2.12	0.49
3:C:70:THR:HA	3:C:74:VAL:CG2	2.41	0.49
4:D:10:TYR:CD1	4:D:10:TYR:N	2.81	0.49
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.48	0.49
4:D:222:MET:HE1	5:E:40:THR:HG23	1.94	0.49
1:A:436:ARG:HH22	3:C:20:ILE:HG22	1.77	0.49
2:B:140:LEU:C	2:B:142:PRO:HD2	2.32	0.49
2:B:152:PHE:HA	2:B:157:THR:HG21	1.94	0.49
2:B:67:HIS:O	2:B:70:ARG:HB3	2.12	0.49
3:C:220:PRO:HG2	3:C:223:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:344:VAL:HB	3:C:349:ILE:HD11	1.95	0.49
6:F:61:ARG:NH1	6:F:61:ARG:HG3	2.28	0.49
7:G:25:PRO:HG2	7:G:26:PHE:HD1	1.77	0.49
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.46	0.49
1:A:443:TRP:O	1:A:445:ARG:N	2.36	0.49
2:B:385:GLN:C	2:B:387:LEU:H	2.16	0.49
2:B:429:ASN:O	2:B:431:GLY:N	2.46	0.49
4:D:235:LEU:CD1	6:F:64:ARG:HA	2.43	0.49
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.95	0.49
7:G:34:VAL:N	7:G:35:PRO:CD	2.76	0.49
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.13	0.48
2:B:385:GLN:C	2:B:387:LEU:N	2.66	0.48
3:C:163:GLU:HB3	3:C:169:PHE:CD1	2.48	0.48
3:C:207:ASN:C	3:C:207:ASN:HD22	2.15	0.48
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.95	0.48
3:C:60:THR:HG23	3:C:136:TRP:CZ3	2.48	0.48
3:C:81:ARG:HG3	3:C:81:ARG:HH11	1.77	0.48
4:D:215:LEU:HD11	5:E:47:VAL:HG23	1.95	0.48
7:G:49:ALA:O	7:G:50:PRO:C	2.51	0.48
3:C:215:ASP:HB3	7:G:7:LEU:HB3	1.93	0.48
1:A:152:TYR:HA	1:A:155:ALA:HB3	1.94	0.48
2:B:120:MET:O	2:B:121:GLU:C	2.51	0.48
3:C:133:VAL:O	3:C:136:TRP:HD1	1.96	0.48
3:C:138:GLN:HA	3:C:138:GLN:NE2	2.28	0.48
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.48	0.48
1:A:45:SER:HB3	1:A:167:VAL:HA	1.96	0.48
1:A:369:LEU:HD22	1:A:375:VAL:HA	1.95	0.48
1:A:374:PRO:O	1:A:377:GLU:HB3	2.13	0.48
1:A:397:GLU:O	1:A:398:ARG:C	2.51	0.48
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.95	0.48
5:E:9:ASN:CG	5:E:11:SER:HB3	2.32	0.48
2:B:399:LEU:O	2:B:402:ILE:HG22	2.14	0.48
2:B:429:ASN:C	2:B:431:GLY:H	2.17	0.48
3:C:127:THR:HG22	3:C:186:LEU:CB	2.41	0.48
3:C:42:LEU:CD2	3:C:190:ILE:HG22	2.43	0.48
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.94	0.48
3:C:238:THR:CB	4:D:212:MET:HG3	2.43	0.48
5:E:14:ARG:O	5:E:15:ARG:C	2.52	0.48
1:A:85:HIS:CG	9:I:314:UNK:HG1	2.49	0.48
2:B:84:LYS:O	2:B:88:GLY:N	2.44	0.48
3:C:167:GLY:CA	3:C:174:PRO:HB2	2.44	0.48
3:C:196:ILE:O	3:C:199:THR:HB	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:181:GLN:HE21	4:D:181:GLN:C	2.16	0.48
4:D:44:ASP:O	4:D:90:TYR:CD2	2.63	0.48
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.94	0.48
1:A:240:GLN:HB2	1:A:422:VAL:HG12	1.93	0.48
3:C:157:ILE:O	3:C:161:LEU:HB2	2.12	0.48
3:C:207:ASN:C	3:C:207:ASN:ND2	2.65	0.48
3:C:361:THR:HA	3:C:365:ILE:HG22	1.95	0.48
5:E:65:SER:C	5:E:67:ASP:N	2.67	0.48
1:A:58:PHE:HD1	1:A:58:PHE:O	1.97	0.48
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.14	0.48
3:C:283:ARG:NH2	3:C:342:GLN:O	2.46	0.48
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.96	0.48
6:F:101:ARG:CB	6:F:104:ARG:HH21	2.27	0.48
1:A:30:SER:O	1:A:202:GLY:HA2	2.13	0.48
1:A:444:LEU:O	1:A:445:ARG:C	2.52	0.48
2:B:113:ARG:HG3	2:B:114:ASP:H	1.77	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.44	0.48
2:B:131:GLU:O	2:B:132:PHE:C	2.51	0.48
4:D:214:LEU:O	4:D:217:PRO:HG2	2.14	0.48
5:E:83:GLU:HG3	5:E:100:HIS:NE2	2.29	0.48
10:J:61:ASN:O	10:J:62:LYS:CB	2.62	0.48
1:A:46:ARG:HG2	1:A:231:LEU:HD13	1.94	0.48
3:C:19:LEU:HD12	3:C:19:LEU:N	2.28	0.48
4:D:98:PRO:HG2	4:D:99:GLU:OE2	2.13	0.48
5:E:55:VAL:O	5:E:59:VAL:HG23	2.13	0.48
2:B:143:GLN:CD	2:B:146:ILE:HD11	2.33	0.48
2:B:275:LEU:O	2:B:279:LEU:HB2	2.13	0.48
3:C:285:ILE:N	3:C:286:PRO:HD3	2.29	0.48
4:D:165:TYR:H	4:D:168:VAL:CG2	2.26	0.48
3:C:219:ILE:HD13	4:D:230:LEU:CD1	2.43	0.48
5:E:136:ILE:HB	5:E:181:GLU:HB3	1.94	0.48
4:D:232:SER:HB2	7:G:23:GLN:OE1	2.14	0.48
2:B:353:SER:C	2:B:355:GLU:H	2.17	0.47
2:B:395:PRO:C	2:B:398:VAL:HG12	2.35	0.47
3:C:182:LEU:CD2	16:C:385:SIG:H381	2.44	0.47
3:C:342:GLN:CA	3:C:342:GLN:HE21	2.11	0.47
4:D:51:LEU:O	4:D:54:VAL:HG12	2.14	0.47
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.35	0.47
1:A:166:SER:HG	5:E:3:THR:HG23	1.73	0.47
2:B:111:CYS:SG	2:B:119:LEU:HD23	2.54	0.47
2:B:406:ALA:C	2:B:408:ALA:N	2.66	0.47
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:62:MET:CG	5:E:63:SER:N	2.77	0.47
8:H:68:CYS:O	8:H:69:VAL:C	2.53	0.47
8:H:73:LEU:HD21	8:H:77:LEU:HD11	1.96	0.47
1:A:287:GLY:CA	1:A:299:VAL:HG11	2.44	0.47
2:B:89:ILE:CD1	2:B:96:LEU:HD12	2.44	0.47
4:D:158:ILE:HG22	4:D:160:MET:N	2.14	0.47
4:D:235:LEU:O	4:D:236:ALA:HB2	2.15	0.47
5:E:171:ILE:HG12	5:E:176:ALA:HB3	1.96	0.47
5:E:52:LYS:CD	5:E:52:LYS:C	2.82	0.47
2:B:170:ASN:N	2:B:170:ASN:HD22	2.12	0.47
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.43	0.47
2:B:250:ASP:O	2:B:251:SER:HB3	2.15	0.47
4:D:147:LEU:N	4:D:147:LEU:HD22	2.29	0.47
7:G:63:THR:O	7:G:64:GLN:C	2.52	0.47
8:H:50:THR:HG22	8:H:52:GLU:N	2.29	0.47
1:A:382:GLU:O	1:A:386:TYR:N	2.43	0.47
2:B:288:GLY:O	2:B:290:ASN:CB	2.63	0.47
3:C:148:THR:HB	3:C:166:TRP:CZ3	2.49	0.47
3:C:167:GLY:H	3:C:175:THR:CA	2.27	0.47
7:G:25:PRO:HG2	7:G:26:PHE:CD1	2.49	0.47
1:A:145:MET:HA	1:A:148:VAL:HG13	1.96	0.47
1:A:152:TYR:O	1:A:155:ALA:HB3	2.13	0.47
1:A:253:VAL:HG11	1:A:335:MET:CE	2.45	0.47
3:C:198:LEU:HD21	12:C:382:HEM:CMA	2.44	0.47
3:C:262:PRO:C	3:C:263:LEU:HD12	2.35	0.47
3:C:32:TRP:CZ3	3:C:209:PRO:HD3	2.49	0.47
6:F:67:ASP:OD1	6:F:71:ARG:CZ	2.62	0.47
1:A:344:ARG:CA	1:A:347:THR:HG22	2.45	0.47
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.47
2:B:225:ASN:O	2:B:226:ILE:HG13	2.14	0.47
2:B:250:ASP:O	2:B:252:LEU:CD2	2.59	0.47
2:B:353:SER:C	2:B:355:GLU:N	2.68	0.47
3:C:356:SER:O	3:C:357:LEU:HB2	2.14	0.47
3:C:92:PHE:CZ	3:C:124:LEU:CD1	2.97	0.47
7:G:60:THR:O	7:G:61:TRP:C	2.52	0.47
2:B:209:LEU:O	2:B:211:VAL:N	2.48	0.47
2:B:96:LEU:CD2	2:B:96:LEU:C	2.83	0.47
3:C:162:VAL:O	3:C:164:TRP:N	2.42	0.47
5:E:153:PHE:CD2	5:E:172:ARG:HG3	2.49	0.47
1:A:306:SER:HB2	9:I:206:UNK:CB	2.45	0.47
10:J:57:HIS:CB	10:J:61:ASN:C	2.72	0.47
1:A:265:PRO:O	1:A:268:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:209:LEU:O	2:B:211:VAL:HG22	2.15	0.47
3:C:78:TRP:CD2	3:C:79:LEU:N	2.83	0.47
4:D:160:MET:HB2	12:D:243:HEM:C1D	2.50	0.47
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.50	0.47
7:G:29:TYR:O	7:G:30:PHE:CB	2.59	0.47
2:B:112:LEU:O	2:B:113:ARG:C	2.54	0.47
15:C:384:PEE:H52	6:F:69:ASN:OD1	2.15	0.47
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.96	0.47
5:E:42:VAL:O	5:E:45:LEU:HB3	2.15	0.47
1:A:431:LEU:HD23	1:A:432:PRO:N	2.30	0.47
2:B:277:HIS:CE1	2:B:364:LEU:CD2	2.97	0.47
1:A:436:ARG:HH11	3:C:223:PRO:HD2	1.80	0.47
3:C:295:LEU:HD11	16:C:385:SIG:H273	1.97	0.47
4:D:75:ASN:ND2	4:D:79:GLU:H	2.13	0.47
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.20	0.47
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46
1:A:235:ARG:HD3	5:E:21:SER:N	2.28	0.46
4:D:192:TRP:CD1	4:D:192:TRP:C	2.86	0.46
7:G:71:ARG:NH2	8:H:60:ASP:OD2	2.49	0.46
1:A:100:LYS:HB2	1:A:100:LYS:HZ2	1.80	0.46
1:A:420:PRO:HD3	1:A:441:MET:HG3	1.96	0.46
2:B:199:PHE:C	2:B:204:MET:HE3	2.35	0.46
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.49	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.51	0.46
3:C:353:GLN:HA	3:C:356:SER:HB3	1.97	0.46
3:C:40:VAL:HG11	3:C:233:LEU:HD21	1.96	0.46
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.50	0.46
5:E:18:ASP:HB3	5:E:28:SER:OG	2.15	0.46
2:B:166:ALA:O	2:B:242:GLY:HA3	2.15	0.46
2:B:264:ILE:C	2:B:266:GLY:H	2.18	0.46
2:B:82:SER:O	2:B:85:ILE:HG22	2.15	0.46
3:C:354:MET:HE3	3:C:354:MET:HA	1.94	0.46
4:D:138:PRO:HD3	8:H:58:LEU:CD2	2.46	0.46
10:J:32:GLU:O	10:J:33:ARG:C	2.53	0.46
1:A:250:LEU:CD2	1:A:251:ALA:N	2.77	0.46
2:B:307:PHE:CD2	2:B:308:ASP:N	2.83	0.46
2:B:307:PHE:CG	2:B:308:ASP:N	2.80	0.46
3:C:167:GLY:N	3:C:175:THR:HG22	2.31	0.46
4:D:165:TYR:CZ	4:D:168:VAL:HG22	2.50	0.46
5:E:57:GLN:O	5:E:59:VAL:N	2.47	0.46
7:G:78:VAL:HG12	7:G:78:VAL:O	2.15	0.46
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:248:ASN:HD21	2:B:428:GLY:CA	2.26	0.46
2:B:275:LEU:HD12	2:B:275:LEU:O	2.15	0.46
3:C:211:GLY:CA	3:C:315:THR:HG23	2.46	0.46
10:J:52:TRP:O	10:J:56:LYS:N	2.45	0.46
1:A:161:THR:HG21	1:A:235:ARG:N	2.29	0.46
1:A:64:PHE:O	1:A:75:LEU:HD23	2.15	0.46
3:C:103:LEU:C	3:C:103:LEU:HD13	2.35	0.46
3:C:168:GLY:O	3:C:169:PHE:HD1	1.98	0.46
3:C:30:ALA:C	3:C:32:TRP:H	2.19	0.46
3:C:369:THR:O	3:C:370:ILE:C	2.54	0.46
3:C:95:ILE:CG2	3:C:96:PHE:N	2.78	0.46
5:E:188:THR:CG2	5:E:194:ILE:HD12	2.45	0.46
1:A:436:ARG:HD3	3:C:223:PRO:HG3	1.98	0.46
3:C:102:GLY:HA2	3:C:107:SER:HB2	1.97	0.46
3:C:113:THR:O	3:C:197:HIS:CE1	2.69	0.46
7:G:26:PHE:N	7:G:26:PHE:CD1	2.68	0.46
1:A:120:CYS:HB3	1:A:122:LEU:HD21	1.97	0.46
1:A:39:VAL:HG22	1:A:41:ILE:HD13	1.98	0.46
2:B:170:ASN:O	2:B:171:ALA:O	2.33	0.46
3:C:147:ILE:O	3:C:150:LEU:CB	2.63	0.46
3:C:210:LEU:HB3	3:C:212:ILE:HG12	1.97	0.46
4:D:160:MET:HB2	12:D:243:HEM:C2D	2.51	0.46
5:E:32:ARG:HH22	7:G:25:PRO:HD2	1.81	0.46
5:E:36:SER:OG	7:G:21:PHE:HE1	1.99	0.46
1:A:106:VAL:HG13	1:A:208:LEU:HD13	1.98	0.46
1:A:399:LEU:HA	1:A:402:VAL:HG23	1.97	0.46
2:B:342:ASN:O	2:B:345:LYS:HB3	2.16	0.46
2:B:92:VAL:HG12	2:B:92:VAL:O	2.14	0.46
3:C:207:ASN:HB3	12:C:382:HEM:O1D	2.16	0.46
3:C:234:THR:HB	4:D:216:VAL:HG12	1.97	0.46
4:D:233:ARG:HB3	6:F:71:ARG:NH2	2.30	0.46
10:J:13:LEU:HG	10:J:23:THR:HG21	1.98	0.46
1:A:197:LEU:HD23	1:A:216:PHE:HE2	1.80	0.46
2:B:47:ILE:HG22	2:B:48:GLY:N	2.31	0.46
4:D:113:LEU:HD12	4:D:113:LEU:N	2.30	0.46
5:E:25:SER:O	5:E:26:ARG:O	2.34	0.46
5:E:38:LEU:O	5:E:42:VAL:HG23	2.16	0.46
2:B:162:ASN:O	2:B:163:LEU:C	2.54	0.45
2:B:38:LEU:O	2:B:38:LEU:HG	2.15	0.45
2:B:436:VAL:C	2:B:438:GLU:H	2.19	0.45
3:C:146:VAL:CG2	3:C:147:ILE:N	2.78	0.45
3:C:287:ASN:OD1	3:C:289:LEU:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:46:ILE:O	3:C:50:LEU:HB2	2.16	0.45
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.50	0.45
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.43	0.45
6:F:89:TYR:CD1	6:F:89:TYR:C	2.90	0.45
2:B:405:VAL:CG1	2:B:406:ALA:N	2.79	0.45
2:B:424:MET:HG2	2:B:425:ALA:N	2.31	0.45
4:D:149:PHE:CE2	4:D:151:PRO:HD3	2.51	0.45
6:F:29:TYR:HB2	6:F:31:LEU:HD21	1.98	0.45
6:F:70:MET:SD	6:F:70:MET:C	2.95	0.45
5:E:45:LEU:HD21	10:J:28:ALA:N	2.30	0.45
1:A:129:LYS:O	1:A:133:VAL:HG23	2.15	0.45
1:A:430:GLN:O	1:A:430:GLN:HG2	2.16	0.45
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.98	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45
3:C:324:THR:O	3:C:325:LEU:C	2.55	0.45
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.52	0.45
5:E:118:ARG:NH1	5:E:174:GLY:O	2.38	0.45
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.52	0.45
1:A:266:ASP:C	1:A:268:VAL:H	2.18	0.45
1:A:332:ASP:O	1:A:333:ASP:C	2.53	0.45
1:A:394:GLU:O	1:A:395:TRP:C	2.54	0.45
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.97	0.45
2:B:152:PHE:HA	2:B:157:THR:CG2	2.47	0.45
2:B:372:VAL:O	2:B:378:PHE:HB2	2.16	0.45
3:C:130:VAL:CG1	3:C:183:HIS:HB2	2.47	0.45
3:C:285:ILE:O	3:C:285:ILE:HG13	2.17	0.45
3:C:369:THR:O	3:C:371:GLY:N	2.49	0.45
3:C:72:ARG:NE	4:D:115:TYR:OH	2.50	0.45
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.51	0.45
4:D:213:GLY:O	4:D:217:PRO:CD	2.64	0.45
5:E:128:LYS:HB2	5:E:187:PHE:CE2	2.52	0.45
5:E:29:ASP:N	5:E:30:PRO:HD2	2.31	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45
4:D:235:LEU:HD12	6:F:64:ARG:HA	1.98	0.45
1:A:349:ILE:HD12	1:A:407:VAL:HG11	1.99	0.45
1:A:33:PRO:CG	1:A:34:THR:H	2.20	0.45
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.99	0.45
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.16	0.45
3:C:277:PHE:CD2	3:C:278:ALA:N	2.85	0.45
3:C:350:ILE:HA	3:C:353:GLN:HE21	1.81	0.45
4:D:113:LEU:CD1	4:D:113:LEU:N	2.80	0.45
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.46	0.45
7:G:71:ARG:CZ	8:H:56:GLU:OE2	2.65	0.45
1:A:105:ASP:O	1:A:106:VAL:C	2.55	0.45
2:B:135:TRP:CD1	2:B:135:TRP:N	2.84	0.45
3:C:101:ARG:HE	3:C:102:GLY:HA2	1.81	0.45
3:C:12:LEU:HD23	3:C:12:LEU:C	2.37	0.45
1:A:436:ARG:HD3	3:C:223:PRO:CG	2.47	0.45
3:C:354:MET:O	3:C:357:LEU:HB3	2.16	0.45
4:D:232:SER:O	4:D:233:ARG:O	2.34	0.45
6:F:96:GLU:OE1	6:F:96:GLU:HA	2.16	0.45
1:A:210:GLU:O	1:A:214:LYS:HB2	2.17	0.45
1:A:346:CYS:HB2	1:A:412:SER:HB3	1.99	0.45
3:C:166:TRP:O	3:C:167:GLY:O	2.34	0.45
8:H:15:ASP:C	8:H:17:LEU:N	2.68	0.45
2:B:137:VAL:CG2	2:B:138:ALA:H	2.30	0.45
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.99	0.45
2:B:56:ARG:NH1	2:B:172:LEU:HD13	2.32	0.45
1:A:292:SER:O	1:A:295:ALA:HB3	2.17	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.98	0.45
4:D:34:LYS:O	4:D:34:LYS:HG2	2.15	0.45
4:D:57:THR:HG22	4:D:58:GLU:N	2.32	0.45
5:E:134:ILE:HD12	5:E:185:TYR:CD1	2.52	0.45
1:A:127:ILE:HG22	1:A:128:GLU:N	2.32	0.45
1:A:444:LEU:C	1:A:445:ARG:O	2.53	0.45
2:B:225:ASN:O	2:B:226:ILE:CG1	2.65	0.45
2:B:200:THR:HG22	2:B:226:ILE:HG21	1.99	0.45
2:B:24:LEU:HD11	2:B:392:TYR:CD2	2.51	0.45
3:C:101:ARG:HD2	3:C:101:ARG:O	2.16	0.45
3:C:323:GLN:O	3:C:326:PHE:HB3	2.17	0.45
3:C:82:ASN:HD22	3:C:82:ASN:N	2.15	0.45
4:D:124:GLU:O	4:D:125:ASP:C	2.55	0.45
4:D:37:CYS:O	4:D:39:SER:N	2.50	0.45
6:F:71:ARG:O	6:F:72:GLN:HB2	2.17	0.45
5:E:16:PRO:CD	7:G:22:GLU:O	2.65	0.45
1:A:178:SER:O	1:A:182:LEU:HD23	2.17	0.44
2:B:38:LEU:HD12	2:B:38:LEU:C	2.37	0.44
4:D:168:VAL:HG12	4:D:168:VAL:O	2.17	0.44
4:D:72:ASP:O	4:D:73:GLY:O	2.34	0.44
6:F:12:TRP:CA	6:F:12:TRP:CE3	3.00	0.44
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.99	0.44
1:A:381:ARG:O	1:A:382:GLU:C	2.56	0.44
2:B:217:LYS:C	2:B:219:VAL:N	2.70	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:238:THR:N	3:C:239:PRO:CD	2.80	0.44
3:C:349:ILE:CG2	3:C:350:ILE:HD13	2.44	0.44
3:C:359:TYR:HD2	3:C:360:PHE:CE1	2.34	0.44
4:D:102:ARG:NH1	4:D:109:LEU:CB	2.77	0.44
5:E:15:ARG:HA	5:E:16:PRO:HD3	1.79	0.44
6:F:102:LYS:HB3	6:F:102:LYS:HE2	1.72	0.44
10:J:57:HIS:CE1	10:J:62:LYS:OXT	2.70	0.44
1:A:382:GLU:CG	1:A:389:ARG:HA	2.39	0.44
2:B:225:ASN:C	2:B:226:ILE:HG13	2.38	0.44
1:A:100:LYS:HG3	2:B:370:MET:CE	2.48	0.44
3:C:295:LEU:CG	16:C:385:SIG:H273	2.47	0.44
14:C:383:U10:C1M	14:C:383:U10:H8	2.47	0.44
4:D:33:TYR:HA	4:D:37:CYS:SG	2.58	0.44
1:A:65:LYS:HZ1	9:I:311:UNK:HA	1.77	0.44
1:A:178:SER:O	1:A:179:ARG:C	2.55	0.44
3:C:282:LEU:C	3:C:282:LEU:CD1	2.86	0.44
3:C:349:ILE:HG22	3:C:350:ILE:N	2.32	0.44
3:C:95:ILE:HD13	3:C:121:LEU:HD12	2.00	0.44
5:E:121:GLN:HA	5:E:125:GLU:OE2	2.17	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
1:A:294:LEU:O	1:A:298:ALA:HB2	2.18	0.44
2:B:157:THR:HG23	2:B:158:HIS:N	2.32	0.44
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.32	0.44
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.44
3:C:154:ILE:HG22	3:C:157:ILE:HG22	2.00	0.44
3:C:247:SER:O	3:C:250:LEU:HB2	2.17	0.44
3:C:139:MET:HE2	3:C:255:GLU:HB3	2.00	0.44
3:C:267:PRO:O	3:C:268:HIS:HB2	2.17	0.44
7:G:73:ASN:O	7:G:74:PRO:C	2.56	0.44
10:J:13:LEU:HA	10:J:19:THR:HG22	1.98	0.44
1:A:140:GLU:O	1:A:142:ASP:N	2.51	0.44
1:A:290:SER:HB3	2:B:90:GLU:OE1	2.18	0.44
4:D:37:CYS:C	4:D:39:SER:H	2.21	0.44
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.99	0.44
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.53	0.44
7:G:57:LEU:CD2	7:G:57:LEU:H	2.31	0.44
1:A:111:GLU:HB2	1:A:215:HIS:CD2	2.52	0.44
1:A:153:LEU:HD21	1:A:319:LEU:HD13	1.98	0.44
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.86	0.44
2:B:112:LEU:HD23	2:B:112:LEU:N	2.33	0.44
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.44
3:C:30:ALA:O	3:C:32:TRP:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:95:TYR:CG	4:D:101:ALA:HB2	2.52	0.44
6:F:59:MET:HA	6:F:59:MET:HE2	1.97	0.44
6:F:71:ARG:O	6:F:72:GLN:CB	2.65	0.44
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.81	0.44
10:J:38:GLY:O	10:J:42:ILE:HG13	2.18	0.44
10:J:52:TRP:O	10:J:56:LYS:HB2	2.18	0.44
2:B:199:PHE:CA	2:B:204:MET:HE2	2.46	0.44
2:B:213:HIS:HD2	2:B:213:HIS:O	2.01	0.44
2:B:258:VAL:CG1	2:B:322:PHE:N	2.75	0.44
3:C:100:GLY:O	3:C:101:ARG:C	2.56	0.44
3:C:132:TYR:HA	12:C:381:HEM:HAA2	2.00	0.44
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.00	0.44
2:B:111:CYS:C	2:B:112:LEU:HD23	2.37	0.44
2:B:253:VAL:HG12	2:B:254:HIS:N	2.33	0.44
3:C:133:VAL:HG13	3:C:140:SER:O	2.18	0.44
3:C:148:THR:HG22	3:C:162:VAL:HG13	2.00	0.44
3:C:87:GLY:O	3:C:88:ALA:C	2.56	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.52	0.44
7:G:24:ARG:HA	7:G:25:PRO:HD2	1.57	0.44
8:H:50:THR:CG2	8:H:52:GLU:H	2.31	0.44
2:B:207:VAL:HG12	2:B:208:GLY:N	2.33	0.43
2:B:120:MET:HE2	2:B:219:VAL:HG11	2.00	0.43
3:C:130:VAL:HA	3:C:133:VAL:CG2	2.47	0.43
3:C:142:TRP:CE2	3:C:265:THR:HG22	2.52	0.43
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.13	0.43
3:C:45:GLN:HB3	12:C:381:HEM:HAB	2.00	0.43
4:D:148:TYR:CD1	4:D:148:TYR:N	2.86	0.43
4:D:29:GLY:O	4:D:32:VAL:HG12	2.18	0.43
5:E:188:THR:HG21	5:E:194:ILE:HD12	2.00	0.43
1:A:252:HIS:HB3	1:A:323:TYR:CE1	2.44	0.43
1:A:158:PHE:CZ	1:A:319:LEU:HD21	2.53	0.43
2:B:219:VAL:C	2:B:221:GLU:N	2.71	0.43
2:B:280:GLY:O	2:B:281:ALA:C	2.56	0.43
2:B:89:ILE:CD1	2:B:96:LEU:HB2	2.45	0.43
3:C:361:THR:C	3:C:363:LEU:N	2.71	0.43
3:C:38:LEU:HD21	3:C:95:ILE:N	2.34	0.43
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.52	0.43
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.33	0.43
8:H:47:ARG:HD2	8:H:49:GLN:H	1.83	0.43
2:B:325:TYR:OH	9:I:119:UNK:HA	2.18	0.43
1:A:228:VAL:HA	1:A:229:PRO:HD2	1.82	0.43
3:C:214:SER:HA	6:F:66:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:354:MET:HE2	3:C:354:MET:HA	1.96	0.43
4:D:197:GLU:O	4:D:199:ASP:N	2.51	0.43
5:E:76:ILE:HD13	5:E:98:VAL:HG21	2.00	0.43
6:F:73:GLN:OE1	7:G:36:ASN:ND2	2.51	0.43
1:A:17:SER:OG	1:A:209:LEU:CD2	2.67	0.43
1:A:45:SER:CA	1:A:48:GLU:HG3	2.46	0.43
1:A:4:TYR:O	1:A:5:ALA:C	2.56	0.43
2:B:279:LEU:HD11	2:B:344:VAL:HG13	2.00	0.43
2:B:436:VAL:C	2:B:438:GLU:N	2.72	0.43
3:C:132:TYR:O	3:C:135:PRO:HD2	2.17	0.43
3:C:328:LEU:HA	3:C:328:LEU:HD12	1.83	0.43
4:D:28:ARG:CD	4:D:171:PHE:CD2	3.01	0.43
10:J:57:HIS:C	10:J:59:TYR:N	2.72	0.43
1:A:126:GLN:O	1:A:130:GLU:HG2	2.19	0.43
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.83	0.43
1:A:281:ASP:O	1:A:284:TYR:CD1	2.71	0.43
14:C:383:U10:H161	14:C:383:U10:H121	1.89	0.43
5:E:148:ALA:HB2	5:E:156:TYR:HE1	1.82	0.43
10:J:13:LEU:H	10:J:13:LEU:CD1	2.31	0.43
1:A:365:LEU:HD21	1:A:395:TRP:CG	2.53	0.43
1:A:438:ARG:CD	1:A:438:ARG:C	2.87	0.43
1:A:53:ASN:HD22	1:A:54:GLY:N	2.15	0.43
2:B:111:CYS:SG	2:B:119:LEU:CD2	3.07	0.43
3:C:235:LEU:C	3:C:237:LEU:H	2.22	0.43
5:E:171:ILE:HD11	5:E:173:LYS:O	2.18	0.43
1:A:156:THR:CA	5:E:7:VAL:HG21	2.47	0.43
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.54	0.43
1:A:35:CYS:HB2	1:A:200:ALA:O	2.17	0.43
2:B:22:GLN:O	2:B:23:ASP:C	2.57	0.43
6:F:73:GLN:HA	7:G:39:ARG:HH12	1.83	0.43
2:B:111:CYS:C	2:B:112:LEU:CD2	2.87	0.43
3:C:134:LEU:HD21	3:C:180:PHE:HD1	1.83	0.43
3:C:261:ASN:ND2	3:C:264:VAL:CB	2.82	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.89	0.43
1:A:310:PHE:CE1	1:A:322:PHE:N	2.87	0.43
1:A:344:ARG:HH11	1:A:344:ARG:HG3	1.83	0.43
2:B:130:PRO:CB	2:B:132:PHE:CE1	3.02	0.43
2:B:137:VAL:C	2:B:139:ASP:H	2.22	0.43
2:B:170:ASN:O	2:B:173:ALA:HB3	2.19	0.43
2:B:253:VAL:CG1	2:B:254:HIS:N	2.81	0.43
2:B:371:SER:O	2:B:372:VAL:HG23	2.19	0.43
2:B:45:SER:OG	2:B:116:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:295:LEU:O	3:C:296:ALA:C	2.56	0.43
4:D:138:PRO:HD3	8:H:58:LEU:HD22	2.01	0.43
5:E:83:GLU:HG3	5:E:100:HIS:CE1	2.53	0.43
2:B:259:ALA:O	2:B:260:GLU:C	2.58	0.43
2:B:82:SER:C	2:B:85:ILE:HG22	2.39	0.43
3:C:108:TYR:HB2	3:C:306:PRO:HG3	2.00	0.43
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.83	0.43
3:C:171:VAL:HA	3:C:175:THR:HG21	2.01	0.43
3:C:210:LEU:HA	3:C:210:LEU:HD23	1.76	0.43
3:C:58:ALA:O	3:C:59:ASP:HB2	2.19	0.43
3:C:5:ILE:HA	3:C:8:SER:OG	2.19	0.43
5:E:26:ARG:O	5:E:27:GLU:CG	2.67	0.43
4:D:235:LEU:HD22	6:F:63:LYS:HE2	2.00	0.43
7:G:71:ARG:NH2	8:H:56:GLU:OE2	2.52	0.43
8:H:35:GLU:O	8:H:39:LEU:CD1	2.67	0.43
10:J:36:ASP:O	10:J:37:GLN:C	2.56	0.43
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.81	0.42
1:A:19:LEU:HB2	1:A:21:ASN:HB3	2.00	0.42
3:C:250:LEU:HB3	3:C:251:LEU:HD12	2.01	0.42
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.42
2:B:189:VAL:O	2:B:191:LEU:N	2.52	0.42
3:C:366:LEU:N	3:C:366:LEU:HD22	2.33	0.42
3:C:88:ALA:O	3:C:91:PHE:HB3	2.19	0.42
4:D:105:ASN:O	4:D:107:GLY:N	2.52	0.42
4:D:153:PHE:HB2	4:D:158:ILE:HD11	2.01	0.42
4:D:47:ALA:HB2	4:D:90:TYR:HA	2.02	0.42
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.87	0.42
7:G:71:ARG:HH21	8:H:56:GLU:CG	2.32	0.42
1:A:120:CYS:CB	1:A:122:LEU:HD21	2.50	0.42
2:B:170:ASN:O	2:B:171:ALA:C	2.57	0.42
2:B:71:LEU:C	2:B:73:SER:H	2.22	0.42
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.54	0.42
3:C:24:ALA:O	3:C:218:LYS:HA	2.20	0.42
3:C:43:MET:CE	3:C:43:MET:CA	2.96	0.42
5:E:91:TRP:O	5:E:94:LYS:O	2.37	0.42
7:G:40:ARG:O	7:G:41:LEU:C	2.56	0.42
1:A:274:ASN:O	1:A:309:THR:HG21	2.20	0.42
2:B:120:MET:O	2:B:123:LEU:N	2.52	0.42
2:B:22:GLN:O	2:B:23:ASP:O	2.37	0.42
2:B:258:VAL:HA	2:B:322:PHE:O	2.20	0.42
3:C:158:GLY:O	3:C:160:THR:N	2.52	0.42
4:D:217:PRO:O	4:D:220:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.18	0.42
6:F:45:GLU:HA	6:F:45:GLU:OE1	2.19	0.42
8:H:66:ASP:HA	8:H:69:VAL:HG23	2.00	0.42
10:J:46:ILE:O	10:J:46:ILE:HG22	2.20	0.42
1:A:5:ALA:O	1:A:8:LEU:HB2	2.20	0.42
2:B:105:MET:CE	2:B:107:TYR:HE1	2.32	0.42
2:B:226:ILE:HG22	2:B:227:ARG:N	2.34	0.42
2:B:277:HIS:HD2	2:B:363:LYS:CB	2.32	0.42
3:C:101:ARG:NE	3:C:102:GLY:N	2.67	0.42
3:C:20:ILE:O	3:C:21:ASP:CB	2.63	0.42
3:C:349:ILE:HG22	3:C:353:GLN:NE2	2.35	0.42
4:D:158:ILE:CG2	4:D:159:GLY:H	2.27	0.42
6:F:31:LEU:N	6:F:31:LEU:CD2	2.81	0.42
6:F:39:GLU:O	6:F:44:LYS:HE3	2.19	0.42
8:H:57:GLU:N	8:H:57:GLU:OE1	2.43	0.42
2:B:340:ALA:O	2:B:344:VAL:HG23	2.19	0.42
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.54	0.42
3:C:148:THR:C	3:C:150:LEU:N	2.72	0.42
3:C:158:GLY:C	3:C:160:THR:N	2.71	0.42
3:C:163:GLU:OE1	3:C:169:PHE:CE1	2.73	0.42
1:A:283:THR:HG21	9:I:114:UNK:CB	2.48	0.42
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.42
1:A:40:TRP:CZ3	1:A:377:GLU:CD	2.93	0.42
1:A:39:VAL:HG22	1:A:41:ILE:CD1	2.49	0.42
1:A:429:GLU:OE1	7:G:7:LEU:HD23	2.20	0.42
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.54	0.42
3:C:27:ASN:HA	6:F:70:MET:HB2	2.01	0.42
4:D:16:GLY:HA2	4:D:17:PRO:HD2	1.83	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.42
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.42
5:E:148:ALA:HB2	5:E:156:TYR:CE1	2.55	0.42
5:E:14:ARG:O	5:E:15:ARG:O	2.37	0.42
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.48	0.42
10:J:9:LEU:O	10:J:13:LEU:HB2	2.19	0.42
1:A:268:VAL:O	1:A:272:VAL:HG23	2.20	0.42
2:B:69:LEU:CD1	2:B:105:MET:HE1	2.38	0.42
2:B:371:SER:O	2:B:372:VAL:CG2	2.67	0.42
2:B:397:THR:HA	2:B:400:GLN:CB	2.49	0.42
2:B:435:PHE:HD1	2:B:438:GLU:OE2	2.03	0.42
3:C:111:LYS:HE3	3:C:307:PHE:CE1	2.55	0.42
3:C:111:LYS:HE3	3:C:307:PHE:HE1	1.85	0.42
3:C:233:LEU:HD13	3:C:233:LEU:C	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:187:PRO:HG2	12:C:381:HEM:CMC	2.50	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.55	0.42
4:D:98:PRO:HG2	4:D:99:GLU:H	1.85	0.42
5:E:113:GLU:CD	5:E:116:GLN:HG3	2.40	0.42
7:G:57:LEU:O	7:G:58:LEU:C	2.58	0.42
9:I:205:UNK:O	9:I:207:UNK:N	2.53	0.42
10:J:57:HIS:CB	10:J:61:ASN:O	2.67	0.42
1:A:240:GLN:HB2	1:A:422:VAL:CG1	2.50	0.42
1:A:362:ARG:CG	1:A:399:LEU:HD11	2.49	0.42
1:A:240:GLN:OE1	1:A:434:TYR:HB2	2.20	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.84	0.42
1:A:64:PHE:C	1:A:66:GLY:H	2.23	0.42
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.55	0.42
6:F:96:GLU:OE1	6:F:99:ARG:NE	2.53	0.42
4:D:234:LYS:O	7:G:15:THR:HA	2.19	0.42
1:A:59:LEU:CD1	1:A:186:LEU:HD11	2.49	0.42
1:A:46:ARG:NH1	1:A:316:GLU:OE2	2.43	0.42
1:A:391:PRO:C	1:A:393:GLU:N	2.72	0.42
2:B:371:SER:C	2:B:372:VAL:HG23	2.40	0.42
2:B:395:PRO:CA	2:B:398:VAL:HG12	2.48	0.42
3:C:346:HIS:O	3:C:347:PRO:C	2.58	0.42
4:D:43:MET:HE3	4:D:46:VAL:HG21	2.02	0.42
4:D:68:VAL:HG21	4:D:92:PRO:HG2	2.02	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.73	0.42
5:E:16:PRO:HA	5:E:17:PRO:HD2	1.90	0.42
5:E:134:ILE:HD12	5:E:185:TYR:CG	2.55	0.42
7:G:49:ALA:N	7:G:50:PRO:HD2	2.35	0.42
1:A:163:LEU:HG	1:A:234:CYS:SG	2.60	0.41
2:B:268:GLU:HG2	2:B:268:GLU:O	2.19	0.41
3:C:27:ASN:CA	6:F:70:MET:HB2	2.50	0.41
3:C:364:LEU:HD12	3:C:364:LEU:N	2.35	0.41
5:E:171:ILE:N	5:E:179:ASN:OD1	2.46	0.41
7:G:38:TRP:C	7:G:40:ARG:N	2.73	0.41
9:I:107:UNK:HA	9:I:115:UNK:O	2.20	0.41
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.55	0.41
1:A:64:PHE:O	1:A:66:GLY:N	2.52	0.41
2:B:146:ILE:CG1	2:B:147:ASP:N	2.79	0.41
2:B:180:ASP:O	2:B:182:ARG:N	2.54	0.41
3:C:156:TYR:C	3:C:158:GLY:H	2.23	0.41
3:C:282:LEU:HD22	3:C:291:GLY:O	2.19	0.41
4:D:29:GLY:O	4:D:30:PHE:C	2.58	0.41
4:D:43:MET:HE2	4:D:46:VAL:CB	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:54:VAL:HG21	4:D:192:TRP:CE3	2.55	0.41
2:B:111:CYS:SG	2:B:112:LEU:N	2.92	0.41
2:B:144:LEU:O	2:B:145:LYS:C	2.59	0.41
2:B:264:ILE:HD11	2:B:317:SER:HA	2.01	0.41
3:C:131:GLY:O	3:C:134:LEU:N	2.46	0.41
3:C:162:VAL:O	3:C:165:ALA:N	2.53	0.41
3:C:167:GLY:HA3	3:C:174:PRO:CG	2.50	0.41
3:C:167:GLY:HA3	3:C:175:THR:HG22	2.01	0.41
3:C:125:MET:HB3	16:C:385:SIG:H281	2.02	0.41
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.41
4:D:175:THR:HA	4:D:176:PRO:HD3	1.82	0.41
5:E:13:TYR:C	5:E:14:ARG:HD3	2.38	0.41
5:E:171:ILE:O	5:E:171:ILE:HG23	2.18	0.41
5:E:175:PRO:O	5:E:176:ALA:C	2.58	0.41
8:H:44:VAL:C	8:H:46:SER:H	2.23	0.41
8:H:72:LYS:O	8:H:75:ASN:ND2	2.54	0.41
1:A:169:GLY:O	5:E:3:THR:HG21	2.20	0.41
1:A:408:ARG:O	1:A:409:GLU:C	2.58	0.41
2:B:33:LEU:HD23	2:B:220:ALA:HB1	2.02	0.41
2:B:221:GLU:HG3	2:B:222:GLN:N	2.36	0.41
2:B:353:SER:OG	2:B:355:GLU:HB3	2.20	0.41
3:C:103:LEU:HD12	3:C:326:PHE:CE1	2.56	0.41
3:C:104:TYR:O	3:C:105:TYR:CG	2.73	0.41
3:C:106:GLY:C	3:C:108:TYR:N	2.73	0.41
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.49	0.41
3:C:355:ALA:O	3:C:357:LEU:N	2.53	0.41
3:C:51:LEU:HA	3:C:51:LEU:HD12	1.74	0.41
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.41
8:H:47:ARG:CD	8:H:48:SER:N	2.82	0.41
4:D:151:PRO:HB2	8:H:59:PHE:HE1	1.84	0.41
4:D:150:ASN:O	4:D:156:GLN:HA	2.21	0.41
5:E:78:LEU:HD13	5:E:132:TRP:NE1	2.34	0.41
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.85	0.41
15:C:384:PEE:O5	7:G:48:VAL:HG21	2.19	0.41
8:H:15:ASP:C	8:H:17:LEU:H	2.23	0.41
10:J:54:HIS:O	10:J:57:HIS:NE2	2.53	0.41
1:A:46:ARG:CD	1:A:231:LEU:HD13	2.50	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.66	0.41
1:A:65:LYS:CD	1:A:65:LYS:N	2.83	0.41
2:B:150:VAL:HA	2:B:153:GLN:HG3	2.01	0.41
2:B:277:HIS:CE1	2:B:364:LEU:HD21	2.56	0.41
2:B:436:VAL:HG23	2:B:437:ASP:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:62:ASN:O	2:B:63:LEU:C	2.58	0.41
4:D:230:LEU:HB3	6:F:70:MET:HE3	2.01	0.41
5:E:129:LYS:HA	5:E:130:PRO:HD3	1.87	0.41
3:C:377:MET:HE2	6:F:20:TYR:HB2	2.02	0.41
10:J:23:THR:O	10:J:27:GLY:N	2.46	0.41
1:A:382:GLU:HG2	1:A:390:ILE:H	1.85	0.41
2:B:111:CYS:O	2:B:112:LEU:CB	2.68	0.41
2:B:248:ASN:ND2	2:B:249:GLY:N	2.61	0.41
2:B:330:ALA:O	2:B:333:ALA:CB	2.68	0.41
3:C:113:THR:CG2	3:C:201:LEU:HA	2.48	0.41
3:C:246:PHE:O	4:D:201:ARG:NH1	2.54	0.41
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.56	0.41
3:C:373:LEU:CD2	3:C:373:LEU:C	2.89	0.41
4:D:227:TRP:O	4:D:228:SER:C	2.58	0.41
5:E:25:SER:C	5:E:26:ARG:O	2.56	0.41
6:F:34:ASP:O	6:F:37:ILE:HG13	2.21	0.41
1:A:39:VAL:HG13	1:A:39:VAL:O	2.20	0.41
2:B:280:GLY:C	2:B:282:ASN:H	2.24	0.41
3:C:220:PRO:O	3:C:221:PHE:C	2.58	0.41
3:C:31:TRP:HZ3	15:C:384:PEE:H152	1.86	0.41
4:D:113:LEU:HA	4:D:116:ILE:HB	2.02	0.41
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.41
8:H:73:LEU:C	8:H:73:LEU:CD2	2.88	0.41
1:A:153:LEU:C	1:A:153:LEU:CD2	2.86	0.41
1:A:158:PHE:O	1:A:159:GLN:C	2.59	0.41
1:A:23:VAL:N	1:A:192:ALA:HB1	2.34	0.41
2:B:198:HIS:CD2	2:B:203:ARG:NH2	2.88	0.41
2:B:436:VAL:O	2:B:438:GLU:N	2.54	0.41
3:C:26:SER:HA	3:C:219:ILE:HD11	2.02	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.56	0.41
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.55	0.41
2:B:101:THR:CG2	2:B:102:ARG:N	2.81	0.41
2:B:277:HIS:CD2	2:B:363:LYS:HB2	2.56	0.41
2:B:409:ASP:OD1	2:B:409:ASP:N	2.54	0.41
3:C:167:GLY:HA3	3:C:174:PRO:HG2	2.02	0.41
3:C:319:ARG:HH22	3:C:371:GLY:CA	2.30	0.41
3:C:34:PHE:CZ	3:C:97:LEU:HD13	2.56	0.41
16:C:385:SIG:H23	16:C:385:SIG:H343	1.79	0.41
6:F:34:ASP:OD1	6:F:34:ASP:N	2.54	0.41
5:E:32:ARG:NH2	7:G:25:PRO:HD2	2.36	0.41
1:A:253:VAL:O	1:A:323:TYR:HA	2.21	0.41
1:A:366:VAL:C	1:A:368:HIS:N	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:64:PHE:CZ	1:A:86:LEU:HG	2.56	0.41
2:B:200:THR:HG22	2:B:226:ILE:CG2	2.51	0.41
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.51	0.41
4:D:86:LYS:N	4:D:89:ASP:OD1	2.49	0.41
5:E:163:SER:HA	5:E:174:GLY:HA3	2.03	0.41
5:E:46:GLY:O	5:E:49:TYR:HB3	2.21	0.41
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.56	0.41
3:C:27:ASN:ND2	6:F:69:ASN:HD22	2.18	0.41
7:G:55:PHE:O	7:G:56:TYR:C	2.60	0.41
1:A:56:GLY:CA	1:A:185:TYR:CE2	2.97	0.40
1:A:388:ARG:N	1:A:388:ARG:HD3	2.31	0.40
2:B:280:GLY:O	2:B:282:ASN:N	2.54	0.40
2:B:405:VAL:HG11	2:B:409:ASP:CG	2.41	0.40
3:C:9:HIS:O	3:C:11:LEU:N	2.54	0.40
3:C:346:HIS:C	3:C:346:HIS:ND1	2.74	0.40
3:C:50:LEU:HD12	12:C:381:HEM:HBC1	2.02	0.40
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.01	0.40
4:D:81:PHE:C	4:D:81:PHE:CD1	2.94	0.40
8:H:47:ARG:CD	8:H:48:SER:H	2.22	0.40
1:A:192:ALA:N	1:A:193:PRO:HD2	2.35	0.40
1:A:245:GLU:C	1:A:247:GLY:H	2.24	0.40
1:A:365:LEU:HD21	1:A:395:TRP:HB3	2.03	0.40
1:A:65:LYS:NZ	9:I:311:UNK:CA	2.77	0.40
2:B:77:THR:CB	2:B:125:ASN:HB3	2.51	0.40
2:B:34:VAL:HG11	2:B:386:ALA:O	2.21	0.40
3:C:13:LYS:HE2	3:C:17:ASN:ND2	2.36	0.40
3:C:172:ASP:N	3:C:175:THR:HG23	2.19	0.40
3:C:211:GLY:HA3	3:C:315:THR:HG23	2.03	0.40
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.51	0.40
3:C:295:LEU:HA	3:C:295:LEU:HD12	1.82	0.40
3:C:202:HIS:HE1	14:C:383:U10:H1M3	1.86	0.40
4:D:207:LYS:O	4:D:211:MET:HG2	2.21	0.40
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.86	0.40
5:E:81:ILE:HD13	5:E:98:VAL:CG1	2.51	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.97	0.40
1:A:253:VAL:HG11	1:A:335:MET:HE2	2.02	0.40
1:A:356:ARG:O	1:A:357:GLY:C	2.59	0.40
1:A:405:ARG:HH11	1:A:405:ARG:HG2	1.85	0.40
2:B:47:ILE:HD11	2:B:116:VAL:HG12	2.03	0.40
2:B:206:LEU:O	2:B:216:LEU:HD21	2.21	0.40
2:B:19:PRO:O	2:B:21:PRO:HD3	2.21	0.40
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:37:SER:O	2:B:38:LEU:CB	2.69	0.40
3:C:292:VAL:O	3:C:295:LEU:HB3	2.22	0.40
3:C:361:THR:O	3:C:362:ILE:C	2.57	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.89	0.40
6:F:87:VAL:O	6:F:87:VAL:HG23	2.21	0.40
3:C:327:TRP:HB2	7:G:51:PRO:HG3	2.03	0.40
8:H:66:ASP:HA	8:H:69:VAL:HB	2.04	0.40
1:A:110:VAL:HA	1:A:113:LEU:HD12	2.03	0.40
1:A:346:CYS:HB3	1:A:411:CYS:HB3	2.03	0.40
1:A:40:TRP:CE3	1:A:96:ALA:HB2	2.57	0.40
3:C:163:GLU:HB3	3:C:169:PHE:CE1	2.57	0.40
3:C:114:TRP:HE3	12:C:382:HEM:HMD1	1.87	0.40
3:C:59:ASP:O	3:C:60:THR:C	2.60	0.40
4:D:147:LEU:N	4:D:147:LEU:CD2	2.84	0.40
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.85	0.40
7:G:18:LEU:O	7:G:19:SER:C	2.59	0.40
7:G:79:ASN:N	7:G:79:ASN:ND2	2.69	0.40
1:A:40:TRP:N	1:A:40:TRP:CD1	2.89	0.40
2:B:367:LYS:O	2:B:371:SER:HB2	2.21	0.40
3:C:222:HIS:O	3:C:224:TYR:N	2.55	0.40
3:C:310:LYS:HB3	3:C:372:THR:HG23	2.04	0.40
3:C:91:PHE:CE1	3:C:124:LEU:HG	2.56	0.40
4:D:195:GLU:OE2	4:D:201:ARG:NH2	2.55	0.40
4:D:78:GLY:O	4:D:79:GLU:CG	2.68	0.40
8:H:69:VAL:CG1	8:H:73:LEU:HD12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/446 (99%)	337 (77%)	85 (19%)	18 (4%)	4 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	404/422 (96%)	295 (73%)	78 (19%)	31 (8%)	1	22
3	C	377/380 (99%)	278 (74%)	68 (18%)	31 (8%)	1	21
4	D	239/241 (99%)	194 (81%)	34 (14%)	11 (5%)	4	39
5	E	194/196 (99%)	151 (78%)	28 (14%)	15 (8%)	1	22
6	F	98/109 (90%)	84 (86%)	12 (12%)	2 (2%)	11	63
7	G	76/81 (94%)	52 (68%)	18 (24%)	6 (8%)	1	22
8	H	64/78 (82%)	56 (88%)	7 (11%)	1 (2%)	14	68
10	J	57/62 (92%)	32 (56%)	20 (35%)	5 (9%)	1	19
All	All	1949/2015 (97%)	1479 (76%)	350 (18%)	120 (6%)	2	30

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	284	TYR
2	B	19	PRO
2	B	20	HIS
2	B	23	ASP
2	B	38	LEU
2	B	113	ARG
2	B	132	PHE
2	B	170	ASN
2	B	171	ALA
2	B	228	GLY
2	B	233	SER
2	B	290	ASN
2	B	410	VAL
3	C	5	ILE
3	C	111	LYS
3	C	167	GLY
3	C	208	ASN
3	C	222	HIS
3	C	284	SER
3	C	349	ILE
3	C	357	LEU
4	D	73	GLY
4	D	75	ASN
4	D	198	HIS
4	D	233	ARG

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Mol	Chain	Res	Type
5	E	11	SER
5	E	21	SER
5	E	58	PHE
5	E	72	SER
7	G	27	PRO
7	G	43	ALA
10	J	5	LEU
10	J	56	LYS
10	J	61	ASN
1	A	65	LYS
1	A	128	GLU
1	A	289	HIS
1	A	291	SER
2	B	210	GLY
2	B	218	ASN
2	B	229	GLY
2	B	261	SER
2	B	372	VAL
2	B	386	ALA
2	B	430	LEU
3	C	58	ALA
3	C	164	TRP
3	C	170	SER
4	D	38	SER
4	D	78	GLY
4	D	106	ASN
4	D	236	ALA
5	E	15	ARG
5	E	17	PRO
5	E	26	ARG
5	E	66	ALA
7	G	33	GLY
1	A	55	ALA
1	A	56	GLY
1	A	72	GLN
1	A	103	SER
1	A	141	ASN
1	A	267	LEU
1	A	285	GLY
2	B	63	LEU
2	B	111	CYS
2	B	181	TYR

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Mol	Chain	Res	Type
2	B	190	GLU
2	B	330	ALA
2	B	371	SER
2	B	407	ASP
3	C	31	TRP
3	C	105	TYR
3	C	207	ASN
3	C	286	PRO
5	E	30	PRO
6	F	53	ASN
10	J	60	GLU
1	A	71	PRO
1	A	292	SER
2	B	83	PHE
2	B	260	GLU
2	B	406	ALA
3	C	4	ASN
3	C	63	ALA
3	C	156	TYR
3	C	159	HIS
3	C	224	TYR
3	C	379	ASN
4	D	240	PRO
5	E	27	GLU
5	E	61	SER
1	A	286	GLY
1	A	382	GLU
1	A	398	ARG
2	B	404	ALA
3	C	10	PRO
3	C	202	HIS
3	C	321	LEU
3	C	359	TYR
5	E	62	MET
5	E	70	ALA
7	G	74	PRO
8	H	65	ARG
10	J	15	ARG
3	C	274	TYR
4	D	176	PRO
5	E	71	MET
5	E	177	PRO

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Mol	Chain	Res	Type
6	F	19	TRP
2	B	249	GLY
3	C	158	GLY
3	C	205	GLY
3	C	352	GLY
7	G	26	PHE
3	C	157	ILE
3	C	259	PRO
4	D	133	GLY
7	G	50	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/376 (96%)	333 (93%)	26 (7%)	21	67
2	B	307/336 (91%)	286 (93%)	21 (7%)	22	70
3	C	326/329 (99%)	298 (91%)	28 (9%)	15	58
4	D	201/207 (97%)	193 (96%)	8 (4%)	42	84
5	E	165/169 (98%)	153 (93%)	12 (7%)	20	66
6	F	90/98 (92%)	80 (89%)	10 (11%)	9	42
7	G	60/72 (83%)	53 (88%)	7 (12%)	8	38
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	40 (98%)	1 (2%)	61	92
All	All	1600/1713 (93%)	1487 (93%)	113 (7%)	21	67

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	58	PHE
1	A	69	ASN
1	A	100	LYS
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	148	VAL
1	A	168	GLU
1	A	182	LEU
1	A	220	PRO
1	A	226	ASP
1	A	250	LEU
1	A	279	HIS
1	A	307	PHE
1	A	316	GLU
1	A	333	ASP
1	A	342	TRP
1	A	361	LEU
1	A	368	HIS
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP
1	A	409	GLU
1	A	438	ARG
1	A	443	TRP
1	A	444	LEU
2	B	21	PRO
2	B	56	ARG
2	B	57	TYR
2	B	62	ASN
2	B	109	VAL
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	193	ASP
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN
2	B	252	LEU
2	B	325	TYR
2	B	351	ASN
2	B	378	PHE
2	B	402	ILE
2	B	407	ASP
2	B	409	ASP
2	B	437	ASP

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Mol	Chain	Res	Type
3	C	4	ASN
3	C	21	ASP
3	C	32	TRP
3	C	43	MET
3	C	104	TYR
3	C	129	PHE
3	C	133	VAL
3	C	136	TRP
3	C	145	THR
3	C	149	ASN
3	C	152	SER
3	C	164	TRP
3	C	166	TRP
3	C	175	THR
3	C	184	PHE
3	C	207	ASN
3	C	208	ASN
3	C	216	SER
3	C	219	ILE
3	C	258	THR
3	C	259	PRO
3	C	272	GLU
3	C	285	ILE
3	C	307	PHE
3	C	325	LEU
3	C	333	LEU
3	C	342	GLN
3	C	350	ILE
4	D	75	ASN
4	D	82	MET
4	D	136	GLU
4	D	163	PRO
4	D	181	GLN
4	D	192	TRP
4	D	209	LEU
4	D	224	ARG
5	E	9	ASN
5	E	11	SER
5	E	27	GLU
5	E	32	ARG
5	E	36	SER
5	E	45	LEU

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Mol	Chain	Res	Type
5	E	52	LYS
5	E	79	SER
5	E	81	ILE
5	E	113	GLU
5	E	136	ILE
5	E	191	ASP
6	F	12	TRP
6	F	31	LEU
6	F	34	ASP
6	F	37	ILE
6	F	59	MET
6	F	64	ARG
6	F	70	MET
6	F	75	LEU
6	F	81	THR
6	F	107	TRP
7	G	4	PHE
7	G	16	TYR
7	G	22	GLU
7	G	26	PHE
7	G	27	PRO
7	G	41	LEU
7	G	77	TYR
10	J	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	85	HIS
1	A	118	GLN
1	A	141	ASN
1	A	151	ASN
1	A	165	GLN
1	A	274	ASN
1	A	301	ASN
1	A	339	GLN
2	B	22	GLN
2	B	62	ASN
2	B	225	ASN

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Mol	Chain	Res	Type
2	B	248	ASN
2	B	277	HIS
2	B	342	ASN
2	B	343	GLN
2	B	351	ASN
2	B	356	ASN
2	B	421	GLN
2	B	429	ASN
3	C	4	ASN
3	C	16	ASN
3	C	17	ASN
3	C	82	ASN
3	C	86	ASN
3	C	138	GLN
3	C	207	ASN
3	C	261	ASN
3	C	323	GLN
3	C	332	ASN
3	C	342	GLN
3	C	353	GLN
4	D	35	GLN
4	D	75	ASN
4	D	105	ASN
4	D	156	GLN
4	D	225	HIS
5	E	9	ASN
5	E	57	GLN
5	E	86	ASN
6	F	69	ASN
7	G	64	GLN
7	G	79	ASN
8	H	75	ASN
10	J	57	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
12	HEM	C	381	3	42,50,50	3.11	9 (21%)	27,82,82	2.56	10 (37%)
12	HEM	C	382	3	42,50,50	3.32	11 (26%)	27,82,82	2.65	10 (37%)
14	U10	C	383	-	29,29,63	3.58	7 (24%)	37,38,79	2.14	9 (24%)
15	PEE	C	384	-	48,48,50	2.51	12 (25%)	53,53,55	4.23	25 (47%)
16	SIG	C	385	-	36,36,36	2.80	13 (36%)	48,50,50	2.38	14 (29%)
11	BOG	D	242	-	20,20,20	1.12	2 (10%)	25,25,25	0.84	1 (4%)
12	HEM	D	243	4	42,50,50	3.37	13 (30%)	27,82,82	3.11	9 (33%)
13	FES	E	197	5	0,4,4	0.00	-	0,4,4	0.00	-
15	PEE	E	198	-	48,48,50	2.58	11 (22%)	53,53,55	4.23	23 (43%)

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
12	HEM	C	381	3	-	0/14/114/114	0/0/8/8
12	HEM	C	382	3	-	0/14/114/114	0/0/8/8
14	U10	C	383	-	-	0/23/47/87	0/1/1/1
15	PEE	C	384	-	1/1/4/4	0/52/52/54	0/0/0/0
16	SIG	C	385	-	-	0/29/30/30	0/2/2/2
11	BOG	D	242	-	-	0/11/31/31	0/1/1/1
12	HEM	D	243	4	-	0/14/114/114	0/0/8/8
13	FES	E	197	5	-	0/0/4/4	0/1/1/1
15	PEE	E	198	-	1/1/4/4	0/52/52/54	0/0/0/0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	C3C-C2C	-14.88	1.33	1.45
14	C	383	U10	C13-C14	14.73	1.62	1.32
12	D	243	HEM	C3B-C2B	-12.32	1.33	1.45
12	C	381	HEM	C3B-C2B	-12.29	1.33	1.45
12	D	243	HEM	C3C-C2C	-11.95	1.36	1.45
15	E	198	PEE	O5-C30	11.63	1.57	1.22
15	C	384	PEE	O5-C30	11.15	1.55	1.22
12	C	382	HEM	C3B-C2B	-9.63	1.36	1.45
12	C	381	HEM	C3C-C2C	-9.10	1.38	1.45
16	C	385	SIG	C37-C36	7.79	1.37	1.33
15	E	198	PEE	C26-C25	7.60	1.58	1.55
14	C	383	U10	C22-C21	-6.88	1.52	1.55
15	C	384	PEE	O2-C10	5.90	1.52	1.34
16	C	385	SIG	C20-C8	5.73	1.59	1.50
16	C	385	SIG	C10-C4	5.66	1.49	1.41
16	C	385	SIG	C2-C3	5.64	1.45	1.41
14	C	383	U10	C6-C1	5.62	1.48	1.35
12	C	382	HEM	CMB-C2B	5.59	1.54	1.45
12	C	381	HEM	CMD-C2D	5.45	1.54	1.45
16	C	385	SIG	O7-C8	5.44	1.41	1.35
12	C	381	HEM	CMB-C2B	5.29	1.54	1.45
12	C	381	HEM	CMC-C2C	5.27	1.54	1.45
15	C	384	PEE	C46-C45	5.01	1.57	1.55
12	C	382	HEM	CMC-C2C	4.85	1.53	1.45
12	D	243	HEM	CMB-C2B	4.77	1.53	1.45
14	C	383	U10	C7-C6	4.71	1.60	1.51
15	E	198	PEE	O2-C10	4.62	1.48	1.34
12	D	243	HEM	CMD-C2D	4.42	1.52	1.45
12	D	243	HEM	C3C-CAC	4.17	1.54	1.40
15	C	384	PEE	C11-C10	4.09	1.63	1.50
12	C	382	HEM	CMD-C2D	4.05	1.52	1.45
12	C	381	HEM	CHC-C4B	-4.04	1.35	1.39
12	D	243	HEM	CBB-CAB	3.96	1.51	1.29
12	D	243	HEM	CBC-CAC	3.91	1.51	1.29
12	D	243	HEM	C3D-C2D	-3.84	1.33	1.43
16	C	385	SIG	O13-C1	3.67	1.43	1.37
15	E	198	PEE	C11-C10	3.61	1.61	1.50
12	C	382	HEM	C3D-C2D	-3.60	1.34	1.43
12	C	381	HEM	C3D-C2D	-3.55	1.34	1.43
16	C	385	SIG	O7-C3	3.53	1.42	1.36
14	C	383	U10	C3-C2	-3.53	1.38	1.48
12	C	381	HEM	C1B-C2B	3.40	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	243	HEM	CMC-C2C	3.40	1.51	1.45
15	E	198	PEE	C46-C45	3.40	1.56	1.55
15	C	384	PEE	C26-C25	3.31	1.56	1.55
16	C	385	SIG	O14-C5	3.29	1.43	1.36
15	C	384	PEE	C31-C30	-3.13	1.41	1.50
12	D	243	HEM	C3B-CAB	3.13	1.50	1.40
16	C	385	SIG	C6-C1	3.00	1.44	1.38
12	D	243	HEM	C1C-NC	2.99	1.41	1.33
15	E	198	PEE	C31-C30	-2.98	1.41	1.50
14	C	383	U10	C8-C9	2.90	1.38	1.32
16	C	385	SIG	C24-C23	-2.85	1.47	1.54
15	E	198	PEE	C22-C21	-2.84	1.34	1.51
16	C	385	SIG	C31-C30	2.80	1.52	1.44
16	C	385	SIG	C21-C22	2.77	1.62	1.54
15	E	198	PEE	C42-C41	-2.76	1.34	1.51
15	C	384	PEE	C42-C41	-2.74	1.35	1.51
15	C	384	PEE	C22-C21	-2.68	1.35	1.51
16	C	385	SIG	C9-C8	2.62	1.42	1.39
12	C	382	HEM	CAA-C2A	2.62	1.56	1.52
15	C	384	PEE	C1-C2	2.59	1.58	1.50
12	C	382	HEM	C4D-ND	2.52	1.40	1.33
12	C	382	HEM	C1B-C2B	2.50	1.47	1.45
11	D	242	BOG	O5-C1	2.47	1.48	1.41
11	D	242	BOG	C4-C5	2.44	1.58	1.53
12	D	243	HEM	C4A-C3A	2.41	1.47	1.43
12	C	382	HEM	C1C-NC	2.40	1.39	1.33
14	C	383	U10	C21-C19	2.34	1.54	1.51
12	C	381	HEM	CAA-C2A	-2.30	1.48	1.52
15	E	198	PEE	C5-C4	2.26	1.57	1.50
15	C	384	PEE	P-O3P	2.23	1.69	1.59
15	E	198	PEE	C1-C2	2.14	1.56	1.50
15	C	384	PEE	C5-C4	2.13	1.57	1.50
15	E	198	PEE	O2-C2	-2.11	1.41	1.46
15	C	384	PEE	O2-C2	-2.10	1.41	1.46
12	D	243	HEM	C1B-C2B	-2.08	1.43	1.45
12	C	382	HEM	C3B-C4B	2.06	1.50	1.45

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	384	PEE	O4-C10-C11	-17.93	51.07	123.78
15	E	198	PEE	O4-C10-C11	-17.89	51.22	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	198	PEE	O3-C30-C31	12.96	151.56	111.90
15	C	384	PEE	O3-C30-C31	12.89	151.35	111.90
15	E	198	PEE	O3-C30-O5	-10.86	95.11	123.48
15	C	384	PEE	O3-C30-O5	-10.86	95.11	123.48
16	C	385	SIG	C20-C8-C9	9.21	131.53	120.42
12	D	243	HEM	C4A-C3A-C2A	-8.74	100.92	107.00
15	E	198	PEE	O2-C2-C3	7.83	137.47	108.50
12	C	382	HEM	CBA-CAA-C2A	7.69	125.43	112.63
15	C	384	PEE	O2-C2-C3	7.49	136.21	108.50
15	E	198	PEE	O2-C10-C11	7.18	126.85	111.54
15	C	384	PEE	O2-C10-C11	7.07	126.60	111.54
12	D	243	HEM	C3A-C4A-NA	6.88	114.09	109.50
12	D	243	HEM	CBA-CAA-C2A	6.57	123.57	112.63
12	C	381	HEM	CAD-C3D-C4D	6.28	134.46	125.60
15	E	198	PEE	C12-C11-C10	-6.18	89.54	113.51
14	C	383	U10	C12-C13-C14	-5.67	115.54	127.81
15	C	384	PEE	C12-C11-C10	-5.62	91.70	113.51
15	E	198	PEE	O2-C10-O4	-5.50	108.98	123.66
15	C	384	PEE	O2-C10-O4	-5.49	109.01	123.66
16	C	385	SIG	C21-C20-C8	5.43	126.95	113.35
12	D	243	HEM	CAD-C3D-C4D	5.35	133.14	125.60
12	C	381	HEM	CBA-CAA-C2A	-5.35	103.73	112.63
12	C	382	HEM	C4A-NA-C1A	-5.28	101.36	107.93
12	C	382	HEM	C3A-C4A-NA	5.04	112.86	109.50
15	C	384	PEE	O3-C3-C2	5.02	121.99	108.80
15	E	198	PEE	O3-C3-C2	4.85	121.55	108.80
14	C	383	U10	C15-C14-C13	-4.69	114.19	123.52
14	C	383	U10	C10-C9-C8	-4.56	114.45	123.52
12	C	381	HEM	C3A-C4A-NA	4.55	112.54	109.50
16	C	385	SIG	C39-C36-C32	-4.54	110.75	118.09
16	C	385	SIG	C21-C22-C23	4.41	119.41	111.73
12	C	381	HEM	C4A-NA-C1A	-4.36	102.51	107.93
14	C	383	U10	C15-C14-C16	4.34	121.98	115.39
12	C	381	HEM	CBD-CAD-C3D	4.12	123.47	114.51
16	C	385	SIG	O7-C3-C2	4.00	120.86	115.97
16	C	385	SIG	C27-C22-C23	-3.98	104.99	112.22
16	C	385	SIG	C33-C9-C10	-3.83	114.65	121.04
12	C	382	HEM	C1A-C2A-C3A	-3.68	103.11	106.92
15	C	384	PEE	C4-C5-N	3.67	117.74	110.92
14	C	383	U10	C1-C6-C5	-3.66	115.66	120.26
12	D	243	HEM	C4A-NA-C1A	-3.60	103.45	107.93
14	C	383	U10	O2-C2-C3	-3.56	113.06	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	198	PEE	C4-C5-N	3.32	117.08	110.92
15	C	384	PEE	O3P-C1-C2	3.30	119.21	108.54
12	C	381	HEM	CAD-C3D-C2D	-3.26	118.87	127.19
15	E	198	PEE	O3P-C1-C2	3.15	118.73	108.54
16	C	385	SIG	C33-C9-C8	3.14	126.79	122.09
15	C	384	PEE	C14-C13-C12	-3.07	98.28	114.56
15	C	384	PEE	C42-C41-C40	3.02	130.59	114.56
15	E	198	PEE	C22-C21-C20	2.98	130.37	114.56
14	C	383	U10	C10-C9-C11	2.94	119.85	115.39
12	D	243	HEM	C1A-C2A-C3A	2.93	109.95	106.92
15	E	198	PEE	C34-C33-C32	-2.92	99.04	114.56
15	E	198	PEE	C42-C41-C40	2.92	130.08	114.56
12	C	382	HEM	CAD-C3D-C4D	2.90	129.69	125.60
15	C	384	PEE	C46-C45-C44	-2.89	104.67	112.94
15	C	384	PEE	O4P-P-O3P	2.89	112.92	104.68
15	E	198	PEE	C33-C32-C31	2.88	123.95	113.28
15	C	384	PEE	C33-C32-C31	2.85	123.82	113.28
12	C	382	HEM	C2A-C1A-NA	2.82	113.66	109.73
12	C	381	HEM	C4A-C3A-C2A	-2.82	105.03	107.00
12	C	382	HEM	CAA-C2A-C1A	2.76	133.82	125.50
11	D	242	BOG	C1'-O1-C1	2.75	118.77	113.91
15	E	198	PEE	C46-C45-C44	-2.68	105.29	112.94
15	C	384	PEE	C34-C33-C32	-2.67	100.39	114.56
12	D	243	HEM	CAD-C3D-C2D	-2.66	120.40	127.19
15	E	198	PEE	C26-C25-C24	-2.65	105.36	112.94
15	E	198	PEE	C14-C13-C12	-2.63	100.58	114.56
15	C	384	PEE	C22-C21-C20	2.61	128.44	114.56
12	D	243	HEM	CAA-C2A-C1A	-2.61	117.62	125.50
16	C	385	SIG	C20-C21-C22	2.58	118.31	114.60
15	E	198	PEE	O5-C30-C31	-2.58	113.32	123.78
15	C	384	PEE	O5-C30-C31	-2.56	113.41	123.78
15	E	198	PEE	C3-C2-C1	-2.55	106.00	111.86
14	C	383	U10	C3-C2-C1	2.50	122.72	117.87
15	E	198	PEE	C3-O3-C30	-2.44	110.03	116.99
15	E	198	PEE	O4P-C4-C5	-2.41	105.48	109.37
14	C	383	U10	C11-C9-C8	2.41	125.69	121.06
15	C	384	PEE	O2-C2-C1	2.33	117.11	108.50
16	C	385	SIG	C10-C4-C5	-2.32	121.37	125.08
16	C	385	SIG	C5-C4-C3	2.32	120.36	114.94
15	E	198	PEE	C36-C35-C34	-2.31	102.32	114.56
12	C	381	HEM	CMC-C2C-C3C	2.29	129.67	124.26
15	C	384	PEE	C3-C2-C1	-2.29	106.61	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	384	PEE	C26-C25-C24	-2.27	106.45	112.94
15	C	384	PEE	O4P-C4-C5	-2.25	105.74	109.37
15	C	384	PEE	C3-O3-C30	-2.24	110.60	116.99
15	C	384	PEE	C23-C24-C25	2.21	122.64	113.73
15	C	384	PEE	C16-C15-C14	-2.18	102.99	114.56
16	C	385	SIG	O7-C3-C4	-2.18	119.02	121.17
15	E	198	PEE	O2-C2-C1	2.17	116.52	108.50
16	C	385	SIG	C6-C1-C2	-2.14	118.38	120.56
12	C	382	HEM	CAA-C2A-C3A	-2.10	123.00	129.00
12	C	381	HEM	CMB-C2B-C1B	2.10	133.71	124.07
12	C	381	HEM	CMB-C2B-C3B	-2.08	121.43	126.21
12	C	382	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
16	C	385	SIG	O7-C8-C20	-2.04	109.21	112.08
12	C	382	HEM	CBD-CAD-C3D	2.02	118.90	114.51
12	D	243	HEM	CMD-C2D-C3D	-2.00	120.68	129.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	E	198	PEE	C2
15	C	384	PEE	C2

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/446 (99%)	7.66	432 (97%) 0 0	12, 58, 89, 100	0
2	B	406/422 (96%)	7.68	396 (97%) 0 0	36, 71, 100, 100	0
3	C	379/380 (99%)	7.39	377 (99%) 0 0	4, 32, 71, 91	0
4	D	241/241 (100%)	7.51	238 (98%) 0 0	10, 41, 77, 100	0
5	E	196/196 (100%)	6.74	181 (92%) 0 0	17, 76, 100, 100	0
6	F	100/109 (91%)	7.69	100 (100%) 0 0	18, 42, 74, 99	0
7	G	78/81 (96%)	7.61	78 (100%) 0 0	26, 54, 89, 100	0
8	H	66/78 (84%)	8.55	66 (100%) 0 0	27, 67, 86, 88	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	7.77	56 (94%) 0 0	37, 53, 86, 100	0
All	All	1967/2048 (96%)	7.53	1924 (97%) 0 0	4, 55, 98, 100	0

All (1924) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	30	PRO	23.0
2	B	44	GLY	19.7
2	B	222	GLN	19.6
7	G	44	CYS	19.5
1	A	269	ALA	19.3
2	B	366	ALA	19.1
5	E	22	THR	19.0
1	A	74	ALA	18.5
2	B	287	ARG	18.1
5	E	108	GLN	17.1
1	A	160	GLY	16.8
3	C	377	MET	16.6
2	B	334	GLY	16.5
2	B	358	GLN	16.5

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Mol	Chain	Res	Type	RSRZ
2	B	266	GLY	16.4
2	B	271	ALA	16.4
5	E	121	GLN	16.3
1	A	376	CYS	16.3
1	A	72	GLN	16.0
5	E	151	GLY	16.0
6	F	78	GLU	15.9
1	A	7	ALA	15.8
2	B	24	LEU	15.7
5	E	144	CYS	15.7
2	B	269	ALA	15.7
1	A	4	TYR	15.7
4	D	40	CYS	15.6
2	B	178	CYS	15.5
1	A	82	MET	15.5
7	G	64	GLN	15.5
5	E	160	CYS	15.4
1	A	71	PRO	15.4
8	H	56	GLU	15.4
1	A	329	MET	15.3
1	A	346	CYS	15.2
2	B	255	ALA	15.1
4	D	103	ALA	15.1
1	A	271	GLN	15.0
2	B	251	SER	14.9
3	C	364	LEU	14.8
2	B	258	VAL	14.8
1	A	233	LYS	14.8
2	B	149	ALA	14.7
2	B	20	HIS	14.7
3	C	220	PRO	14.7
1	A	127	ILE	14.7
2	B	374	SER	14.6
2	B	281	ALA	14.5
1	A	411	CYS	14.5
3	C	198	LEU	14.5
3	C	138	GLN	14.5
5	E	80	ASP	14.5
1	A	120	CYS	14.5
2	B	413	ALA	14.4
2	B	412	LYS	14.4
2	B	64	GLY	14.4

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Mol	Chain	Res	Type	RSRZ
4	D	60	GLU	14.4
1	A	304	CYS	14.3
2	B	141	GLN	14.3
2	B	397	THR	14.2
1	A	234	CYS	14.2
2	B	21	PRO	14.2
8	H	28	GLU	14.1
1	A	67	THR	14.0
2	B	143	GLN	14.0
2	B	184	GLY	14.0
1	A	130	GLU	13.9
3	C	313	GLN	13.9
2	B	90	GLU	13.9
6	F	84	GLU	13.9
10	J	41	ALA	13.9
2	B	120	MET	13.8
2	B	185	LYS	13.8
1	A	204	GLU	13.8
2	B	80	ALA	13.7
1	A	246	ASP	13.6
1	A	83	GLY	13.6
4	D	133	GLY	13.6
1	A	86	LEU	13.6
1	A	335	MET	13.6
5	E	44	THR	13.6
2	B	105	MET	13.5
5	E	46	GLY	13.5
1	A	73	ASN	13.5
3	C	380	TYR	13.5
8	H	55	THR	13.4
10	J	12	LEU	13.4
1	A	164	ALA	13.4
8	H	27	LEU	13.4
8	H	63	HIS	13.3
2	B	233	SER	13.3
3	C	71	CYS	13.2
1	A	156	THR	13.2
2	B	363	LYS	13.2
4	D	124	GLU	13.2
8	H	54	CYS	13.1
7	G	51	PRO	13.1
3	C	202	HIS	13.1

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Mol	Chain	Res	Type	RSRZ
1	A	144	SER	13.0
8	H	68	CYS	13.0
4	D	37	CYS	13.0
2	B	395	PRO	13.0
8	H	52	GLU	13.0
6	F	85	GLU	13.0
3	C	155	PRO	13.0
1	A	373	THR	13.0
6	F	91	GLU	13.0
1	A	14	THR	13.0
1	A	209	LEU	13.0
1	A	109	ALA	12.9
4	D	184	LYS	12.9
5	E	179	ASN	12.9
3	C	250	LEU	12.9
1	A	32	GLN	12.9
2	B	205	ALA	12.9
5	E	139	CYS	12.8
3	C	143	GLY	12.8
2	B	318	ASP	12.8
1	A	267	LEU	12.8
2	B	139	ASP	12.7
1	A	137	GLU	12.7
1	A	262	TRP	12.7
1	A	388	ARG	12.7
8	H	22	GLU	12.7
4	D	6	HIS	12.7
5	E	86	ASN	12.7
7	G	5	GLY	12.7
10	J	59	TYR	12.7
8	H	18	THR	12.7
2	B	345	LYS	12.6
2	B	29	LEU	12.6
4	D	94	PRO	12.6
5	E	148	ALA	12.6
3	C	122	LEU	12.6
2	B	106	ALA	12.6
3	C	93	ILE	12.6
6	F	76	PRO	12.6
2	B	210	GLY	12.6
4	D	179	MET	12.6
5	E	177	PRO	12.5

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Mol	Chain	Res	Type	RSRZ
2	B	329	GLN	12.5
4	D	105	ASN	12.5
4	D	212	MET	12.5
2	B	339	ALA	12.5
6	F	106	GLU	12.5
10	J	7	ALA	12.5
6	F	51	PRO	12.5
3	C	69	HIS	12.5
3	C	94	CYS	12.5
1	A	429	GLU	12.5
2	B	323	GLY	12.5
5	E	172	ARG	12.5
1	A	383	LEU	12.5
4	D	58	GLU	12.4
10	J	45	HIS	12.5
1	A	321	GLY	12.4
5	E	50	ALA	12.4
2	B	373	GLU	12.4
1	A	18	GLN	12.4
1	A	347	THR	12.4
4	D	51	LEU	12.4
1	A	162	GLY	12.4
4	D	14	HIS	12.4
1	A	338	LEU	12.4
2	B	47	ILE	12.4
7	G	79	ASN	12.3
1	A	125	SER	12.3
7	G	43	ALA	12.3
1	A	353	GLU	12.3
3	C	154	ILE	12.3
3	C	306	PRO	12.2
2	B	406	ALA	12.2
2	B	433	THR	12.2
4	D	234	LYS	12.2
4	D	16	GLY	12.2
2	B	108	THR	12.1
1	A	39	VAL	12.1
4	D	35	GLN	12.1
4	D	114	SER	12.1
8	H	30	CYS	12.1
5	E	9	ASN	12.1
4	D	195	GLU	12.1

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Mol	Chain	Res	Type	RSRZ
6	F	33	ARG	12.1
3	C	110	TYR	12.1
4	D	20	SER	12.1
2	B	45	SER	12.1
7	G	55	PHE	12.0
1	A	431	LEU	12.0
2	B	306	PRO	12.0
2	B	148	LYS	12.0
3	C	21	ASP	12.0
8	H	33	ALA	12.0
10	J	19	THR	12.0
3	C	205	GLY	12.0
4	D	154	PRO	11.9
1	A	66	GLY	11.9
10	J	40	ASP	11.9
2	B	388	ALA	11.9
2	B	325	TYR	11.9
3	C	147	ILE	11.9
3	C	238	THR	11.9
1	A	94	HIS	11.9
8	H	35	GLU	11.8
10	J	39	ALA	11.8
3	C	286	PRO	11.8
2	B	91	ALA	11.8
2	B	43	PRO	11.8
2	B	418	VAL	11.8
1	A	352	SER	11.8
2	B	27	THR	11.8
3	C	43	MET	11.8
1	A	20	ASP	11.8
3	C	161	LEU	11.8
4	D	78	GLY	11.7
6	F	38	TYR	11.7
3	C	160	THR	11.7
5	E	166	ASP	11.7
8	H	57	GLU	11.7
1	A	318	GLY	11.7
2	B	380	GLU	11.7
5	E	133	VAL	11.7
1	A	230	THR	11.6
2	B	77	THR	11.6
4	D	101	ALA	11.6

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Mol	Chain	Res	Type	RSRZ
3	C	302	LEU	11.6
4	D	22	ASP	11.6
3	C	41	CYS	11.6
1	A	38	GLY	11.6
1	A	140	GLU	11.6
1	A	218	GLY	11.6
4	D	156	GLN	11.6
3	C	183	HIS	11.5
3	C	289	LEU	11.5
4	D	82	MET	11.5
2	B	50	PHE	11.5
3	C	268	HIS	11.5
8	H	77	LEU	11.5
7	G	35	PRO	11.5
2	B	415	LYS	11.5
10	J	8	ARG	11.5
5	E	55	VAL	11.5
6	F	34	ASP	11.4
1	A	240	GLN	11.4
2	B	154	ASN	11.4
2	B	187	THR	11.4
2	B	231	GLY	11.4
7	G	47	ARG	11.4
2	B	246	GLU	11.4
1	A	424	GLY	11.4
2	B	279	LEU	11.4
4	D	52	VAL	11.4
1	A	96	ALA	11.3
5	E	15	ARG	11.3
3	C	7	LYS	11.3
1	A	432	PRO	11.3
2	B	288	GLY	11.3
1	A	258	GLU	11.3
1	A	401	GLU	11.3
3	C	335	ILE	11.3
1	A	211	LEU	11.2
1	A	311	SER	11.2
1	A	325	VAL	11.2
1	A	326	CYS	11.2
1	A	385	THR	11.2
2	B	214	PRO	11.2
1	A	118	GLN	11.2

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Mol	Chain	Res	Type	RSRZ
5	E	49	TYR	11.2
7	G	6	HIS	11.2
4	D	239	PRO	11.2
3	C	106	GLY	11.2
6	F	17	ARG	11.2
2	B	317	SER	11.1
2	B	428	GLY	11.1
4	D	138	PRO	11.1
2	B	438	GLU	11.1
1	A	419	CYS	11.1
6	F	41	ASP	11.1
2	B	263	ALA	11.1
5	E	48	ALA	11.0
6	F	59	MET	11.0
7	G	46	LEU	11.0
5	E	158	CYS	11.0
1	A	322	PHE	11.0
5	E	122	HIS	11.0
4	D	85	GLY	11.0
2	B	268	GLU	11.0
4	D	4	GLU	11.0
3	C	323	GLN	11.0
3	C	252	GLY	10.9
4	D	187	CYS	10.9
1	A	116	ILE	10.9
3	C	45	GLN	10.9
1	A	17	SER	10.9
1	A	313	CYS	10.9
2	B	181	TYR	10.9
7	G	23	GLN	10.9
5	E	93	GLY	10.8
2	B	338	LYS	10.8
2	B	310	SER	10.8
3	C	153	ALA	10.8
8	H	64	ALA	10.8
10	J	6	THR	10.8
2	B	285	VAL	10.8
3	C	239	PRO	10.8
8	H	32	LYS	10.8
3	C	78	TRP	10.8
8	H	60	ASP	10.8
1	A	266	ASP	10.8

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Mol	Chain	Res	Type	RSRZ
8	H	67	HIS	10.8
3	C	240	PHE	10.8
2	B	259	ALA	10.8
4	D	188	THR	10.8
4	D	72	ASP	10.7
1	A	417	ASP	10.7
3	C	47	LEU	10.7
3	C	261	ASN	10.7
2	B	72	ALA	10.7
7	G	52	PHE	10.7
3	C	347	PRO	10.7
2	B	227	ARG	10.7
3	C	127	THR	10.7
3	C	333	LEU	10.7
5	E	42	VAL	10.7
6	F	90	LEU	10.7
8	H	38	GLU	10.6
2	B	364	LEU	10.6
4	D	203	ARG	10.6
3	C	378	LEU	10.6
2	B	138	ALA	10.6
3	C	233	LEU	10.6
4	D	125	ASP	10.6
3	C	189	ALA	10.6
5	E	51	ALA	10.6
3	C	115	ASN	10.6
1	A	259	GLY	10.6
10	J	30	LEU	10.6
7	G	27	PRO	10.6
10	J	9	LEU	10.6
5	E	87	MET	10.5
5	E	40	THR	10.5
2	B	54	GLY	10.5
3	C	126	ALA	10.5
5	E	116	GLN	10.5
3	C	352	GLY	10.5
3	C	81	ARG	10.5
3	C	369	THR	10.5
3	C	199	THR	10.5
1	A	147	GLU	10.5
3	C	322	SER	10.5
2	B	69	LEU	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	297	ILE	10.5
5	E	185	TYR	10.5
7	G	31	SER	10.5
2	B	165	ALA	10.5
4	D	137	PRO	10.5
8	H	53	ASP	10.4
2	B	155	PRO	10.4
1	A	405	ARG	10.4
1	A	89	TYR	10.4
6	F	32	MET	10.4
5	E	62	MET	10.4
1	A	189	HIS	10.4
2	B	423	SER	10.4
6	F	98	ILE	10.4
2	B	436	VAL	10.4
4	D	93	LYS	10.3
3	C	215	ASP	10.3
2	B	147	ASP	10.3
6	F	36	THR	10.3
10	J	32	GLU	10.3
5	E	38	LEU	10.3
2	B	277	HIS	10.3
3	C	297	ALA	10.3
10	J	36	ASP	10.3
3	C	357	LEU	10.3
10	J	25	VAL	10.3
3	C	67	VAL	10.3
4	D	67	GLU	10.3
2	B	348	ALA	10.3
3	C	350	ILE	10.3
7	G	62	GLY	10.3
1	A	92	ARG	10.2
3	C	304	LEU	10.2
8	H	58	LEU	10.2
1	A	107	PRO	10.2
10	J	23	THR	10.2
1	A	319	LEU	10.2
1	A	334	MET	10.2
3	C	203	GLU	10.2
6	F	35	ASP	10.2
4	D	123	GLY	10.2
1	A	78	GLU	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	GLN	10.2
6	F	40	ASN	10.2
5	E	170	ARG	10.2
2	B	355	GLU	10.2
3	C	150	LEU	10.2
4	D	121	HIS	10.2
1	A	256	ALA	10.2
3	C	29	SER	10.1
4	D	197	GLU	10.1
1	A	15	GLN	10.1
5	E	18	ASP	10.1
3	C	111	LYS	10.1
1	A	387	GLY	10.1
4	D	99	GLU	10.1
4	D	236	ALA	10.1
3	C	293	LEU	10.1
4	D	111	PRO	10.1
2	B	320	GLY	10.1
3	C	371	GLY	10.1
3	C	354	MET	10.1
8	H	17	LEU	10.1
1	A	340	GLY	10.1
2	B	136	GLU	10.0
3	C	242	THR	10.0
1	A	415	ILE	10.0
10	J	33	ARG	10.0
1	A	333	ASP	10.0
3	C	31	TRP	10.0
4	D	240	PRO	10.0
1	A	143	THR	10.0
1	A	195	MET	9.9
2	B	243	GLU	9.9
1	A	180	ALA	9.9
3	C	353	GLN	9.9
6	F	30	GLY	9.9
2	B	359	ALA	9.9
1	A	273	ALA	9.9
4	D	220	TYR	9.9
2	B	145	LYS	9.9
3	C	187	PRO	9.9
10	J	38	GLY	9.9
2	B	22	GLN	9.9

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Mol	Chain	Res	Type	RSRZ
3	C	294	ALA	9.9
4	D	174	GLY	9.9
8	H	40	CYS	9.9
3	C	100	GLY	9.8
6	F	57	ASP	9.8
1	A	87	ASN	9.8
3	C	337	THR	9.8
7	G	12	HIS	9.8
3	C	256	ASN	9.8
7	G	8	THR	9.8
2	B	370	MET	9.8
5	E	107	ASP	9.8
5	E	27	GLU	9.8
7	G	24	ARG	9.8
4	D	126	TYR	9.8
3	C	346	HIS	9.8
6	F	68	LEU	9.8
4	D	23	HIS	9.8
4	D	44	ASP	9.7
5	E	37	TYR	9.7
3	C	344	VAL	9.7
1	A	56	GLY	9.7
6	F	75	LEU	9.7
3	C	25	PRO	9.7
10	J	37	GLN	9.7
3	C	55	HIS	9.7
2	B	162	ASN	9.7
1	A	341	GLN	9.7
6	F	16	ILE	9.6
1	A	49	SER	9.6
1	A	348	SER	9.6
2	B	176	LEU	9.6
6	F	101	ARG	9.6
2	B	58	GLU	9.6
1	A	19	LEU	9.6
3	C	157	ILE	9.6
7	G	28	HIS	9.6
4	D	55	CYS	9.6
1	A	169	GLY	9.6
5	E	8	PRO	9.6
1	A	370	ASP	9.6
4	D	196	PRO	9.6

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Mol	Chain	Res	Type	RSRZ
3	C	23	PRO	9.5
3	C	230	ILE	9.5
8	H	21	ARG	9.5
2	B	92	VAL	9.5
5	E	23	LYS	9.5
10	J	42	ILE	9.5
1	A	196	VAL	9.5
4	D	241	LYS	9.5
2	B	36	ALA	9.5
3	C	12	LEU	9.5
6	F	83	TYR	9.5
2	B	275	LEU	9.5
3	C	271	PRO	9.5
6	F	95	LYS	9.5
4	D	176	PRO	9.5
2	B	385	GLN	9.5
6	F	67	ASP	9.5
3	C	4	ASN	9.4
3	C	139	MET	9.4
3	C	361	THR	9.4
6	F	88	PRO	9.4
1	A	351	GLU	9.4
2	B	375	SER	9.4
2	B	254	HIS	9.4
2	B	134	PRO	9.4
3	C	234	THR	9.4
4	D	194	ALA	9.4
2	B	59	ASN	9.4
2	B	270	ASN	9.4
6	F	39	GLU	9.3
2	B	73	SER	9.3
2	B	76	THR	9.3
1	A	374	PRO	9.3
2	B	340	ALA	9.3
2	B	419	SER	9.3
10	J	4	THR	9.3
5	E	99	ARG	9.3
4	D	208	MET	9.3
2	B	427	SER	9.3
5	E	192	MET	9.3
1	A	386	TYR	9.3
3	C	298	SER	9.3

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Mol	Chain	Res	Type	RSRZ
2	B	256	ALA	9.3
3	C	194	THR	9.3
4	D	211	MET	9.3
6	F	10	SER	9.2
6	F	45	GLU	9.2
10	J	53	LYS	9.2
3	C	332	ASN	9.2
8	H	47	ARG	9.2
2	B	351	ASN	9.2
4	D	226	LYS	9.2
1	A	305	GLN	9.2
3	C	77	GLY	9.2
8	H	65	ARG	9.2
4	D	177	ALA	9.2
10	J	13	LEU	9.2
6	F	47	ILE	9.2
6	F	108	ASP	9.2
1	A	161	THR	9.2
3	C	253	ASP	9.2
4	D	130	LEU	9.2
1	A	80	GLU	9.2
3	C	24	ALA	9.2
5	E	152	ASP	9.2
5	E	149	ASN	9.2
3	C	65	SER	9.2
1	A	59	LEU	9.2
3	C	280	ALA	9.2
4	D	38	SER	9.2
1	A	426	GLY	9.2
1	A	261	GLY	9.2
1	A	248	LEU	9.2
7	G	3	GLN	9.2
2	B	84	LYS	9.1
7	G	65	GLU	9.1
3	C	37	LEU	9.1
4	D	131	LEU	9.1
2	B	389	ALA	9.1
2	B	68	LEU	9.1
3	C	320	PRO	9.1
10	J	43	TYR	9.1
2	B	208	GLY	9.1
8	H	71	HIS	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	228	GLY	9.1
3	C	57	THR	9.1
3	C	89	SER	9.1
5	E	14	ARG	9.1
3	C	255	GLU	9.1
3	C	300	LEU	9.1
3	C	212	ILE	9.1
4	D	29	GLY	9.1
1	A	270	LEU	9.1
1	A	212	ALA	9.1
2	B	130	PRO	9.1
3	C	279	TYR	9.1
2	B	377	GLY	9.1
7	G	57	LEU	9.0
1	A	188	THR	9.0
4	D	192	TRP	9.0
1	A	112	LEU	9.0
5	E	59	VAL	9.0
4	D	1	SER	9.0
5	E	100	HIS	9.0
1	A	288	LEU	9.0
4	D	221	TYR	9.0
8	H	15	ASP	9.0
1	A	121	SER	9.0
1	A	285	GLY	9.0
6	F	93	TYR	9.0
1	A	315	SER	9.0
1	A	41	ILE	9.0
5	E	104	LYS	9.0
3	C	331	ALA	9.0
7	G	68	LYS	9.0
1	A	69	ASN	9.0
1	A	225	ASP	8.9
8	H	66	ASP	8.9
2	B	48	GLY	8.9
2	B	280	GLY	8.9
2	B	276	GLN	8.9
6	F	105	GLU	8.9
4	D	135	CYS	8.9
4	D	200	HIS	8.9
7	G	26	PHE	8.9
3	C	309	HIS	8.9

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Mol	Chain	Res	Type	RSRZ
10	J	22	LEU	8.9
3	C	237	LEU	8.9
6	F	79	GLN	8.9
2	B	242	GLY	8.9
1	A	425	PRO	8.9
5	E	28	SER	8.9
7	G	33	GLY	8.9
8	H	49	GLN	8.9
4	D	19	SER	8.9
1	A	217	GLY	8.9
5	E	156	TYR	8.9
2	B	110	GLU	8.9
7	G	17	SER	8.9
3	C	318	PHE	8.9
2	B	290	ASN	8.8
4	D	48	TYR	8.8
4	D	198	HIS	8.8
8	H	72	LYS	8.8
2	B	60	SER	8.8
3	C	276	LEU	8.8
4	D	21	LEU	8.8
1	A	237	THR	8.8
1	A	21	ASN	8.8
2	B	191	LEU	8.8
1	A	142	ASP	8.8
2	B	332	TYR	8.8
2	B	113	ARG	8.8
1	A	177	LEU	8.8
3	C	262	PRO	8.8
4	D	95	TYR	8.8
4	D	193	ALA	8.8
1	A	55	ALA	8.8
10	J	34	ALA	8.8
5	E	178	LEU	8.8
3	C	375	ASN	8.8
4	D	209	LEU	8.8
1	A	155	ALA	8.8
8	H	75	ASN	8.8
10	J	18	SER	8.8
5	E	56	THR	8.8
1	A	433	ASP	8.8
2	B	164	HIS	8.7

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Mol	Chain	Res	Type	RSRZ
2	B	112	LEU	8.7
2	B	392	TYR	8.7
3	C	97	LEU	8.7
2	B	315	SER	8.7
4	D	69	GLU	8.7
2	B	376	GLU	8.7
3	C	49	GLY	8.7
1	A	439	SER	8.7
4	D	205	GLY	8.7
1	A	23	VAL	8.7
6	F	28	LYS	8.7
1	A	390	ILE	8.7
3	C	79	LEU	8.7
3	C	290	GLY	8.7
4	D	75	ASN	8.7
1	A	202	GLY	8.7
3	C	225	TYR	8.7
1	A	360	PHE	8.6
1	A	389	ARG	8.6
2	B	23	ASP	8.6
2	B	107	TYR	8.6
4	D	134	TYR	8.6
7	G	66	PHE	8.6
8	H	26	GLN	8.6
1	A	145	MET	8.6
5	E	45	LEU	8.6
3	C	249	ASN	8.6
3	C	148	THR	8.6
2	B	409	ASP	8.6
3	C	36	SER	8.6
4	D	116	ILE	8.6
7	G	56	TYR	8.6
1	A	382	GLU	8.6
1	A	430	GLN	8.6
2	B	109	VAL	8.6
3	C	103	LEU	8.6
3	C	292	VAL	8.6
4	D	43	MET	8.6
3	C	128	ALA	8.6
4	D	182	VAL	8.6
5	E	95	PRO	8.5
2	B	346	THR	8.5

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Mol	Chain	Res	Type	RSRZ
3	C	251	LEU	8.5
6	F	73	GLN	8.5
6	F	80	TRP	8.5
3	C	53	ALA	8.5
4	D	219	VAL	8.5
1	A	176	LYS	8.5
1	A	90	SER	8.5
7	G	30	PHE	8.5
2	B	272	PHE	8.5
4	D	161	ALA	8.5
4	D	190	LEU	8.5
1	A	414	TYR	8.5
3	C	259	PRO	8.5
1	A	263	ALA	8.5
5	E	82	PRO	8.5
1	A	422	VAL	8.5
7	G	18	LEU	8.5
3	C	86	ASN	8.5
5	E	76	ILE	8.5
1	A	123	GLU	8.5
1	A	102	LEU	8.5
7	G	45	ILE	8.5
3	C	272	GLU	8.4
4	D	50	HIS	8.4
2	B	125	ASN	8.4
2	B	284	HIS	8.4
1	A	221	PHE	8.4
1	A	75	LEU	8.4
3	C	117	GLY	8.4
5	E	106	ILE	8.4
6	F	42	ASP	8.4
3	C	316	MET	8.4
1	A	339	GLN	8.4
2	B	390	GLY	8.4
1	A	31	SER	8.4
3	C	99	ILE	8.4
4	D	160	MET	8.4
1	A	235	ARG	8.4
1	A	372	THR	8.4
2	B	238	LYS	8.4
2	B	378	PHE	8.4
1	A	28	GLU	8.4

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Mol	Chain	Res	Type	RSRZ
3	C	87	GLY	8.4
3	C	116	THR	8.4
1	A	254	ALA	8.3
3	C	14	MET	8.3
1	A	151	ASN	8.3
1	A	423	ALA	8.3
4	D	109	LEU	8.3
2	B	426	ALA	8.3
4	D	88	SER	8.3
7	G	58	LEU	8.3
2	B	371	SER	8.3
7	G	59	TYR	8.3
1	A	170	PRO	8.3
3	C	195	ILE	8.3
6	F	15	GLY	8.3
1	A	60	GLU	8.3
3	C	151	PHE	8.3
4	D	13	SER	8.3
3	C	19	LEU	8.3
3	C	360	PHE	8.3
4	D	166	ASN	8.3
7	G	29	TYR	8.3
3	C	144	ALA	8.3
1	A	260	PRO	8.3
7	G	40	ARG	8.3
1	A	441	MET	8.3
3	C	265	THR	8.3
3	C	315	THR	8.3
8	H	48	SER	8.3
5	E	67	ASP	8.3
7	G	74	PRO	8.3
4	D	26	ILE	8.3
5	E	36	SER	8.3
3	C	40	VAL	8.2
3	C	156	TYR	8.2
6	F	24	ALA	8.2
1	A	10	SER	8.2
4	D	235	LEU	8.2
2	B	216	LEU	8.2
5	E	165	TYR	8.2
1	A	343	MET	8.2
3	C	236	MET	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	221	GLU	8.2
3	C	244	ALA	8.2
5	E	146	PRO	8.2
2	B	215	VAL	8.2
3	C	224	TYR	8.2
7	G	19	SER	8.2
7	G	73	ASN	8.2
1	A	286	GLY	8.2
2	B	53	ALA	8.1
3	C	98	HIS	8.1
3	C	206	SER	8.1
3	C	95	ILE	8.1
6	F	64	ARG	8.1
1	A	375	VAL	8.1
3	C	269	ILE	8.1
2	B	28	LYS	8.1
2	B	219	VAL	8.1
1	A	98	TYR	8.1
1	A	396	GLU	8.1
4	D	172	ASP	8.1
8	H	50	THR	8.1
2	B	128	THR	8.1
3	C	82	ASN	8.1
1	A	378	ASP	8.1
3	C	338	TRP	8.1
4	D	162	PRO	8.1
3	C	33	ASN	8.1
3	C	221	PHE	8.1
1	A	182	LEU	8.1
2	B	235	ALA	8.1
3	C	125	MET	8.1
2	B	414	ALA	8.1
6	F	22	ASN	8.1
5	E	78	LEU	8.1
5	E	6	LYS	8.1
3	C	370	ILE	8.0
3	C	20	ILE	8.0
5	E	153	PHE	8.0
1	A	358	LYS	8.0
2	B	115	ASP	8.0
3	C	60	THR	8.0
2	B	260	GLU	8.0

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Mol	Chain	Res	Type	RSRZ
2	B	61	SER	8.0
5	E	143	GLY	8.0
1	A	309	THR	8.0
1	A	349	ILE	8.0
2	B	75	LEU	8.0
3	C	341	SER	8.0
8	H	39	LEU	8.0
1	A	48	GLU	8.0
1	A	6	GLN	8.0
1	A	368	HIS	8.0
3	C	105	TYR	8.0
6	F	37	ILE	8.0
2	B	379	LEU	7.9
4	D	112	ASP	7.9
2	B	63	LEU	7.9
3	C	254	PRO	7.9
4	D	92	PRO	7.9
1	A	403	ASP	7.9
4	D	108	ALA	7.9
1	A	93	GLU	7.9
3	C	84	HIS	7.9
1	A	172	GLU	7.9
1	A	134	ILE	7.9
4	D	170	GLU	7.9
5	E	35	PHE	7.9
1	A	168	GLU	7.9
3	C	301	ILE	7.9
4	D	41	HIS	7.9
2	B	352	VAL	7.9
4	D	173	ASP	7.9
2	B	257	ILE	7.9
2	B	218	ASN	7.9
1	A	365	LEU	7.9
1	A	420	PRO	7.8
1	A	165	GLN	7.8
7	G	77	TYR	7.8
1	A	302	LYS	7.8
2	B	146	ILE	7.8
7	G	13	LEU	7.8
1	A	398	ARG	7.8
4	D	90	TYR	7.8
3	C	305	ILE	7.8

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Mol	Chain	Res	Type	RSRZ
3	C	231	LEU	7.8
2	B	121	GLU	7.8
3	C	196	ILE	7.8
1	A	367	SER	7.8
2	B	437	ASP	7.8
4	D	191	ARG	7.8
5	E	75	GLU	7.8
2	B	240	ARG	7.8
3	C	307	PHE	7.8
4	D	71	GLN	7.7
2	B	118	ILE	7.7
1	A	276	ILE	7.7
8	H	34	ARG	7.7
2	B	381	GLU	7.7
2	B	411	ILE	7.7
2	B	253	VAL	7.7
6	F	104	ARG	7.7
3	C	51	LEU	7.7
1	A	11	VAL	7.7
5	E	7	VAL	7.7
2	B	140	LEU	7.7
2	B	116	VAL	7.7
1	A	175	ARG	7.7
1	A	47	TYR	7.7
1	A	152	TYR	7.7
3	C	186	LEU	7.7
5	E	173	LYS	7.7
2	B	157	THR	7.7
1	A	364	ALA	7.7
3	C	296	ALA	7.7
1	A	324	PHE	7.7
3	C	287	ASN	7.7
1	A	81	SER	7.7
2	B	71	LEU	7.7
1	A	185	TYR	7.6
4	D	12	TRP	7.6
5	E	189	SER	7.6
1	A	295	ALA	7.6
2	B	39	GLU	7.6
1	A	310	PHE	7.6
4	D	54	VAL	7.6
2	B	264	ILE	7.6

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Mol	Chain	Res	Type	RSRZ
5	E	110	ALA	7.6
1	A	434	TYR	7.6
3	C	182	LEU	7.6
10	J	26	VAL	7.6
5	E	102	THR	7.6
6	F	103	GLU	7.6
1	A	114	ALA	7.6
4	D	34	LYS	7.6
1	A	150	PHE	7.6
4	D	96	PRO	7.6
2	B	404	ALA	7.6
1	A	158	PHE	7.6
5	E	24	SER	7.6
5	E	115	SER	7.6
3	C	26	SER	7.6
8	H	41	ASP	7.6
3	C	170	SER	7.6
6	F	82	LYS	7.6
1	A	131	ARG	7.6
1	A	62	LEU	7.5
4	D	127	VAL	7.5
3	C	68	ALA	7.5
4	D	31	GLN	7.5
5	E	150	ALA	7.5
10	J	44	GLU	7.5
3	C	281	ILE	7.5
3	C	273	TRP	7.5
3	C	355	ALA	7.5
5	E	113	GLU	7.5
5	E	124	LEU	7.5
2	B	273	SER	7.5
2	B	195	VAL	7.5
2	B	420	ARG	7.5
4	D	63	ALA	7.5
10	J	28	ALA	7.5
1	A	312	ILE	7.5
4	D	89	ASP	7.5
1	A	45	SER	7.5
1	A	228	VAL	7.5
1	A	163	LEU	7.5
1	A	301	ASN	7.5
4	D	7	PRO	7.5

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Mol	Chain	Res	Type	RSRZ
4	D	204	MET	7.5
1	A	37	VAL	7.4
4	D	186	VAL	7.4
8	H	51	GLU	7.4
4	D	169	LEU	7.4
5	E	68	VAL	7.4
7	G	50	PRO	7.4
3	C	197	HIS	7.4
3	C	214	SER	7.4
3	C	30	ALA	7.4
1	A	289	HIS	7.4
5	E	188	THR	7.4
2	B	198	HIS	7.4
1	A	443	TRP	7.4
6	F	89	TYR	7.4
2	B	57	TYR	7.4
1	A	99	ILE	7.4
3	C	38	LEU	7.4
1	A	247	GLY	7.4
6	F	61	ARG	7.4
3	C	367	PHE	7.4
3	C	373	LEU	7.4
1	A	438	ARG	7.4
1	A	300	THR	7.4
3	C	275	PHE	7.4
1	A	33	PRO	7.4
2	B	189	VAL	7.4
8	H	43	ARG	7.4
3	C	210	LEU	7.4
3	C	348	PHE	7.3
2	B	398	VAL	7.3
2	B	368	TYR	7.3
3	C	141	PHE	7.3
4	D	228	SER	7.3
5	E	77	LYS	7.3
1	A	239	SER	7.3
1	A	265	PRO	7.3
4	D	100	ALA	7.3
3	C	123	THR	7.3
2	B	89	ILE	7.3
4	D	15	ARG	7.3
2	B	307	PHE	7.3

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Mol	Chain	Res	Type	RSRZ
6	F	77	LYS	7.3
5	E	119	ASP	7.3
10	J	10	TYR	7.3
2	B	321	LEU	7.3
4	D	119	ALA	7.3
6	F	92	PRO	7.3
1	A	252	HIS	7.3
3	C	334	LEU	7.3
4	D	189	PHE	7.3
5	E	74	ILE	7.3
4	D	120	ARG	7.3
1	A	296	SER	7.2
1	A	342	TRP	7.2
3	C	229	ASP	7.2
2	B	179	PRO	7.2
3	C	169	PHE	7.2
3	C	39	ALA	7.2
4	D	76	GLU	7.2
4	D	213	GLY	7.2
2	B	46	THR	7.2
1	A	253	VAL	7.2
3	C	336	LEU	7.2
7	G	42	ARG	7.2
5	E	31	SER	7.2
4	D	222	MET	7.2
3	C	342	GLN	7.2
2	B	18	PRO	7.2
2	B	177	TYR	7.2
3	C	266	PRO	7.2
4	D	144	ARG	7.2
5	E	13	TYR	7.2
1	A	186	LEU	7.2
6	F	71	ARG	7.2
5	E	66	ALA	7.2
8	H	23	GLN	7.2
8	H	59	PHE	7.2
2	B	405	VAL	7.2
8	H	31	VAL	7.1
4	D	5	LEU	7.1
1	A	159	GLN	7.1
7	G	78	VAL	7.1
1	A	245	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
2	B	117	GLU	7.1
2	B	341	TYR	7.1
6	F	19	TRP	7.1
1	A	251	ALA	7.1
1	A	50	GLU	7.1
1	A	29	GLN	7.1
2	B	237	ALA	7.1
2	B	399	LEU	7.1
5	E	71	MET	7.1
4	D	70	VAL	7.1
2	B	131	GLU	7.1
4	D	163	PRO	7.1
3	C	140	SER	7.1
2	B	209	LEU	7.1
2	B	400	GLN	7.1
1	A	409	GLU	7.1
6	F	107	TRP	7.1
4	D	47	ALA	7.1
10	J	57	HIS	7.1
10	J	14	PHE	7.1
10	J	17	THR	7.1
2	B	247	GLN	7.1
6	F	69	ASN	7.0
1	A	8	LEU	7.0
4	D	223	LYS	7.0
4	D	53	GLY	7.0
4	D	77	ASP	7.0
1	A	108	LYS	7.0
3	C	311	SER	7.0
5	E	30	PRO	7.0
3	C	295	LEU	7.0
2	B	74	SER	7.0
1	A	184	GLU	7.0
2	B	396	SER	7.0
5	E	4	ASP	7.0
1	A	207	GLN	7.0
7	G	38	TRP	7.0
5	E	123	ASP	7.0
2	B	132	PHE	6.9
4	D	57	THR	6.9
2	B	100	SER	6.9
5	E	94	LYS	6.9

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Mol	Chain	Res	Type	RSRZ
8	H	76	SER	6.9
1	A	191	THR	6.9
1	A	24	ARG	6.9
2	B	408	ALA	6.9
4	D	49	ARG	6.9
3	C	102	GLY	6.9
4	D	98	PRO	6.9
2	B	193	ASP	6.9
2	B	262	ALA	6.9
4	D	132	THR	6.9
5	E	114	VAL	6.9
1	A	336	PHE	6.8
2	B	102	ARG	6.8
1	A	199	ALA	6.8
3	C	345	GLU	6.8
5	E	184	SER	6.8
3	C	88	ALA	6.8
1	A	154	HIS	6.8
2	B	309	VAL	6.8
4	D	122	GLY	6.8
3	C	42	LEU	6.8
1	A	406	MET	6.8
1	A	404	ALA	6.8
4	D	210	LEU	6.8
3	C	191	ALA	6.8
1	A	138	LEU	6.8
2	B	160	ILE	6.8
2	B	430	LEU	6.8
10	J	54	HIS	6.8
1	A	115	ASP	6.7
1	A	179	ARG	6.7
1	A	292	SER	6.7
5	E	103	LYS	6.7
6	F	31	LEU	6.7
4	D	217	PRO	6.7
2	B	220	ALA	6.7
3	C	56	TYR	6.7
1	A	52	ASN	6.7
1	A	444	LEU	6.7
10	J	11	SER	6.7
4	D	158	ILE	6.7
3	C	35	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	6.7
10	J	35	PHE	6.7
4	D	30	PHE	6.7
3	C	211	GLY	6.7
4	D	110	PRO	6.7
1	A	9	GLN	6.7
4	D	97	ASN	6.7
10	J	5	LEU	6.7
1	A	283	THR	6.7
2	B	421	GLN	6.7
3	C	288	LYS	6.7
3	C	232	GLY	6.6
2	B	26	ILE	6.6
3	C	164	TRP	6.6
3	C	260	ALA	6.6
5	E	32	ARG	6.6
2	B	79	GLY	6.6
1	A	316	GLU	6.6
3	C	363	LEU	6.6
10	J	21	ALA	6.6
3	C	303	PHE	6.6
5	E	159	PRO	6.6
2	B	150	VAL	6.6
3	C	32	TRP	6.6
2	B	123	LEU	6.6
2	B	403	ASP	6.6
8	H	19	THR	6.6
6	F	52	GLU	6.6
1	A	279	HIS	6.6
1	A	190	TYR	6.6
2	B	183	ILE	6.6
1	A	61	HIS	6.5
3	C	181	ALA	6.5
1	A	407	VAL	6.5
2	B	344	VAL	6.5
5	E	98	VAL	6.5
2	B	410	VAL	6.5
1	A	36	THR	6.5
3	C	217	ASP	6.5
4	D	214	LEU	6.5
3	C	359	TYR	6.5
6	F	44	LYS	6.5

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Mol	Chain	Res	Type	RSRZ
4	D	150	ASN	6.5
6	F	13	LEU	6.5
1	A	337	VAL	6.5
1	A	129	LYS	6.5
2	B	87	ARG	6.5
3	C	188	PHE	6.5
2	B	55	SER	6.5
1	A	122	LEU	6.5
4	D	91	PHE	6.5
3	C	379	ASN	6.5
1	A	306	SER	6.5
1	A	13	GLU	6.5
1	A	40	TRP	6.5
2	B	435	PHE	6.5
3	C	90	PHE	6.5
3	C	130	VAL	6.5
1	A	205	HIS	6.5
2	B	93	GLY	6.4
2	B	186	VAL	6.4
3	C	158	GLY	6.4
4	D	199	ASP	6.4
1	A	257	VAL	6.4
1	A	103	SER	6.4
10	J	51	LEU	6.4
5	E	25	SER	6.4
5	E	92	ARG	6.4
2	B	99	GLU	6.4
1	A	53	ASN	6.4
1	A	135	VAL	6.4
2	B	159	VAL	6.4
1	A	213	GLN	6.4
4	D	153	PHE	6.4
1	A	54	GLY	6.4
3	C	228	LYS	6.4
5	E	33	LYS	6.4
2	B	35	ILE	6.4
3	C	218	LYS	6.4
6	F	70	MET	6.4
6	F	74	ILE	6.4
10	J	47	ASN	6.4
3	C	362	ILE	6.4
1	A	427	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
5	E	43	THR	6.4
4	D	118	ARG	6.4
2	B	333	ALA	6.4
5	E	19	ASP	6.3
5	E	34	GLY	6.3
3	C	235	LEU	6.3
3	C	152	SER	6.3
3	C	243	LEU	6.3
8	H	74	PHE	6.3
1	A	26	ALA	6.3
1	A	298	ALA	6.3
4	D	233	ARG	6.3
3	C	101	ARG	6.3
5	E	128	LYS	6.3
1	A	293	PRO	6.3
5	E	17	PRO	6.3
10	J	24	ILE	6.3
2	B	156	GLN	6.3
6	F	20	TYR	6.3
1	A	128	GLU	6.3
3	C	314	ARG	6.3
3	C	50	LEU	6.3
1	A	111	GLU	6.3
4	D	128	PHE	6.3
4	D	145	GLU	6.3
1	A	181	ASP	6.3
3	C	112	GLU	6.2
1	A	238	GLY	6.2
1	A	206	GLN	6.2
3	C	46	ILE	6.2
4	D	155	GLY	6.2
1	A	106	VAL	6.2
1	A	146	ARG	6.2
4	D	79	GLU	6.2
6	F	58	ARG	6.2
1	A	397	GLU	6.2
4	D	28	ARG	6.2
3	C	213	SER	6.2
2	B	194	PHE	6.2
5	E	183	PRO	6.2
6	F	62	ILE	6.2
7	G	4	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	173	ASN	6.2
6	F	14	GLU	6.2
3	C	343	PRO	6.2
3	C	317	THR	6.1
4	D	143	VAL	6.1
2	B	171	ALA	6.1
4	D	115	TYR	6.1
2	B	394	PRO	6.1
5	E	10	PHE	6.1
3	C	177	THR	6.1
2	B	180	ASP	6.1
3	C	319	ARG	6.1
3	C	11	LEU	6.1
1	A	183	THR	6.1
3	C	327	TRP	6.1
2	B	190	GLU	6.1
3	C	5	ILE	6.1
1	A	359	ASN	6.1
1	A	88	ALA	6.1
4	D	107	GLY	6.1
10	J	49	GLY	6.1
2	B	169	ARG	6.1
4	D	106	ASN	6.1
3	C	75	GLN	6.1
3	C	277	PHE	6.1
6	F	50	LEU	6.1
1	A	224	ASP	6.1
2	B	196	GLN	6.1
3	C	145	THR	6.1
3	C	17	ASN	6.1
4	D	74	PRO	6.1
1	A	445	ARG	6.1
1	A	84	ALA	6.0
3	C	324	THR	6.0
4	D	141	VAL	6.0
3	C	310	LYS	6.0
5	E	39	VAL	6.0
1	A	363	ASN	6.0
5	E	85	LYS	6.0
7	G	67	GLU	6.0
10	J	58	LYS	6.0
2	B	239	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	265	GLY	6.0
1	A	124	ASP	6.0
6	F	43	VAL	6.0
8	H	13	LEU	6.0
5	E	147	ILE	6.0
5	E	176	ALA	6.0
3	C	171	VAL	6.0
4	D	201	ARG	6.0
1	A	208	LEU	6.0
1	A	287	GLY	6.0
3	C	113	THR	6.0
2	B	82	SER	6.0
1	A	294	LEU	6.0
5	E	63	SER	6.0
1	A	244	ARG	6.0
8	H	20	VAL	6.0
2	B	119	LEU	6.0
5	E	2	HIS	6.0
1	A	141	ASN	6.0
1	A	290	SER	6.0
3	C	119	ILE	6.0
3	C	267	PRO	6.0
3	C	325	LEU	6.0
2	B	133	ARG	6.0
2	B	365	LYS	6.0
7	G	32	LYS	6.0
7	G	54	ALA	6.0
3	C	166	TRP	5.9
2	B	319	SER	5.9
3	C	133	VAL	5.9
4	D	65	ALA	5.9
1	A	241	ILE	5.9
5	E	53	ASN	5.9
5	E	194	ILE	5.9
4	D	46	VAL	5.9
3	C	180	PHE	5.9
1	A	25	VAL	5.9
1	A	153	LEU	5.9
1	A	236	PHE	5.9
2	B	250	ASP	5.9
3	C	114	TRP	5.9
4	D	17	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
3	C	358	SER	5.9
1	A	394	GLU	5.9
2	B	343	GLN	5.9
4	D	8	PRO	5.9
2	B	407	ASP	5.9
4	D	227	TRP	5.9
2	B	326	THR	5.9
1	A	437	ILE	5.9
8	H	46	SER	5.9
6	F	48	ARG	5.9
2	B	62	ASN	5.9
3	C	109	LEU	5.9
1	A	242	ARG	5.9
2	B	103	GLU	5.9
4	D	218	LEU	5.9
2	B	286	LYS	5.8
1	A	280	TYR	5.8
5	E	60	SER	5.8
2	B	163	LEU	5.8
3	C	227	PHE	5.8
1	A	400	ALA	5.8
7	G	49	ALA	5.8
3	C	64	PHE	5.8
1	A	178	SER	5.8
3	C	92	PHE	5.8
1	A	200	ALA	5.8
3	C	137	GLY	5.8
4	D	142	SER	5.8
5	E	131	GLU	5.8
7	G	69	SER	5.7
8	H	42	GLU	5.7
1	A	232	SER	5.7
4	D	152	TYR	5.7
1	A	51	LYS	5.7
6	F	60	PHE	5.7
2	B	248	ASN	5.7
3	C	247	SER	5.7
4	D	167	ASP	5.7
8	H	78	LYS	5.7
1	A	418	GLN	5.7
4	D	183	ALA	5.7
1	A	222	THR	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	5.7
1	A	440	GLY	5.7
2	B	267	ALA	5.7
2	B	335	GLN	5.7
2	B	201	SER	5.7
6	F	56	ASP	5.7
1	A	393	GLU	5.7
1	A	117	VAL	5.7
2	B	232	LEU	5.7
3	C	284	SER	5.7
1	A	126	GLN	5.7
1	A	16	VAL	5.7
1	A	44	GLY	5.6
2	B	31	ASN	5.6
3	C	104	TYR	5.6
4	D	62	LYS	5.6
1	A	377	GLU	5.6
5	E	20	TYR	5.6
4	D	146	GLY	5.6
6	F	54	LEU	5.6
3	C	175	THR	5.6
3	C	258	THR	5.6
10	J	29	LEU	5.6
2	B	19	PRO	5.6
8	H	14	VAL	5.6
6	F	55	TYR	5.6
3	C	135	PRO	5.6
3	C	222	HIS	5.6
1	A	412	SER	5.6
3	C	248	PRO	5.6
5	E	61	SER	5.6
6	F	18	LYS	5.6
2	B	151	ALA	5.6
4	D	9	SER	5.6
2	B	204	MET	5.6
2	B	65	THR	5.6
6	F	53	ASN	5.6
3	C	85	ALA	5.5
4	D	68	VAL	5.5
1	A	63	ALA	5.5
3	C	136	TRP	5.5
1	A	167	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	431	GLY	5.5
6	F	26	PHE	5.5
7	G	48	VAL	5.5
3	C	15	ILE	5.5
4	D	185	ASP	5.5
4	D	59	ASP	5.5
6	F	87	VAL	5.5
3	C	219	ILE	5.5
4	D	136	GLU	5.5
2	B	81	SER	5.5
5	E	127	VAL	5.5
1	A	416	TYR	5.5
1	A	139	GLN	5.5
2	B	94	GLY	5.5
1	A	356	ARG	5.5
4	D	202	LYS	5.5
7	G	21	PHE	5.5
3	C	61	SER	5.4
4	D	18	LEU	5.4
2	B	230	LEU	5.4
2	B	328	SER	5.4
3	C	108	TYR	5.4
1	A	219	VAL	5.4
3	C	330	VAL	5.4
3	C	339	ILE	5.4
6	F	81	THR	5.4
2	B	137	VAL	5.4
1	A	133	VAL	5.4
2	B	336	VAL	5.4
1	A	68	LYS	5.4
1	A	392	LEU	5.4
2	B	386	ALA	5.4
4	D	168	VAL	5.4
4	D	32	VAL	5.4
3	C	201	LEU	5.4
3	C	365	ILE	5.4
4	D	238	ARG	5.3
3	C	167	GLY	5.3
1	A	320	PHE	5.3
3	C	6	ARG	5.3
4	D	181	GLN	5.3
6	F	12	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
6	F	109	LYS	5.3
2	B	142	PRO	5.3
2	B	367	LYS	5.3
1	A	57	TYR	5.3
2	B	369	LEU	5.3
2	B	111	CYS	5.3
3	C	62	LEU	5.3
3	C	193	ILE	5.3
10	J	31	PHE	5.3
2	B	234	GLY	5.3
7	G	39	ARG	5.3
1	A	249	PRO	5.3
1	A	395	TRP	5.3
2	B	387	LEU	5.3
4	D	66	GLU	5.3
2	B	314	ALA	5.3
1	A	277	ILE	5.3
1	A	226	ASP	5.3
6	F	100	GLU	5.3
7	G	61	TRP	5.3
2	B	356	ASN	5.2
3	C	83	LEU	5.2
3	C	121	LEU	5.2
3	C	58	ALA	5.2
2	B	153	GLN	5.2
8	H	25	GLU	5.2
7	G	41	LEU	5.2
3	C	366	LEU	5.2
1	A	350	SER	5.2
1	A	91	SER	5.2
2	B	202	ALA	5.2
1	A	231	LEU	5.2
1	A	100	LYS	5.2
2	B	66	SER	5.2
3	C	376	LYS	5.2
2	B	197	ASN	5.2
1	A	391	PRO	5.2
2	B	127	THR	5.2
3	C	76	TYR	5.2
2	B	135	TRP	5.1
1	A	361	LEU	5.1
4	D	164	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
4	D	215	LEU	5.1
3	C	349	ILE	5.1
1	A	214	LYS	5.1
2	B	167	ALA	5.1
6	F	97	VAL	5.1
4	D	11	PRO	5.1
2	B	175	SER	5.1
2	B	424	MET	5.1
7	G	25	PRO	5.1
2	B	316	TYR	5.1
3	C	245	LEU	5.1
1	A	314	TYR	5.1
1	A	46	ARG	5.1
1	A	402	VAL	5.1
2	B	161	GLU	5.1
4	D	80	MET	5.1
5	E	140	THR	5.1
8	H	24	CYS	5.1
1	A	43	ALA	5.1
4	D	39	SER	5.1
4	D	229	VAL	5.1
6	F	29	TYR	5.1
3	C	270	LYS	5.0
1	A	317	THR	5.0
2	B	337	ILE	5.0
4	D	33	TYR	5.0
7	G	53	LEU	5.0
1	A	64	PHE	5.0
2	B	383	GLY	5.0
4	D	64	LEU	5.0
2	B	324	PHE	5.0
3	C	131	GLY	5.0
1	A	268	VAL	5.0
5	E	169	GLY	5.0
8	H	61	PHE	5.0
6	F	21	TYR	5.0
1	A	332	ASP	5.0
3	C	9	HIS	5.0
3	C	278	ALA	5.0
3	C	73	ASN	5.0
5	E	29	ASP	5.0
8	H	73	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
3	C	356	SER	5.0
3	C	124	LEU	5.0
1	A	85	HIS	5.0
2	B	322	PHE	5.0
2	B	40	ASN	5.0
1	A	264	HIS	5.0
3	C	74	VAL	5.0
2	B	199	PHE	5.0
1	A	119	ASN	5.0
1	A	215	HIS	5.0
7	G	10	VAL	4.9
1	A	435	ASN	4.9
7	G	34	VAL	4.9
3	C	146	VAL	4.9
3	C	226	SER	4.9
2	B	384	SER	4.9
1	A	97	TYR	4.9
3	C	120	LEU	4.9
2	B	83	PHE	4.9
6	F	49	ARG	4.9
3	C	207	ASN	4.9
4	D	232	SER	4.9
5	E	157	TYR	4.9
10	J	46	ILE	4.9
2	B	86	THR	4.9
2	B	98	VAL	4.9
1	A	330	SER	4.9
7	G	14	ILE	4.9
8	H	29	LYS	4.9
2	B	114	ASP	4.9
3	C	44	THR	4.9
1	A	362	ARG	4.9
1	A	381	ARG	4.8
1	A	77	LYS	4.8
2	B	213	HIS	4.8
5	E	57	GLN	4.8
1	A	105	ASP	4.8
1	A	132	ASP	4.8
6	F	63	LYS	4.8
4	D	104	ALA	4.8
2	B	245	ARG	4.8
2	B	244	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	4.8
7	G	75	ALA	4.8
2	B	252	LEU	4.8
3	C	274	TYR	4.8
1	A	278	GLY	4.8
1	A	410	VAL	4.8
4	D	45	TYR	4.8
5	E	171	ILE	4.8
1	A	104	LYS	4.7
2	B	78	LYS	4.7
4	D	27	ARG	4.7
6	F	72	GLN	4.7
5	E	52	LYS	4.7
2	B	168	TYR	4.7
4	D	224	ARG	4.7
1	A	408	ARG	4.7
5	E	16	PRO	4.7
3	C	66	SER	4.7
5	E	190	ASP	4.7
5	E	1	SER	4.7
3	C	96	PHE	4.7
4	D	149	PHE	4.7
6	F	46	ALA	4.7
5	E	72	SER	4.7
10	J	27	GLY	4.7
4	D	207	LYS	4.7
3	C	174	PRO	4.6
7	G	2	ARG	4.6
8	H	37	LEU	4.6
3	C	48	THR	4.6
3	C	149	ASN	4.6
6	F	94	LEU	4.6
4	D	157	ALA	4.6
4	D	117	VAL	4.6
5	E	54	VAL	4.6
2	B	422	LYS	4.6
3	C	165	ALA	4.6
3	C	173	ASN	4.6
1	A	220	PRO	4.6
3	C	223	PRO	4.5
2	B	70	ARG	4.5
4	D	113	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	41	TYR	4.5
2	B	353	SER	4.5
2	B	416	LYS	4.5
3	C	374	GLU	4.5
3	C	132	TYR	4.5
3	C	28	ILE	4.5
1	A	355	LEU	4.5
3	C	34	PHE	4.5
1	A	70	ARG	4.5
5	E	26	ARG	4.5
4	D	129	SER	4.5
5	E	81	ILE	4.5
10	J	62	LYS	4.5
2	B	354	ASN	4.5
1	A	282	ARG	4.5
8	H	45	SER	4.5
3	C	299	VAL	4.5
8	H	62	LEU	4.5
2	B	25	GLU	4.4
10	J	50	LYS	4.4
10	J	60	GLU	4.4
1	A	34	THR	4.4
4	D	25	SER	4.4
4	D	73	GLY	4.4
4	D	151	PRO	4.4
4	D	175	THR	4.4
2	B	170	ASN	4.4
1	A	229	PRO	4.4
2	B	172	LEU	4.4
5	E	64	ALA	4.4
3	C	159	HIS	4.4
1	A	136	ARG	4.4
3	C	308	LEU	4.4
2	B	101	THR	4.4
1	A	284	TYR	4.4
2	B	425	ALA	4.4
2	B	429	ASN	4.4
5	E	168	SER	4.4
3	C	291	GLY	4.4
5	E	73	LYS	4.4
5	E	161	HIS	4.4
2	B	173	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	329	LEU	4.3
2	B	274	VAL	4.3
2	B	311	ALA	4.3
5	E	117	LEU	4.3
5	E	11	SER	4.3
3	C	200	PHE	4.3
3	C	185	LEU	4.3
7	G	11	ARG	4.3
4	D	2	ASP	4.3
6	F	86	ASP	4.3
1	A	327	ASP	4.3
4	D	180	SER	4.3
2	B	382	VAL	4.3
3	C	372	THR	4.3
7	G	16	TYR	4.3
8	H	36	ARG	4.3
5	E	181	GLU	4.3
7	G	63	THR	4.3
3	C	326	PHE	4.3
1	A	274	ASN	4.3
2	B	206	LEU	4.3
7	G	9	ARG	4.3
2	B	249	GLY	4.3
7	G	76	ALA	4.3
3	C	54	MET	4.2
1	A	79	VAL	4.2
3	C	172	ASP	4.2
1	A	30	SER	4.2
2	B	158	HIS	4.2
4	D	178	THR	4.2
3	C	351	ILE	4.2
3	C	2	ALA	4.2
2	B	32	GLY	4.2
2	B	350	GLY	4.2
10	J	52	TRP	4.2
2	B	362	ASN	4.2
4	D	159	GLY	4.2
5	E	193	VAL	4.2
5	E	155	GLY	4.2
1	A	65	LYS	4.2
1	A	223	TYR	4.1
3	C	321	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	4.1
3	C	216	SER	4.1
2	B	223	LEU	4.1
2	B	192	HIS	4.1
6	F	96	GLU	4.1
8	H	70	ALA	4.1
1	A	255	ILE	4.1
5	E	91	TRP	4.1
5	E	154	GLY	4.1
3	C	282	LEU	4.1
1	A	166	SER	4.1
1	A	187	SER	4.0
3	C	72	ARG	4.0
2	B	330	ALA	4.0
3	C	59	ASP	4.0
5	E	58	PHE	4.0
7	G	37	VAL	4.0
3	C	3	PRO	4.0
7	G	60	THR	4.0
1	A	369	LEU	4.0
3	C	22	LEU	4.0
3	C	209	PRO	4.0
2	B	96	LEU	4.0
2	B	226	ILE	4.0
2	B	391	SER	4.0
2	B	56	ARG	4.0
1	A	291	SER	4.0
2	B	129	ALA	4.0
2	B	327	ILE	4.0
1	A	5	ALA	4.0
2	B	313	ASN	4.0
3	C	285	ILE	4.0
2	B	236	LYS	3.9
5	E	5	ILE	3.9
2	B	188	SER	3.9
2	B	95	LYS	3.9
1	A	331	ILE	3.9
3	C	178	ARG	3.9
5	E	12	ASP	3.9
1	A	210	GLU	3.9
2	B	308	ASP	3.9
2	B	217	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	129	PHE	3.9
2	B	439	LEU	3.9
5	E	79	SER	3.9
2	B	283	PRO	3.9
3	C	27	ASN	3.9
1	A	272	VAL	3.9
2	B	126	VAL	3.9
2	B	124	LEU	3.9
3	C	264	VAL	3.9
2	B	34	VAL	3.9
5	E	69	LEU	3.9
1	A	197	LEU	3.8
2	B	342	ASN	3.8
3	C	312	LYS	3.8
2	B	174	ASP	3.8
1	A	357	GLY	3.8
1	A	413	LYS	3.8
3	C	70	THR	3.8
4	D	230	LEU	3.8
2	B	211	VAL	3.8
3	C	107	SER	3.8
1	A	442	PHE	3.8
2	B	49	VAL	3.8
1	A	203	VAL	3.8
6	F	27	ASN	3.8
4	D	102	ARG	3.8
6	F	65	ALA	3.8
1	A	371	GLY	3.8
1	A	101	ALA	3.8
1	A	148	VAL	3.8
1	A	157	ALA	3.8
10	J	15	ARG	3.8
5	E	191	ASP	3.8
1	A	22	GLY	3.7
1	A	307	PHE	3.7
3	C	63	ALA	3.7
4	D	81	PHE	3.7
4	D	87	LEU	3.7
1	A	436	ARG	3.7
2	B	67	HIS	3.7
1	A	354	VAL	3.7
6	F	25	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
10	J	55	ILE	3.6
3	C	10	PRO	3.6
7	G	20	PRO	3.6
4	D	165	TYR	3.6
4	D	225	HIS	3.6
4	D	206	LEU	3.6
8	H	44	VAL	3.6
2	B	207	VAL	3.6
3	C	80	ILE	3.6
5	E	3	THR	3.5
1	A	380	GLY	3.5
3	C	263	LEU	3.5
5	E	186	GLU	3.5
5	E	130	PRO	3.5
3	C	241	LEU	3.5
5	E	89	PHE	3.5
2	B	122	PHE	3.5
3	C	16	ASN	3.5
7	G	7	LEU	3.5
5	E	88	ALA	3.5
8	H	69	VAL	3.4
1	A	198	ALA	3.4
3	C	179	PHE	3.4
2	B	401	GLN	3.4
2	B	97	SER	3.4
2	B	434	PRO	3.4
3	C	142	TRP	3.4
4	D	148	TYR	3.4
7	G	71	ARG	3.4
1	A	171	SER	3.4
5	E	129	LYS	3.4
2	B	38	LEU	3.4
2	B	372	VAL	3.4
7	G	15	THR	3.4
2	B	85	ILE	3.4
3	C	204	SER	3.4
3	C	18	SER	3.4
1	A	149	VAL	3.4
1	A	27	SER	3.3
5	E	195	VAL	3.3
4	D	3	LEU	3.3
4	D	10	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	231	LYS	3.3
2	B	347	ILE	3.3
5	E	126	ARG	3.3
1	A	250	LEU	3.3
4	D	83	ARG	3.3
1	A	328	ARG	3.3
2	B	104	ASN	3.3
6	F	11	ARG	3.3
3	C	163	GLU	3.3
5	E	125	GLU	3.3
7	G	36	ASN	3.3
4	D	42	SER	3.3
1	A	95	THR	3.2
3	C	257	PHE	3.2
5	E	163	SER	3.2
3	C	246	PHE	3.2
2	B	229	GLY	3.2
2	B	357	VAL	3.2
4	D	24	THR	3.1
2	B	152	PHE	3.1
7	G	70	LYS	3.1
5	E	145	VAL	3.1
2	B	52	LYS	3.1
3	C	176	LEU	3.1
2	B	51	ILE	3.1
5	E	134	ILE	3.1
1	A	379	ILE	3.1
5	E	65	SER	3.1
6	F	102	LYS	3.0
3	C	52	LEU	3.0
3	C	134	LEU	3.0
5	E	162	GLY	3.0
5	E	164	HIS	3.0
5	E	41	ALA	3.0
1	A	299	VAL	3.0
5	E	21	SER	2.9
3	C	283	ARG	2.9
4	D	216	VAL	2.9
1	A	243	HIS	2.9
1	A	344	ARG	2.9
5	E	180	LEU	2.9
5	E	97	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	132	TRP	2.9
3	C	91	PHE	2.9
4	D	84	PRO	2.9
5	E	70	ALA	2.9
3	C	340	GLY	2.9
4	D	86	LYS	2.9
1	A	12	PRO	2.8
7	G	22	GLU	2.8
1	A	323	TYR	2.8
4	D	140	GLY	2.8
2	B	88	GLY	2.8
3	C	184	PHE	2.8
1	A	421	ALA	2.8
10	J	48	GLU	2.8
1	A	275	ALA	2.8
5	E	118	ARG	2.8
5	E	111	ALA	2.7
10	J	16	ARG	2.7
3	C	328	LEU	2.7
2	B	278	VAL	2.7
5	E	135	LEU	2.7
1	A	58	PHE	2.7
3	C	118	VAL	2.7
1	A	193	PRO	2.7
2	B	361	LYS	2.7
2	B	182	ARG	2.6
2	B	144	LEU	2.6
4	D	237	TYR	2.6
2	B	166	ALA	2.6
1	A	428	ILE	2.6
3	C	192	GLY	2.6
3	C	190	ILE	2.5
4	D	171	PHE	2.5
2	B	203	ARG	2.5
1	A	345	LEU	2.5
6	F	23	ALA	2.5
4	D	36	VAL	2.4
2	B	432	HIS	2.4
7	G	72	LYS	2.4
5	E	167	ALA	2.4
3	C	368	PRO	2.4
6	F	99	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	331	ALA	2.3
5	E	47	VAL	2.3
1	A	303	LEU	2.3
2	B	261	SER	2.2
2	B	312	PHE	2.2
5	E	138	VAL	2.2
2	B	33	LEU	2.2
2	B	393	ASN	2.2
4	D	56	TYR	2.1
3	C	208	ASN	2.1
2	B	225	ASN	2.1
8	H	16	PRO	2.1
5	E	109	GLU	2.1
5	E	96	LEU	2.1
3	C	8	SER	2.1
1	A	192	ALA	2.1
5	E	105	GLU	2.1
6	F	66	LEU	2.0
1	A	76	GLU	2.0
3	C	13	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
13	FES	E	197	4/4	2.66	2.15	59,60,64,65	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	HEM	D	243	43/43	1.86	0.54	10,21,32,35	0
12	HEM	C	381	43/43	1.58	0.24	6,24,32,43	0
12	HEM	C	382	43/43	1.54	-0.01	8,20,32,41	0
15	PEE	C	384	49/51	1.59	-0.11	42,58,76,87	0
11	BOG	D	242	20/20	1.58	-0.12	35,68,81,81	0
16	SIG	C	385	35/35	1.39	-0.49	2,17,26,29	0
15	PEE	E	198	49/51	1.41	-0.57	43,80,98,100	0
14	U10	C	383	29/63	1.13	-1.22	72,88,100,100	0

6.5 Other polymers

There are no such residues in this entry.